wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 10:11 AM JST

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

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

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

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

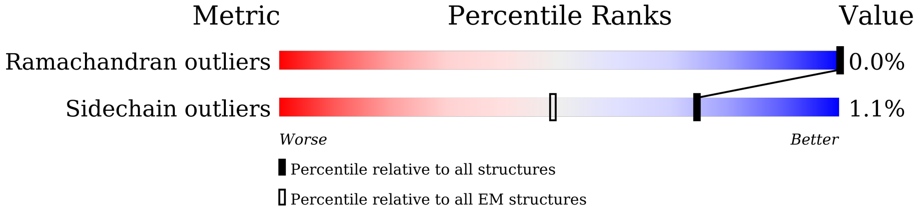
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

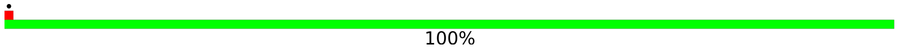
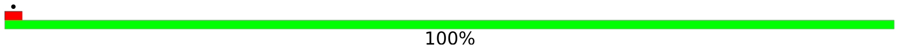
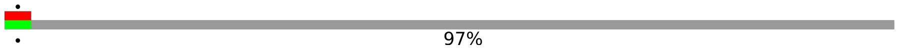
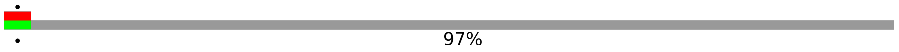
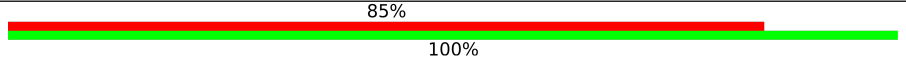
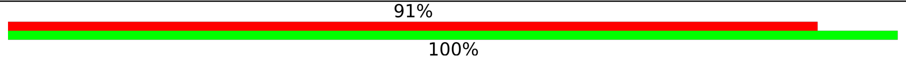
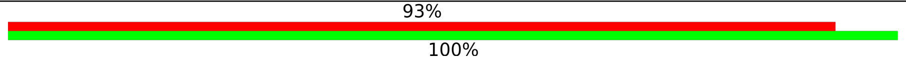
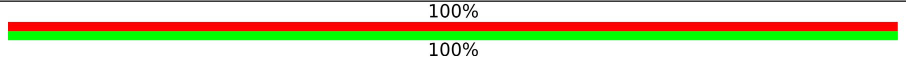
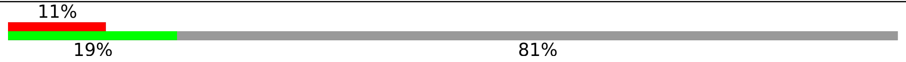
The reported resolution of this entry is 3.02 Å.

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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	U1	98	
1	u1	98	
2	U2	3634	
2	u2	3634	
3	U3	34	
3	u3	34	
4	U4	30	
4	u4	30	
5	U5	172	

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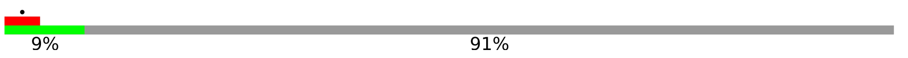
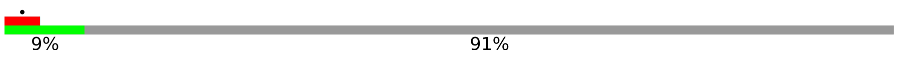
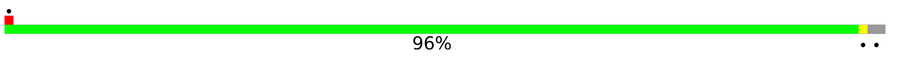
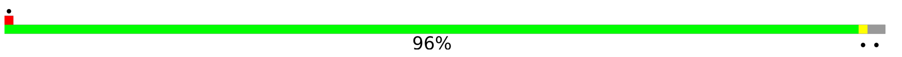
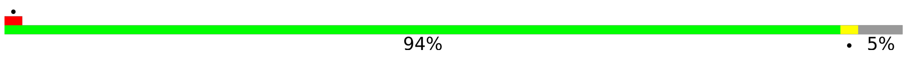
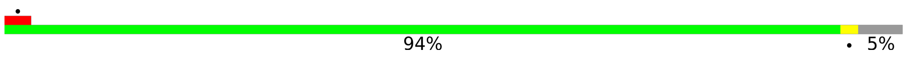
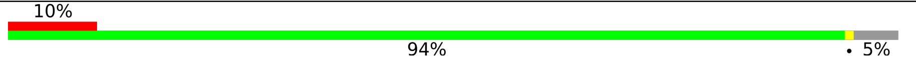
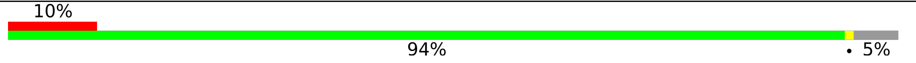
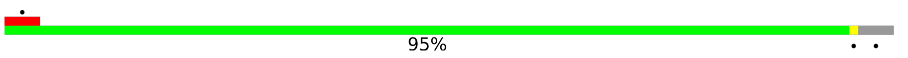
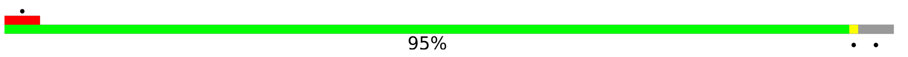
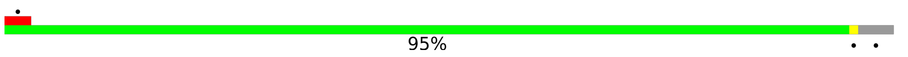
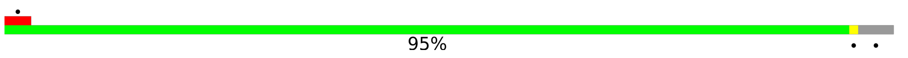
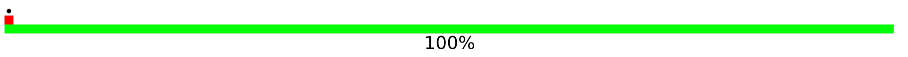
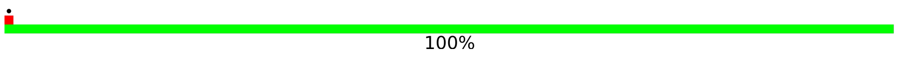
6	U6	478	
6	u6	478	
7	C1	688	
7	c1	688	
8	C2	604	
8	c2	604	
9	C3	594	
9	c3	594	
10	5B	637	
10	5b	637	
11	6A	130	
11	6a	130	
12	6B	230	
12	6b	230	
13	6L	88	
13	6l	88	
14	6C	103	
14	6c	103	
15	7A	133	
15	7a	133	
16	7C	236	
16	7c	236	
17	7L	990	
17	7l	990	

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Mol	Chain	Length	Quality of chain
18	M1	346	• 99% •
18	m1	346	• 99% •
19	M2	318	99% •
19	m2	318	• 99% •
20	M3	330	• 99% •
20	m3	330	• 99% •
21	T1	72	97% •
21	t1	72	97% •
22	T2	72	• 88% 12%
22	t2	72	• 88% 12%
23	T3	93	5% 89% 11%
23	t3	93	5% 89% 11%
24	T4	68	• 82% • 16%
24	t4	68	• 82% • 16%
25	T5	81	5% 78% 22%
25	t5	81	5% 78% 22%
26	T6	72	7% 97% •
26	t6	72	6% 97% •
27	BP	380	• 100%
27	bp	380	• 100%
28	FS	188	• 99% •
28	fs	188	• 99% •
29	AC	127	• 77% • 21%
29	ac	127	• 77% • 21%
30	Y7	453	21% 74% • 25%

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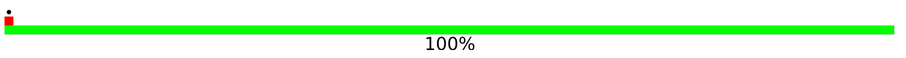
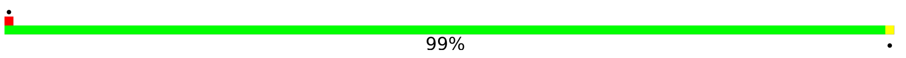
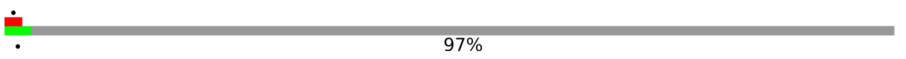
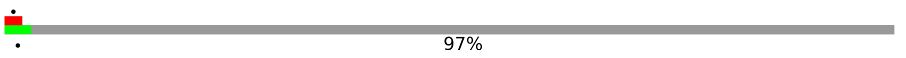
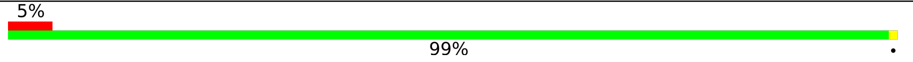
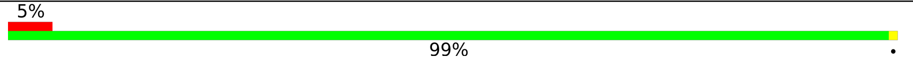
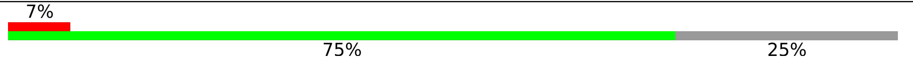
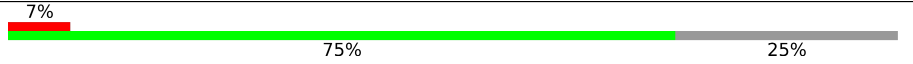
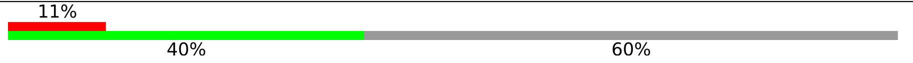
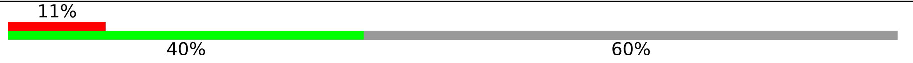
Mol	Chain	Length	Quality of chain
30	y7	453	
31	Y0	89	
31	y0	89	
32	Y5	190	
32	y5	190	
33	A	490	
33	a	490	
34	B	473	
34	b	473	
35	C	1471	
35	c	1471	
36	D	402	
36	d	402	
37	E	385	
37	e	385	
38	F	348	
38	f	348	
39	G	318	
39	g	318	
40	H	318	
40	h	318	
41	I	252	
41	i	252	
42	J	234	
42	j	234	

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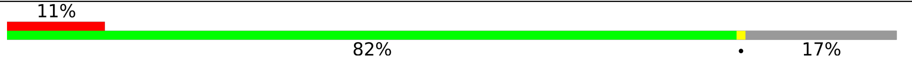
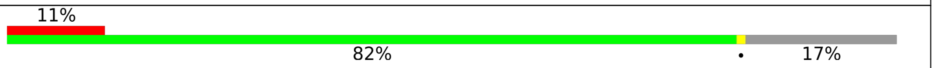
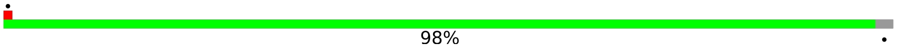
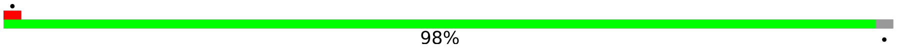
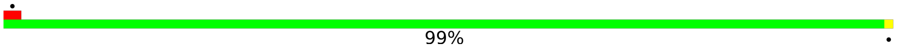
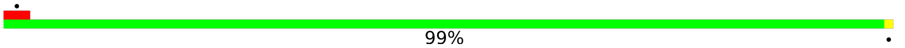
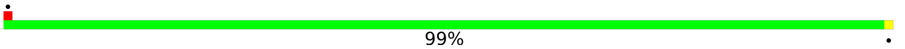
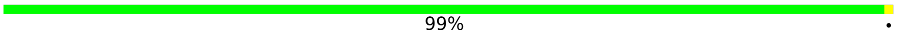
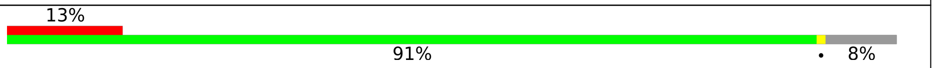
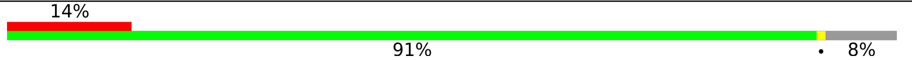
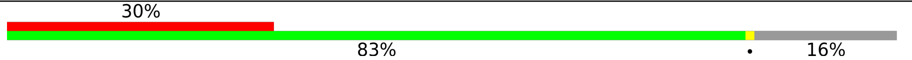
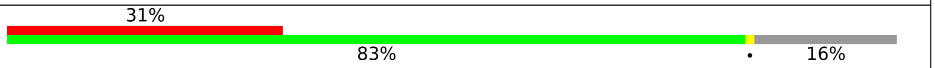
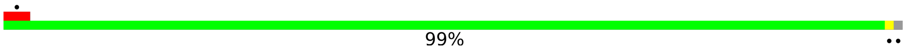
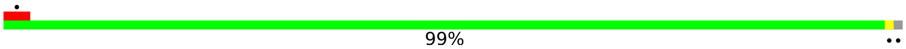
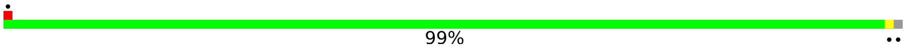
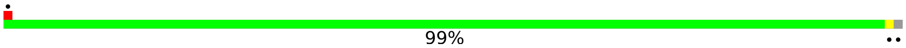
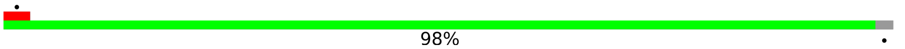
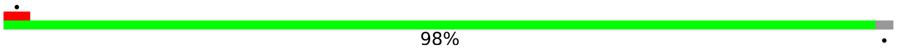
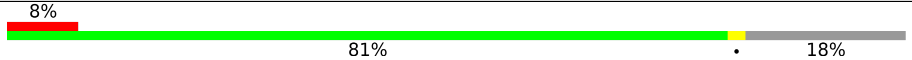
Mol	Chain	Length	Quality of chain
43	K	231	
43	k	231	
44	L	222	
44	l	222	
45	M	220	
45	m	220	
46	N	210	
46	n	210	
47	O	193	
47	o	193	
48	P	175	
48	p	175	
49	Q	173	
49	q	173	
50	R	173	
50	r	173	
51	S	170	
51	s	170	
52	T	158	
52	t	158	
53	U	154	
53	u	154	
54	V	149	
54	v	149	
55	W	124	

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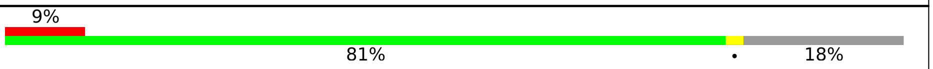
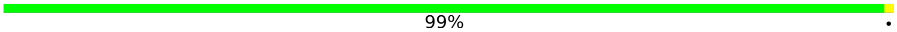
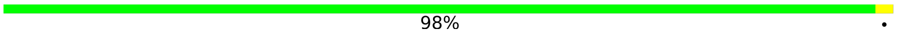
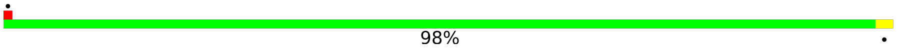
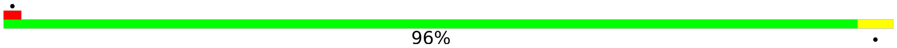
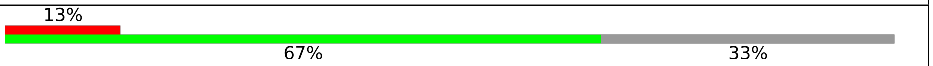
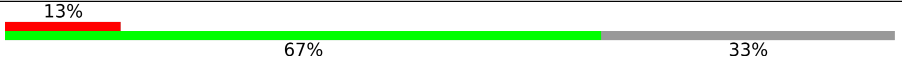
Mol	Chain	Length	Quality of chain
55	w	124	
56	X	122	
56	x	122	
57	Y	105	
57	y	105	
58	Z	90	
58	z	90	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	HEA	C1	701	X	-	-	-
59	HEA	C1	702	X	-	-	-
59	HEA	c1	701	X	-	-	-
59	HEA	c1	702	X	-	-	-

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 490	C 294	N 98	O 98	0	0
1	u1	98	Total 490	C 294	N 98	O 98	0	0

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

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

- Molecule 3 is a protein called Unknown peptide.

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

- Molecule 4 is a protein called Unknown peptide.

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

- Molecule 5 is a protein called Uncharacterized protein.

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

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

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

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

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

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

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

- Molecule 9 is a protein called Ymf68.

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6B	221	Total 1904	C 1234	N 311	O 346	S 13	0	0
12	6b	221	Total 1904	C 1234	N 311	O 346	S 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 638	C 408	N 108	O 116	S 6	0	0
13	6l	77	Total 638	C 408	N 108	O 116	S 6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 1509	C 978	N 260	O 257	S 14	0	0
28	fs	188	Total 1509	C 978	N 260	O 257	S 14	0	0

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

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

- Molecule 30 is a protein called Ymf67.

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

- Molecule 31 is a protein called Ymf70.

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

- Molecule 32 is a protein called Ymf75.

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

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called TraB family protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 1165 732 204 224 5	0	0
51	s	143	Total C N O S 1165 732 204 224 5	0	0

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

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

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

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

- 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 1234 802 217 213 2	0	0
54	v	146	Total C N O S 1234 802 217 213 2	0	0

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

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

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

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

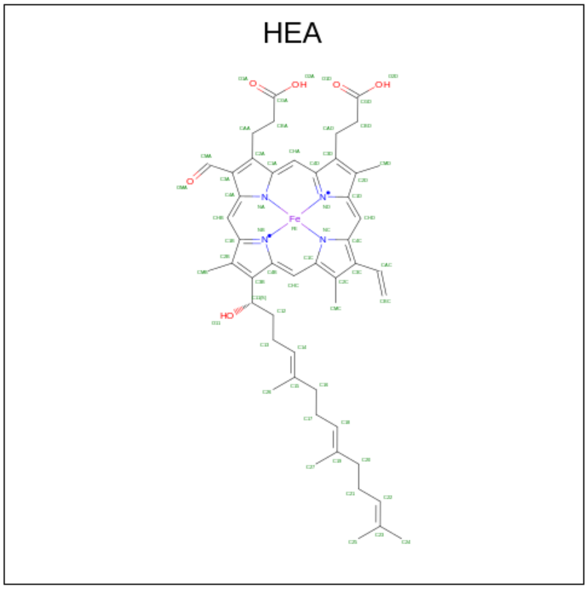
- Molecule 57 is a protein called Cytochrome c oxidase subunit TT25.

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

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

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

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



Mol	Chain	Residues	Atoms	AltConf
59	C1	1	Total C Fe N O 120 98 2 8 12	0
59	C1	1	Total C Fe N O 120 98 2 8 12	0
59	c1	1	Total C Fe N O 120 98 2 8 12	0
59	c1	1	Total C Fe N O 120 98 2 8 12	0

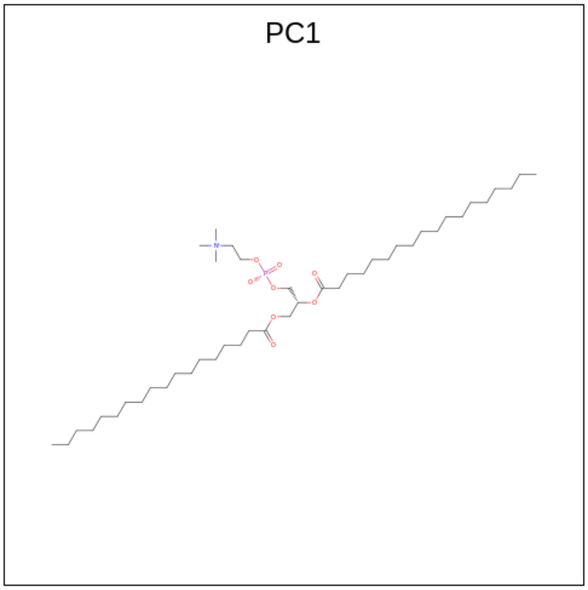
- Molecule 60 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- 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 1 1	0
61	c1	1	Total Mg 1 1	0

- Molecule 62 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
62	C1	1	49	39	1	8	1	0
62	C3	1	163	123	4	32	4	0
62	C3	1	163	123	4	32	4	0
62	C3	1	163	123	4	32	4	0
62	C3	1	163	123	4	32	4	0
62	7C	1	97	77	2	16	2	0
62	7C	1	97	77	2	16	2	0
62	M1	1	35	25	1	8	1	0
62	M2	1	127	97	3	24	3	0
62	M2	1	127	97	3	24	3	0
62	M2	1	127	97	3	24	3	0
62	A	1	86	66	2	16	2	0
62	A	1	86	66	2	16	2	0
62	J	1	37	27	1	8	1	0

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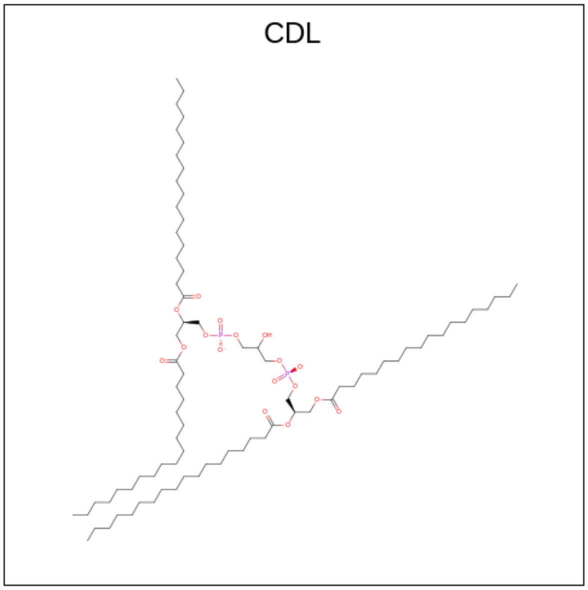
Mol	Chain	Residues	Atoms	AltConf
62	N	1	Total C N O P 68 48 2 16 2	0
62	N	1	Total C N O P 68 48 2 16 2	0
62	V	1	Total C N O P 54 44 1 8 1	0
62	c1	1	Total C N O P 49 39 1 8 1	0
62	c3	1	Total C N O P 163 123 4 32 4	0
62	c3	1	Total C N O P 163 123 4 32 4	0
62	c3	1	Total C N O P 163 123 4 32 4	0
62	c3	1	Total C N O P 163 123 4 32 4	0
62	7c	1	Total C N O P 43 33 1 8 1	0
62	m1	1	Total C N O P 89 69 2 16 2	0
62	m1	1	Total C N O P 89 69 2 16 2	0
62	m2	1	Total C N O P 127 97 3 24 3	0
62	m2	1	Total C N O P 127 97 3 24 3	0
62	m2	1	Total C N O P 127 97 3 24 3	0
62	a	1	Total C N O P 86 66 2 16 2	0
62	a	1	Total C N O P 86 66 2 16 2	0
62	j	1	Total C N O P 37 27 1 8 1	0
62	n	1	Total C N O P 68 48 2 16 2	0
62	n	1	Total C N O P 68 48 2 16 2	0
62	v	1	Total C N O P 54 44 1 8 1	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
63	C1	1	124	86	34	4	0
63	C1	1	124	86	34	4	0
63	C3	1	68	49	17	2	0
63	5B	1	216	159	51	6	0
63	5B	1	216	159	51	6	0
63	5B	1	216	159	51	6	0
63	7A	1	167	129	34	4	0
63	7A	1	167	129	34	4	0
63	7C	1	136	98	34	4	0
63	7C	1	136	98	34	4	0
63	M1	1	227	170	51	6	0
63	M1	1	227	170	51	6	0
63	M1	1	227	170	51	6	0
63	M2	1	194	137	51	6	0

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Mol	Chain	Residues	Atoms	AltConf
63	M2	1	Total C O P 194 137 51 6	0
63	M2	1	Total C O P 194 137 51 6	0
63	M3	1	Total C O P 208 151 51 6	0
63	M3	1	Total C O P 208 151 51 6	0
63	M3	1	Total C O P 208 151 51 6	0
63	Y7	1	Total C O P 65 46 17 2	0
63	Y0	1	Total C O P 64 45 17 2	0
63	Y5	1	Total C O P 81 62 17 2	0
63	A	1	Total C O P 51 32 17 2	0
63	B	1	Total C O P 62 43 17 2	0
63	E	1	Total C O P 132 94 34 4	0
63	E	1	Total C O P 132 94 34 4	0
63	F	1	Total C O P 100 81 17 2	0
63	J	1	Total C O P 70 51 17 2	0
63	L	1	Total C O P 74 55 17 2	0
63	N	1	Total C O P 95 76 17 2	0
63	T	1	Total C O P 143 105 34 4	0
63	T	1	Total C O P 143 105 34 4	0
63	U	1	Total C O P 82 63 17 2	0
63	V	1	Total C O P 91 72 17 2	0
63	c1	1	Total C O P 124 86 34 4	0

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Mol	Chain	Residues	Atoms	AltConf
63	c1	1	Total C O P 124 86 34 4	0
63	c3	1	Total C O P 68 49 17 2	0
63	5b	1	Total C O P 154 116 34 4	0
63	5b	1	Total C O P 154 116 34 4	0
63	7a	1	Total C O P 167 129 34 4	0
63	7a	1	Total C O P 167 129 34 4	0
63	7c	1	Total C O P 136 98 34 4	0
63	7c	1	Total C O P 136 98 34 4	0
63	m1	1	Total C O P 227 170 51 6	0
63	m1	1	Total C O P 227 170 51 6	0
63	m1	1	Total C O P 227 170 51 6	0
63	m2	1	Total C O P 194 137 51 6	0
63	m2	1	Total C O P 194 137 51 6	0
63	m2	1	Total C O P 194 137 51 6	0
63	m3	1	Total C O P 208 151 51 6	0
63	m3	1	Total C O P 208 151 51 6	0
63	m3	1	Total C O P 208 151 51 6	0
63	y7	1	Total C O P 65 46 17 2	0
63	y0	1	Total C O P 64 45 17 2	0
63	y5	1	Total C O P 81 62 17 2	0
63	a	1	Total C O P 51 32 17 2	0

