



Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 09:12 PM EST

PDB ID : 7W5Z
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 Full wwPDB EM Validation 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:

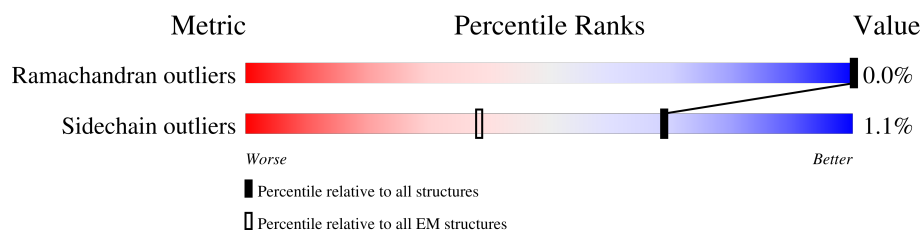
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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.




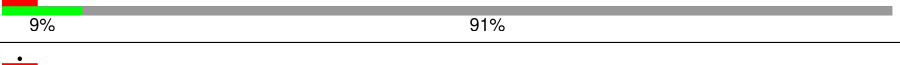
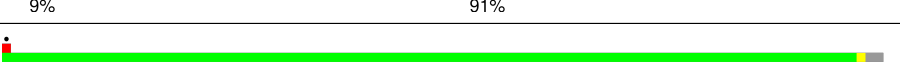
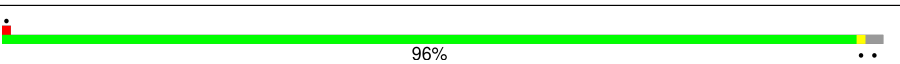
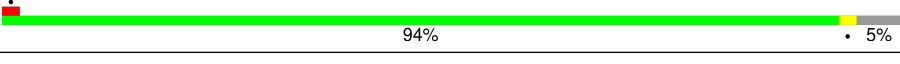
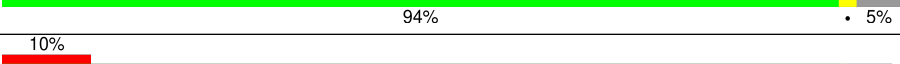
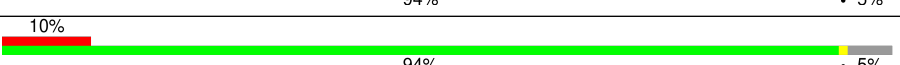

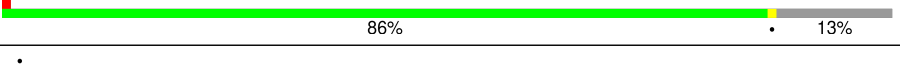
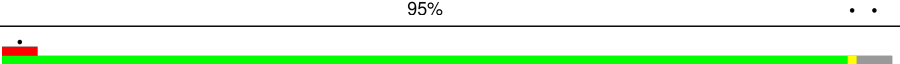
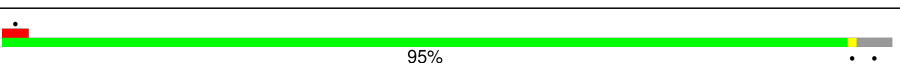
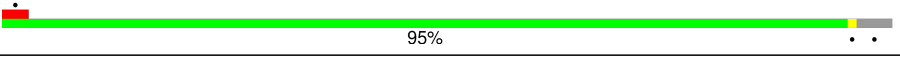

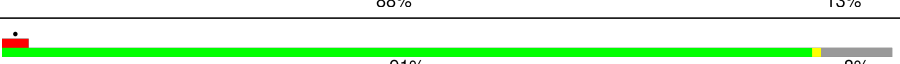
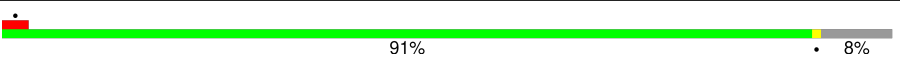
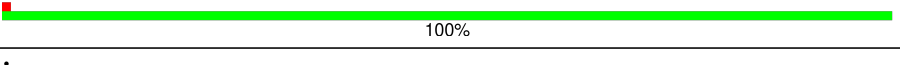
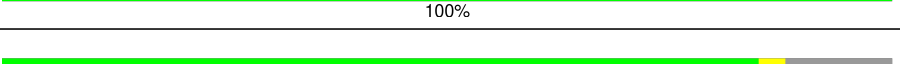
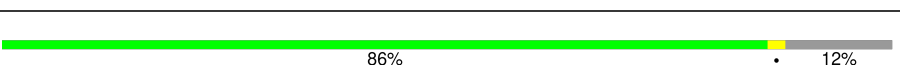





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	100%
1	u1	98	100%
2	U2	3634	97%
2	u2	3634	97%
3	U3	34	85% 100%
3	u3	34	91% 100%
4	U4	30	93% 100%
4	u4	30	100%
5	U5	172	11% 19% 81%

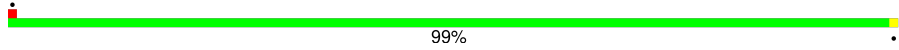
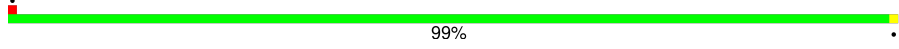
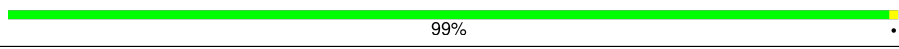
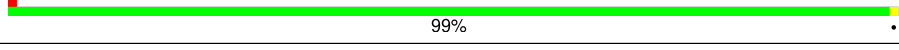
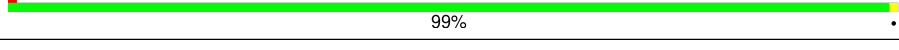
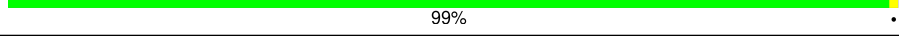
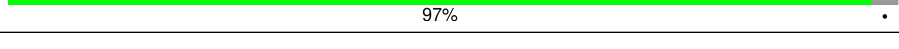
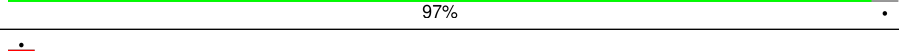
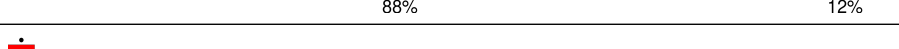
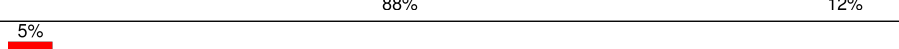
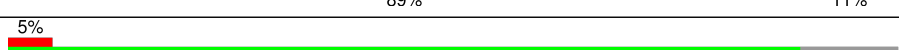

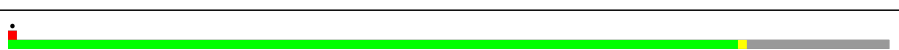

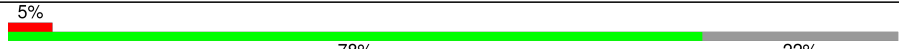
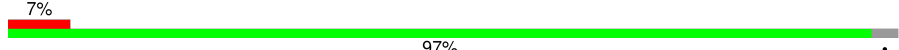



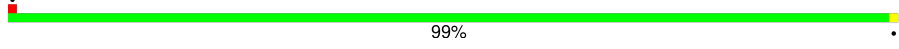
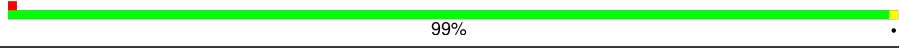
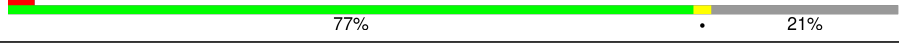



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Mol	Chain	Length	Quality of chain
5	u5	172	
6	U6	478	
6	u6	478	
7	C1	688	
7	c1	688	
8	C2	604	
8	c2	604	
9	C3	594	
9	c3	594	
10	5B	637	
10	5b	637	
11	6A	130	
11	6a	130	
12	6B	230	
12	6b	230	
13	6L	88	
13	6l	88	
14	6C	103	
14	6c	103	
15	7A	133	
15	7a	133	
16	7C	236	
16	7c	236	
17	7L	990	
17	7l	990	


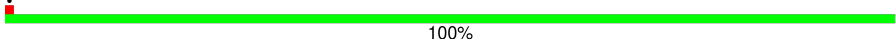
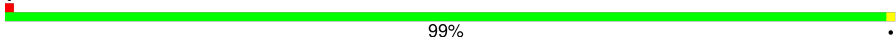
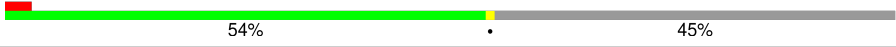
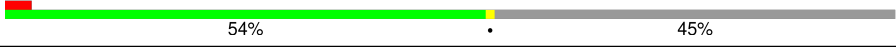
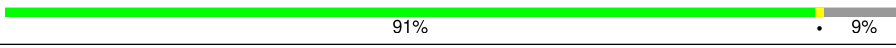

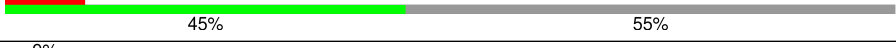

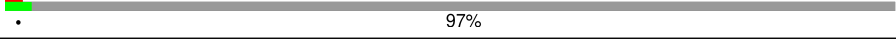
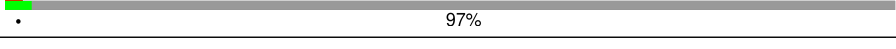

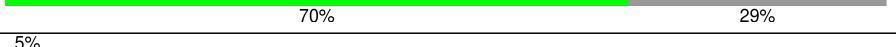
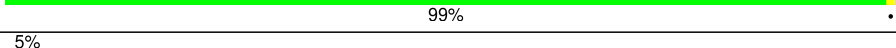
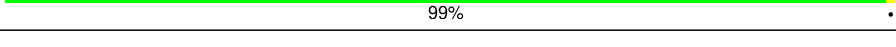
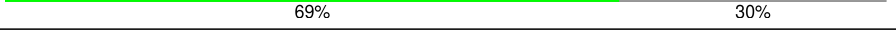
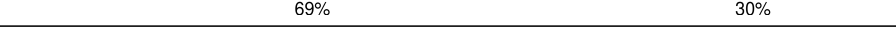

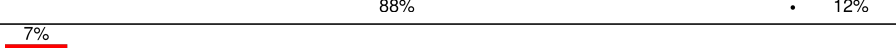
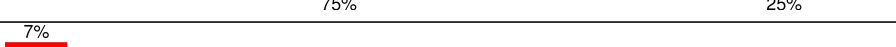
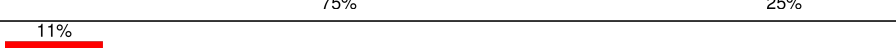




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Mol	Chain	Length	Quality of chain
18	M1	346	
18	m1	346	
19	M2	318	
19	m2	318	
20	M3	330	
20	m3	330	
21	T1	72	
21	t1	72	
22	T2	72	
22	t2	72	
23	T3	93	
23	t3	93	
24	T4	68	
24	t4	68	
25	T5	81	
25	t5	81	
26	T6	72	
26	t6	72	
27	BP	380	
27	bp	380	
28	FS	188	
28	fs	188	
29	AC	127	
29	ac	127	
30	Y7	453	







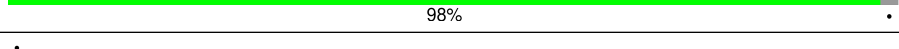
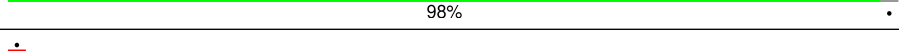
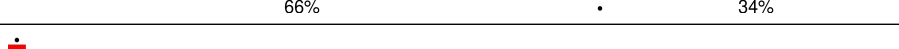
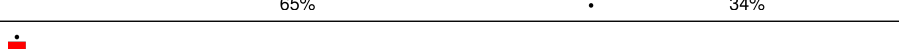
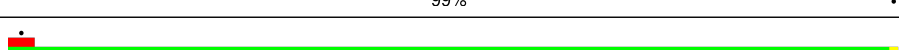
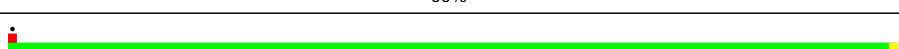
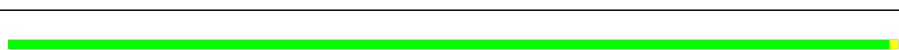
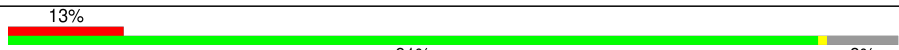
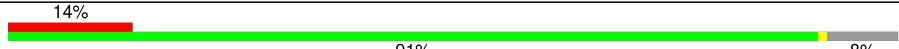


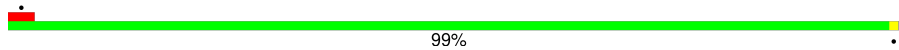
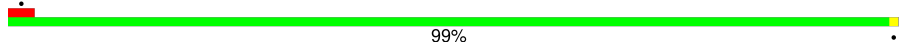
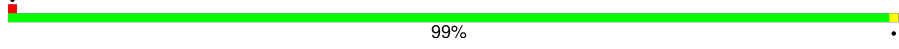
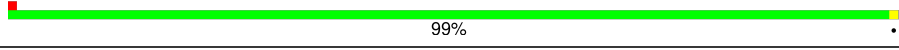
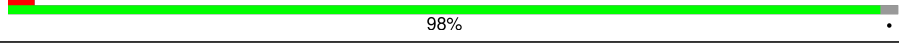
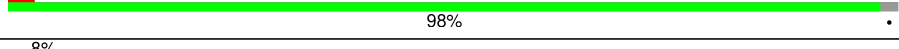


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Mol	Chain	Length	Quality of chain
30	y7	453	
31	Y0	89	
31	y0	89	
32	Y5	190	
32	y5	190	
33	A	490	
33	a	490	
34	B	473	
34	b	473	
35	C	1471	
35	c	1471	
36	D	402	
36	d	402	
37	E	385	
37	e	385	
38	F	348	
38	f	348	
39	G	318	
39	g	318	
40	H	318	
40	h	318	
41	I	252	
41	i	252	
42	J	234	
42	j	234	


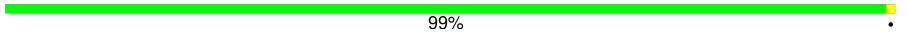
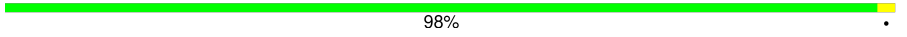
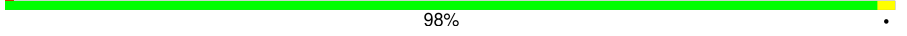
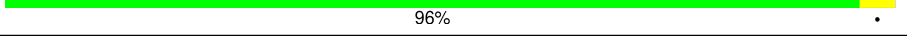


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Mol	Chain	Length	Quality of chain
43	K	231	
43	k	231	
44	L	222	
44	l	222	
45	M	220	
45	m	220	
46	N	210	
46	n	210	
47	O	193	
47	o	193	
48	P	175	
48	p	175	
49	Q	173	
49	q	173	
50	R	173	
50	r	173	
51	S	170	
51	s	170	
52	T	158	
52	t	158	
53	U	154	
53	u	154	
54	V	149	
54	v	149	
55	W	124	

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Mol	Chain	Length	Quality of chain
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	
			4624	2915	778	912	2	17	0
									0

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

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

- 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		
			1904	1234	311	346	13	0	0
12	6b	221	Total	C	N	O	S		
			1904	1234	311	346	13	0	0

- 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		
			638	408	108	116	6	0	0
13	6l	77	Total	C	N	O	S		
			638	408	108	116	6	0	0

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

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

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

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

- 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		

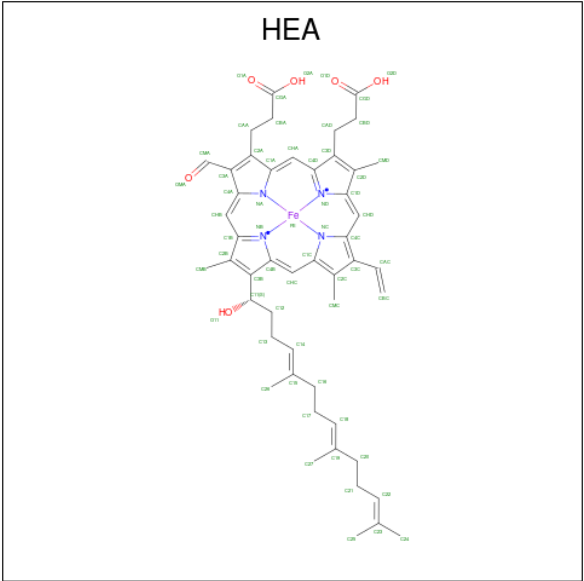
- Molecule 57 is a protein called Cytochrome c oxidase subunit TT25.

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 (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (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	

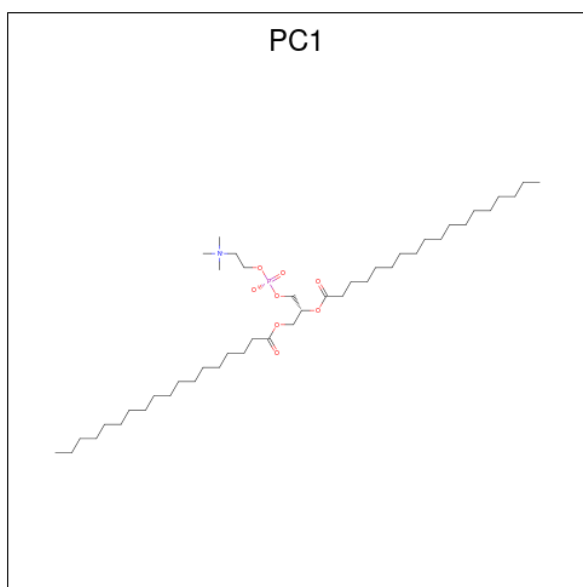
- Molecule 60 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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 (three-letter code: 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 (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



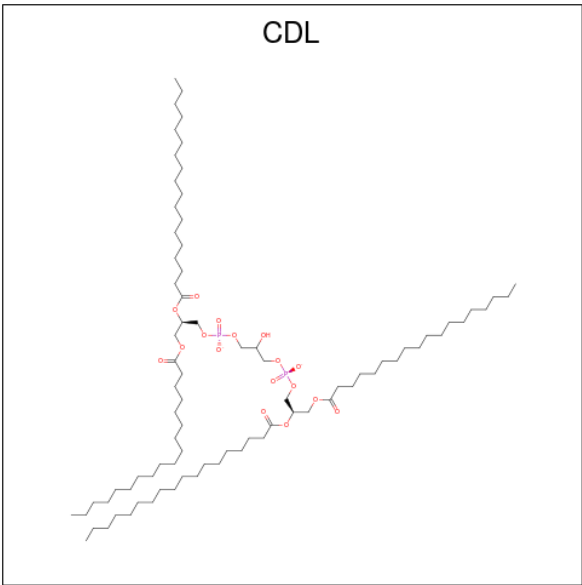
Mol	Chain	Residues	Atoms					AltConf
62	C1	1	Total	C	N	O	P	0
			49	39	1	8	1	
62	C3	1	Total	C	N	O	P	0
			52	42	1	8	1	
62	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
62	C3	1	Total	C	N	O	P	0
			31	21	1	8	1	
62	C3	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	7C	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	7C	1	Total	C	N	O	P	0
			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 (three-letter code: 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	

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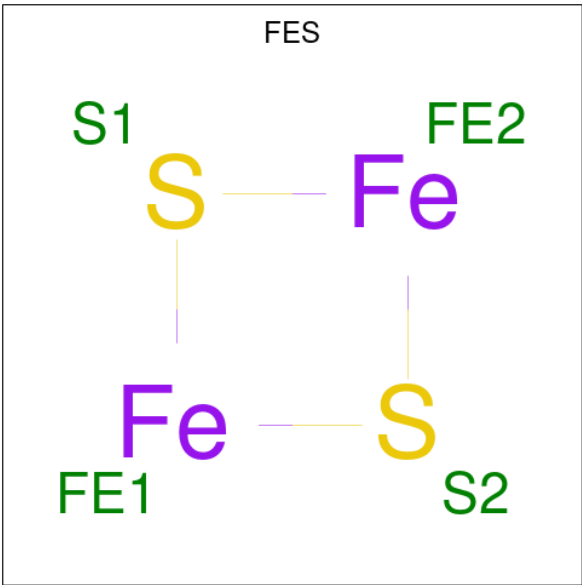
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Mol	Chain	Residues	Atoms				AltConf
63	b	1	Total	C	O	P	0
			62	43	17	2	
63	e	1	Total	C	O	P	0
			60	41	17	2	
63	e	1	Total	C	O	P	0
			72	53	17	2	
63	f	1	Total	C	O	P	0
			100	81	17	2	
63	j	1	Total	C	O	P	0
			70	51	17	2	
63	k	1	Total	C	O	P	0
			62	43	17	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 (three-letter code: 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 (three-letter code: 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	





- Molecule 2: Transmembrane protein, putative

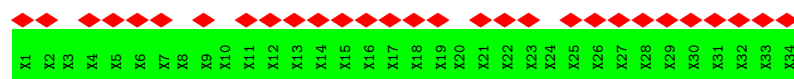
Chain u2: 97%

[illegible]

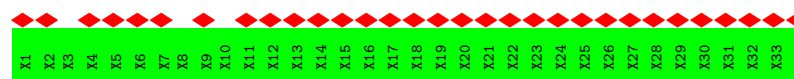




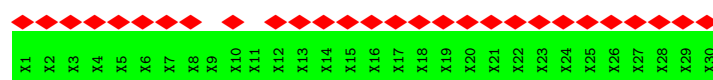




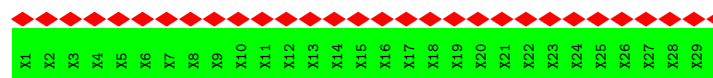
• Molecule 3: Unknown peptide



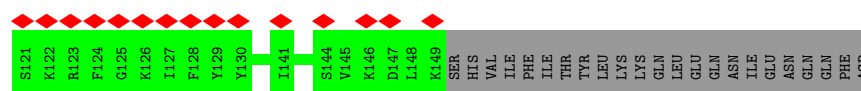
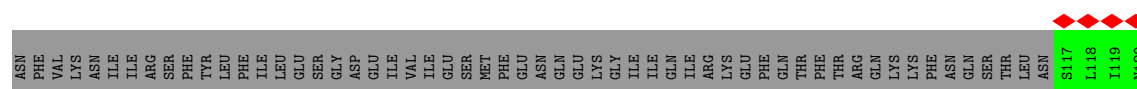
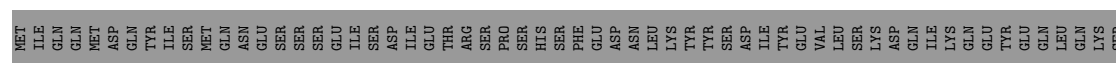
• Molecule 4: Unknown peptide



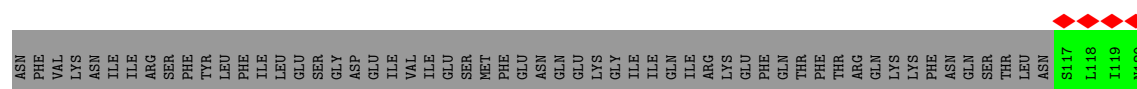
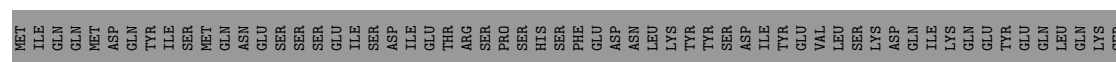
• Molecule 4: Unknown peptide



• Molecule 5: Uncharacterized protein

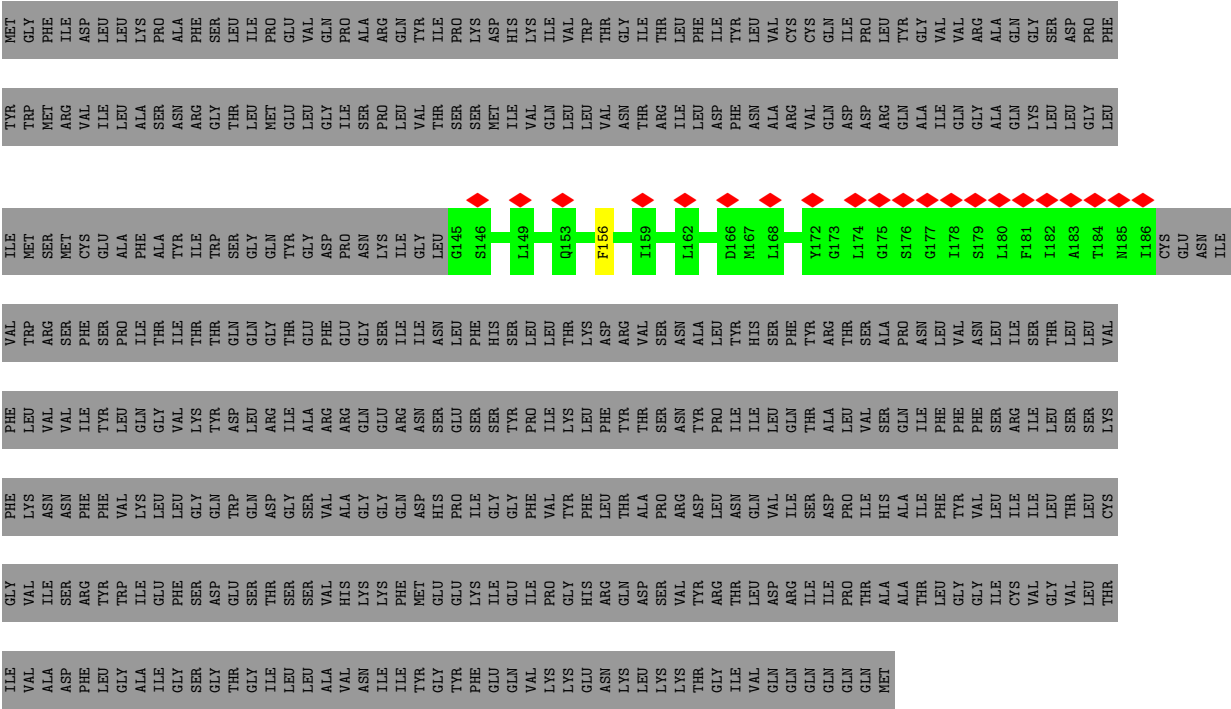


• Molecule 5: Uncharacterized protein





• Molecule 6: Protein transporter Sec61 alpha subunit



• Molecule 6: Protein transporter Sec61 alpha subunit



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

• Molecule 7: Cytochrome c oxidase subunit 1

Chain C1:  96%

MET TRP VAL ASP PHE ILE ASP GLN THR LYS SER SER LEU LYS VAL SER V16 Y57 R164 N189 D190 K217 K263 C264 S265 T275 R318 R329 F404 T414 Y432 F503 H591 M621 R672 E687 LYS

• Molecule 7: Cytochrome c oxidase subunit 1

Chain c1:  96%

MET TRP VAL ASP PHE ILE ASP GLN THR LYS SER SER LEU LYS VAL SER V16 Y57 R164 N189 D190 K217 K263 C264 S265 T275 F310 R318 R329 T414 Y432 F503 H591 D592 M621 R672 E687 LYS

• Molecule 8: Cytochrome c oxidase subunit 2

Chain C2:  94% • 5%

H1 R59 G75 K76 W77 G78 D79 F80 K210 S211 L212 F224 D228 L229 Y230 D234 Y238 D242 D274 F291 T335 R348 L409 Y431 LYS ASP ASP ASN GLY ASN LYS T439 D440 L441 V501 D526 T536 H559 K583 MET LEU

ASN THR VAL SER ARG LYS ARG PHE GLU THR HIS TYR GLU LEU ARG LYS SER TRP

• Molecule 8: Cytochrome c oxidase subunit 2

Chain c2:  94% • 5%

H1 R59 G75 K76 W77 G78 D79 F80 L81 A82 K210 F224 D228 L229 Y230 Y238 D242 D274 F291 D333 Y334 T335 R348 L409 Y431 LYS ASP ASP ASN GLY ASN LYS T439 D440 L441 V501 D526 T536 H559 K583 MET LEU

ASN THR VAL SER ARG LYS ARG PHE GLU THR HIS TYR GLU LEU ARG LYS SER TRP

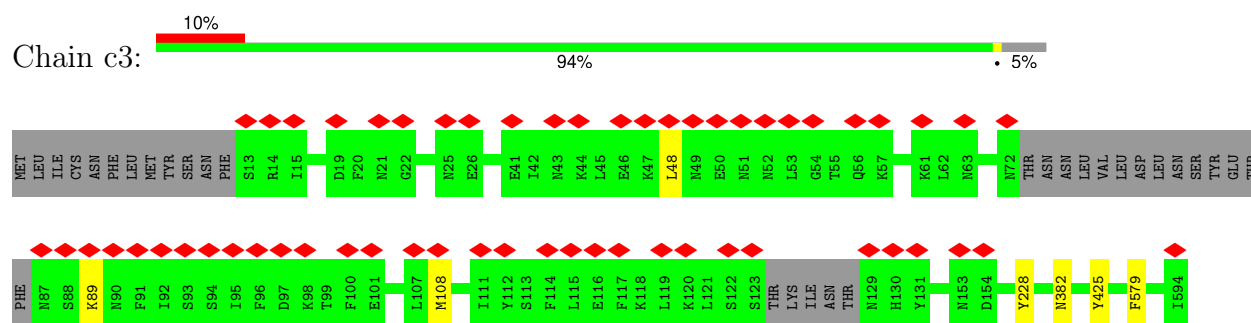
• Molecule 9: Ymf68

Chain C3:  94% • 5%

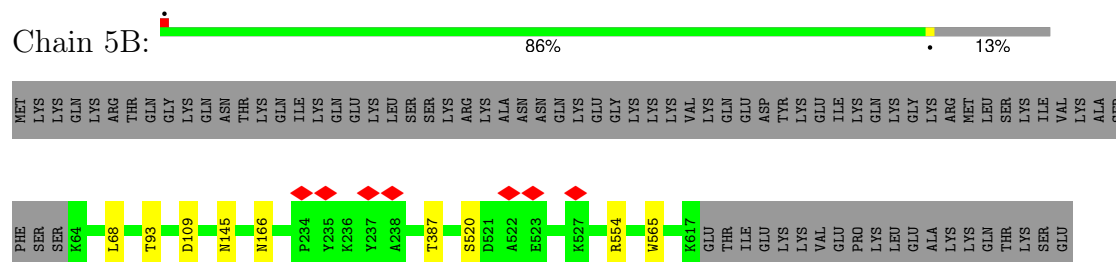
MET LEU ILE CYS ASN PHE LEU MET TYR SER ASN PHE S13 R14 I15 D19 F20 N21 G22 N25 E26 E41 I42 M43 K44 L45 E46 K47 L48 M49 E50 N51 N52 L53 Q54 T55 Q56 K57 K61 L62 M63 D69 N72 THR ASN ASN LEU VAL LEU ASP MET LEU ASN SER TYR

GLU THR PHE M87 S88 K89 N90 F91 I92 S93 S94 I95 F96 D97 K98 T99 F100 E101 L107 M108 I111 Y112 S113 F114 L115 E116 L119 K120 L121 S122 S123 THR LYS ILE ASN THR M129 H130 Y131 M143 M153 D154 Y228 N382 Y425 F579 I594

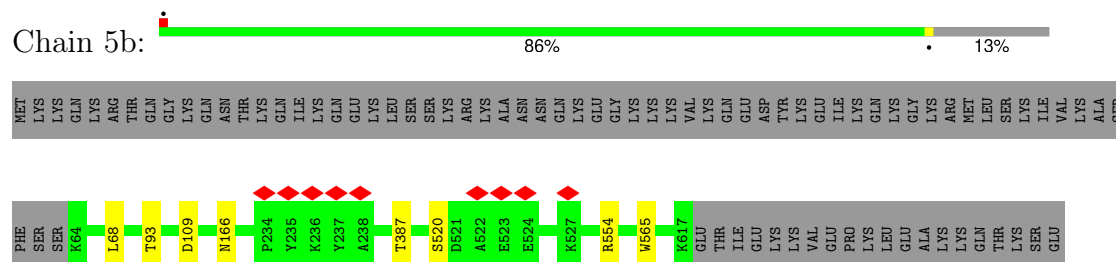
• Molecule 9: Ymf68



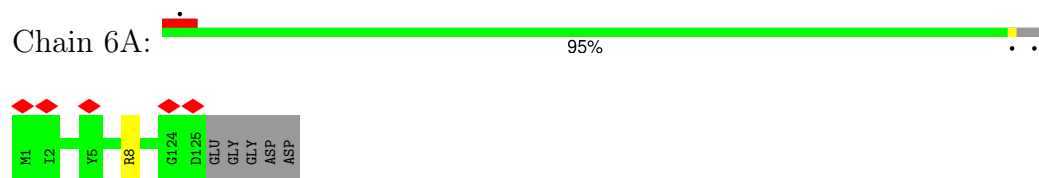
- Molecule 10: Cytochrome C oxidase subunit Vb protein



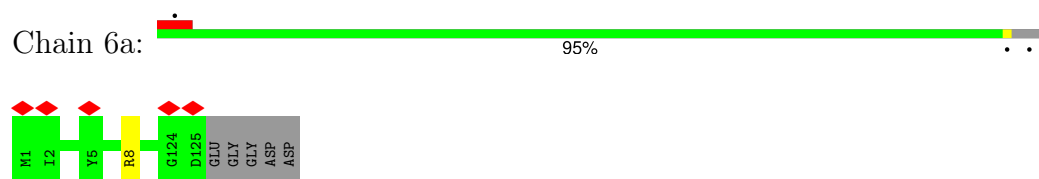
- Molecule 10: Cytochrome C oxidase subunit Vb protein



- Molecule 11: Transmembrane protein, putative

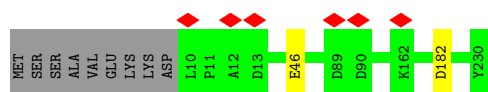


- Molecule 11: Transmembrane protein, putative



- Molecule 12: Cytochrome c oxidase subunit 6B

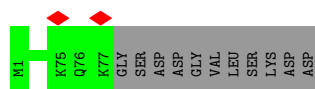




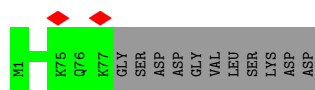
- Molecule 12: Cytochrome c oxidase subunit 6B



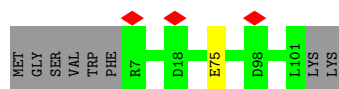
- Molecule 13: Cytochrome c oxidase subunit 6B-like



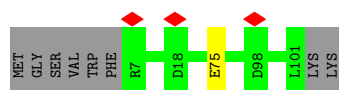
- Molecule 13: Cytochrome c oxidase subunit 6B-like



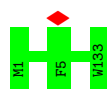
- Molecule 14: Transmembrane protein, putative



- Molecule 14: Transmembrane protein, putative

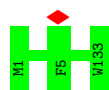


- Molecule 15: Transmembrane protein, putative




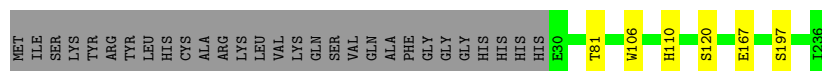
- Molecule 15: Transmembrane protein, putative

Chain 7a:  100%




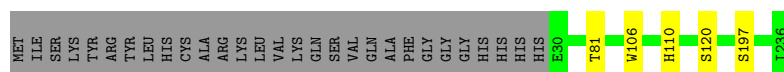
- Molecule 16: Cytochrome c oxidase subunit 7C

Chain 7C:  85% 12%



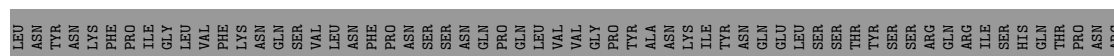
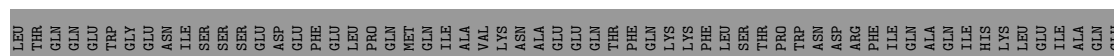
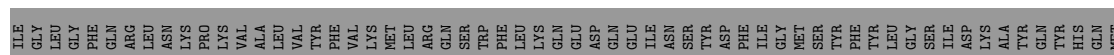
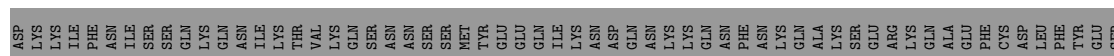
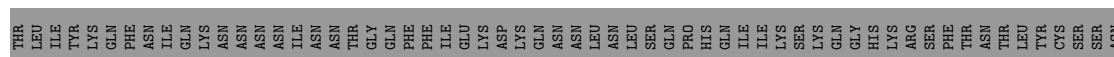
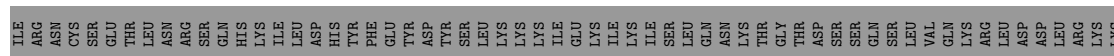
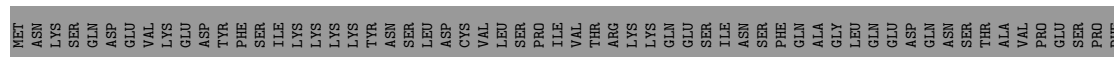
- Molecule 16: Cytochrome c oxidase subunit 7C

Chain 7c:  86% 12%

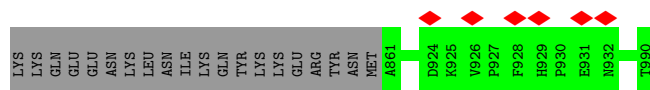


- Molecule 17: CTF/NF-I domain-containing protein

Chain 7L:  13% 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



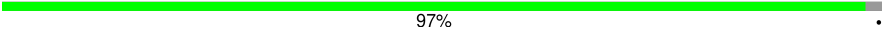
- Molecule 20: Carrier protein



- Molecule 20: Carrier protein



- Molecule 21: Tim10/DDP family zinc finger protein

Chain T1:  97%




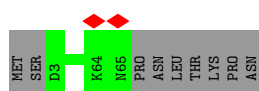
- Molecule 21: Tim10/DDP family zinc finger protein

Chain t1:  97%




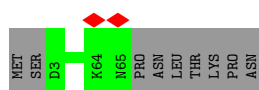
- Molecule 22: Cytochrome c oxidase small TIM subunit 2

Chain T2:  88% 12%




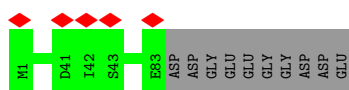
- Molecule 22: Cytochrome c oxidase small TIM subunit 2

Chain t2:  88% 12%




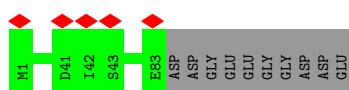
- Molecule 23: Cytochrome c oxidase small TIM subunit 3

Chain T3:  5% 89% 11%




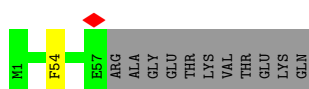
- Molecule 23: Cytochrome c oxidase small TIM subunit 3

Chain t3:  5% 89% 11%

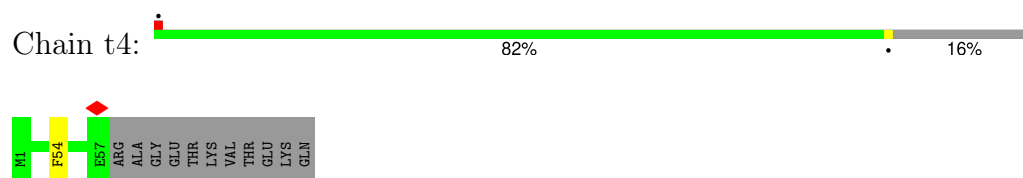


- Molecule 24: Cytochrome c oxidase small TIM subunit 4

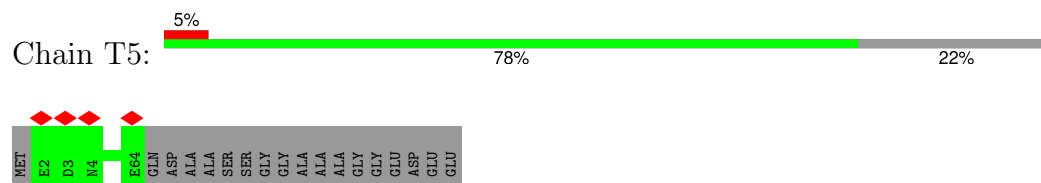
Chain T4:  82% 16%



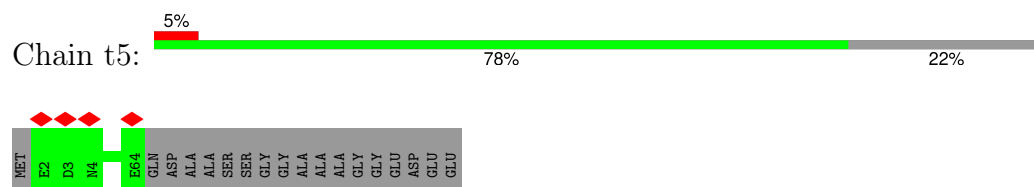
- Molecule 24: Cytochrome c oxidase small TIM subunit 4



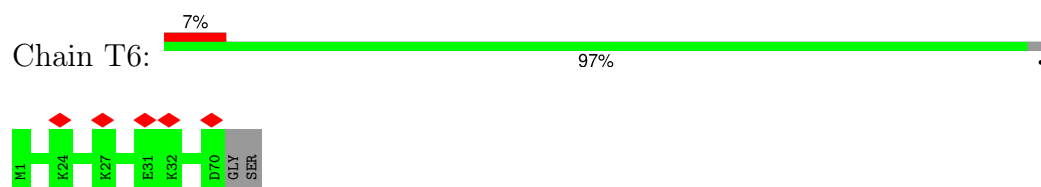
- Molecule 25: Cytochrome c oxidase small TIM subunit 5



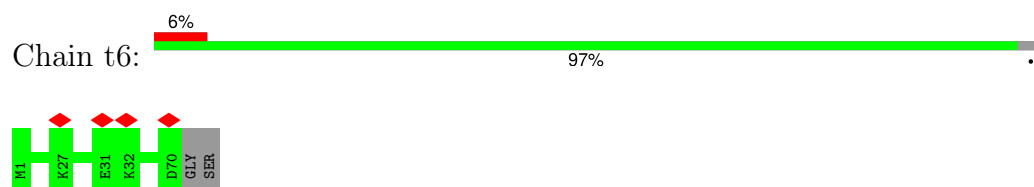
- Molecule 25: Cytochrome c oxidase small TIM subunit 5



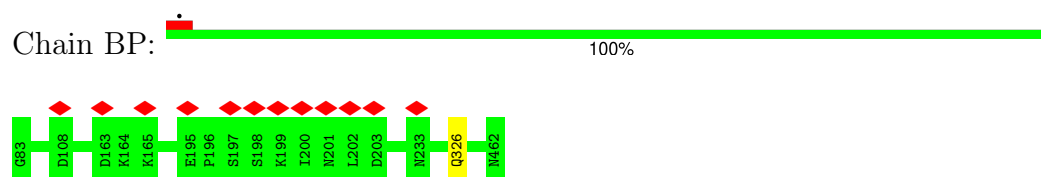
- Molecule 26: Cytochrome c oxidase small TIM subunit 6



- Molecule 26: Cytochrome c oxidase small TIM subunit 6

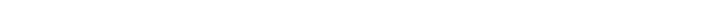


- Molecule 27: Chromosome condensation regulator RCC1 repeat protein



- Molecule 27: Chromosome condensation regulator RCC1 repeat protein



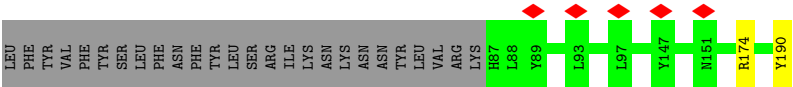
Chain v7: 

Chain Y0: 100%

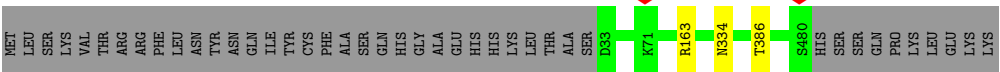
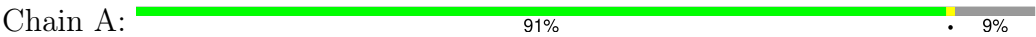
Chain v0:  99%

Chain Y5:  54% 45%

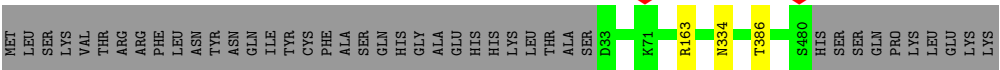
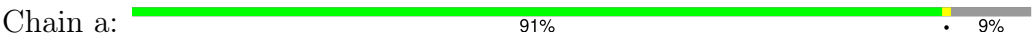
Chain v5:  54% 45%



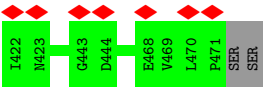
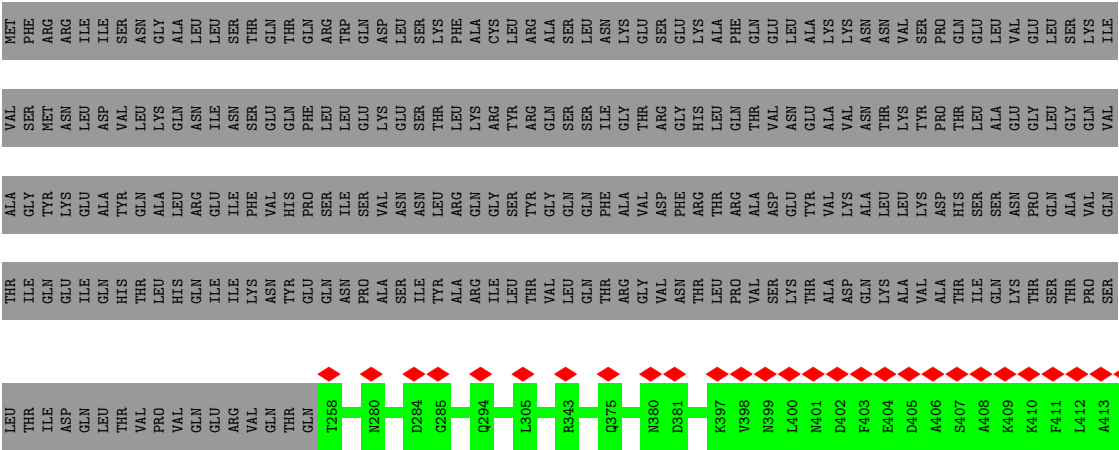
• Molecule 33: Transmembrane protein, putative



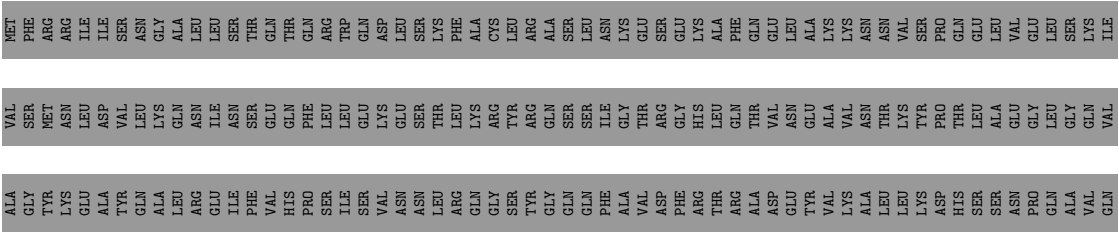
• Molecule 33: Transmembrane protein, putative



• Molecule 34: Protein phosphatase 2C, putative



• Molecule 34: Protein phosphatase 2C, putative



LYS	GLN	TYR	ILE	PHE	SER	THR	VAL	F429	F430	F438	L439	G440	I441	K445	R446	S447	I450	V451	Y452	M453	P454	M455	H456	M457	L458	L459	T460	Y461	C462	F463	M464	M465	L466	F468	F469	K470	V471	M472	G473	I474	SER	SER	LYS	LYS	LYS	GLY	PHE	ASP	TYR	VAL	PHE	THR	THR	LEU	LYS	GLU
ASN	GLU	LYS	THR	HIS	ILE	VAL	THR	ILE	LEU	GLN	VAL	THR	GLY	PHE	SER	VAL	ALA	ILE	GLY	TRP	TYR	PHE	ILE	GLY	VAL	VAL	ASN	ASP	ASN	GLN	THR	ASN	TRP	ILE	SER	GLU	GLY	VAL	TYR	TYR	GLN	LYS	TYR	ILE	LYS	GLY	ASP	THR	VAL	PHE	THR	THR	LEU	LYS	GLU	
ILE	TYR	TRP	TRP	ILE	THR	THR	MET	THR	THR	ASP	GLY	ASP	ILE	SER	THR	ALA	ASN	ILE	TYR	ILE	SER	ILE	VAL	MET	LEU	VAL	CYS	VAL	PHE	ALA	TYR	ILE	ASN	ASN	GLN	VAL	ILE	ILE	ILE	SER	ASN	LYS	VAL	THR	GLN	ILE	THR	VAL	GLU	ASP						
ASP	LYS	ILE	THR	THR	MET	GLN	ARG	TYR	ASN	ARG	LYS	VAL	ILE	ILE	ILE	LEU	LYS	VAL	LEU	ARG	LYS	THR	GLY	ALA	GLN	ARG	ASN	ASP	ASP	LYS	GLN	ALA	GLY	ASP	ILE	ILE	ILE	LEU	SER	ASN	LYS	VAL	THR	GLU	THR	ILE	THR	VAL	GLU	GLU						
ILE	ASN	SER	ILE	ILE	ASN	LYS	PHE	ASN	PHE	PHE	SER	ASN	SER	LYS	THR	THR	GLY	VAL	PHE	LYS	THR	THR	VAL	LEU	ASN	PRO	GLY	ILE	ILE	PHE	ARG	GLU	GLN	ASN	ILE	ASP	MET	SER	ILE	THR	TYR	GLY	VAL	ILE	THR	VAL	GLU	VAL								
TYR	GLN	GLN	SER	VAL	GLN	LYS	GLN	ASP	ASP	THR	ILE	GLN	THR	GLN	ASN	THR	PHE	LYS	GLY	GLY	PHE	PHE	GLY	LEU	LEU	ARG	LYS	ALA	SER	ALA	SER	SER	ILE	THR	THR	LYS	THR	ARG	GLU	GLU	THR	ILE	ILE	GLN	TYR	ILE	GLN	VAL								
ASN	ASN	GLU	ASN	TYR	GLY	ARG	PHE	LYS	ASN	GLN	GLN	VAL	PHE	LYS	GLY	PRO	LEU	LEU	HIS	CYS	TYR	ASN	CYS	LEU	LYS	ILE	GLY	HIS	ILE	SER	CYS	PRO	LYS	THR	ASN	LYS	ASN	GLN	THR	ASN	GLN	THR	ASN	GLY	VAL	TYR	SER									
SER	PHE	GLN	GLN	ARG	ILE	ILE	PHE	ASP	ASP	THR	LYS	ASN	THR	LYS	PRO	LEU	ASN	ASN	GLN	ASN	VAL	VAL	LYS	ILE	LEU	GLN	ASN	GLN	ASP	ASN	ASN	ILE	PRO	LYS	THR	ASN	GLY	ASN	GLY	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR			
ASN	SER	GLU	ASP	GLU	ASP	ASN	ASP	GLU	TYR	GLY	GLU	GLY	ALA	SER	SER	THR	GLN	ASN	ASN	PHE	ASN	ASN	ASN	LYS	LYS	ASN	ASN	ASN	ASN	ASN	ASN	ALA	LEU	LYS	LYS	GLN	LYS	GLY	VAL	VAL	LYS	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN					
ASN	ASN	GLN	ILE	CYS	GLU	ASN	ILE	SER	SER	LEU	ASN	ASN	TYR	CYS	ASN	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLU	ILE	LYS	ASN	TYR	VAL	VAL	SER	PHE	ASN	ASN	LEU	SER	GLN	LYS	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN				
GLN	ASN	LEU	GLU	GLN	ASN	ASN	ASN	PHE	ASN	ASN	GLN	HIS	SER	LYS	SER	GLN	ASP	SER	SER	GLU	GLN	GLN	GLN	ASN	ILE	LYS	ASN	TYR	VAL	VAL	SER	PHE	ASN	ASN	VAL	ASP	GLY	ASN	GLY	THR	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN					
ARG	LYS	SER	GLN	LYS	GLN	GLN	GLN	ILE	ASN	ASN	THR	ASP	ILE	LYS	LEU	THR	LYS	GLN	GLN	THR	GLN	GLN	GLN	SER	LYS	ALA	ASN	GLN	GLN	GLN	GLN	LYS	MET	ASN	PRO	SER	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN			
ASN	LEU	LYS	GLY	GLN	GLN	GLN	PHE	ASN	ASN	ASN	ARG	VAL	SER	LYS	LEU	LEU	ASN	ASN	HIS	ASN	GLN	ASN	ASN	LYS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN			
HIS	SER	SER	GLN	ASN	ILE	LEU	PRO	GLN	ILE	GLN	LYS	ASN	GLN	LYS	ALA	ASP	LYS	LYS	LYS	GLY	ASN	PHE	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN			
ASN	LEU	SER	GLN	ILE	LYS	THR	LYS	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN				
ARG	SER	GLN	ILE	LEU	LEU	LEU	ASN	PRO	GLN	GLN	LYS	LEU	THR	SER	VAL	GLY	ARG	MET	GLY	ASN	SER	PHE	ARG	GLU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU			
LEU	LYS	LEU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN		
TYR	GLY	VAL	SER	LYS	ARG	GLY	GLY	GLN	PRO	CYS	ASN	LYS	ASN	ASN	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	

● Molecule 36: SURF1-like protein



- Molecule 36: SURF1-like protein

Chain d:

70% 29%

MET TYR GLU GLY ARG TRP LYS MET VAL ASN GLN ILE LYS GLN ASP ILE GLU LEU ILE LEU ARG GLN MET ASN GLU ARG ILE HIS ALA MET LYS LYS LYS TYR ASN GLU LEU LYS GLY ILE LYS GLN LYS CYS ILE ASP LEU ILE ASP TYR ALA LYS GLN

● Molecule 37: TraB family protein

Chain E:

5%

99%

M1 T53 E82 D92 T111 L112 S113 L114 D115 N116 T117 I118 R119 N120 L121 D176 P186 D254 D267 W280 E297 K381 H384 HIS

● Molecule 37: TraB family protein

Chain e:

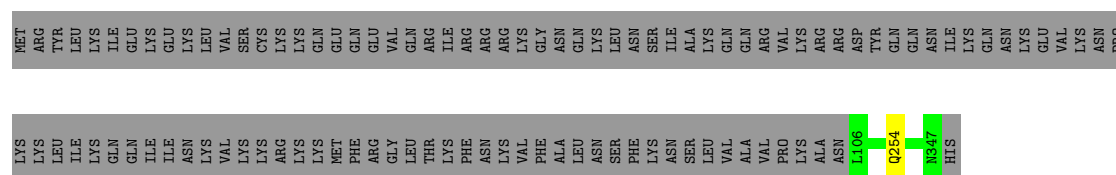
5%

99%


M1 T53 E82 D92 T111 L112 S113 L114 D115 N116 T117 I118 R119 N120 L121 D176 P186 D254 D267 W280 E297 D378 K381 P382 K383 H384 HIS

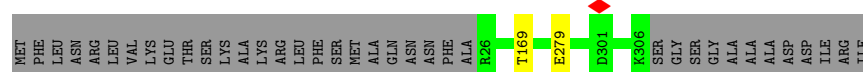
[illegible]

Chain f:  69% 30%




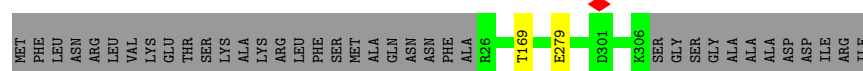
- Molecule 39: Cytochrome c oxidase subunit TT7

Chain G:  88% 12%




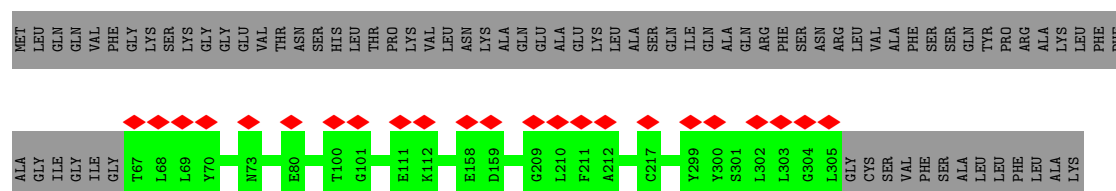
- Molecule 39: Cytochrome c oxidase subunit TT7

Chain g:  88% 12%




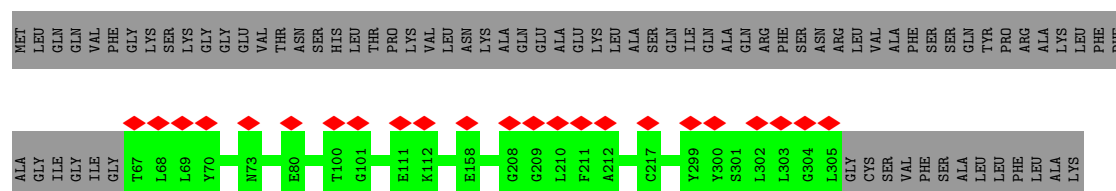
- Molecule 40: SURF1-like protein

Chain H:  7% 75% 25%



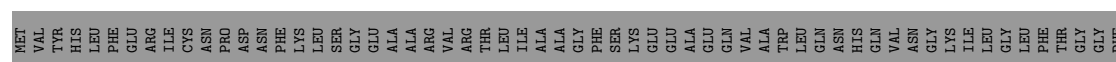
- Molecule 40: SURF1-like protein

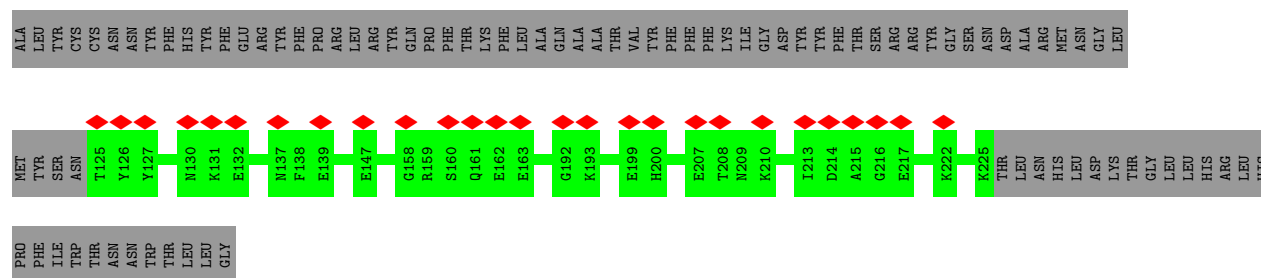
Chain h:  7% 75% 25%



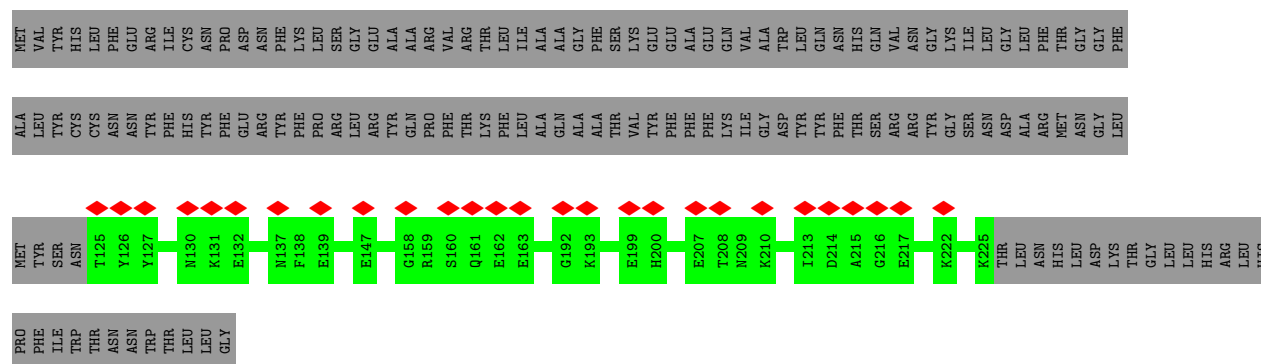
- Molecule 41: Cytochrome c oxidase subunit TT9

Chain I:  11% 40% 60%

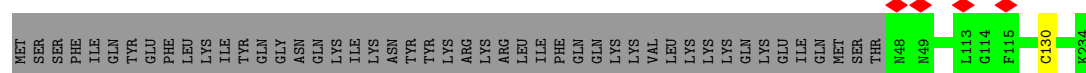
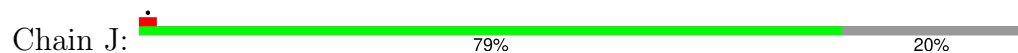




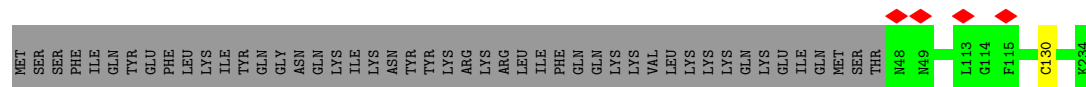
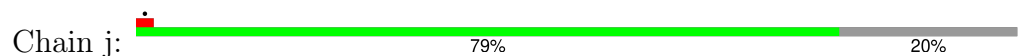
- Molecule 41: Cytochrome c oxidase subunit TT9



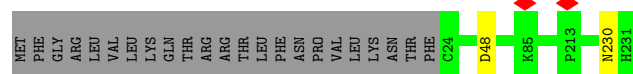
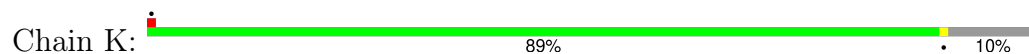
- Molecule 42: Cytochrome c oxidase subunit TT10



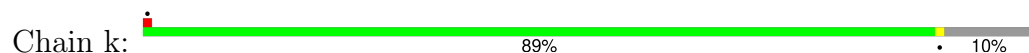
- Molecule 42: Cytochrome c oxidase subunit TT10

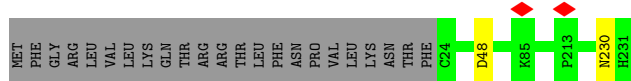


- Molecule 43: Cytochrome c oxidase subunit TT11

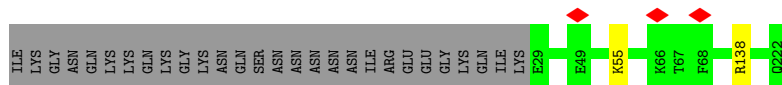
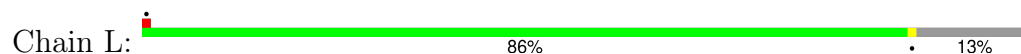


- Molecule 43: Cytochrome c oxidase subunit TT11

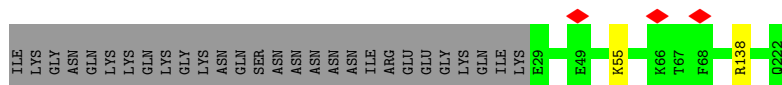
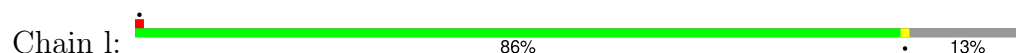




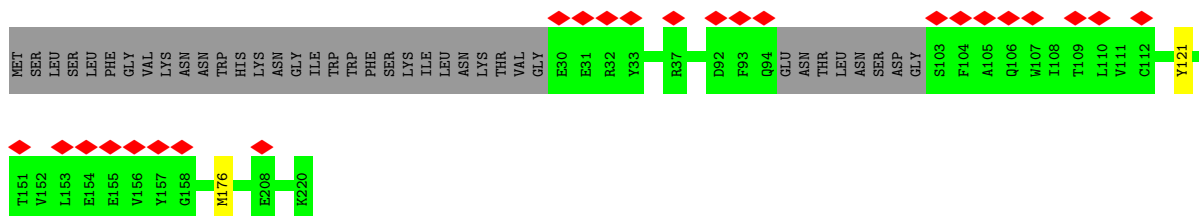
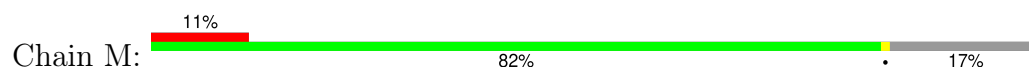
- Molecule 44: Cytochrome c oxidase subunit TT12



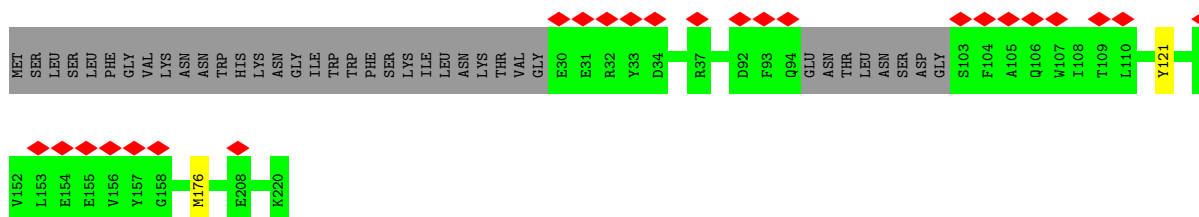
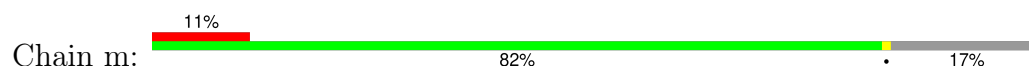
- Molecule 44: Cytochrome c oxidase subunit TT12



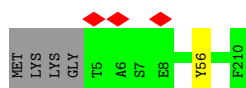
- Molecule 45: Transmembrane protein, putative



- Molecule 45: Transmembrane protein, putative



- Molecule 46: Transmembrane protein, putative



- Molecule 46: Transmembrane protein, putative

- Chain 0:  66% 34%

MET	LYS	GLU	LYS	ILE	PHE	ASN	GLU	LEU	THR	ARG	LYS	MET	LYS	ARG	LYS	GLU	ILE	SER	ALA	LYS	ILE	GLN	ARG	GLU	GLU	ASN	LYS	GLN	ILE	ILE	ILE	ARG	GLN	ASN	LYS	TYR	ILE	GLN	SER	ILE	GLN	GLY	ILE	GLN	GLU	ARG	LYS	LYS	LYS	TYR	LEU	LEU	VAL.
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Chain o:  65% 34%

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

Sequence logo for the 1000th iteration. The y-axis shows amino acid frequencies: MET, ALA, THR, GLN, ASN, V66, E67, E68, M69, N163, Y193. The x-axis shows positions 1000, 1001, 1002, 1003, 1004, 1005, 1006, 1007, 1008, 1009, 1010. The logo shows a strong preference for V66, E67, E68, and M69 at positions 1000-1003, and N163 and Y193 at positions 1008-1009.