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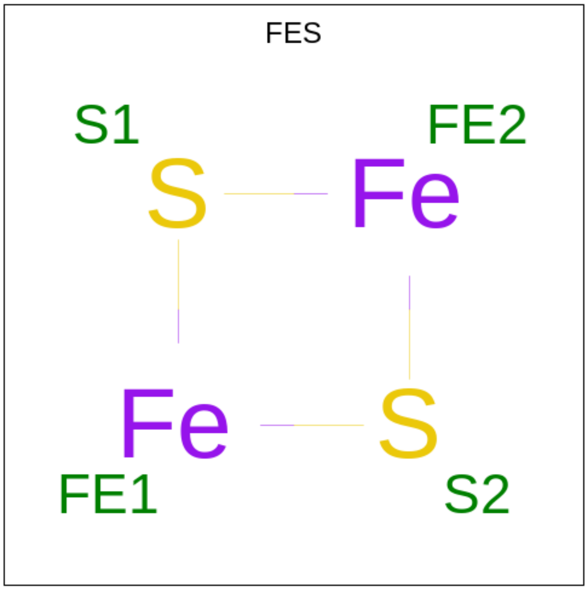
Mol	Chain	Residues	Atoms	AltConf
63	b	1	Total C O P 62 43 17 2	0
63	e	1	Total C O P 132 94 34 4	0
63	e	1	Total C O P 132 94 34 4	0
63	f	1	Total C O P 100 81 17 2	0
63	j	1	Total C O P 70 51 17 2	0
63	k	1	Total C O P 62 43 17 2	0
63	l	1	Total C O P 74 55 17 2	0
63	n	1	Total C O P 95 76 17 2	0
63	t	1	Total C O P 143 105 34 4	0
63	t	1	Total C O P 143 105 34 4	0
63	u	1	Total C O P 82 63 17 2	0
63	v	1	Total C O P 91 72 17 2	0

- 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 1 1	0
64	M	1	Total Zn 1 1	0
64	5b	1	Total Zn 1 1	0
64	m	1	Total Zn 1 1	0

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

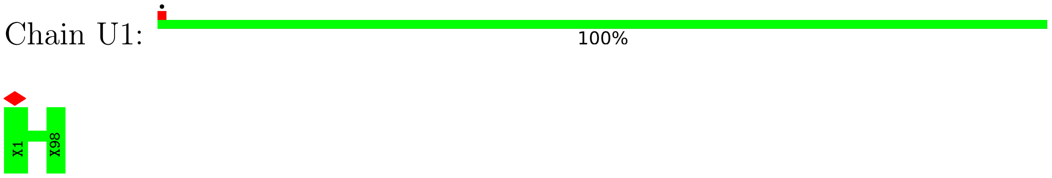


Mol	Chain	Residues	Atoms	AltConf
65	FS	1	Total Fe S 8 4 4	0
65	FS	1	Total Fe S 8 4 4	0
65	fs	1	Total Fe S 8 4 4	0
65	fs	1	Total Fe S 8 4 4	0

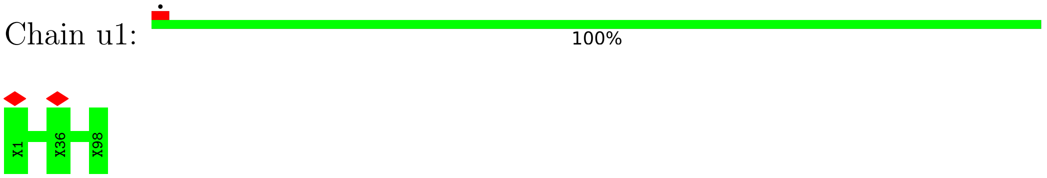
3 Residue-property plots ⓘ

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

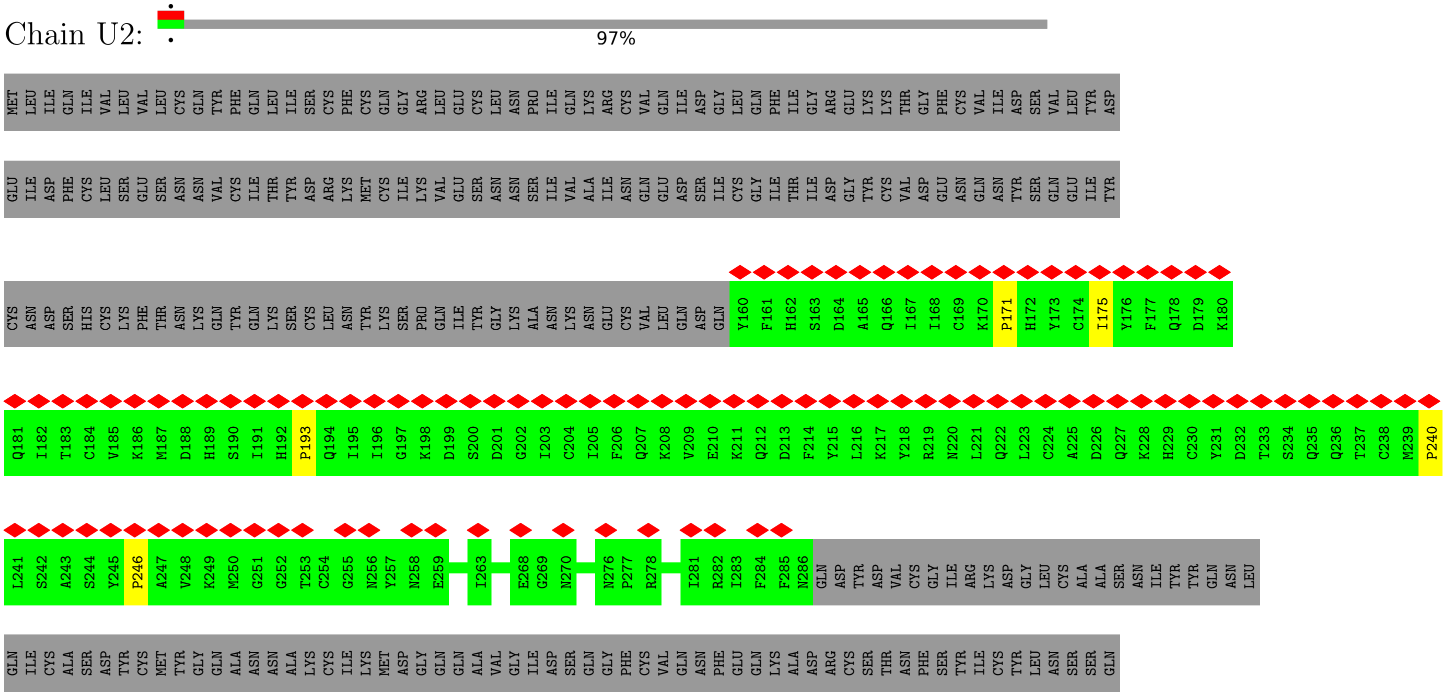
- Molecule 1: Unknown peptide



- Molecule 1: Unknown peptide



- Molecule 2: Transmembrane protein, putative



ILE CYS ILE ASN LEU GLN GLY TYR GLN ASN TYR CYS GLN GLN ALA ASN LYS CYS TYR GLU PHE SER LEU GLN GLN TYR ILE GLY ARG ASP ILE TYR TYR TYR CYS ILE GLN SER GLU GLN SER LEU GLN PRO GLN ASN VAL GLN ASN CYS LEU GLN ASN PRO SER TYR ILE CYS GLN LYS

ARG ASP GLY THR MET CYS VAL TYR TYR TYR GLN ILE PRO THR TYR PHE THR TYR LEU GLY TYR ILE ASN SER SER GLY TYR CYS ALA GLN GLU GLY TYR GLN THR TYR THR SER GLN PRO GLN PHE GLN THR ILE THR ASN LEU ASN PRO ASN PHE CYS GLN ASP ASP SER TYR VAL ILE

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

CYS GLY LEU VAL GLN GLN SER SER ALA ILE GLU CYS ALA TYR ASP GLN ASP TYR CYS ILE TYR ASN SER ILE CYS TYR ASN LEU SER ASP GLN ASN ILE GLN THR SER GLY ILE ASP TYR TYR GLY ASN CYS LEU GLN ARG GLY LYS TYR TYR GLN ASN TRP LYS LYS CYS SER VAL ASN

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

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

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

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

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

ASN ASN PRO SER GLN GLN GLY CYS PHE GLU LEU ASP GLY ASP ILE ASN ARG ALA GLY ILE ASP SER LYS GLY ASN CYS LEU GLN GLN ASP LEU PRO ASN ALA VAL ARG CYS SER PRO GLY GLN PHE CYS LEU ASN ASP LYS PHE GLY ASN ALA CYS GLN SER LEU LEU LEU SER PHE LYS

ASN ASN ARG PHE ALA ARG GLN LYS GLY THR GLY VAL CYS LEU SER TYR ILE ASP PRO SER GLN PHE LYS GLY ASP ASN ILE ASP ILE CYS VAL LYS GLY SER CYS LYS TYR SER ASP PRO LYS ASN LEU ASP PHE CYS PHE SER LEU GLY GLN LEU ALA PHE GLY ASN GLN VAL VAL GLY

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

THR CYS GLN ASP ILE ASN MET PRO ASN SER MET GLY CYS LEU TYR GLY LEU TYR CYS ILE ASN PRO ASN ASP GLY TYR LYS CYS VAL LEU MET ASN ASP ASP ASN LYS ILE GLY ARG SER LEU VAL ASN GLN GLN CYS LEU GLN GLN GLY GLU LEU ILE ALA ASN TYR CYS GLN PRO ASP

PHE CYS ILE LEU ASN GLY ALA CYS VAL PRO LEU SER ASN LYS PHE PRO GLY LYS GLU ASN GLN THR GLN LYS CYS LEU PRO GLU GLN ILE GLU GLY GLN TYR GLY ALA SER ASN CYS TYR LYS GLU GLY PHE CYS LEU ILE ILE ASN PRO GLN ASN GLN LEU ALA SER CYS TYR GLN LEU

ASP TYR SER ASN PRO ASN THR ILE GLY ILE GLN ILE ASP THR GLN HIS CYS LEU LYS GLU GLY GLU THR VAL ALA ILE MET CYS ALA TYR GLU LYS TYR CYS ILE ASP PRO VAL SER GLN SER CYS LYS ILE GLN ASP ILE LYS GLN GLY TYR CYS LEU GLY LYS ASN GLY MET CYS ALA

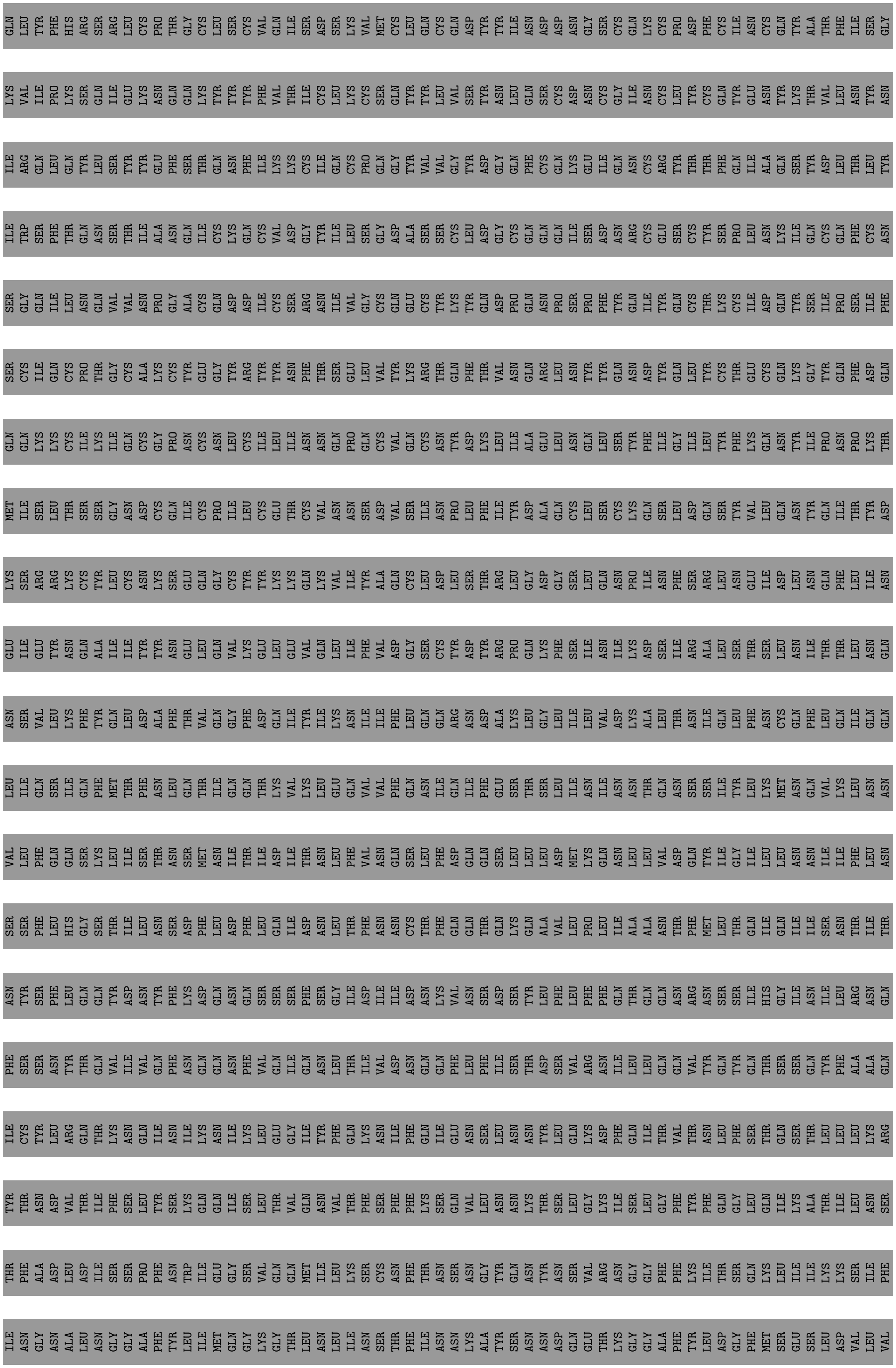
LYS ASN GLY SER CYS VAL TYR CYS GLN VAL SER GLN CYS LEU THR ASN GLN ASN SER GLY THR CYS ILE ASP LEU GLN GLN PRO PRO ALA LEU PHE CYS LYS ASP ILE ASN VAL HIS SER GLU ASN ILE PHE ILE GLN ASN GLN LYS GLY ILE CYS GLN TYR LEU ASN SER GLY GLN CYS

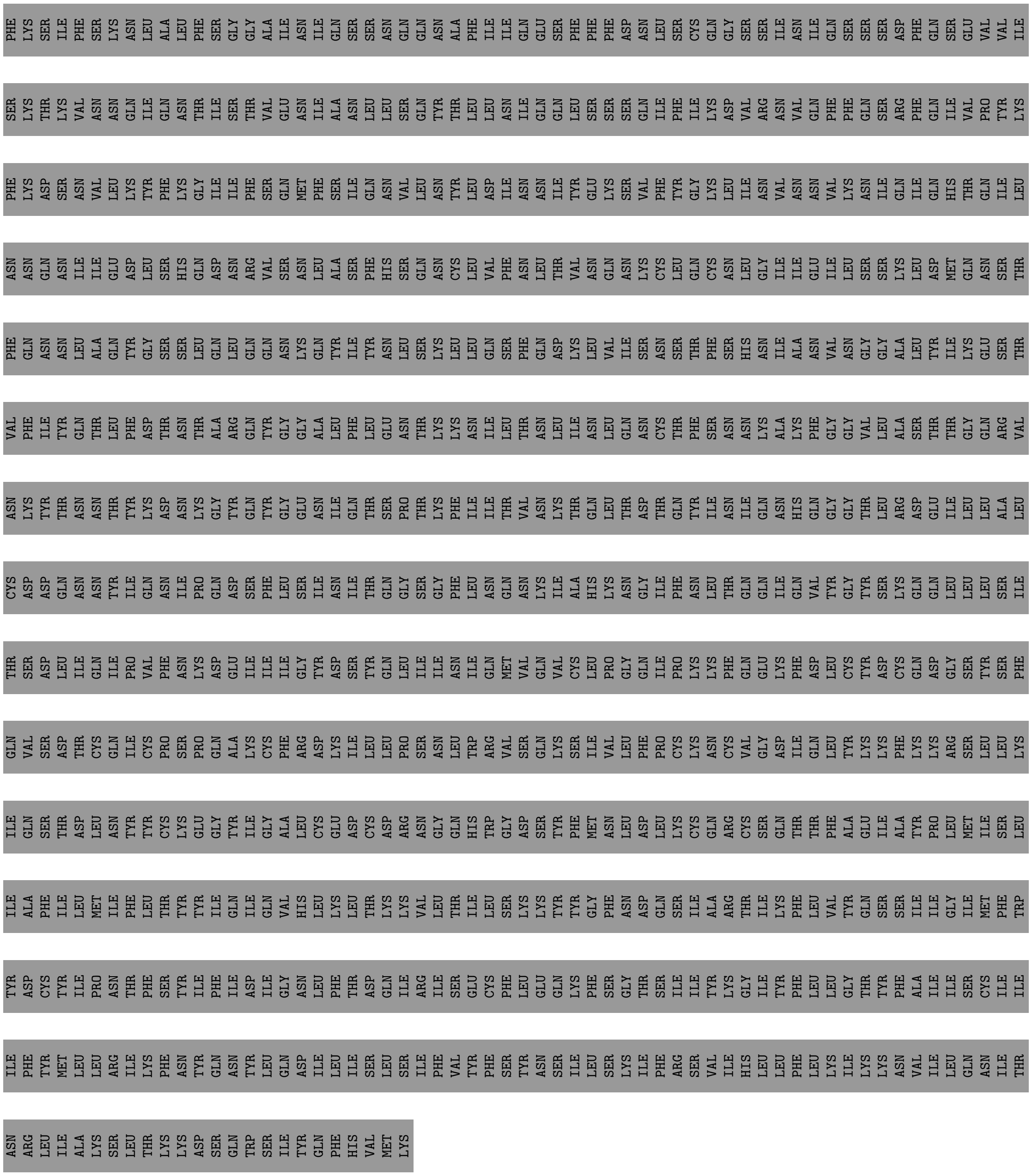
ASP ILE CYS PRO GLU ASN TYR CYS LYS PHE ASN ASN MET CYS PHE GLY SER GLN ASP LEU LEU LYS ILE LEU LYS GLY ASN GLN CYS PHE VAL TYR VAL PRO LYS LEU LYS THR CYS GLN ILE GLN ASP LEU ASN THR PRO ASN SER GLN GLY ASN MET ASN CYS MET ASN ASN LYS GLY

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

GLN SER ILE PRO SER LEU LYS CYS PRO LYS GLY CYS PHE SER CYS ASN SER PRO ASN PHE CYS THR GLN CYS ILE GLU GLY PHE PHE LEU TYR GLN ASP THR SER ASN GLN GLN PHE CYS ILE GLN CYS GLN LYS GLN ILE ILE GLN ASP ASN THR LEU LYS ILE TYR TYR ASN GLN ILE

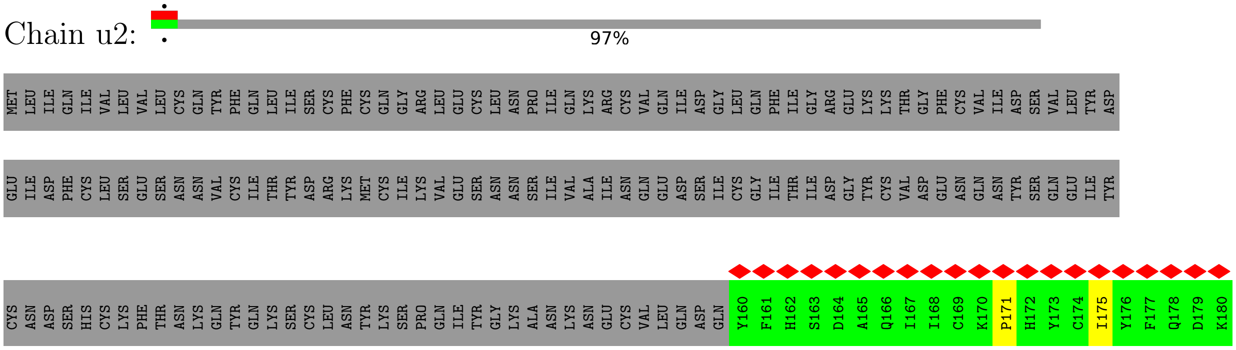
PRO THR TYR SER CYS LEU ASP CYS SER SER GLU TYR GLY THR TRP ASN GLN ILE SER SER LYS TYR ARG ASN CYS GLN ASN PHE ILE VAL LYS LEU ASP ASN LEU LEU GLN ILE THR SER GLN LYS TYR ALA ALA GLN ASN TYR ILE ILE SER PRO ILE SER THR THR GLN ALA PRO TYR

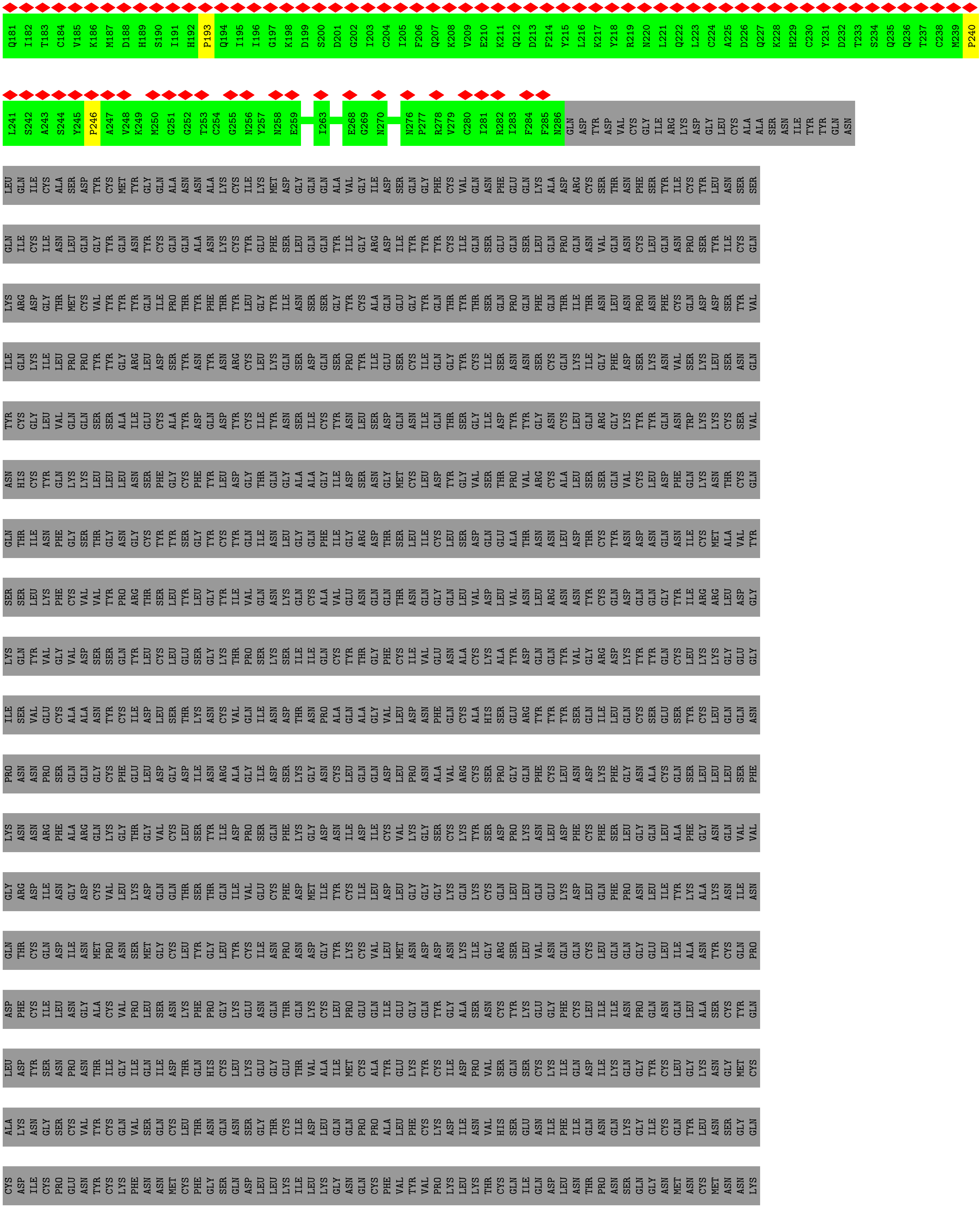

GLN LEU TYR PHE HIS ARG SER ARG LEU CYS PRO THR GLY CYS LEU SER CYS VAL GLN ILE SER ASP SER LYS VAL MET CYS LEU GLN CYS GLN ASP TYR TYR ILE ASN ASP ASP ASN GLY SER CYS GLN LYS CYS PRO ASP PHE CYS ILE ASN CYS GLN TYR ALA THR PHE ILE SER GLY
LYS VAL ILE PRO LYS SER GLN ILE GLU LYS ASN GLN GLN LYS TYR TYR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



- Molecule 2: Transmembrane protein, putative

Chain u2:





Q181 I182 T183 C184 V185 K186 M187 D188 H189 S190 I191 H192 P193 Q194 I195 I196 G197 K198 D199 S200 D201 G202 I203 C204 I205 F206 Q207 K208 V209 E210 K211 Q212 D213 F214 Y215 L216 K217 Y218 R219 N220 L221 Q222 L223 C224 A225 D226 Q227 K228 H229 C230 Y231 D232 T233 S234 Q235 Q236 T237 C238 M239 P240