- Chain P: 99%

Diagram illustrating the structure of the 16S rRNA gene, showing segments M1, F90, K128, E151, V152, D153, P154, R155, E159, and H175. Red diamonds are placed above the segments K128, V152, P154, and E159.

- Chain p:

- Chain Q: 

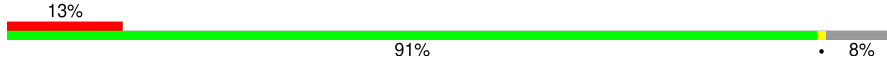
Diagram illustrating the structure of a protein with four domains: M1 (green), H70 (yellow), R128 (yellow), and K172/F173 (green). Red diamonds are positioned above the M1 and K172/F173 domains.

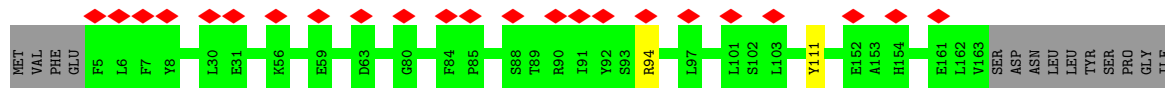
- 

Chain q:  99%




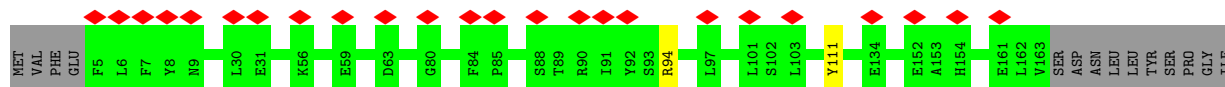
- Molecule 50: Cytochrome c oxidase subunit TT18

Chain R:  91% 13% 8%




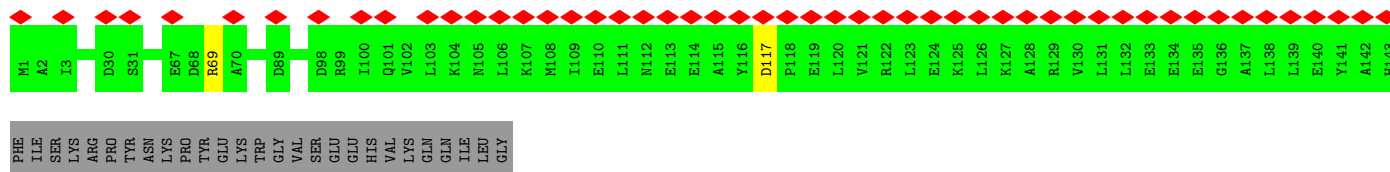
- Molecule 50: Cytochrome c oxidase subunit TT18

Chain r:  91% 14% 8%




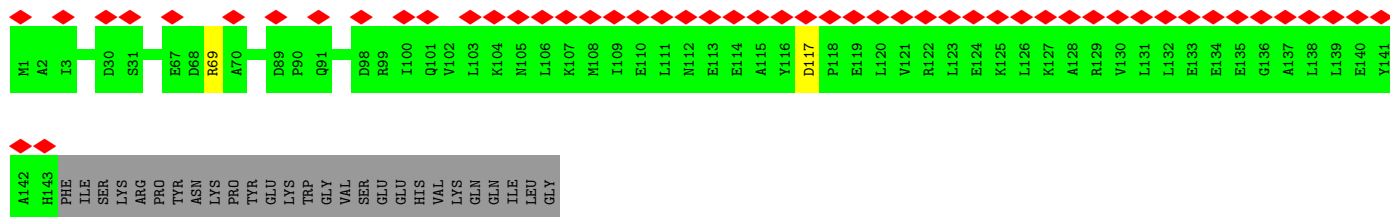
- Molecule 51: Cytochrome c oxidase subunit TT19

Chain S:  83% 30% 16%



- Molecule 51: Cytochrome c oxidase subunit TT19

Chain s:  83% 31% 16%



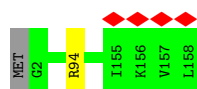
- Molecule 52: Transmembrane protein, putative

Chain T:  99%



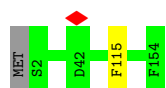
- Molecule 52: Transmembrane protein, putative

Chain t:  99%



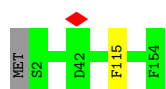
- Molecule 53: Transmembrane protein, putative

Chain U:  99%



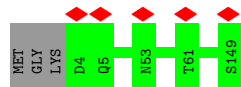
- Molecule 53: Transmembrane protein, putative

Chain u:  99%



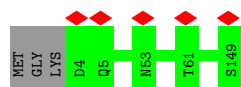
- Molecule 54: Cytochrome c oxidase subunit TT22

Chain V:  98%




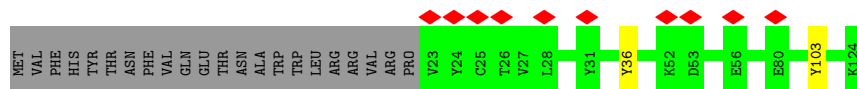
- Molecule 54: Cytochrome c oxidase subunit TT22

Chain v:  98%




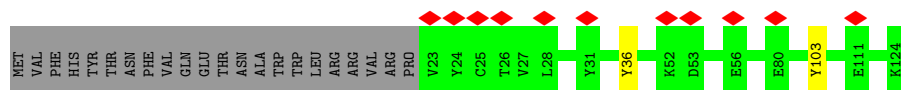
- Molecule 55: Transmembrane protein, putative

Chain W:  8% 81% 18%



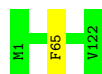
- Molecule 55: Transmembrane protein, putative

Chain w:  9% 81% 18%



- Molecule 56: Transmembrane protein, putative

Chain X:  99%



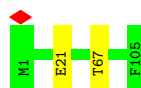
- Molecule 56: Transmembrane protein, putative

Chain x:  98%



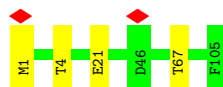
- Molecule 57: Cytochrome c oxidase subunit TT25

Chain Y:  98%



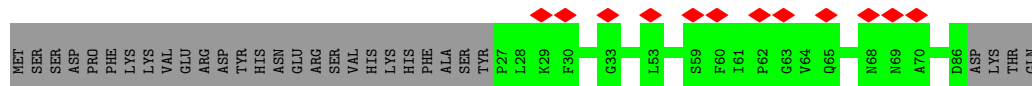
- Molecule 57: Cytochrome c oxidase subunit TT25

Chain y:  96%



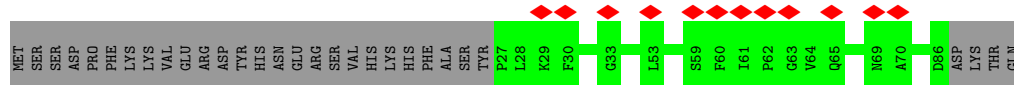
- Molecule 58: Cytochrome c oxidase subunit TT26

Chain Z:  13% 67% 33%



- Molecule 58: Cytochrome c oxidase subunit TT26

Chain z:  13% 67% 33%



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 (Å)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CU, MG, ZN, FES, CDL, TPO, FME, PC1, SEP, HEA

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	0.26	0/749	0.56	4/1031 (0.4%)
2	u2	0.25	0/749	0.56	4/1031 (0.4%)
5	U5	0.25	0/247	0.37	0/335
5	u5	0.25	0/247	0.36	0/335
6	U6	0.27	0/276	0.37	0/373
6	u6	0.26	0/276	0.35	0/373
7	C1	0.29	0/5752	0.47	0/7801
7	c1	0.29	0/5752	0.47	0/7801
8	C2	0.27	0/5027	0.47	0/6818
8	c2	0.27	0/5027	0.47	0/6818
9	C3	0.29	0/5098	0.44	0/6922
9	c3	0.29	0/5098	0.44	0/6922
10	5B	0.28	0/4706	0.46	0/6349
10	5b	0.28	0/4706	0.45	0/6349
11	6A	0.28	0/1107	0.44	0/1500
11	6a	0.28	0/1107	0.44	0/1500
12	6B	0.29	0/1968	0.46	0/2662
12	6b	0.29	0/1968	0.46	0/2662
13	6L	0.27	0/641	0.42	0/861
13	6l	0.26	0/641	0.42	0/861
14	6C	0.28	0/873	0.46	0/1184
14	6c	0.27	0/873	0.46	0/1184
15	7A	0.30	0/1198	0.48	0/1621
15	7a	0.30	0/1198	0.48	0/1621
16	7C	0.28	0/1830	0.44	0/2487
16	7c	0.28	0/1830	0.44	0/2487
17	7L	0.27	0/1099	0.44	0/1495
17	7l	0.28	0/1099	0.44	0/1495
18	M1	0.29	0/2958	0.46	0/4013
18	m1	0.29	0/2958	0.46	0/4013
19	M2	0.27	0/2621	0.47	0/3554
19	m2	0.28	0/2621	0.47	0/3554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	M3	0.27	0/2689	0.44	0/3657
20	m3	0.27	0/2689	0.45	0/3657
21	T1	0.26	0/546	0.41	0/735
21	t1	0.26	0/546	0.41	0/735
22	T2	0.26	0/518	0.44	0/694
22	t2	0.26	0/518	0.44	0/694
23	T3	0.26	0/662	0.43	0/888
23	t3	0.26	0/662	0.44	0/888
24	T4	0.29	0/483	0.44	0/652
24	t4	0.30	0/483	0.44	0/652
25	T5	0.27	0/523	0.43	0/705
25	t5	0.27	0/523	0.43	0/705
26	T6	0.27	0/565	0.42	0/760
26	t6	0.27	0/565	0.42	0/760
27	BP	0.28	0/2984	0.47	0/4047
27	bp	0.28	0/2984	0.47	0/4047
28	FS	0.29	0/1562	0.46	0/2123
28	fs	0.29	0/1562	0.46	0/2123
29	AC	0.26	0/836	0.48	0/1133
29	ac	0.26	0/836	0.48	0/1133
30	Y7	0.28	0/2968	0.40	0/4014
30	y7	0.28	0/2968	0.40	0/4014
31	Y0	0.29	0/793	0.45	0/1077
31	y0	0.29	0/793	0.44	0/1077
32	Y5	0.28	0/951	0.39	0/1284
32	y5	0.28	0/951	0.39	0/1284
33	A	0.29	0/3863	0.46	0/5258
33	a	0.29	0/3863	0.46	0/5258
34	B	0.25	0/1712	0.44	0/2318
34	b	0.26	0/1712	0.44	0/2318
35	C	0.27	0/393	0.43	0/531
35	c	0.27	0/393	0.43	0/531
36	D	0.28	0/2394	0.47	0/3254
36	d	0.27	0/2394	0.47	0/3254
37	E	0.27	0/3258	0.46	0/4425
37	e	0.27	0/3258	0.46	0/4425
38	F	0.28	0/2066	0.45	0/2809
38	f	0.28	0/2066	0.45	0/2809
39	G	0.29	0/2439	0.47	0/3328
39	g	0.29	0/2439	0.47	0/3328
40	H	0.26	0/1960	0.47	0/2656
40	h	0.27	0/1960	0.47	0/2656
41	I	0.24	0/873	0.44	0/1173

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	i	0.24	0/873	0.43	0/1173
42	J	0.26	0/1621	0.46	0/2201
42	j	0.26	0/1621	0.46	0/2201
43	K	0.26	0/1755	0.44	0/2376
43	k	0.26	0/1755	0.43	0/2376
44	L	0.26	0/1718	0.44	0/2333
44	l	0.26	0/1718	0.44	0/2333
45	M	0.28	0/1640	0.45	0/2227
45	m	0.27	0/1640	0.45	0/2227
46	N	0.28	0/1770	0.43	0/2391
46	n	0.28	0/1770	0.43	0/2391
47	O	0.27	0/1090	0.46	0/1466
47	o	0.27	0/1090	0.45	0/1466
48	P	0.26	0/1428	0.45	0/1931
48	p	0.26	0/1428	0.44	0/1931
49	Q	0.29	0/1478	0.48	0/2005
49	q	0.29	0/1478	0.48	0/2005
50	R	0.25	0/1336	0.42	0/1808
50	r	0.25	0/1336	0.42	0/1808
51	S	0.24	0/1178	0.43	0/1588
51	s	0.25	0/1178	0.44	0/1588
52	T	0.28	0/1367	0.46	0/1853
52	t	0.28	0/1367	0.46	0/1853
53	U	0.27	0/1335	0.46	0/1794
53	u	0.27	0/1335	0.46	0/1794
54	V	0.28	0/1277	0.47	0/1735
54	v	0.28	0/1277	0.47	0/1735
55	W	0.26	0/933	0.43	0/1266
55	w	0.26	0/933	0.43	0/1266
56	X	0.28	0/1043	0.45	0/1413
56	x	0.28	0/1043	0.45	0/1413
57	Y	0.28	0/882	0.46	0/1192
57	y	0.29	0/882	0.46	0/1192
58	Z	0.25	0/491	0.44	0/664
58	z	0.25	0/491	0.44	0/664
All	All	0.28	0/187060	0.45	8/253540 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U2	171	PRO	N-CA-CB	5.87	110.34	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	u2	171	PRO	N-CA-CB	5.87	110.34	103.30
2	U2	193	PRO	N-CA-CB	5.71	110.15	103.30
2	U2	240	PRO	N-CA-CB	5.68	110.12	103.30
2	u2	246	PRO	N-CA-CB	5.68	110.12	103.30
2	u2	193	PRO	N-CA-CB	5.68	110.12	103.30
2	U2	246	PRO	N-CA-CB	5.68	110.12	103.30
2	u2	240	PRO	N-CA-CB	5.68	110.11	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U2	125/3634 (3%)	115 (92%)	9 (7%)	1 (1%)	16	49
2	u2	125/3634 (3%)	114 (91%)	10 (8%)	1 (1%)	16	49
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	25	58
6	u6	24/419 (6%)	23 (96%)	1 (4%)	25	58
7	C1	597/613 (97%)	588 (98%)	9 (2%)	60	82
7	c1	597/613 (97%)	587 (98%)	10 (2%)	56	80
8	C2	542/569 (95%)	531 (98%)	11 (2%)	50	77
8	c2	542/569 (95%)	531 (98%)	11 (2%)	50	77
9	C3	534/565 (94%)	527 (99%)	7 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	c3	534/565 (94%)	527 (99%)	7 (1%)	65	84
10	5B	502/579 (87%)	495 (99%)	7 (1%)	62	83
10	5b	502/579 (87%)	496 (99%)	6 (1%)	67	85
11	6A	113/116 (97%)	112 (99%)	1 (1%)	75	89
11	6a	113/116 (97%)	112 (99%)	1 (1%)	75	89
12	6B	199/207 (96%)	197 (99%)	2 (1%)	73	88
12	6b	199/207 (96%)	196 (98%)	3 (2%)	60	82
13	6L	71/80 (89%)	71 (100%)	0	100	100
13	6l	71/80 (89%)	71 (100%)	0	100	100
14	6C	81/88 (92%)	80 (99%)	1 (1%)	67	85
14	6c	81/88 (92%)	80 (99%)	1 (1%)	67	85
15	7A	119/119 (100%)	119 (100%)	0	100	100
15	7a	119/119 (100%)	119 (100%)	0	100	100
16	7C	193/217 (89%)	189 (98%)	4 (2%)	48	76
16	7c	193/217 (89%)	190 (98%)	3 (2%)	58	81
17	7L	121/943 (13%)	121 (100%)	0	100	100
17	7l	121/943 (13%)	121 (100%)	0	100	100
18	M1	294/294 (100%)	292 (99%)	2 (1%)	81	91
18	m1	294/294 (100%)	292 (99%)	2 (1%)	81	91
19	M2	259/259 (100%)	256 (99%)	3 (1%)	67	85
19	m2	259/259 (100%)	256 (99%)	3 (1%)	67	85
20	M3	275/276 (100%)	272 (99%)	3 (1%)	70	87
20	m3	275/276 (100%)	272 (99%)	3 (1%)	70	87
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%)	52 (98%)	1 (2%)	52	78
24	t4	53/62 (86%)	52 (98%)	1 (2%)	52	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
26	t6	61/62 (98%)	61 (100%)	0	100	100
27	BP	308/308 (100%)	307 (100%)	1 (0%)	91	96
27	bp	308/308 (100%)	307 (100%)	1 (0%)	91	96
28	FS	164/164 (100%)	163 (99%)	1 (1%)	84	92
28	fs	164/164 (100%)	162 (99%)	2 (1%)	67	85
29	AC	87/113 (77%)	85 (98%)	2 (2%)	45	74
29	ac	87/113 (77%)	85 (98%)	2 (2%)	45	74
30	Y7	328/442 (74%)	324 (99%)	4 (1%)	67	85
30	y7	328/442 (74%)	323 (98%)	5 (2%)	60	82
31	Y0	83/83 (100%)	83 (100%)	0	100	100
31	y0	83/83 (100%)	82 (99%)	1 (1%)	67	85
32	Y5	101/185 (55%)	99 (98%)	2 (2%)	50	77
32	y5	101/185 (55%)	99 (98%)	2 (2%)	50	77
33	A	409/447 (92%)	406 (99%)	3 (1%)	81	91
33	a	409/447 (92%)	406 (99%)	3 (1%)	81	91
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%)	7	28
35	c	44/1405 (3%)	40 (91%)	4 (9%)	7	28
36	D	250/358 (70%)	248 (99%)	2 (1%)	79	90
36	d	250/358 (70%)	248 (99%)	2 (1%)	79	90
37	E	341/342 (100%)	338 (99%)	3 (1%)	75	89
37	e	341/342 (100%)	338 (99%)	3 (1%)	75	89
38	F	218/318 (69%)	217 (100%)	1 (0%)	86	94
38	f	218/318 (69%)	217 (100%)	1 (0%)	86	94
39	G	260/289 (90%)	258 (99%)	2 (1%)	79	90
39	g	260/289 (90%)	258 (99%)	2 (1%)	79	90
40	H	209/272 (77%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	h	209/272 (77%)	209 (100%)	0	100	100
41	I	90/219 (41%)	90 (100%)	0	100	100
41	i	90/219 (41%)	90 (100%)	0	100	100
42	J	170/216 (79%)	169 (99%)	1 (1%)	84	92
42	j	170/216 (79%)	169 (99%)	1 (1%)	84	92
43	K	191/213 (90%)	189 (99%)	2 (1%)	73	88
43	k	191/213 (90%)	189 (99%)	2 (1%)	73	88
44	L	181/206 (88%)	179 (99%)	2 (1%)	70	87
44	l	181/206 (88%)	179 (99%)	2 (1%)	70	87
45	M	166/199 (83%)	164 (99%)	2 (1%)	67	85
45	m	166/199 (83%)	164 (99%)	2 (1%)	67	85
46	N	178/181 (98%)	177 (99%)	1 (1%)	84	92
46	n	178/181 (98%)	177 (99%)	1 (1%)	84	92
47	O	119/180 (66%)	118 (99%)	1 (1%)	79	90
47	o	119/180 (66%)	117 (98%)	2 (2%)	56	80
48	P	156/156 (100%)	154 (99%)	2 (1%)	65	84
48	p	156/156 (100%)	155 (99%)	1 (1%)	84	92
49	Q	157/157 (100%)	155 (99%)	2 (1%)	65	84
49	q	157/157 (100%)	155 (99%)	2 (1%)	65	84
50	R	144/157 (92%)	142 (99%)	2 (1%)	62	83
50	r	144/157 (92%)	142 (99%)	2 (1%)	62	83
51	S	129/154 (84%)	127 (98%)	2 (2%)	58	81
51	s	129/154 (84%)	127 (98%)	2 (2%)	58	81
52	T	138/139 (99%)	137 (99%)	1 (1%)	81	91
52	t	138/139 (99%)	137 (99%)	1 (1%)	81	91
53	U	137/138 (99%)	136 (99%)	1 (1%)	81	91
53	u	137/138 (99%)	136 (99%)	1 (1%)	81	91
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%)	90 (98%)	2 (2%)	47	75
55	w	92/113 (81%)	90 (98%)	2 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	X	105/105 (100%)	104 (99%)	1 (1%)	73	88
56	x	105/105 (100%)	103 (98%)	2 (2%)	52	78
57	Y	88/88 (100%)	86 (98%)	2 (2%)	45	74
57	y	88/88 (100%)	84 (96%)	4 (4%)	23	56
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%)	19298 (99%)	208 (1%)	69	87

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	U6	156	PHE
7	C1	57	TYR
7	C1	164	ARG
7	C1	275	THR
7	C1	404	PHE
7	C1	414	THR
7	C1	503	PHE
7	C1	591	HIS
7	C1	621	MET
7	C1	672	ARG
8	C2	59	ARG
8	C2	224	PHE
8	C2	238	TYR
8	C2	291	PHE
8	C2	335	THR
8	C2	348	ARG
8	C2	409	ILE
8	C2	501	VAL
8	C2	526	ASP
8	C2	536	THR
8	C2	559	HIS
9	C3	48	LEU
9	C3	89	LYS
9	C3	108	MET
9	C3	228	TYR
9	C3	382	ASN
9	C3	425	TYR
9	C3	579	PHE
10	5B	68	LEU

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Mol	Chain	Res	Type
10	5B	93	THR
10	5B	109	ASP
10	5B	145	ASN
10	5B	166	ASN
10	5B	554	ARG
10	5B	565	TRP
11	6A	8	ARG
12	6B	46	GLU
12	6B	182	ASP
14	6C	75	GLU
16	7C	81	THR
16	7C	106	TRP
16	7C	110	HIS
16	7C	167	GLU
18	M1	14	LEU
18	M1	329	THR
19	M2	2	ASN
19	M2	3	TYR
19	M2	40	ARG
20	M3	34	GLN
20	M3	77	ASP
20	M3	206	ARG
24	T4	54	PHE
27	BP	326	GLN
28	FS	18	LEU
29	AC	33	TYR
29	AC	112	ASP
30	Y7	208	LEU
30	Y7	400	TYR
30	Y7	406	HIS
30	Y7	453	PHE
32	Y5	174	ARG
32	Y5	190	TYR
33	A	163	ARG
33	A	334	ASN
33	A	386	THR
35	C	460	THR
35	C	463	PHE
35	C	464	ASN
35	C	468	PHE
36	D	166	VAL
36	D	186	ARG

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Mol	Chain	Res	Type
37	E	53	THR
37	E	280	TRP
37	E	381	LYS
38	F	254	GLN
39	G	169	THR
39	G	279	GLU
42	J	130	CYS
43	K	48	ASP
43	K	230	ASN
44	L	55	LYS
44	L	138	ARG
45	M	121	TYR
45	M	176	MET
46	N	56	TYR
47	O	163	ASN
48	P	90	PHE
48	P	151	GLU
49	Q	70	HIS
49	Q	128	ARG
50	R	94	ARG
50	R	111	TYR
51	S	69	ARG
51	S	117	ASP
52	T	94	ARG
53	U	115	PHE
55	W	36	TYR
55	W	103	TYR
56	X	65	PHE
57	Y	21	GLU
57	Y	67	THR
6	u6	156	PHE
7	c1	57	TYR
7	c1	164	ARG
7	c1	275	THR
7	c1	310	PHE
7	c1	414	THR
7	c1	503	PHE
7	c1	591	HIS
7	c1	592	ASP
7	c1	621	MET
7	c1	672	ARG
8	c2	59	ARG

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Mol	Chain	Res	Type
8	c2	224	PHE
8	c2	238	TYR
8	c2	291	PHE
8	c2	335	THR
8	c2	348	ARG
8	c2	409	ILE
8	c2	501	VAL
8	c2	526	ASP
8	c2	536	THR
8	c2	559	HIS
9	c3	48	LEU
9	c3	89	LYS
9	c3	108	MET
9	c3	228	TYR
9	c3	382	ASN
9	c3	425	TYR
9	c3	579	PHE
10	5b	68	LEU
10	5b	93	THR
10	5b	109	ASP
10	5b	166	ASN
10	5b	554	ARG
10	5b	565	TRP
11	6a	8	ARG
12	6b	46	GLU
12	6b	133	CYS
12	6b	182	ASP
14	6c	75	GLU
16	7c	81	THR
16	7c	106	TRP
16	7c	110	HIS
18	m1	14	LEU
18	m1	329	THR
19	m2	3	TYR
19	m2	40	ARG
19	m2	107	THR
20	m3	34	GLN
20	m3	77	ASP
20	m3	206	ARG
24	t4	54	PHE
27	bp	326	GLN
28	fs	1	MET

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Mol	Chain	Res	Type
28	fs	18	LEU
29	ac	33	TYR
29	ac	112	ASP
30	y7	106	LYS
30	y7	208	LEU
30	y7	400	TYR
30	y7	406	HIS
30	y7	453	PHE
31	y0	52	GLU
32	y5	174	ARG
32	y5	190	TYR
33	a	163	ARG
33	a	334	ASN
33	a	386	THR
36	d	166	VAL
36	d	186	ARG
37	e	53	THR
37	e	280	TRP
37	e	381	LYS
38	f	254	GLN
39	g	169	THR
39	g	279	GLU
42	j	130	CYS
43	k	48	ASP
43	k	230	ASN
44	l	55	LYS
44	l	138	ARG
45	m	121	TYR
45	m	176	MET
46	n	56	TYR
47	o	68	GLU
47	o	163	ASN
48	p	90	PHE
49	q	70	HIS
49	q	128	ARG
50	r	94	ARG
50	r	111	TYR
51	s	69	ARG
51	s	117	ASP
52	t	94	ARG
53	u	115	PHE
55	w	36	TYR

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Mol	Chain	Res	Type
55	w	103	TYR
56	x	65	PHE
56	x	119	LYS
57	y	1	MET
57	y	4	THR
57	y	21	GLU
57	y	67	THR
35	c	460	THR
35	c	463	PHE
35	c	464	ASN
35	c	468	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
8	C2	96	ASN
9	C3	575	GLN
10	5B	164	GLN
18	M1	120	ASN
27	BP	260	ASN
27	BP	283	ASN
30	Y7	118	ASN
30	Y7	172	ASN
30	Y7	191	ASN
35	C	456	HIS
38	F	254	GLN
8	c2	96	ASN
9	c3	33	ASN
18	m1	120	ASN
27	bp	260	ASN
27	bp	283	ASN
30	y7	118	ASN
30	y7	172	ASN
30	y7	191	ASN
38	f	254	GLN
39	g	55	GLN
43	k	30	GLN
48	p	36	ASN
48	p	75	GLN
35	c	456	HIS

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

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
19	FME	M2	1	19	-	4/7/9/11	-
15	FME	7a	1	15	-	4/7/9/11	-
16	SEP	7c	197	16	-	0/6/8/10	-
16	SEP	7C	197	16	-	2/6/8/10	-
15	FME	7A	1	15	-	4/7/9/11	-
24	FME	T4	1	24	-	4/7/9/11	-
37	FME	e	1	37	-	5/7/9/11	-
37	FME	E	1	37	-	5/7/9/11	-
16	SEP	7C	120	16	-	0/6/8/10	-
26	FME	T6	1	26	-	5/7/9/11	-
13	FME	6l	1	13	-	6/7/9/11	-
10	SEP	5B	520	10	-	3/6/8/10	-
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	-
24	FME	t4	1	24	-	4/7/9/11	-
31	FME	y0	1	31	-	5/7/9/11	-
16	SEP	7c	120	16	-	0/6/8/10	-
48	FME	p	1	48	-	3/7/9/11	-
26	FME	t6	1	26	-	5/7/9/11	-
10	SEP	5b	520	10	-	3/6/8/10	-
13	FME	6L	1	13	-	5/7/9/11	-
19	FME	m2	1	19	-	4/7/9/11	-
10	TPO	5B	387	10	-	1/9/11/13	-

All (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	3.42	1.61	1.50
16	7C	120	SEP	P-O1P	3.41	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7c	197	SEP	P-O1P	3.39	1.61	1.50

All (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	106.98	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
16	7c	120	SEP	OG-CB-CA	2.84	110.91	108.14
10	5b	520	SEP	OG-CB-CA	2.75	110.82	108.14
10	5B	520	SEP	OG-CB-CA	2.66	110.73	108.14

There are no chirality outliers.

All (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
13	6L	1	FME	N-CA-CB-CG
13	6L	1	FME	C-CA-CB-CG
13	6L	1	FME	O-C-CA-CB
15	7A	1	FME	O1-CN-N-CA
15	7A	1	FME	C-CA-CB-CG
15	7A	1	FME	O-C-CA-CB
16	7C	197	SEP	CB-OG-P-O1P
16	7C	197	SEP	CB-OG-P-O2P
19	M2	1	FME	O1-CN-N-CA
19	M2	1	FME	N-CA-CB-CG
24	T4	1	FME	O1-CN-N-CA
24	T4	1	FME	CB-CA-N-CN
26	T6	1	FME	O1-CN-N-CA
26	T6	1	FME	CB-CA-N-CN
31	Y0	1	FME	O1-CN-N-CA
31	Y0	1	FME	C-CA-CB-CG
37	E	1	FME	O1-CN-N-CA
37	E	1	FME	CB-CA-N-CN
37	E	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
48	P	1	FME	O1-CN-N-CA
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
13	6l	1	FME	CB-CA-N-CN
13	6l	1	FME	C-CA-CB-CG
13	6l	1	FME	O-C-CA-CB
15	7a	1	FME	O1-CN-N-CA
15	7a	1	FME	C-CA-CB-CG
15	7a	1	FME	O-C-CA-CB
19	m2	1	FME	O1-CN-N-CA
19	m2	1	FME	N-CA-CB-CG
24	t4	1	FME	O1-CN-N-CA
24	t4	1	FME	CB-CA-N-CN
26	t6	1	FME	O1-CN-N-CA
26	t6	1	FME	CB-CA-N-CN
31	y0	1	FME	O1-CN-N-CA
31	y0	1	FME	C-CA-CB-CG
37	e	1	FME	O1-CN-N-CA
37	e	1	FME	CB-CA-N-CN
37	e	1	FME	N-CA-CB-CG
48	p	1	FME	O1-CN-N-CA
31	y0	1	FME	CA-CB-CG-SD
13	6L	1	FME	CA-CB-CG-SD
31	Y0	1	FME	CA-CB-CG-SD
15	7A	1	FME	N-CA-CB-CG
13	6l	1	FME	N-CA-CB-CG
15	7a	1	FME	N-CA-CB-CG
37	E	1	FME	CB-CG-SD-CE
48	P	1	FME	N-CA-CB-CG
24	t4	1	FME	N-CA-CB-CG
31	y0	1	FME	N-CA-CB-CG
48	p	1	FME	N-CA-CB-CG
24	t4	1	FME	CB-CG-SD-CE
37	e	1	FME	CB-CG-SD-CE
24	T4	1	FME	CB-CG-SD-CE
13	6l	1	FME	CB-CG-SD-CE
24	T4	1	FME	N-CA-CB-CG
26	T6	1	FME	CB-CG-SD-CE
19	M2	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
37	E	1	FME	C-CA-CB-CG
19	m2	1	FME	C-CA-CB-CG
26	t6	1	FME	C-CA-CB-CG
37	e	1	FME	C-CA-CB-CG
19	M2	1	FME	CB-CA-N-CN
31	Y0	1	FME	CB-CA-N-CN
19	m2	1	FME	CB-CA-N-CN
26	t6	1	FME	N-CA-CB-CG
26	t6	1	FME	CB-CG-SD-CE
26	T6	1	FME	C-CA-CB-CG
26	T6	1	FME	N-CA-CB-CG
48	P	1	FME	CB-CA-N-CN
48	p	1	FME	CB-CA-N-CN
31	Y0	1	FME	N-CA-CB-CG
31	y0	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
59	HEA	C1	702	7	58,67,67	1.17	5 (8%)	63,103,103	1.62	15 (23%)
63	CDL	c1	706	-	58,58,99	0.38	0	64,70,111	0.41	0
63	CDL	M1	401	-	94,94,99	0.31	0	100,106,111	0.32	0
62	PC1	A	501	-	44,44,53	0.31	0	50,52,61	0.36	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	7c	302	-	50,50,99	0.41	0	56,62,111	0.34	0
62	PC1	a	501	-	44,44,53	0.31	0	50,52,61	0.36	0
63	CDL	a	503	-	50,50,99	0.41	0	56,62,111	0.51	0
63	CDL	v	201	-	90,90,99	0.32	0	96,102,111	0.37	0
63	CDL	7c	301	-	84,84,99	0.32	0	90,96,111	0.34	0
63	CDL	7C	301	-	84,84,99	0.32	0	90,96,111	0.34	0
62	PC1	C3	602	-	38,38,53	0.33	0	44,46,61	0.34	0
62	PC1	m1	402	-	53,53,53	0.29	0	59,61,61	0.35	0
63	CDL	5b	703	-	66,66,99	0.36	0	72,78,111	0.33	0
62	PC1	c1	705	-	48,48,53	0.31	0	54,56,61	0.31	0
63	CDL	M3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
63	CDL	y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
62	PC1	C3	601	-	51,51,53	0.29	0	57,59,61	0.38	0
63	CDL	M3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
63	CDL	M2	401	-	53,53,99	0.40	0	59,65,111	0.39	0
63	CDL	Y0	101	-	63,63,99	0.37	0	69,75,111	0.34	0
63	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.33	0
63	CDL	M1	403	-	65,65,99	0.36	0	71,77,111	0.30	0
62	PC1	n	301	-	31,31,53	0.36	0	37,39,61	0.36	0
63	CDL	M3	401	-	93,93,99	0.30	0	99,105,111	0.34	0
63	CDL	5B	703	-	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
62	PC1	A	502	-	40,40,53	0.33	0	46,48,61	0.39	0
63	CDL	Y7	501	-	64,64,99	0.37	0	70,76,111	0.37	0
62	PC1	M2	402	-	31,31,53	0.37	0	37,39,61	0.37	0
62	PC1	M1	404	-	34,34,53	0.35	0	40,42,61	0.33	0
63	CDL	5B	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	m1	403	-	65,65,99	0.36	0	71,77,111	0.32	0
62	PC1	7C	304	-	42,42,53	0.32	0	48,50,61	0.30	0
63	CDL	C3	604	-	67,67,99	0.36	0	73,79,111	0.30	0
63	CDL	T	201	-	67,67,99	0.36	0	73,79,111	0.35	0
63	CDL	t	202	-	74,74,99	0.34	0	80,86,111	0.35	0
62	PC1	J	302	-	36,36,53	0.34	0	42,44,61	0.33	0
62	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.38	0
63	CDL	k	301	-	61,61,99	0.37	0	67,73,111	0.33	0
63	CDL	m2	401	-	53,53,99	0.40	0	59,65,111	0.40	0
59	HEA	c1	701	7	58,67,67	1.12	5 (8%)	63,103,103	1.61	15 (23%)
63	CDL	7a	202	-	99,99,99	0.30	0	105,111,111	0.30	0
63	CDL	l	301	-	73,73,99	0.34	0	79,85,111	0.29	0
63	CDL	T	202	-	74,74,99	0.34	0	80,86,111	0.35	0
63	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.30	0
62	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	PC1	v	202	-	53,53,53	0.29	0	59,61,61	0.33	0
63	CDL	E	401	-	59,59,99	0.38	0	65,71,111	0.38	0
63	CDL	c1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
63	CDL	f	401	-	99,99,99	0.29	0	105,111,111	0.35	0
65	FES	fs	201	28	0,4,4	-	-	-		
63	CDL	U	201	-	81,81,99	0.32	0	87,93,111	0.32	0
62	PC1	m2	405	-	40,40,53	0.33	0	46,48,61	0.33	0
63	CDL	m2	404	-	73,73,99	0.34	0	79,85,111	0.35	0
62	PC1	m1	405	-	34,34,53	0.35	0	40,42,61	0.32	0
63	CDL	m1	404	-	65,65,99	0.36	0	71,77,111	0.30	0
62	PC1	j	302	-	36,36,53	0.34	0	42,44,61	0.33	0
63	CDL	m3	401	-	93,93,99	0.30	0	99,105,111	0.33	0
59	HEA	C1	701	7	58,67,67	1.12	5 (8%)	63,103,103	1.62	15 (23%)
62	PC1	C3	605	-	40,40,53	0.33	0	46,48,61	0.42	0
62	PC1	7c	303	-	42,42,53	0.32	0	48,50,61	0.30	0
65	FES	fs	202	28	0,4,4	-	-	-		
63	CDL	F	401	-	99,99,99	0.29	0	105,111,111	0.36	0
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
62	PC1	M2	406	-	53,53,53	0.29	0	59,61,61	0.28	0
62	PC1	7C	302	-	53,53,53	0.29	0	59,61,61	0.36	0
62	PC1	m2	402	-	31,31,53	0.37	0	37,39,61	0.37	0
63	CDL	t	201	-	67,67,99	0.36	0	73,79,111	0.35	0
65	FES	FS	201	28	0,4,4	-	-	-		
62	PC1	c3	602	-	38,38,53	0.33	0	44,46,61	0.34	0
63	CDL	C1	706	-	58,58,99	0.38	0	64,70,111	0.40	0
63	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0
63	CDL	V	201	-	90,90,99	0.32	0	96,102,111	0.37	0
62	PC1	N	302	-	35,35,53	0.36	0	41,43,61	0.35	0
63	CDL	7A	202	-	99,99,99	0.30	0	105,111,111	0.29	0
63	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	a	502	-	40,40,53	0.34	0	46,48,61	0.40	0
65	FES	FS	202	28	0,4,4	-	-	-		
62	PC1	c3	605	-	40,40,53	0.33	0	46,48,61	0.42	0
62	PC1	C1	705	-	48,48,53	0.31	0	54,56,61	0.31	0
63	CDL	u	201	-	81,81,99	0.32	0	87,93,111	0.32	0
63	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.35	0
63	CDL	5B	704	-	66,66,99	0.36	0	72,78,111	0.34	0
63	CDL	e	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.32	0
62	PC1	m2	406	-	53,53,53	0.29	0	59,61,61	0.28	0
63	CDL	Y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
63	CDL	5b	702	-	86,86,99	0.32	0	92,98,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.39	0
63	CDL	e	401	-	59,59,99	0.38	0	65,71,111	0.38	0
63	CDL	c3	604	-	67,67,99	0.36	0	73,79,111	0.31	0
63	CDL	N	303	-	94,94,99	0.31	0	100,106,111	0.36	0
59	HEA	c1	702	7	58,67,67	1.17	5 (8%)	63,103,103	1.62	16 (25%)
63	CDL	7a	201	-	66,66,99	0.36	0	72,78,111	0.38	0
63	CDL	m1	401	-	94,94,99	0.31	0	100,106,111	0.32	0
63	CDL	7C	303	-	50,50,99	0.41	0	56,62,111	0.35	0
62	PC1	N	301	-	31,31,53	0.36	0	37,39,61	0.36	0
63	CDL	E	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	y0	101	-	63,63,99	0.37	0	69,75,111	0.34	0
62	PC1	V	202	-	53,53,53	0.29	0	59,61,61	0.33	0
63	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.30	0
63	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
63	CDL	m3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
63	CDL	m3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
63	CDL	A	503	-	50,50,99	0.41	0	56,62,111	0.50	0
63	CDL	n	303	-	94,94,99	0.31	0	100,106,111	0.37	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
59	HEA	C1	702	7	-	10/32/76/76	-
63	CDL	c1	706	-	-	19/69/69/110	-
63	CDL	M1	401	-	-	27/105/105/110	-
62	PC1	A	501	-	-	11/48/48/57	-
62	PC1	n	302	-	-	4/39/39/57	-
63	CDL	7c	302	-	-	15/61/61/110	-
62	PC1	a	501	-	-	13/48/48/57	-
63	CDL	a	503	-	-	12/61/61/110	-
63	CDL	v	201	-	-	13/101/101/110	-
63	CDL	7c	301	-	-	24/95/95/110	-
63	CDL	7C	301	-	-	22/95/95/110	-
62	PC1	C3	602	-	-	10/42/42/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	m1	402	-	-	16/57/57/57	-
63	CDL	5b	703	-	-	11/77/77/110	-
62	PC1	c1	705	-	-	9/52/52/57	-
63	CDL	M3	403	-	-	17/73/73/110	-
63	CDL	y5	201	-	-	15/91/91/110	-
62	PC1	C3	601	-	-	12/55/55/57	-
63	CDL	M3	402	-	-	13/61/61/110	-
63	CDL	M2	401	-	-	15/64/64/110	-
63	CDL	Y0	101	-	-	17/74/74/110	-
63	CDL	b	501	-	-	14/72/72/110	-
63	CDL	M1	403	-	-	9/76/76/110	-
62	PC1	n	301	-	-	13/35/35/57	-
63	CDL	M3	401	-	-	20/104/104/110	-
63	CDL	5B	703	-	-	14/72/72/110	-
63	CDL	7A	201	-	-	12/77/77/110	-
62	PC1	A	502	-	-	11/44/44/57	-
63	CDL	Y7	501	-	-	11/75/75/110	-
62	PC1	M2	402	-	-	4/35/35/57	-
62	PC1	M1	404	-	-	8/38/38/57	-
63	CDL	5B	702	-	-	23/97/97/110	-
63	CDL	m1	403	-	-	15/76/76/110	-
62	PC1	7C	304	-	-	12/46/46/57	-
63	CDL	C3	604	-	-	9/78/78/110	-
63	CDL	T	201	-	-	12/78/78/110	-
63	CDL	t	202	-	-	14/85/85/110	-
62	PC1	J	302	-	-	7/40/40/57	-
62	PC1	c3	601	-	-	12/55/55/57	-
63	CDL	k	301	-	-	14/72/72/110	-
63	CDL	m2	401	-	-	18/64/64/110	-
59	HEA	c1	701	7	-	16/32/76/76	-
63	CDL	7a	202	-	-	23/110/110/110	-
63	CDL	l	301	-	-	21/84/84/110	-
63	CDL	T	202	-	-	13/85/85/110	-
63	CDL	j	301	-	-	13/80/80/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	C3	603	-	-	10/34/34/57	-
62	PC1	v	202	-	-	9/57/57/57	-
63	CDL	E	401	-	-	17/70/70/110	-
63	CDL	c1	707	-	-	10/75/75/110	-
63	CDL	f	401	-	-	17/110/110/110	-
65	FES	fs	201	28	-	-	0/1/1/1
63	CDL	U	201	-	-	17/92/92/110	-
62	PC1	m2	405	-	-	6/44/44/57	-
63	CDL	m2	404	-	-	16/84/84/110	-
62	PC1	m1	405	-	-	8/38/38/57	-
63	CDL	m1	404	-	-	10/76/76/110	-
62	PC1	j	302	-	-	8/40/40/57	-
63	CDL	m3	401	-	-	19/104/104/110	-
59	HEA	C1	701	7	-	15/32/76/76	-
62	PC1	C3	605	-	-	10/44/44/57	-
62	PC1	7c	303	-	-	13/46/46/57	-
65	FES	fs	202	28	-	-	0/1/1/1
63	CDL	F	401	-	-	19/110/110/110	-
62	PC1	M2	405	-	-	11/44/44/57	-
63	CDL	y7	501	-	-	10/75/75/110	-
62	PC1	M2	406	-	-	8/57/57/57	-
62	PC1	7C	302	-	-	17/57/57/57	-
62	PC1	m2	402	-	-	3/35/35/57	-
63	CDL	t	201	-	-	10/78/78/110	-
65	FES	FS	201	28	-	-	0/1/1/1
62	PC1	c3	602	-	-	9/42/42/57	-
63	CDL	C1	706	-	-	17/69/69/110	-
63	CDL	L	301	-	-	21/84/84/110	-
63	CDL	V	201	-	-	14/101/101/110	-
62	PC1	N	302	-	-	4/39/39/57	-
63	CDL	7A	202	-	-	19/110/110/110	-
63	CDL	B	501	-	-	14/72/72/110	-
62	PC1	a	502	-	-	9/44/44/57	-
65	FES	FS	202	28	-	-	0/1/1/1
62	PC1	c3	605	-	-	9/44/44/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	C1	705	-	-	12/52/52/57	-
63	CDL	u	201	-	-	15/92/92/110	-
63	CDL	M2	404	-	-	17/84/84/110	-
63	CDL	5B	704	-	-	9/77/77/110	-
63	CDL	e	402	-	-	14/82/82/110	-
63	CDL	m2	403	-	-	15/76/76/110	-
62	PC1	m2	406	-	-	8/57/57/57	-
63	CDL	Y5	201	-	-	16/91/91/110	-
63	CDL	5b	702	-	-	23/97/97/110	-
62	PC1	c3	603	-	-	10/34/34/57	-
63	CDL	e	401	-	-	16/70/70/110	-
63	CDL	c3	604	-	-	9/78/78/110	-
63	CDL	N	303	-	-	22/105/105/110	-
59	HEA	c1	702	7	-	11/32/76/76	-
63	CDL	7a	201	-	-	13/77/77/110	-
63	CDL	m1	401	-	-	26/105/105/110	-
63	CDL	7C	303	-	-	15/61/61/110	-
62	PC1	N	301	-	-	13/35/35/57	-
63	CDL	E	402	-	-	14/82/82/110	-
63	CDL	M1	402	-	-	15/76/76/110	-
63	CDL	y0	101	-	-	21/74/74/110	-
62	PC1	V	202	-	-	10/57/57/57	-
63	CDL	J	301	-	-	12/80/80/110	-
63	CDL	C1	707	-	-	11/75/75/110	-
63	CDL	m3	403	-	-	18/73/73/110	-
63	CDL	m3	402	-	-	13/61/61/110	-
63	CDL	A	503	-	-	8/61/61/110	-
63	CDL	n	303	-	-	22/105/105/110	-
63	CDL	M2	403	-	-	15/76/76/110	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	702	HEA	C3A-C2A	-3.76	1.35	1.40
59	C1	702	HEA	C3A-C2A	-3.73	1.35	1.40
59	c1	702	HEA	C4D-C3D	3.26	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	C1	702	HEA	C4D-C3D	3.25	1.50	1.45
59	c1	701	HEA	C3A-C2A	-2.96	1.36	1.40
59	C1	701	HEA	C4D-C3D	2.94	1.50	1.45
59	C1	701	HEA	C1D-ND	-2.92	1.35	1.40
59	c1	701	HEA	C1D-ND	-2.92	1.35	1.40
59	c1	701	HEA	C4D-C3D	2.91	1.50	1.45
59	C1	701	HEA	C3A-C2A	-2.90	1.36	1.40
59	c1	702	HEA	C1D-ND	-2.82	1.35	1.40
59	C1	702	HEA	C1D-ND	-2.80	1.35	1.40
59	C1	701	HEA	C4B-NB	-2.44	1.36	1.40
59	c1	701	HEA	C4B-NB	-2.43	1.36	1.40
59	c1	702	HEA	C4B-NB	-2.41	1.36	1.40
59	C1	702	HEA	C4B-NB	-2.41	1.36	1.40
59	C1	702	HEA	C3C-C2C	-2.31	1.37	1.40
59	c1	702	HEA	C3C-C2C	-2.27	1.37	1.40
59	c1	701	HEA	C3C-C2C	-2.14	1.37	1.40
59	C1	701	HEA	C3C-C2C	-2.10	1.37	1.40

All (61) 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	CMC-C2C-C1C	-3.40	123.47	128.46
59	C1	702	HEA	CMC-C2C-C1C	-3.35	123.54	128.46
59	C1	702	HEA	C13-C14-C15	-3.30	120.06	127.62
59	c1	702	HEA	C13-C14-C15	-3.27	120.13	127.62
59	C1	701	HEA	C4B-NB-C1B	3.21	109.01	105.21
59	C1	702	HEA	C17-C18-C19	-3.20	120.29	127.62
59	c1	702	HEA	C17-C18-C19	-3.19	120.33	127.62
59	c1	701	HEA	CAA-CBA-CGA	-3.17	105.30	113.83
59	C1	701	HEA	CAA-CBA-CGA	-3.17	105.30	113.83
59	c1	701	HEA	C4B-NB-C1B	3.12	108.90	105.21
59	C1	701	HEA	C13-C14-C15	-2.96	120.84	127.62
59	C1	701	HEA	C1D-ND-C4D	2.92	108.67	105.21
59	c1	701	HEA	C13-C14-C15	-2.92	120.94	127.62
59	c1	701	HEA	C17-C18-C19	-2.91	120.95	127.62
59	C1	701	HEA	C17-C18-C19	-2.90	120.99	127.62
59	C1	701	HEA	CMC-C2C-C1C	-2.88	124.24	128.46
59	c1	701	HEA	CMC-C2C-C1C	-2.83	124.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c1	701	HEA	C1D-ND-C4D	2.83	108.56	105.21
59	c1	702	HEA	C1D-ND-C4D	2.73	108.44	105.21
59	C1	702	HEA	C1D-ND-C4D	2.69	108.39	105.21
59	C1	702	HEA	C26-C15-C16	2.60	119.73	115.23
59	c1	701	HEA	C27-C19-C20	2.55	119.65	115.23
59	c1	702	HEA	C26-C15-C16	2.52	119.61	115.23
59	c1	702	HEA	C3D-C4D-ND	-2.49	107.94	110.35
59	C1	702	HEA	C3D-C4D-ND	-2.45	107.98	110.35
59	C1	701	HEA	C27-C19-C20	2.45	119.48	115.23
59	C1	702	HEA	C4D-CHA-C1A	2.36	125.67	122.56
59	c1	702	HEA	C27-C19-C20	2.35	119.31	115.23
59	C1	701	HEA	CMB-C2B-C3B	-2.33	125.78	130.28
59	c1	702	HEA	C4D-CHA-C1A	2.32	125.63	122.56
59	C1	702	HEA	C27-C19-C20	2.32	119.25	115.23
59	C1	701	HEA	C3D-C4D-ND	-2.32	108.11	110.35
59	c1	701	HEA	CMB-C2B-C3B	-2.30	125.83	130.28
59	C1	701	HEA	C26-C15-C16	2.29	119.21	115.23
59	C1	701	HEA	CBA-CAA-C2A	2.29	116.33	112.55
59	C1	702	HEA	CMB-C2B-C3B	-2.28	125.88	130.28
59	c1	702	HEA	CMB-C2B-C3B	-2.25	125.92	130.28
59	c1	701	HEA	C26-C15-C16	2.25	119.14	115.23
59	c1	701	HEA	C3D-C4D-ND	-2.25	108.18	110.35
59	c1	701	HEA	CBA-CAA-C2A	2.23	116.22	112.55
59	C1	702	HEA	CAA-CBA-CGA	-2.19	107.92	113.83
59	c1	702	HEA	CAD-CBD-CGD	-2.18	107.87	113.67
59	C1	702	HEA	CAD-CBD-CGD	-2.17	107.90	113.67
59	c1	702	HEA	CAD-C3D-C4D	2.17	128.48	124.70
59	C1	702	HEA	C25-C23-C24	2.17	119.58	114.59
59	C1	702	HEA	CAD-C3D-C4D	2.14	128.43	124.70
59	c1	702	HEA	CAA-CBA-CGA	-2.14	108.07	113.83
59	c1	702	HEA	C21-C22-C23	-2.14	120.52	127.64
59	C1	702	HEA	C21-C22-C23	-2.13	120.55	127.64
59	c1	702	HEA	C25-C23-C24	2.12	119.47	114.59
59	C1	701	HEA	C3B-C4B-NB	-2.08	107.45	109.84
59	c1	701	HEA	C21-C22-C23	-2.07	120.73	127.64
59	C1	701	HEA	CAD-CBD-CGD	-2.07	108.18	113.67
59	c1	701	HEA	CAD-CBD-CGD	-2.05	108.22	113.67
59	C1	701	HEA	C21-C22-C23	-2.05	120.80	127.64
59	c1	701	HEA	C3B-C4B-NB	-2.02	107.52	109.84
59	c1	702	HEA	OMA-CMA-C3A	-2.01	120.03	124.80

There are no chirality outliers.

All (1445) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	C1	701	HEA	C1A-C2A-CAA-CBA
59	C1	701	HEA	C3A-C2A-CAA-CBA
59	C1	701	HEA	C26-C15-C16-C17
59	C1	701	HEA	C15-C16-C17-C18
59	C1	701	HEA	C17-C18-C19-C20
59	C1	701	HEA	C17-C18-C19-C27
59	C1	702	HEA	C13-C14-C15-C16
59	C1	702	HEA	C13-C14-C15-C26
59	C1	702	HEA	C17-C18-C19-C27
59	c1	701	HEA	C1A-C2A-CAA-CBA
59	c1	701	HEA	C3A-C2A-CAA-CBA
59	c1	701	HEA	C15-C16-C17-C18
59	c1	701	HEA	C17-C18-C19-C20
59	c1	701	HEA	C17-C18-C19-C27
59	c1	702	HEA	C13-C14-C15-C16
59	c1	702	HEA	C13-C14-C15-C26
59	c1	702	HEA	C17-C18-C19-C27
62	C1	705	PC1	C11-O13-P-O12
62	C3	601	PC1	C1-O11-P-O14
62	C3	601	PC1	C1-O11-P-O13
62	C3	601	PC1	C2-C1-O11-P
62	C3	602	PC1	C1-O11-P-O12
62	C3	602	PC1	O21-C2-C3-O31
62	C3	603	PC1	C11-O13-P-O12
62	7C	302	PC1	C11-O13-P-O14
62	7C	302	PC1	C11-O13-P-O11
62	7C	302	PC1	C1-O11-P-O12
62	7C	302	PC1	C1-O11-P-O14
62	7C	302	PC1	C1-O11-P-O13
62	7C	304	PC1	C11-O13-P-O12
62	7C	304	PC1	C11-O13-P-O14
62	7C	304	PC1	C11-O13-P-O11
62	7C	304	PC1	C1-O11-P-O14
62	M1	404	PC1	C11-O13-P-O12
62	M1	404	PC1	C11-O13-P-O11
62	M2	405	PC1	C11-O13-P-O12
62	M2	406	PC1	C1-O11-P-O12
62	M2	406	PC1	C1-O11-P-O13
62	A	501	PC1	C11-O13-P-O12
62	A	501	PC1	C11-O13-P-O11
62	A	501	PC1	C1-O11-P-O12
62	A	501	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
62	A	501	PC1	C2-C1-O11-P
62	A	502	PC1	C11-O13-P-O11
62	A	502	PC1	C1-O11-P-O13
62	J	302	PC1	C1-O11-P-O12
62	J	302	PC1	C1-O11-P-O14
62	J	302	PC1	C1-O11-P-O13
62	N	301	PC1	C11-O13-P-O14
62	N	301	PC1	C1-O11-P-O12
62	N	301	PC1	C1-O11-P-O14
62	N	302	PC1	C1-O11-P-O13
62	N	302	PC1	O13-C11-C12-N
62	V	202	PC1	C11-O13-P-O12
62	V	202	PC1	C11-O13-P-O14
62	V	202	PC1	C11-O13-P-O11
62	V	202	PC1	C1-O11-P-O14
62	V	202	PC1	C1-O11-P-O13
62	c1	705	PC1	C11-O13-P-O12
62	c1	705	PC1	C11-O13-P-O11
62	c3	601	PC1	C1-O11-P-O14
62	c3	601	PC1	C1-O11-P-O13
62	c3	601	PC1	C2-C1-O11-P
62	c3	602	PC1	C1-O11-P-O12
62	c3	602	PC1	C1-O11-P-O13
62	c3	602	PC1	O21-C2-C3-O31
62	c3	603	PC1	C11-O13-P-O12
62	c3	603	PC1	C11-O13-P-O11
62	7c	303	PC1	C11-O13-P-O12
62	7c	303	PC1	C11-O13-P-O14
62	7c	303	PC1	C11-O13-P-O11
62	7c	303	PC1	C1-O11-P-O14
62	7c	303	PC1	C1-O11-P-O13
62	m1	402	PC1	C11-O13-P-O12
62	m1	402	PC1	C11-O13-P-O14
62	m1	402	PC1	C11-O13-P-O11
62	m1	402	PC1	C1-O11-P-O12
62	m1	402	PC1	C1-O11-P-O14
62	m1	402	PC1	C1-O11-P-O13
62	m1	405	PC1	C11-O13-P-O12
62	m1	405	PC1	C11-O13-P-O14
62	m1	405	PC1	C11-O13-P-O11
62	m2	405	PC1	C11-O13-P-O11
62	m2	406	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
62	m2	406	PC1	C1-O11-P-O13
62	a	501	PC1	C11-O13-P-O12
62	a	501	PC1	C1-O11-P-O12
62	a	502	PC1	C11-O13-P-O11
62	a	502	PC1	C1-O11-P-O13
62	j	302	PC1	C1-O11-P-O12
62	j	302	PC1	C1-O11-P-O14
62	j	302	PC1	C1-O11-P-O13
62	n	301	PC1	C11-O13-P-O14
62	n	301	PC1	C1-O11-P-O12
62	n	301	PC1	C1-O11-P-O14
62	n	302	PC1	C1-O11-P-O13
62	n	302	PC1	O13-C11-C12-N
62	v	202	PC1	C11-O13-P-O12
62	v	202	PC1	C1-O11-P-O14
62	v	202	PC1	C1-O11-P-O13
63	C1	706	CDL	CA2-OA2-PA1-OA3
63	C1	706	CDL	CA2-OA2-PA1-OA5
63	C1	706	CDL	CA3-OA5-PA1-OA2
63	C1	706	CDL	CB2-OB2-PB2-OB3
63	C1	706	CDL	CB3-OB5-PB2-OB2
63	C1	706	CDL	CB3-OB5-PB2-OB3
63	C1	707	CDL	CA2-OA2-PA1-OA3
63	C1	707	CDL	CA3-OA5-PA1-OA2
63	C1	707	CDL	CA3-OA5-PA1-OA3
63	C1	707	CDL	CA3-OA5-PA1-OA4
63	C3	604	CDL	CA2-OA2-PA1-OA3
63	C3	604	CDL	CA2-OA2-PA1-OA4
63	C3	604	CDL	CA2-OA2-PA1-OA5
63	5B	702	CDL	CA2-C1-CB2-OB2
63	5B	702	CDL	CA2-OA2-PA1-OA3
63	5B	702	CDL	CA2-OA2-PA1-OA4
63	5B	702	CDL	CA2-OA2-PA1-OA5
63	5B	702	CDL	CA3-OA5-PA1-OA2
63	5B	702	CDL	CA3-OA5-PA1-OA3
63	5B	702	CDL	CA3-OA5-PA1-OA4
63	5B	703	CDL	CA2-OA2-PA1-OA3
63	5B	703	CDL	CA2-OA2-PA1-OA5
63	5B	703	CDL	CA3-OA5-PA1-OA4
63	5B	704	CDL	CA3-OA5-PA1-OA2
63	5B	704	CDL	CB2-OB2-PB2-OB3
63	7A	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
63	7A	201	CDL	CA2-OA2-PA1-OA5
63	7A	201	CDL	CB2-OB2-PB2-OB4
63	7A	201	CDL	CB2-OB2-PB2-OB5
63	7A	202	CDL	CA3-OA5-PA1-OA3
63	7A	202	CDL	CB2-OB2-PB2-OB3
63	7A	202	CDL	CB2-OB2-PB2-OB5
63	7C	301	CDL	CA3-OA5-PA1-OA2
63	7C	301	CDL	CA3-OA5-PA1-OA3
63	7C	301	CDL	CB2-OB2-PB2-OB4
63	7C	301	CDL	CB3-OB5-PB2-OB2
63	7C	301	CDL	CB3-OB5-PB2-OB3
63	7C	301	CDL	CB3-OB5-PB2-OB4
63	7C	303	CDL	CA2-OA2-PA1-OA3
63	7C	303	CDL	CA2-OA2-PA1-OA4
63	7C	303	CDL	CA2-OA2-PA1-OA5
63	7C	303	CDL	CA3-OA5-PA1-OA2
63	7C	303	CDL	CA3-OA5-PA1-OA3
63	7C	303	CDL	CA3-OA5-PA1-OA4
63	7C	303	CDL	CB2-OB2-PB2-OB3
63	M1	401	CDL	CA2-OA2-PA1-OA4
63	M1	401	CDL	CB2-OB2-PB2-OB4
63	M1	401	CDL	CB3-OB5-PB2-OB2
63	M1	401	CDL	CB3-OB5-PB2-OB3
63	M1	401	CDL	CB3-OB5-PB2-OB4
63	M1	403	CDL	CA2-OA2-PA1-OA3
63	M1	403	CDL	CA3-OA5-PA1-OA2
63	M1	403	CDL	CA3-OA5-PA1-OA3
63	M1	403	CDL	CA3-OA5-PA1-OA4
63	M1	403	CDL	CB2-OB2-PB2-OB4
63	M2	401	CDL	CA2-OA2-PA1-OA3
63	M2	401	CDL	CA3-OA5-PA1-OA4
63	M2	401	CDL	CB3-OB5-PB2-OB3
63	M2	403	CDL	CA2-OA2-PA1-OA3
63	M2	403	CDL	CA2-OA2-PA1-OA4
63	M2	403	CDL	CA2-OA2-PA1-OA5
63	M2	403	CDL	CB2-OB2-PB2-OB5
63	M2	403	CDL	CB3-OB5-PB2-OB2
63	M2	404	CDL	CA2-OA2-PA1-OA3
63	M2	404	CDL	CA2-OA2-PA1-OA5
63	M2	404	CDL	CB2-OB2-PB2-OB3
63	M2	404	CDL	CB2-OB2-PB2-OB4
63	M2	404	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
63	M3	401	CDL	CB2-OB2-PB2-OB4
63	M3	401	CDL	CB2-OB2-PB2-OB5
63	M3	401	CDL	CB3-OB5-PB2-OB2
63	M3	401	CDL	CB3-OB5-PB2-OB3
63	M3	402	CDL	CA2-OA2-PA1-OA5
63	M3	402	CDL	CA3-OA5-PA1-OA4
63	M3	402	CDL	CB2-OB2-PB2-OB3
63	M3	402	CDL	CB2-OB2-PB2-OB4
63	M3	402	CDL	CB2-OB2-PB2-OB5
63	M3	402	CDL	CB3-OB5-PB2-OB2
63	M3	403	CDL	CA2-OA2-PA1-OA5
63	Y7	501	CDL	CA2-OA2-PA1-OA3
63	Y7	501	CDL	CA2-OA2-PA1-OA4
63	Y7	501	CDL	CA2-OA2-PA1-OA5
63	Y7	501	CDL	CB2-OB2-PB2-OB5
63	Y0	101	CDL	CA2-OA2-PA1-OA5
63	Y0	101	CDL	CA3-OA5-PA1-OA3
63	Y0	101	CDL	CB2-OB2-PB2-OB3
63	Y0	101	CDL	CB3-OB5-PB2-OB2
63	Y0	101	CDL	CB3-OB5-PB2-OB3
63	Y5	201	CDL	CA2-OA2-PA1-OA4
63	Y5	201	CDL	CA2-OA2-PA1-OA5
63	Y5	201	CDL	CA3-OA5-PA1-OA4
63	Y5	201	CDL	CB2-OB2-PB2-OB4
63	Y5	201	CDL	CB3-OB5-PB2-OB3
63	A	503	CDL	CA2-OA2-PA1-OA3
63	A	503	CDL	CB3-OB5-PB2-OB2
63	A	503	CDL	CB3-OB5-PB2-OB3
63	B	501	CDL	CA2-OA2-PA1-OA3
63	B	501	CDL	CA2-OA2-PA1-OA4
63	B	501	CDL	CA2-OA2-PA1-OA5
63	B	501	CDL	CA3-OA5-PA1-OA2
63	B	501	CDL	CA3-OA5-PA1-OA3
63	B	501	CDL	CA3-OA5-PA1-OA4
63	E	401	CDL	CA2-OA2-PA1-OA3
63	E	401	CDL	CA2-OA2-PA1-OA5
63	E	401	CDL	CA3-OA5-PA1-OA2
63	E	401	CDL	CA3-OA5-PA1-OA4
63	E	401	CDL	CB3-OB5-PB2-OB2
63	E	401	CDL	CB3-OB5-PB2-OB3
63	E	402	CDL	CA2-OA2-PA1-OA3
63	E	402	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
63	E	402	CDL	CA2-OA2-PA1-OA5
63	E	402	CDL	CB2-OB2-PB2-OB3
63	F	401	CDL	CA3-OA5-PA1-OA2
63	F	401	CDL	CA3-OA5-PA1-OA3
63	F	401	CDL	CB3-OB5-PB2-OB2
63	F	401	CDL	CB3-OB5-PB2-OB3
63	F	401	CDL	CB3-OB5-PB2-OB4
63	J	301	CDL	CA2-OA2-PA1-OA3
63	L	301	CDL	CA2-OA2-PA1-OA3
63	L	301	CDL	CA2-OA2-PA1-OA5
63	L	301	CDL	CA3-OA5-PA1-OA2
63	L	301	CDL	CA3-OA5-PA1-OA4
63	L	301	CDL	CB2-OB2-PB2-OB5
63	L	301	CDL	CB3-OB5-PB2-OB2
63	L	301	CDL	CB3-OB5-PB2-OB3
63	N	303	CDL	CA2-OA2-PA1-OA4
63	N	303	CDL	CA2-OA2-PA1-OA5
63	N	303	CDL	CA3-OA5-PA1-OA2
63	N	303	CDL	CA3-OA5-PA1-OA3
63	N	303	CDL	CA3-OA5-PA1-OA4
63	N	303	CDL	CB2-OB2-PB2-OB3
63	N	303	CDL	CB2-OB2-PB2-OB4
63	N	303	CDL	CB2-OB2-PB2-OB5
63	N	303	CDL	CB3-OB5-PB2-OB2
63	N	303	CDL	CB3-OB5-PB2-OB3
63	N	303	CDL	CB3-OB5-PB2-OB4
63	T	201	CDL	CA2-OA2-PA1-OA5
63	T	201	CDL	CB2-OB2-PB2-OB3
63	T	201	CDL	CB2-OB2-PB2-OB5
63	T	201	CDL	CB3-OB5-PB2-OB3
63	T	202	CDL	CB3-OB5-PB2-OB2
63	T	202	CDL	CB3-OB5-PB2-OB3
63	T	202	CDL	CB3-OB5-PB2-OB4
63	U	201	CDL	CA3-OA5-PA1-OA2
63	U	201	CDL	CA3-OA5-PA1-OA3
63	U	201	CDL	CA3-OA5-PA1-OA4
63	U	201	CDL	CB3-OB5-PB2-OB2
63	V	201	CDL	CB2-OB2-PB2-OB3
63	V	201	CDL	CB3-OB5-PB2-OB2
63	V	201	CDL	CB3-OB5-PB2-OB3
63	c1	706	CDL	CA2-OA2-PA1-OA3
63	c1	706	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
63	c1	706	CDL	CA3-OA5-PA1-OA2
63	c1	706	CDL	CB2-OB2-PB2-OB3
63	c1	706	CDL	CB2-OB2-PB2-OB5
63	c1	706	CDL	CB3-OB5-PB2-OB2
63	c1	706	CDL	CB3-OB5-PB2-OB3
63	c1	707	CDL	CA2-OA2-PA1-OA3
63	c1	707	CDL	CA3-OA5-PA1-OA2
63	c1	707	CDL	CA3-OA5-PA1-OA3
63	c1	707	CDL	CA3-OA5-PA1-OA4
63	c3	604	CDL	CA2-OA2-PA1-OA3
63	c3	604	CDL	CA2-OA2-PA1-OA4
63	c3	604	CDL	CA2-OA2-PA1-OA5
63	5b	702	CDL	CA2-OA2-PA1-OA3
63	5b	702	CDL	CA2-OA2-PA1-OA4
63	5b	702	CDL	CA2-OA2-PA1-OA5
63	5b	702	CDL	CA3-OA5-PA1-OA2
63	5b	702	CDL	CA3-OA5-PA1-OA3
63	5b	702	CDL	CA3-OA5-PA1-OA4
63	5b	702	CDL	CB3-OB5-PB2-OB2
63	5b	702	CDL	CB3-OB5-PB2-OB4
63	5b	703	CDL	CA3-OA5-PA1-OA2
63	5b	703	CDL	CB2-OB2-PB2-OB3
63	7a	201	CDL	CA2-OA2-PA1-OA4
63	7a	201	CDL	CA2-OA2-PA1-OA5
63	7a	201	CDL	CB2-OB2-PB2-OB4
63	7a	201	CDL	CB2-OB2-PB2-OB5
63	7a	202	CDL	CA2-OA2-PA1-OA4
63	7a	202	CDL	CA3-OA5-PA1-OA3
63	7a	202	CDL	CB2-OB2-PB2-OB3
63	7a	202	CDL	CB2-OB2-PB2-OB5
63	7c	301	CDL	CA3-OA5-PA1-OA2
63	7c	301	CDL	CA3-OA5-PA1-OA3
63	7c	301	CDL	CB2-OB2-PB2-OB3
63	7c	301	CDL	CB2-OB2-PB2-OB4
63	7c	301	CDL	CB2-OB2-PB2-OB5
63	7c	301	CDL	CB3-OB5-PB2-OB2
63	7c	301	CDL	CB3-OB5-PB2-OB4
63	7c	302	CDL	CA2-OA2-PA1-OA3
63	7c	302	CDL	CA2-OA2-PA1-OA4
63	7c	302	CDL	CA2-OA2-PA1-OA5
63	7c	302	CDL	CA3-OA5-PA1-OA2
63	7c	302	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
63	7c	302	CDL	CA3-OA5-PA1-OA4
63	7c	302	CDL	CB2-OB2-PB2-OB3
63	m1	401	CDL	CA2-OA2-PA1-OA4
63	m1	401	CDL	CB2-OB2-PB2-OB4
63	m1	401	CDL	CB2-OB2-PB2-OB5
63	m1	401	CDL	CB3-OB5-PB2-OB2
63	m1	401	CDL	CB3-OB5-PB2-OB3
63	m1	401	CDL	CB3-OB5-PB2-OB4
63	m1	404	CDL	CA2-OA2-PA1-OA3
63	m1	404	CDL	CA3-OA5-PA1-OA2
63	m1	404	CDL	CA3-OA5-PA1-OA3
63	m1	404	CDL	CA3-OA5-PA1-OA4
63	m1	404	CDL	CB2-OB2-PB2-OB4
63	m2	401	CDL	CA2-OA2-PA1-OA3
63	m2	401	CDL	CA2-OA2-PA1-OA5
63	m2	401	CDL	CA3-OA5-PA1-OA4
63	m2	401	CDL	CB3-OB5-PB2-OB2
63	m2	401	CDL	CB3-OB5-PB2-OB3
63	m2	403	CDL	CA2-OA2-PA1-OA3
63	m2	403	CDL	CA2-OA2-PA1-OA4
63	m2	403	CDL	CA2-OA2-PA1-OA5
63	m2	403	CDL	CB2-OB2-PB2-OB5
63	m2	404	CDL	CA2-OA2-PA1-OA3
63	m2	404	CDL	CA2-OA2-PA1-OA5
63	m2	404	CDL	CB2-OB2-PB2-OB3
63	m2	404	CDL	CB2-OB2-PB2-OB4
63	m2	404	CDL	CB2-OB2-PB2-OB5
63	m3	401	CDL	CB2-OB2-PB2-OB4
63	m3	401	CDL	CB2-OB2-PB2-OB5
63	m3	401	CDL	CB3-OB5-PB2-OB2
63	m3	401	CDL	CB3-OB5-PB2-OB3
63	m3	401	CDL	CB3-OB5-PB2-OB4
63	m3	402	CDL	CA2-OA2-PA1-OA5
63	m3	402	CDL	CA3-OA5-PA1-OA2
63	m3	402	CDL	CA3-OA5-PA1-OA3
63	m3	402	CDL	CA3-OA5-PA1-OA4
63	m3	402	CDL	CB2-OB2-PB2-OB3
63	m3	402	CDL	CB2-OB2-PB2-OB4
63	m3	402	CDL	CB2-OB2-PB2-OB5
63	m3	402	CDL	CB3-OB5-PB2-OB2
63	m3	403	CDL	CA2-OA2-PA1-OA5
63	y7	501	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
63	y7	501	CDL	CA2-OA2-PA1-OA4
63	y7	501	CDL	CA2-OA2-PA1-OA5
63	y7	501	CDL	CB2-OB2-PB2-OB5
63	y0	101	CDL	CA2-OA2-PA1-OA4
63	y0	101	CDL	CA2-OA2-PA1-OA5
63	y0	101	CDL	CA3-OA5-PA1-OA3
63	y0	101	CDL	CB2-OB2-PB2-OB3
63	y0	101	CDL	CB3-OB5-PB2-OB2
63	y0	101	CDL	CB3-OB5-PB2-OB3
63	y5	201	CDL	CA2-OA2-PA1-OA4
63	y5	201	CDL	CA2-OA2-PA1-OA5
63	y5	201	CDL	CA3-OA5-PA1-OA4
63	y5	201	CDL	CB2-OB2-PB2-OB4
63	y5	201	CDL	CB2-OB2-PB2-OB5
63	y5	201	CDL	CB3-OB5-PB2-OB2
63	y5	201	CDL	CB3-OB5-PB2-OB3
63	a	503	CDL	CA2-OA2-PA1-OA3
63	a	503	CDL	CB2-OB2-PB2-OB4
63	a	503	CDL	CB3-OB5-PB2-OB3
63	b	501	CDL	CA2-OA2-PA1-OA3
63	b	501	CDL	CA2-OA2-PA1-OA4
63	b	501	CDL	CA2-OA2-PA1-OA5
63	b	501	CDL	CA3-OA5-PA1-OA2
63	b	501	CDL	CA3-OA5-PA1-OA3
63	b	501	CDL	CA3-OA5-PA1-OA4
63	e	401	CDL	CA2-OA2-PA1-OA3
63	e	401	CDL	CA2-OA2-PA1-OA5
63	e	401	CDL	CA3-OA5-PA1-OA2
63	e	401	CDL	CA3-OA5-PA1-OA4
63	e	401	CDL	CB3-OB5-PB2-OB2
63	e	401	CDL	CB3-OB5-PB2-OB3
63	e	402	CDL	CA2-OA2-PA1-OA3
63	e	402	CDL	CA2-OA2-PA1-OA4
63	e	402	CDL	CA2-OA2-PA1-OA5
63	e	402	CDL	CB3-OB5-PB2-OB4
63	f	401	CDL	CA2-C1-CB2-OB2
63	f	401	CDL	CA3-OA5-PA1-OA3
63	f	401	CDL	CB3-OB5-PB2-OB2
63	f	401	CDL	CB3-OB5-PB2-OB3
63	f	401	CDL	CB3-OB5-PB2-OB4
63	k	301	CDL	CA2-OA2-PA1-OA3
63	k	301	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
63	k	301	CDL	CA3-OA5-PA1-OA4
63	l	301	CDL	CA2-OA2-PA1-OA3
63	l	301	CDL	CA2-OA2-PA1-OA5
63	l	301	CDL	CA3-OA5-PA1-OA2
63	l	301	CDL	CA3-OA5-PA1-OA4
63	l	301	CDL	CB2-OB2-PB2-OB5
63	l	301	CDL	CB3-OB5-PB2-OB2
63	l	301	CDL	CB3-OB5-PB2-OB3
63	n	303	CDL	CA2-OA2-PA1-OA4
63	n	303	CDL	CA2-OA2-PA1-OA5
63	n	303	CDL	CA3-OA5-PA1-OA2
63	n	303	CDL	CA3-OA5-PA1-OA3
63	n	303	CDL	CA3-OA5-PA1-OA4
63	n	303	CDL	CB2-OB2-PB2-OB3
63	n	303	CDL	CB2-OB2-PB2-OB4
63	n	303	CDL	CB2-OB2-PB2-OB5
63	n	303	CDL	CB3-OB5-PB2-OB2
63	n	303	CDL	CB3-OB5-PB2-OB3
63	n	303	CDL	CB3-OB5-PB2-OB4
63	t	201	CDL	CA2-OA2-PA1-OA5
63	t	201	CDL	CB2-OB2-PB2-OB3
63	t	201	CDL	CB3-OB5-PB2-OB3
63	t	202	CDL	CB3-OB5-PB2-OB2
63	t	202	CDL	CB3-OB5-PB2-OB3
63	t	202	CDL	CB3-OB5-PB2-OB4
63	u	201	CDL	CA3-OA5-PA1-OA2
63	u	201	CDL	CA3-OA5-PA1-OA3
63	u	201	CDL	CA3-OA5-PA1-OA4
63	u	201	CDL	CB2-OB2-PB2-OB3
63	u	201	CDL	CB2-OB2-PB2-OB5
63	u	201	CDL	CB3-OB5-PB2-OB2
63	u	201	CDL	CB3-OB5-PB2-OB3
63	u	201	CDL	CB3-OB5-PB2-OB4
63	v	201	CDL	CB2-OB2-PB2-OB3
63	v	201	CDL	CB3-OB5-PB2-OB2
63	v	201	CDL	CB3-OB5-PB2-OB3
59	c1	701	HEA	C21-C22-C23-C25
59	C1	701	HEA	C18-C19-C20-C21
59	c1	701	HEA	C18-C19-C20-C21
63	5B	702	CDL	O1-C1-CB2-OB2
63	F	401	CDL	O1-C1-CB2-OB2
63	5b	702	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
63	f	401	CDL	O1-C1-CB2-OB2
59	C1	701	HEA	C21-C22-C23-C25
59	c1	701	HEA	C26-C15-C16-C17
59	c1	701	HEA	C14-C15-C16-C17
59	c1	702	HEA	C18-C19-C20-C21
62	a	501	PC1	C2-C1-O11-P
63	M1	401	CDL	C1-CB2-OB2-PB2
63	m1	401	CDL	C1-CB2-OB2-PB2
59	C1	702	HEA	C17-C18-C19-C20
59	c1	702	HEA	C17-C18-C19-C20
63	5b	702	CDL	CA2-C1-CB2-OB2
62	C3	601	PC1	C11-C12-N-C13
62	c3	601	PC1	C11-C12-N-C13
59	C1	701	HEA	C14-C15-C16-C17
59	C1	702	HEA	C18-C19-C20-C21
63	5b	702	CDL	OB5-CB3-CB4-OB6
62	C3	602	PC1	C21-C22-C23-C24
62	V	202	PC1	C31-C32-C33-C34
62	v	202	PC1	C31-C32-C33-C34
62	c3	602	PC1	C21-C22-C23-C24
63	v	201	CDL	CB5-C51-C52-C53
62	C3	601	PC1	C11-C12-N-C14
62	J	302	PC1	C11-C12-N-C15
62	c3	602	PC1	C11-C12-N-C15
62	j	302	PC1	C11-C12-N-C15
62	M2	406	PC1	C21-C22-C23-C24
62	m2	406	PC1	C21-C22-C23-C24
63	U	201	CDL	CB5-C51-C52-C53
63	V	201	CDL	CB5-C51-C52-C53
63	u	201	CDL	CB5-C51-C52-C53
63	C3	604	CDL	CA7-C31-C32-C33
63	M1	401	CDL	CB7-C71-C72-C73
63	m1	401	CDL	CB7-C71-C72-C73
63	c3	604	CDL	CA7-C31-C32-C33
63	F	401	CDL	CA2-C1-CB2-OB2
62	C3	602	PC1	C11-C12-N-C15
62	C3	605	PC1	C11-C12-N-C15
62	7C	302	PC1	C11-C12-N-C15
62	M2	405	PC1	C11-C12-N-C13
62	M2	405	PC1	C11-C12-N-C14
62	N	301	PC1	C11-C12-N-C14
62	c3	601	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
62	c3	605	PC1	C11-C12-N-C15
62	m1	402	PC1	C11-C12-N-C15
62	n	301	PC1	C11-C12-N-C14
63	Y0	101	CDL	O1-C1-CA2-OA2
63	M1	401	CDL	CB5-C51-C52-C53
63	Y0	101	CDL	CA4-CA3-OA5-PA1
63	7A	202	CDL	C76-C77-C78-C79
63	7a	202	CDL	CA7-C31-C32-C33
59	C1	701	HEA	O11-C11-C12-C13
59	c1	701	HEA	O11-C11-C12-C13
62	M2	405	PC1	C11-C12-N-C15
62	J	302	PC1	C11-C12-N-C14
63	e	402	CDL	C54-C55-C56-C57
63	7A	202	CDL	C52-C53-C54-C55
63	M2	403	CDL	C11-C12-C13-C14
63	m2	403	CDL	C11-C12-C13-C14
63	m3	401	CDL	CA5-C11-C12-C13
63	7a	202	CDL	OB5-CB3-CB4-CB6
63	J	301	CDL	O1-C1-CA2-OA2
63	j	301	CDL	O1-C1-CA2-OA2
59	c1	701	HEA	C21-C22-C23-C24
63	7A	202	CDL	CA7-C31-C32-C33
63	M3	401	CDL	CA5-C11-C12-C13
63	E	401	CDL	CA5-C11-C12-C13
63	e	401	CDL	CA5-C11-C12-C13
63	7a	202	CDL	C76-C77-C78-C79
63	7a	202	CDL	C52-C53-C54-C55
63	M1	401	CDL	C77-C78-C79-C80
63	m1	401	CDL	C77-C78-C79-C80
63	C3	604	CDL	CB5-C51-C52-C53
63	5B	703	CDL	CA5-C11-C12-C13
63	k	301	CDL	CA5-C11-C12-C13
62	7C	304	PC1	C22-C23-C24-C25
63	V	201	CDL	C56-C57-C58-C59
63	n	303	CDL	C39-C40-C41-C42
63	N	303	CDL	C39-C40-C41-C42
63	t	202	CDL	C75-C76-C77-C78
63	E	402	CDL	C54-C55-C56-C57
62	C3	601	PC1	C11-C12-N-C15
62	C3	602	PC1	C11-C12-N-C13
62	C3	605	PC1	C11-C12-N-C13
62	7C	302	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
62	c3	601	PC1	C11-C12-N-C15
62	c3	602	PC1	C11-C12-N-C13
62	m1	402	PC1	C11-C12-N-C14
62	j	302	PC1	C11-C12-N-C13
62	j	302	PC1	C11-C12-N-C14
63	T	202	CDL	C75-C76-C77-C78
63	5B	702	CDL	C73-C74-C75-C76
63	7A	202	CDL	C62-C63-C64-C65
63	7a	202	CDL	C62-C63-C64-C65
63	m3	401	CDL	C58-C59-C60-C61
62	7c	303	PC1	C22-C23-C24-C25
63	M3	401	CDL	C73-C74-C75-C76
62	v	202	PC1	C3B-C3C-C3D-C3E
63	5b	702	CDL	C73-C74-C75-C76
62	V	202	PC1	C3B-C3C-C3D-C3E
63	m3	401	CDL	C72-C73-C74-C75
62	V	202	PC1	C3E-C3F-C3G-C3H
63	m1	401	CDL	CB5-C51-C52-C53
63	7C	301	CDL	C81-C82-C83-C84
63	f	401	CDL	CB7-C71-C72-C73
59	c1	701	HEA	C27-C19-C20-C21
62	C3	602	PC1	C11-C12-N-C14
62	C3	605	PC1	C11-C12-N-C14
62	7C	302	PC1	C11-C12-N-C13
62	J	302	PC1	C11-C12-N-C13
62	N	301	PC1	C11-C12-N-C13
62	N	301	PC1	C11-C12-N-C15
62	c3	602	PC1	C11-C12-N-C14
62	c3	605	PC1	C11-C12-N-C13
62	c3	605	PC1	C11-C12-N-C14
62	7c	303	PC1	C11-C12-N-C13
62	m1	402	PC1	C11-C12-N-C13
62	n	301	PC1	C11-C12-N-C13
62	n	301	PC1	C11-C12-N-C15
59	c1	702	HEA	C21-C22-C23-C25
63	m3	401	CDL	C73-C74-C75-C76
63	J	301	CDL	C52-C53-C54-C55
62	7C	304	PC1	C31-C32-C33-C34
63	T	202	CDL	C14-C15-C16-C17
63	7c	301	CDL	C81-C82-C83-C84
63	t	202	CDL	C14-C15-C16-C17
63	Y5	201	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
63	y0	101	CDL	CA4-CA3-OA5-PA1
63	y5	201	CDL	CA4-CA3-OA5-PA1
63	U	201	CDL	C74-C75-C76-C77
62	7C	302	PC1	C2B-C2C-C2D-C2E
59	C1	701	HEA	C21-C22-C23-C24
63	j	301	CDL	C52-C53-C54-C55
63	v	201	CDL	C56-C57-C58-C59
63	y5	201	CDL	C41-C42-C43-C44
62	7C	304	PC1	C11-C12-N-C13
63	Y5	201	CDL	C41-C42-C43-C44
63	5B	703	CDL	OB5-CB3-CB4-CB6
63	5B	704	CDL	OB5-CB3-CB4-CB6
63	Y0	101	CDL	OA5-CA3-CA4-CA6
63	N	303	CDL	OA5-CA3-CA4-CA6
63	c1	706	CDL	OB5-CB3-CB4-CB6
63	5b	703	CDL	OB5-CB3-CB4-CB6
63	m2	403	CDL	OB5-CB3-CB4-CB6
63	y0	101	CDL	OA5-CA3-CA4-CA6
63	f	401	CDL	OB5-CB3-CB4-CB6
63	M3	401	CDL	C72-C73-C74-C75
63	F	401	CDL	CB7-C71-C72-C73
62	m1	402	PC1	C2B-C2C-C2D-C2E
63	M3	401	CDL	C58-C59-C60-C61
62	7c	303	PC1	C31-C32-C33-C34
63	u	201	CDL	C74-C75-C76-C77
63	j	301	CDL	C16-C17-C18-C19
63	M1	402	CDL	C71-C72-C73-C74
63	M1	402	CDL	C51-C52-C53-C54
63	c3	604	CDL	CB5-C51-C52-C53
62	C3	602	PC1	C1-C2-C3-O31
62	c3	602	PC1	C1-C2-C3-O31
63	M1	402	CDL	CA3-CA4-CA6-OA8
63	m1	403	CDL	CA3-CA4-CA6-OA8
63	m3	401	CDL	CB3-CB4-CB6-OB8
63	b	501	CDL	CB3-CB4-CB6-OB8
62	n	302	PC1	C33-C34-C35-C36
63	m1	403	CDL	C71-C72-C73-C74
63	m1	403	CDL	C51-C52-C53-C54
62	C3	605	PC1	C21-C22-C23-C24
62	N	302	PC1	C33-C34-C35-C36
63	5B	702	CDL	OB5-CB3-CB4-OB6
63	M3	403	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
63	N	303	CDL	OB5-CB3-CB4-OB6
63	m1	403	CDL	OB5-CB3-CB4-OB6
63	m3	403	CDL	OB5-CB3-CB4-OB6
63	j	301	CDL	OB5-CB3-CB4-OB6
63	J	301	CDL	C16-C17-C18-C19
63	7c	301	CDL	C34-C35-C36-C37
62	7c	303	PC1	C11-C12-N-C15
63	7a	202	CDL	C32-C31-CA7-OA8
59	C1	701	HEA	C3B-C11-C12-C13
59	c1	701	HEA	C3B-C11-C12-C13
63	t	201	CDL	C19-C20-C21-C22
62	c3	605	PC1	C21-C22-C23-C24
63	v	201	CDL	C74-C75-C76-C77
63	Y5	201	CDL	C39-C40-C41-C42
63	m3	401	CDL	C52-C53-C54-C55
63	y5	201	CDL	C39-C40-C41-C42
63	7C	301	CDL	C34-C35-C36-C37
63	M1	401	CDL	CB4-CB3-OB5-PB2
63	F	401	CDL	CB4-CB3-OB5-PB2
63	T	202	CDL	CA4-CA3-OA5-PA1
63	7a	201	CDL	CB4-CB3-OB5-PB2
63	m1	401	CDL	CB4-CB3-OB5-PB2
63	t	202	CDL	CA4-CA3-OA5-PA1
62	N	301	PC1	C23-C24-C25-C26
63	V	201	CDL	C74-C75-C76-C77
62	v	202	PC1	C3E-C3F-C3G-C3H
63	V	201	CDL	C53-C54-C55-C56
63	m2	404	CDL	C34-C35-C36-C37
63	7A	202	CDL	OB5-CB3-CB4-CB6
63	M2	401	CDL	OB5-CB3-CB4-CB6
63	B	501	CDL	OB5-CB3-CB4-CB6
63	F	401	CDL	OB5-CB3-CB4-CB6
63	J	301	CDL	OB5-CB3-CB4-CB6
63	5b	702	CDL	OB5-CB3-CB4-CB6
63	y7	501	CDL	OB5-CB3-CB4-CB6
63	b	501	CDL	OB5-CB3-CB4-CB6
63	n	303	CDL	OA5-CA3-CA4-CA6
62	n	301	PC1	C23-C24-C25-C26
63	m3	403	CDL	O1-C1-CA2-OA2
63	v	201	CDL	C53-C54-C55-C56
63	T	201	CDL	C19-C20-C21-C22
63	m1	401	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
63	M3	401	CDL	C32-C33-C34-C35
63	M1	401	CDL	C74-C75-C76-C77
62	m1	402	PC1	C24-C25-C26-C27
63	M2	404	CDL	C34-C35-C36-C37
63	7A	201	CDL	CA5-C11-C12-C13
63	7a	201	CDL	CA5-C11-C12-C13
63	m2	404	CDL	CA7-C31-C32-C33
63	M3	401	CDL	C52-C53-C54-C55
63	7C	301	CDL	CA3-CA4-CA6-OA8
63	M1	402	CDL	CB3-CB4-CB6-OB8
63	M3	401	CDL	CB3-CB4-CB6-OB8
63	B	501	CDL	CB3-CB4-CB6-OB8
63	7c	301	CDL	CA3-CA4-CA6-OA8
63	N	303	CDL	C42-C43-C44-C45
63	n	303	CDL	C44-C45-C46-C47
63	N	303	CDL	C44-C45-C46-C47
63	n	303	CDL	C42-C43-C44-C45
62	7C	304	PC1	C11-C12-N-C15
63	C1	706	CDL	OB5-CB3-CB4-OB6
63	M2	403	CDL	OB5-CB3-CB4-OB6
63	F	401	CDL	OB5-CB3-CB4-OB6
63	J	301	CDL	OB5-CB3-CB4-OB6
63	5b	702	CDL	OA5-CA3-CA4-OA6
63	7a	202	CDL	OB5-CB3-CB4-OB6
63	m2	403	CDL	OB5-CB3-CB4-OB6
63	M3	403	CDL	O1-C1-CA2-OA2
63	5B	702	CDL	C1-CB2-OB2-PB2
63	7A	201	CDL	CB4-CB3-OB5-PB2
63	B	501	CDL	CB4-CB3-OB5-PB2
63	L	301	CDL	CA4-CA3-OA5-PA1
63	5b	702	CDL	C1-CB2-OB2-PB2
63	b	501	CDL	CB4-CB3-OB5-PB2
63	f	401	CDL	CB4-CB3-OB5-PB2
63	l	301	CDL	CA4-CA3-OA5-PA1
63	m3	401	CDL	C32-C33-C34-C35
63	7C	303	CDL	OA6-CA4-CA6-OA8
63	E	402	CDL	OA6-CA4-CA6-OA8
63	7c	301	CDL	OA6-CA4-CA6-OA8
63	7c	302	CDL	OA6-CA4-CA6-OA8
63	e	402	CDL	OA6-CA4-CA6-OA8
63	F	401	CDL	C80-C81-C82-C83
62	C1	705	PC1	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
62	M2	406	PC1	C11-C12-N-C14
62	c1	705	PC1	C3B-C3C-C3D-C3E
62	m1	402	PC1	C29-C2A-C2B-C2C
63	f	401	CDL	C80-C81-C82-C83
62	C3	601	PC1	O31-C31-C32-C33
62	m1	402	PC1	C3B-C3C-C3D-C3E
63	7c	301	CDL	CA2-C1-CB2-OB2
63	T	202	CDL	C56-C57-C58-C59
63	7A	202	CDL	C32-C31-CA7-OA8
62	7C	302	PC1	C24-C25-C26-C27
63	C1	706	CDL	OB5-CB3-CB4-CB6
63	5B	702	CDL	OA5-CA3-CA4-CA6
63	M2	403	CDL	OB5-CB3-CB4-CB6
63	Y7	501	CDL	OB5-CB3-CB4-CB6
63	5b	702	CDL	OA5-CA3-CA4-CA6
63	m2	401	CDL	OB5-CB3-CB4-CB6
63	m3	403	CDL	OB5-CB3-CB4-CB6
63	j	301	CDL	OB5-CB3-CB4-CB6
63	k	301	CDL	OB5-CB3-CB4-CB6
63	n	303	CDL	OB5-CB3-CB4-CB6
63	t	202	CDL	OB5-CB3-CB4-CB6
63	M2	403	CDL	C52-C53-C54-C55
63	n	303	CDL	CB7-C71-C72-C73
62	c1	705	PC1	C39-C3A-C3B-C3C
59	C1	701	HEA	C27-C19-C20-C21
62	7C	302	PC1	C29-C2A-C2B-C2C
63	y0	101	CDL	O1-C1-CA2-OA2
63	m1	403	CDL	CB7-C71-C72-C73
63	M1	401	CDL	C19-C20-C21-C22
63	t	202	CDL	C56-C57-C58-C59
63	m3	401	CDL	C20-C21-C22-C23
63	7A	202	CDL	OB5-CB3-CB4-OB6
63	7C	301	CDL	OB5-CB3-CB4-OB6
63	M1	402	CDL	OB5-CB3-CB4-OB6
63	M2	401	CDL	OB5-CB3-CB4-OB6
63	Y7	501	CDL	OB5-CB3-CB4-OB6
63	5b	703	CDL	OB5-CB3-CB4-OB6
63	m2	401	CDL	OB5-CB3-CB4-OB6
63	m3	403	CDL	OA5-CA3-CA4-OA6
63	b	501	CDL	OB5-CB3-CB4-OB6
63	f	401	CDL	OB5-CB3-CB4-OB6
63	n	303	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
63	E	402	CDL	CA3-CA4-CA6-OA8
63	e	402	CDL	CA3-CA4-CA6-OA8
62	C1	705	PC1	C39-C3A-C3B-C3C
63	m2	403	CDL	C52-C53-C54-C55
63	7C	301	CDL	OA6-CA4-CA6-OA8
63	M1	402	CDL	OB6-CB4-CB6-OB8
63	b	501	CDL	OB6-CB4-CB6-OB8
63	l	301	CDL	OB6-CB4-CB6-OB8
62	M2	406	PC1	C11-C12-N-C15
62	m2	402	PC1	C11-C12-N-C13
62	m2	402	PC1	C11-C12-N-C15
62	m2	406	PC1	C11-C12-N-C14
62	m2	406	PC1	C11-C12-N-C15
62	m2	405	PC1	C32-C33-C34-C35
63	V	201	CDL	C51-C52-C53-C54
63	7C	301	CDL	CA5-C11-C12-C13
63	v	201	CDL	C51-C52-C53-C54
62	C3	603	PC1	O13-C11-C12-N
62	M2	402	PC1	O13-C11-C12-N
62	M2	405	PC1	O13-C11-C12-N
62	A	501	PC1	O13-C11-C12-N
62	A	502	PC1	O13-C11-C12-N
62	V	202	PC1	O13-C11-C12-N
62	c3	603	PC1	O13-C11-C12-N
62	m2	405	PC1	O13-C11-C12-N
62	a	501	PC1	O13-C11-C12-N
62	a	502	PC1	O13-C11-C12-N
62	v	202	PC1	O13-C11-C12-N
63	m1	401	CDL	C19-C20-C21-C22
62	7C	302	PC1	C3B-C3C-C3D-C3E
63	7c	301	CDL	CA5-C11-C12-C13
63	M3	401	CDL	C20-C21-C22-C23
63	U	201	CDL	C32-C33-C34-C35
63	7C	301	CDL	C53-C54-C55-C56
63	u	201	CDL	C53-C54-C55-C56
62	M1	404	PC1	O11-C1-C2-C3
63	7C	303	CDL	OA5-CA3-CA4-CA6
63	M1	402	CDL	OB5-CB3-CB4-CB6
63	M3	403	CDL	OA5-CA3-CA4-CA6
63	M3	403	CDL	OB5-CB3-CB4-CB6
63	N	303	CDL	OB5-CB3-CB4-CB6
63	T	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
63	7c	302	CDL	OA5-CA3-CA4-CA6
63	m1	403	CDL	OB5-CB3-CB4-CB6
63	m3	403	CDL	OA5-CA3-CA4-CA6
63	U	201	CDL	C53-C54-C55-C56
63	7c	301	CDL	C35-C36-C37-C38
63	u	201	CDL	C32-C33-C34-C35
63	7a	202	CDL	C21-C22-C23-C24
63	7C	301	CDL	C35-C36-C37-C38
63	7c	301	CDL	C53-C54-C55-C56
63	M2	404	CDL	C1-CA2-OA2-PA1
63	A	503	CDL	CA4-CA3-OA5-PA1
63	l	301	CDL	C1-CA2-OA2-PA1
62	M1	404	PC1	O11-C1-C2-O21
62	m1	405	PC1	O11-C1-C2-O21
63	C1	706	CDL	OA5-CA3-CA4-OA6
63	5B	702	CDL	OA5-CA3-CA4-OA6
63	5B	703	CDL	OB5-CB3-CB4-OB6
63	5B	704	CDL	OB5-CB3-CB4-OB6
63	7C	303	CDL	OA5-CA3-CA4-OA6
63	M3	403	CDL	OA5-CA3-CA4-OA6
63	B	501	CDL	OB5-CB3-CB4-OB6
63	N	303	CDL	OA5-CA3-CA4-OA6
63	T	202	CDL	OB5-CB3-CB4-OB6
63	c1	706	CDL	OA5-CA3-CA4-OA6
63	c1	706	CDL	OB5-CB3-CB4-OB6
63	7c	302	CDL	OA5-CA3-CA4-OA6
63	y7	501	CDL	OB5-CB3-CB4-OB6
63	y0	101	CDL	OA5-CA3-CA4-OA6
63	k	301	CDL	OB5-CB3-CB4-OB6
63	n	303	CDL	OA5-CA3-CA4-OA6
63	t	202	CDL	OB5-CB3-CB4-OB6
63	m1	401	CDL	C61-C62-C63-C64
63	M3	401	CDL	C23-C24-C25-C26
62	7c	303	PC1	C11-C12-N-C14
62	m1	405	PC1	C11-C12-N-C13
63	M3	403	CDL	CA5-C11-C12-C13
63	M1	402	CDL	OA6-CA4-CA6-OA8
63	M3	401	CDL	OB6-CB4-CB6-OB8
63	B	501	CDL	OB6-CB4-CB6-OB8
63	L	301	CDL	OB6-CB4-CB6-OB8
63	m3	401	CDL	OB6-CB4-CB6-OB8
63	M3	403	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
63	M3	403	CDL	CB2-C1-CA2-OA2
63	m3	403	CDL	CB2-C1-CA2-OA2
63	M2	404	CDL	CB3-CB4-CB6-OB8
63	m1	403	CDL	CB3-CB4-CB6-OB8
63	m2	404	CDL	CB3-CB4-CB6-OB8
63	M3	403	CDL	C71-C72-C73-C74
63	m3	403	CDL	C74-C75-C76-C77
62	C1	705	PC1	C26-C27-C28-C29
62	M2	405	PC1	C32-C33-C34-C35
63	u	201	CDL	C55-C56-C57-C58
63	7A	202	CDL	C21-C22-C23-C24
63	F	401	CDL	C36-C37-C38-C39
63	U	201	CDL	C55-C56-C57-C58
62	C1	705	PC1	C11-O13-P-O14
62	C1	705	PC1	C11-O13-P-O11
62	C1	705	PC1	C11-C12-N-C14
62	C3	601	PC1	C1-O11-P-O12
62	C3	602	PC1	C1-O11-P-O14
62	C3	602	PC1	C1-O11-P-O13
62	C3	603	PC1	C11-O13-P-O14
62	C3	603	PC1	C11-O13-P-O11
62	C3	603	PC1	C1-O11-P-O12
62	C3	603	PC1	C1-O11-P-O14
62	C3	603	PC1	C1-O11-P-O13
62	7C	302	PC1	C11-O13-P-O12
62	7C	304	PC1	C1-O11-P-O13
62	7C	304	PC1	C11-C12-N-C14
62	M1	404	PC1	C11-O13-P-O14
62	M2	402	PC1	C11-C12-N-C15
62	M2	405	PC1	C11-O13-P-O14
62	M2	405	PC1	C11-O13-P-O11
62	A	502	PC1	C11-O13-P-O14
62	A	502	PC1	C1-O11-P-O14
62	N	301	PC1	C11-O13-P-O12
62	N	301	PC1	C11-O13-P-O11
62	N	301	PC1	C1-O11-P-O13
62	V	202	PC1	C1-O11-P-O12
62	c1	705	PC1	C11-O13-P-O14
62	c3	601	PC1	C1-O11-P-O12
62	c3	602	PC1	C1-O11-P-O14
62	c3	603	PC1	C11-O13-P-O14
62	c3	603	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
62	c3	603	PC1	C1-O11-P-O14
62	c3	603	PC1	C1-O11-P-O13
62	a	501	PC1	C1-O11-P-O13
62	a	502	PC1	C11-O13-P-O14
62	a	502	PC1	C1-O11-P-O14
62	n	301	PC1	C11-O13-P-O12
62	n	301	PC1	C11-O13-P-O11
62	n	301	PC1	C1-O11-P-O13
62	v	202	PC1	C11-O13-P-O14
62	v	202	PC1	C11-O13-P-O11
63	C1	706	CDL	CA3-OA5-PA1-OA3
63	C1	706	CDL	CB3-OB5-PB2-OB4
63	C1	707	CDL	CA2-OA2-PA1-OA5
63	5B	702	CDL	CB2-OB2-PB2-OB3
63	5B	702	CDL	CB3-OB5-PB2-OB2
63	5B	702	CDL	CB3-OB5-PB2-OB3
63	5B	702	CDL	CB3-OB5-PB2-OB4
63	5B	703	CDL	CA2-OA2-PA1-OA4
63	5B	703	CDL	CA3-OA5-PA1-OA2
63	5B	703	CDL	CA3-OA5-PA1-OA3
63	5B	703	CDL	CB3-OB5-PB2-OB3
63	5B	704	CDL	CA3-OA5-PA1-OA3
63	7A	202	CDL	CA3-OA5-PA1-OA2
63	7A	202	CDL	CB2-OB2-PB2-OB4
63	7A	202	CDL	CB3-OB5-PB2-OB3
63	7C	301	CDL	CB2-OB2-PB2-OB3
63	7C	301	CDL	CB2-OB2-PB2-OB5
63	7C	303	CDL	CB2-OB2-PB2-OB4
63	M1	401	CDL	CA2-OA2-PA1-OA3
63	M1	401	CDL	CA2-OA2-PA1-OA5
63	M1	401	CDL	CB2-OB2-PB2-OB3
63	M1	401	CDL	CB2-OB2-PB2-OB5
63	M1	403	CDL	CA2-OA2-PA1-OA5
63	M1	403	CDL	CB2-OB2-PB2-OB3
63	M1	403	CDL	CB2-OB2-PB2-OB5
63	M2	401	CDL	CA2-OA2-PA1-OA4
63	M2	401	CDL	CA2-OA2-PA1-OA5
63	M2	401	CDL	CA3-OA5-PA1-OA2
63	M2	401	CDL	CA3-OA5-PA1-OA3
63	M2	401	CDL	CB2-OB2-PB2-OB3
63	M2	401	CDL	CB3-OB5-PB2-OB2
63	M2	401	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
63	M2	403	CDL	CA3-OA5-PA1-OA3
63	M2	403	CDL	CB2-OB2-PB2-OB3
63	M2	404	CDL	CA2-OA2-PA1-OA4
63	M3	401	CDL	CB3-OB5-PB2-OB4
63	M3	402	CDL	CA2-OA2-PA1-OA3
63	M3	402	CDL	CA3-OA5-PA1-OA2
63	M3	402	CDL	CA3-OA5-PA1-OA3
63	M3	402	CDL	CB3-OB5-PB2-OB3
63	M3	403	CDL	CA2-OA2-PA1-OA3
63	M3	403	CDL	CA3-OA5-PA1-OA3
63	Y7	501	CDL	CB2-OB2-PB2-OB3
63	Y0	101	CDL	CA3-OA5-PA1-OA2
63	Y0	101	CDL	CB2-OB2-PB2-OB5
63	Y0	101	CDL	CB3-OB5-PB2-OB4
63	Y5	201	CDL	CA3-OA5-PA1-OA2
63	Y5	201	CDL	CA3-OA5-PA1-OA3
63	Y5	201	CDL	CB2-OB2-PB2-OB3
63	Y5	201	CDL	CB2-OB2-PB2-OB5
63	Y5	201	CDL	CB3-OB5-PB2-OB2
63	A	503	CDL	CB3-OB5-PB2-OB4
63	E	401	CDL	CA2-OA2-PA1-OA4
63	E	401	CDL	CB3-OB5-PB2-OB4
63	F	401	CDL	CA3-OA5-PA1-OA4
63	J	301	CDL	CA2-OA2-PA1-OA4
63	J	301	CDL	CA2-OA2-PA1-OA5
63	J	301	CDL	CB2-OB2-PB2-OB3
63	L	301	CDL	CA2-OA2-PA1-OA4
63	L	301	CDL	CB2-OB2-PB2-OB3
63	T	201	CDL	CA2-OA2-PA1-OA3
63	T	201	CDL	CB2-OB2-PB2-OB4
63	U	201	CDL	CB2-OB2-PB2-OB3
63	U	201	CDL	CB2-OB2-PB2-OB4
63	U	201	CDL	CB2-OB2-PB2-OB5
63	U	201	CDL	CB3-OB5-PB2-OB3
63	V	201	CDL	CB3-OB5-PB2-OB4
63	c1	706	CDL	CA3-OA5-PA1-OA3
63	c1	706	CDL	CB2-OB2-PB2-OB4
63	c1	706	CDL	CB3-OB5-PB2-OB4
63	c1	707	CDL	CA2-OA2-PA1-OA5
63	5b	702	CDL	CB3-OB5-PB2-OB3
63	5b	703	CDL	CA3-OA5-PA1-OA3
63	5b	703	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
63	7a	201	CDL	CB3-OB5-PB2-OB3
63	7a	202	CDL	CA3-OA5-PA1-OA2
63	7a	202	CDL	CA3-OA5-PA1-OA4
63	7a	202	CDL	CB2-OB2-PB2-OB4
63	7a	202	CDL	CB3-OB5-PB2-OB3
63	7c	301	CDL	CB3-OB5-PB2-OB3
63	7c	302	CDL	CB2-OB2-PB2-OB5
63	m1	401	CDL	CA2-OA2-PA1-OA3
63	m1	401	CDL	CA2-OA2-PA1-OA5
63	m1	401	CDL	CB2-OB2-PB2-OB3
63	m1	404	CDL	CA2-OA2-PA1-OA5
63	m1	404	CDL	CB2-OB2-PB2-OB3
63	m1	404	CDL	CB2-OB2-PB2-OB5
63	m1	404	CDL	CB3-OB5-PB2-OB3
63	m2	401	CDL	CA2-OA2-PA1-OA4
63	m2	401	CDL	CA3-OA5-PA1-OA2
63	m2	401	CDL	CA3-OA5-PA1-OA3
63	m2	401	CDL	CB2-OB2-PB2-OB3
63	m2	403	CDL	CA3-OA5-PA1-OA3
63	m2	403	CDL	CB2-OB2-PB2-OB3
63	m2	403	CDL	CB3-OB5-PB2-OB2
63	m2	404	CDL	CA2-OA2-PA1-OA4
63	m3	402	CDL	CA2-OA2-PA1-OA3
63	m3	402	CDL	CB3-OB5-PB2-OB3
63	m3	403	CDL	CA2-OA2-PA1-OA3
63	m3	403	CDL	CA3-OA5-PA1-OA3
63	y7	501	CDL	CB2-OB2-PB2-OB3
63	y0	101	CDL	CA2-OA2-PA1-OA3
63	y0	101	CDL	CA3-OA5-PA1-OA2
63	y0	101	CDL	CA3-OA5-PA1-OA4
63	y0	101	CDL	CB2-OB2-PB2-OB5
63	y0	101	CDL	CB3-OB5-PB2-OB4
63	y5	201	CDL	CA3-OA5-PA1-OA2
63	y5	201	CDL	CA3-OA5-PA1-OA3
63	y5	201	CDL	CB2-OB2-PB2-OB3
63	a	503	CDL	CA2-OA2-PA1-OA5
63	a	503	CDL	CB2-OB2-PB2-OB5
63	a	503	CDL	CB3-OB5-PB2-OB2
63	a	503	CDL	CB3-OB5-PB2-OB4
63	e	401	CDL	CA2-OA2-PA1-OA4
63	e	401	CDL	CB3-OB5-PB2-OB4
63	e	402	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
63	j	301	CDL	CA2-OA2-PA1-OA3
63	j	301	CDL	CA2-OA2-PA1-OA4
63	j	301	CDL	CA2-OA2-PA1-OA5
63	j	301	CDL	CB2-OB2-PB2-OB3
63	k	301	CDL	CA2-OA2-PA1-OA4
63	k	301	CDL	CA3-OA5-PA1-OA2
63	k	301	CDL	CA3-OA5-PA1-OA3
63	k	301	CDL	CB3-OB5-PB2-OB3
63	l	301	CDL	CA2-OA2-PA1-OA4
63	l	301	CDL	CB2-OB2-PB2-OB3
63	t	201	CDL	CA2-OA2-PA1-OA3
63	t	201	CDL	CB2-OB2-PB2-OB5
63	v	201	CDL	CB3-OB5-PB2-OB4
63	M1	401	CDL	C61-C62-C63-C64
63	m3	401	CDL	C23-C24-C25-C26
62	M2	405	PC1	C2-C1-O11-P
63	M2	401	CDL	CB4-CB3-OB5-PB2
63	M2	404	CDL	CA4-CA3-OA5-PA1
63	M2	404	CDL	CB4-CB3-OB5-PB2
63	M3	403	CDL	C1-CB2-OB2-PB2
63	Y7	501	CDL	CB4-CB3-OB5-PB2
63	B	501	CDL	C1-CA2-OA2-PA1
63	E	401	CDL	CA4-CA3-OA5-PA1
63	E	401	CDL	C1-CB2-OB2-PB2
63	J	301	CDL	C1-CA2-OA2-PA1
63	L	301	CDL	C1-CA2-OA2-PA1
63	L	301	CDL	CB4-CB3-OB5-PB2
63	N	303	CDL	CA4-CA3-OA5-PA1
63	7c	302	CDL	C1-CA2-OA2-PA1
63	m2	401	CDL	CB4-CB3-OB5-PB2
63	m2	404	CDL	C1-CA2-OA2-PA1
63	m2	404	CDL	CA4-CA3-OA5-PA1
63	m2	404	CDL	CB4-CB3-OB5-PB2
63	m3	403	CDL	C1-CB2-OB2-PB2
63	y7	501	CDL	CB4-CB3-OB5-PB2
63	a	503	CDL	CA4-CA3-OA5-PA1
63	e	401	CDL	C1-CA2-OA2-PA1
63	e	401	CDL	CA4-CA3-OA5-PA1
63	e	401	CDL	C1-CB2-OB2-PB2
63	j	301	CDL	C1-CA2-OA2-PA1
63	l	301	CDL	CB4-CB3-OB5-PB2
63	n	303	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
63	m3	403	CDL	CA5-C11-C12-C13
62	c1	705	PC1	C2A-C2B-C2C-C2D
63	m1	401	CDL	C18-C19-C20-C21
63	M1	401	CDL	C18-C19-C20-C21
63	y7	501	CDL	CA6-CA4-OA6-CA5
63	M1	401	CDL	C72-C71-CB7-OB8
62	C1	705	PC1	C2A-C2B-C2C-C2D
63	L	301	CDL	C12-C13-C14-C15
63	m3	403	CDL	C71-C72-C73-C74
62	7C	304	PC1	C2A-C2B-C2C-C2D
62	M2	406	PC1	C11-C12-N-C13
62	m1	405	PC1	C11-C12-N-C14
62	A	501	PC1	O11-C1-C2-C3
62	a	501	PC1	O11-C1-C2-C3
63	e	402	CDL	OB5-CB3-CB4-CB6
62	7c	303	PC1	C2A-C2B-C2C-C2D
63	N	303	CDL	CB7-C71-C72-C73
63	5b	703	CDL	CA7-C31-C32-C33
63	C1	707	CDL	OB5-CB3-CB4-OB6
63	Y0	101	CDL	OA5-CA3-CA4-OA6
63	c1	707	CDL	OB5-CB3-CB4-OB6
63	M1	401	CDL	C52-C51-CB5-OB6
63	B	501	CDL	C51-C52-C53-C54
63	5b	702	CDL	C35-C36-C37-C38
63	7C	303	CDL	C1-CA2-OA2-PA1
63	M1	403	CDL	CB4-CB3-OB5-PB2
63	m3	402	CDL	C1-CA2-OA2-PA1
63	b	501	CDL	C1-CA2-OA2-PA1
63	5B	702	CDL	C35-C36-C37-C38
63	v	201	CDL	C16-C17-C18-C19
63	m1	403	CDL	OA6-CA4-CA6-OA8
63	m1	403	CDL	OB6-CB4-CB6-OB8
62	c3	601	PC1	O31-C31-C32-C33
63	m1	401	CDL	C52-C51-CB5-OB6
62	c1	705	PC1	C26-C27-C28-C29
63	m3	403	CDL	C73-C74-C75-C76
62	N	301	PC1	C21-C22-C23-C24
63	F	401	CDL	C52-C53-C54-C55
63	M3	403	CDL	C73-C74-C75-C76
63	y0	101	CDL	C52-C51-CB5-OB6
63	L	301	CDL	CB3-CB4-CB6-OB8
63	l	301	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
63	5B	704	CDL	C72-C71-CB7-OB8
63	f	401	CDL	C36-C37-C38-C39
63	c1	706	CDL	CA7-C31-C32-C33
62	C3	601	PC1	C39-C3A-C3B-C3C
63	e	402	CDL	C53-C54-C55-C56
63	5B	704	CDL	CA7-C31-C32-C33
63	7c	301	CDL	C82-C83-C84-C85
63	7C	301	CDL	CA2-C1-CB2-OB2
63	E	401	CDL	C1-CA2-OA2-PA1
63	M2	404	CDL	CA7-C31-C32-C33
63	f	401	CDL	C52-C53-C54-C55
63	5B	702	CDL	CA7-C31-C32-C33
63	m1	401	CDL	C51-C52-C53-C54
62	C3	605	PC1	C35-C36-C37-C38
62	c3	601	PC1	C38-C39-C3A-C3B
63	V	201	CDL	C16-C17-C18-C19
63	C1	706	CDL	CA7-C31-C32-C33
63	Y0	101	CDL	C72-C71-CB7-OB8
63	m1	403	CDL	C11-C12-C13-C14
63	E	402	CDL	C53-C54-C55-C56
62	M2	402	PC1	C11-C12-N-C13
62	m2	402	PC1	C11-C12-N-C14
62	m2	406	PC1	C11-C12-N-C13
63	C1	706	CDL	C52-C51-CB5-OB6
63	7a	202	CDL	C32-C31-CA7-OA9
63	l	301	CDL	C12-C13-C14-C15
63	A	503	CDL	OB6-CB4-CB6-OB8
63	5b	703	CDL	C71-C72-C73-C74
63	m3	401	CDL	C53-C54-C55-C56
63	m1	403	CDL	C31-C32-C33-C34
63	b	501	CDL	C51-C52-C53-C54
62	m2	405	PC1	C2-C1-O11-P
63	7C	303	CDL	CB4-CB3-OB5-PB2
63	7c	302	CDL	CB4-CB3-OB5-PB2
63	Y0	101	CDL	C52-C51-CB5-OB6
63	y0	101	CDL	C72-C71-CB7-OB8
63	M1	402	CDL	C31-C32-C33-C34
62	m2	406	PC1	C2E-C2F-C2G-C2H
63	l	301	CDL	C22-C23-C24-C25
63	A	503	CDL	CB3-CB4-CB6-OB8
63	M3	401	CDL	C36-C37-C38-C39
62	C3	601	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
62	c3	601	PC1	C39-C3A-C3B-C3C
63	7a	202	CDL	C40-C41-C42-C43
62	C3	601	PC1	C1-C2-O21-C21
62	C3	605	PC1	C1-C2-O21-C21
62	A	502	PC1	C3-C2-O21-C21
62	c3	601	PC1	C1-C2-O21-C21
62	c3	605	PC1	C1-C2-O21-C21
62	a	502	PC1	C3-C2-O21-C21
63	7A	201	CDL	CA6-CA4-OA6-CA5
63	7C	301	CDL	CB6-CB4-OB6-CB5
63	Y7	501	CDL	CA6-CA4-OA6-CA5
63	A	503	CDL	CA3-CA4-OA6-CA5
63	N	303	CDL	CA6-CA4-OA6-CA5
63	7a	201	CDL	CA6-CA4-OA6-CA5
63	a	503	CDL	CA3-CA4-OA6-CA5
63	n	303	CDL	CA6-CA4-OA6-CA5
63	t	201	CDL	CA6-CA4-OA6-CA5
63	M3	401	CDL	C53-C54-C55-C56
63	m1	401	CDL	C72-C71-CB7-OB8
63	5B	703	CDL	C75-C76-C77-C78
63	M1	402	CDL	CB7-C71-C72-C73
63	L	301	CDL	C14-C15-C16-C17
63	u	201	CDL	C11-C12-C13-C14
63	7c	301	CDL	OB5-CB3-CB4-OB6
63	M1	402	CDL	C11-C12-C13-C14
63	V	201	CDL	O1-C1-CA2-OA2
63	v	201	CDL	O1-C1-CA2-OA2
63	M1	401	CDL	C51-C52-C53-C54
62	m2	406	PC1	C2-C1-O11-P
63	M3	403	CDL	C1-CA2-OA2-PA1
63	m1	404	CDL	CB4-CB3-OB5-PB2
62	m1	405	PC1	O11-C1-C2-C3
63	U	201	CDL	OB5-CB3-CB4-CB6
63	M1	402	CDL	C13-C14-C15-C16
63	U	201	CDL	C11-C12-C13-C14
63	7c	301	CDL	C39-C40-C41-C42
63	m2	401	CDL	OA6-CA4-CA6-OA8
63	a	503	CDL	OB6-CB4-CB6-OB8
62	M2	405	PC1	C24-C25-C26-C27
63	L	301	CDL	C22-C23-C24-C25
59	C1	702	HEA	CAD-CBD-CGD-O1D
63	5B	704	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
62	M1	404	PC1	C11-C12-N-C13
62	m1	405	PC1	C11-C12-N-C15
62	a	501	PC1	C11-C12-N-C15
63	7A	202	CDL	C40-C41-C42-C43
63	m1	403	CDL	C13-C14-C15-C16
59	c1	702	HEA	CAD-CBD-CGD-O1D
62	C3	605	PC1	O31-C31-C32-C33
63	c1	706	CDL	C52-C51-CB5-OB6
63	m3	401	CDL	C51-C52-C53-C54
62	C1	705	PC1	C28-C29-C2A-C2B
62	M2	406	PC1	C2E-C2F-C2G-C2H
62	m1	402	PC1	C39-C3A-C3B-C3C
62	m2	405	PC1	C24-C25-C26-C27
59	C1	701	HEA	CAD-CBD-CGD-O2D
59	c1	701	HEA	CAD-CBD-CGD-O2D
63	c3	604	CDL	C52-C53-C54-C55
62	m2	405	PC1	C22-C23-C24-C25
63	5b	703	CDL	C74-C75-C76-C77
62	M2	406	PC1	C2-C1-O11-P
63	c3	604	CDL	CB4-CB3-OB5-PB2
63	m3	403	CDL	C1-CA2-OA2-PA1
63	t	201	CDL	CA4-CA3-OA5-PA1
62	M2	405	PC1	C22-C23-C24-C25
63	k	301	CDL	C75-C76-C77-C78
63	m3	403	CDL	C16-C17-C18-C19
62	C1	705	PC1	C11-C12-N-C13
63	f	401	CDL	C38-C39-C40-C41
63	M3	401	CDL	C77-C78-C79-C80
63	m3	402	CDL	C53-C54-C55-C56
63	C1	706	CDL	CA3-CA4-CA6-OA8
63	m2	401	CDL	CA3-CA4-CA6-OA8
63	a	503	CDL	CB3-CB4-CB6-OB8
63	t	202	CDL	CB3-CB4-CB6-OB8
63	N	303	CDL	C73-C74-C75-C76
63	l	301	CDL	C14-C15-C16-C17
63	M1	401	CDL	C12-C11-CA5-OA6
62	c3	605	PC1	C36-C37-C38-C39
62	m1	402	PC1	C2A-C2B-C2C-C2D
63	E	401	CDL	OB5-CB3-CB4-OB6
63	U	201	CDL	OB5-CB3-CB4-OB6
63	7C	301	CDL	C82-C83-C84-C85
63	C1	707	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
63	c1	707	CDL	CB7-C71-C72-C73
62	A	501	PC1	C36-C37-C38-C39
62	c3	605	PC1	O31-C31-C32-C33
63	7A	201	CDL	C72-C71-CB7-OB8
63	m1	401	CDL	C12-C11-CA5-OA6
62	c1	705	PC1	C28-C29-C2A-C2B
63	m1	403	CDL	C32-C31-CA7-OA8
63	5B	702	CDL	OB5-CB3-CB4-CB6
63	E	401	CDL	OB5-CB3-CB4-CB6
62	c3	605	PC1	C35-C36-C37-C38
63	5B	702	CDL	C56-C57-C58-C59
63	u	201	CDL	C62-C63-C64-C65
63	C3	604	CDL	CB4-CB3-OB5-PB2
63	5B	703	CDL	C1-CA2-OA2-PA1
63	M3	402	CDL	C1-CA2-OA2-PA1
63	T	201	CDL	CA4-CA3-OA5-PA1
63	k	301	CDL	CB4-CB3-OB5-PB2
63	M3	402	CDL	C53-C54-C55-C56
62	a	501	PC1	C36-C37-C38-C39
63	m3	401	CDL	C36-C37-C38-C39
62	C3	603	PC1	O21-C21-C22-C23
63	M3	403	CDL	C16-C17-C18-C19
62	c3	603	PC1	O21-C21-C22-C23
62	n	301	PC1	C21-C22-C23-C24
62	C1	705	PC1	C11-C12-N-C15
63	M3	401	CDL	C51-C52-C53-C54
63	7a	202	CDL	C41-C42-C43-C44
62	n	302	PC1	O31-C31-C32-C33
63	5b	703	CDL	C72-C71-CB7-OB8
63	7a	201	CDL	C72-C71-CB7-OB8
63	7a	202	CDL	C72-C71-CB7-OB8
63	m3	402	CDL	C32-C31-CA7-OA8
63	n	303	CDL	C73-C74-C75-C76
63	M1	401	CDL	CB3-CB4-OB6-CB5
63	M2	401	CDL	CB3-CB4-OB6-CB5
63	M2	404	CDL	CB3-CB4-OB6-CB5
63	E	402	CDL	CB3-CB4-OB6-CB5
63	T	201	CDL	CA6-CA4-OA6-CA5
63	T	202	CDL	CA6-CA4-OA6-CA5
63	7c	301	CDL	CB6-CB4-OB6-CB5
63	m2	401	CDL	CB3-CB4-OB6-CB5
63	m2	404	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
63	e	402	CDL	CB3-CB4-OB6-CB5
63	t	202	CDL	CA6-CA4-OA6-CA5
62	7C	302	PC1	C39-C3A-C3B-C3C
63	f	401	CDL	C77-C78-C79-C80
62	7C	302	PC1	C2A-C2B-C2C-C2D
63	5b	702	CDL	C56-C57-C58-C59
59	c1	702	HEA	C4D-C3D-CAD-CBD
63	5B	703	CDL	CB4-CB3-OB5-PB2
63	k	301	CDL	C1-CA2-OA2-PA1
63	7c	301	CDL	CB2-C1-CA2-OA2
59	C1	702	HEA	C19-C20-C21-C22
63	7C	303	CDL	CA3-CA4-CA6-OA8
63	7c	302	CDL	CA3-CA4-CA6-OA8
63	M3	401	CDL	C71-C72-C73-C74
63	c1	706	CDL	C32-C31-CA7-OA8
62	c3	605	PC1	C24-C25-C26-C27
63	f	401	CDL	C34-C35-C36-C37
62	A	502	PC1	O31-C31-C32-C33
63	7A	202	CDL	C39-C40-C41-C42
62	A	502	PC1	O21-C2-C3-O31
63	L	301	CDL	C23-C24-C25-C26
62	a	502	PC1	O31-C31-C32-C33
63	M1	402	CDL	C12-C11-CA5-OA6
63	J	301	CDL	C32-C31-CA7-OA8
63	7A	202	CDL	C32-C31-CA7-OA9
63	M1	401	CDL	C78-C79-C80-C81
62	M2	402	PC1	C11-C12-N-C14
62	C3	601	PC1	O32-C31-C32-C33
63	C1	706	CDL	C32-C31-CA7-OA8
63	7a	201	CDL	C32-C31-CA7-OA8
63	T	201	CDL	C24-C25-C26-C27
63	t	201	CDL	C24-C25-C26-C27
63	5b	703	CDL	C83-C84-C85-C86
63	M1	402	CDL	C32-C31-CA7-OA8
63	M2	403	CDL	C72-C71-CB7-OB8
62	7c	303	PC1	C26-C27-C28-C29
63	C3	604	CDL	C1-CB2-OB2-PB2
62	c3	601	PC1	C3A-C3B-C3C-C3D
63	F	401	CDL	C38-C39-C40-C41
59	c1	701	HEA	C19-C20-C21-C22
59	C1	702	HEA	CAA-CBA-CGA-O2A
63	L	301	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
62	c1	705	PC1	O13-C11-C12-N
63	m1	401	CDL	C56-C57-C58-C59
62	A	501	PC1	O31-C31-C32-C33
62	N	302	PC1	O31-C31-C32-C33
63	E	402	CDL	C72-C71-CB7-OB8
63	j	301	CDL	C32-C31-CA7-OA8
62	7C	304	PC1	C2D-C2E-C2F-C2G
59	c1	702	HEA	CAA-CBA-CGA-O2A
63	C3	604	CDL	C12-C11-CA5-OA6
63	m1	403	CDL	C12-C11-CA5-OA6
63	5b	702	CDL	C58-C59-C60-C61
63	l	301	CDL	C13-C14-C15-C16
62	M1	404	PC1	C11-C12-N-C14
63	F	401	CDL	C77-C78-C79-C80
63	c1	707	CDL	C52-C53-C54-C55
63	m2	404	CDL	C33-C34-C35-C36
62	N	301	PC1	O21-C21-C22-C23
62	a	501	PC1	O31-C31-C32-C33
62	n	301	PC1	O21-C21-C22-C23
63	c3	604	CDL	C12-C11-CA5-OA6
63	e	402	CDL	C72-C71-CB7-OB8
63	l	301	CDL	C12-C11-CA5-OA6
63	C1	707	CDL	C52-C53-C54-C55
63	Y5	201	CDL	CB7-C71-C72-C73
63	l	301	CDL	C23-C24-C25-C26
63	M2	404	CDL	C52-C51-CB5-OB6
63	M1	401	CDL	C57-C58-C59-C60
63	7a	202	CDL	C39-C40-C41-C42
63	E	401	CDL	C16-C17-C18-C19
63	7A	201	CDL	C32-C31-CA7-OA8
63	L	301	CDL	C12-C11-CA5-OA6
63	m2	403	CDL	C72-C71-CB7-OB8
63	y0	101	CDL	C12-C11-CA5-OA6
63	t	202	CDL	C12-C11-CA5-OA6
63	5B	704	CDL	C82-C83-C84-C85
63	F	401	CDL	C34-C35-C36-C37
59	C1	701	HEA	C19-C20-C21-C22
63	M2	403	CDL	CA3-CA4-CA6-OA8
63	Y7	501	CDL	CB3-CB4-CB6-OB8
63	c1	706	CDL	CA3-CA4-CA6-OA8
63	m2	403	CDL	CA3-CA4-CA6-OA8
63	y7	501	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
62	a	501	PC1	C11-C12-N-C13
63	T	202	CDL	C12-C11-CA5-OA6
63	m2	404	CDL	C52-C51-CB5-OB6
63	C1	706	CDL	C33-C34-C35-C36
62	j	302	PC1	O21-C2-C3-O31
63	V	201	CDL	OB6-CB4-CB6-OB8
63	v	201	CDL	OB6-CB4-CB6-OB8
63	7a	202	CDL	C60-C61-C62-C63
62	C3	603	PC1	O31-C31-C32-C33
62	7C	302	PC1	O21-C21-C22-C23
63	5B	702	CDL	C58-C59-C60-C61
63	k	301	CDL	C77-C78-C79-C80
63	M2	404	CDL	CA5-C11-C12-C13
63	C1	707	CDL	OB5-CB3-CB4-CB6
63	c1	707	CDL	OB5-CB3-CB4-CB6
59	C1	702	HEA	CAD-CBD-CGD-O2D
62	C3	605	PC1	C24-C25-C26-C27
63	m3	401	CDL	C34-C35-C36-C37
62	a	501	PC1	C2A-C2B-C2C-C2D
63	M2	403	CDL	CB7-C71-C72-C73
63	7A	202	CDL	C60-C61-C62-C63
63	7C	301	CDL	C39-C40-C41-C42
63	Y0	101	CDL	C15-C16-C17-C18
62	A	502	PC1	C1-C2-O21-C21
62	a	502	PC1	C1-C2-O21-C21
63	7A	201	CDL	CA3-CA4-OA6-CA5
63	M1	401	CDL	CB6-CB4-OB6-CB5
63	M2	401	CDL	CB6-CB4-OB6-CB5
63	E	401	CDL	CA3-CA4-OA6-CA5
63	E	401	CDL	CA6-CA4-OA6-CA5
63	E	402	CDL	CB6-CB4-OB6-CB5
63	T	202	CDL	CA3-CA4-OA6-CA5
63	7a	201	CDL	CA3-CA4-OA6-CA5
63	7c	301	CDL	CB3-CB4-OB6-CB5
63	m1	401	CDL	CB3-CB4-OB6-CB5
63	m1	401	CDL	CB6-CB4-OB6-CB5
63	m2	401	CDL	CB6-CB4-OB6-CB5
63	e	401	CDL	CA3-CA4-OA6-CA5
63	e	401	CDL	CA6-CA4-OA6-CA5
63	e	402	CDL	CB6-CB4-OB6-CB5
63	t	202	CDL	CA3-CA4-OA6-CA5
63	7c	302	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
63	M1	401	CDL	C56-C57-C58-C59
59	c1	702	HEA	CAD-CBD-CGD-O2D
63	y5	201	CDL	C72-C71-CB7-OB8
62	C3	605	PC1	C36-C37-C38-C39
63	7C	303	CDL	C51-C52-C53-C54
63	F	401	CDL	C72-C73-C74-C75
63	b	501	CDL	C15-C16-C17-C18
63	T	201	CDL	C32-C31-CA7-OA8
62	c3	603	PC1	O31-C31-C32-C33
63	7A	202	CDL	C72-C71-CB7-OB8
63	c1	707	CDL	C32-C31-CA7-OA8
63	c1	706	CDL	C33-C34-C35-C36
63	M2	403	CDL	C1-CB2-OB2-PB2
63	Y0	101	CDL	CB4-CB3-OB5-PB2
63	E	402	CDL	CA4-CA3-OA5-PA1
62	a	501	PC1	O32-C31-C32-C33
63	J	301	CDL	C32-C31-CA7-OA9
63	j	301	CDL	C32-C31-CA7-OA9
63	C1	707	CDL	C32-C31-CA7-OA8
59	C1	702	HEA	C4D-C3D-CAD-CBD
63	E	402	CDL	C72-C71-CB7-OB9
63	7a	201	CDL	C32-C31-CA7-OA9
63	e	401	CDL	C16-C17-C18-C19
63	m1	401	CDL	C57-C58-C59-C60
63	M3	402	CDL	C32-C31-CA7-OA8
63	Y0	101	CDL	C12-C11-CA5-OA6
63	c3	604	CDL	C12-C11-CA5-OA7
63	m1	403	CDL	C12-C11-CA5-OA7
62	M1	404	PC1	C11-C12-N-C15
62	N	301	PC1	O22-C21-C22-C23
63	M2	404	CDL	C52-C51-CB5-OB7
63	t	202	CDL	C12-C11-CA5-OA7
63	M1	402	CDL	C12-C11-CA5-OA7
63	M2	404	CDL	C33-C34-C35-C36
63	Y7	501	CDL	C71-C72-C73-C74
63	y5	201	CDL	CB7-C71-C72-C73
62	a	502	PC1	O32-C31-C32-C33
63	C1	706	CDL	C32-C31-CA7-OA9
63	5B	703	CDL	C77-C78-C79-C80
62	C3	602	PC1	C28-C29-C2A-C2B
62	A	501	PC1	C2A-C2B-C2C-C2D
59	c1	702	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
63	e	402	CDL	C72-C71-CB7-OB9
63	m2	403	CDL	OA6-CA4-CA6-OA8
63	B	501	CDL	C15-C16-C17-C18
63	5b	702	CDL	C31-C32-C33-C34
62	A	502	PC1	O32-C31-C32-C33
63	C3	604	CDL	C12-C11-CA5-OA7
63	L	301	CDL	C12-C11-CA5-OA7
63	c1	706	CDL	C32-C31-CA7-OA9
63	m2	404	CDL	C52-C51-CB5-OB7
62	J	302	PC1	O31-C31-C32-C33
63	Y5	201	CDL	C72-C71-CB7-OB8
63	y0	101	CDL	C15-C16-C17-C18
62	A	502	PC1	C1-C2-C3-O31
63	E	402	CDL	CB3-CB4-CB6-OB8
63	V	201	CDL	CB3-CB4-CB6-OB8
63	v	201	CDL	CB3-CB4-CB6-OB8
62	C3	605	PC1	C2-C1-O11-P
63	m2	401	CDL	C1-CA2-OA2-PA1
63	m2	403	CDL	C1-CB2-OB2-PB2
63	y0	101	CDL	CB4-CB3-OB5-PB2
63	T	201	CDL	C52-C51-CB5-OB6
63	f	401	CDL	C72-C71-CB7-OB8
63	t	201	CDL	C52-C51-CB5-OB6
62	a	501	PC1	C11-C12-N-C14
59	c1	701	HEA	CAD-CBD-CGD-O1D
62	7C	302	PC1	O22-C21-C22-C23
62	A	501	PC1	O32-C31-C32-C33
62	n	301	PC1	O22-C21-C22-C23
63	l	301	CDL	C12-C11-CA5-OA7
62	m1	402	PC1	O21-C21-C22-C23
63	7A	201	CDL	C12-C11-CA5-OA6
63	7c	301	CDL	C52-C51-CB5-OB6
62	7c	303	PC1	C2D-C2E-C2F-C2G
62	C3	603	PC1	O32-C31-C32-C33
63	m2	401	CDL	C32-C31-CA7-OA8
63	m3	403	CDL	C72-C71-CB7-OB8
63	j	301	CDL	C72-C71-CB7-OB8
63	U	201	CDL	C62-C63-C64-C65
62	C1	705	PC1	C3A-C3B-C3C-C3D
62	c3	603	PC1	O32-C31-C32-C33
63	7A	201	CDL	C32-C31-CA7-OA9
63	T	202	CDL	C12-C11-CA5-OA7