L241 S242 A243 S244 Y245 P246 A247 V248 K249 M250 G251 G252 T253 C254 G255 N256 Y257 N258 E259 I263 E268 G269 N270 N276 P277 R278 V279 C280 I281 R282 I283 F284 F285 N286 GLN ASP TYR ASP VAL CYS GLY ILE ARG LYS ASP GLY LEU CYS ALA ALA SER ASN ILE TYR TYR GLN ASN

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

GLN ILE CYS ILE ASN LEU GLN GLY TYR GLN ASN TYR CYS GLN GLN ALA ASN LYS CYS TYR GLU PHE SER LEU GLN GLN TYR ILE GLY ARG ASP ILE TYR TYR TYR CYS ILE GLN SER GLU GLN SER LEU GLN PRO GLN ASN VAL GLN ASN CYS LEU GLN ASN PRO SER TYR ILE CYS GLN

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

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

TYR CYS GLY LEU VAL GLN GLN SER SER ALA ILE GLU CYS ALA TYR ASP GLN ASP TYR CYS ILE TYR ASN SER ILE CYS TYR ASN LEU SER ASP GLN ASN ILE GLN THR SER GLY ILE ASP TYR TYR GLY ASN CYS LEU GLN ARG GLY LYS TYR TYR GLN ASN TRP LYS LYS CYS SER VAL

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

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

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

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

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

PRO ASN ASN PRO SER GLN GLN GLY CYS PHE GLU LEU ASP GLY ASP ILE ASN ARG ALA GLY ILE ASP SER LYS GLY ASN CYS LEU GLN GLN ASP LEU PRO ASN ALA VAL ARG CYS SER PRO GLY GLN PHE CYS LEU ASN ASP LYS PHE GLY ASN ALA CYS GLN SER LEU LEU LEU SER PHE

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

GLN THR CYS GLN ASP ILE ASN MET PRO ASN SER MET GLY CYS LEU TYR GLY LEU TYR CYS ILE ASN PRO ASN ASP GLY TYR LYS CYS VAL LEU MET ASN ASP ASP ASN LYS ILE GLY ARG SER LEU VAL ASN GLN GLN CYS LEU GLN GLN GLY GLU LEU ILE ALA ASN TYR CYS GLN PRO

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

LEU ASP TYR SER ASN PRO ASN THR ILE GLY ILE GLN ILE ASP THR GLN HIS CYS LEU LYS GLU GLY GLU THR VAL ALA ILE MET CYS ALA TYR GLU LYS TYR CYS ILE ASP PRO VAL SER GLN SER CYS LYS ILE GLN ASP ILE LYS GLN GLY TYR CYS LEU GLY LYS ASN GLY MET CYS

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

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

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

CYS GLN SER ILE PRO SER LEU LYS CYS PRO LYS GLY CYS PHE SER CYS ASN SER PRO ASN PHE CYS THR GLN CYS ILE GLU GLY PHE PHE LEU TYR GLN ASP THR SER ASN GLN GLN PHE CYS ILE GLN CYS GLN LYS GLN ILE ILE GLN ASP ASN THR LEU LYS ILE TYR TYR ASN GLN

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

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

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

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

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

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

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

GLN GLN GLN LYS LYS CYS ILE LYS ILE GLN CYS GLY PRO ASN CYS ASN LEU CYS ILE LEU ILE ASN ASN GLN PRO GLN CYS VAL GLN CYS ASN TYR ASP LYS LEU ILE ALA GLU LEU ASN GLN LEU SER TYR PHE ILE GLY ILE LEU TYR PHE LYS GLN ASN TYR ILE PRO ASN PRO LYS

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

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

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

GLN ASN SER VAL LEU LYS PHE TYR GLN LEU ASP ALA PHE THR VAL GLN GLY PHE ASP GLN ILE TYR ILE LYS ASN ILE ILE PHE LEU GLN GLN ARG ASN ASP ALA LYS LEU GLY LEU ILE LEU VAL ASP LYS ALA LEU THR ASN ILE GLN LEU PHE ASN CYS GLN PHE LEU GLN ILE GLN

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

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

ASN SER SER PHE LEU HIS GLY SER THR ILE LEU ASN SER ASP PHE LEU ASP PHE LEU GLN ILE ASP ASN LEU THR PHE ASN ASN CYS THR PHE GLN GLN THR GLN LYS GLN ALA VAL LEU PRO LEU ILE ALA ALA ASN THR PHE MET LEU THR GLN ILE GLN ILE ILE SER ASN THR ILE

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

GLN PHE SER SER ASN TYR THR GLN VAL ILE VAL GLN PHE ASN GLN GLN ASN PHE VAL GLN ILE GLN ASN LEU THR ILE VAL ASP ASN GLN GLN PHE LEU PHE ILE SER THR ASP SER VAL ARG ASN ILE LEU LEU GLN GLN VAL TYR GLN TYR GLN THR SER SER GLN TYR PHE ALA ALA

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

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

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

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

VAL PHE LYS SER ILE PHE SER LYS ASN LEU ALA LEU PHE SER GLY GLY ALA ILE ASN ILE GLN SER SER ASN GLN GLN ASN ALA PHE ILE ILE GLN GLU SER PHE PHE ASP ASN LEU SER CYS GLN GLY SER SER ILE ASN ILE GLN SER SER SER ASP PHE GLN SER GLU VAL VAL

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

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

LEU ASN ASN GLN ASN ILE ILE GLU ASP LEU SER HIS GLN ASP ASN ARG VAL SER ASN LEU ALA SER PHE HIS SER GLN ASN CYS LEU VAL PHE ASN LEU THR VAL ASN GLN ASN LYS CYS LEU GLN CYS ASN LEU GLY ILE ILE GLU ILE LEU SER SER LYS LEU ASP MET GLN ASN SER

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

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

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

LEU CYS ASP ASP GLN ASN ASN TYR ILE GLN ASN ILE PRO GLN ASP SER PHE LEU SER ILE ASN ILE THR GLN GLY SER GLY PHE LEU ASN GLN ASN LYS ILE ALA HIS LYS ASN GLY ILE PHE ASN LEU THR GLN GLN ILE GLN VAL TYR GLY TYR SER LYS GLN GLN LEU LEU LEU SER

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

PHE GLN VAL SER ASP THR CYS GLN ILE CYS PRO SER PRO GLN ALA LYS CYS PHE ARG ASP LYS ILE LEU LEU PRO SER ASN LEU TRP ARG VAL SER GLN LYS SER ILE VAL LEU PHE PRO CYS LYS ASN CYS VAL GLY ASP ILE GLN LEU TYR LYS LYS PHE LYS LYS ARG SER LEU LEU

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

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

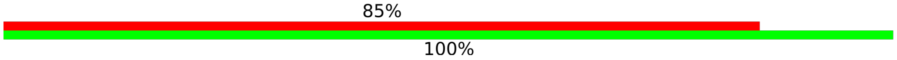
TRP TYR ASP CYS TYR ILE PRO ASN THR PHE SER TYR ILE PHE ILE ASP ILE GLY ASN LEU PHE THR ASP GLN ILE ARG ILE SER GLU CYS PHE LEU GLU GLN LYS PHE SER GLY THR SER ILE ILE TYR LYS GLY ILE TYR PHE LEU LEU GLY THR TYR PHE ALA ILE ILE SER CYS ILE

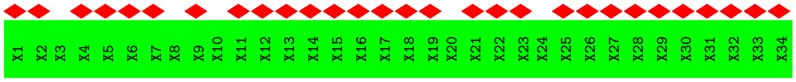
ILE ILE PHE TYR MET LEU LEU ARG ILE LYS PHE ASN TYR GLN ASN TYR LEU GLN ASP ILE LEU ILE SER LEU SER ILE PHE VAL TYR PHE SER TYR ASN SER ILE LEU SER LYS ILE PHE ARG SER VAL ILE HIS LEU LEU PHE LEU LYS ILE LYS LYS ASN VAL ILE LEU GLN ASN ILE

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

- Molecule 3: Unknown peptide

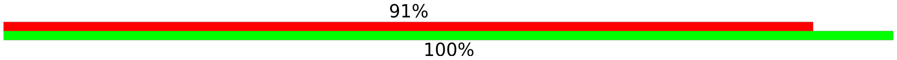
Chain U3:

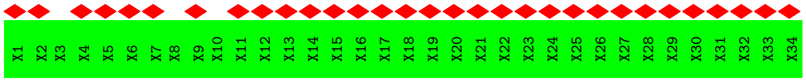




- Molecule 3: Unknown peptide

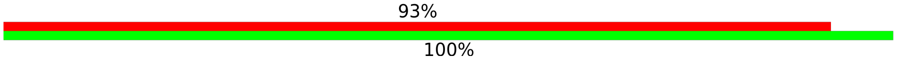
Chain u3:

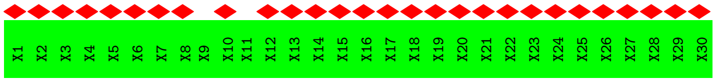




- Molecule 4: Unknown peptide

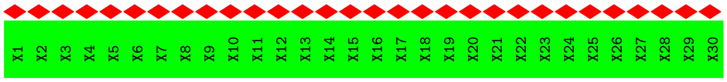
Chain U4:





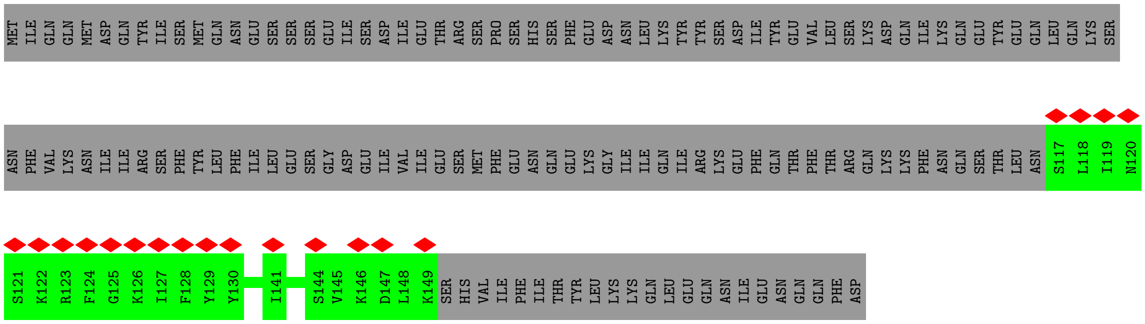
- Molecule 4: Unknown peptide

Chain u4:



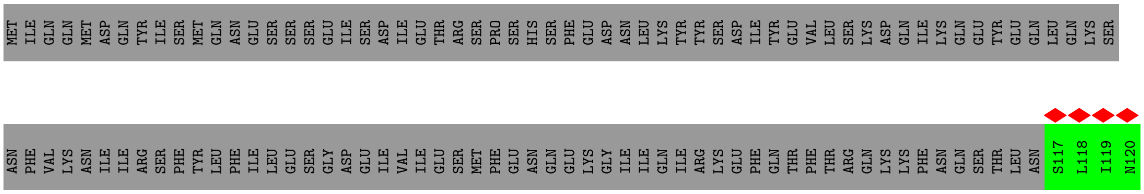
- Molecule 5: Uncharacterized protein

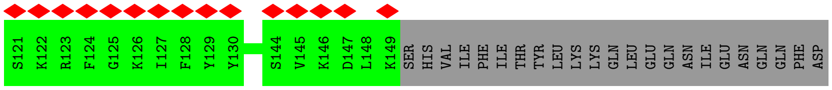
Chain U5:



- Molecule 5: Uncharacterized protein

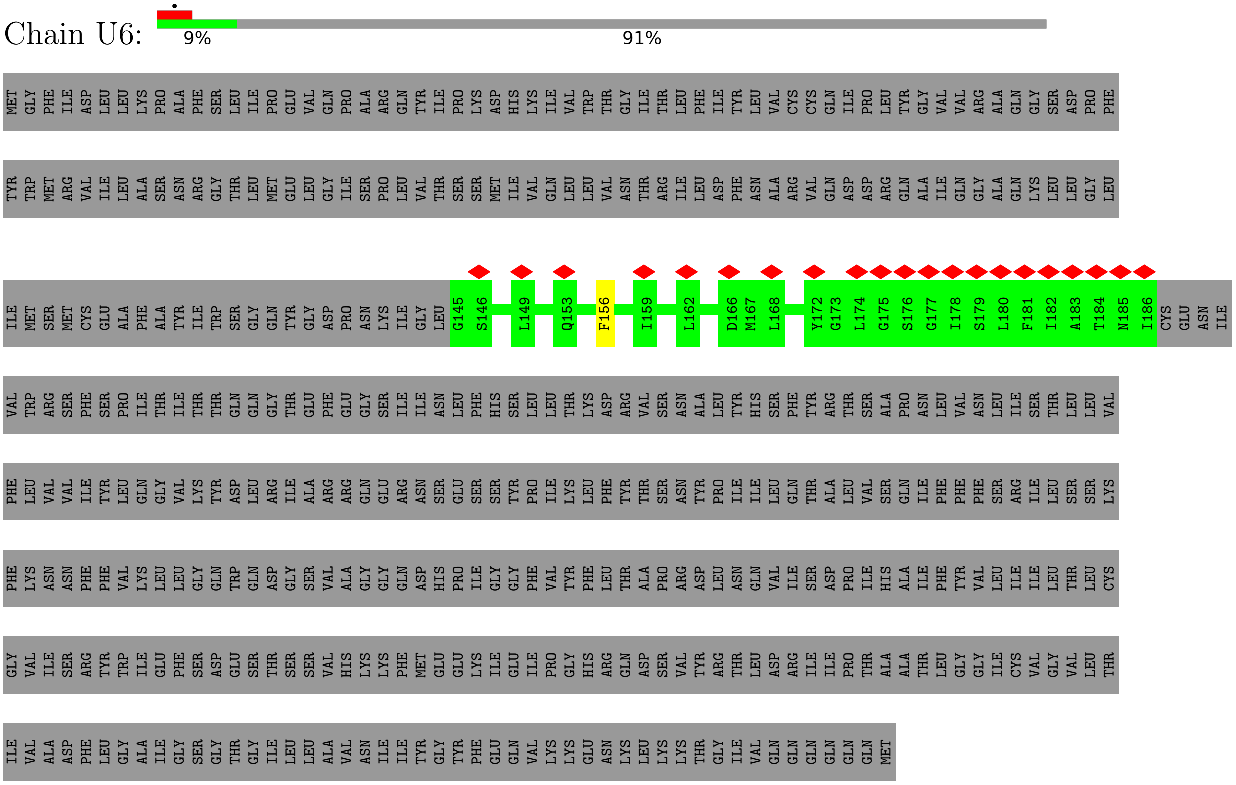
Chain u5:





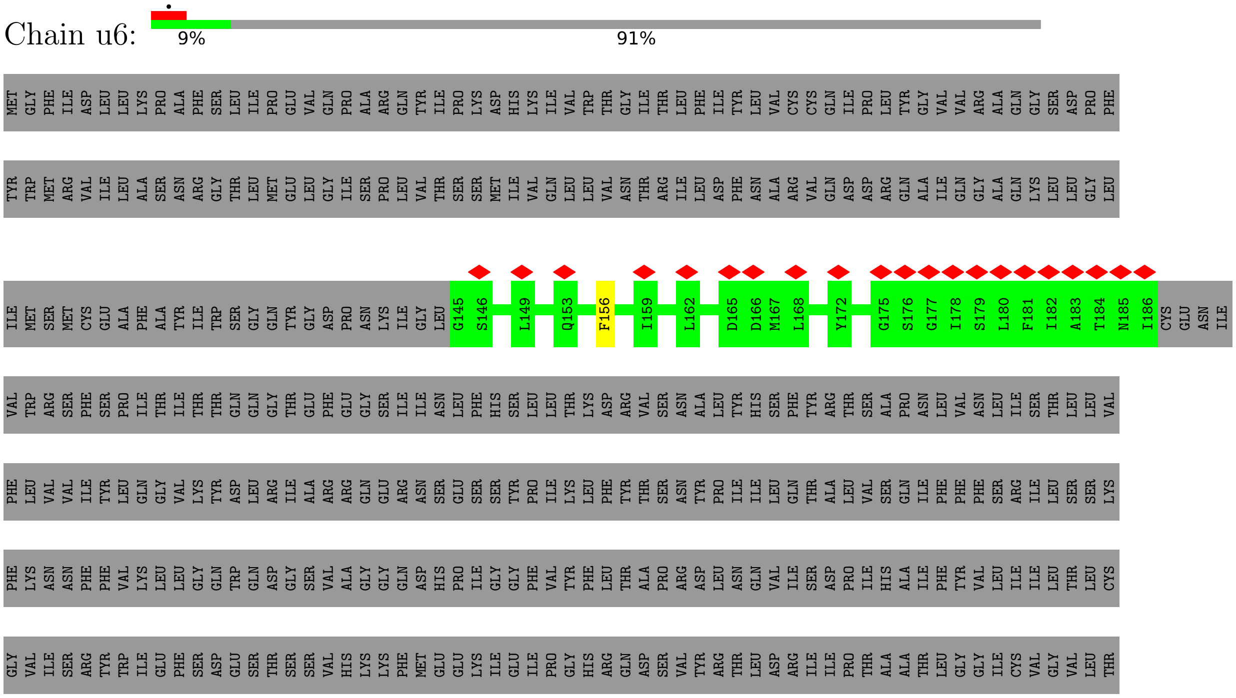
- Molecule 6: Protein transporter Sec61 alpha subunit

Chain U6:



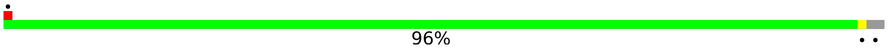
- Molecule 6: Protein transporter Sec61 alpha subunit

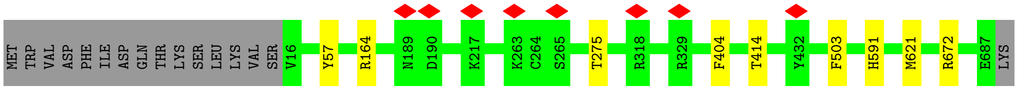
Chain u6:



- Molecule 7: Cytochrome c oxidase subunit 1

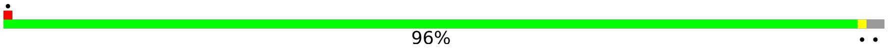
Chain C1:

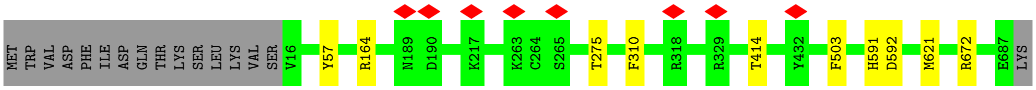




- Molecule 7: Cytochrome c oxidase subunit 1

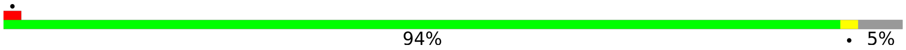
Chain c1:

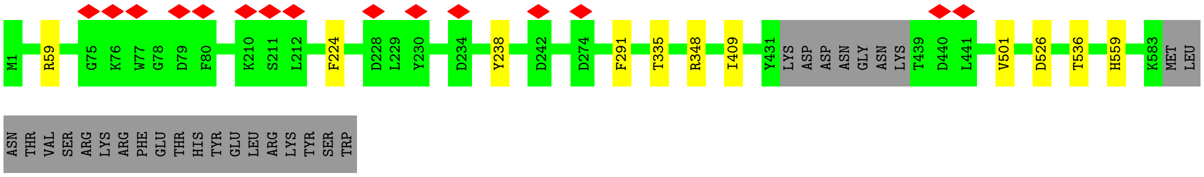




- Molecule 8: Cytochrome c oxidase subunit 2

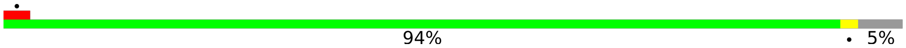
Chain C2:

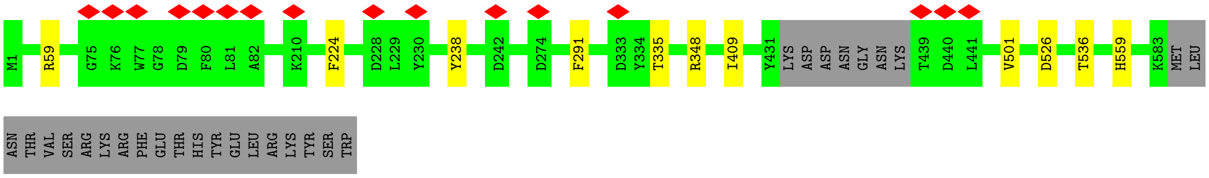




- Molecule 8: Cytochrome c oxidase subunit 2

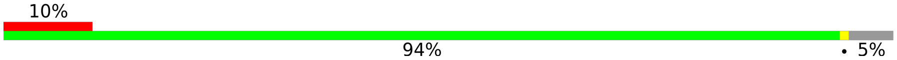
Chain c2:

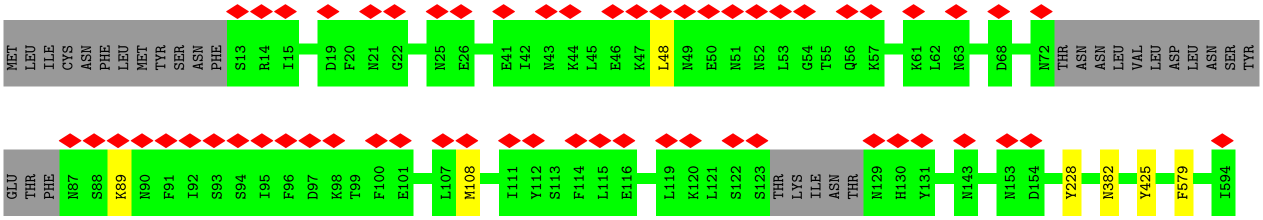




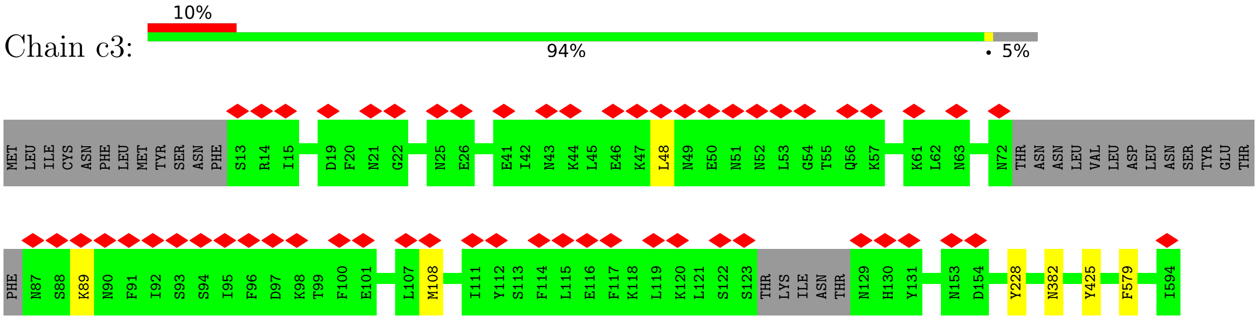
- Molecule 9: Ymf68

Chain C3:

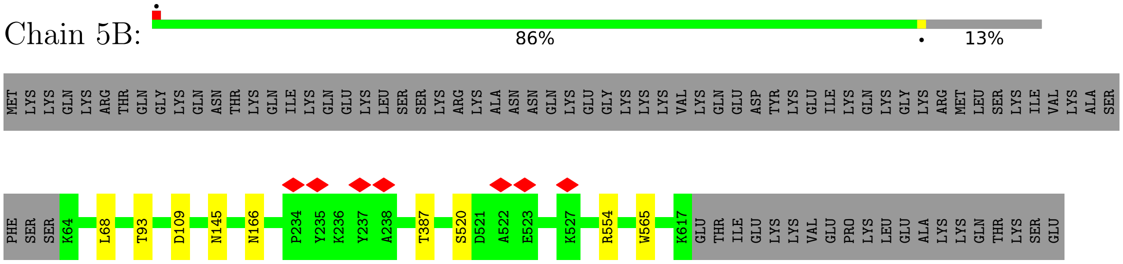




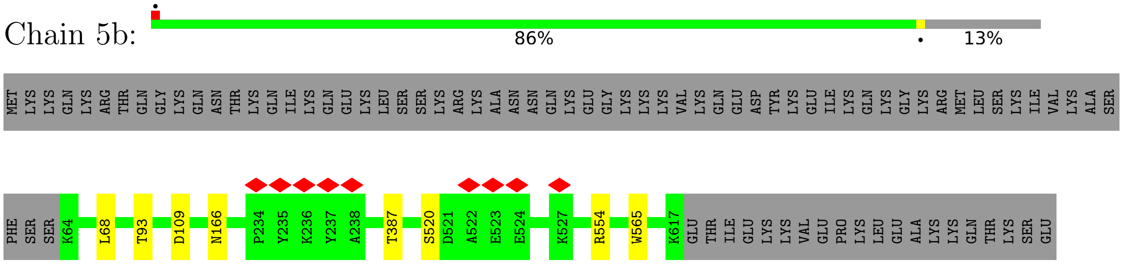
- Molecule 9: Ymf68



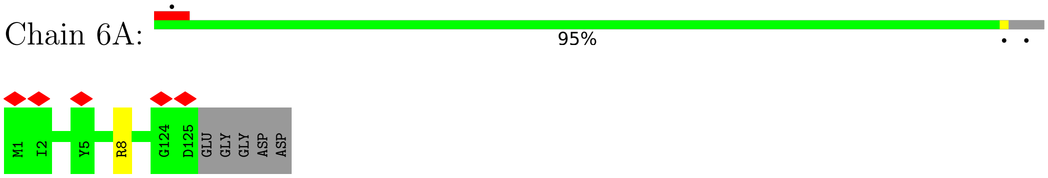
- Molecule 10: Cytochrome C oxidase subunit Vb protein