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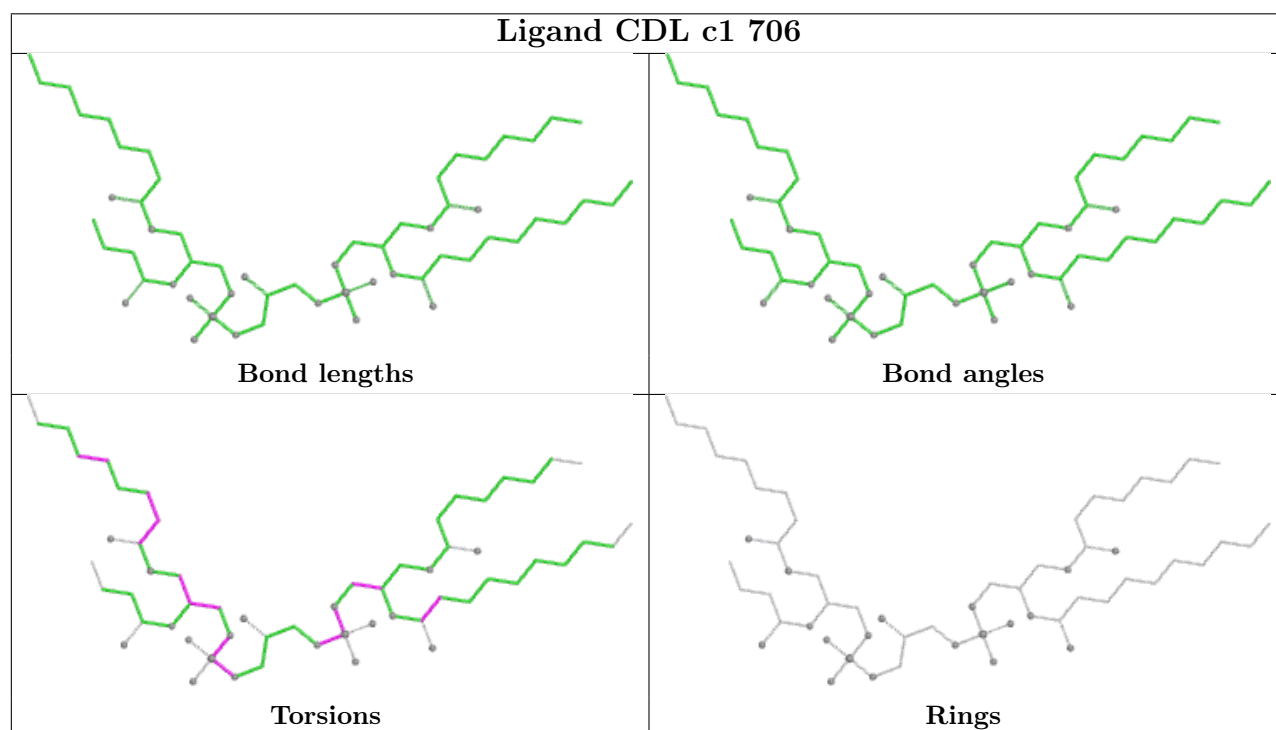
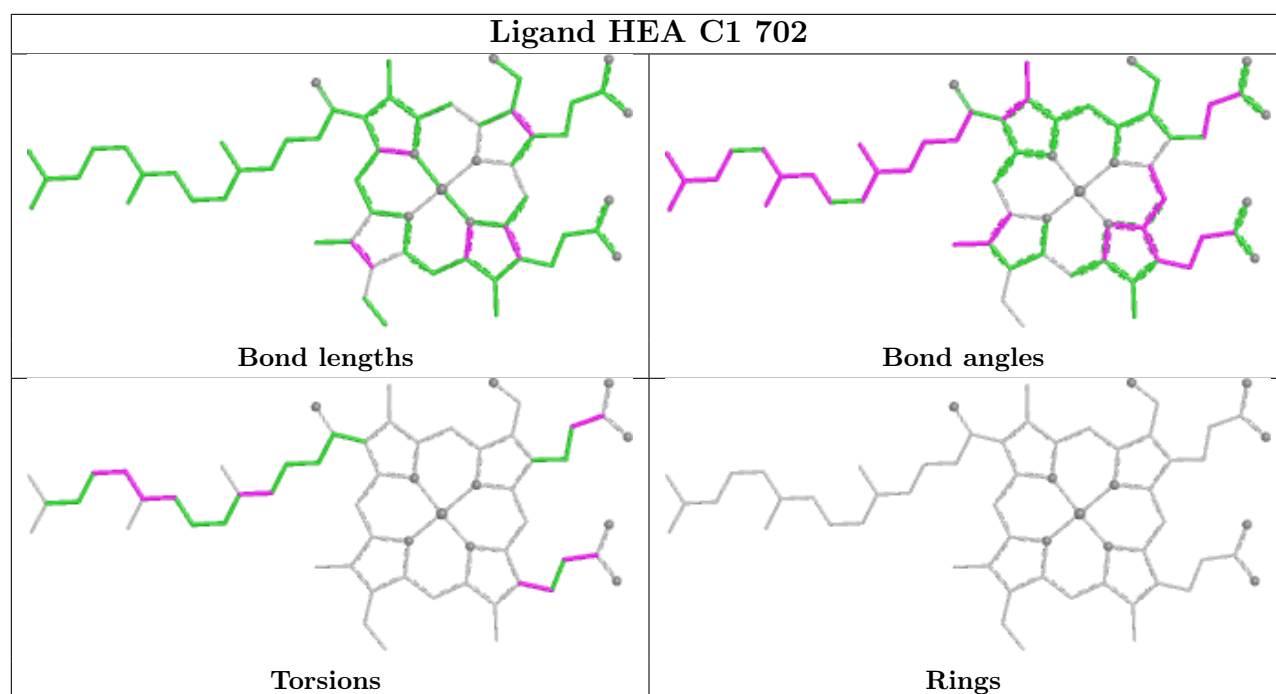
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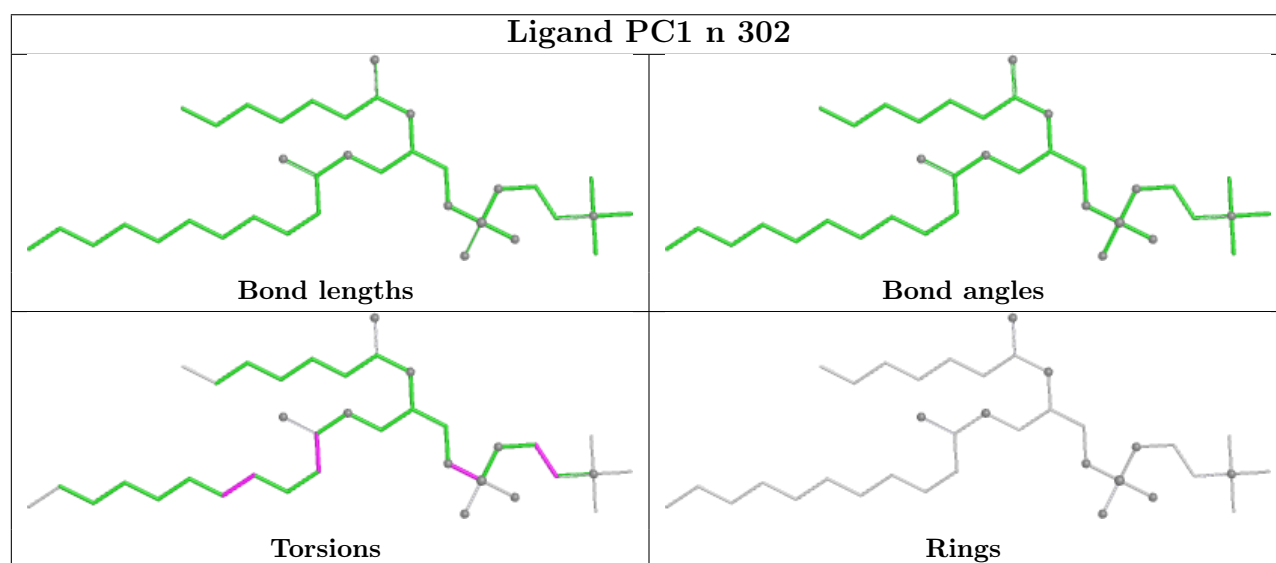
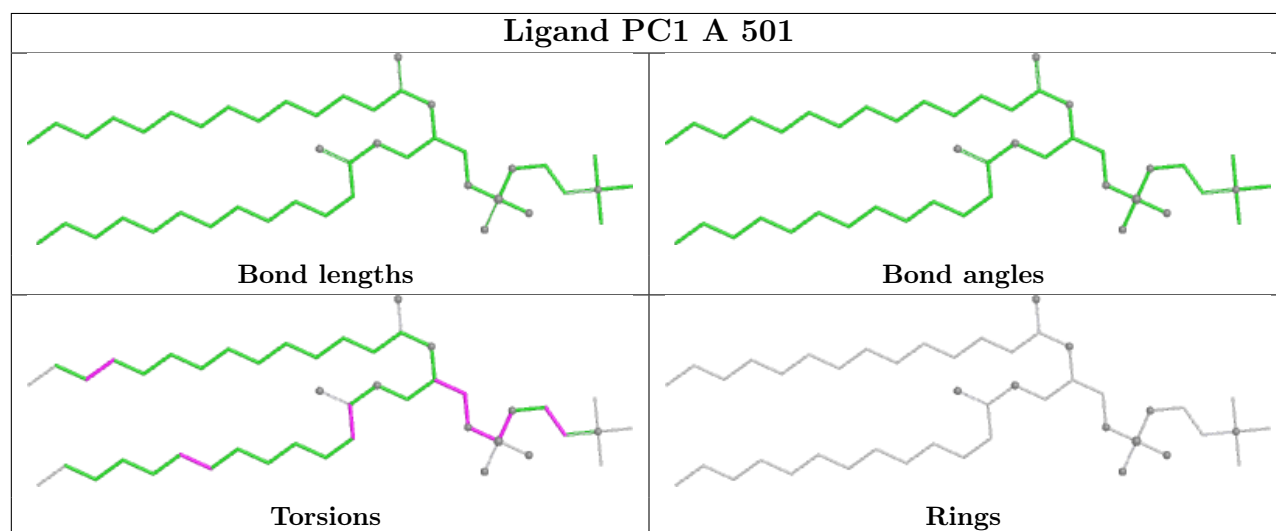
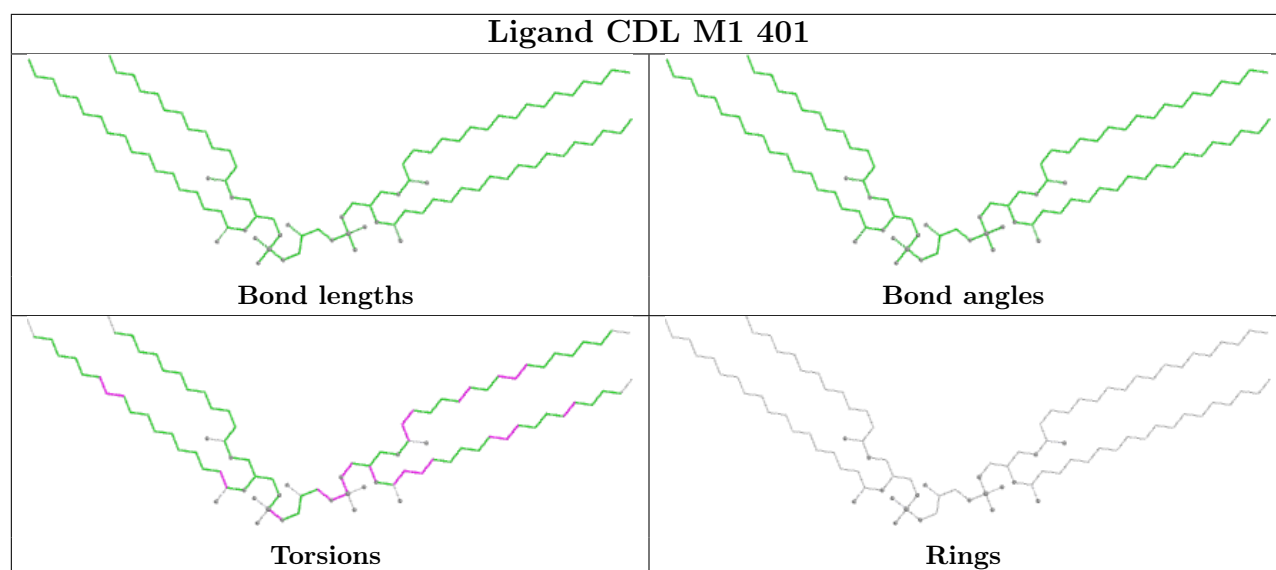
Mol	Chain	Res	Type	Atoms
63	5b	702	CDL	CA7-C31-C32-C33
63	7a	202	CDL	C57-C58-C59-C60
62	j	302	PC1	O31-C31-C32-C33
63	7C	301	CDL	C12-C11-CA5-OA6
63	M3	403	CDL	C72-C71-CB7-OB8
63	7a	201	CDL	C12-C11-CA5-OA6
63	7c	301	CDL	C12-C11-CA5-OA6
63	e	401	CDL	C72-C71-CB7-OB8
63	5B	702	CDL	C11-C12-C13-C14
63	C1	707	CDL	C32-C31-CA7-OA9
63	Y5	201	CDL	C72-C71-CB7-OB9
63	7C	301	CDL	C52-C51-CB5-OB6
63	5b	702	CDL	C12-C11-CA5-OA6
63	m3	403	CDL	C12-C11-CA5-OA6
63	a	503	CDL	C12-C11-CA5-OA6
63	y0	101	CDL	C12-C11-CA5-OA7
63	V	201	CDL	C72-C73-C74-C75

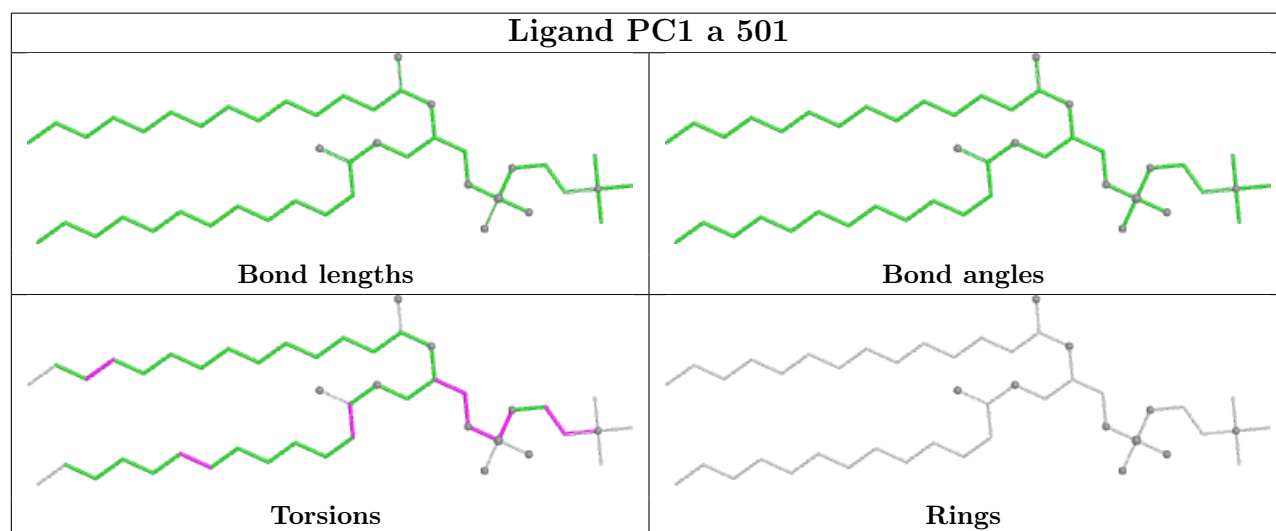
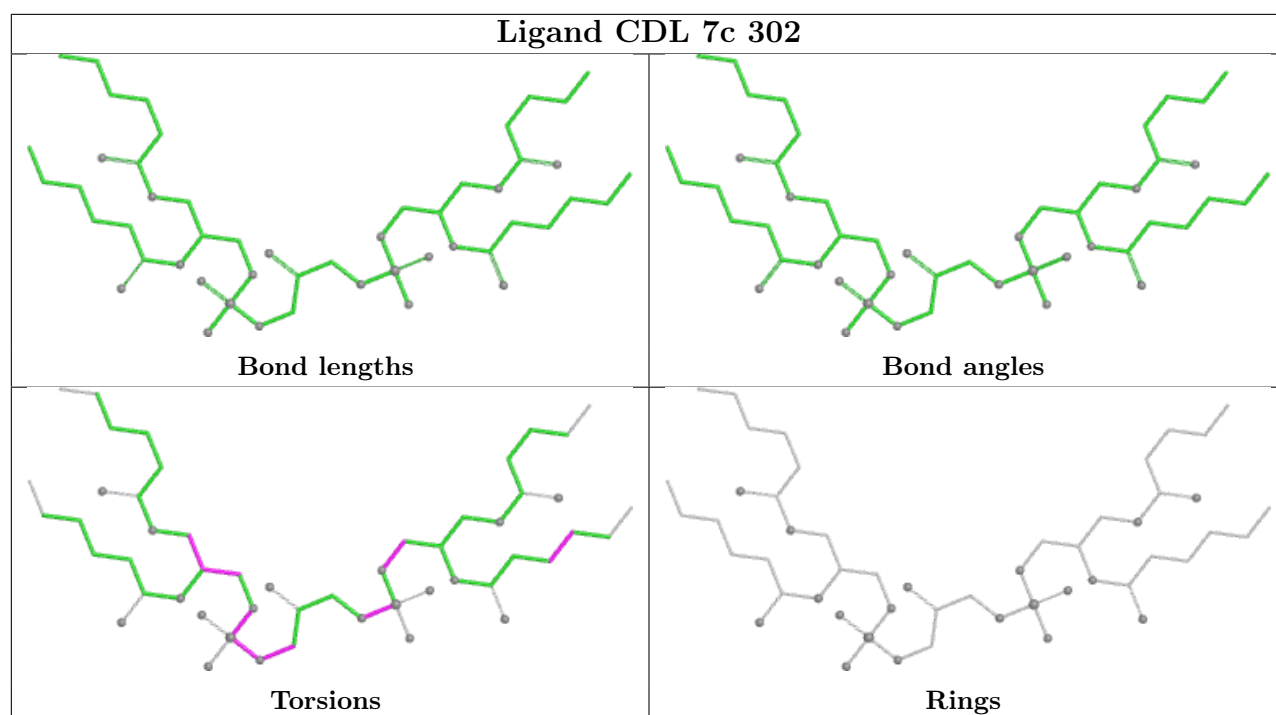
There are no ring outliers.

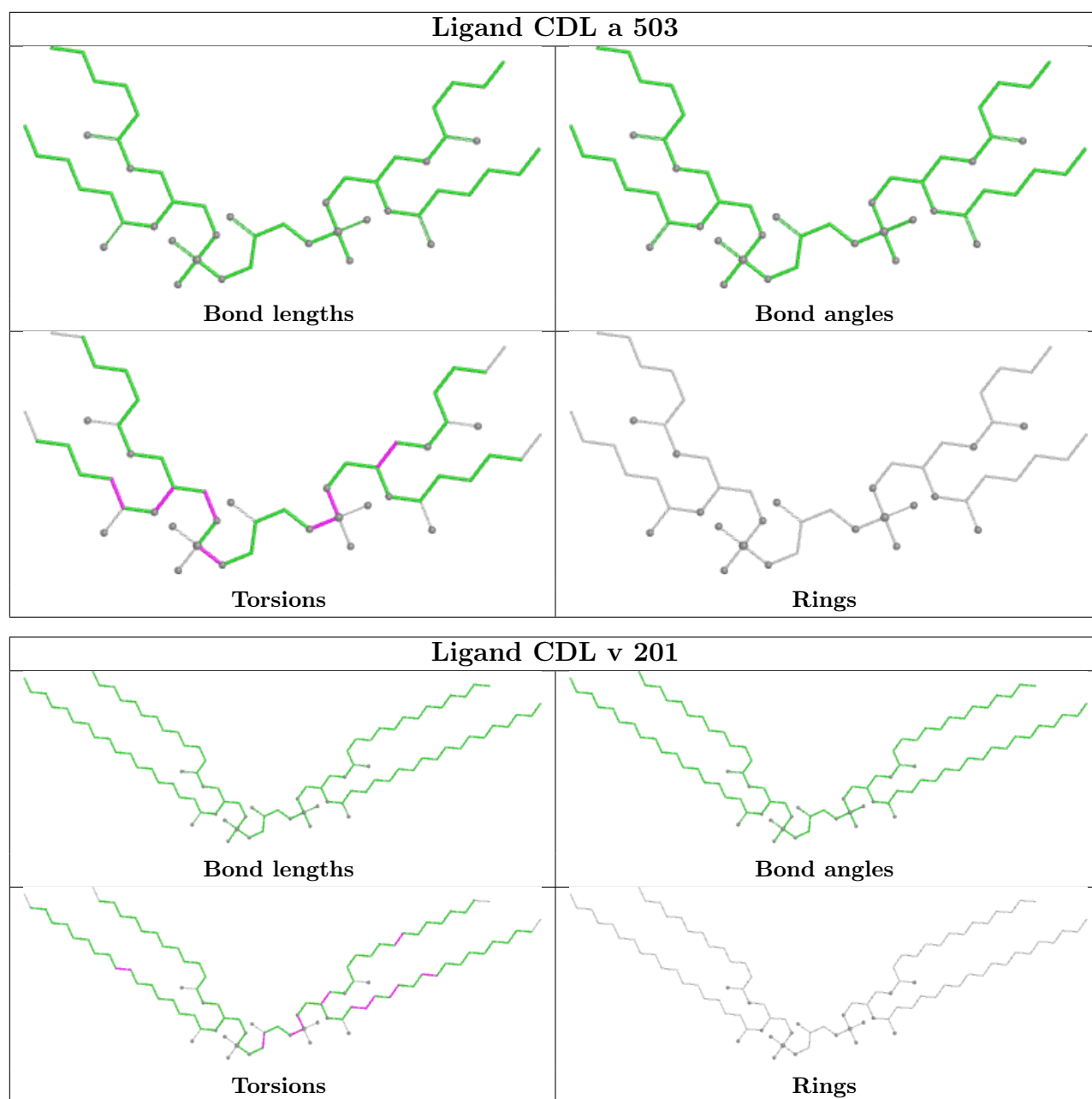
No monomer is involved in short contacts.

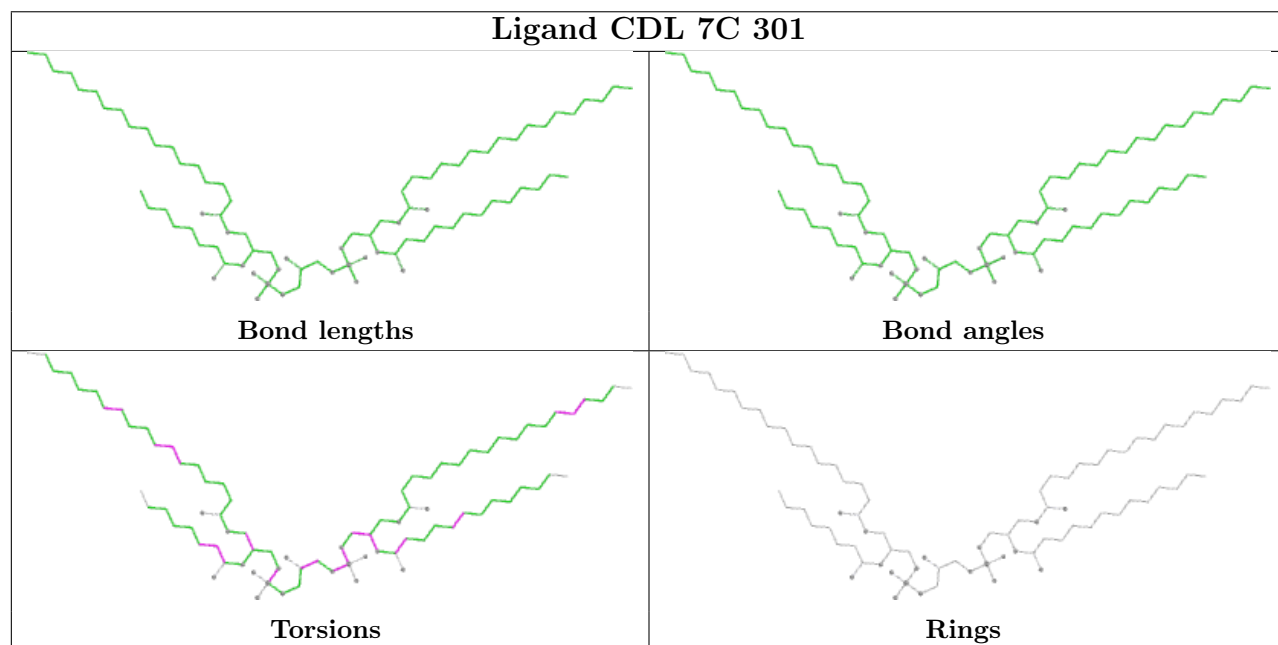
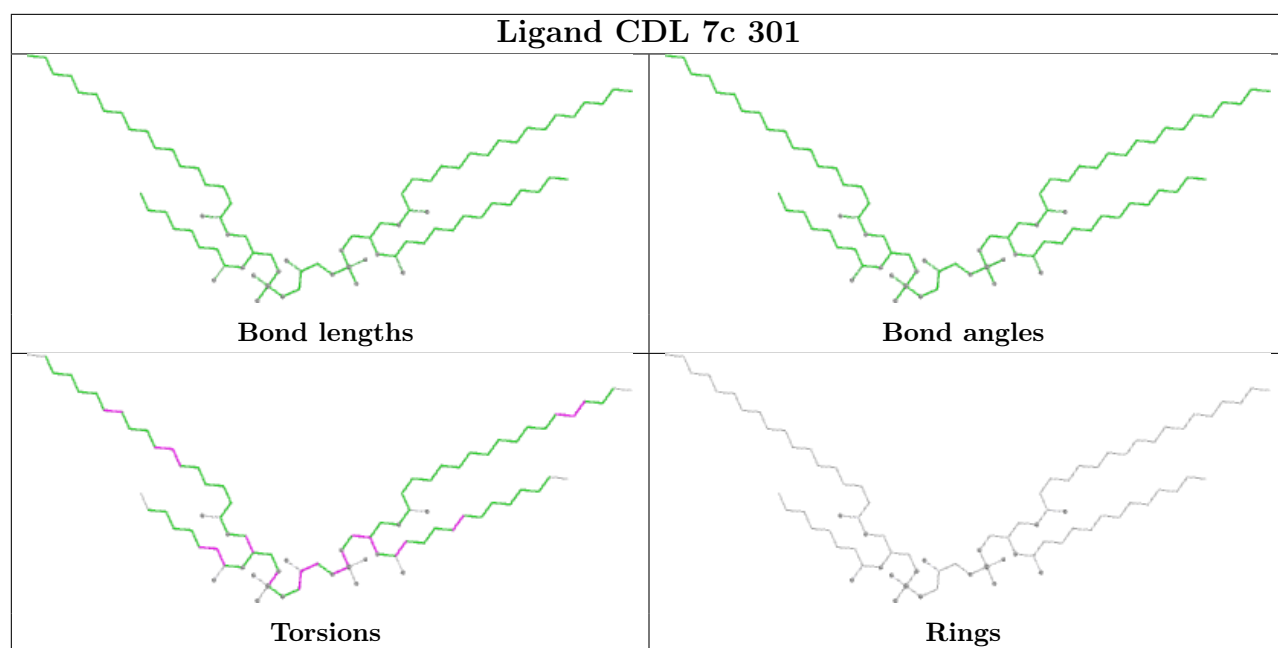
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

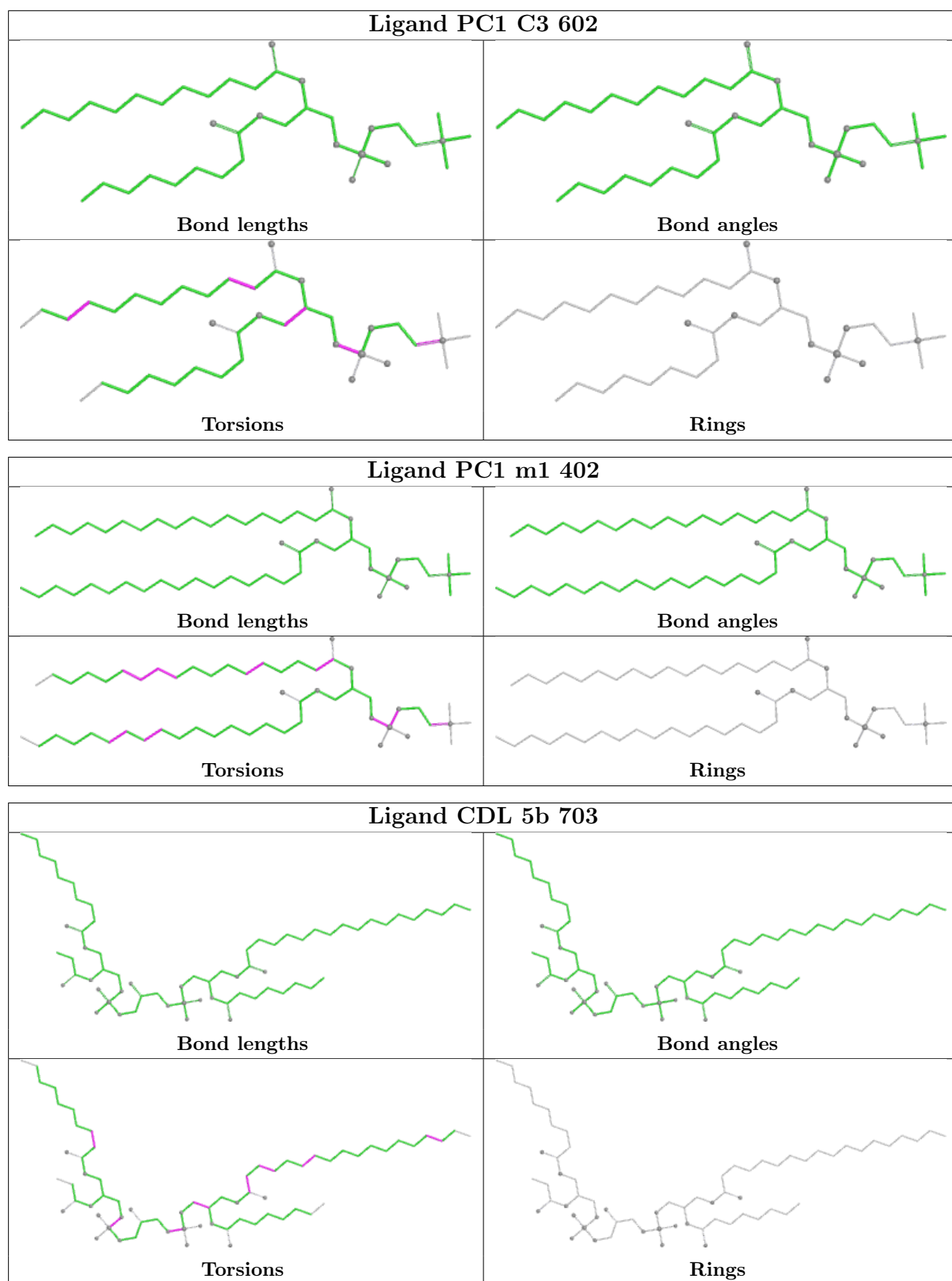


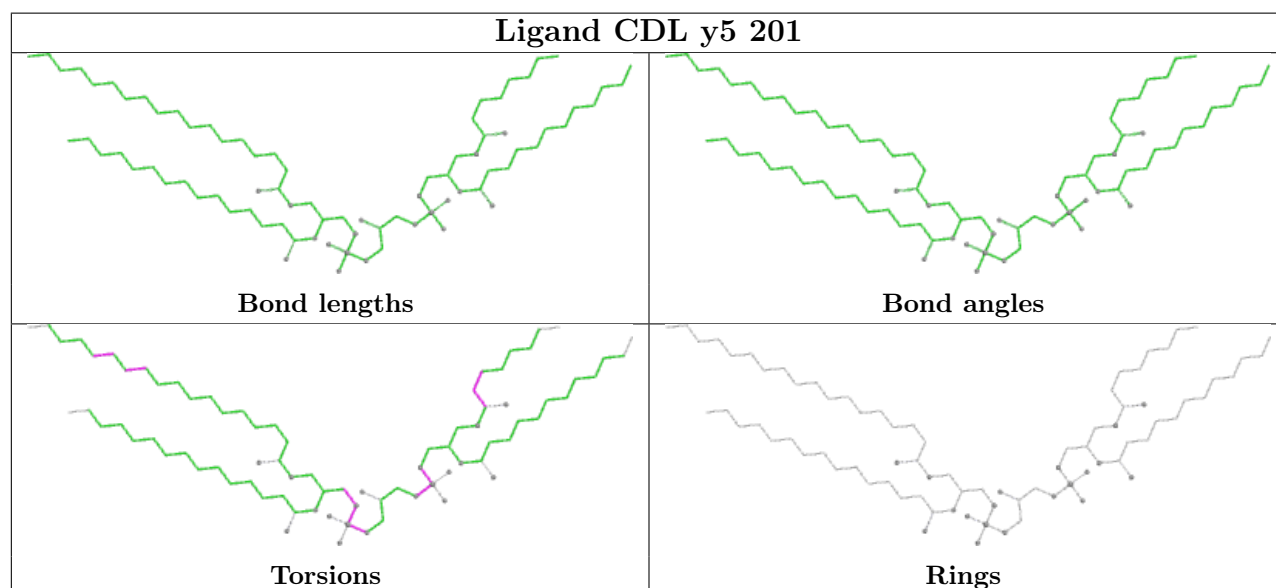
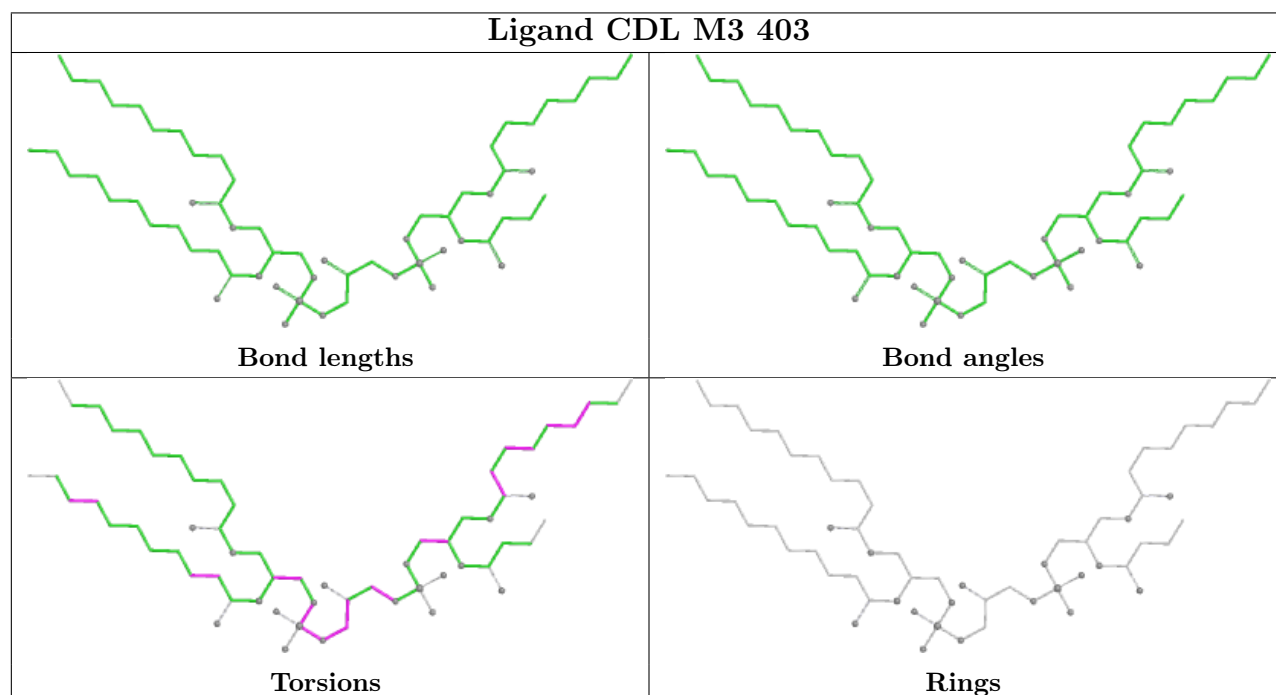
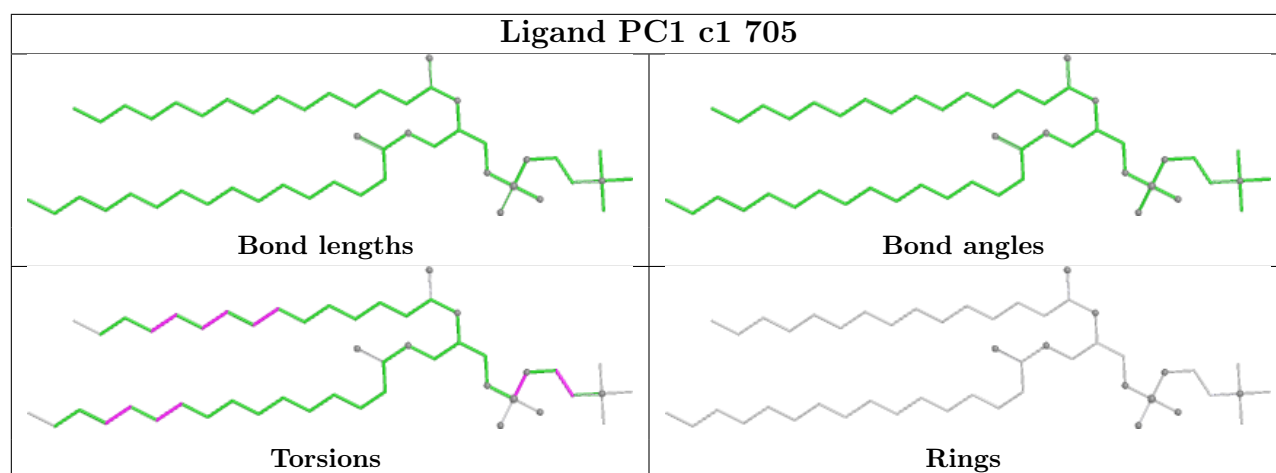