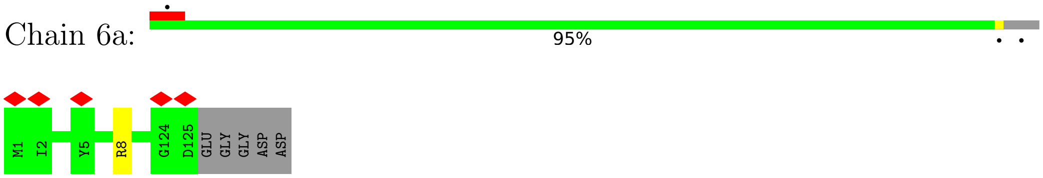
- Molecule 10: Cytochrome C oxidase subunit Vb protein



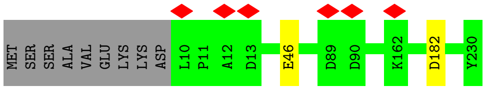
- Molecule 11: Transmembrane protein, putative



- Molecule 11: Transmembrane protein, putative

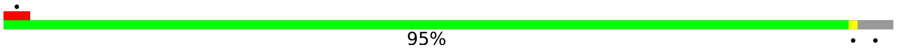


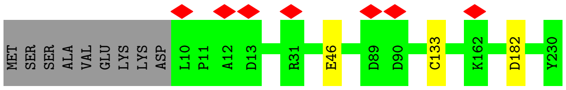
- Molecule 12: Cytochrome c oxidase subunit 6B



- Molecule 12: Cytochrome c oxidase subunit 6B

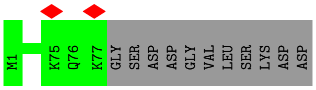
Chain 6b:





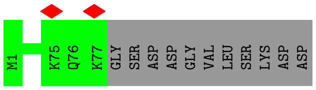
- Molecule 13: Cytochrome c oxidase subunit 6B-like

Chain 6L:



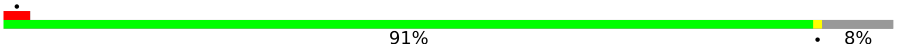
- Molecule 13: Cytochrome c oxidase subunit 6B-like

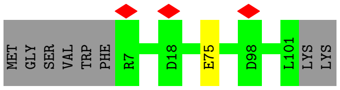
Chain 6l:



- Molecule 14: Transmembrane protein, putative

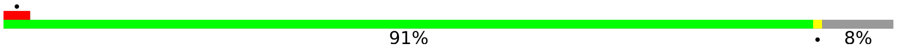
Chain 6C:

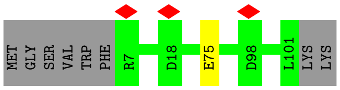




- Molecule 14: Transmembrane protein, putative

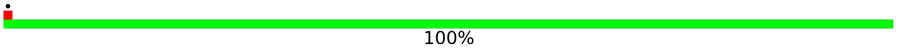
Chain 6c:

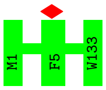




- Molecule 15: Transmembrane protein, putative

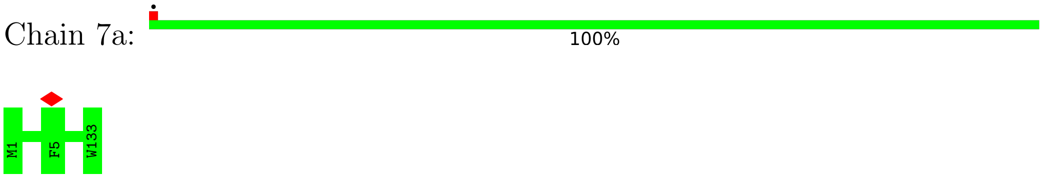
Chain 7A:





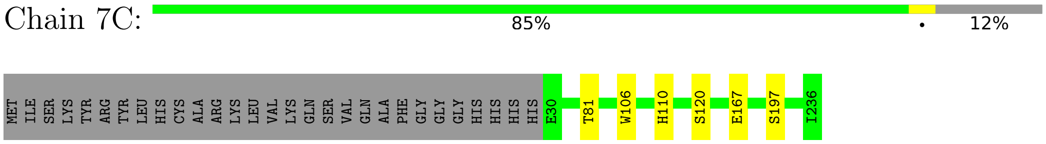
- Molecule 15: Transmembrane protein, putative

Chain 7a:



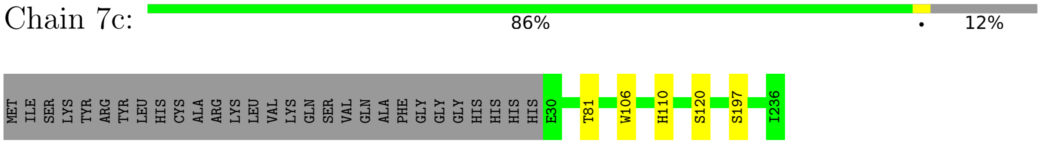
- Molecule 16: Cytochrome c oxidase subunit 7C

Chain 7C:



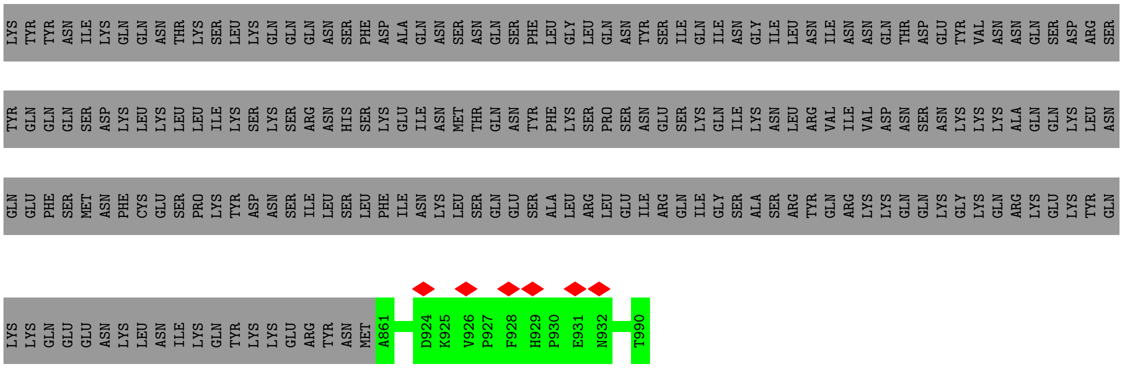
- Molecule 16: Cytochrome c oxidase subunit 7C

Chain 7c:

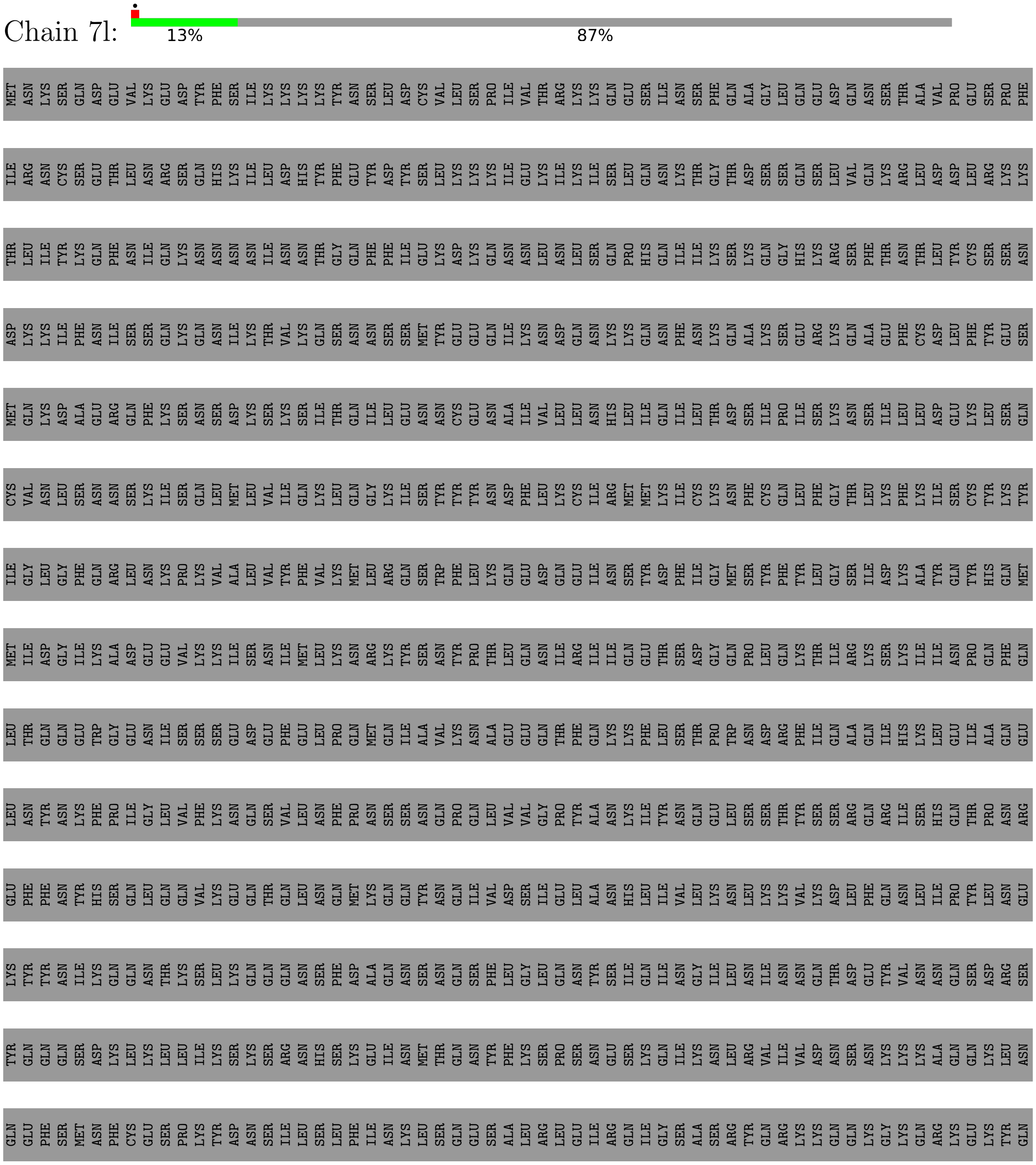


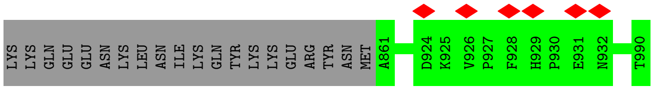
- Molecule 17: CTF/NF-I domain-containing protein

Chain 7L:



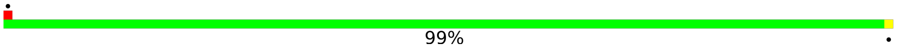
- Molecule 17: CTF/NF-I domain-containing protein

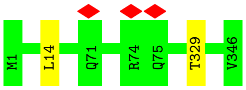




- Molecule 18: Oxoglutarate/malate translocator protein, putative

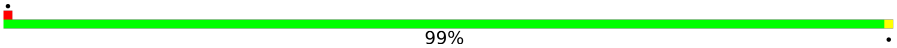
Chain M1:

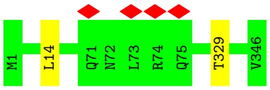




- Molecule 18: Oxoglutarate/malate translocator protein, putative

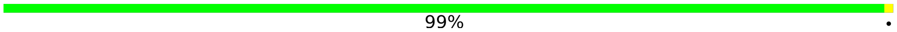
Chain m1:

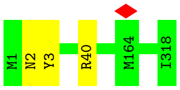




- Molecule 19: 2-oxoglutarate/malate carrier protein

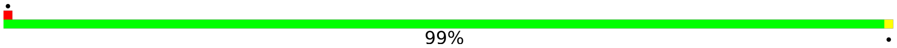
Chain M2:

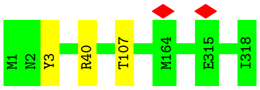




- Molecule 19: 2-oxoglutarate/malate carrier protein

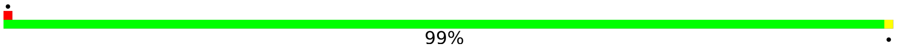
Chain m2:

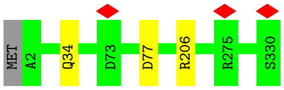




- Molecule 20: Carrier protein

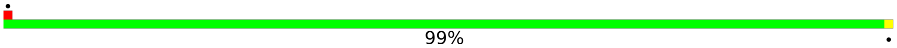
Chain M3:

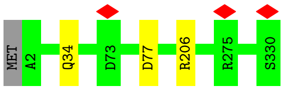




- Molecule 20: Carrier protein

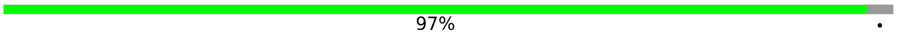
Chain m3:

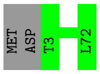




- Molecule 21: Tim10/DDP family zinc finger protein

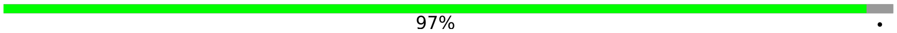
Chain T1:

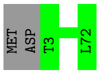




- Molecule 21: Tim10/DDP family zinc finger protein

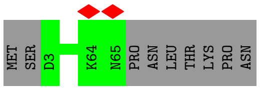
Chain t1:





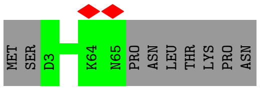
- Molecule 22: Cytochrome c oxidase small TIM subunit 2

Chain T2:



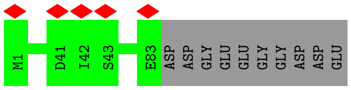
- Molecule 22: Cytochrome c oxidase small TIM subunit 2

Chain t2:



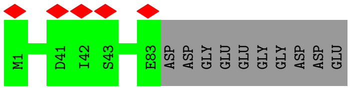
- Molecule 23: Cytochrome c oxidase small TIM subunit 3

Chain T3:



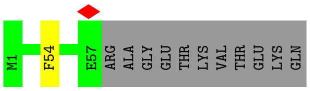
- Molecule 23: Cytochrome c oxidase small TIM subunit 3

Chain t3:



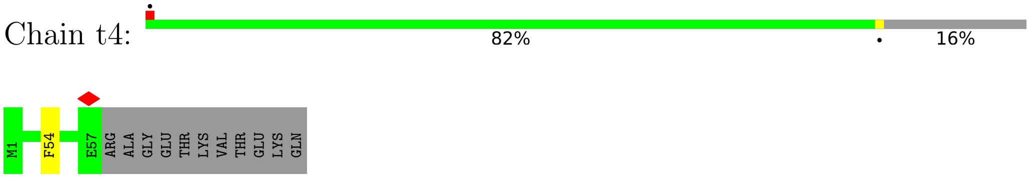
- Molecule 24: Cytochrome c oxidase small TIM subunit 4

Chain T4:



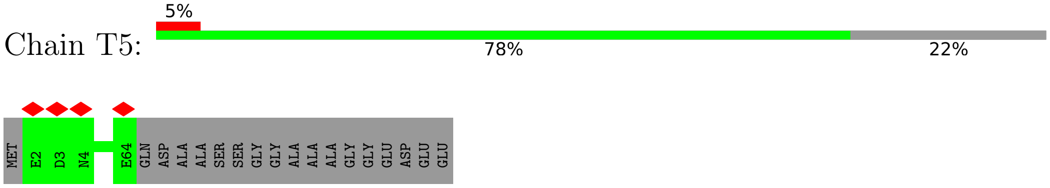
- Molecule 24: Cytochrome c oxidase small TIM subunit 4

Chain t4:



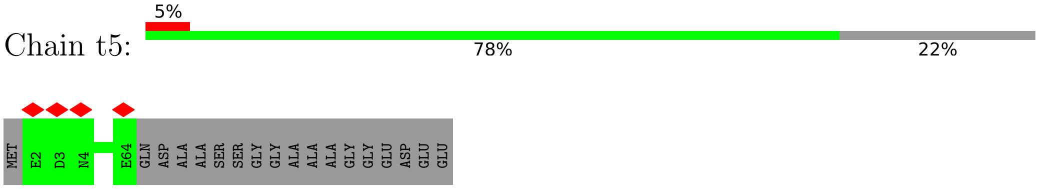
- Molecule 25: Cytochrome c oxidase small TIM subunit 5

Chain T5:



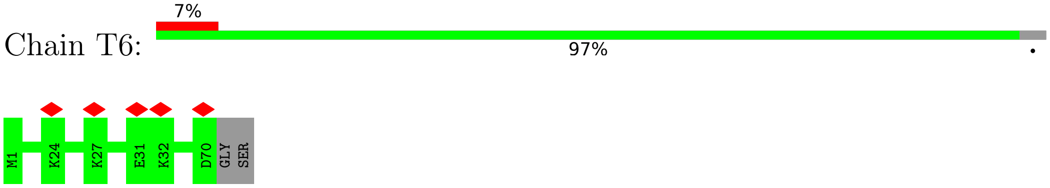
- Molecule 25: Cytochrome c oxidase small TIM subunit 5

Chain t5:



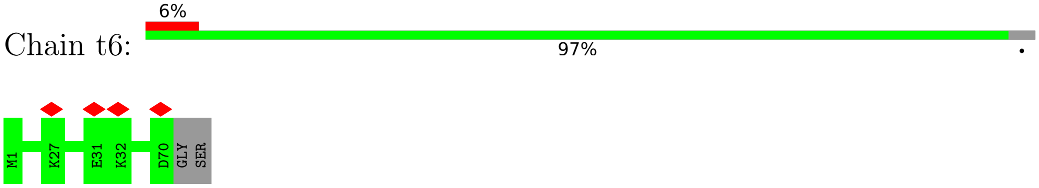
- Molecule 26: Cytochrome c oxidase small TIM subunit 6

Chain T6:



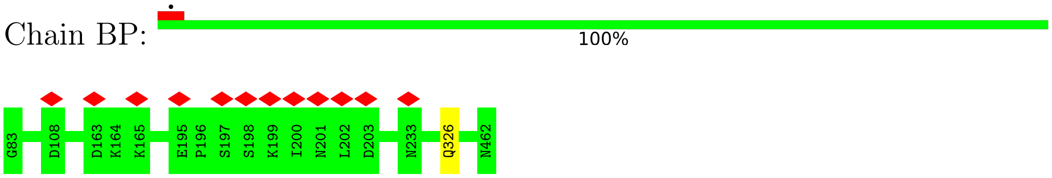
- Molecule 26: Cytochrome c oxidase small TIM subunit 6

Chain t6:



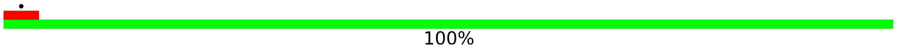
- Molecule 27: Chromosome condensation regulator RCC1 repeat protein

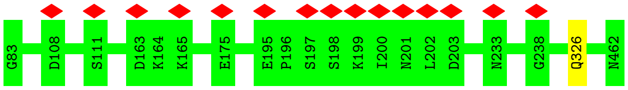
Chain BP:



- Molecule 27: Chromosome condensation regulator RCC1 repeat protein

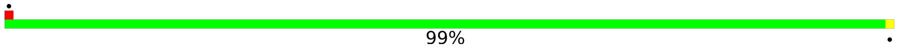
Chain bp:

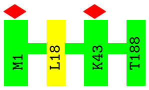




- Molecule 28: Iron-binding zinc finger CDGSH type protein

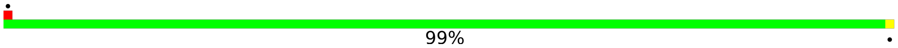
Chain FS:

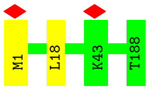




- Molecule 28: Iron-binding zinc finger CDGSH type protein

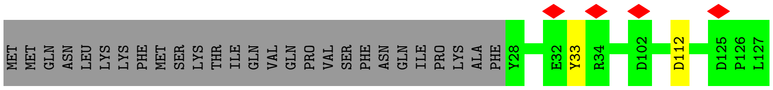
Chain fs:





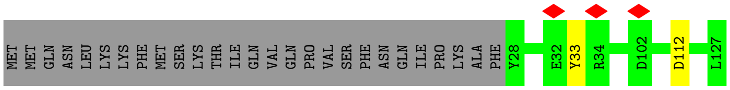
- Molecule 29: Cytochrome c oxidase acyl carrier-like subunit

Chain AC:



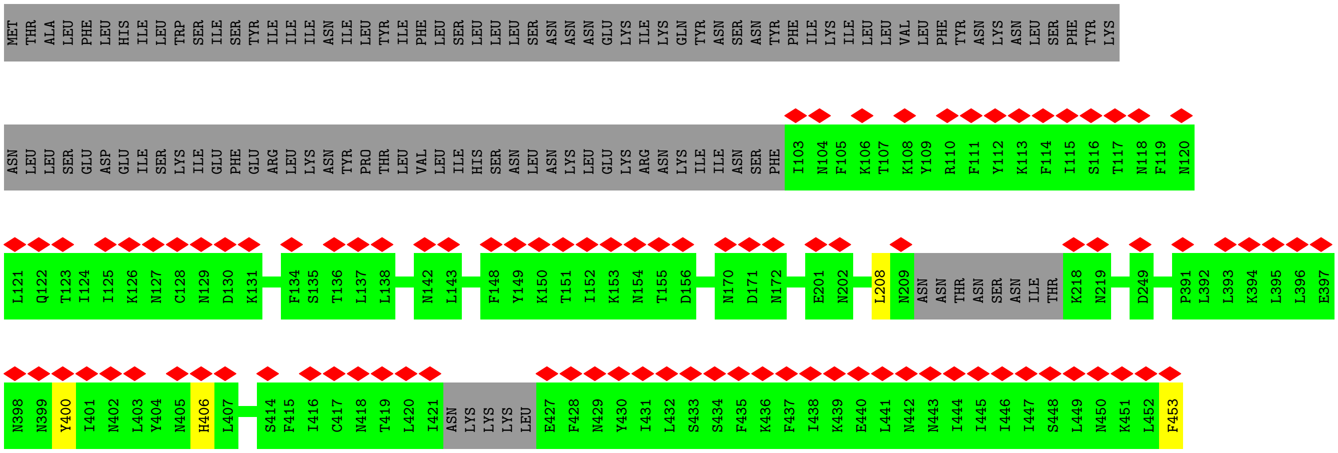
- Molecule 29: Cytochrome c oxidase acyl carrier-like subunit

Chain ac:



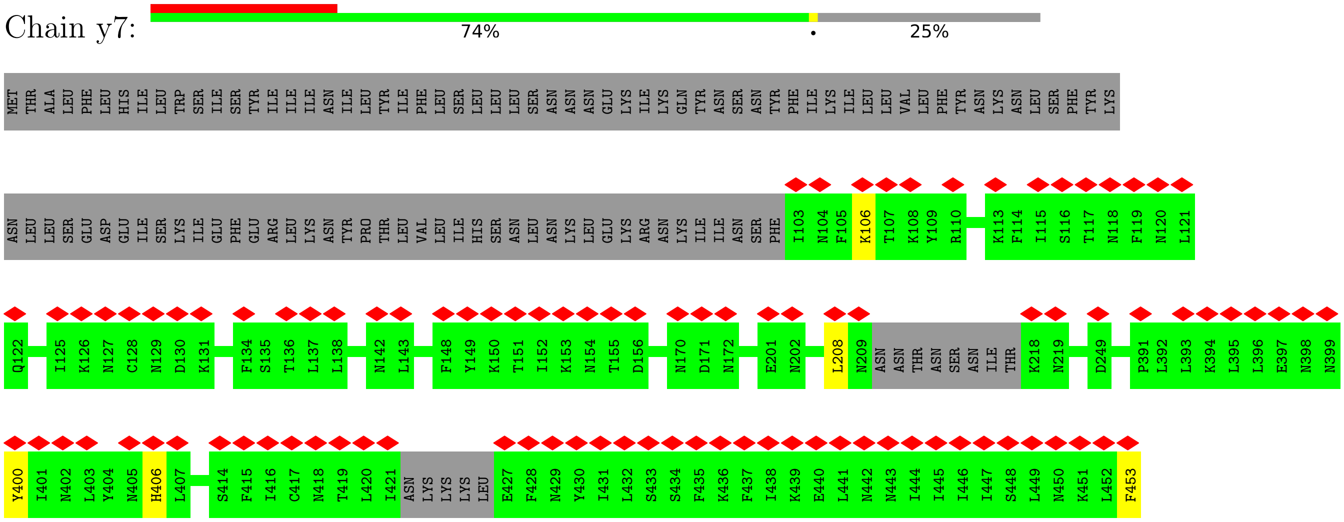
- Molecule 30: Ymf67

Chain Y7:



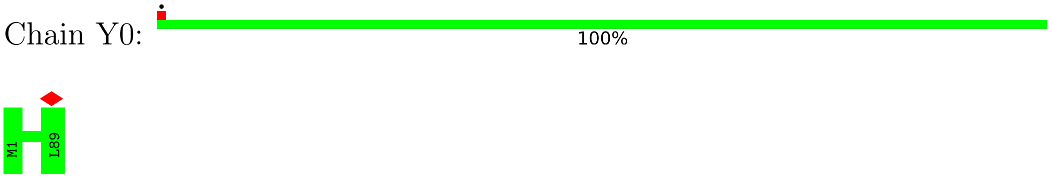
- Molecule 30: Ymf67

Chain y7:



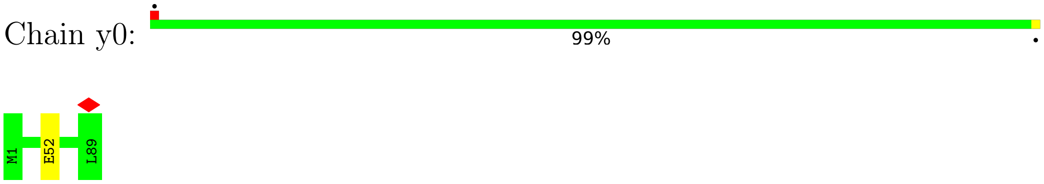
- Molecule 31: Ymf70

Chain Y0:



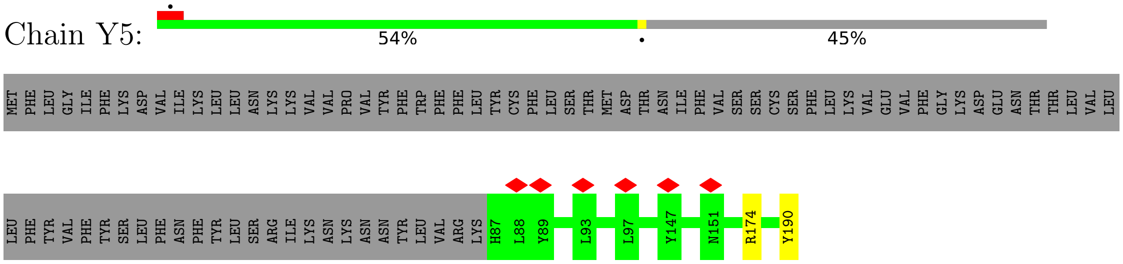
- Molecule 31: Ymf70

Chain y0:



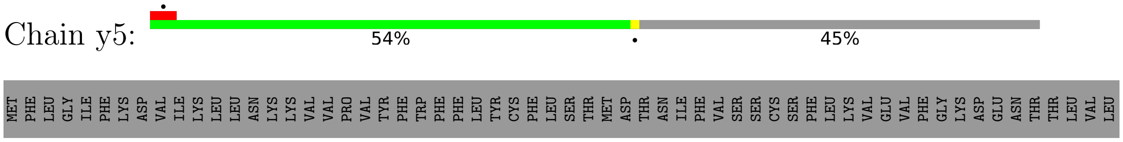
- Molecule 32: Ymf75

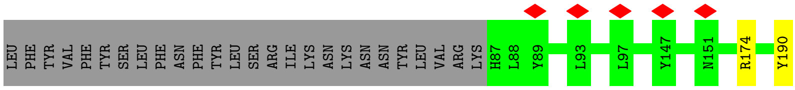
Chain Y5:



- Molecule 32: Ymf75

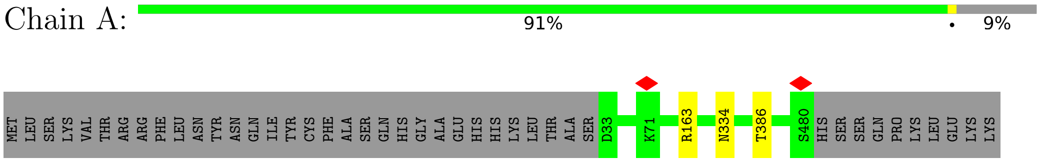
Chain y5:





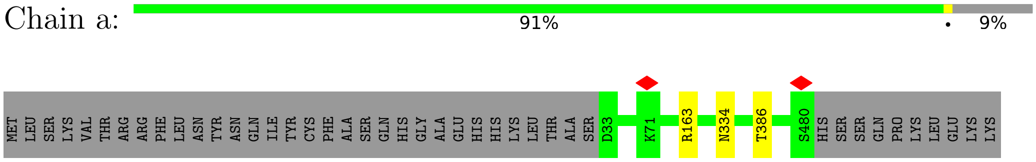
- Molecule 33: Transmembrane protein, putative

Chain A:



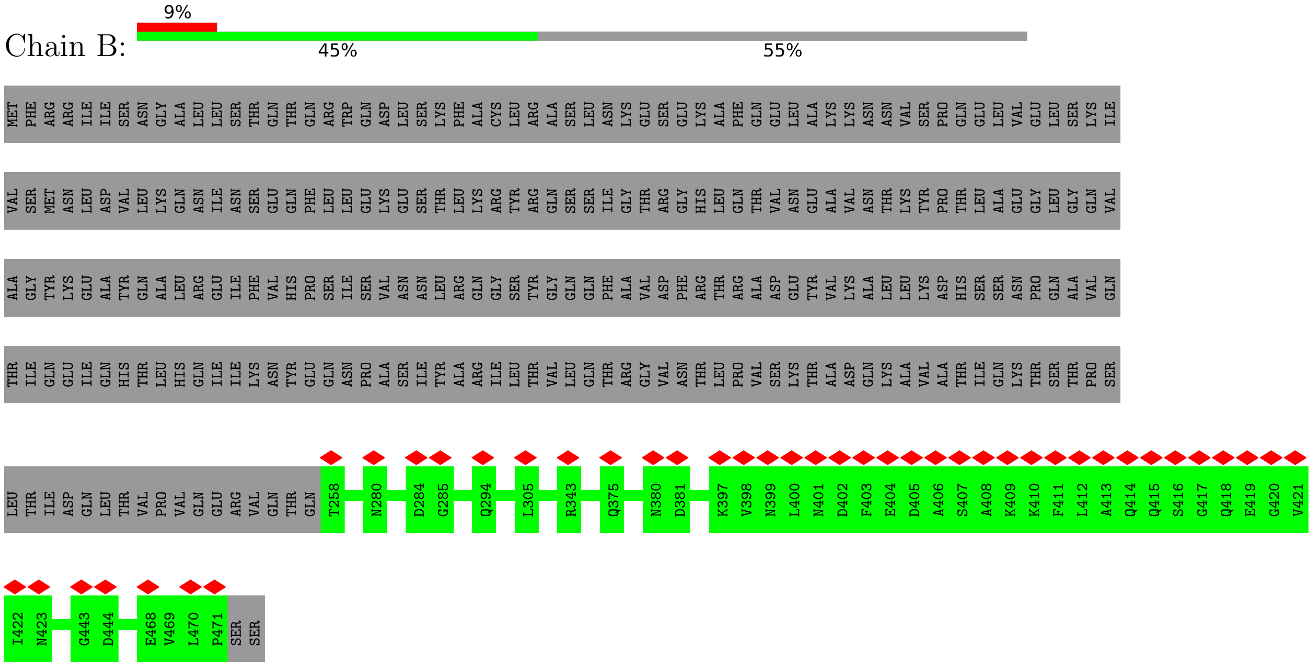
- Molecule 33: Transmembrane protein, putative

Chain a:



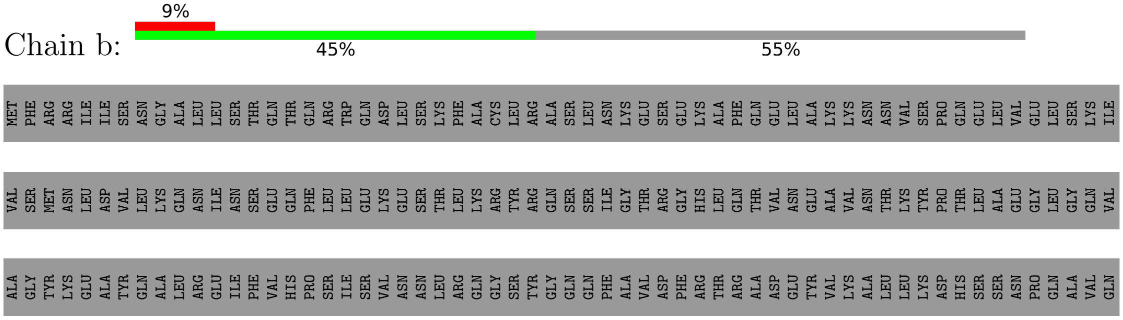
- Molecule 34: Protein phosphatase 2C, putative

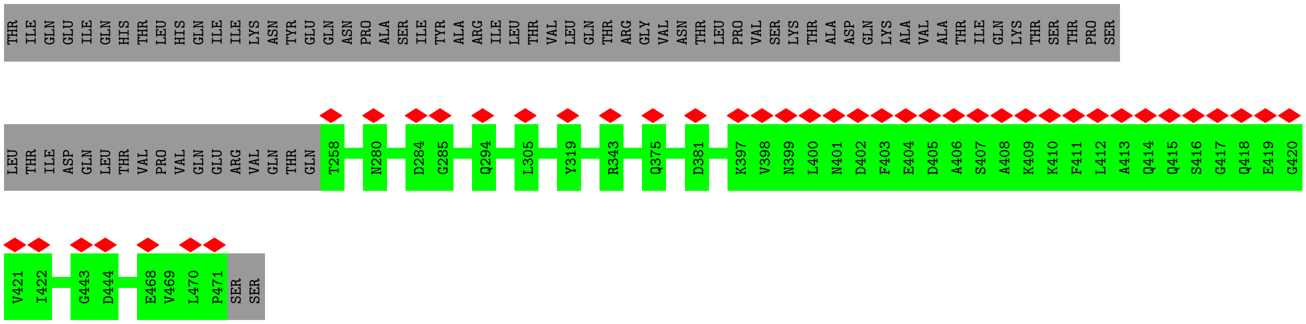
Chain B:



- Molecule 34: Protein phosphatase 2C, putative

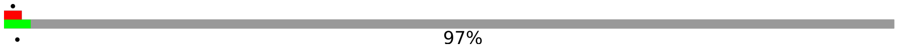
Chain b:

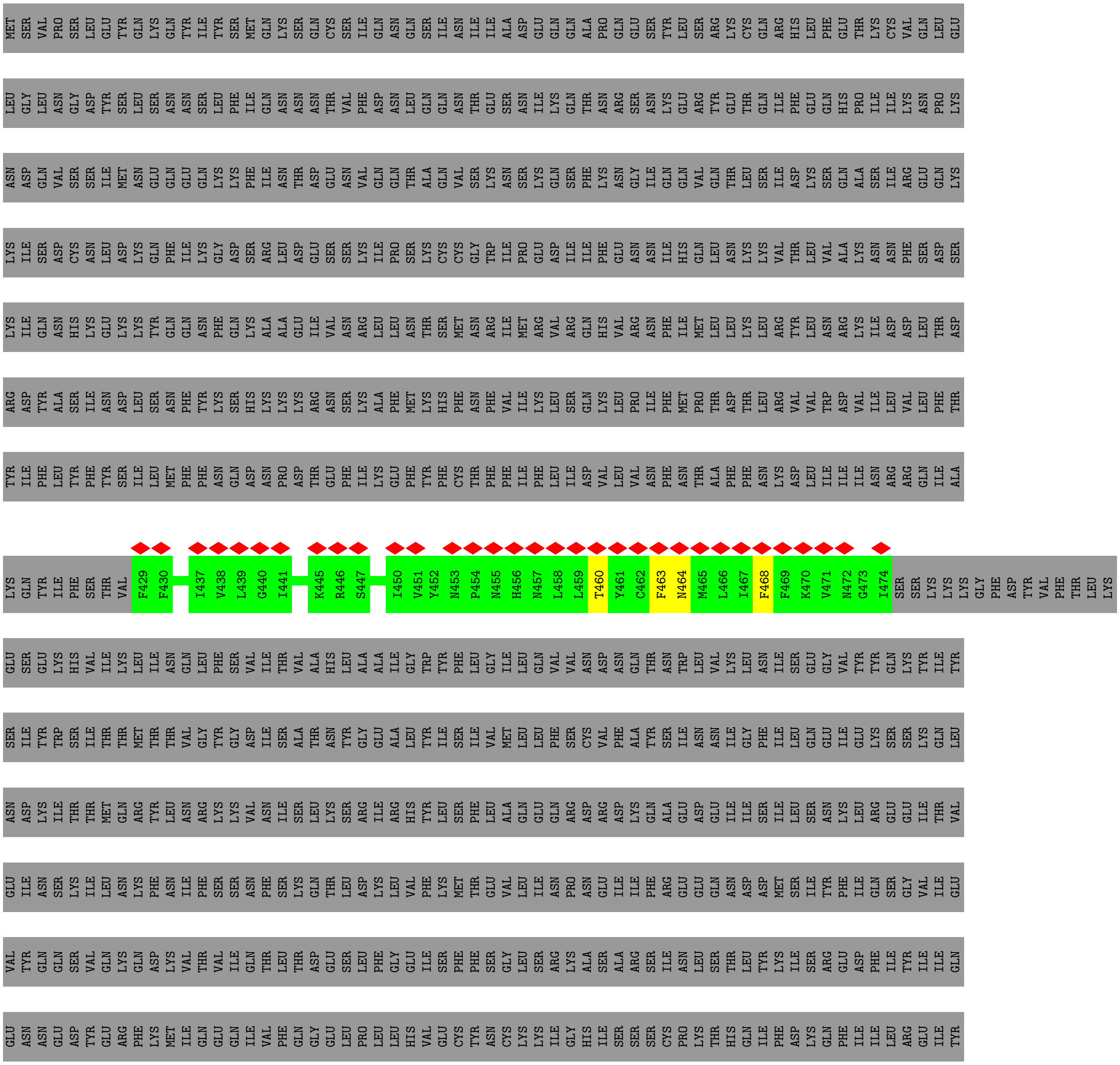




- Molecule 35: Cyclic nucleotide-binding domain protein

Chain C:





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

ASP ASN ASN GLN ILE CYS GLU ASN ILE SER SER ILE LEU ASN SER ASP GLN TYR CYS ASN SER GLN LYS VAL ILE SER ASN ASN ILE ASN ASP ASN LEU GLU ILE LYS LYS SER TYR VAL LYS SER PHE ASN LEU SER ASN ARG GLN LYS SER LEU ASP ASP PHE GLU LYS ILE LYS SER

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

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

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

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

LYS ASN LEU SER GLN ILE LYS THR LYS GLN SER ILE GLY LYS SER SER ILE LEU ASN ALA LEU SER ASN ILE ASN ASN ILE ASP GLY ASN THR ASN ASP LEU ASN ASN LYS ASN ASN ASN SER LYS LEU LEU GLN ALA GLN ASN SER GLN ILE THR ASN GLY ASN GLN LEU GLN ILE VAL

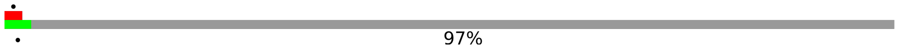
ASP ARG LEU SER LYS LEU LEU LEU ASN PRO GLN LEU PRO LEU LEU LEU LYS LEU THR SER VAL GLY MET SER PHE ARG GLU MET ASN SER ILE ASN SER ASN ASN ALA MET ASP MET PHE ASP LYS MET HIS ASN PHE LYS LYS PHE PHE PRO HIS ASN ASN ILE GLU ASN VAL LEU ASN

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

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

- Molecule 35: Cyclic nucleotide-binding domain protein

Chain c:



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

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

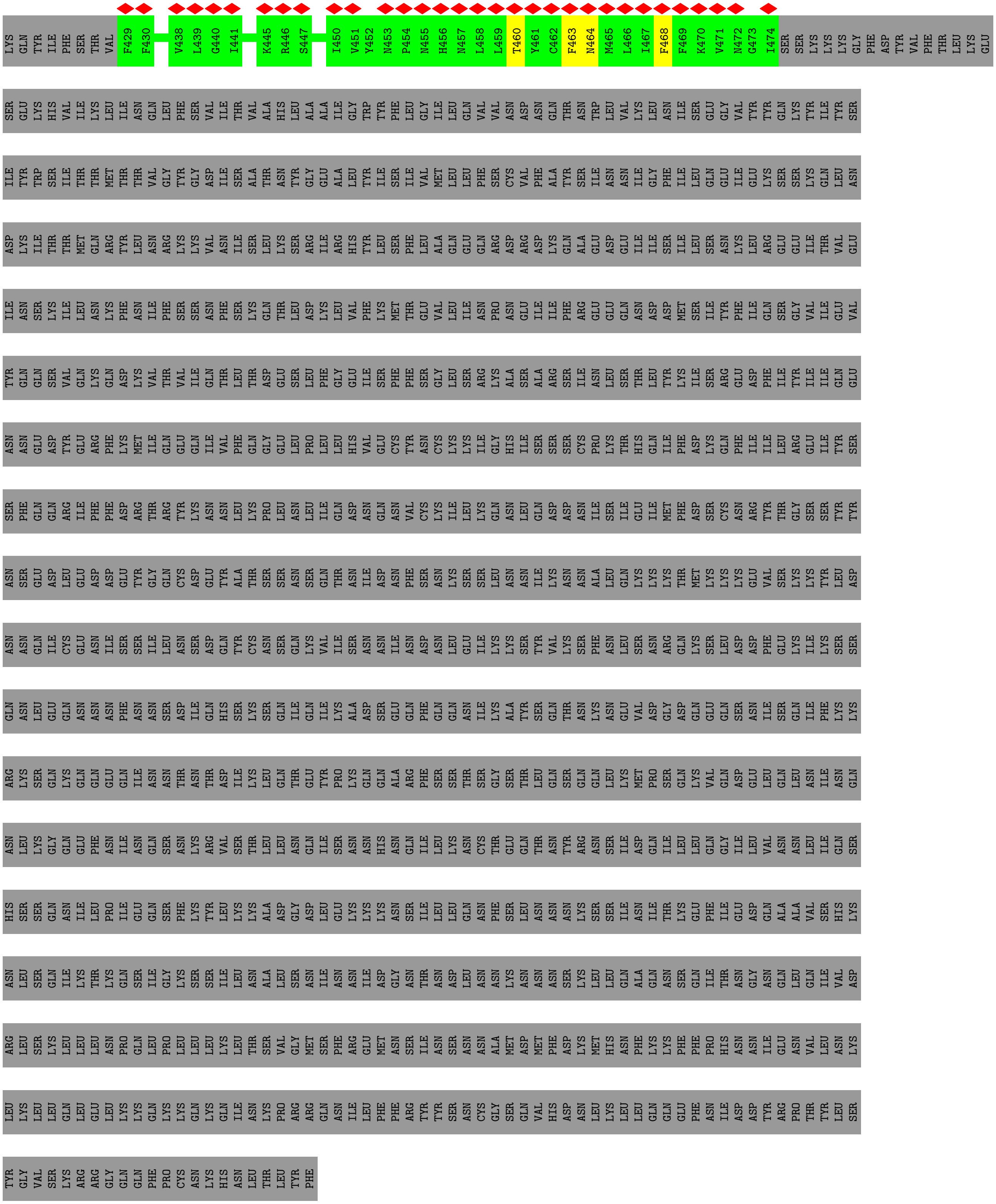
ASN ASP GLN VAL SER SER ILE MET ASN GLU GLN GLU GLN LYS LYS PHE ILE ASN THR ASP GLU ASN VAL GLN GLN THR ALA GLN VAL SER LYS ASN SER LYS GLN SER PHE LYS ASN GLY ILE GLN GLN VAL GLN THR LEU SER ILE ASP LYS SER GLN ALA SER ILE ARG GLU GLN LYS

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

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

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

TYR ILE PHE LEU TYR PHE TYR SER ILE LEU MET PHE PHE ASN GLN ASP ASN PRO ASP THR GLU PHE ILE LYS GLU PHE TYR PHE CYS THR PHE PHE ILE PHE LEU ILE ASP VAL LEU VAL ASN PHE ASN THR ALA PHE PHE ASN LYS ASP LEU ILE ILE ILE ASN ARG ARG GLN ILE ALA



LYS GLN TYR ILE PHE SER THR VAL F429 F430 V438 L439 G440 I441 K445 R446 S447 I450 V451 Y452 N453 P454 N455 H456 N457 L458 L459 T460 Y461 C462 F463 N464 M465 L466 I467 F468 F469 K470 V471 N472 G473 I474 SER SER LYS LYS LYS GLY PHE ASP TYR VAL PHE THR LEU LYS GLU

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

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

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

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

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

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

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

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

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

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

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

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

ASN LEU SER GLN ILE LYS THR LYS GLN SER ILE GLY LYS SER SER ILE LEU ASN ALA LEU SER ASN ILE ASN ASN ILE ASP GLY ASN THR ASN ASP LEU ASN ASN LYS ASN ASN ASN SER LYS LEU LEU GLN ALA GLN ASN SER GLN ILE THR ASN GLY ASN GLN LEU GLN ILE VAL ASP

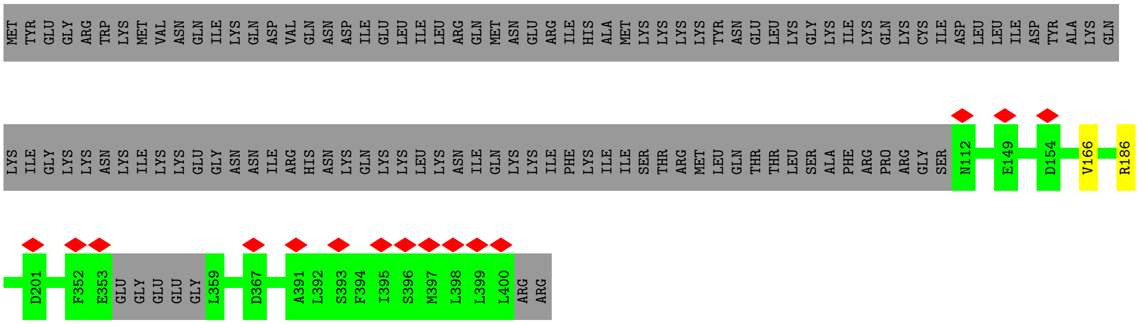
ARG LEU SER LYS LEU LEU LEU ASN PRO GLN LEU PRO LEU LEU LEU LYS LEU THR SER VAL GLY MET SER PHE ARG GLU MET ASN SER ILE ASN SER ASN ASN ALA MET ASP MET PHE ASP LYS MET HIS ASN PHE LYS LYS PHE PHE PRO HIS ASN ASN ILE GLU ASN VAL LEU ASN LYS

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

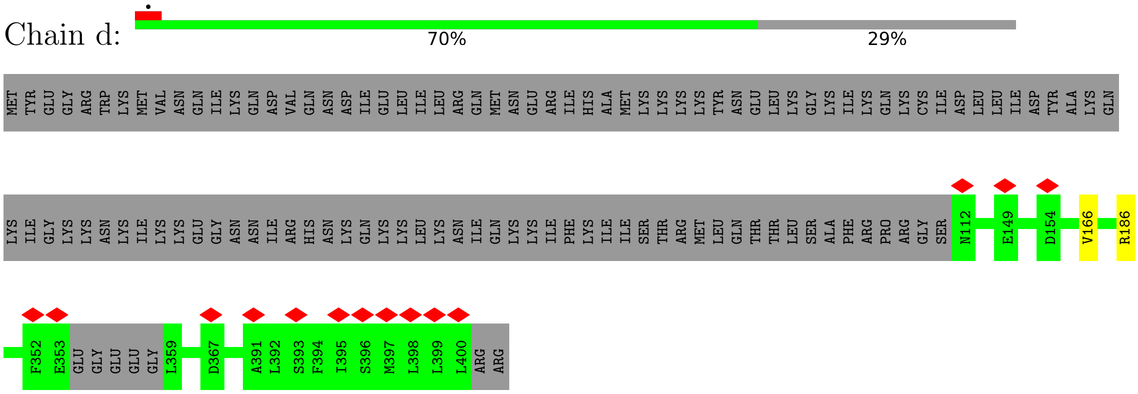
TYR GLY VAL SER LYS ARG ARG GLY GLN GLN PHE PRO CYS ASN LYS HIS ASN LEU THR LEU TYR PHE

- Molecule 36: SURF1-like protein

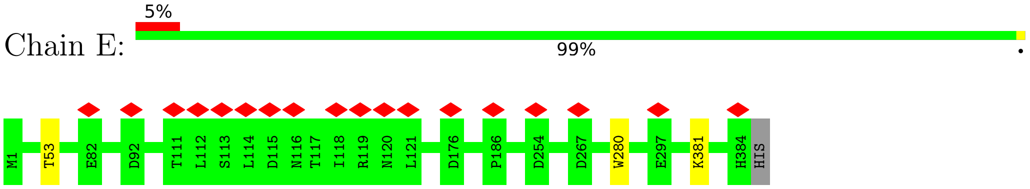
Chain D:



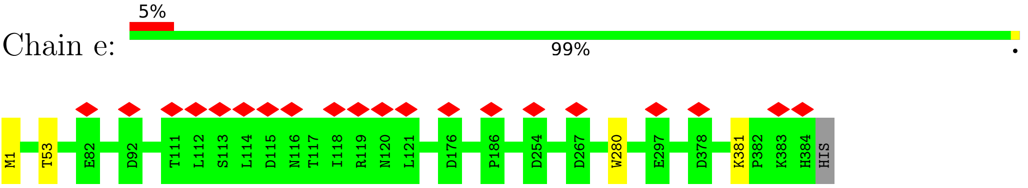
- Molecule 36: SURF1-like protein



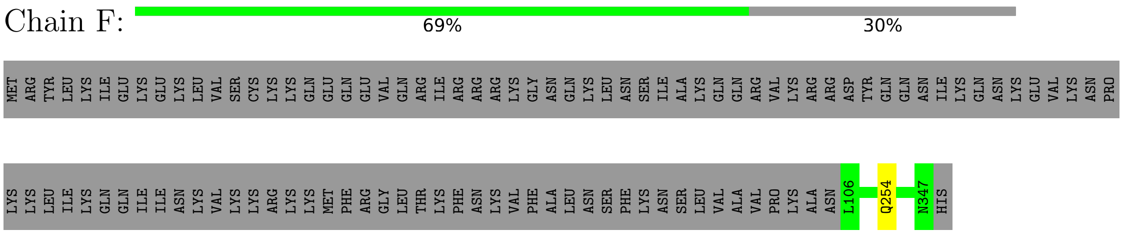
- Molecule 37: TraB family protein



- Molecule 37: TraB family protein

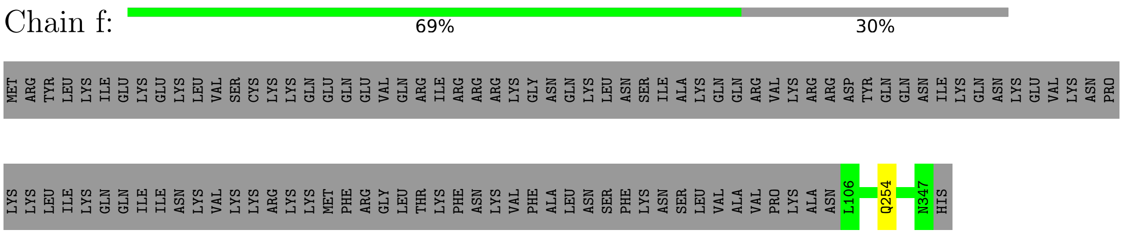


- Molecule 38: Transmembrane protein, putative



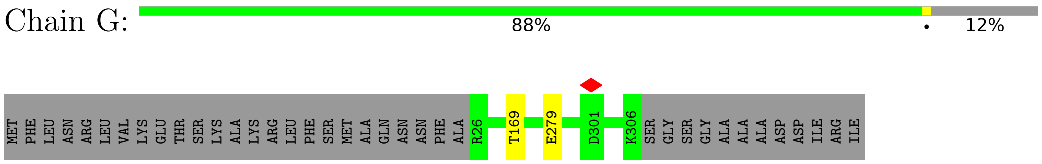
- Molecule 38: Transmembrane protein, putative