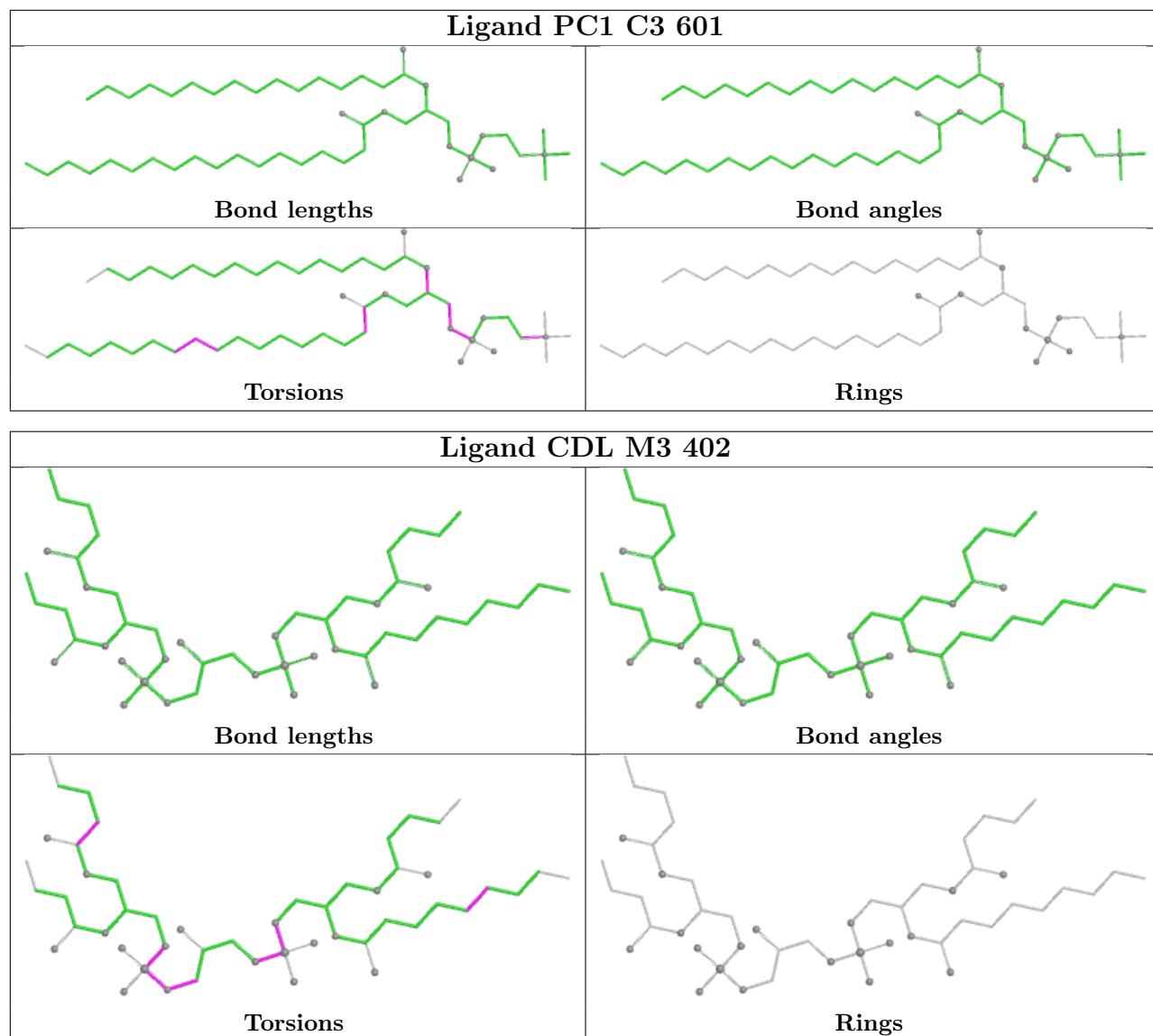


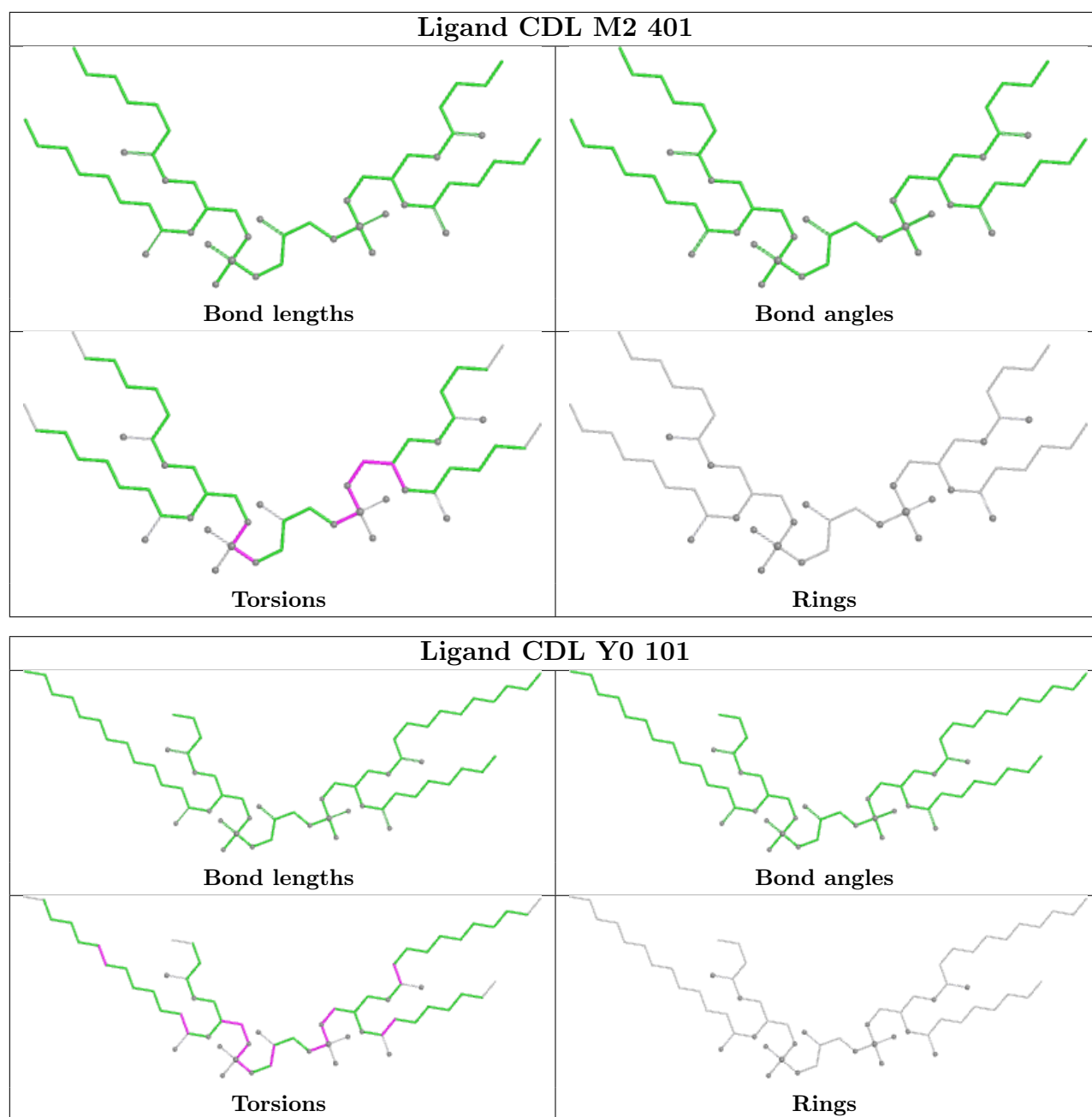


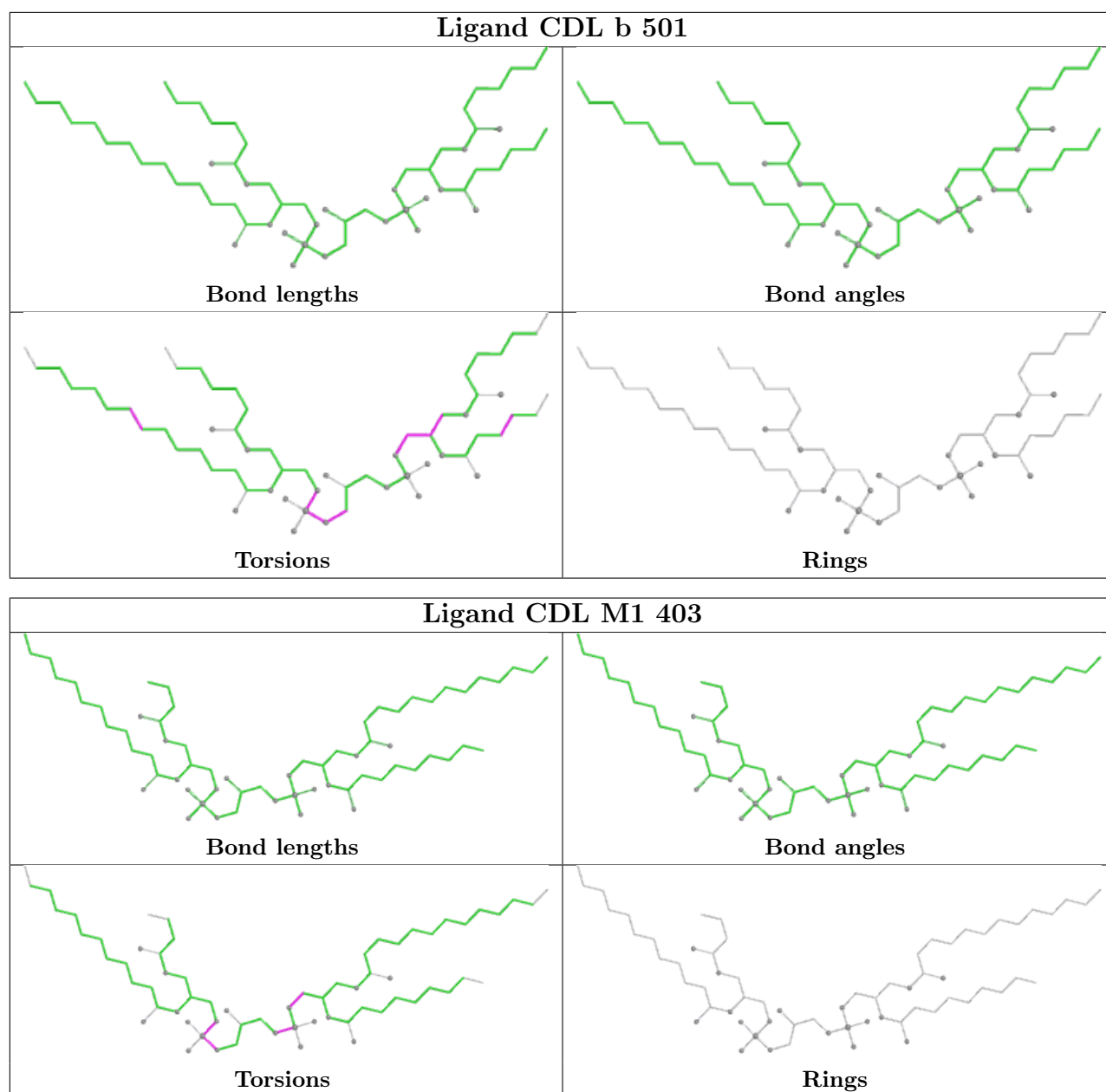


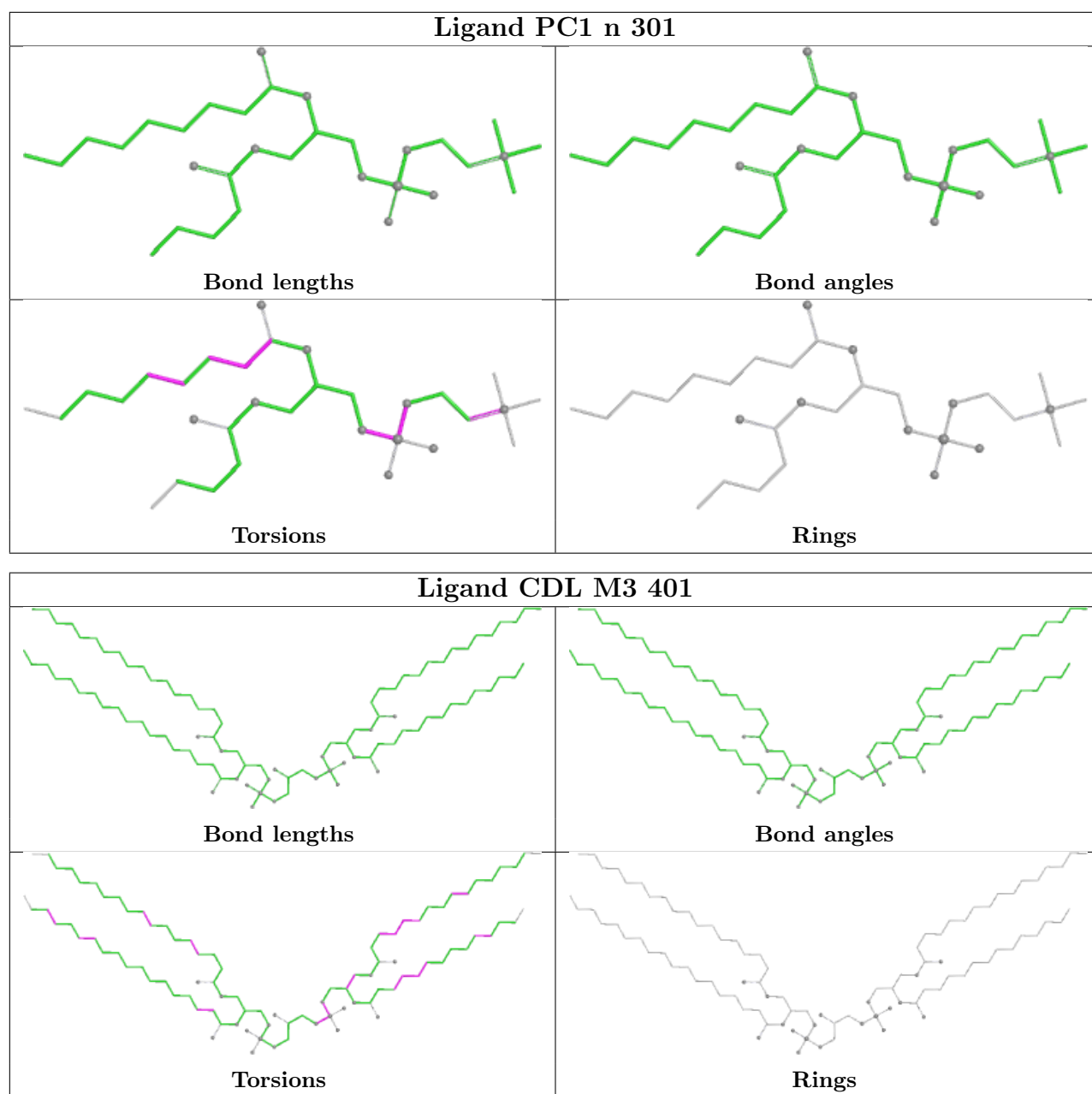


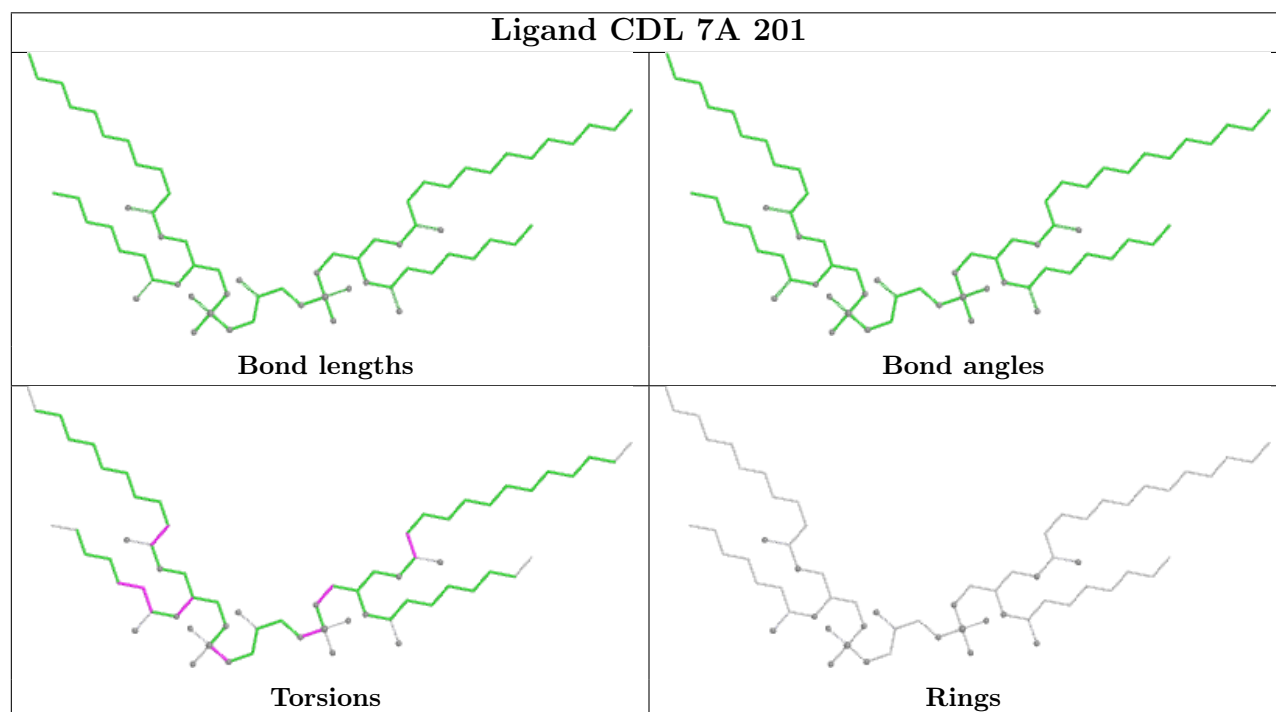
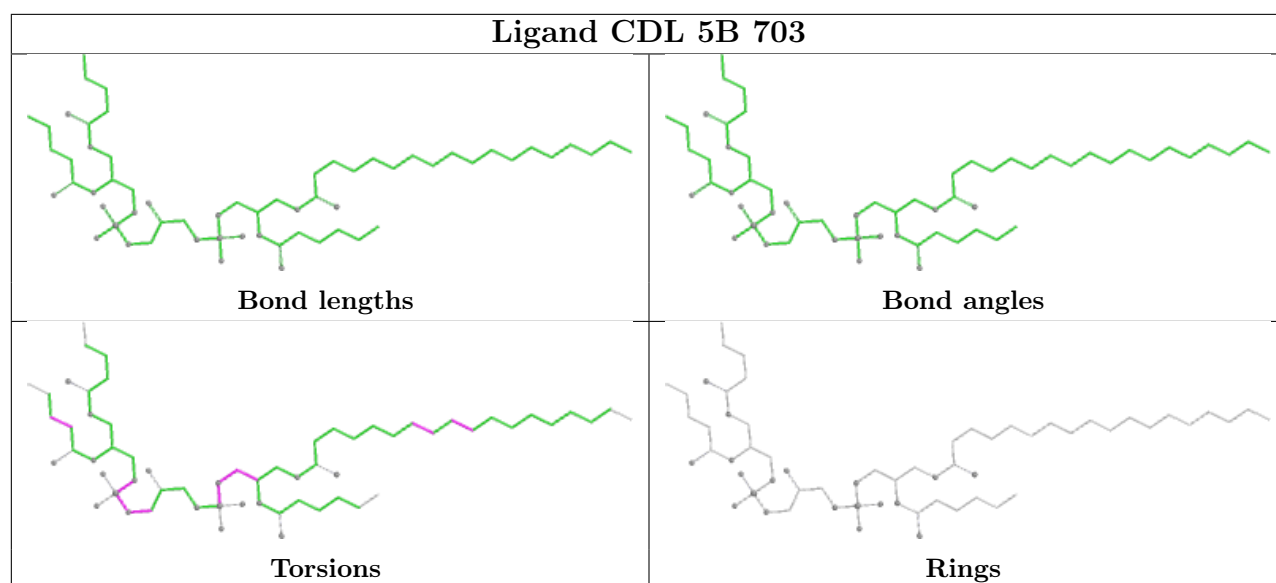


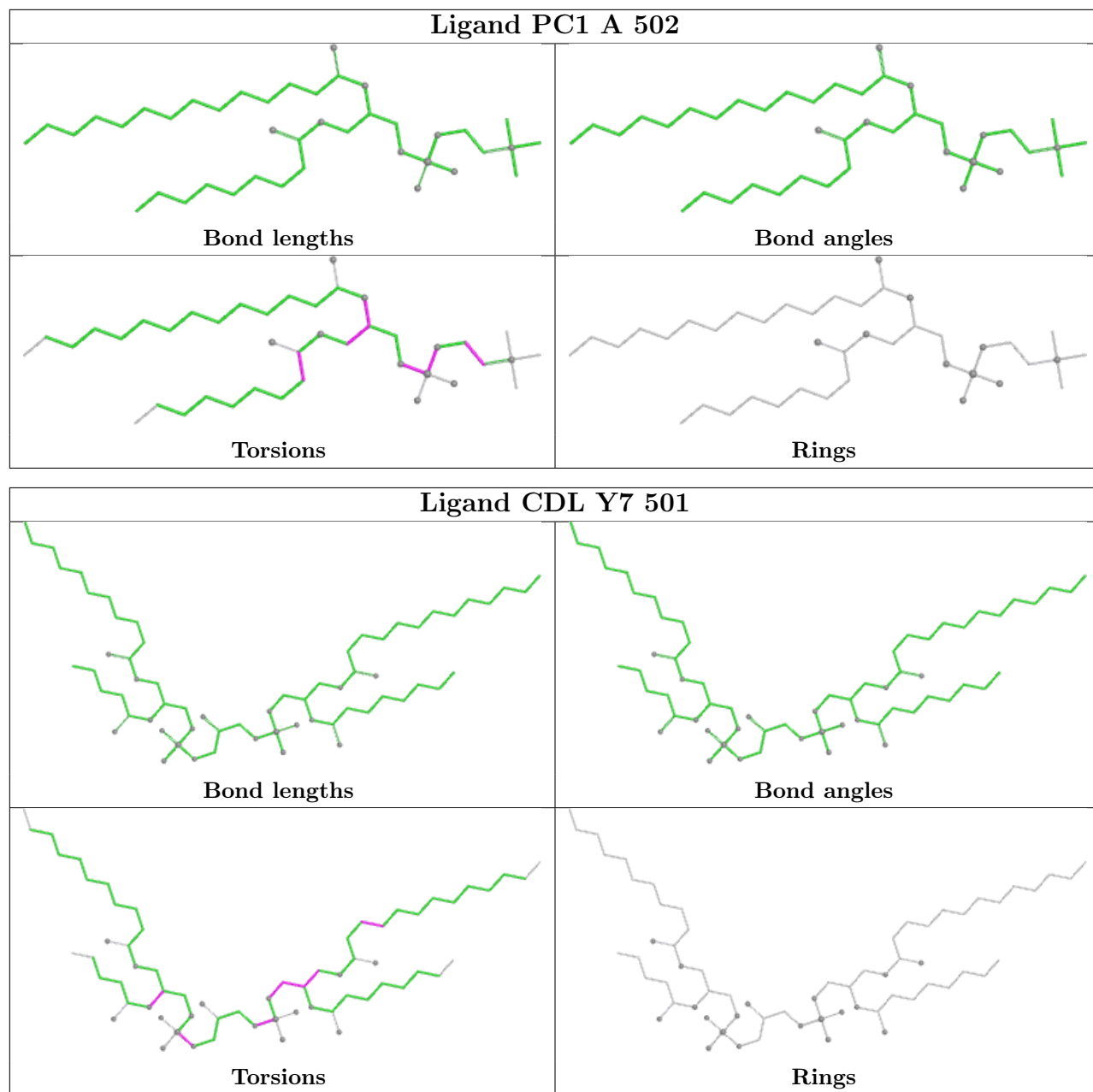


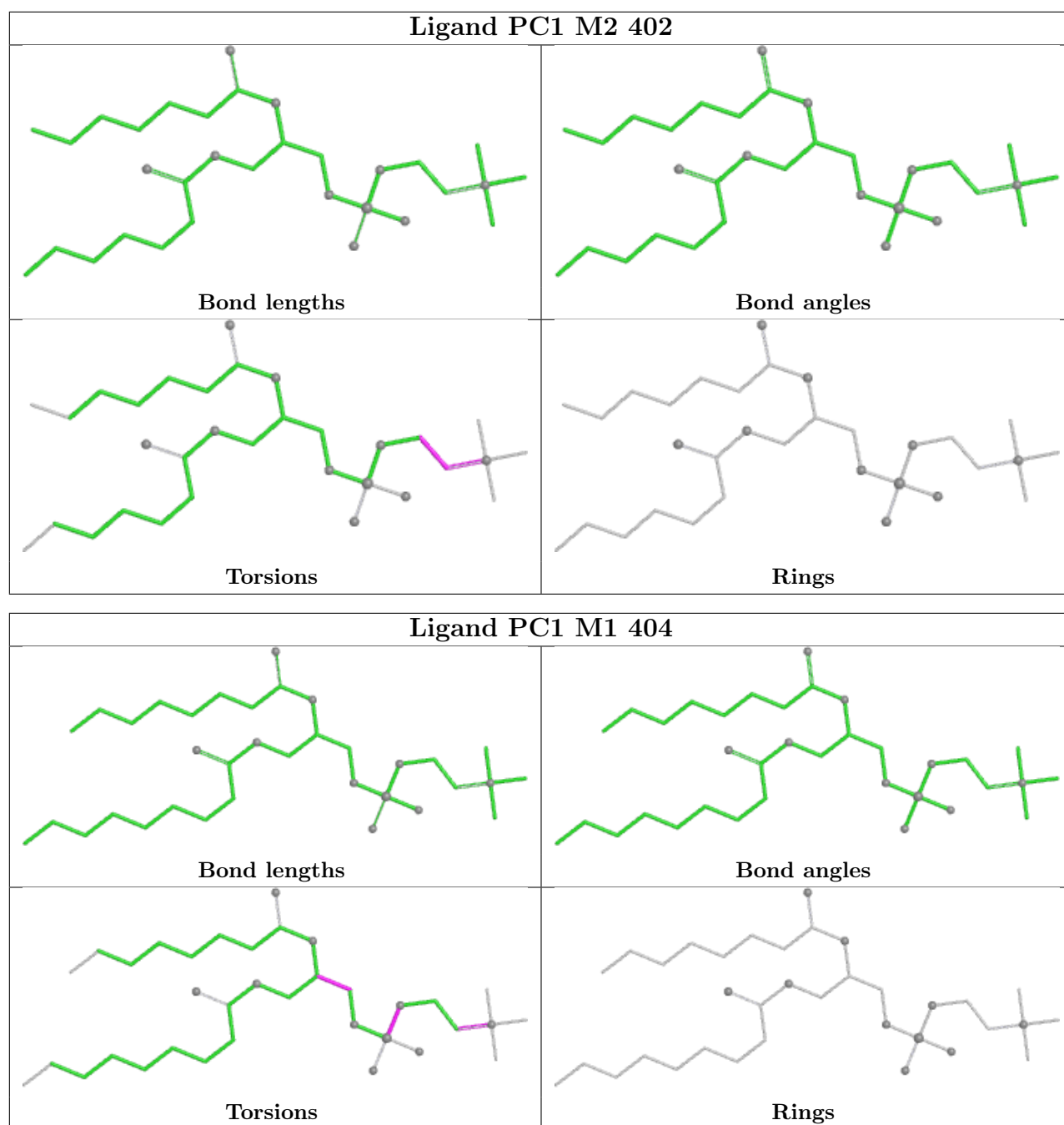


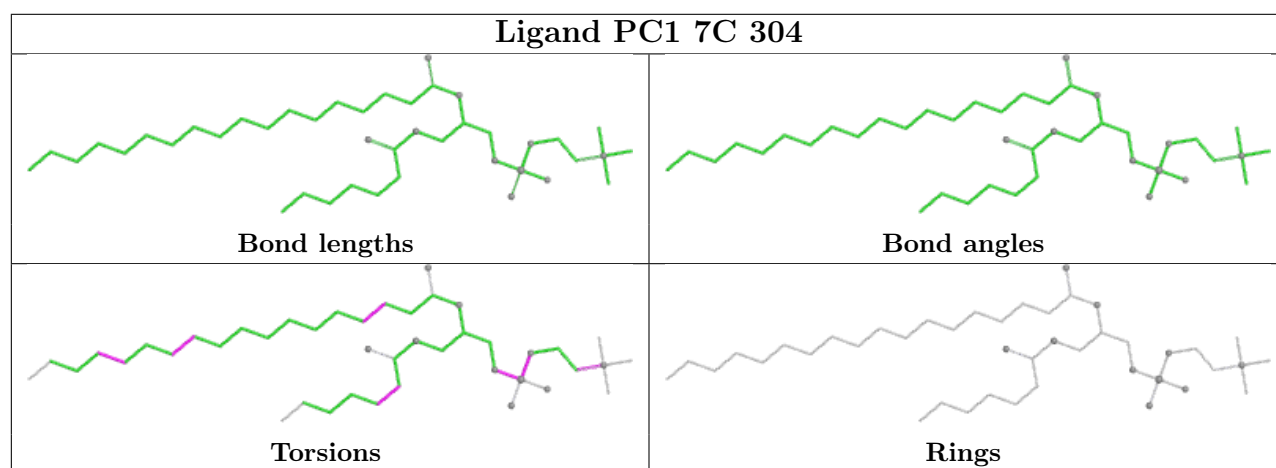
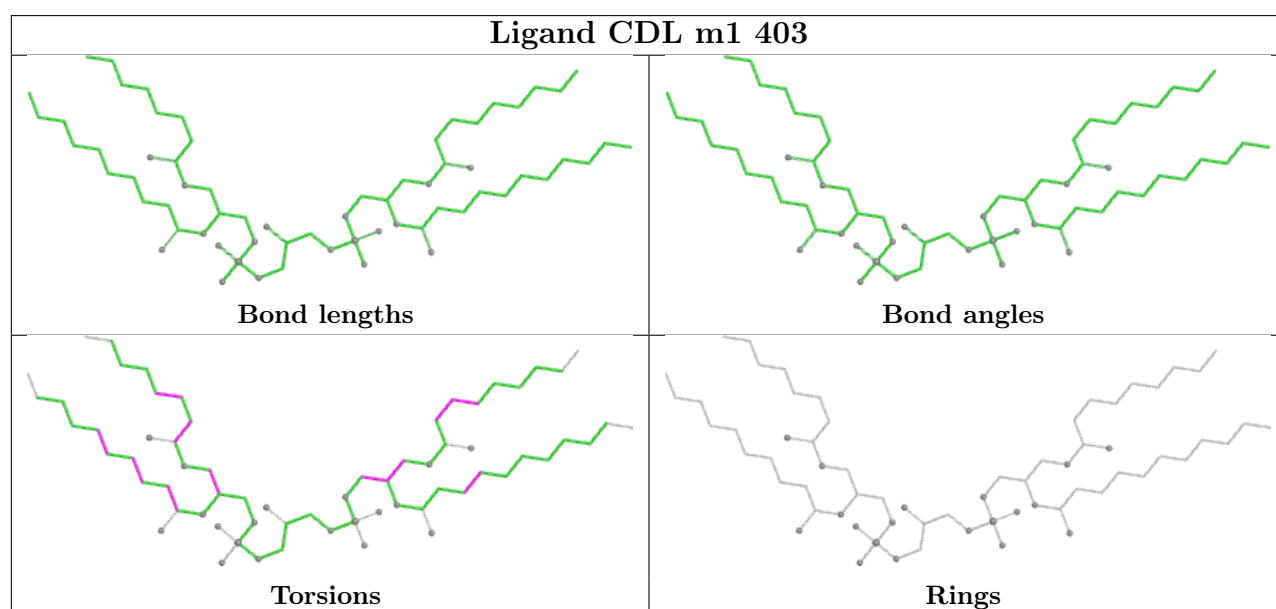
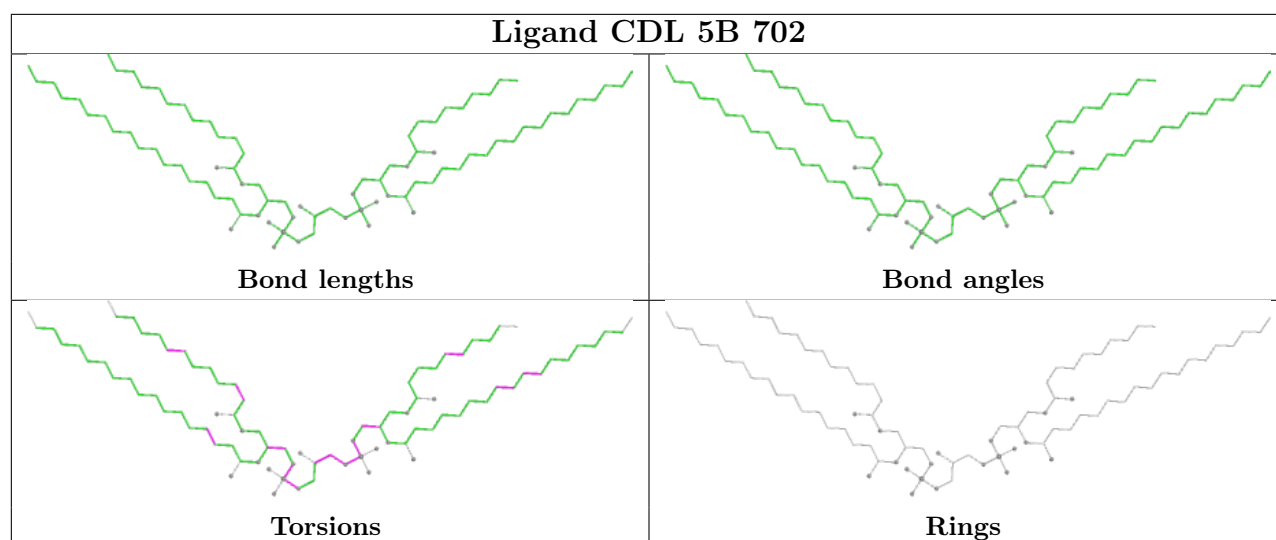


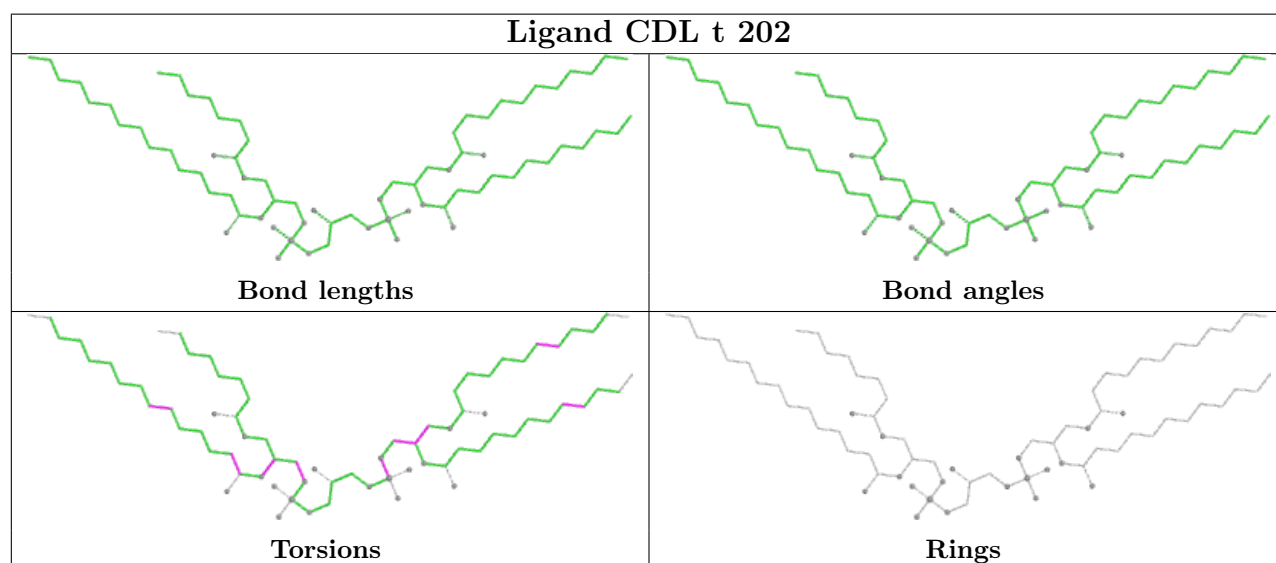
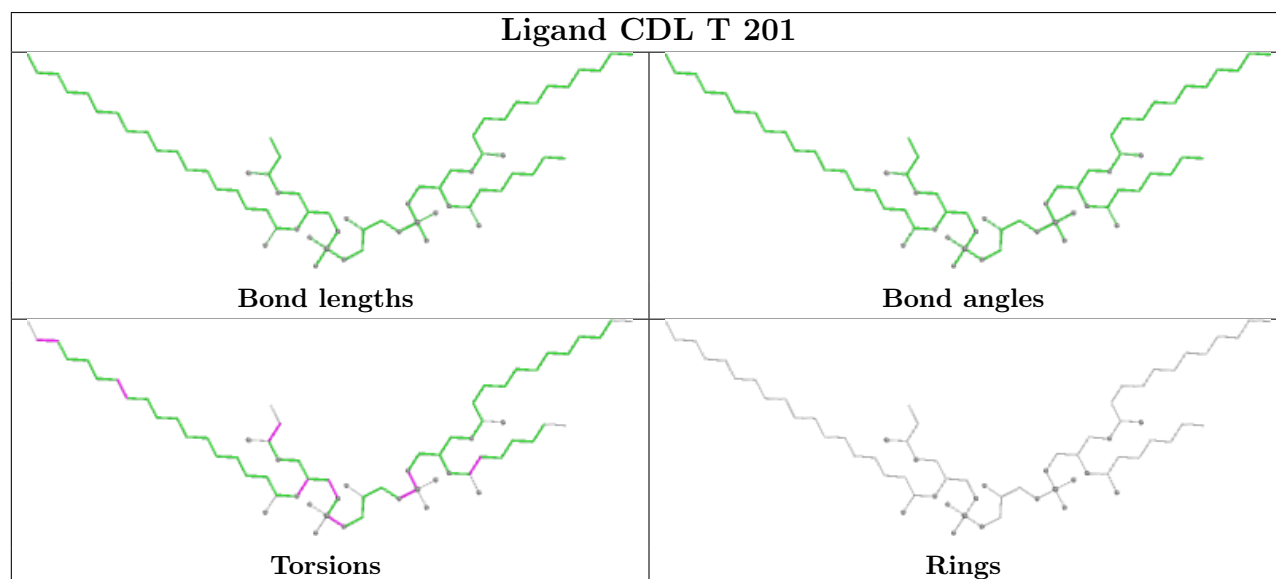
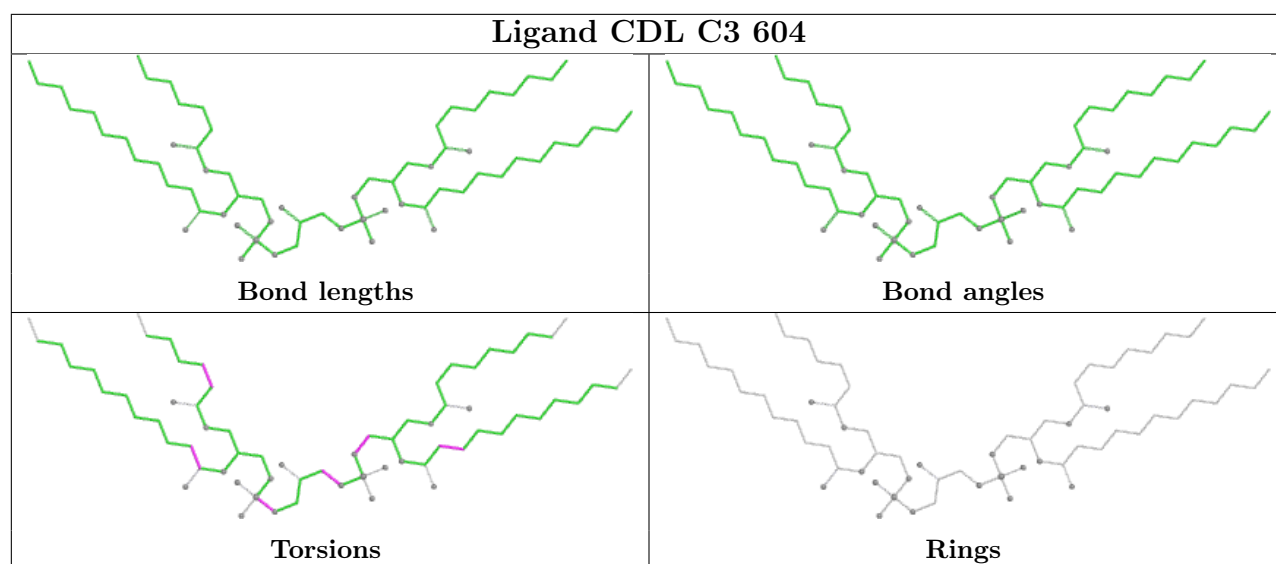


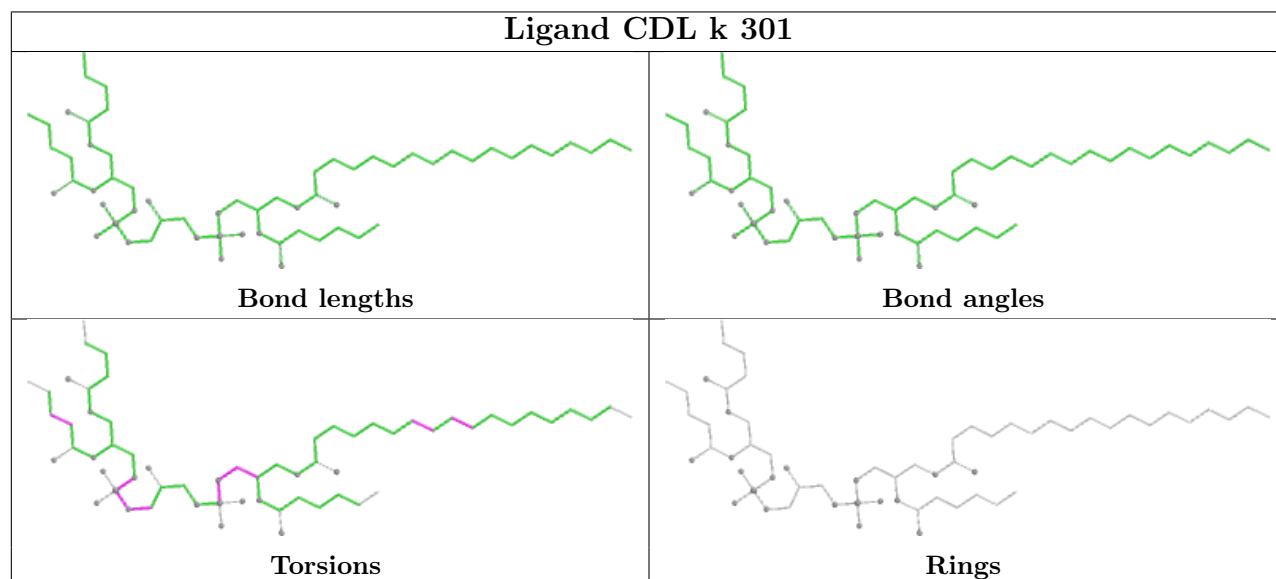
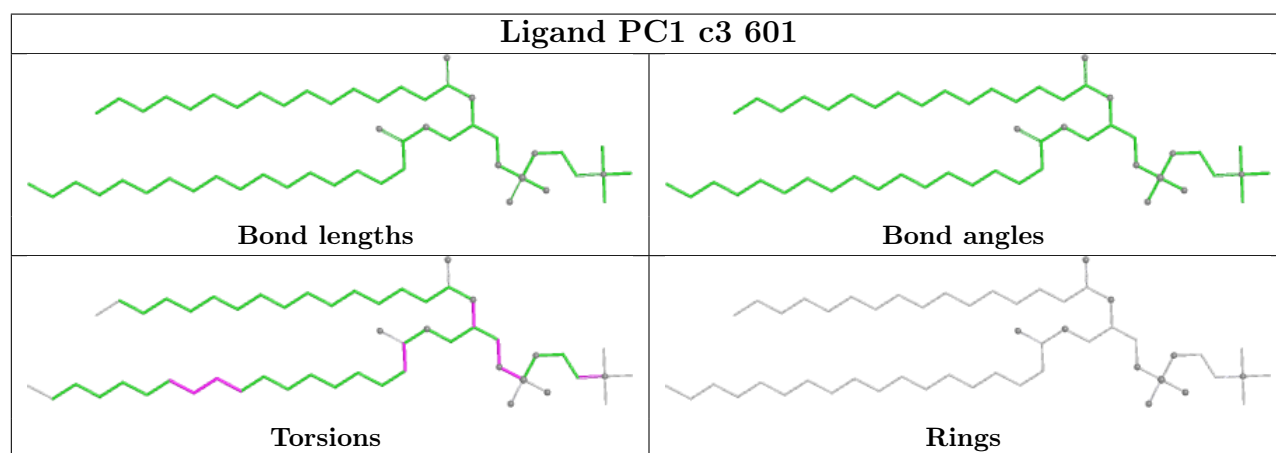
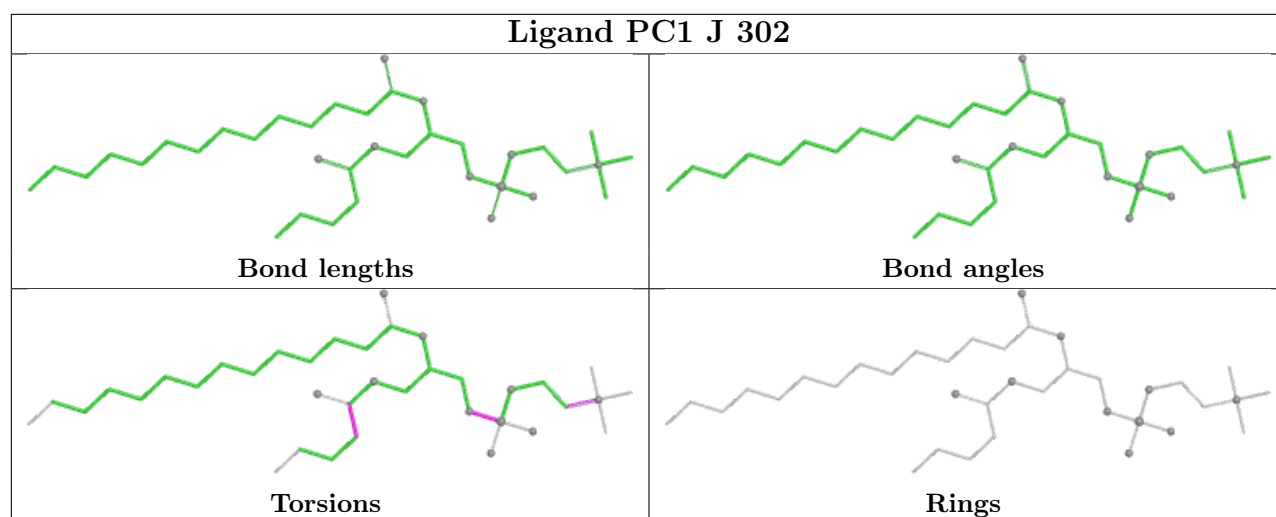


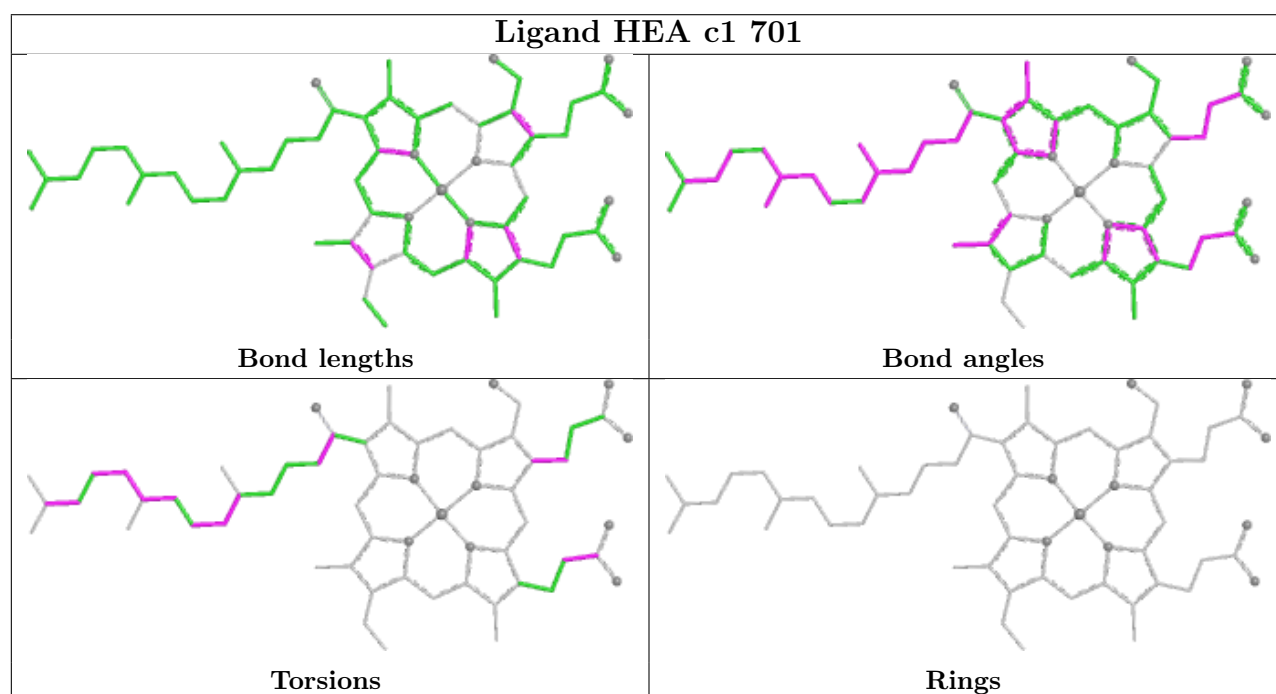
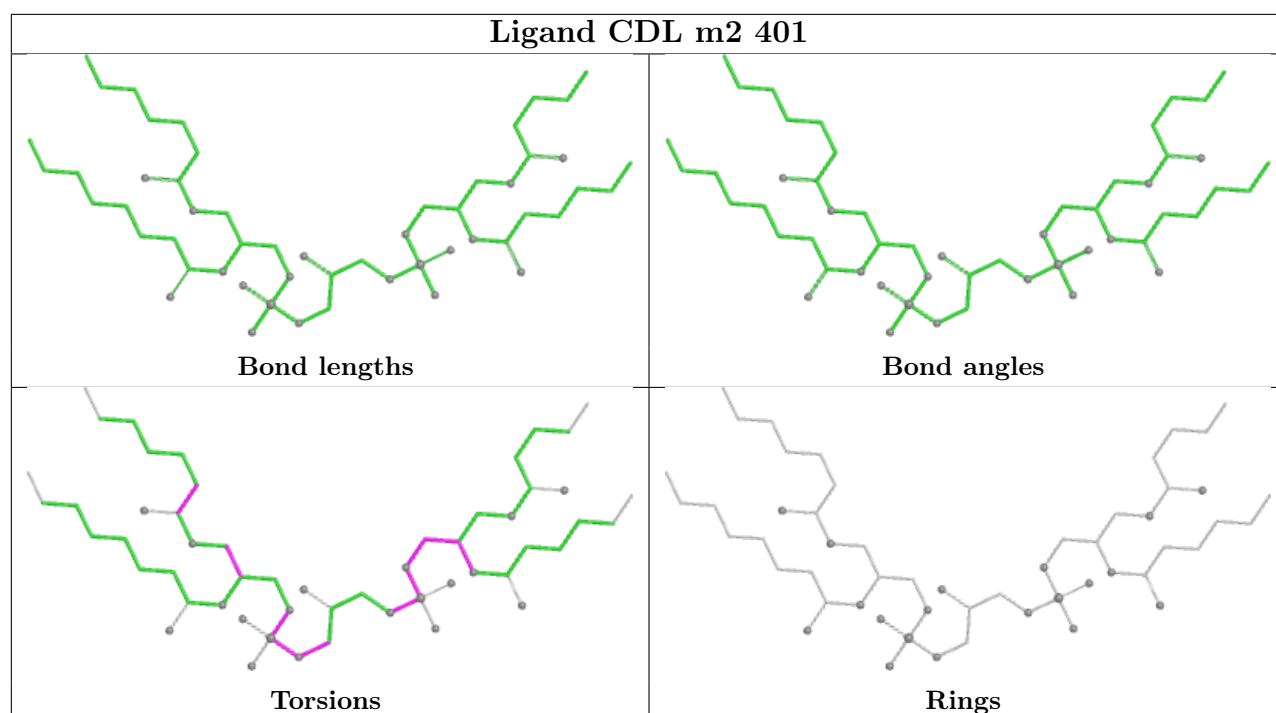