Chain f:



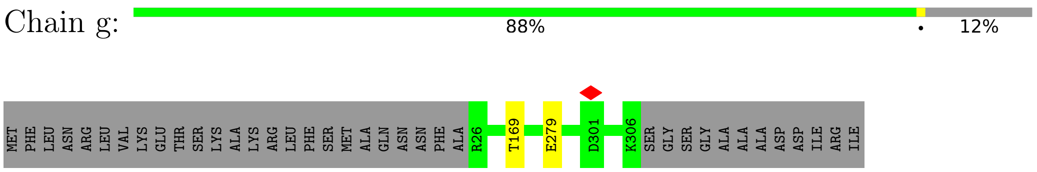
- Molecule 39: Cytochrome c oxidase subunit TT7

Chain G:



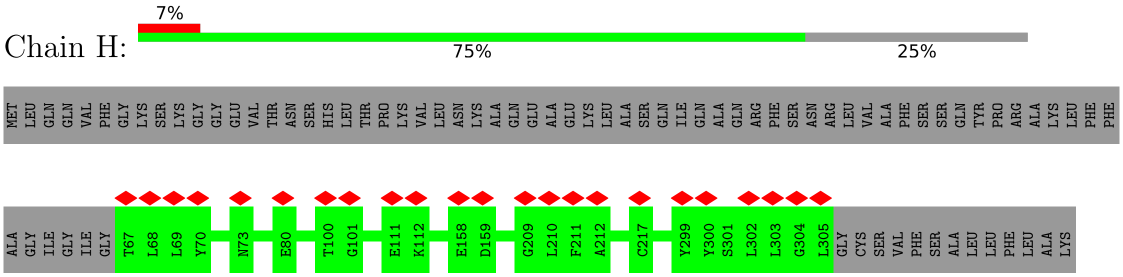
- Molecule 39: Cytochrome c oxidase subunit TT7

Chain g:



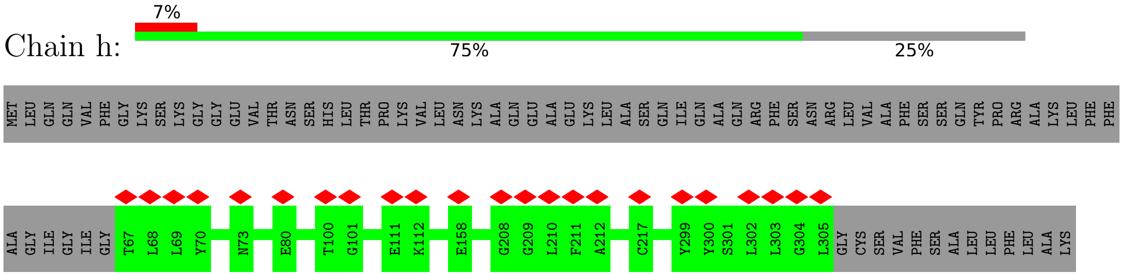
- Molecule 40: SURF1-like protein

Chain H:



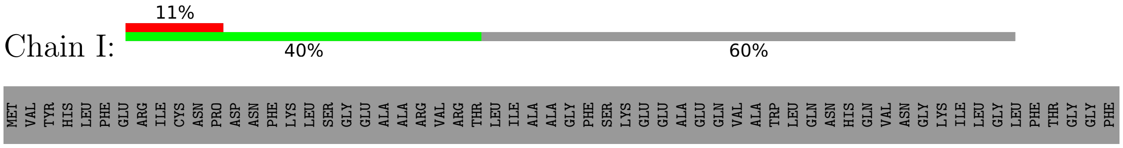
- Molecule 40: SURF1-like protein

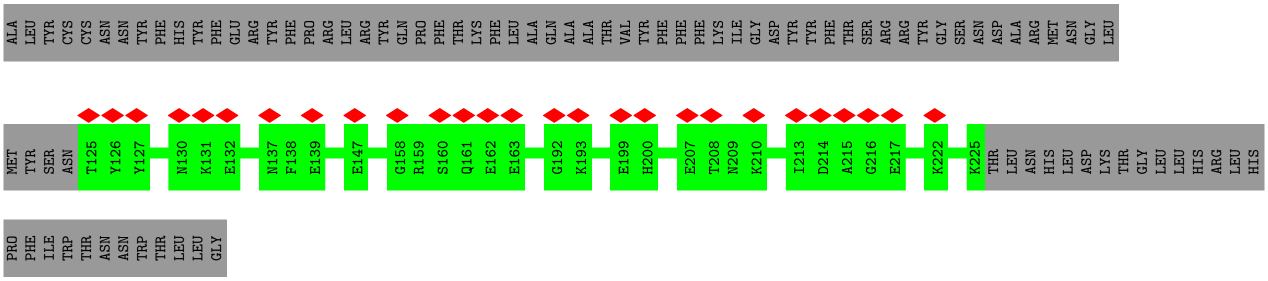
Chain h:



- Molecule 41: Cytochrome c oxidase subunit TT9

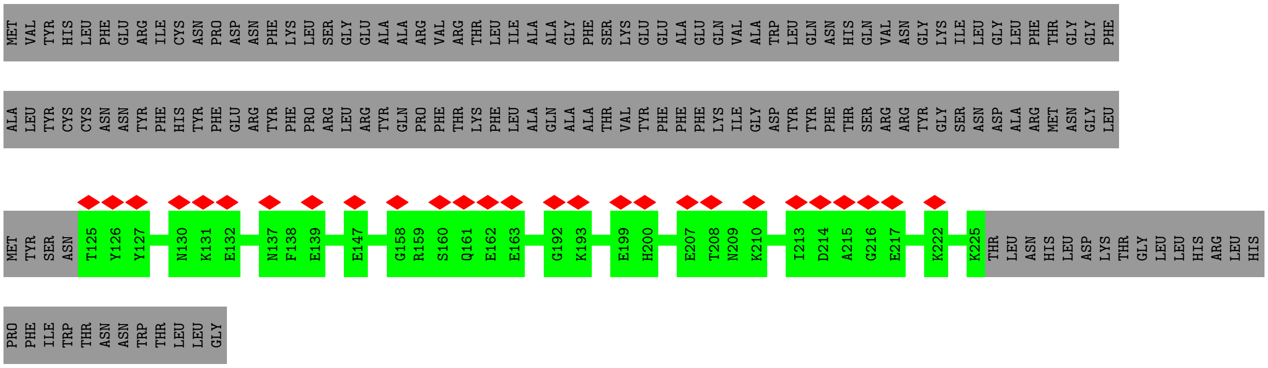
Chain I:





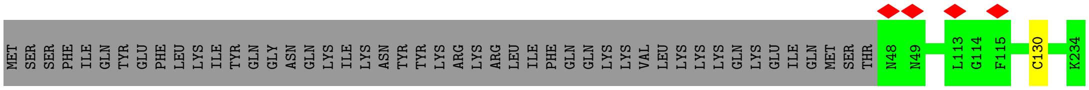
- Molecule 41: Cytochrome c oxidase subunit TT9

Chain i:



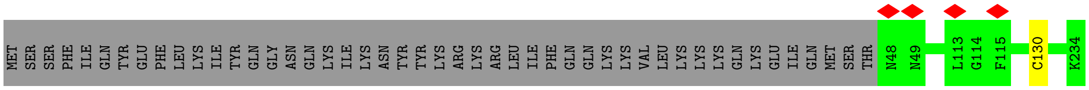
- Molecule 42: Cytochrome c oxidase subunit TT10

Chain J:



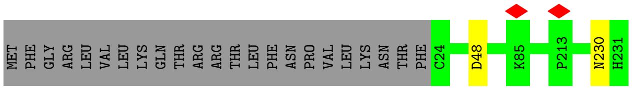
- Molecule 42: Cytochrome c oxidase subunit TT10

Chain j:



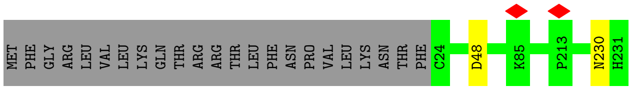
- Molecule 43: Cytochrome c oxidase subunit TT11

Chain K:



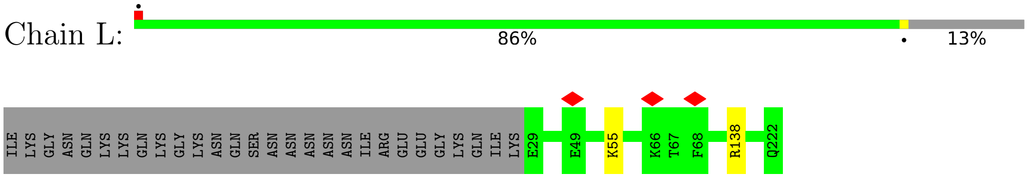
- Molecule 43: Cytochrome c oxidase subunit TT11

Chain k:



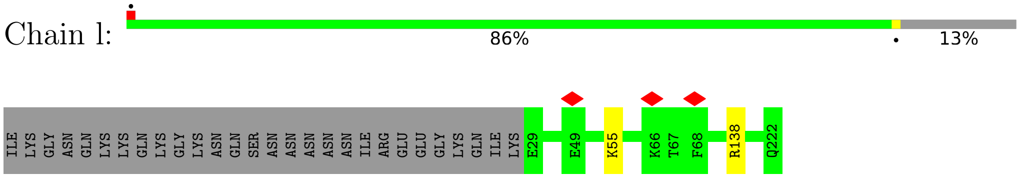
- Molecule 44: Cytochrome c oxidase subunit TT12

Chain L:



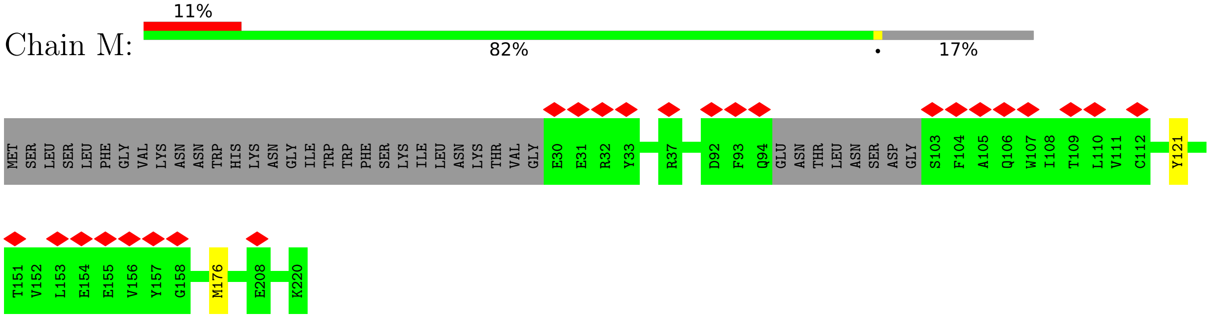
- Molecule 44: Cytochrome c oxidase subunit TT12

Chain l:



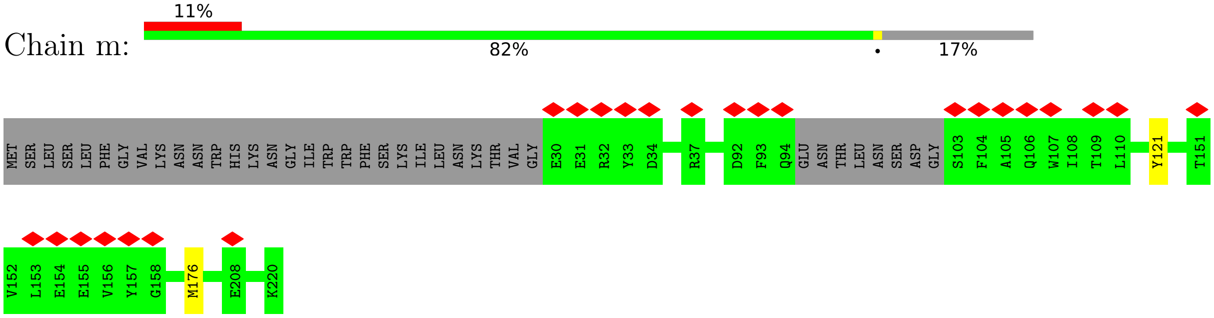
- Molecule 45: Transmembrane protein, putative

Chain M:



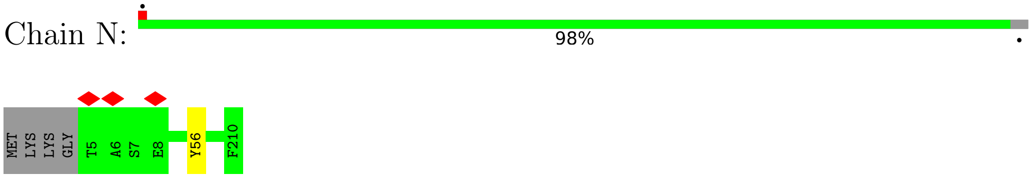
- Molecule 45: Transmembrane protein, putative

Chain m:



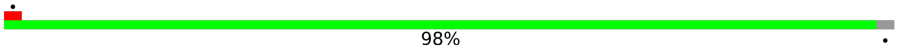
- Molecule 46: Transmembrane protein, putative

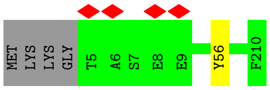
Chain N:



- Molecule 46: Transmembrane protein, putative

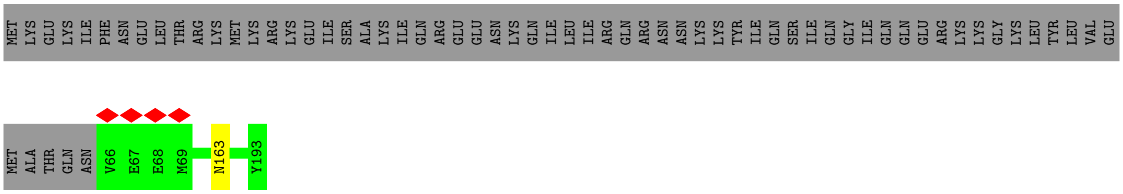
Chain n:





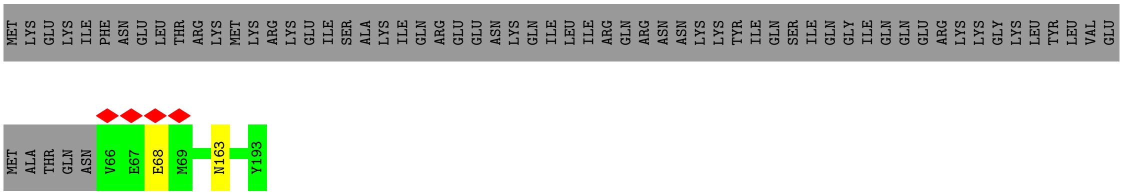
- Molecule 47: Cytochrome c oxidase subunit TT15

Chain O:



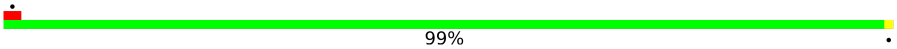
- Molecule 47: Cytochrome c oxidase subunit TT15

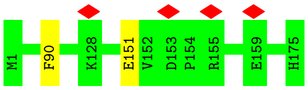
Chain o:



- Molecule 48: Cytochrome c oxidase subunit TT16

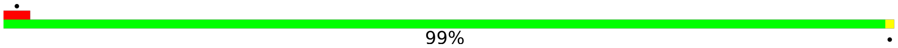
Chain P:

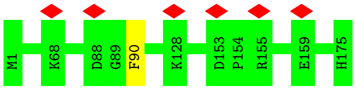




- Molecule 48: Cytochrome c oxidase subunit TT16

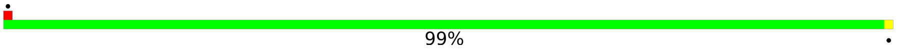
Chain p:

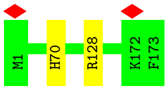




- Molecule 49: Transmembrane protein, putative

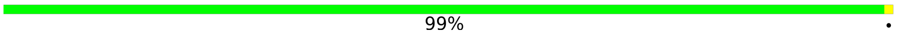
Chain Q:





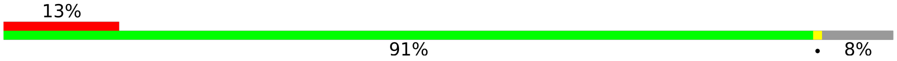
- Molecule 49: Transmembrane protein, putative

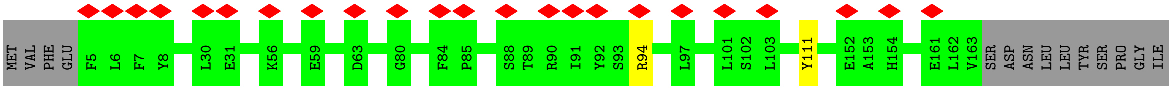
Chain q:



- Molecule 50: Cytochrome c oxidase subunit TT18

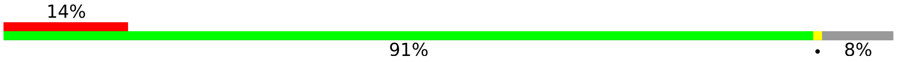
Chain R:

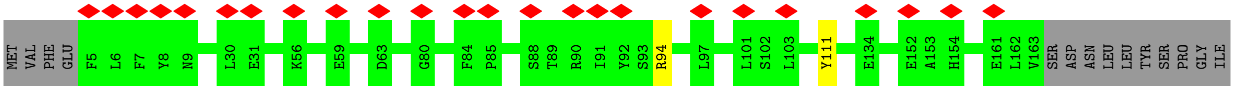




- Molecule 50: Cytochrome c oxidase subunit TT18

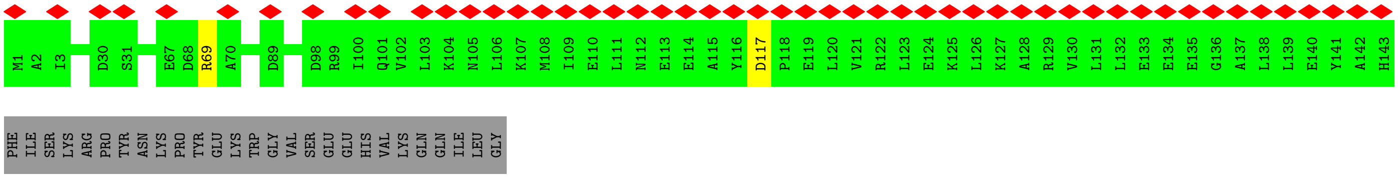
Chain r:





- Molecule 51: Cytochrome c oxidase subunit TT19

Chain S:

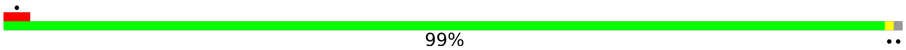


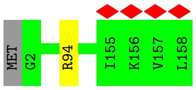
- Molecule 51: Cytochrome c oxidase subunit TT19

Chain s:

- Molecule 52: Transmembrane protein, putative

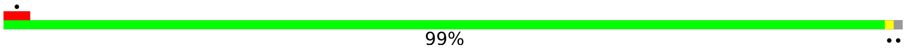
Chain T:

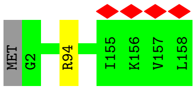




- Molecule 52: Transmembrane protein, putative

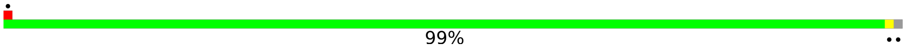
Chain t:

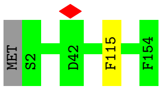




- Molecule 53: Transmembrane protein, putative

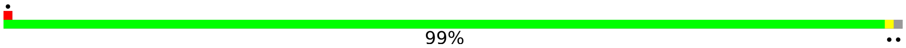
Chain U:

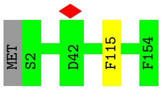




- Molecule 53: Transmembrane protein, putative

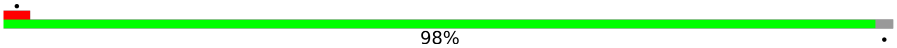
Chain u:

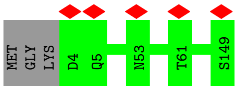




- Molecule 54: Cytochrome c oxidase subunit TT22

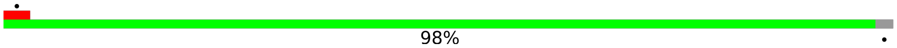
Chain V:

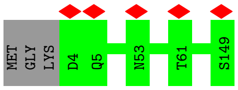




- Molecule 54: Cytochrome c oxidase subunit TT22

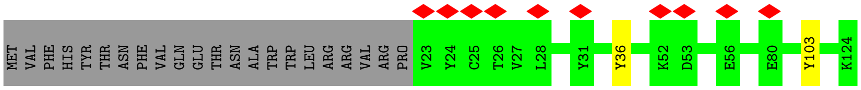
Chain v:





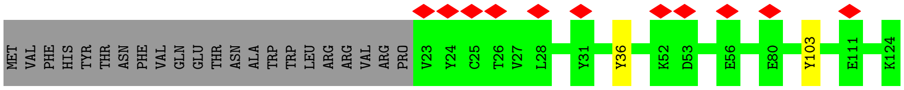
- Molecule 55: Transmembrane protein, putative

Chain W:



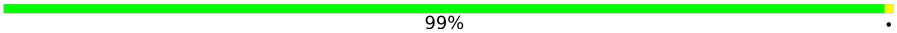
- Molecule 55: Transmembrane protein, putative

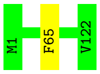
Chain w:



- Molecule 56: Transmembrane protein, putative

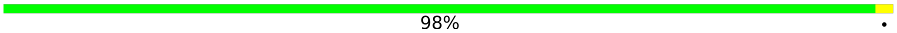
Chain X:





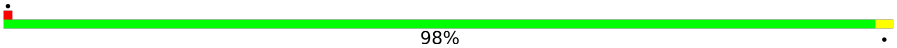
- Molecule 56: Transmembrane protein, putative

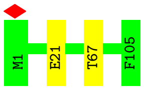
Chain x:



- Molecule 57: Cytochrome c oxidase subunit TT25

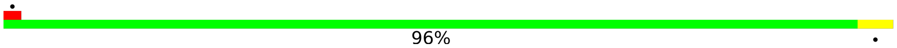
Chain Y:

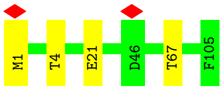




- Molecule 57: Cytochrome c oxidase subunit TT25

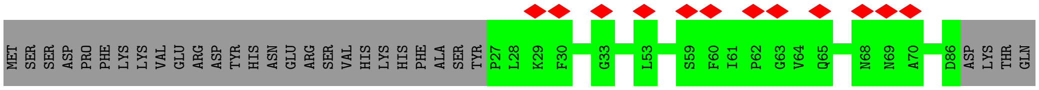
Chain y:





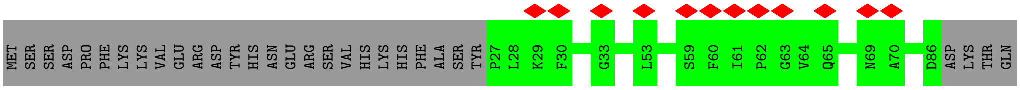
- Molecule 58: Cytochrome c oxidase subunit TT26

Chain Z:



- Molecule 58: Cytochrome c oxidase subunit TT26

Chain z:



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 $(e^-/\text{Å}^2)$	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	5.0	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, ZN, FME, MG, SEP, PC1, CDL, FES, HEA, TPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
2	U2	0.26	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.