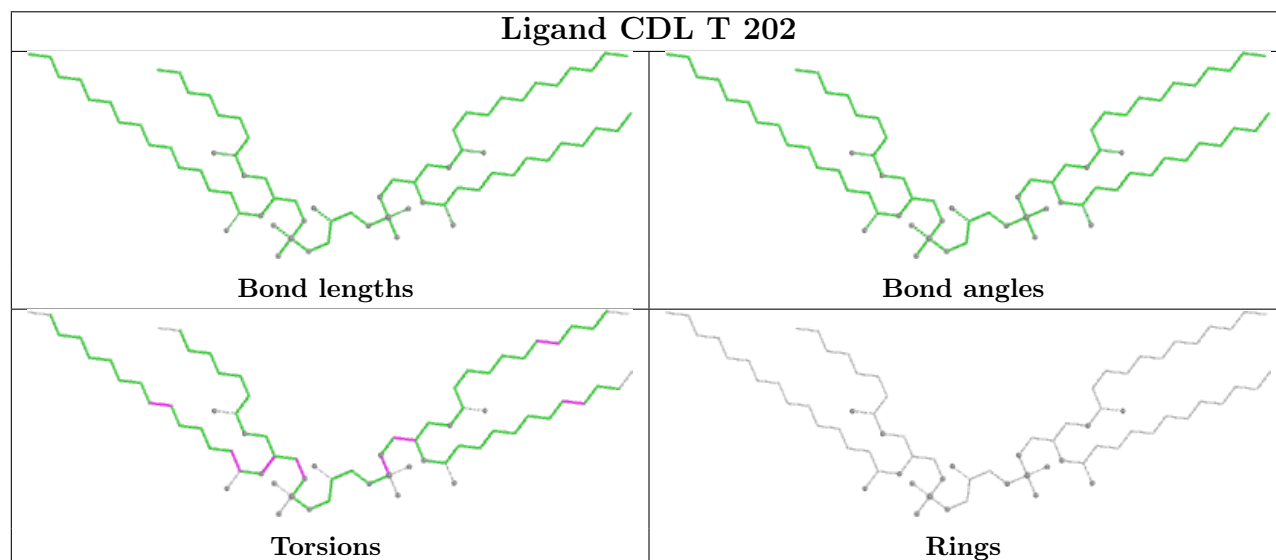
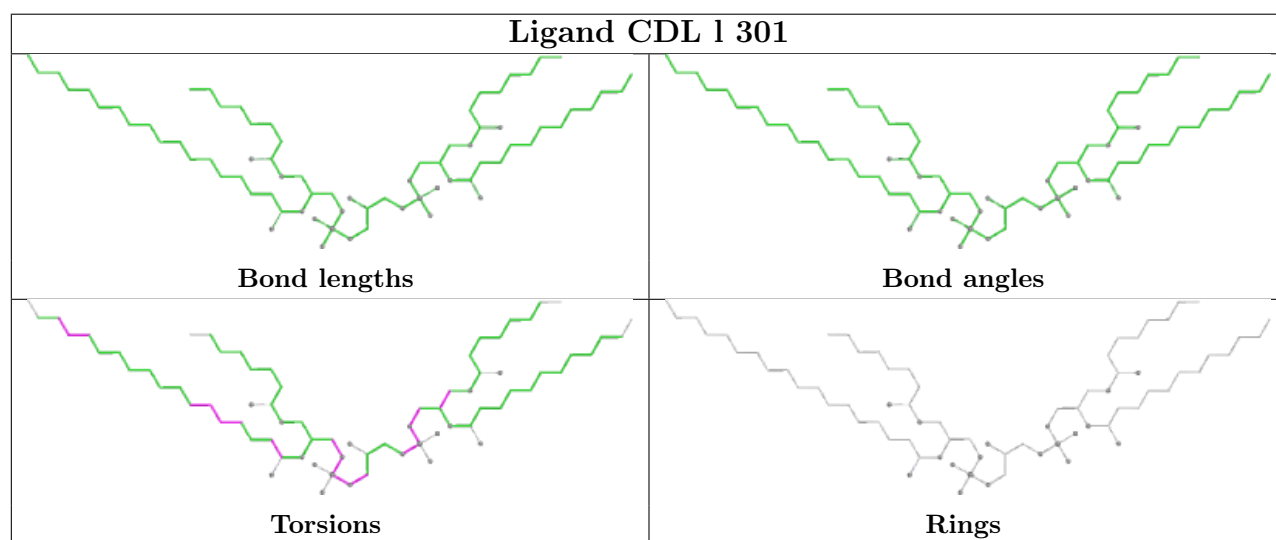
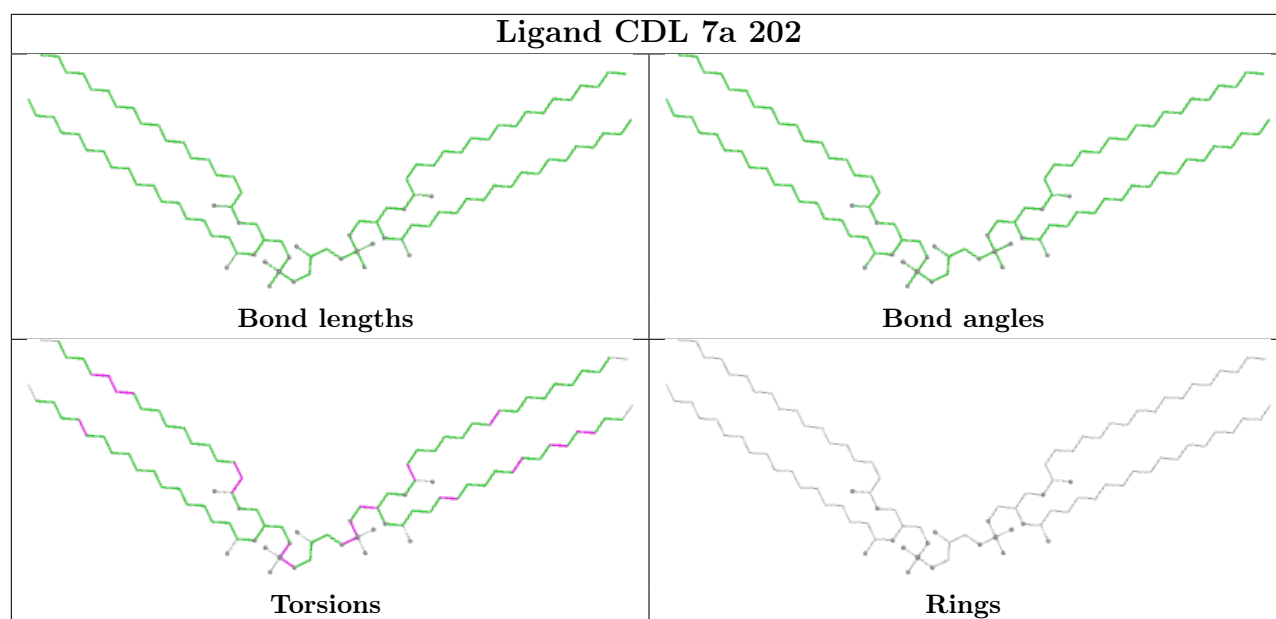


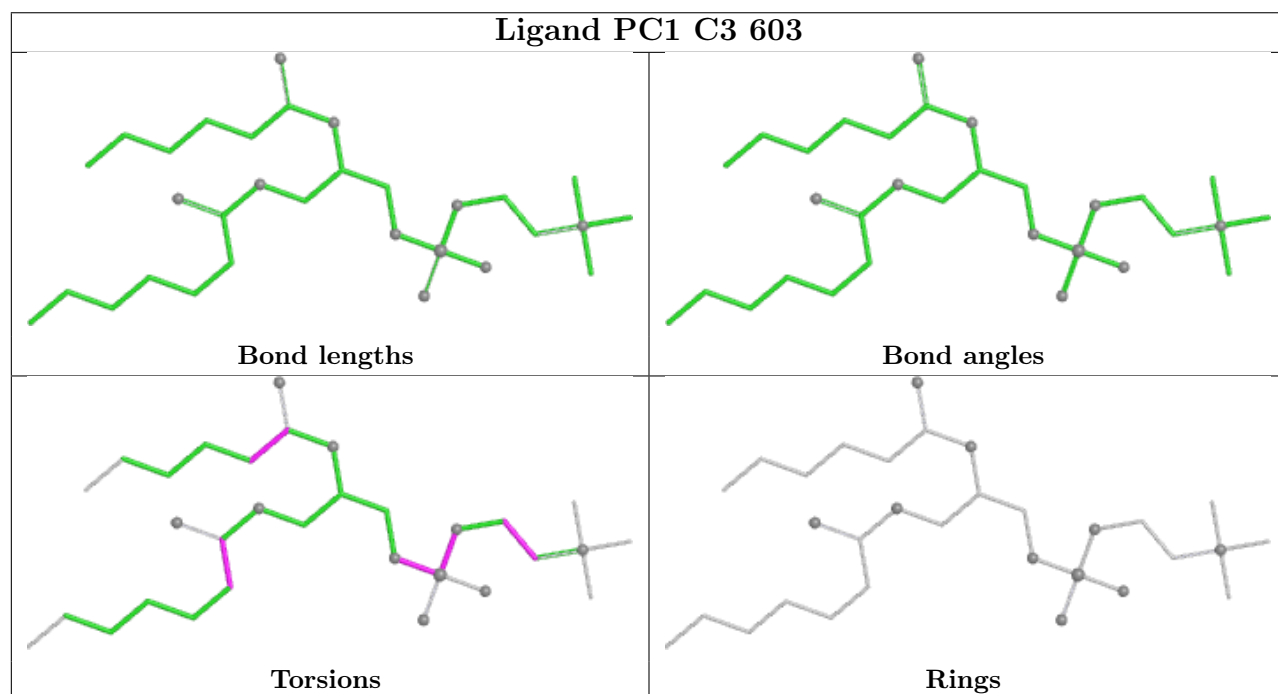
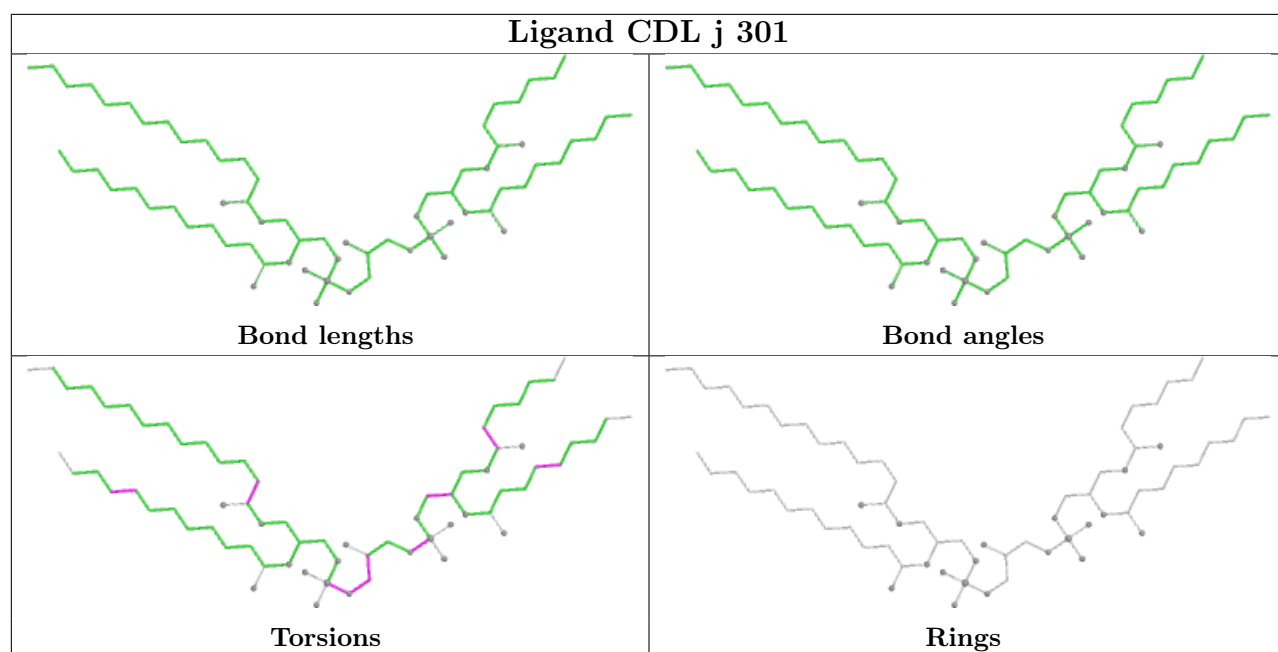


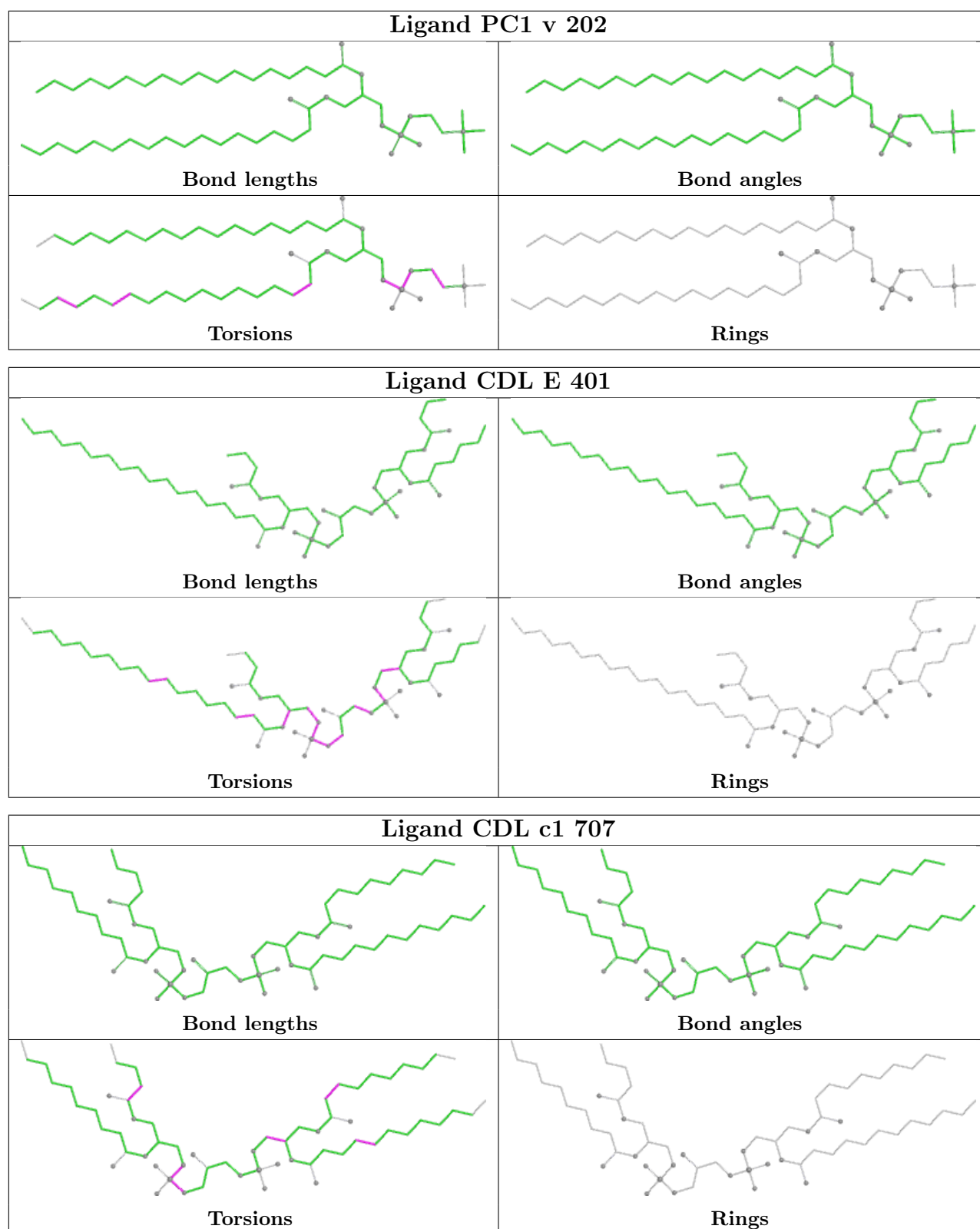


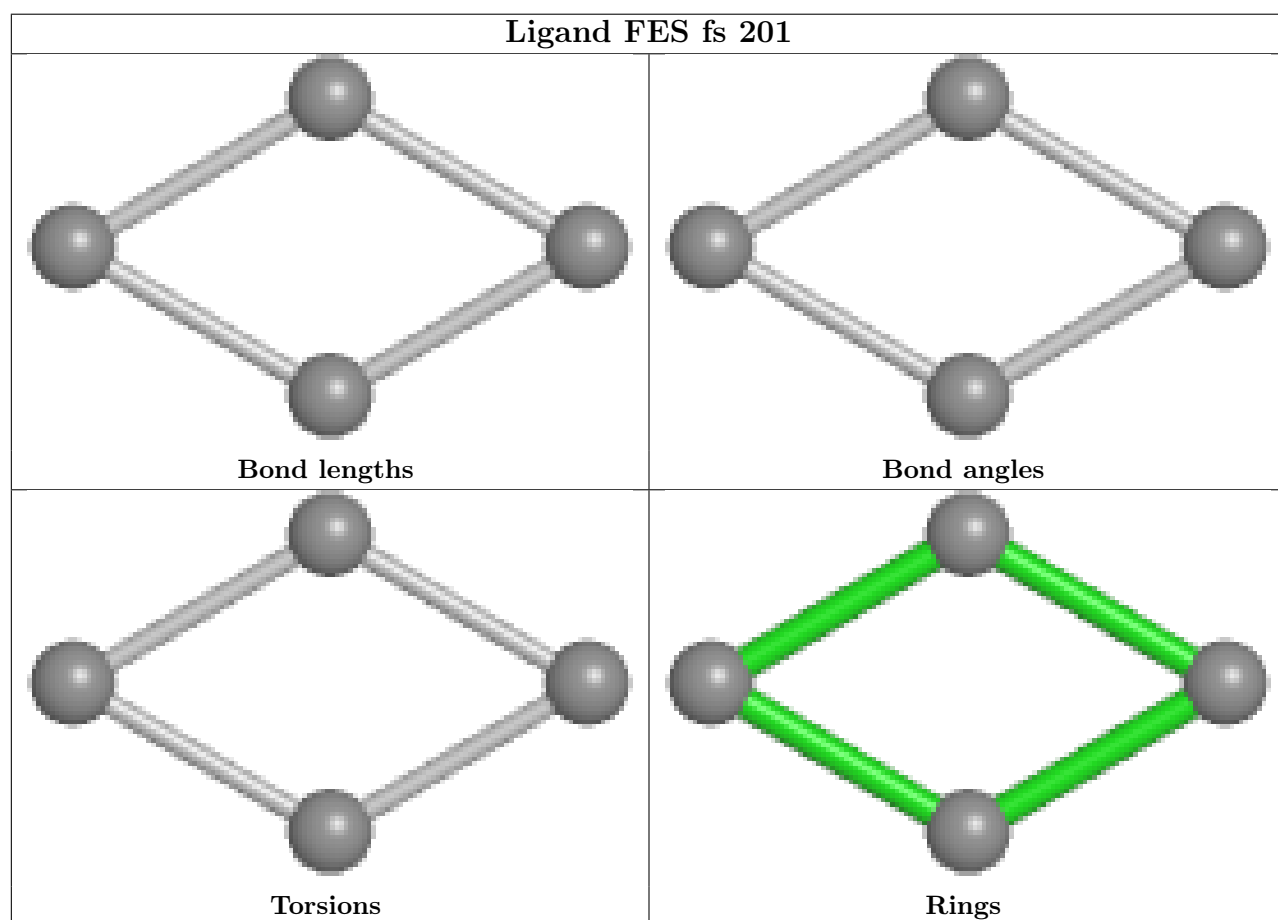
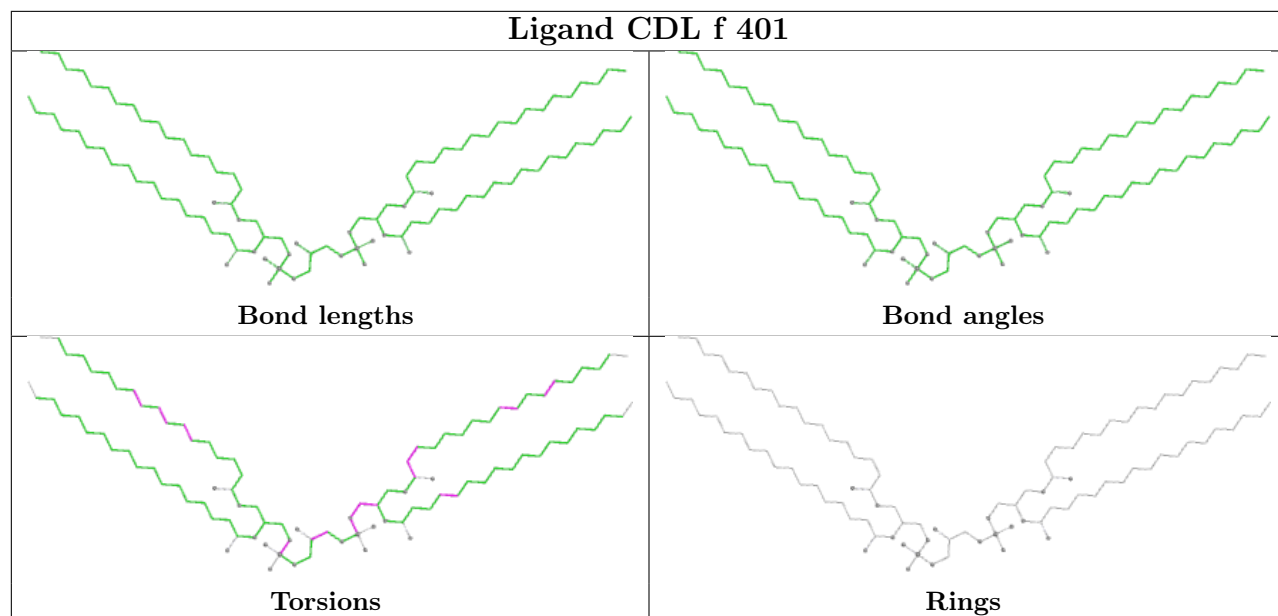


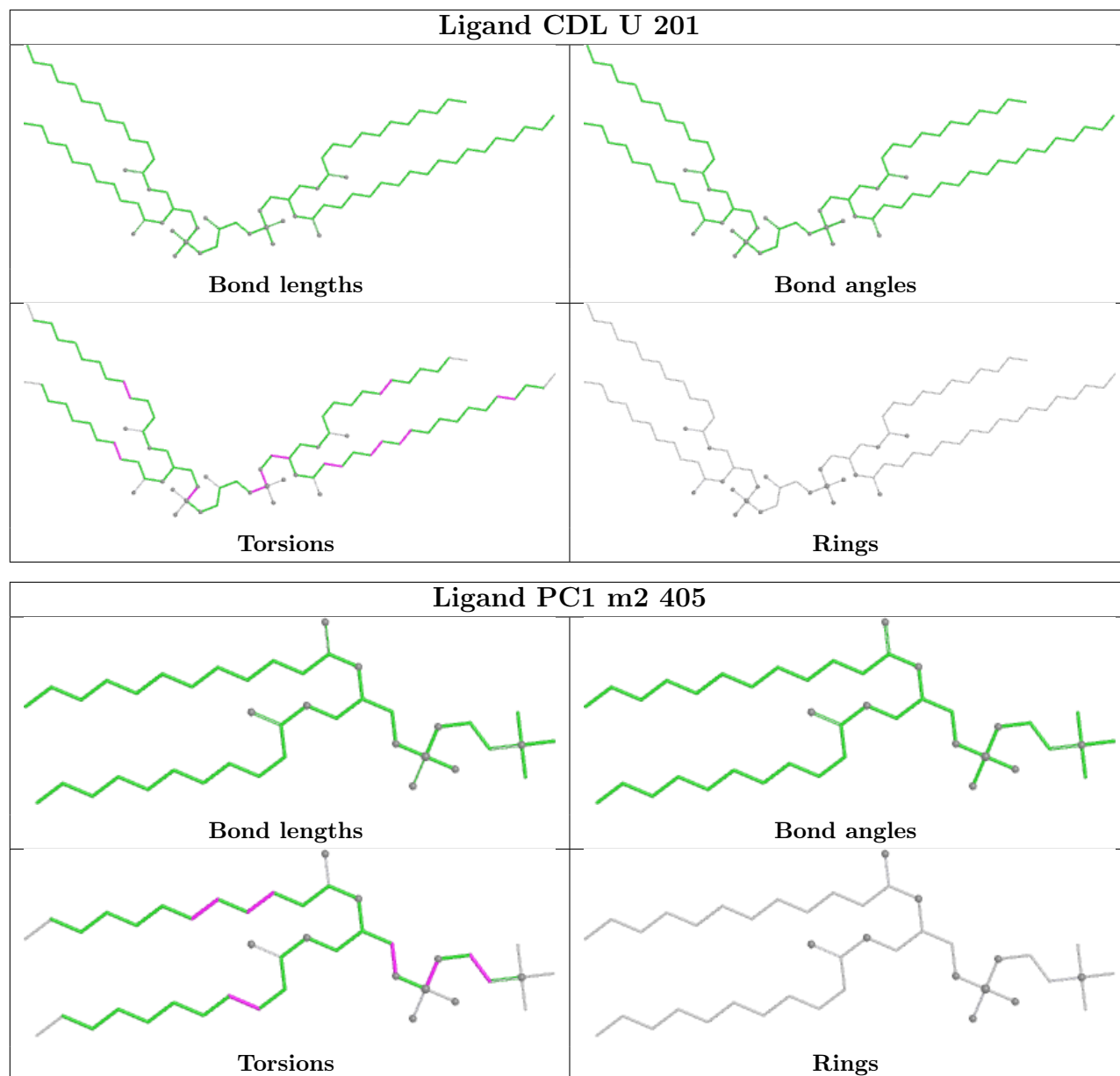


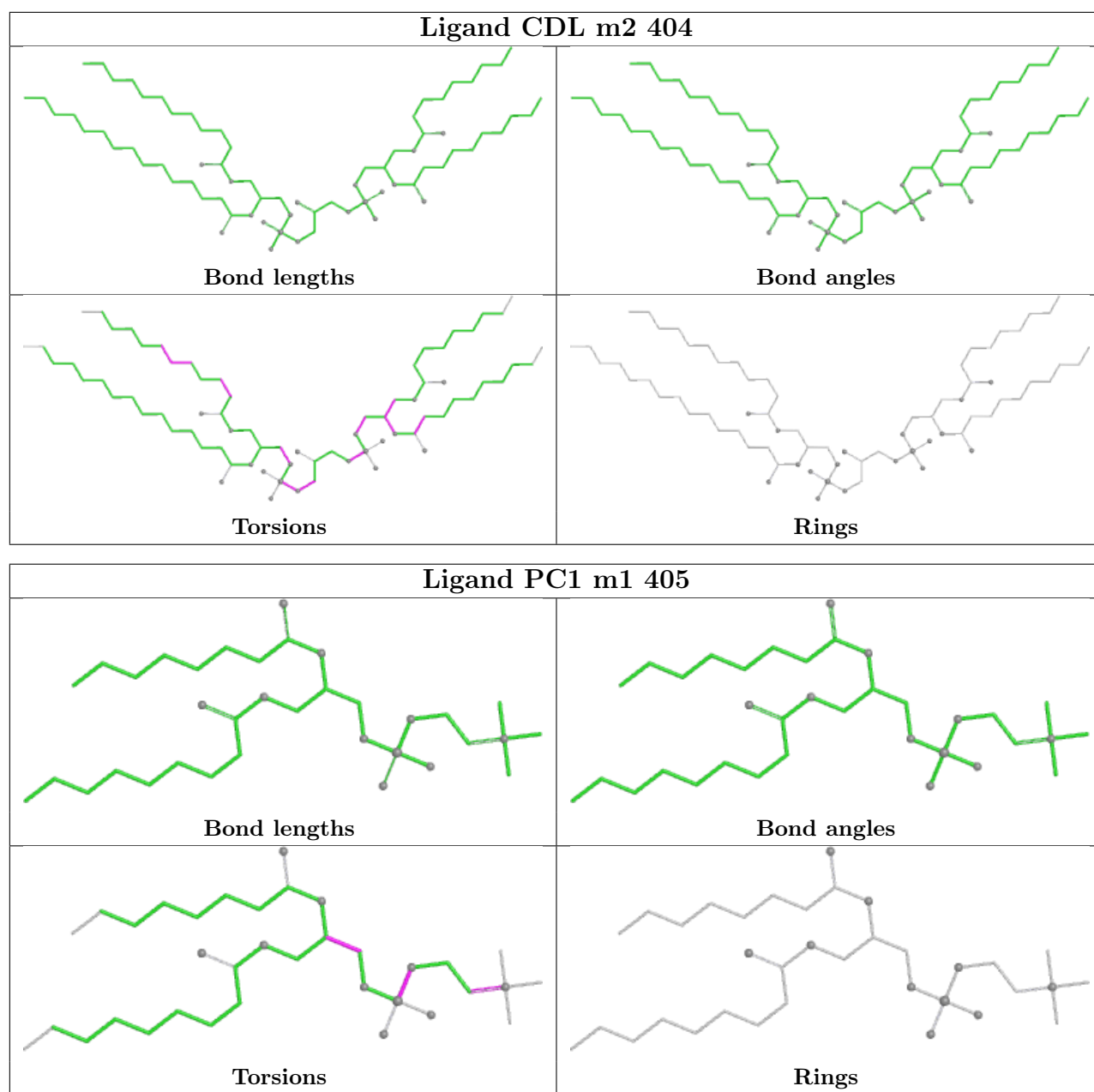


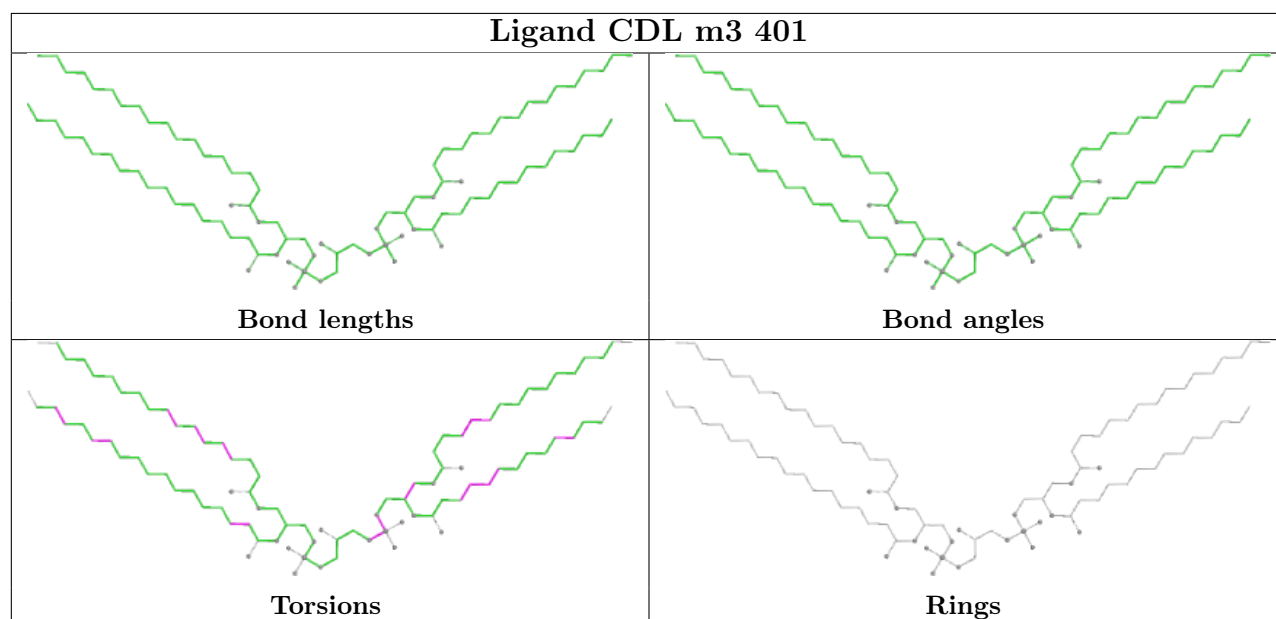
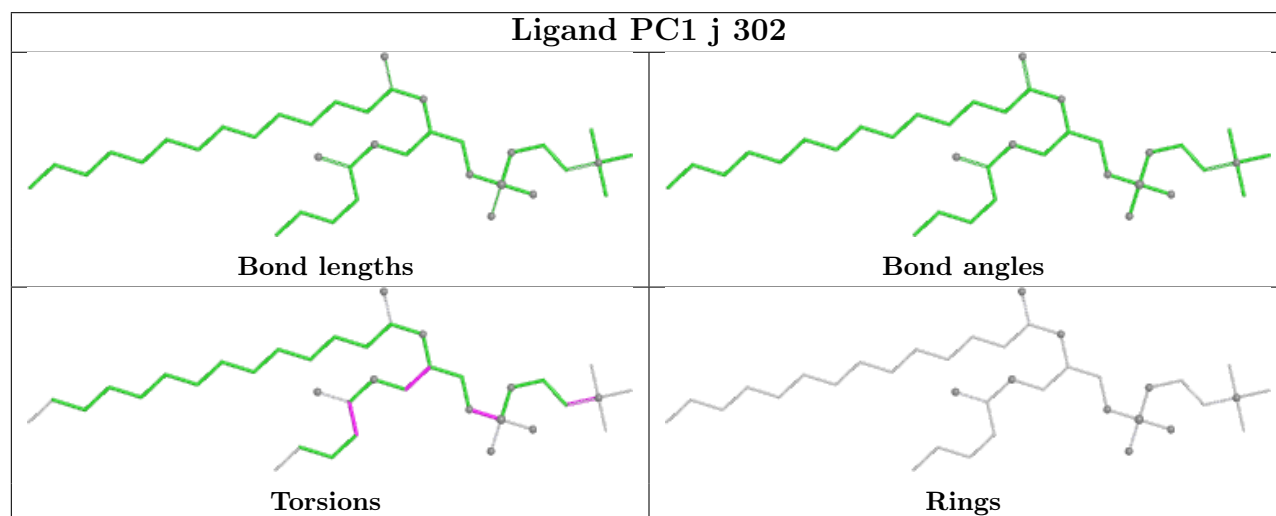
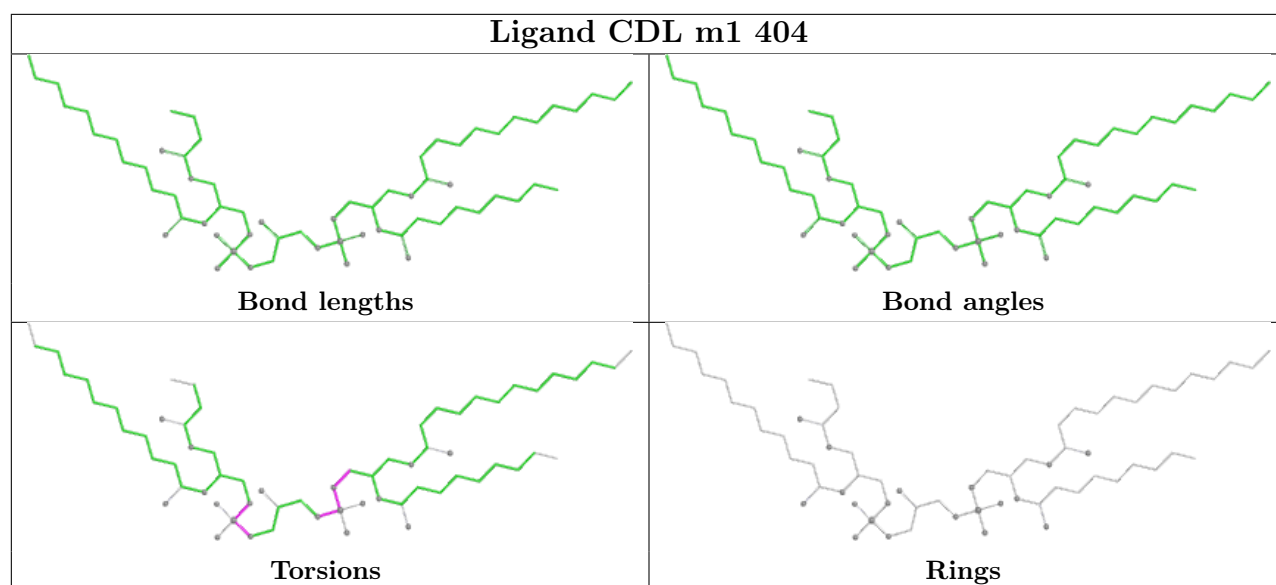


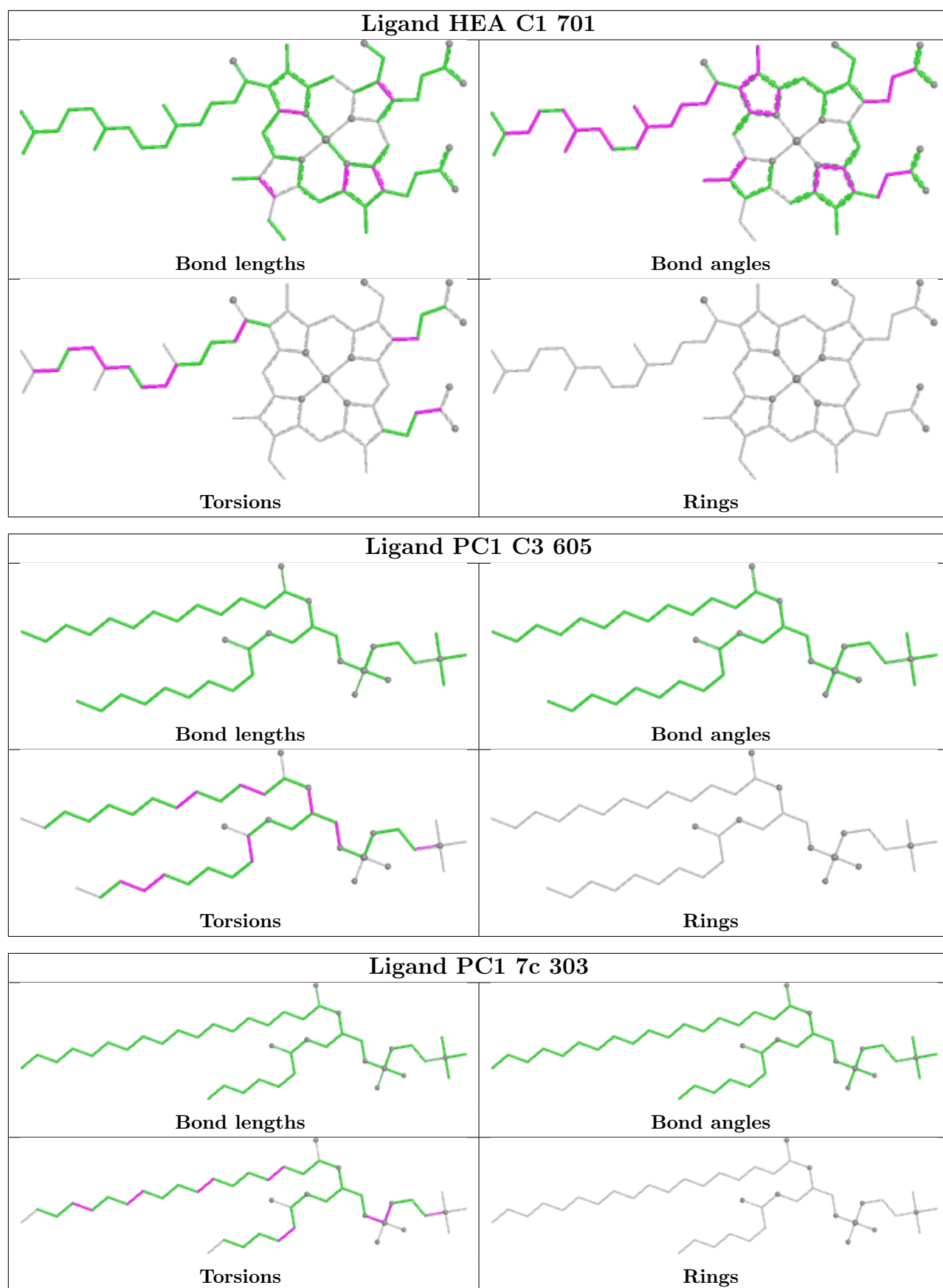


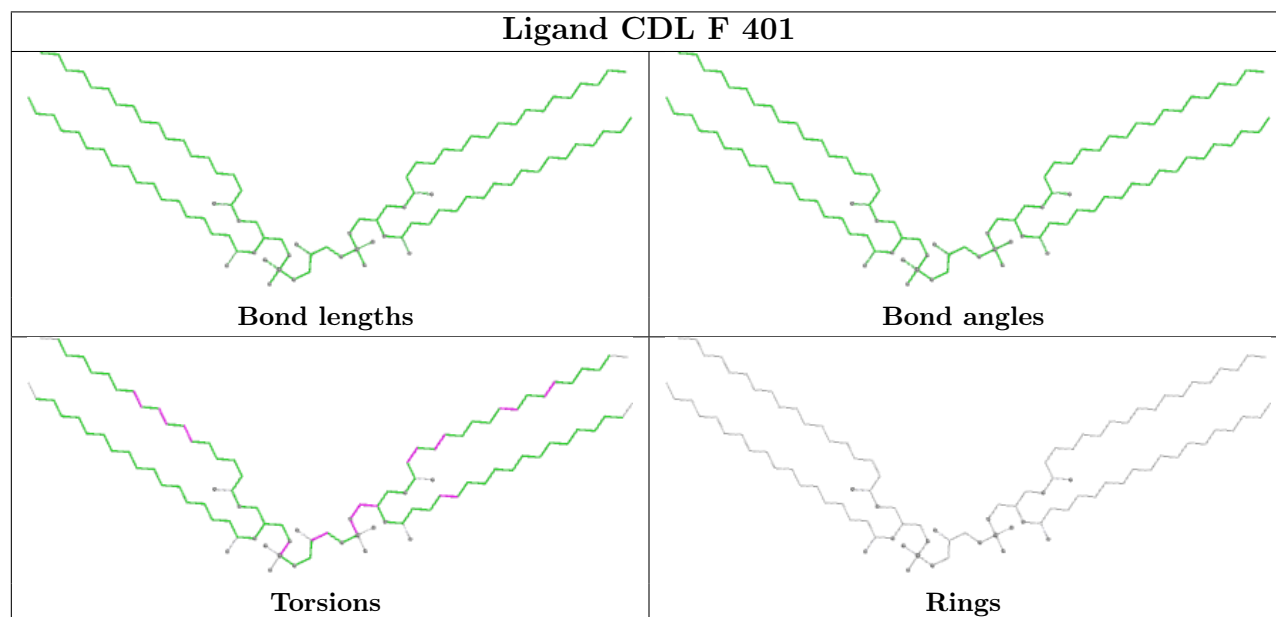
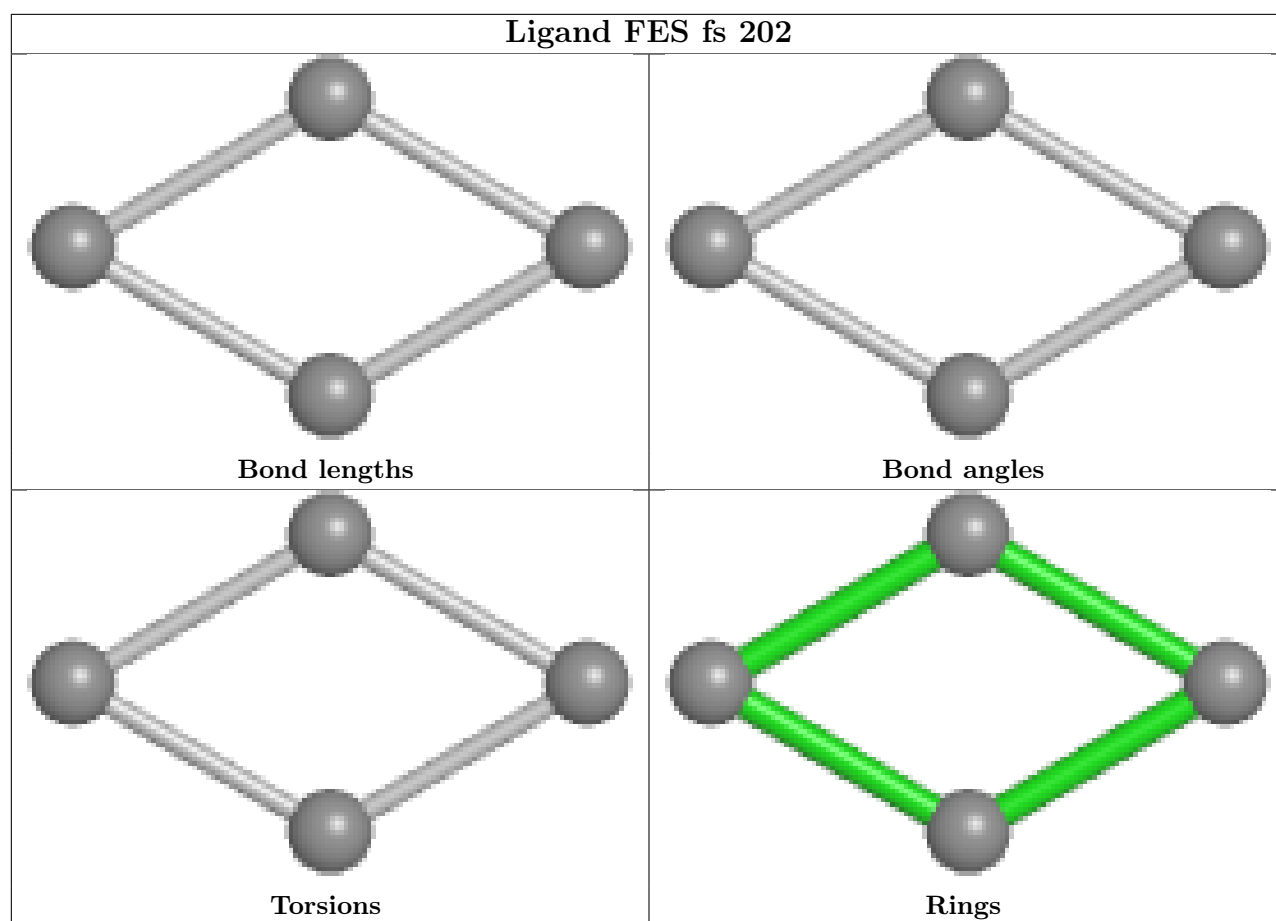


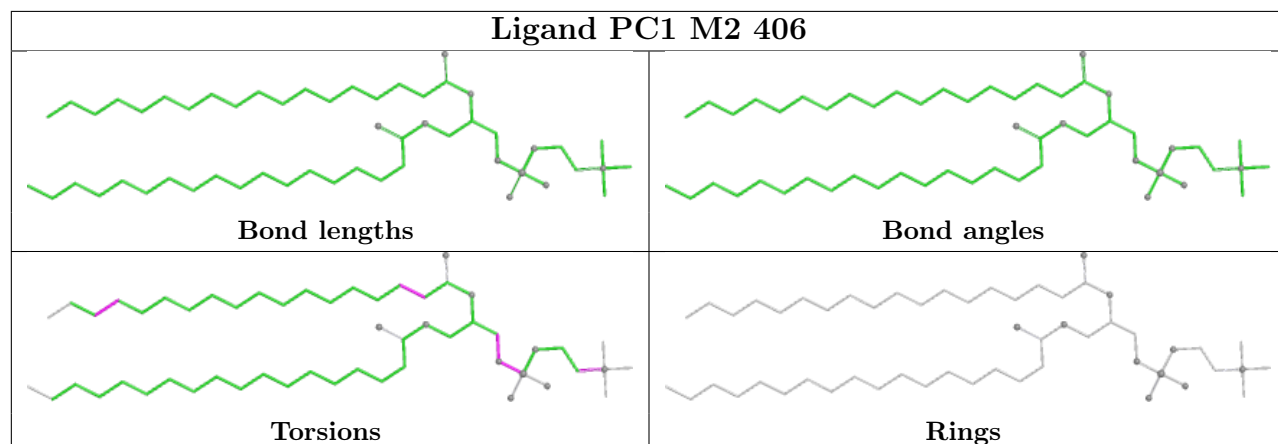
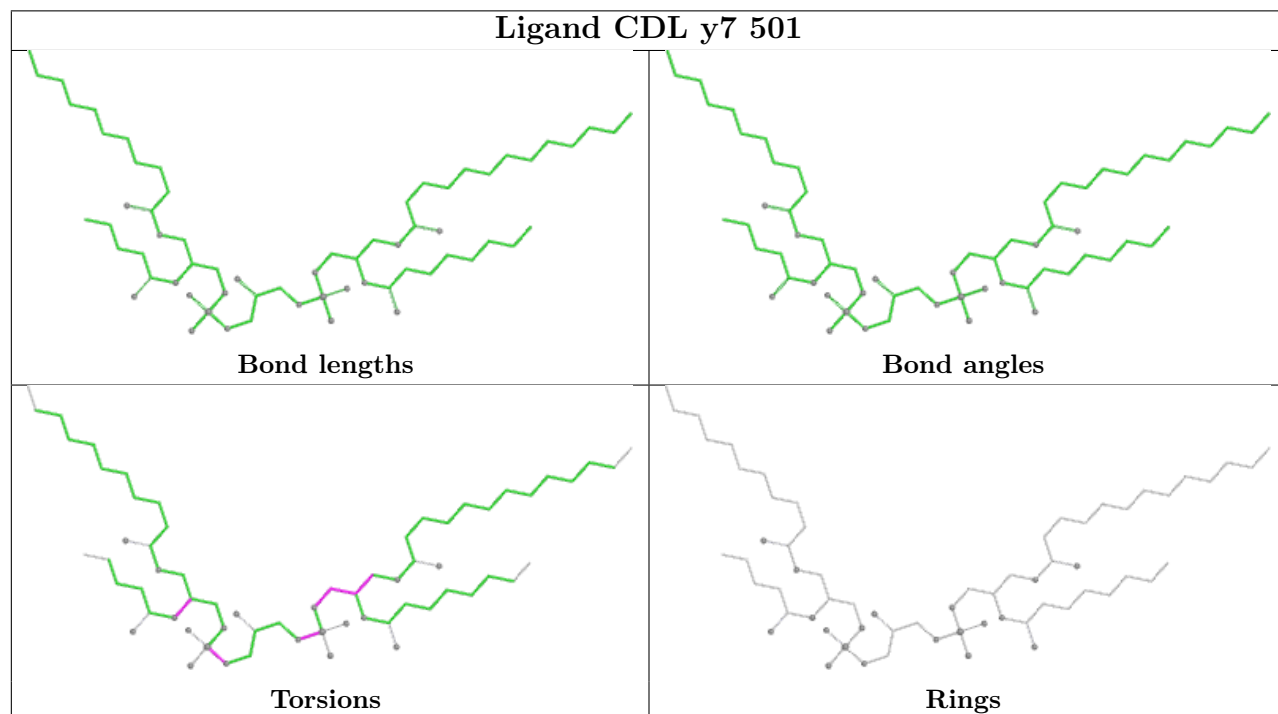
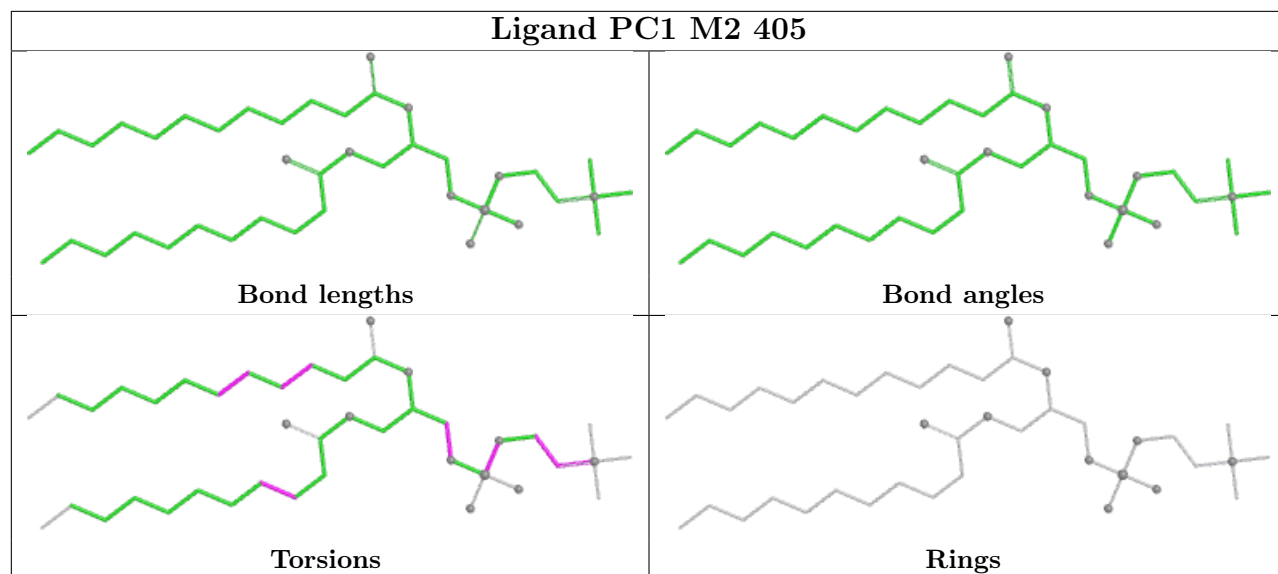


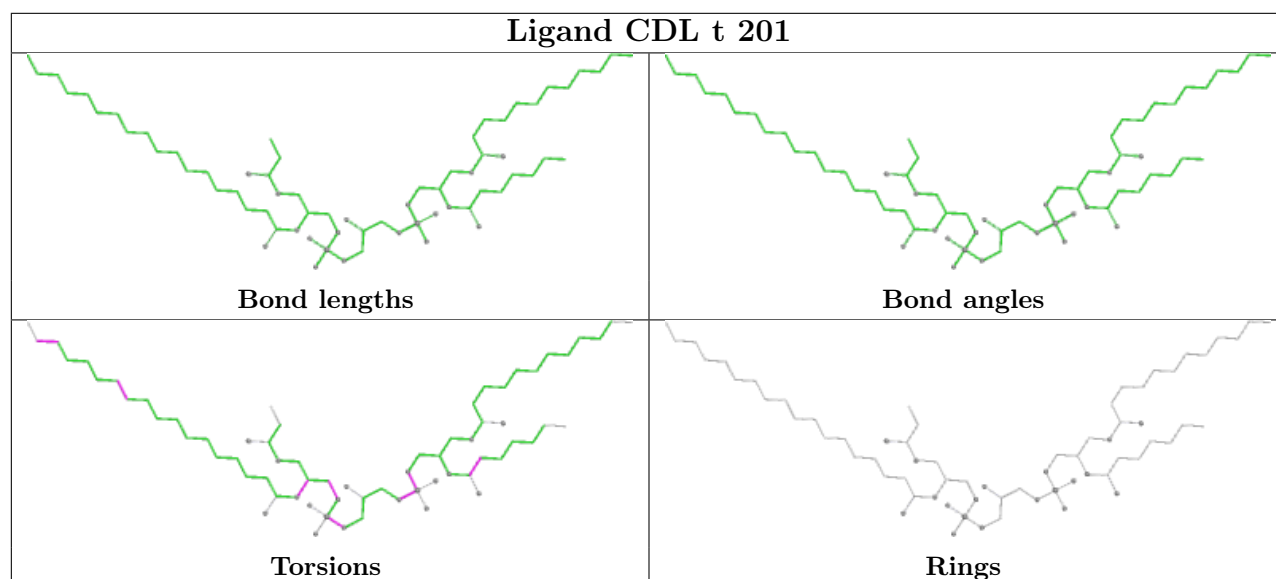
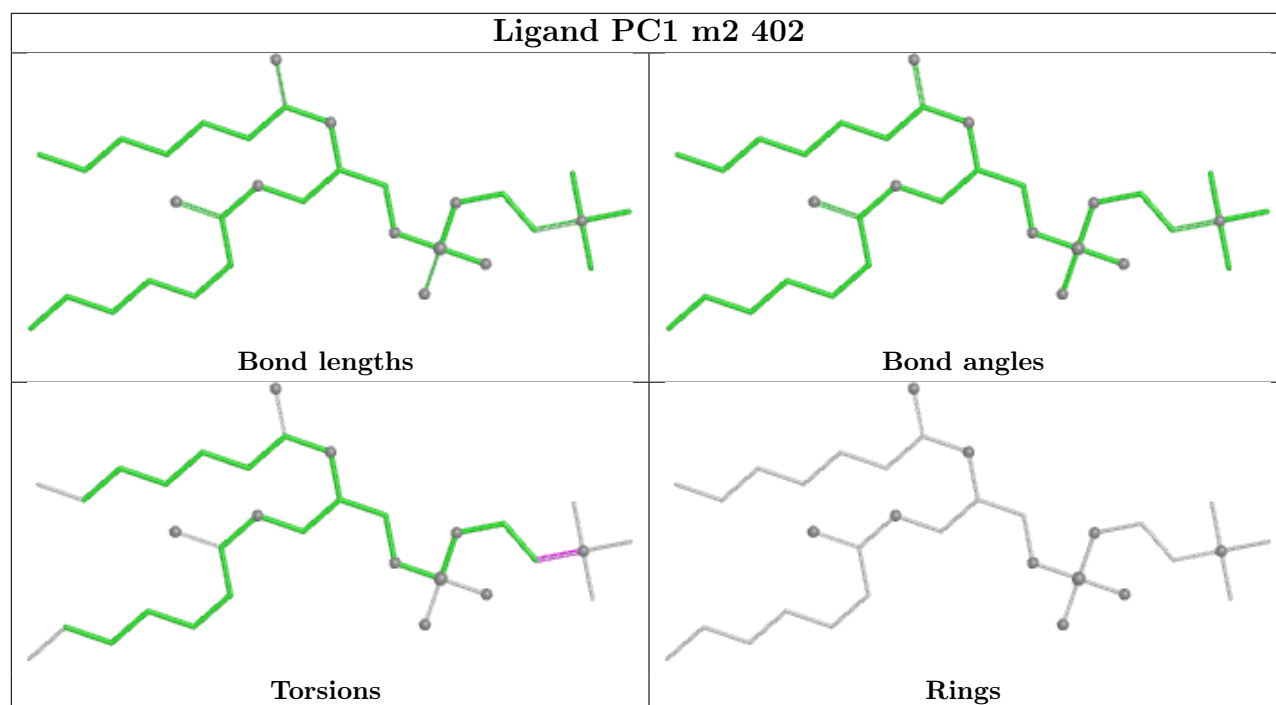
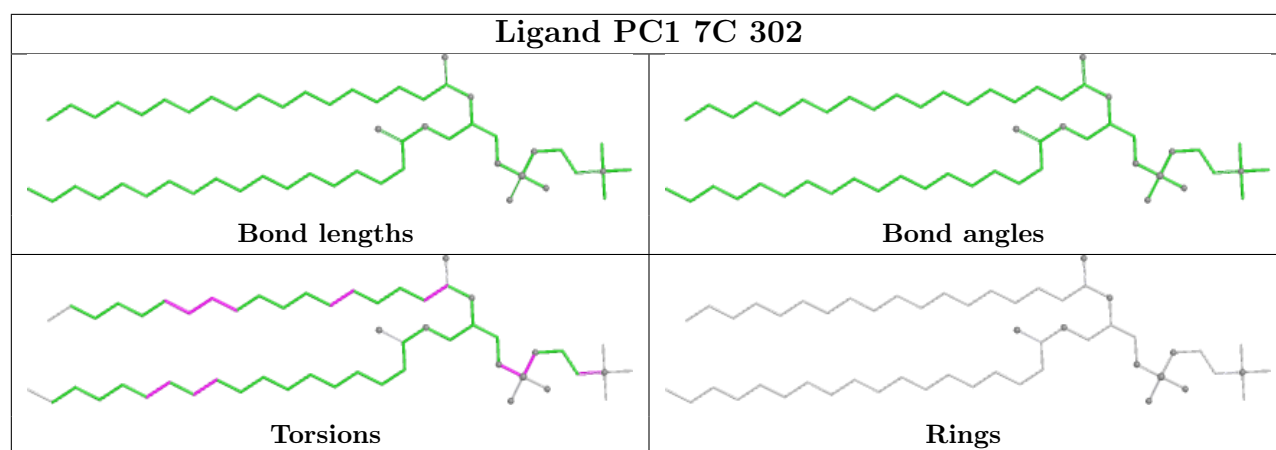


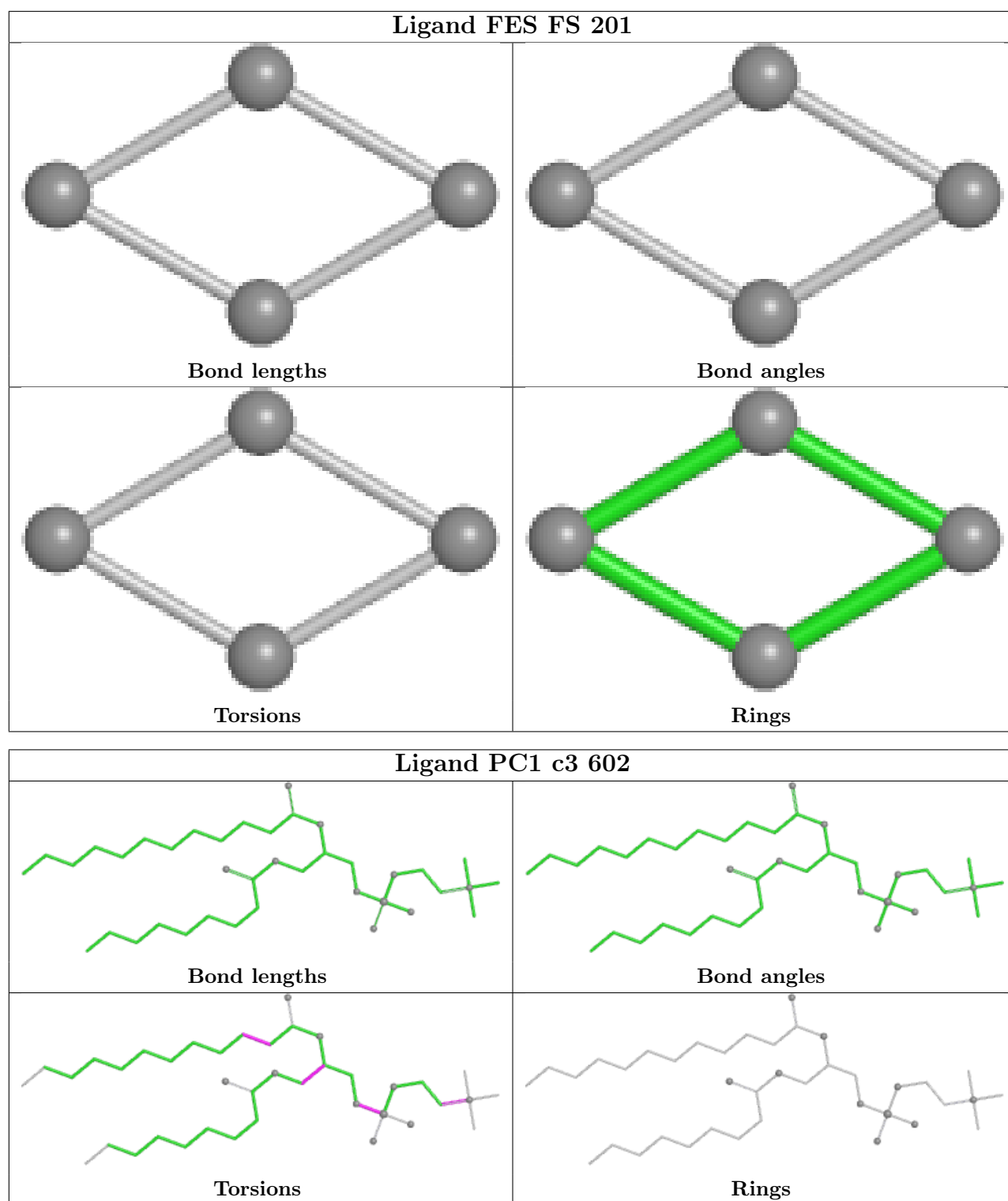


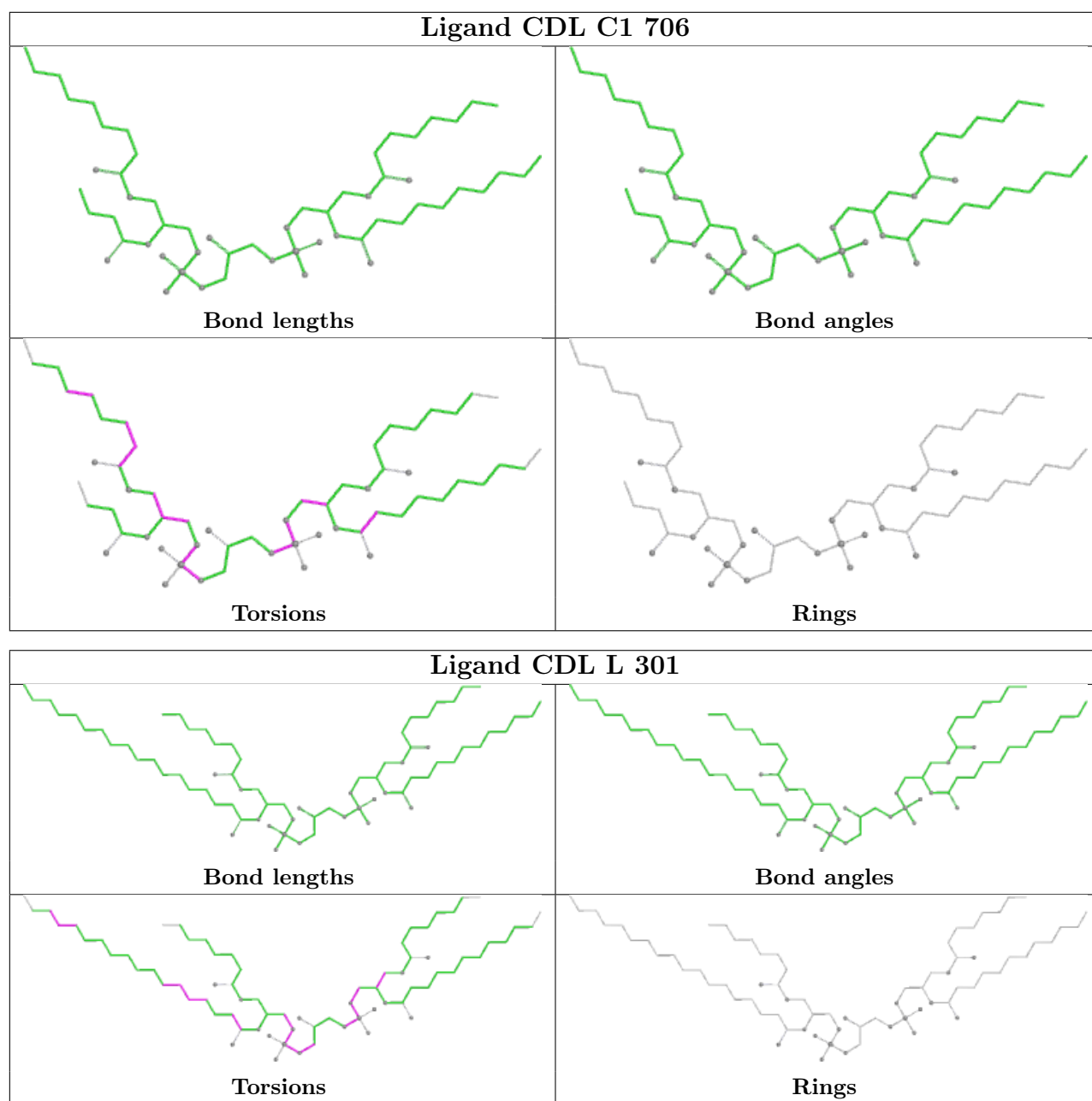


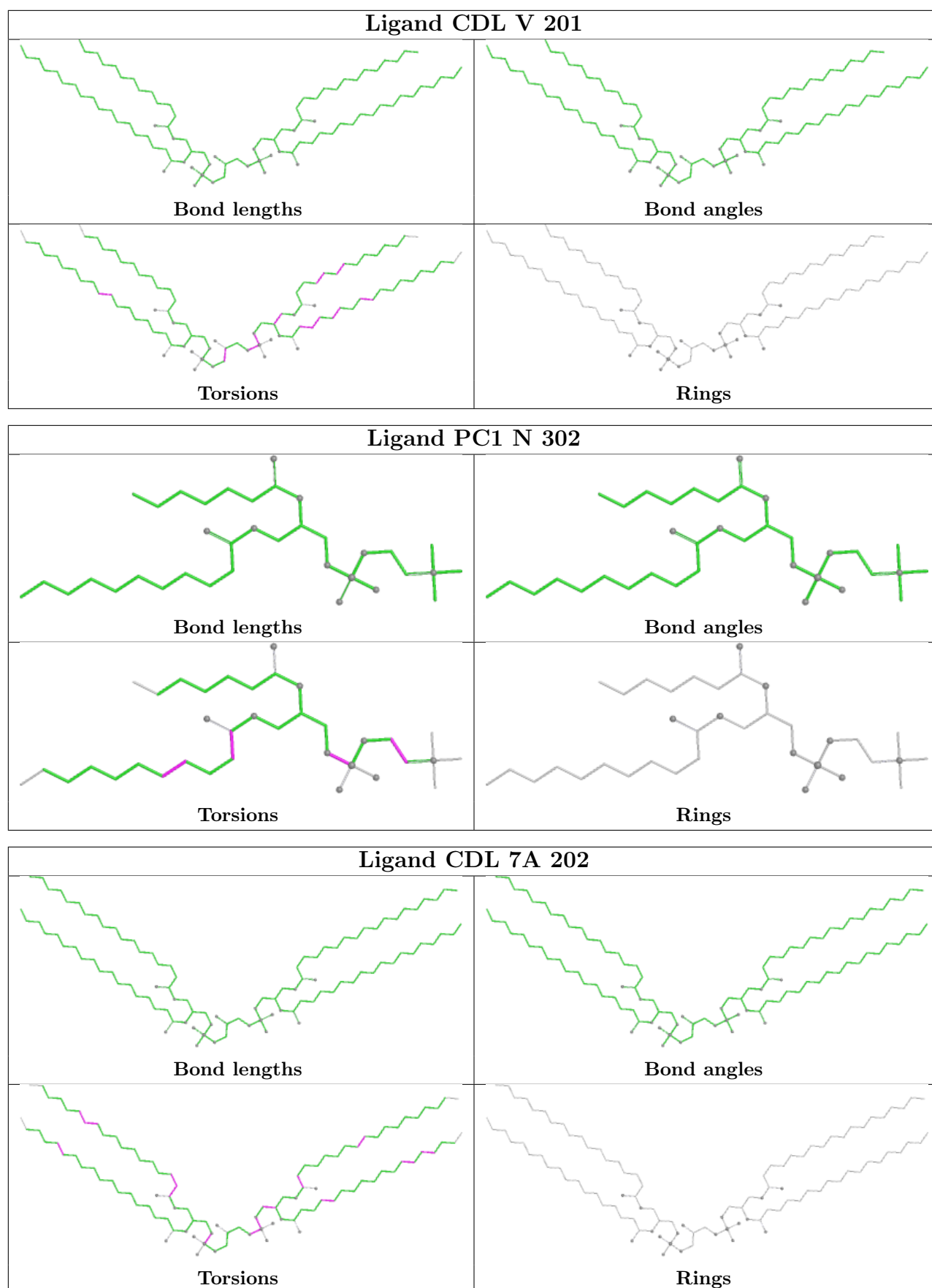


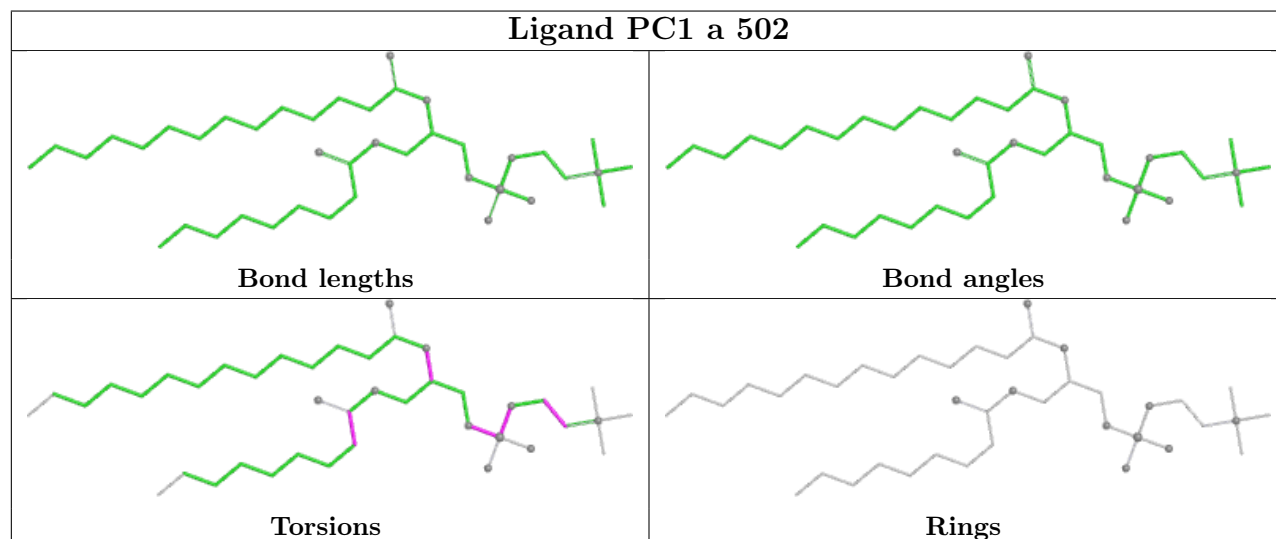
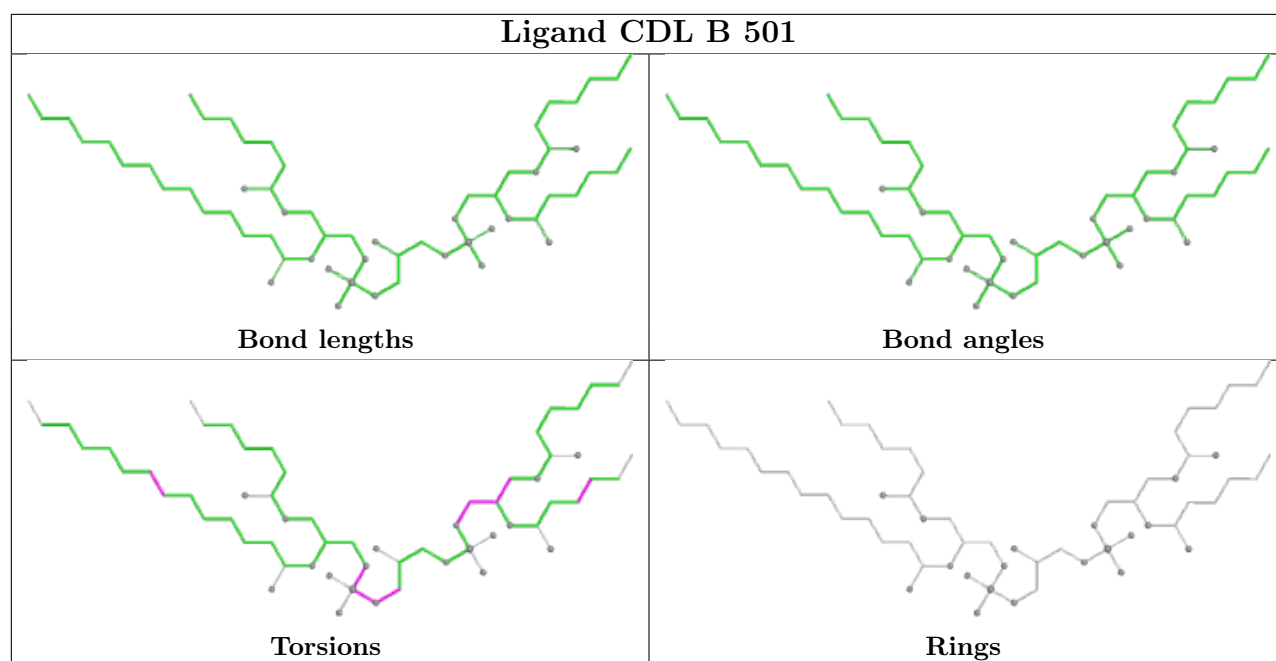


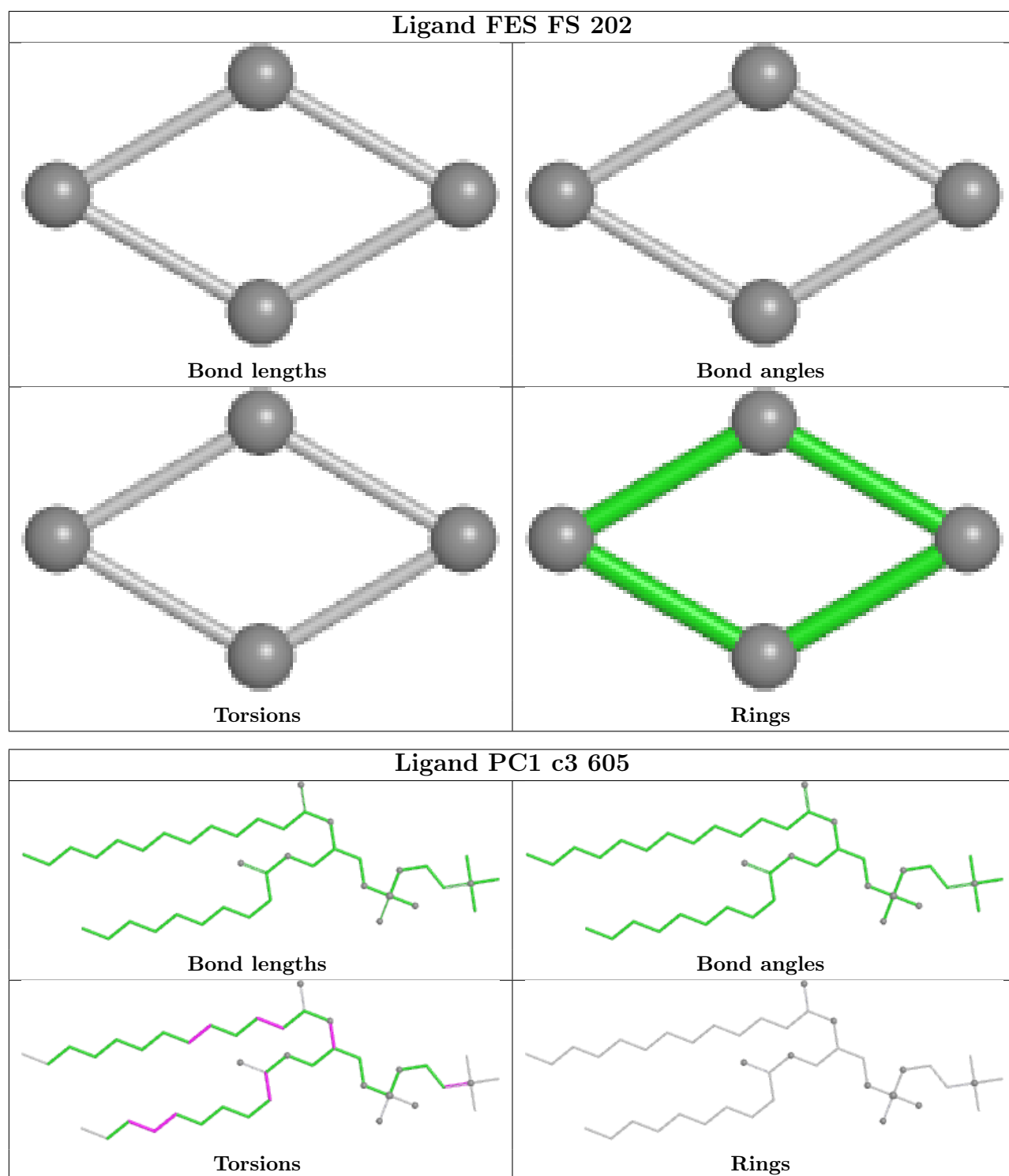


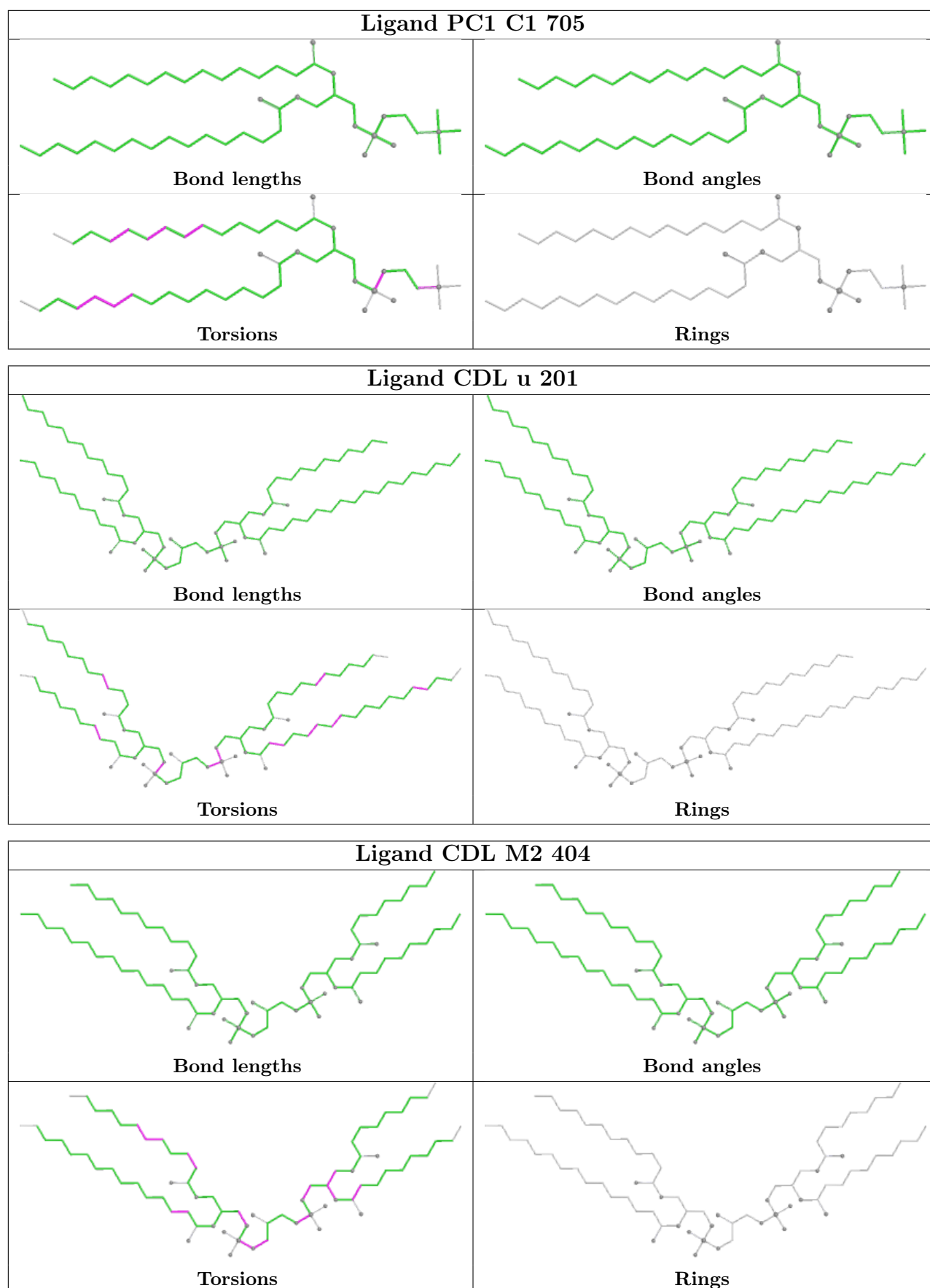


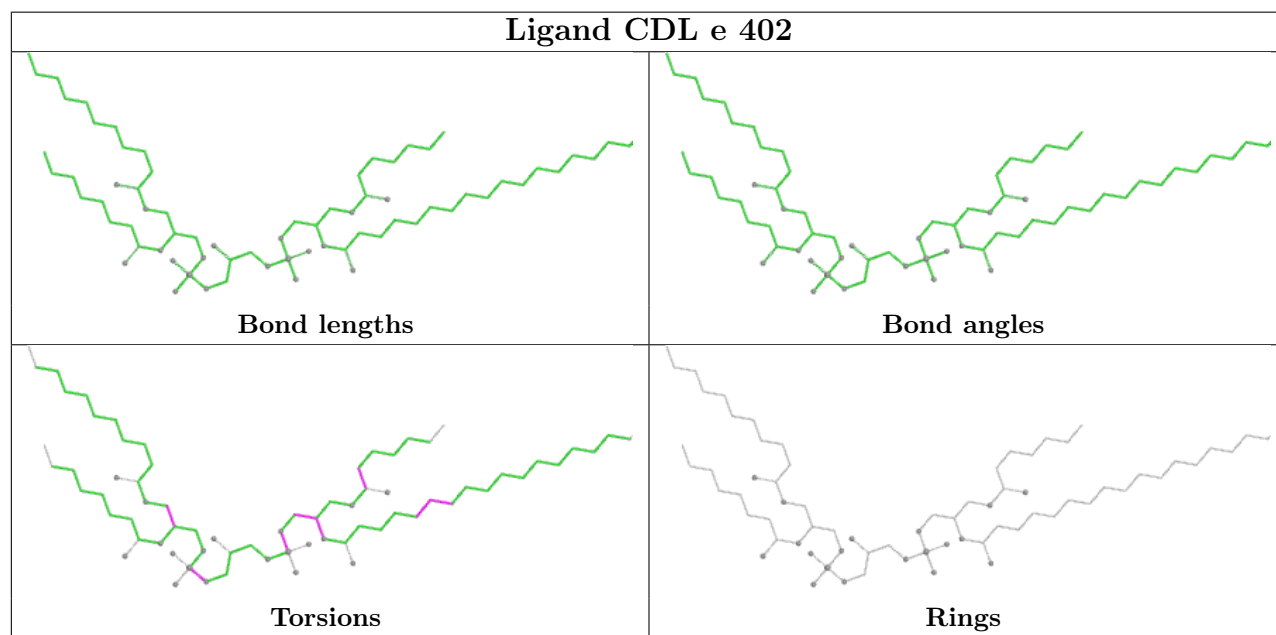
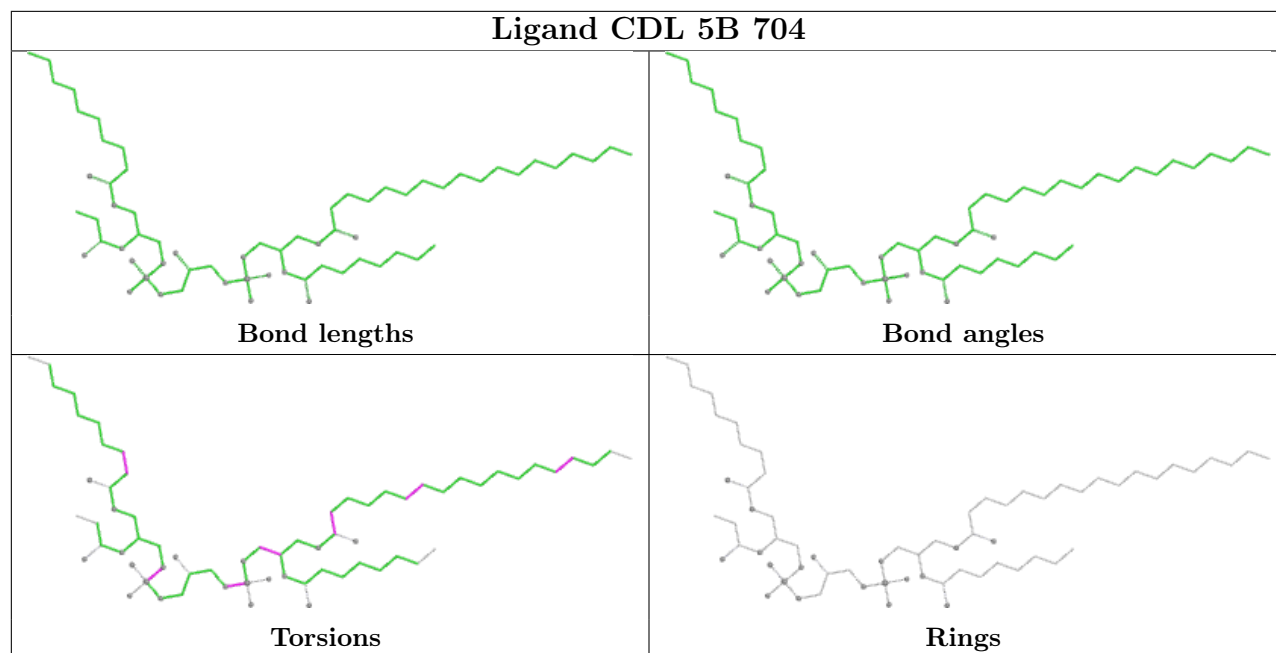


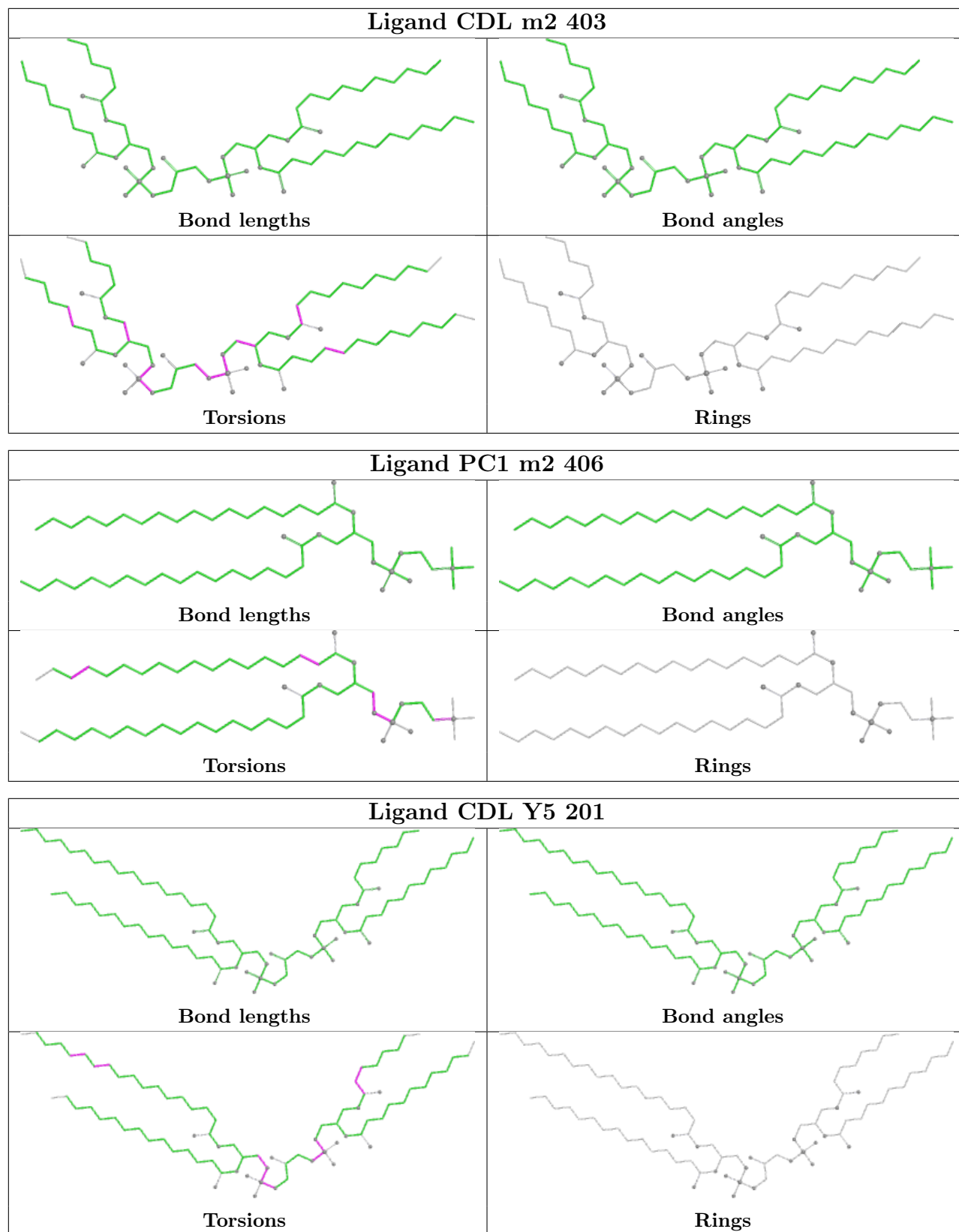


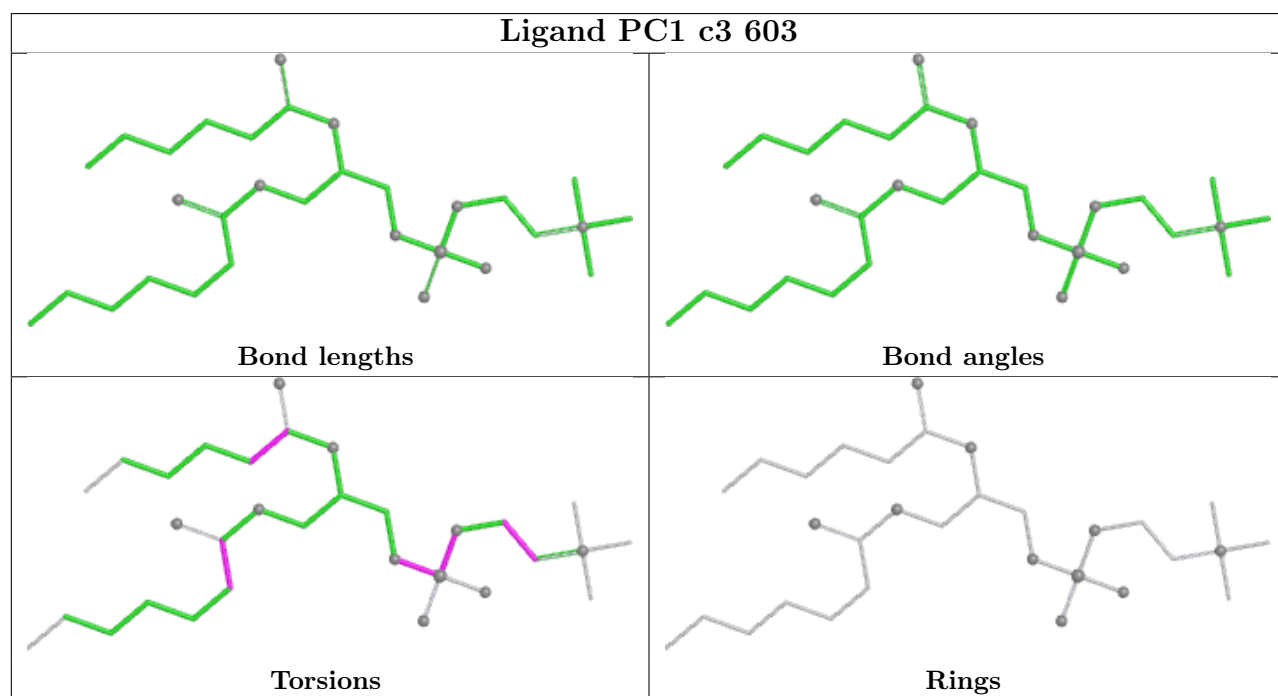
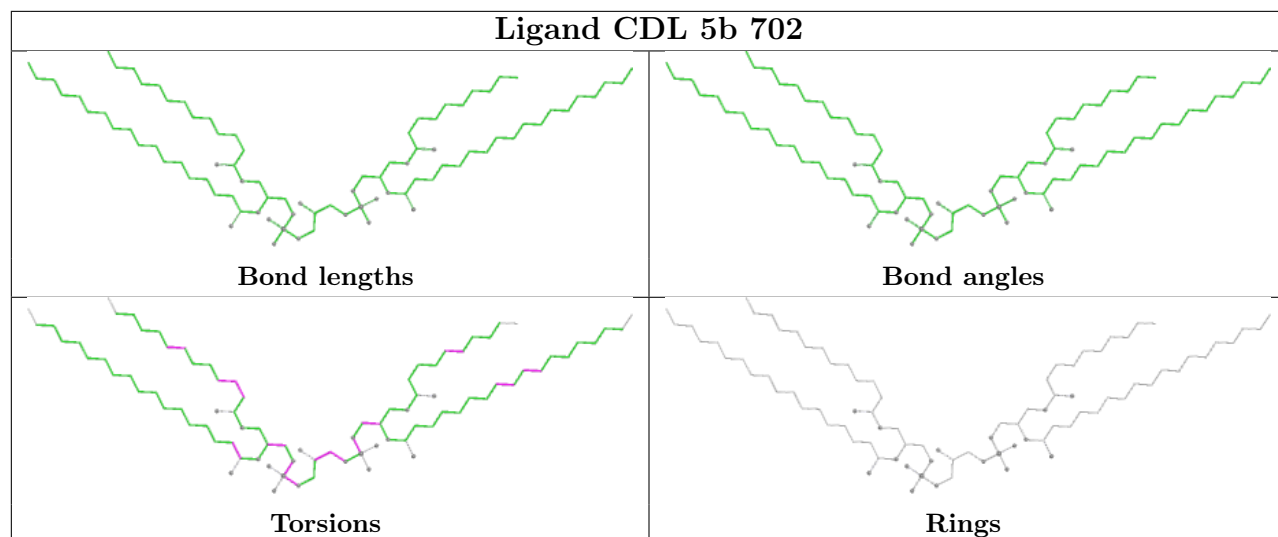


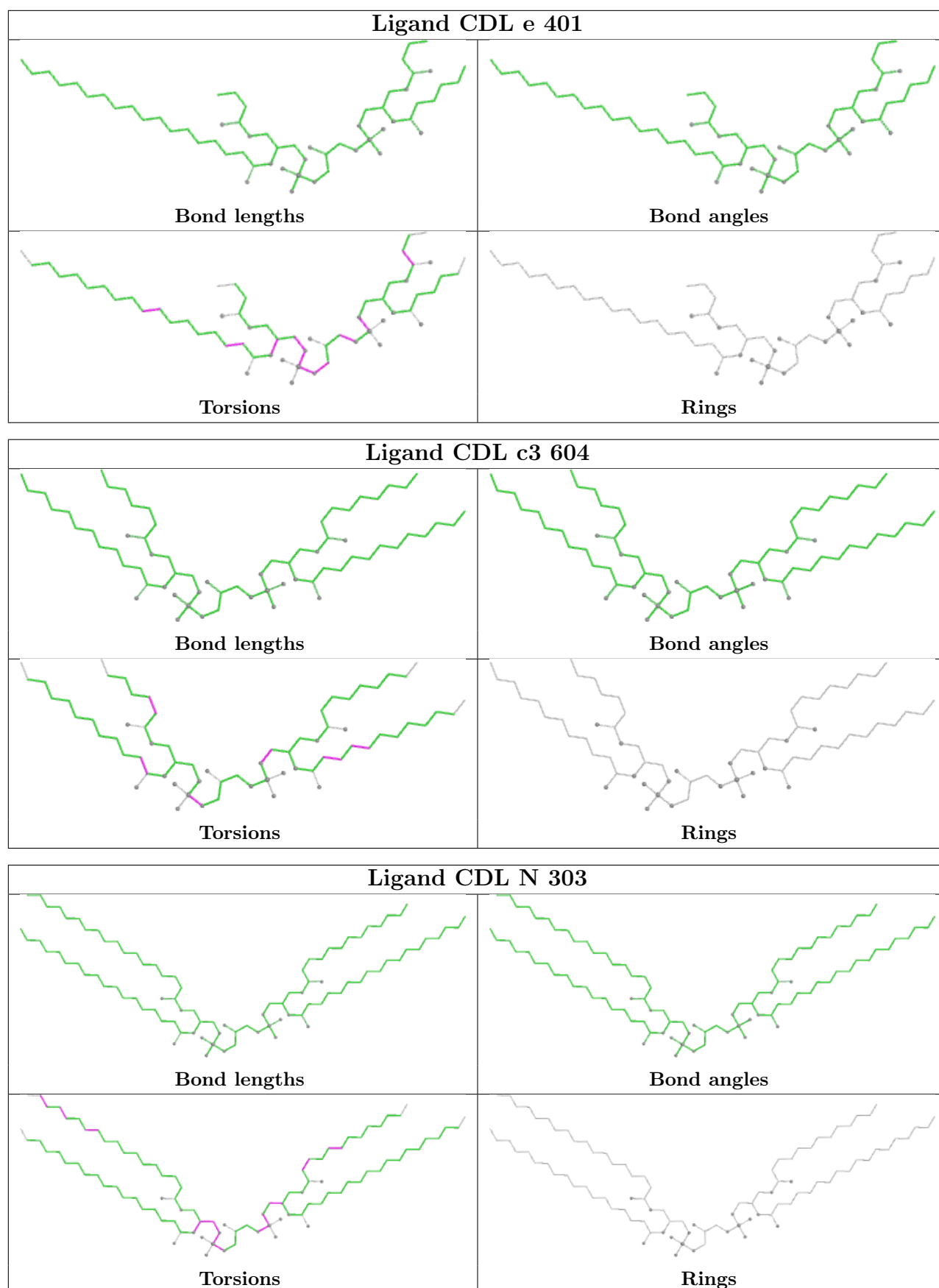


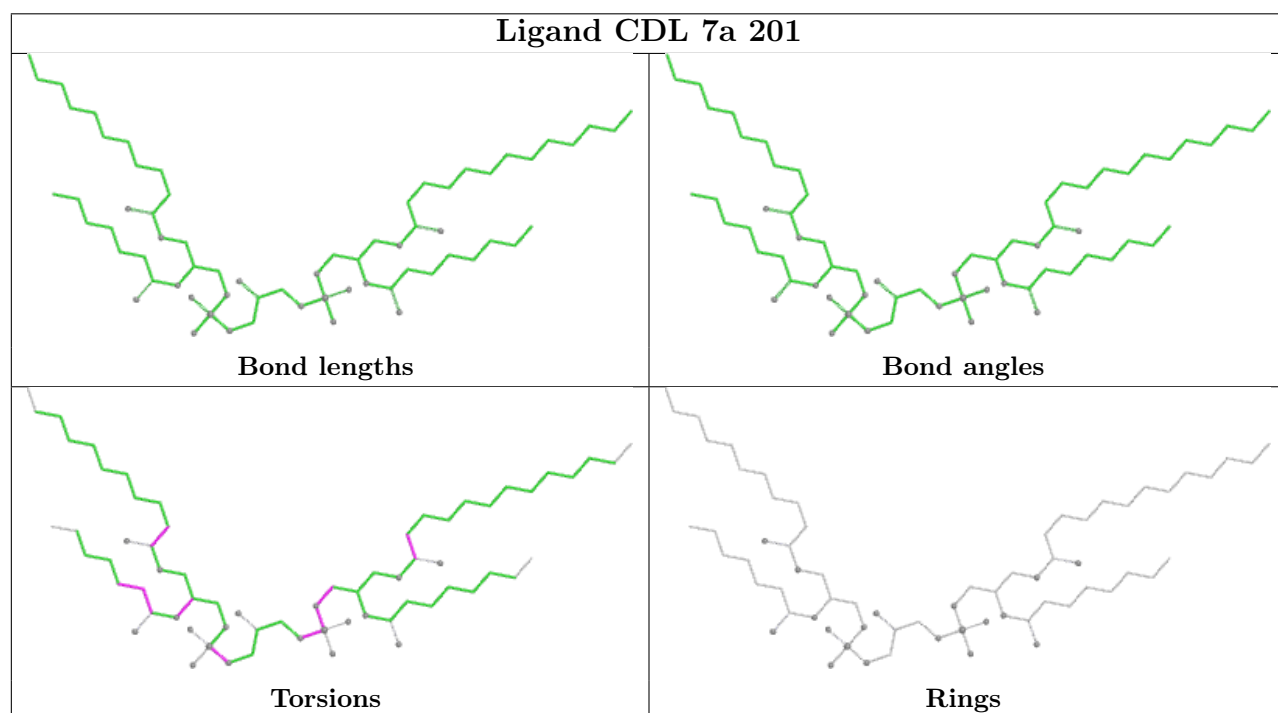
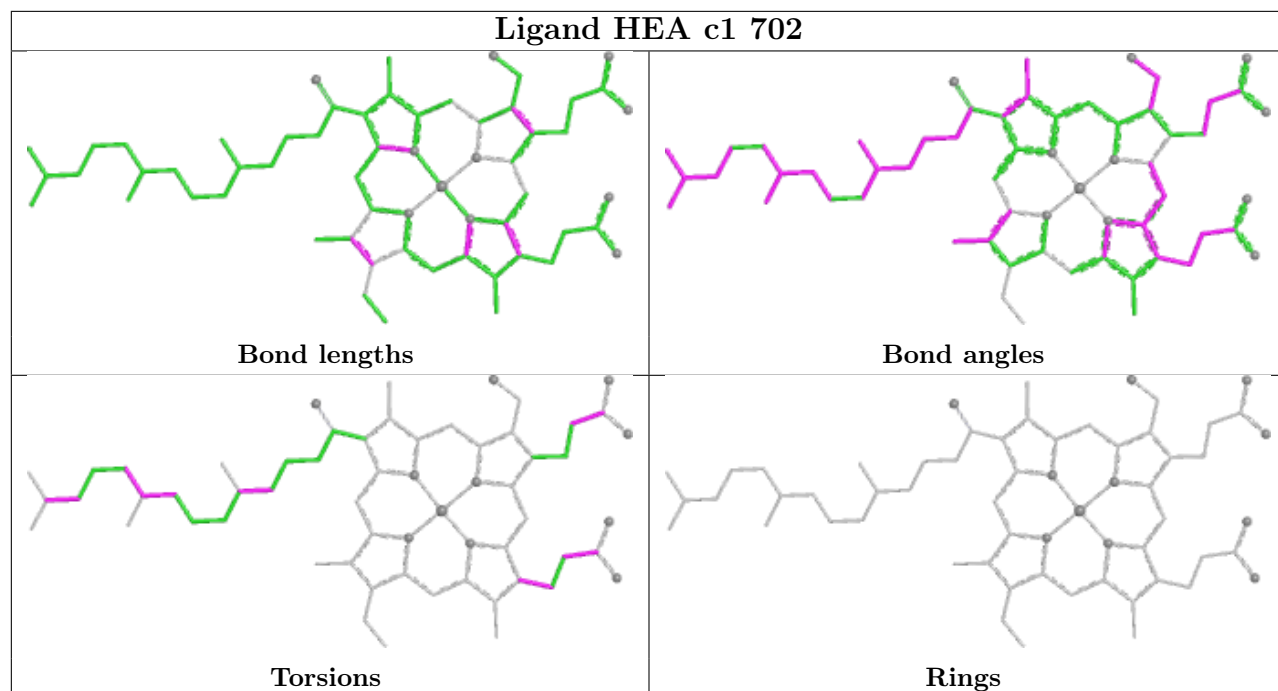


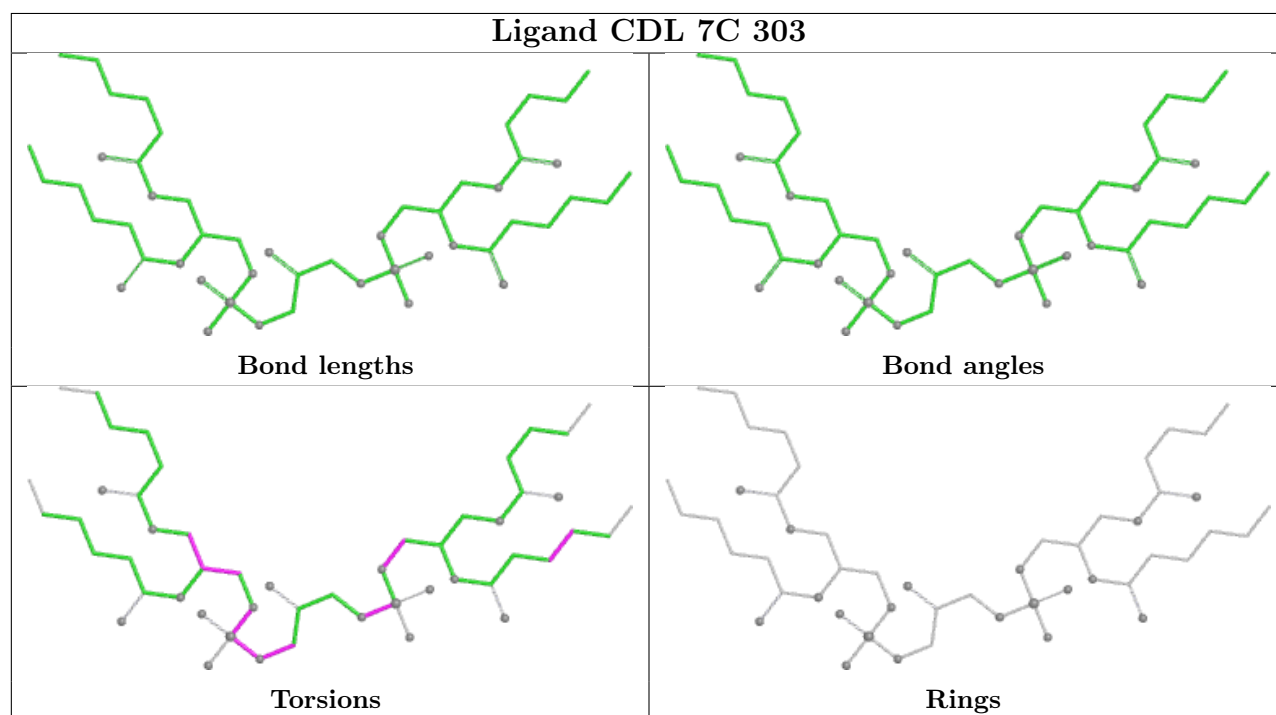
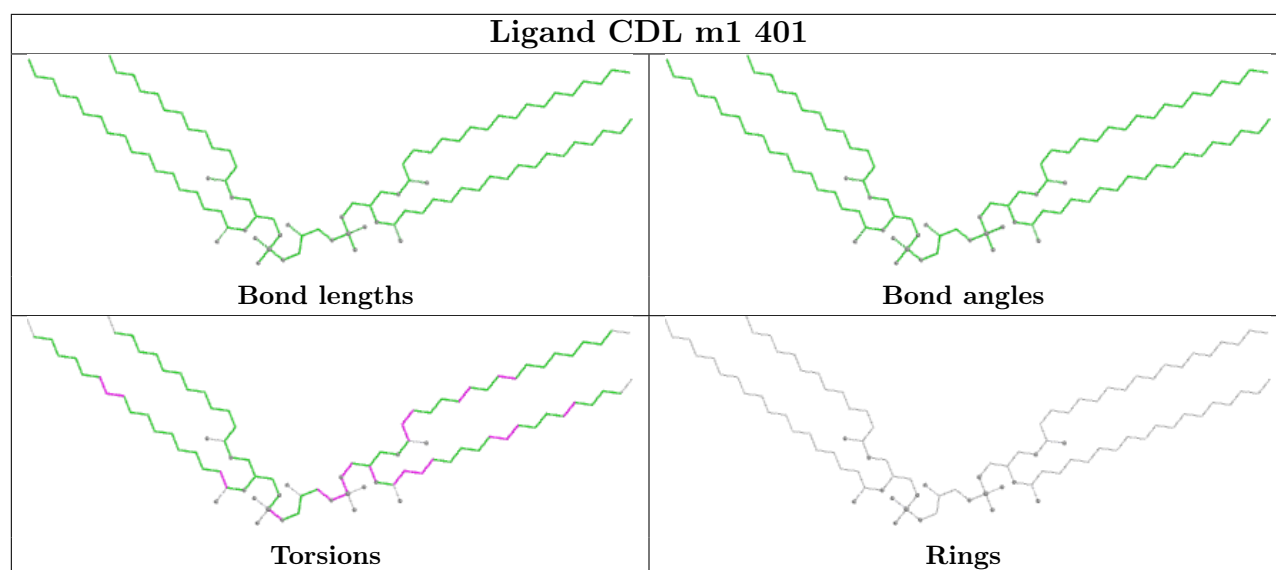


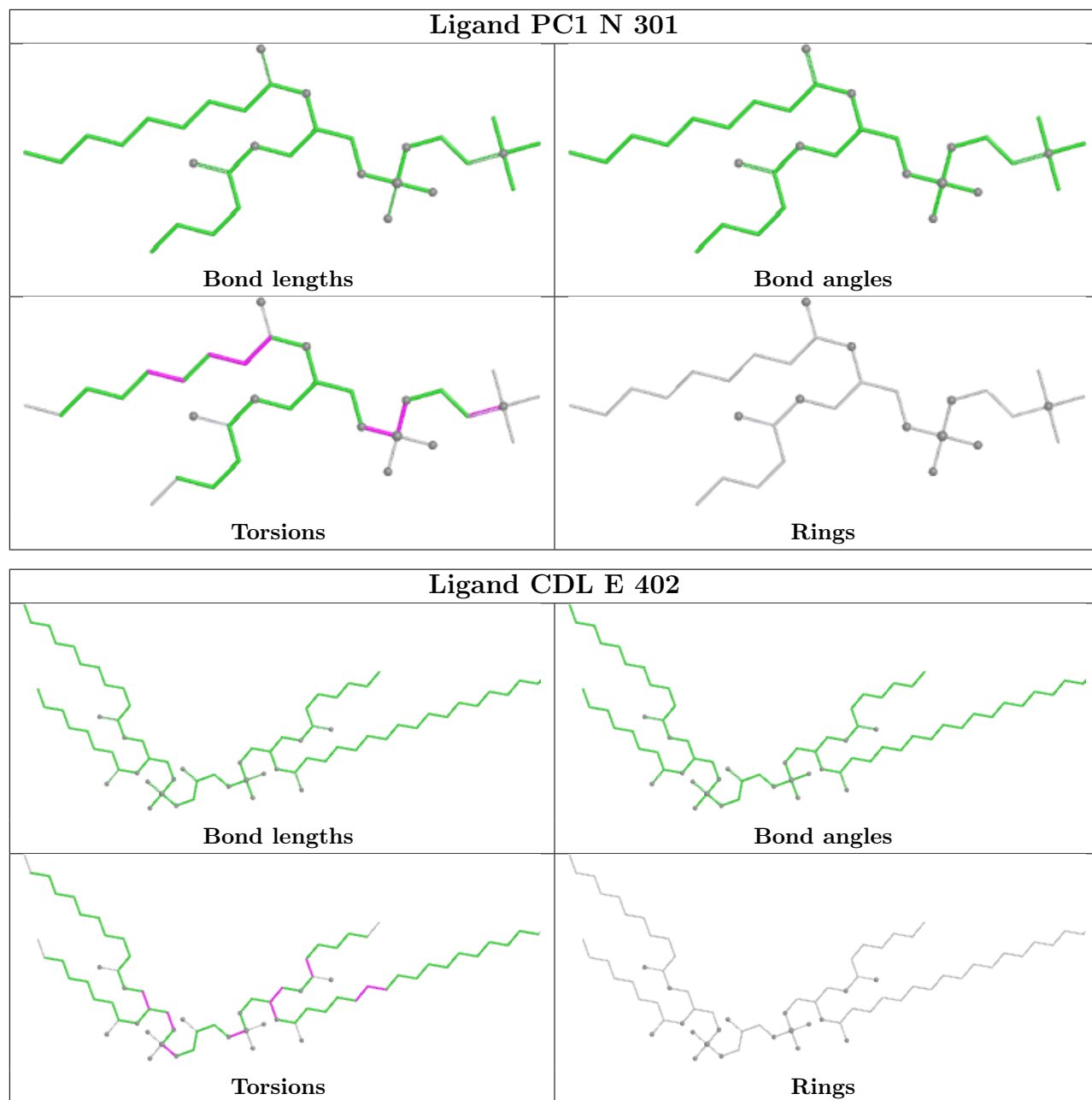


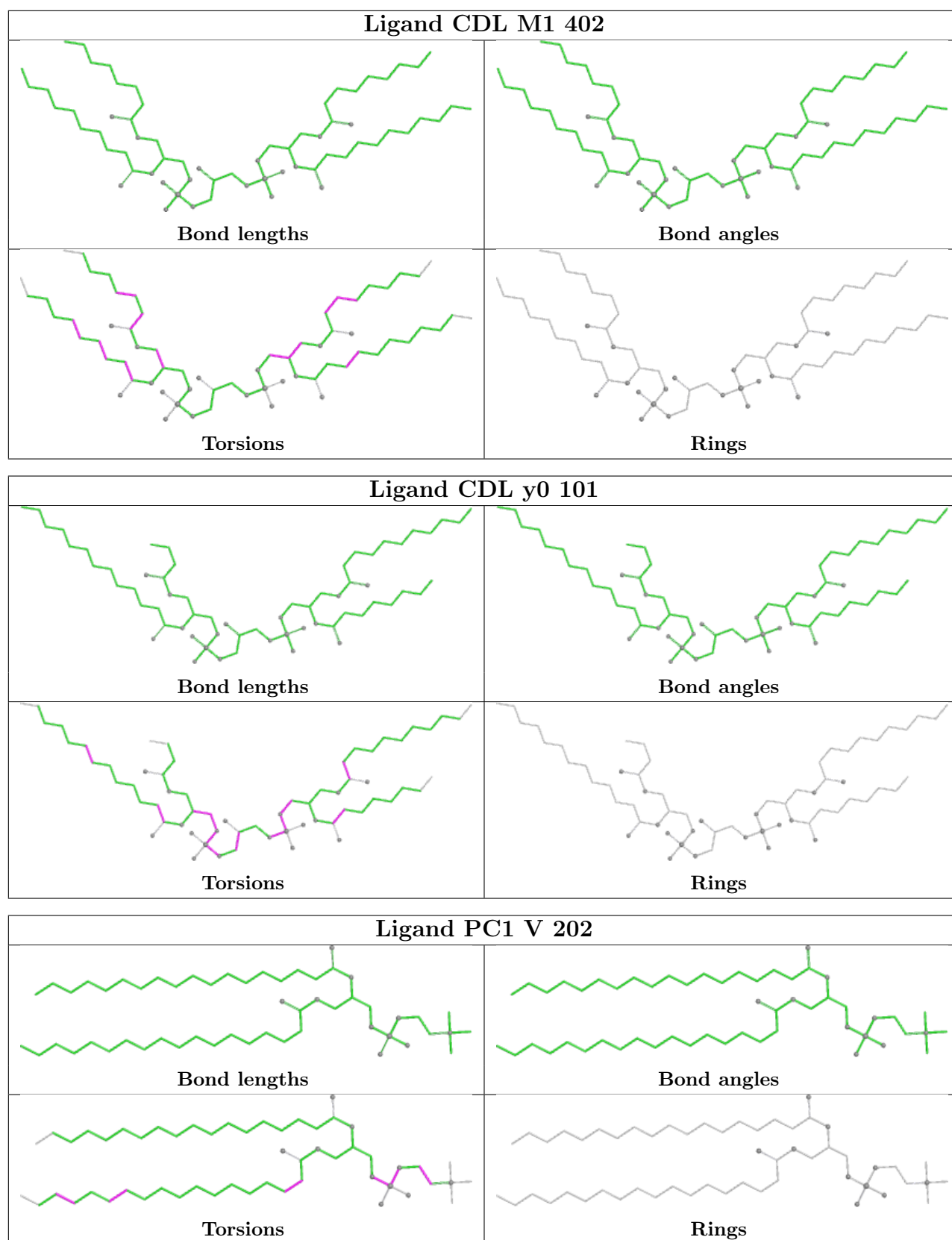


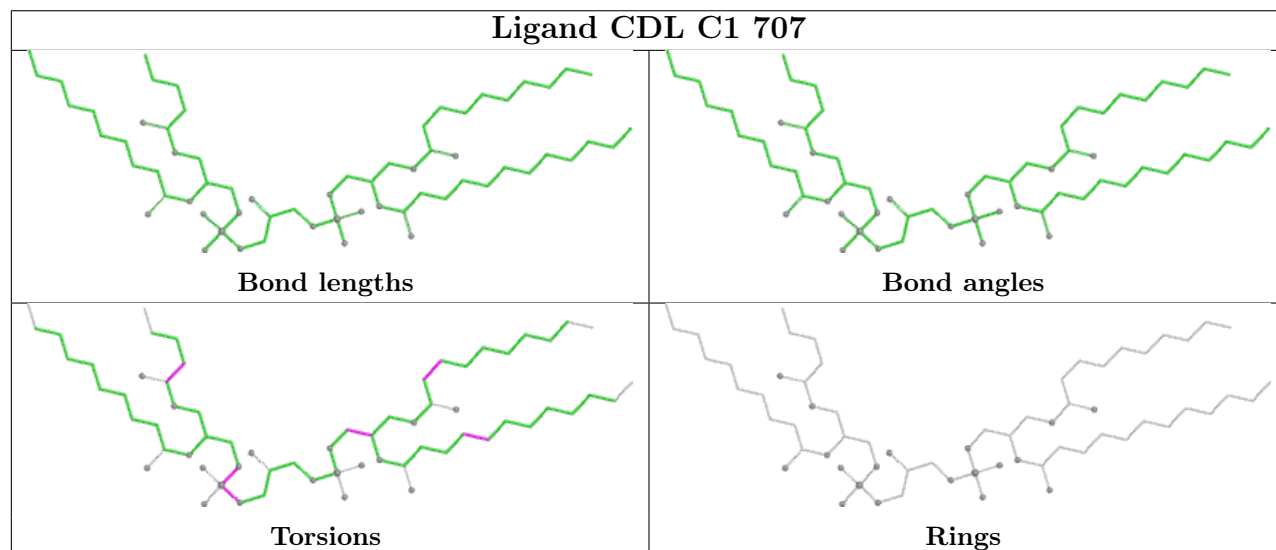
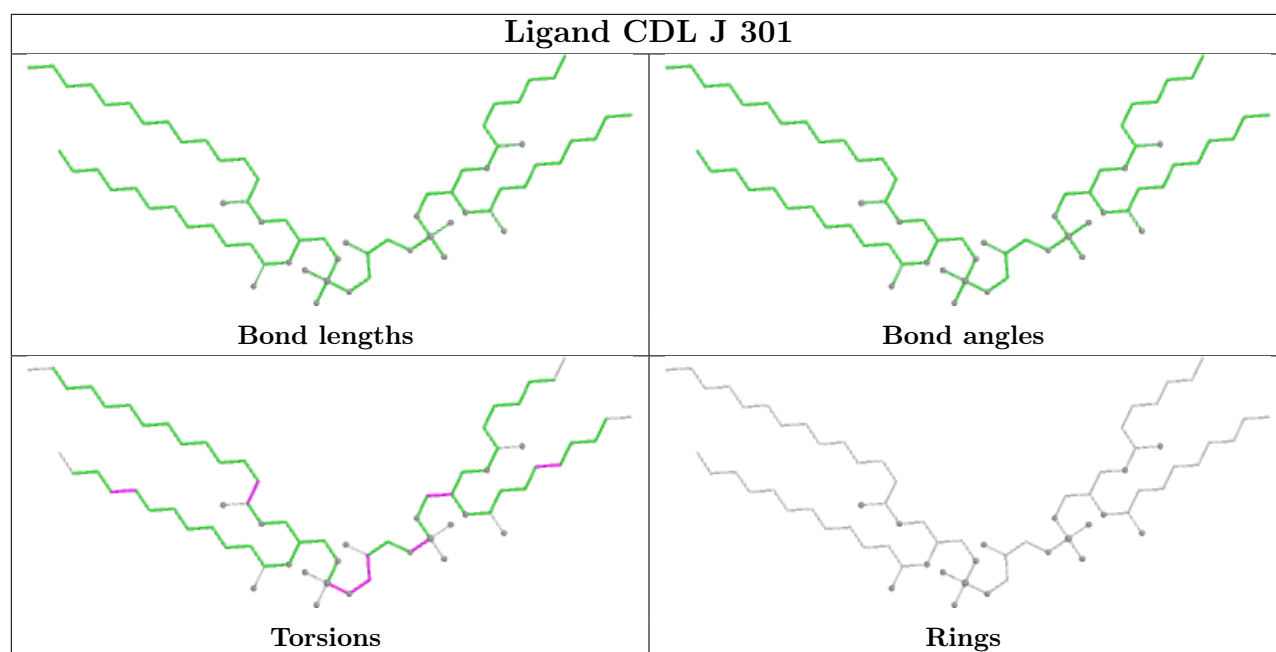


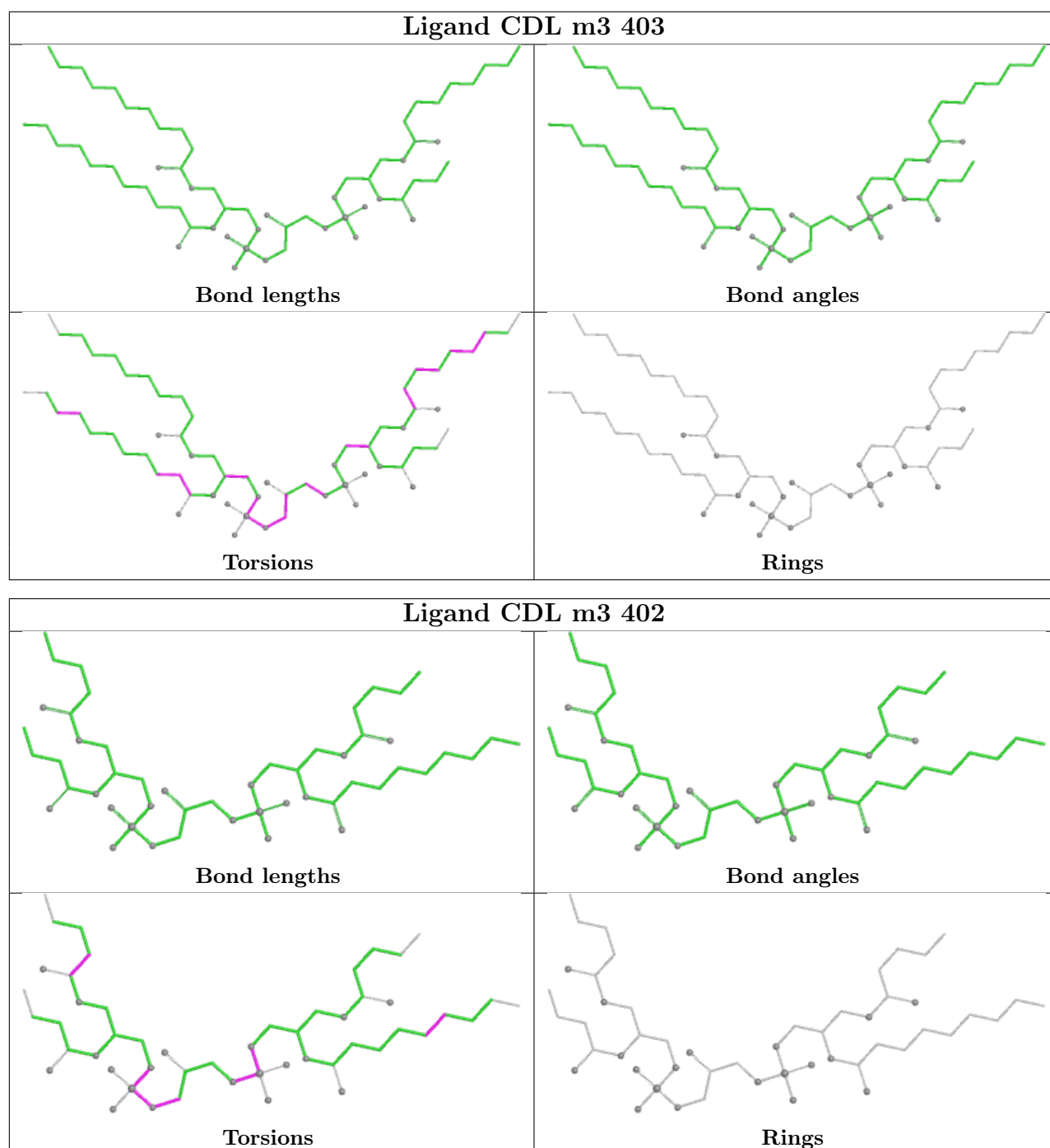


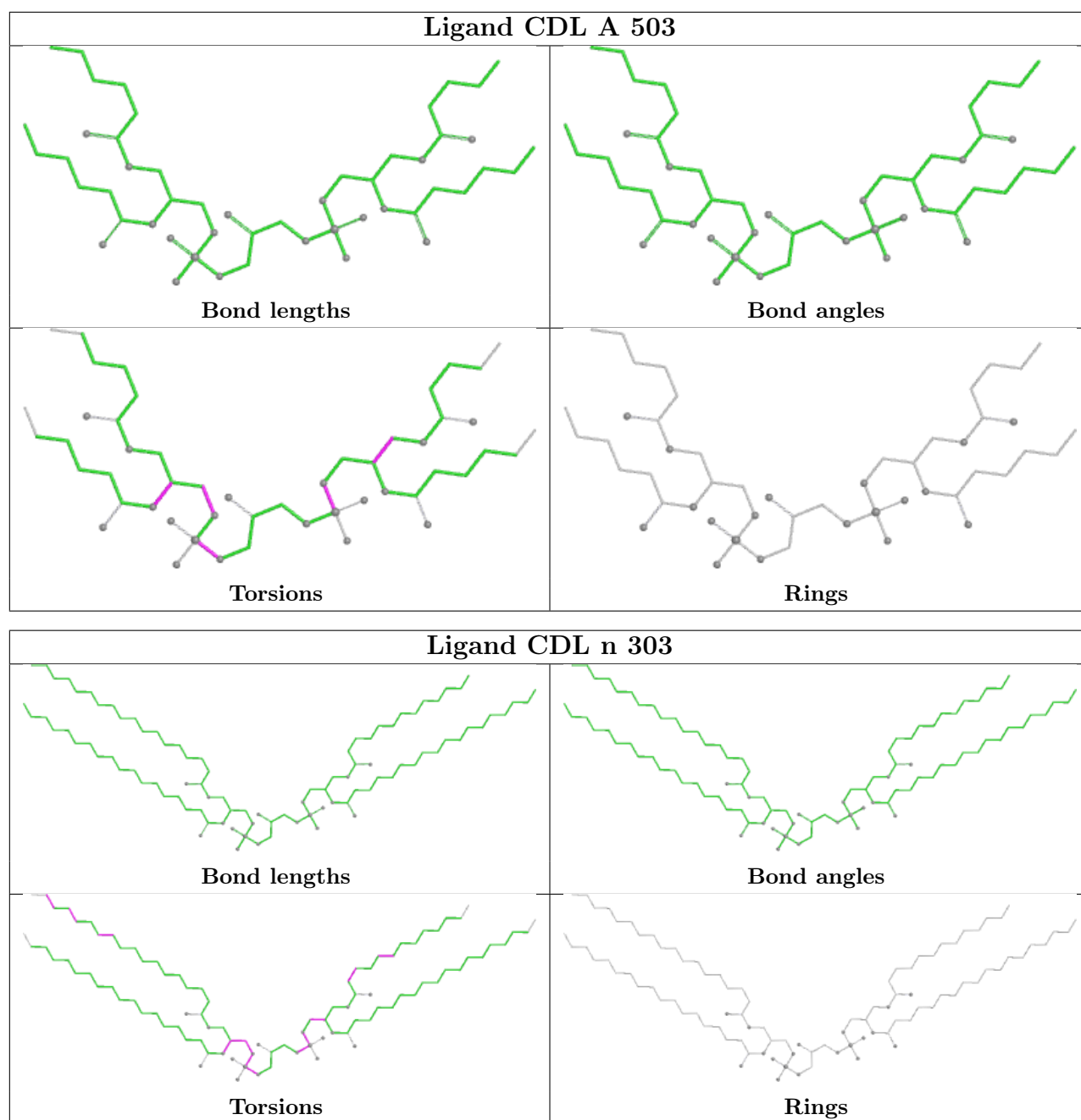


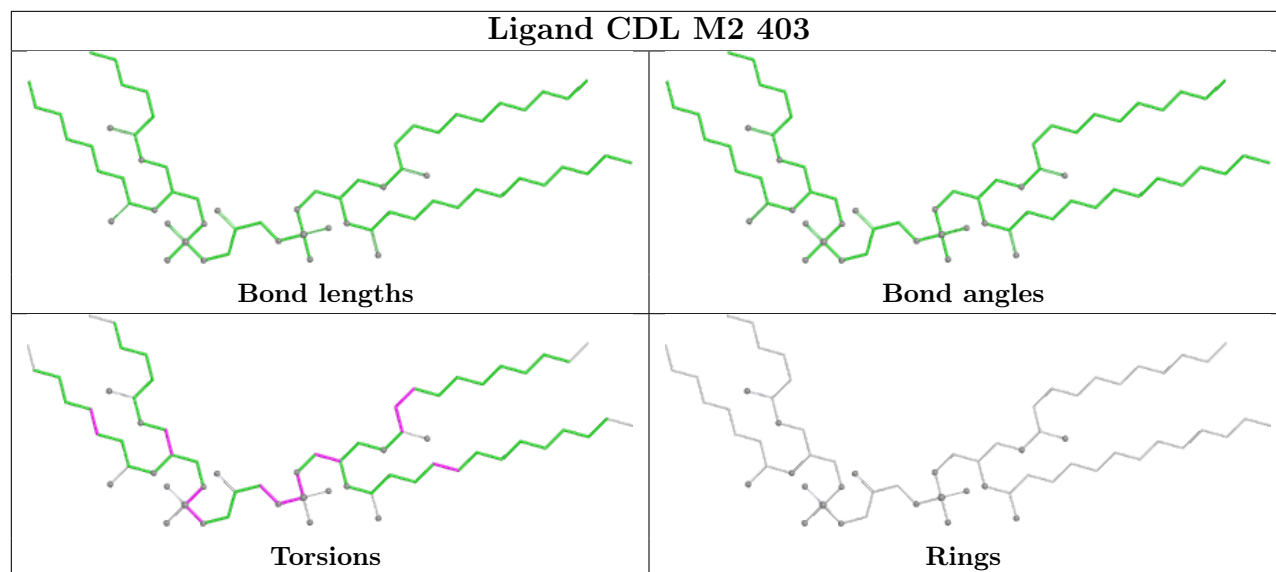












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

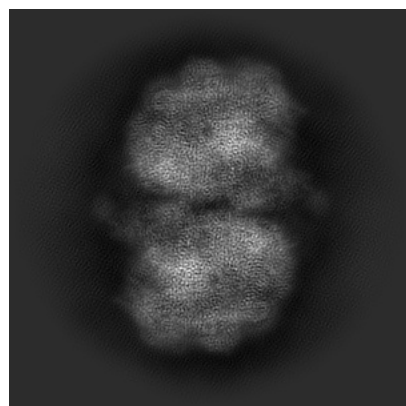
6 Map visualisation [i](#)

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.

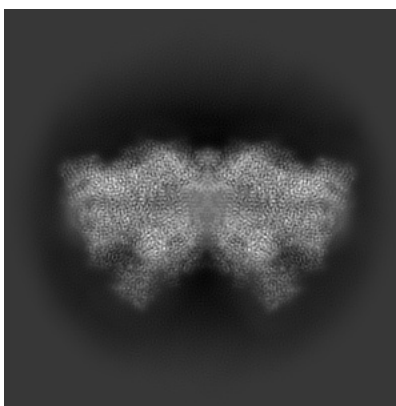
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

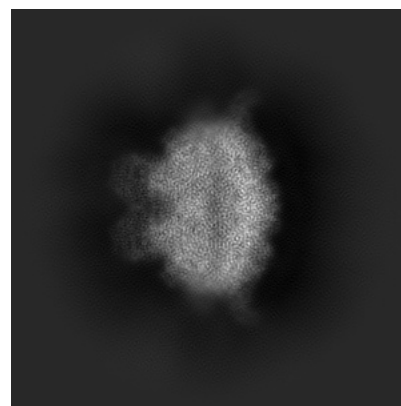
6.1.1 Primary map



X

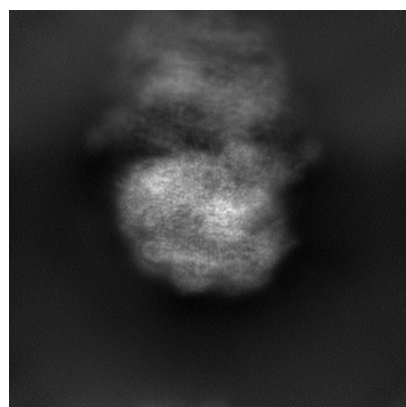


Y

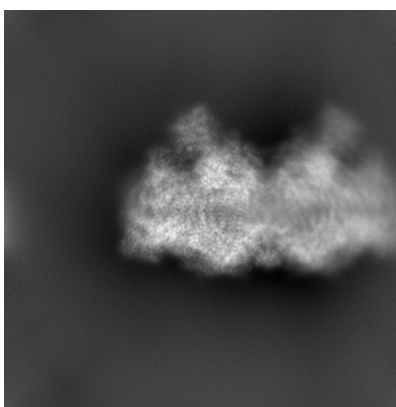


Z

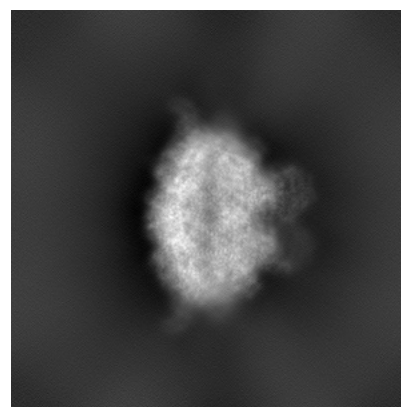
6.1.2 Raw map



X



Y

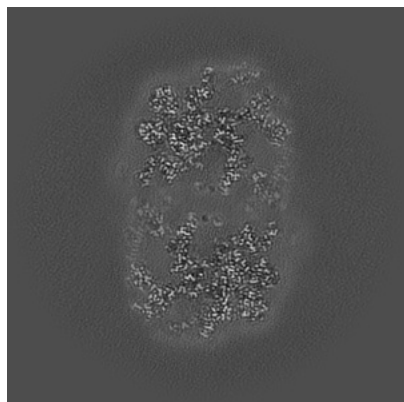


Z

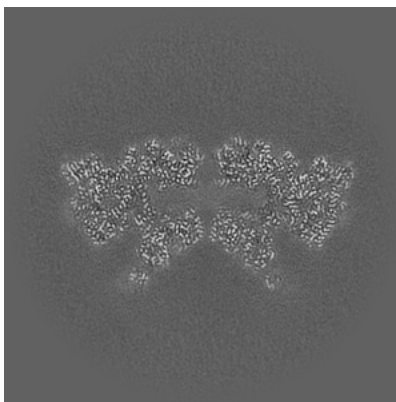
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

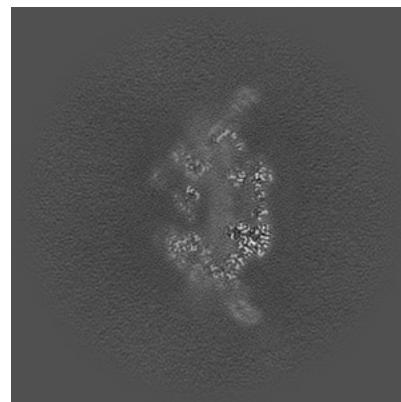
6.2.1 Primary map



X Index: 256

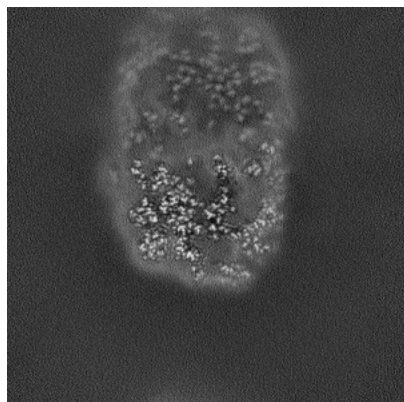


Y Index: 256

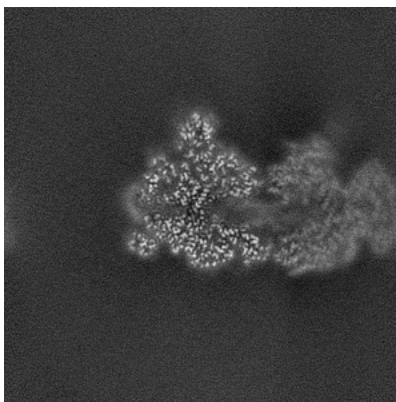


Z Index: 256

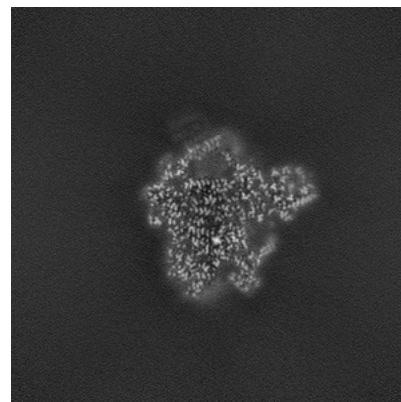
6.2.2 Raw map



X Index: 256



Y Index: 256

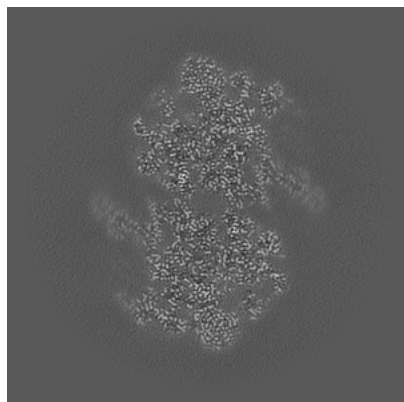


Z Index: 256

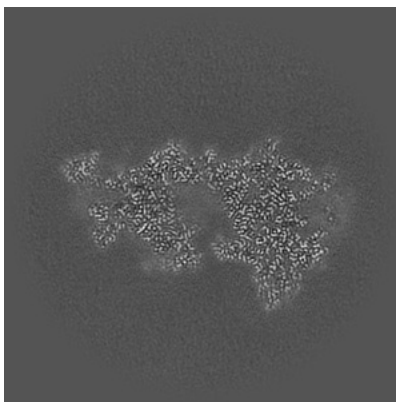
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

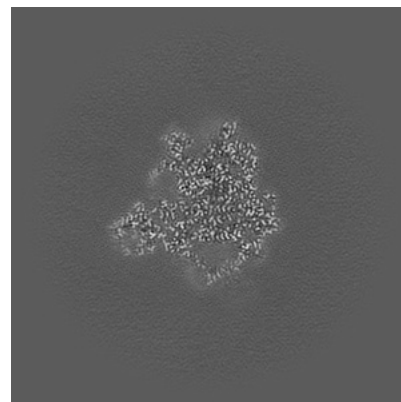
6.3.1 Primary map



X Index: 297

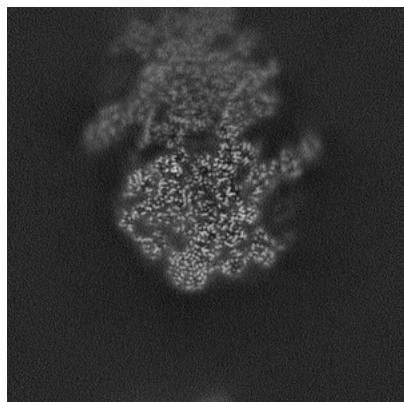


Y Index: 286

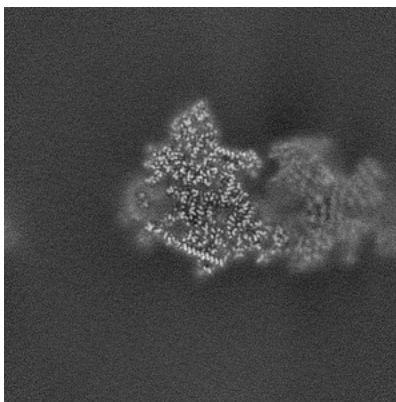


Z Index: 180

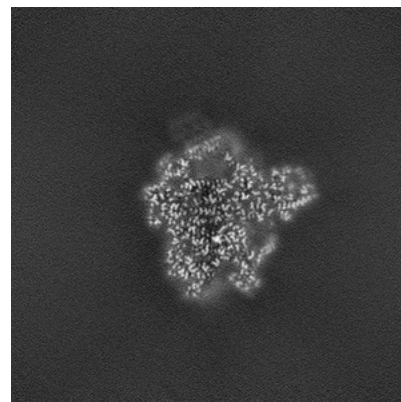
6.3.2 Raw map



X Index: 217



Y Index: 273

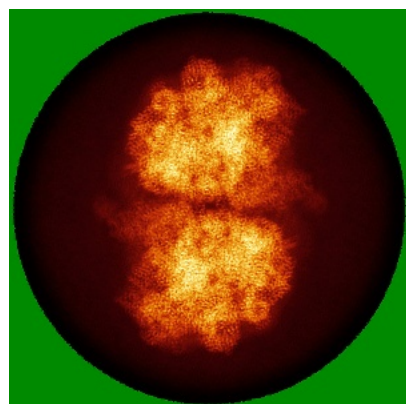


Z Index: 257

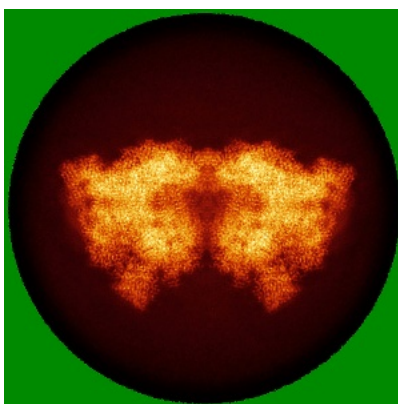
The images above show the largest variance slices of the map in three orthogonal directions.

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

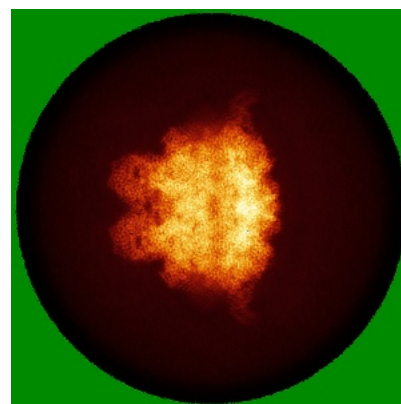
6.4.1 Primary map



X

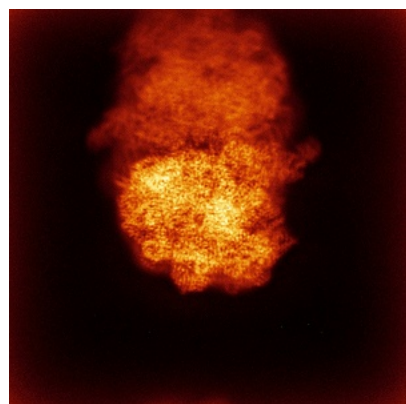


Y

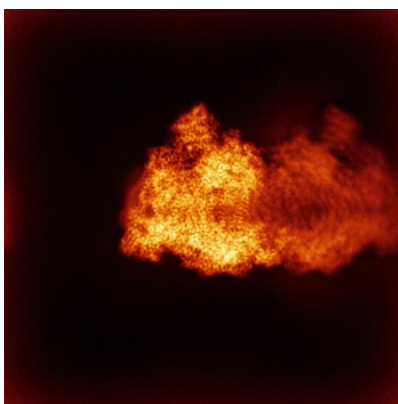


Z

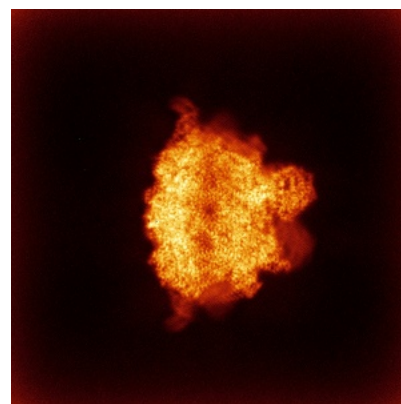
6.4.2 Raw map



X



Y

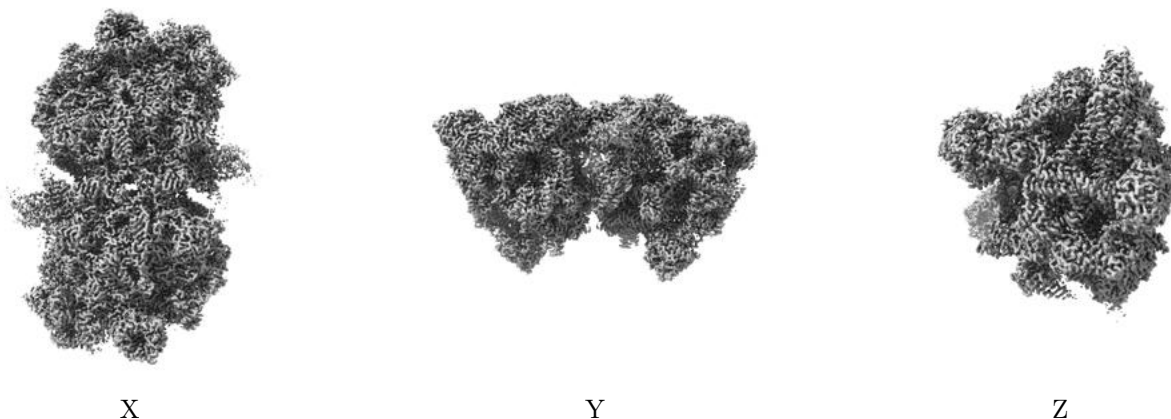


Z

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.

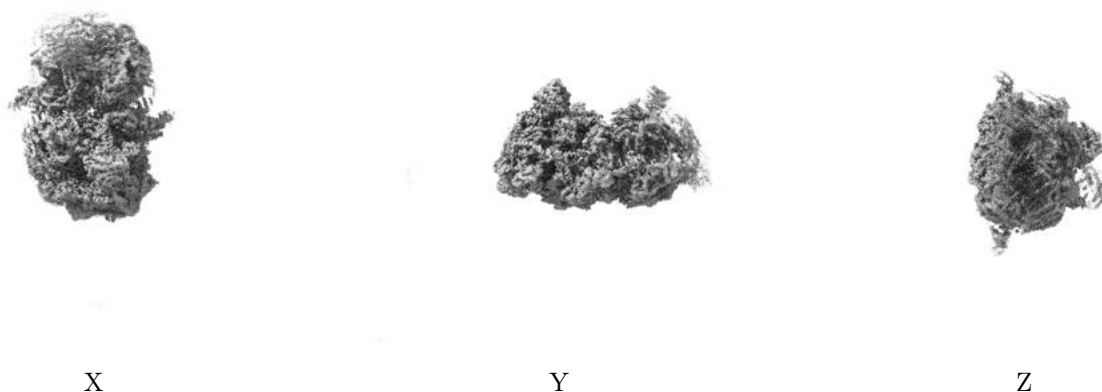
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

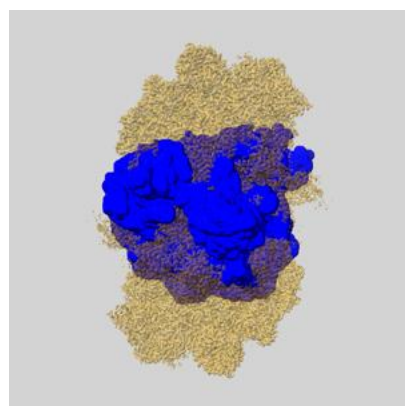
6.6 Mask visualisation [i](#)

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

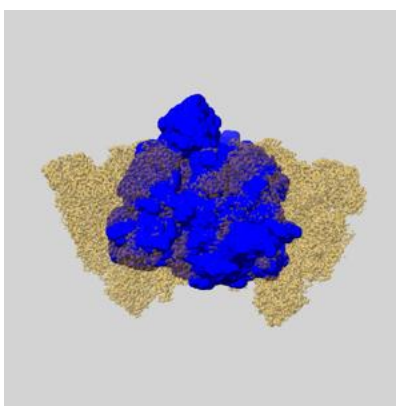
A mask typically either:

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

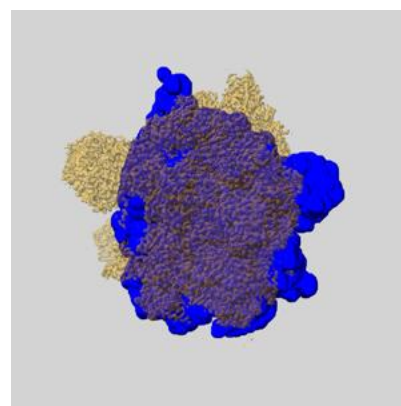
6.6.1 emd_32325_msk_1.map [i](#)



X



Y

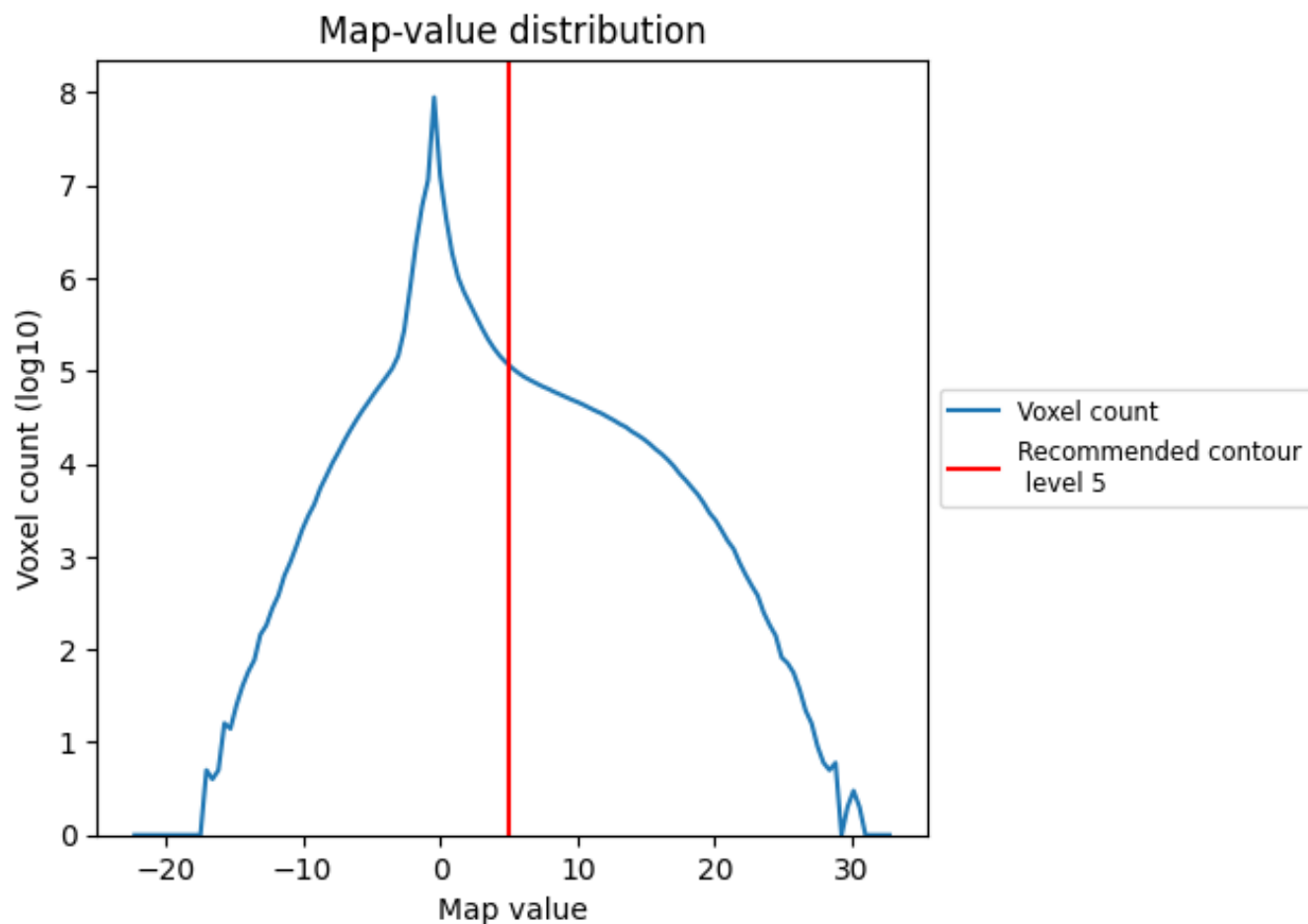


Z

7 Map analysis [i](#)

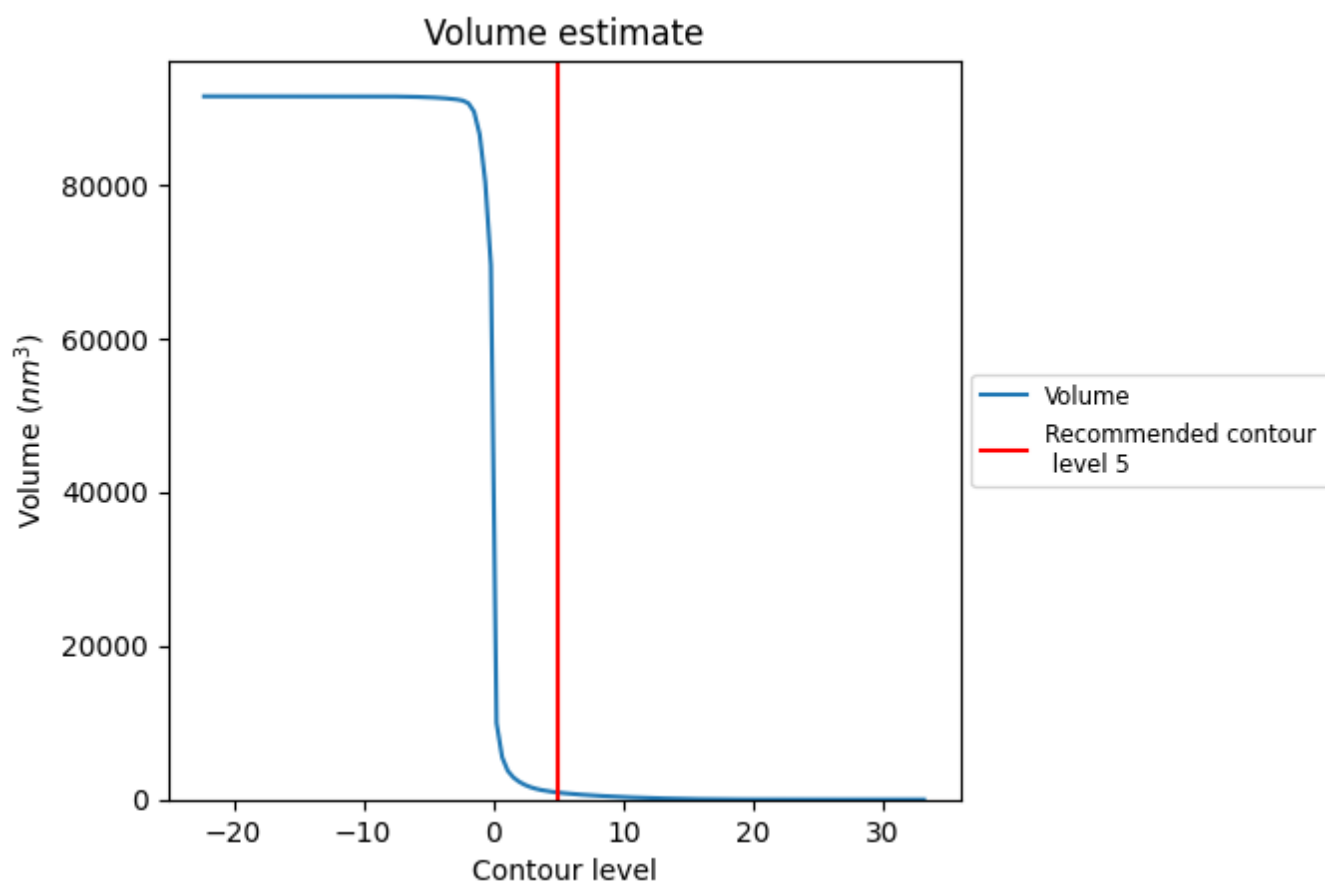
This section contains the results of statistical analysis of the map.

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.

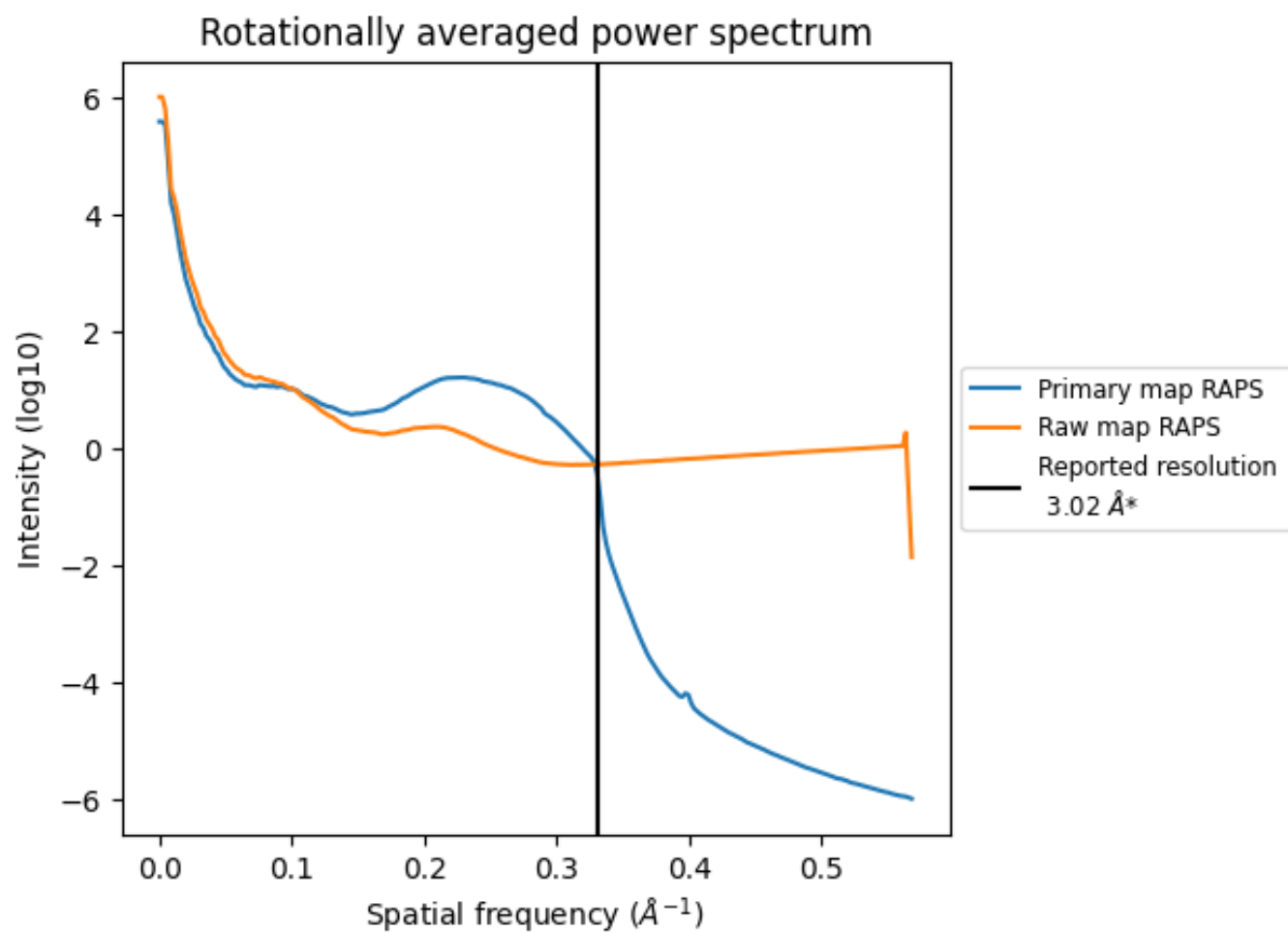
7.2 Volume estimate [i](#)



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 ⓘ

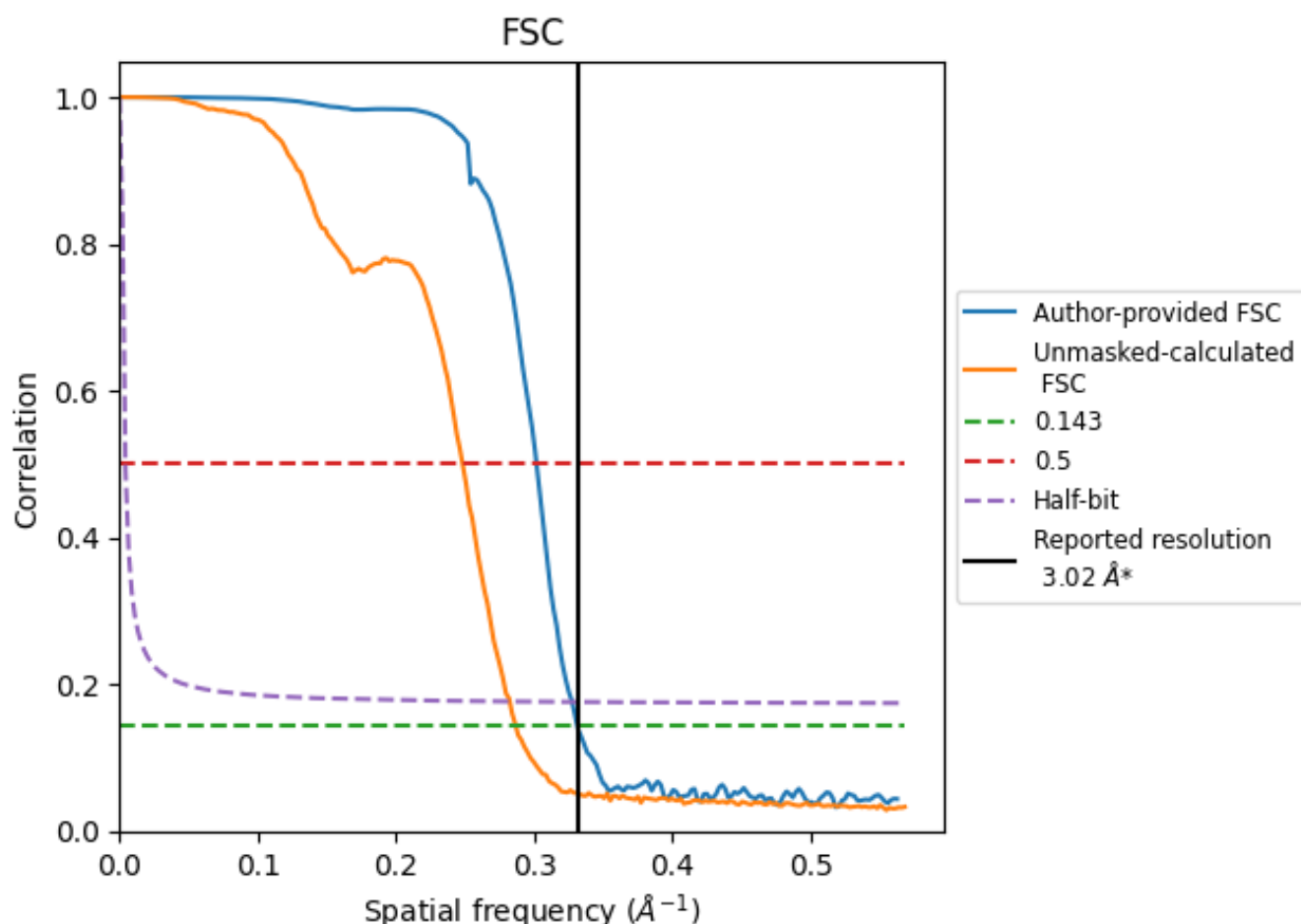


*Reported resolution corresponds to spatial frequency of 0.331 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

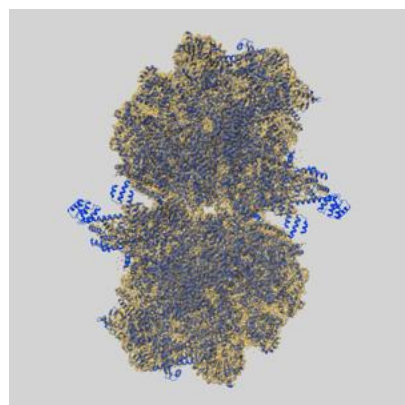
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.31	3.05
Unmasked-calculated*	3.49	4.03	3.54

*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 %

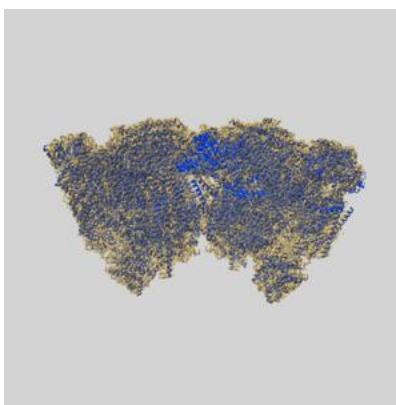
9 Map-model fit [i](#)

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.

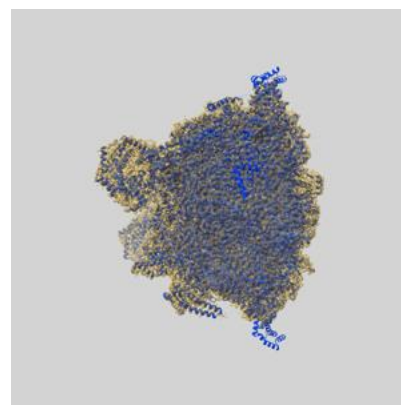
9.1 Map-model overlay [i](#)



X



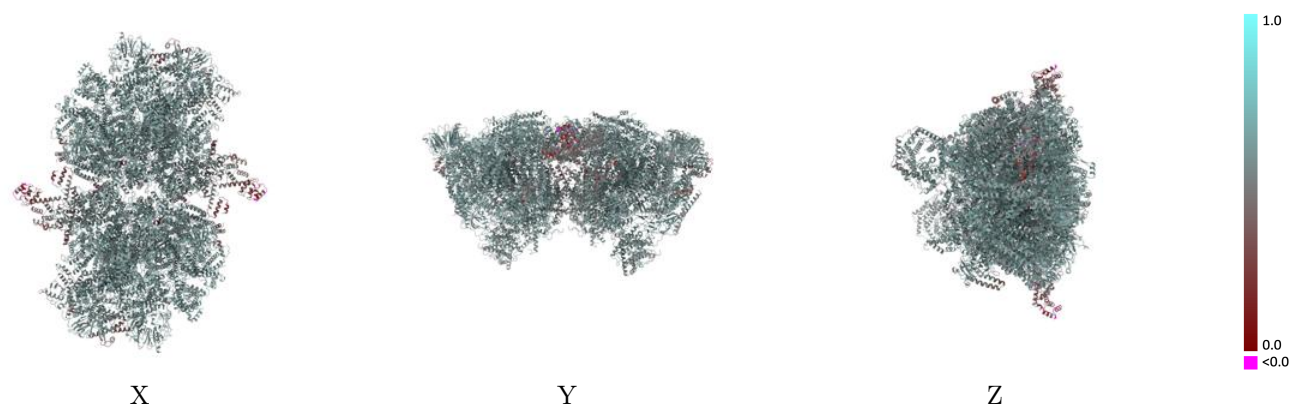
Y



Z

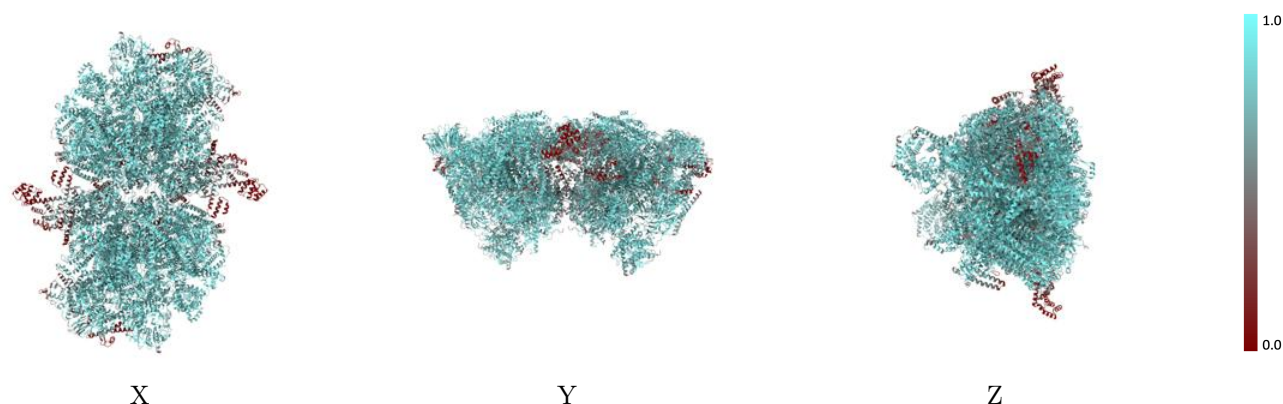
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



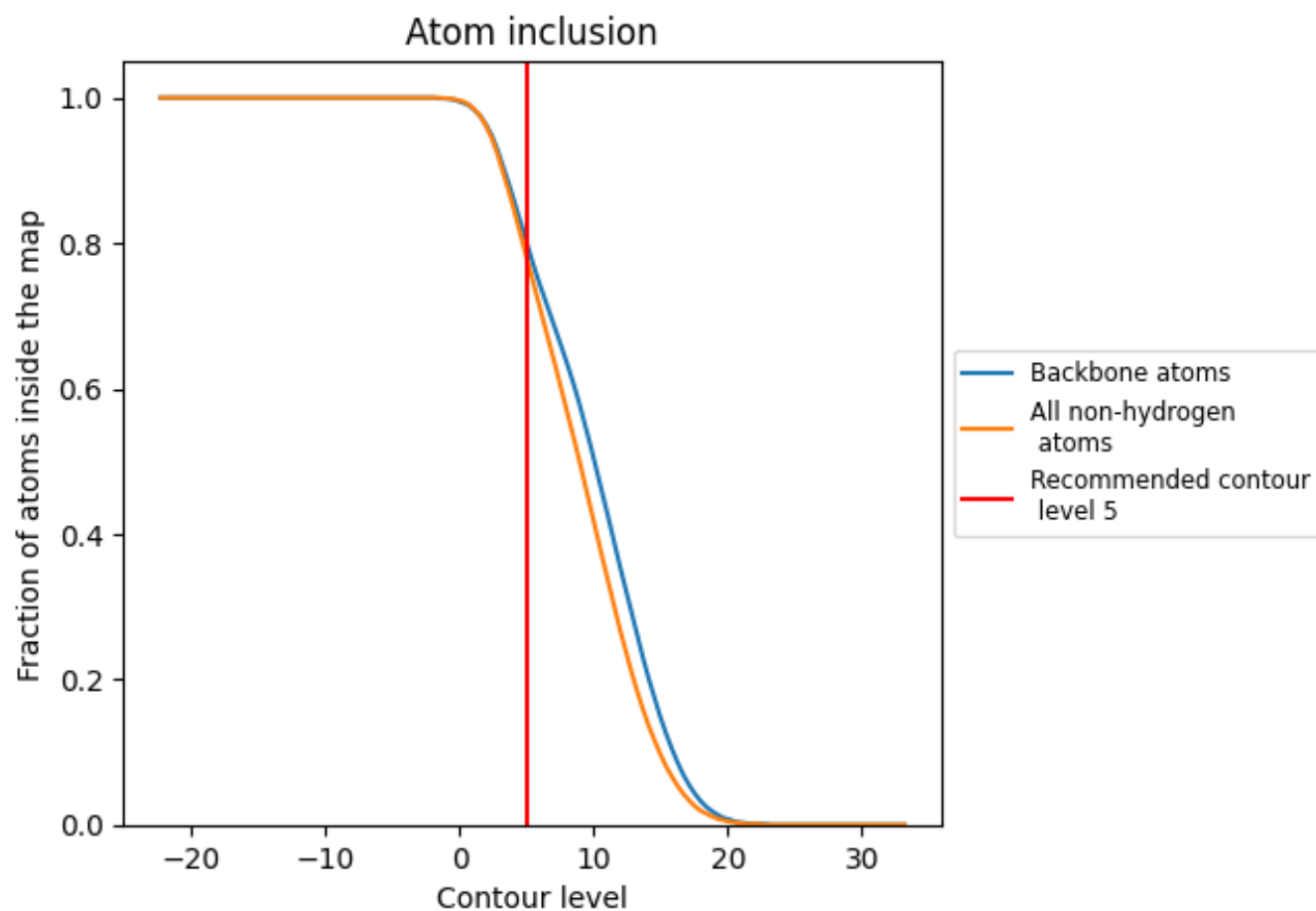
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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