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	19	55
2	u2	125/3634 (3%)	114 (91%)	10 (8%)	1 (1%)	19	55
5	U5	31/172 (18%)	31 (100%)	0	0	100	100
5	u5	31/172 (18%)	31 (100%)	0	0	100	100
6	U6	40/478 (8%)	39 (98%)	1 (2%)	0	100	100
6	u6	40/478 (8%)	39 (98%)	1 (2%)	0	100	100
7	C1	670/688 (97%)	638 (95%)	32 (5%)	0	100	100
7	c1	670/688 (97%)	638 (95%)	32 (5%)	0	100	100
8	C2	572/604 (95%)	547 (96%)	25 (4%)	0	100	100
8	c2	572/604 (95%)	547 (96%)	25 (4%)	0	100	100
9	C3	557/594 (94%)	542 (97%)	15 (3%)	0	100	100
9	c3	557/594 (94%)	543 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
24	t4	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
25	T5	61/81 (75%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
40	H	237/318 (74%)	233 (98%)	4 (2%)	0	100	100
40	h	237/318 (74%)	234 (99%)	3 (1%)	0	100	100

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	65
6	u6	24/419 (6%)	23 (96%)	1 (4%)	30	65
7	C1	597/613 (97%)	588 (98%)	9 (2%)	65	86
7	c1	597/613 (97%)	587 (98%)	10 (2%)	60	85
8	C2	542/569 (95%)	531 (98%)	11 (2%)	55	82
8	c2	542/569 (95%)	531 (98%)	11 (2%)	55	82
9	C3	534/565 (94%)	527 (99%)	7 (1%)	69	88
9	c3	534/565 (94%)	527 (99%)	7 (1%)	69	88
10	5B	502/579 (87%)	495 (99%)	7 (1%)	67	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	5b	502/579 (87%)	496 (99%)	6 (1%)	71	89
11	6A	113/116 (97%)	112 (99%)	1 (1%)	78	92
11	6a	113/116 (97%)	112 (99%)	1 (1%)	78	92
12	6B	199/207 (96%)	197 (99%)	2 (1%)	76	91
12	6b	199/207 (96%)	196 (98%)	3 (2%)	65	86
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%)	71	89
14	6c	81/88 (92%)	80 (99%)	1 (1%)	71	89
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%)	53	81
16	7c	193/217 (89%)	190 (98%)	3 (2%)	62	86
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%)	84	94
18	m1	294/294 (100%)	292 (99%)	2 (1%)	84	94
19	M2	259/259 (100%)	256 (99%)	3 (1%)	71	89
19	m2	259/259 (100%)	256 (99%)	3 (1%)	71	89
20	M3	275/276 (100%)	272 (99%)	3 (1%)	73	90
20	m3	275/276 (100%)	272 (99%)	3 (1%)	73	90
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%)	57	83
24	t4	53/62 (86%)	52 (98%)	1 (2%)	57	83
25	T5	57/66 (86%)	57 (100%)	0	100	100
25	t5	57/66 (86%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	92	97
27	bp	308/308 (100%)	307 (100%)	1 (0%)	92	97
28	FS	164/164 (100%)	163 (99%)	1 (1%)	86	95
28	fs	164/164 (100%)	162 (99%)	2 (1%)	71	89
29	AC	87/113 (77%)	85 (98%)	2 (2%)	50	79
29	ac	87/113 (77%)	85 (98%)	2 (2%)	50	79
30	Y7	328/442 (74%)	324 (99%)	4 (1%)	71	89
30	y7	328/442 (74%)	323 (98%)	5 (2%)	65	86
31	Y0	83/83 (100%)	83 (100%)	0	100	100
31	y0	83/83 (100%)	82 (99%)	1 (1%)	71	89
32	Y5	101/185 (55%)	99 (98%)	2 (2%)	55	82
32	y5	101/185 (55%)	99 (98%)	2 (2%)	55	82
33	A	409/447 (92%)	406 (99%)	3 (1%)	84	94
33	a	409/447 (92%)	406 (99%)	3 (1%)	84	94
34	B	182/413 (44%)	182 (100%)	0	100	100
34	b	182/413 (44%)	182 (100%)	0	100	100
35	C	44/1405 (3%)	40 (91%)	4 (9%)	9	33
35	c	44/1405 (3%)	40 (91%)	4 (9%)	9	33
36	D	250/358 (70%)	248 (99%)	2 (1%)	81	93
36	d	250/358 (70%)	248 (99%)	2 (1%)	81	93
37	E	341/342 (100%)	338 (99%)	3 (1%)	78	92
37	e	341/342 (100%)	338 (99%)	3 (1%)	78	92
38	F	218/318 (69%)	217 (100%)	1 (0%)	88	96
38	f	218/318 (69%)	217 (100%)	1 (0%)	88	96
39	G	260/289 (90%)	258 (99%)	2 (1%)	81	93
39	g	260/289 (90%)	258 (99%)	2 (1%)	81	93
40	H	209/272 (77%)	209 (100%)	0	100	100
40	h	209/272 (77%)	209 (100%)	0	100	100
41	I	90/219 (41%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	i	90/219 (41%)	90 (100%)	0	100	100
42	J	170/216 (79%)	169 (99%)	1 (1%)	86	95
42	j	170/216 (79%)	169 (99%)	1 (1%)	86	95
43	K	191/213 (90%)	189 (99%)	2 (1%)	76	91
43	k	191/213 (90%)	189 (99%)	2 (1%)	76	91
44	L	181/206 (88%)	179 (99%)	2 (1%)	73	90
44	l	181/206 (88%)	179 (99%)	2 (1%)	73	90
45	M	166/199 (83%)	164 (99%)	2 (1%)	71	89
45	m	166/199 (83%)	164 (99%)	2 (1%)	71	89
46	N	178/181 (98%)	177 (99%)	1 (1%)	86	95
46	n	178/181 (98%)	177 (99%)	1 (1%)	86	95
47	O	119/180 (66%)	118 (99%)	1 (1%)	81	93
47	o	119/180 (66%)	117 (98%)	2 (2%)	60	85
48	P	156/156 (100%)	154 (99%)	2 (1%)	69	88
48	p	156/156 (100%)	155 (99%)	1 (1%)	86	95
49	Q	157/157 (100%)	155 (99%)	2 (1%)	69	88
49	q	157/157 (100%)	155 (99%)	2 (1%)	69	88
50	R	144/157 (92%)	142 (99%)	2 (1%)	67	87
50	r	144/157 (92%)	142 (99%)	2 (1%)	67	87
51	S	129/154 (84%)	127 (98%)	2 (2%)	62	86
51	s	129/154 (84%)	127 (98%)	2 (2%)	62	86
52	T	138/139 (99%)	137 (99%)	1 (1%)	84	94
52	t	138/139 (99%)	137 (99%)	1 (1%)	84	94
53	U	137/138 (99%)	136 (99%)	1 (1%)	84	94
53	u	137/138 (99%)	136 (99%)	1 (1%)	84	94
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%)	52	80
55	w	92/113 (81%)	90 (98%)	2 (2%)	52	80
56	X	105/105 (100%)	104 (99%)	1 (1%)	76	91
56	x	105/105 (100%)	103 (98%)	2 (2%)	57	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	Y	88/88 (100%)	86 (98%)	2 (2%)	50	79
57	y	88/88 (100%)	84 (96%)	4 (4%)	27	63
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%)	74	90

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	c2	291	PHE
16	7c	110	HIS
56	x	119	LYS
8	c2	501	VAL
10	5b	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
27	bp	260	ASN
30	y7	172	ASN
35	c	456	HIS
30	y7	118	ASN
30	y7	191	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	TPO	5b	387	10	8,10,11	1.54	1 (12%)	10,14,16	1.90	1 (10%)
31	FME	Y0	1	31	8,9,10	0.96	0	7,9,11	0.86	0
26	FME	t6	1	26	8,9,10	0.93	0	7,9,11	0.78	0
16	SEP	7C	197	16	8,9,10	1.53	1 (12%)	8,12,14	2.20	2 (25%)
19	FME	m2	1	19	8,9,10	0.94	0	7,9,11	0.92	0
10	TPO	5B	387	10	8,10,11	1.03	0	10,14,16	1.88	1 (10%)
13	FME	6L	1	13	8,9,10	0.95	0	7,9,11	0.87	0
31	FME	y0	1	31	8,9,10	0.95	0	7,9,11	0.86	0
24	FME	t4	1	24	8,9,10	0.92	0	7,9,11	0.92	0
48	FME	P	1	48	8,9,10	0.92	0	7,9,11	1.03	0
19	FME	M2	1	19	8,9,10	0.94	0	7,9,11	0.99	0
16	SEP	7c	120	16	8,9,10	1.50	1 (12%)	8,12,14	1.65	2 (25%)
48	FME	p	1	48	8,9,10	0.91	0	7,9,11	1.05	0
16	SEP	7C	120	16	8,9,10	1.49	1 (12%)	8,12,14	1.67	2 (25%)
16	SEP	7c	197	16	8,9,10	1.51	1 (12%)	8,12,14	2.17	2 (25%)
13	FME	6l	1	13	8,9,10	0.93	0	7,9,11	0.93	0
10	SEP	5b	520	10	8,9,10	1.52	1 (12%)	8,12,14	1.62	2 (25%)
15	FME	7A	1	15	8,9,10	0.95	0	7,9,11	0.87	0
15	FME	7a	1	15	8,9,10	0.94	0	7,9,11	0.86	0
37	FME	e	1	37	8,9,10	0.94	0	7,9,11	0.99	1 (14%)
26	FME	T6	1	26	8,9,10	0.93	0	7,9,11	0.80	0
24	FME	T4	1	24	8,9,10	0.92	0	7,9,11	0.89	0
37	FME	E	1	37	8,9,10	0.95	0	7,9,11	0.99	0
10	SEP	5B	520	10	8,9,10	1.52	1 (12%)	8,12,14	1.59	2 (25%)

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
10	TPO	5b	387	10	-	1/9/11/13	-
31	FME	Y0	1	31	-	5/7/9/11	-
26	FME	t6	1	26	-	5/7/9/11	-
16	SEP	7C	197	16	-	2/5/8/10	-
19	FME	m2	1	19	-	4/7/9/11	-
10	TPO	5B	387	10	-	1/9/11/13	-
13	FME	6L	1	13	-	5/7/9/11	-
31	FME	y0	1	31	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	FME	t4	1	24	-	4/7/9/11	-
48	FME	P	1	48	-	3/7/9/11	-
19	FME	M2	1	19	-	4/7/9/11	-
16	SEP	7c	120	16	-	0/5/8/10	-
48	FME	p	1	48	-	3/7/9/11	-
16	SEP	7C	120	16	-	0/5/8/10	-
16	SEP	7c	197	16	-	0/5/8/10	-
13	FME	6l	1	13	-	6/7/9/11	-
10	SEP	5b	520	10	-	3/5/8/10	-
15	FME	7A	1	15	-	5/7/9/11	-
15	FME	7a	1	15	-	4/7/9/11	-
37	FME	e	1	37	-	5/7/9/11	-
26	FME	T6	1	26	-	5/7/9/11	-
24	FME	T4	1	24	-	4/7/9/11	-
37	FME	E	1	37	-	5/7/9/11	-
10	SEP	5B	520	10	-	3/5/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7C	197	SEP	P-O1P	3.34	1.61	1.50
10	5b	520	SEP	P-O1P	3.32	1.61	1.50
10	5B	520	SEP	P-O1P	3.31	1.61	1.50
16	7c	120	SEP	P-O1P	3.29	1.61	1.50
10	5b	387	TPO	P-O1P	3.27	1.61	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	5b	387	TPO	P-OG1-CB	-5.47	106.70	123.21
10	5B	387	TPO	P-OG1-CB	-5.37	106.98	123.21
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	197	SEP	P-OG-CB	-3.93	107.48	118.30

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 122 ligands modelled in this entry, 12 are monoatomic - leaving 110 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
63	CDL	y0	101	-	63,63,99	0.37	0	69,75,111	0.33	0
62	PC1	A	501	-	44,44,53	0.31	0	50,52,61	0.34	0
63	CDL	7C	303	-	50,50,99	0.41	0	56,62,111	0.34	0
62	PC1	M2	405	-	40,40,53	0.33	0	46,48,61	0.33	0
62	PC1	a	502	-	40,40,53	0.34	0	46,48,61	0.38	0
63	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.30	0
63	CDL	k	301	-	61,61,99	0.37	0	67,73,111	0.33	0
59	HEA	c1	702	7	57,67,67	1.19	5 (8%)	61,103,103	1.69	17 (27%)
62	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.37	0
63	CDL	7a	201	-	66,66,99	0.36	0	72,78,111	0.37	0
63	CDL	Y7	501	-	64,64,99	0.37	0	70,76,111	0.36	0
63	CDL	m1	403	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	m2	401	-	53,53,99	0.40	0	59,65,111	0.39	0
62	PC1	m1	402	-	53,53,53	0.29	0	59,61,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
63	CDL	c1	706	-	58,58,99	0.38	0	64,70,111	0.41	0
63	CDL	U	201	-	81,81,99	0.33	0	87,93,111	0.32	0
63	CDL	E	402	-	71,71,99	0.35	0	77,83,111	0.34	0
63	CDL	M3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
65	FES	fs	201	28	0,4,4	-	-	-		
63	CDL	c1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
63	CDL	7C	301	-	84,84,99	0.33	0	90,96,111	0.34	0
62	PC1	C3	602	-	38,38,53	0.34	0	44,46,61	0.32	0
63	CDL	M3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
63	CDL	v	201	-	90,90,99	0.32	0	96,102,111	0.36	0
62	PC1	a	501	-	44,44,53	0.31	0	50,52,61	0.34	0
62	PC1	m2	406	-	53,53,53	0.29	0	59,61,61	0.26	0
63	CDL	7c	302	-	50,50,99	0.41	0	56,62,111	0.34	0
65	FES	fs	202	28	0,4,4	-	-	-		
63	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.33	0
63	CDL	t	202	-	74,74,99	0.35	0	80,86,111	0.35	0
63	CDL	N	303	-	94,94,99	0.31	0	100,106,111	0.36	0
63	CDL	t	201	-	67,67,99	0.36	0	73,79,111	0.35	0
63	CDL	n	303	-	94,94,99	0.31	0	100,106,111	0.37	0
62	PC1	A	502	-	40,40,53	0.33	0	46,48,61	0.37	0
63	CDL	M1	401	-	94,94,99	0.31	0	100,106,111	0.32	0
63	CDL	5b	703	-	66,66,99	0.36	0	72,78,111	0.33	0
65	FES	FS	202	28	0,4,4	-	-	-		
59	HEA	C1	701	7	57,67,67	1.13	6 (10%)	61,103,103	1.69	16 (26%)
59	HEA	c1	701	7	57,67,67	1.14	6 (10%)	61,103,103	1.67	15 (24%)
63	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
63	CDL	y7	501	-	64,64,99	0.37	0	70,76,111	0.36	0
62	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.37	0
63	CDL	7a	202	-	99,99,99	0.30	0	105,111,111	0.30	0
63	CDL	c3	604	-	67,67,99	0.36	0	73,79,111	0.31	0
62	PC1	v	202	-	53,53,53	0.29	0	59,61,61	0.31	0
62	PC1	c3	605	-	40,40,53	0.33	0	46,48,61	0.41	0
62	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.37	0
62	PC1	n	301	-	31,31,53	0.37	0	37,39,61	0.34	0
63	CDL	7A	201	-	66,66,99	0.36	0	72,78,111	0.37	0
62	PC1	N	301	-	31,31,53	0.37	0	37,39,61	0.34	0
63	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.34	0
63	CDL	m3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
62	PC1	N	302	-	35,35,53	0.36	0	41,43,61	0.32	0
65	FES	FS	201	28	0,4,4	-	-	-		
63	CDL	T	202	-	74,74,99	0.35	0	80,86,111	0.34	0
63	CDL	m3	401	-	93,93,99	0.31	0	99,105,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
63	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.31	0
62	PC1	7C	302	-	53,53,53	0.29	0	59,61,61	0.35	0
63	CDL	A	503	-	50,50,99	0.41	0	56,62,111	0.50	0
63	CDL	C1	706	-	58,58,99	0.38	0	64,70,111	0.40	0
63	CDL	5B	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0
62	PC1	J	302	-	36,36,53	0.35	0	42,44,61	0.31	0
62	PC1	C3	601	-	51,51,53	0.30	0	57,59,61	0.36	0
63	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.33	0
63	CDL	E	401	-	59,59,99	0.38	0	65,71,111	0.38	0
63	CDL	M2	401	-	53,53,99	0.40	0	59,65,111	0.39	0
62	PC1	V	202	-	53,53,53	0.29	0	59,61,61	0.31	0
63	CDL	m1	404	-	65,65,99	0.36	0	71,77,111	0.30	0
59	HEA	C1	702	7	57,67,67	1.19	5 (8%)	61,103,103	1.69	17 (27%)
62	PC1	m2	405	-	40,40,53	0.33	0	46,48,61	0.32	0
63	CDL	7c	301	-	84,84,99	0.33	0	90,96,111	0.33	0
63	CDL	5B	704	-	66,66,99	0.36	0	72,78,111	0.34	0
63	CDL	M3	401	-	93,93,99	0.31	0	99,105,111	0.34	0
62	PC1	m2	402	-	31,31,53	0.37	0	37,39,61	0.35	0
63	CDL	m2	404	-	73,73,99	0.35	0	79,85,111	0.34	0
63	CDL	f	401	-	99,99,99	0.30	0	105,111,111	0.35	0
62	PC1	c1	705	-	48,48,53	0.31	0	54,56,61	0.30	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	0.36	0
63	CDL	5b	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
62	PC1	j	302	-	36,36,53	0.35	0	42,44,61	0.31	0
63	CDL	a	503	-	50,50,99	0.41	0	56,62,111	0.50	0
62	PC1	C1	705	-	48,48,53	0.31	0	54,56,61	0.30	0
63	CDL	Y0	101	-	63,63,99	0.37	0	69,75,111	0.33	0
63	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.30	0
63	CDL	m3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
63	CDL	e	401	-	59,59,99	0.38	0	65,71,111	0.38	0
63	CDL	Y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
62	PC1	7c	303	-	42,42,53	0.33	0	48,50,61	0.29	0
63	CDL	u	201	-	81,81,99	0.33	0	87,93,111	0.32	0
63	CDL	5B	703	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	M2	406	-	53,53,53	0.29	0	59,61,61	0.26	0
63	CDL	T	201	-	67,67,99	0.36	0	73,79,111	0.35	0
63	CDL	F	401	-	99,99,99	0.30	0	105,111,111	0.36	0
62	PC1	M1	404	-	34,34,53	0.35	0	40,42,61	0.31	0
62	PC1	c3	602	-	38,38,53	0.34	0	44,46,61	0.32	0
62	PC1	C3	605	-	40,40,53	0.33	0	46,48,61	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
63	CDL	e	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	C3	604	-	67,67,99	0.36	0	73,79,111	0.30	0
63	CDL	M1	403	-	65,65,99	0.36	0	71,77,111	0.30	0
63	CDL	m1	401	-	94,94,99	0.31	0	100,106,111	0.31	0
62	PC1	n	302	-	35,35,53	0.36	0	41,43,61	0.33	0
63	CDL	7A	202	-	99,99,99	0.30	0	105,111,111	0.29	0
62	PC1	7C	304	-	42,42,53	0.33	0	48,50,61	0.29	0
63	CDL	M2	403	-	65,65,99	0.36	0	71,77,111	0.32	0
62	PC1	M2	402	-	31,31,53	0.37	0	37,39,61	0.35	0
62	PC1	m1	405	-	34,34,53	0.35	0	40,42,61	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	CDL	y0	101	-	-	19/74/74/110	-
62	PC1	A	501	-	-	11/48/48/57	-
63	CDL	7C	303	-	-	16/61/61/110	-
62	PC1	M2	405	-	-	11/44/44/57	-
62	PC1	a	502	-	-	9/44/44/57	-
63	CDL	M1	402	-	-	15/76/76/110	-
63	CDL	j	301	-	-	15/80/80/110	-
63	CDL	k	301	-	-	15/72/72/110	-
59	HEA	c1	702	7	3/3/7/16	11/32/76/76	-
62	PC1	C3	603	-	-	10/34/34/57	-
63	CDL	7a	201	-	-	13/77/77/110	-
63	CDL	Y7	501	-	-	14/75/75/110	-
63	CDL	m1	403	-	-	15/76/76/110	-
63	CDL	m2	401	-	-	20/64/64/110	-
62	PC1	m1	402	-	-	16/57/57/57	-
63	CDL	c1	706	-	-	19/69/69/110	-
63	CDL	U	201	-	-	18/92/92/110	-
63	CDL	E	402	-	-	14/82/82/110	-
63	CDL	M3	403	-	-	19/73/73/110	-
65	FES	fs	201	28	-	-	0/1/1/1
63	CDL	c1	707	-	-	12/75/75/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	CDL	7C	301	-	-	24/95/95/110	-
62	PC1	C3	602	-	-	10/42/42/57	-
63	CDL	M3	402	-	-	13/61/61/110	-
63	CDL	v	201	-	-	14/101/101/110	-
62	PC1	a	501	-	-	14/48/48/57	-
62	PC1	m2	406	-	-	9/57/57/57	-
63	CDL	7c	302	-	-	16/61/61/110	-
65	FES	fs	202	28	-	-	0/1/1/1
63	CDL	b	501	-	-	16/72/72/110	-
63	CDL	t	202	-	-	14/85/85/110	-
63	CDL	N	303	-	-	22/105/105/110	-
63	CDL	t	201	-	-	13/78/78/110	-
63	CDL	n	303	-	-	22/105/105/110	-
62	PC1	A	502	-	-	10/44/44/57	-
63	CDL	M1	401	-	-	27/105/105/110	-
63	CDL	5b	703	-	-	12/77/77/110	-
65	FES	FS	202	28	-	-	0/1/1/1
59	HEA	C1	701	7	3/3/7/16	17/32/76/76	-
59	HEA	c1	701	7	3/3/7/16	17/32/76/76	-
63	CDL	C1	707	-	-	12/75/75/110	-
63	CDL	y7	501	-	-	13/75/75/110	-
62	PC1	c3	603	-	-	10/34/34/57	-
63	CDL	7a	202	-	-	23/110/110/110	-
63	CDL	c3	604	-	-	9/78/78/110	-
62	PC1	v	202	-	-	10/57/57/57	-
62	PC1	c3	605	-	-	9/44/44/57	-
62	PC1	c3	601	-	-	12/55/55/57	-
62	PC1	n	301	-	-	13/35/35/57	-
63	CDL	7A	201	-	-	13/77/77/110	-
62	PC1	N	301	-	-	13/35/35/57	-
63	CDL	M2	404	-	-	18/84/84/110	-
63	CDL	m3	403	-	-	19/73/73/110	-
62	PC1	N	302	-	-	7/39/39/57	-
65	FES	FS	201	28	-	-	0/1/1/1
63	CDL	T	202	-	-	13/85/85/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	CDL	m3	401	-	-	19/104/104/110	-
63	CDL	m2	403	-	-	16/76/76/110	-
62	PC1	7C	302	-	-	17/57/57/57	-
63	CDL	A	503	-	-	10/61/61/110	-
63	CDL	C1	706	-	-	18/69/69/110	-
63	CDL	5B	702	-	-	23/97/97/110	-
63	CDL	L	301	-	-	21/84/84/110	-
62	PC1	J	302	-	-	9/40/40/57	-
62	PC1	C3	601	-	-	12/55/55/57	-
63	CDL	B	501	-	-	17/72/72/110	-
63	CDL	E	401	-	-	18/70/70/110	-
63	CDL	M2	401	-	-	16/64/64/110	-
62	PC1	V	202	-	-	10/57/57/57	-
63	CDL	m1	404	-	-	10/76/76/110	-
59	HEA	C1	702	7	3/3/7/16	10/32/76/76	-
62	PC1	m2	405	-	-	7/44/44/57	-
63	CDL	7c	301	-	-	26/95/95/110	-
63	CDL	5B	704	-	-	11/77/77/110	-
63	CDL	M3	401	-	-	20/104/104/110	-
62	PC1	m2	402	-	-	3/35/35/57	-
63	CDL	m2	404	-	-	17/84/84/110	-
63	CDL	f	401	-	-	20/110/110/110	-
62	PC1	c1	705	-	-	8/52/52/57	-
63	CDL	l	301	-	-	22/84/84/110	-
63	CDL	V	201	-	-	14/101/101/110	-
63	CDL	5b	702	-	-	24/97/97/110	-
63	CDL	y5	201	-	-	16/91/91/110	-
62	PC1	j	302	-	-	10/40/40/57	-
63	CDL	a	503	-	-	14/61/61/110	-
62	PC1	C1	705	-	-	11/52/52/57	-
63	CDL	Y0	101	-	-	19/74/74/110	-
63	CDL	J	301	-	-	14/80/80/110	-
63	CDL	m3	402	-	-	13/61/61/110	-
63	CDL	e	401	-	-	16/70/70/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	CDL	Y5	201	-	-	16/91/91/110	-
62	PC1	7c	303	-	-	13/46/46/57	-
63	CDL	u	201	-	-	17/92/92/110	-
63	CDL	5B	703	-	-	14/72/72/110	-
62	PC1	M2	406	-	-	9/57/57/57	-
63	CDL	T	201	-	-	13/78/78/110	-
63	CDL	F	401	-	-	23/110/110/110	-
62	PC1	M1	404	-	-	8/38/38/57	-
62	PC1	c3	602	-	-	9/42/42/57	-
62	PC1	C3	605	-	-	10/44/44/57	-
63	CDL	e	402	-	-	15/82/82/110	-
63	CDL	C3	604	-	-	9/78/78/110	-
63	CDL	M1	403	-	-	10/76/76/110	-
63	CDL	m1	401	-	-	26/105/105/110	-
62	PC1	n	302	-	-	6/39/39/57	-
63	CDL	7A	202	-	-	21/110/110/110	-
62	PC1	7C	304	-	-	12/46/46/57	-
63	CDL	M2	403	-	-	17/76/76/110	-
62	PC1	M2	402	-	-	4/35/35/57	-
62	PC1	m1	405	-	-	8/38/38/57	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	702	HEA	C3A-C2A	-3.67	1.35	1.40
59	C1	702	HEA	C3A-C2A	-3.64	1.35	1.40
59	c1	702	HEA	C4D-C3D	3.21	1.50	1.45
59	C1	702	HEA	C4D-C3D	3.20	1.50	1.45
59	C1	701	HEA	C1D-ND	-2.97	1.35	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	C1	702	HEA	C13-C12-C11	-5.12	106.65	114.35
59	c1	702	HEA	C13-C12-C11	-5.07	106.73	114.35
59	C1	701	HEA	C13-C12-C11	-3.87	108.53	114.35
59	C1	701	HEA	C4B-NB-C1B	3.81	109.01	105.07
59	c1	701	HEA	C13-C12-C11	-3.81	108.63	114.35

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
59	C1	701	HEA	NB
59	C1	701	HEA	NA
59	C1	701	HEA	ND
59	C1	702	HEA	NB
59	C1	702	HEA	NA

5 of 1527 torsion outliers are listed below:

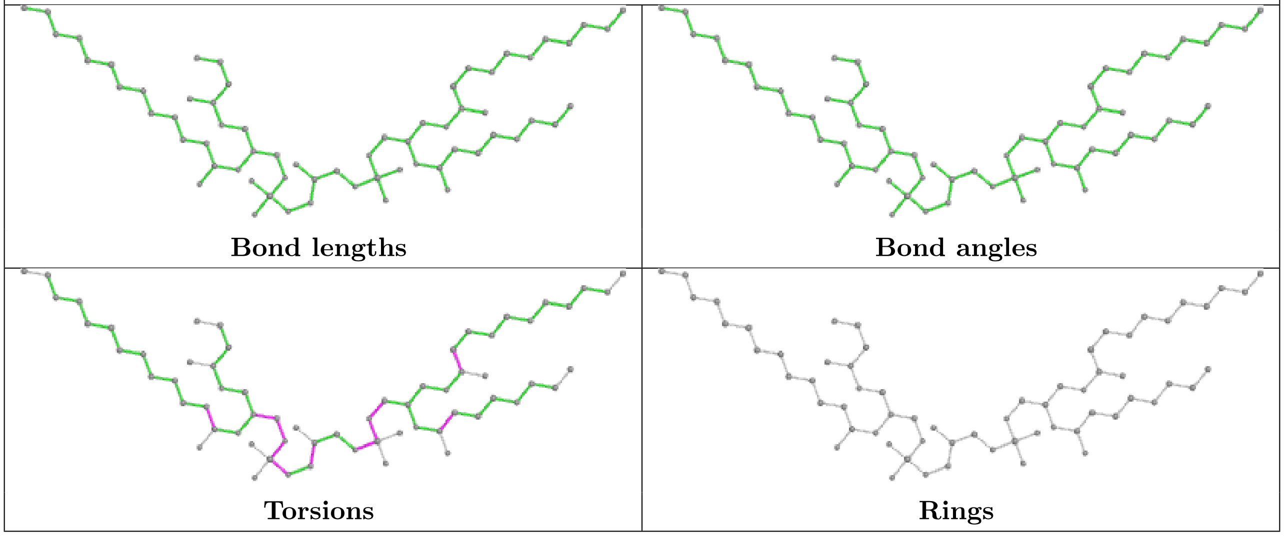
Mol	Chain	Res	Type	Atoms
59	C1	701	HEA	C1A-C2A-CAA-CBA
59	C1	701	HEA	C3A-C2A-CAA-CBA
59	C1	701	HEA	C26-C15-C16-C17
59	C1	701	HEA	C15-C16-C17-C18
59	C1	701	HEA	C17-C18-C19-C20

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand CDL y0 101



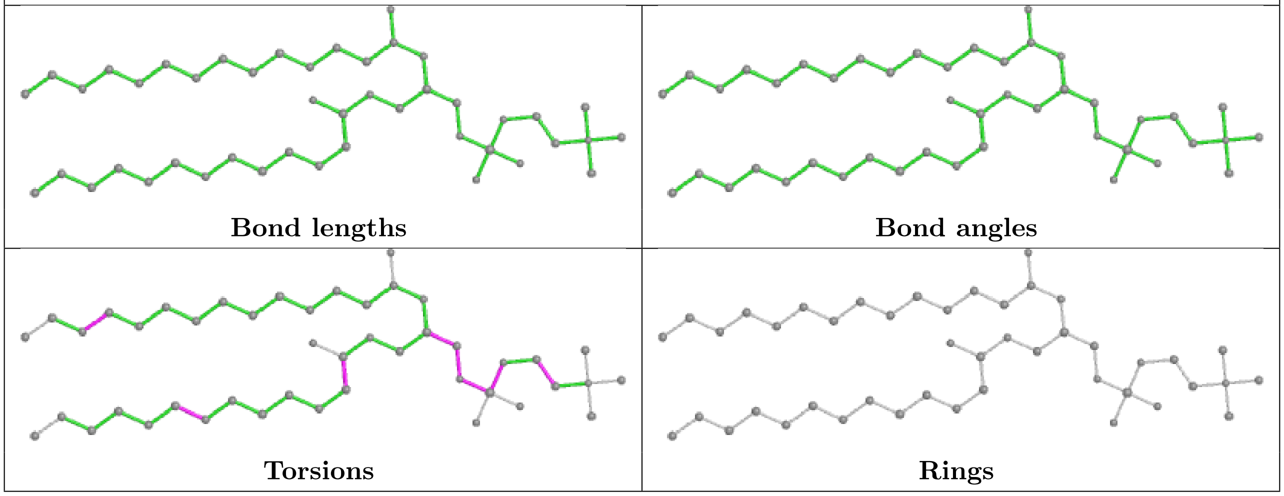
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 501



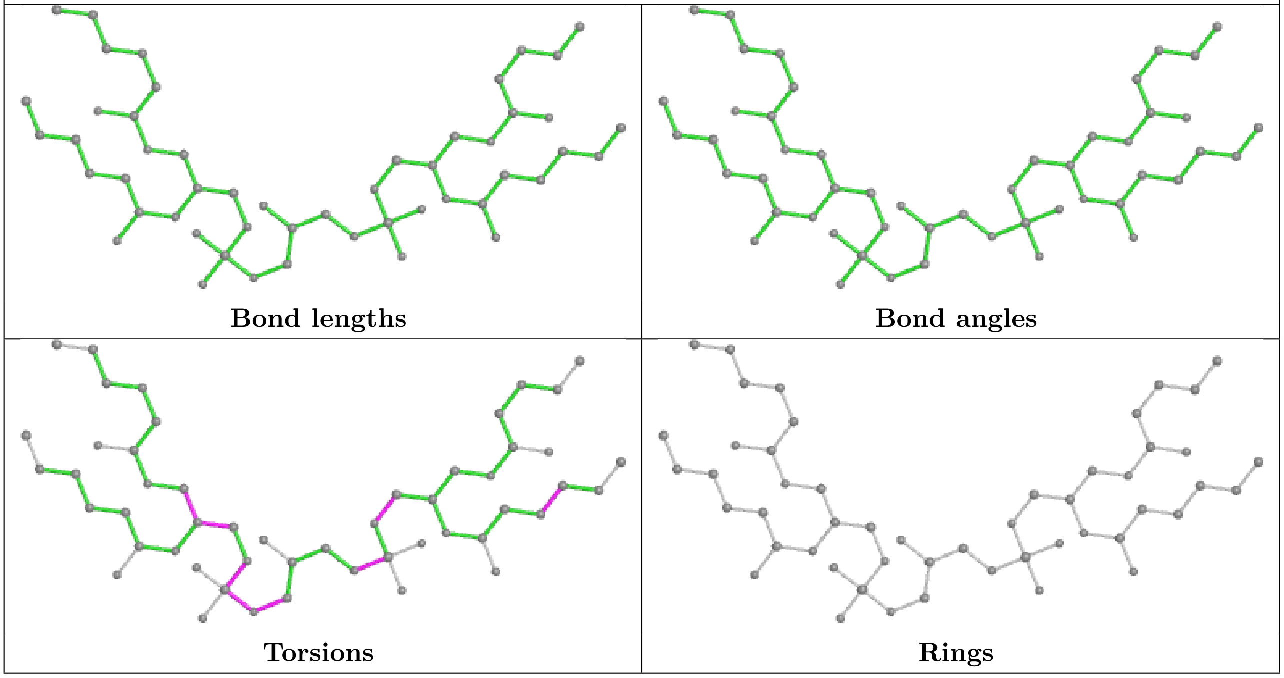
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL 7C 303



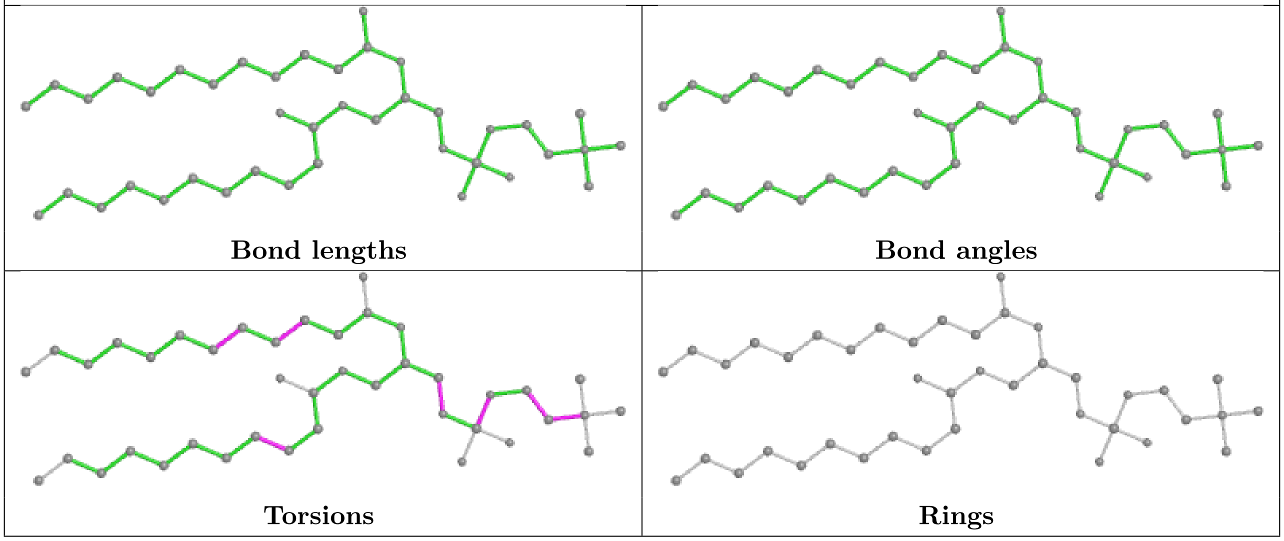
Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 M2 405



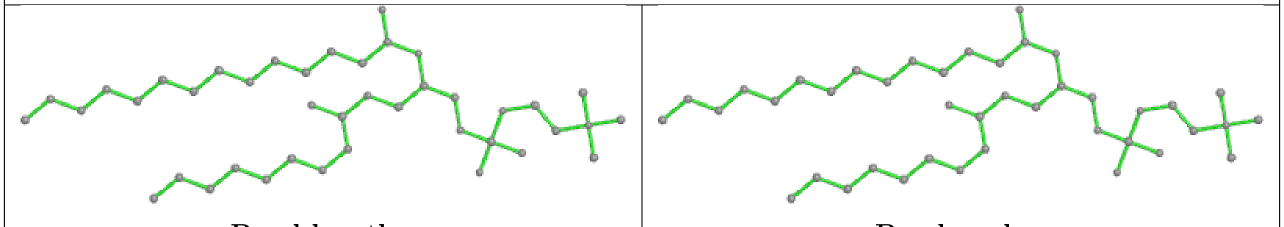
Bond lengths

Bond angles

Torsions

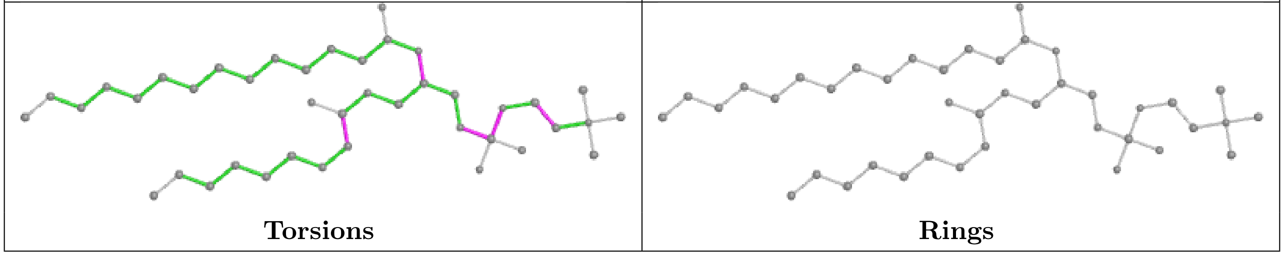
Rings

Ligand PC1 a 502



Bond lengths

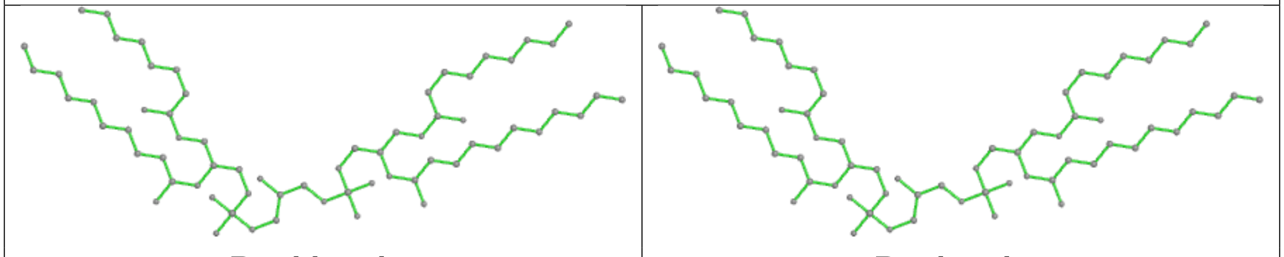
Bond angles



Torsions

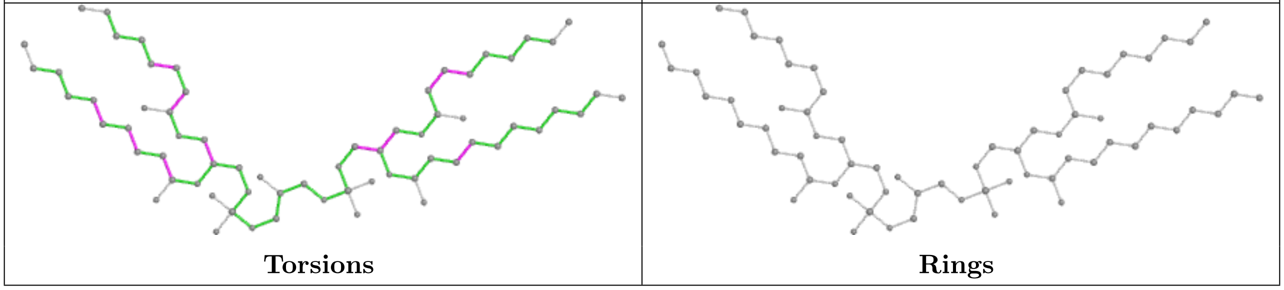
Rings

Ligand CDL M1 402



Bond lengths

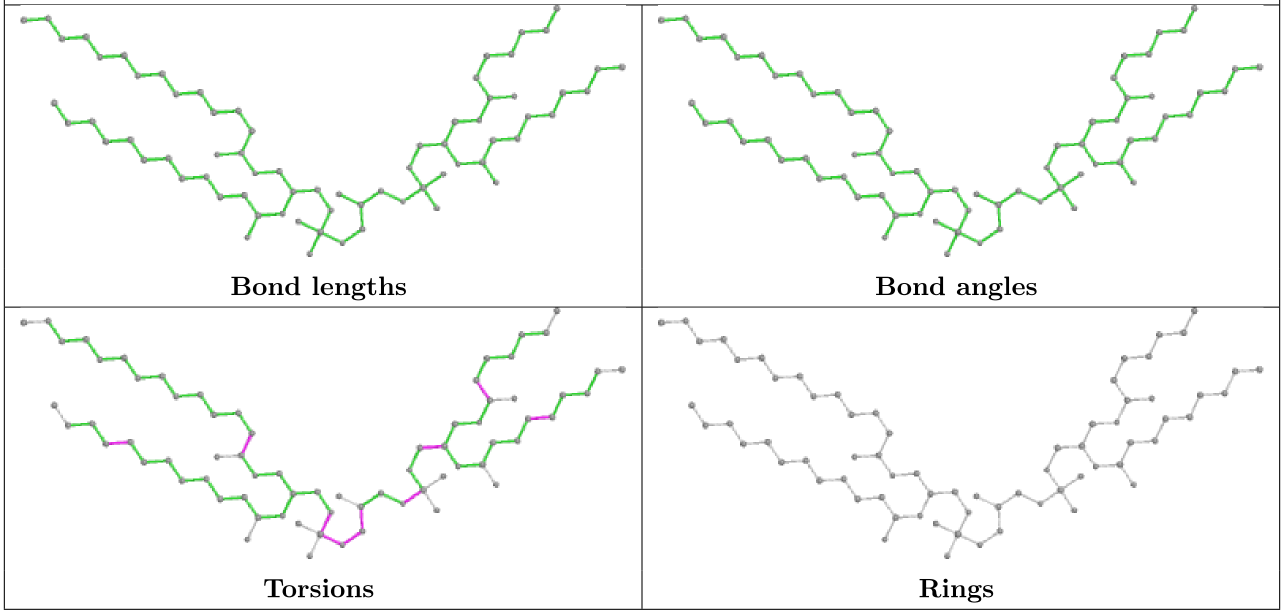
Bond angles



Torsions

Rings

Ligand CDL j 301



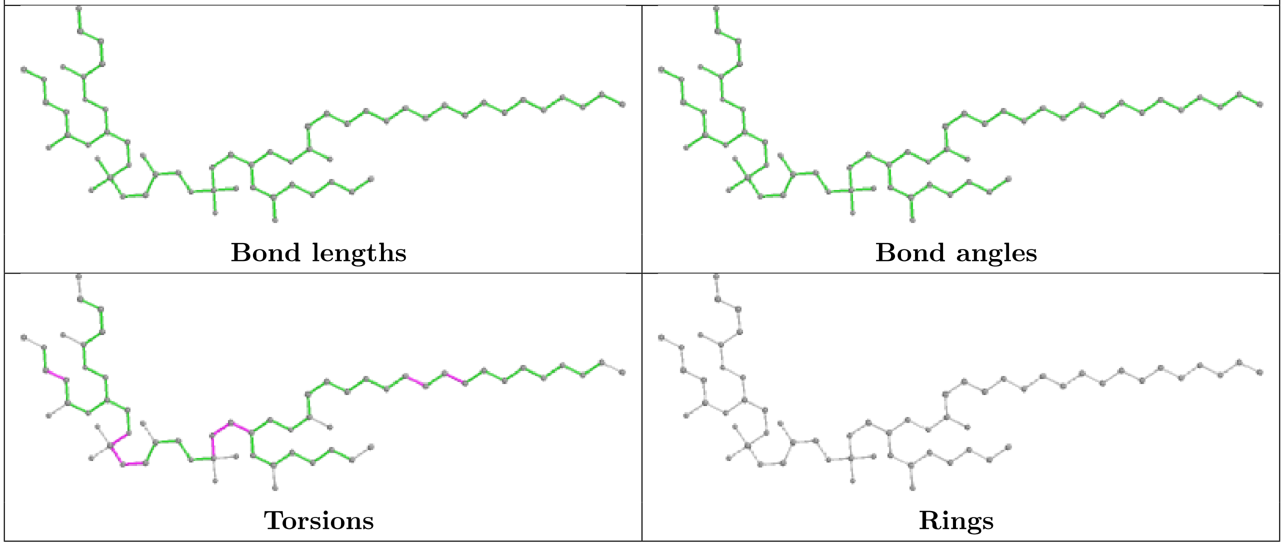
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL k 301



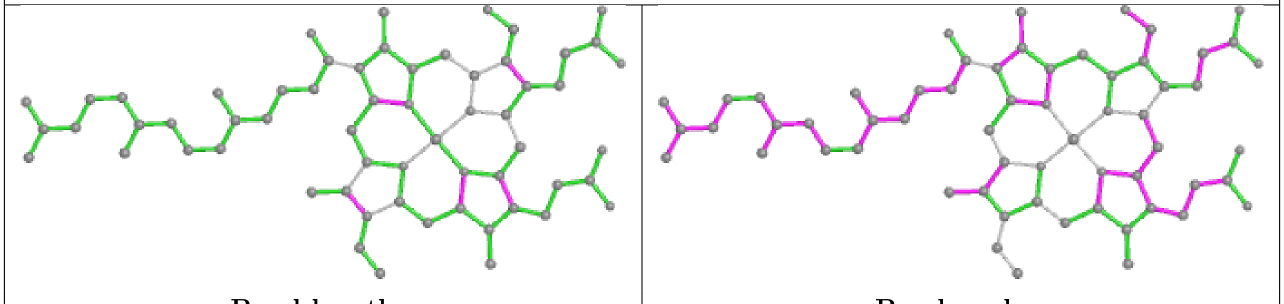
Bond lengths

Bond angles

Torsions

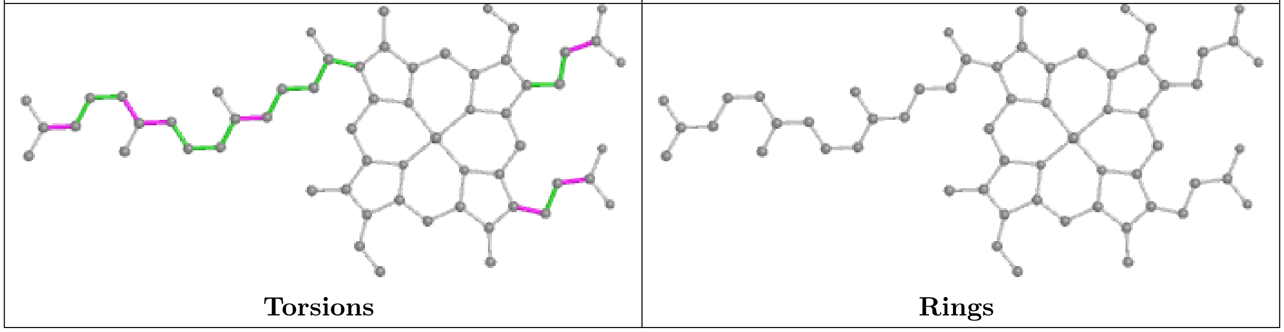
Rings

Ligand HEA c1 702



Bond lengths

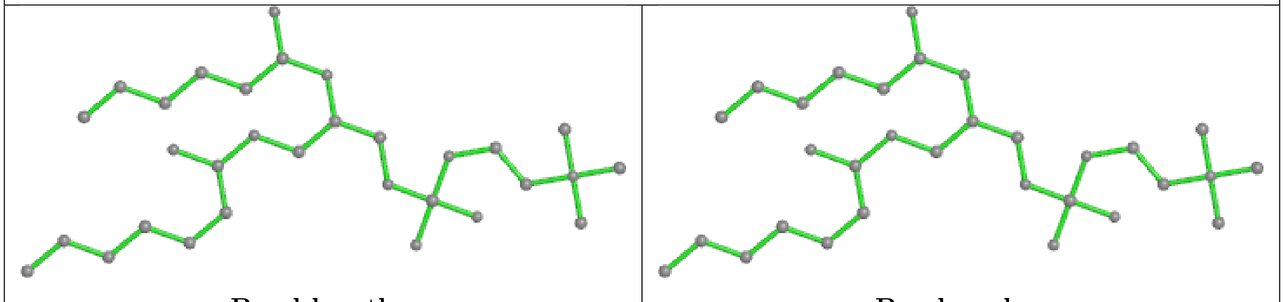
Bond angles



Torsions

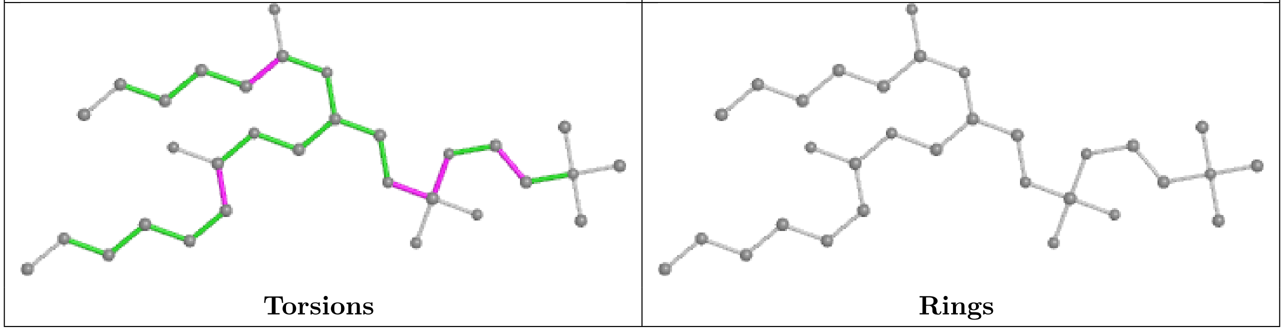
Rings

Ligand PC1 C3 603



Bond lengths

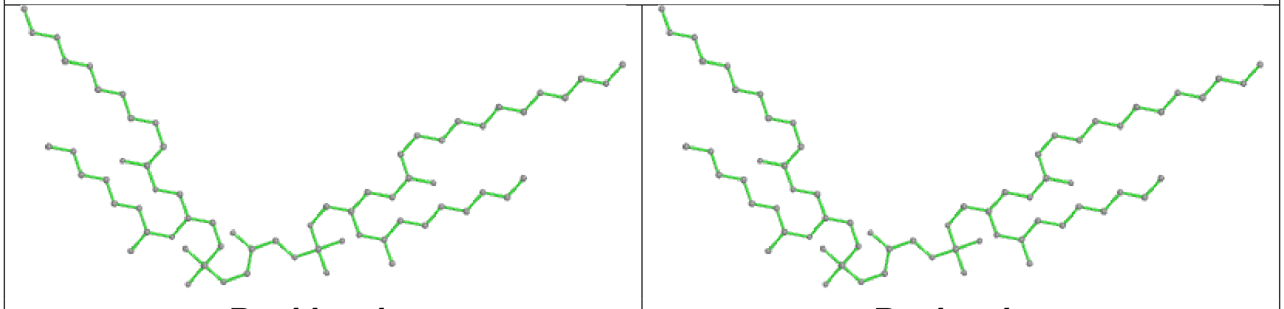
Bond angles



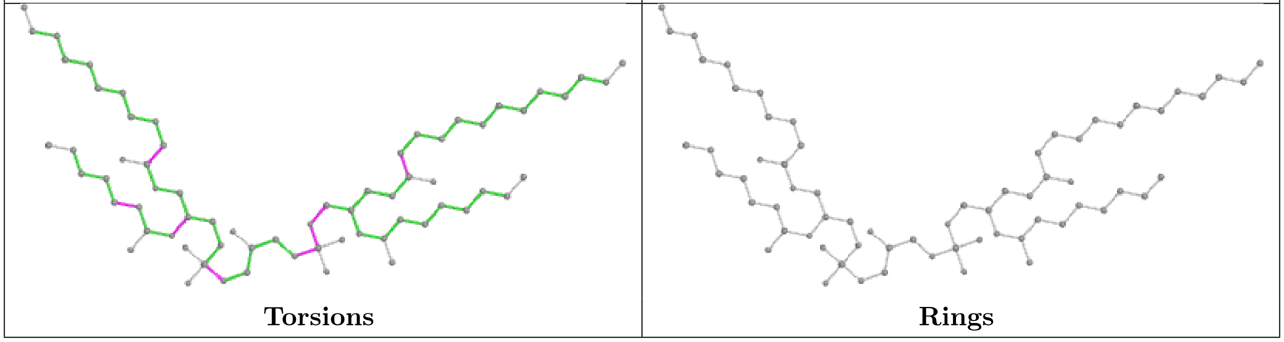
Torsions

Rings

Ligand CDL 7a 201

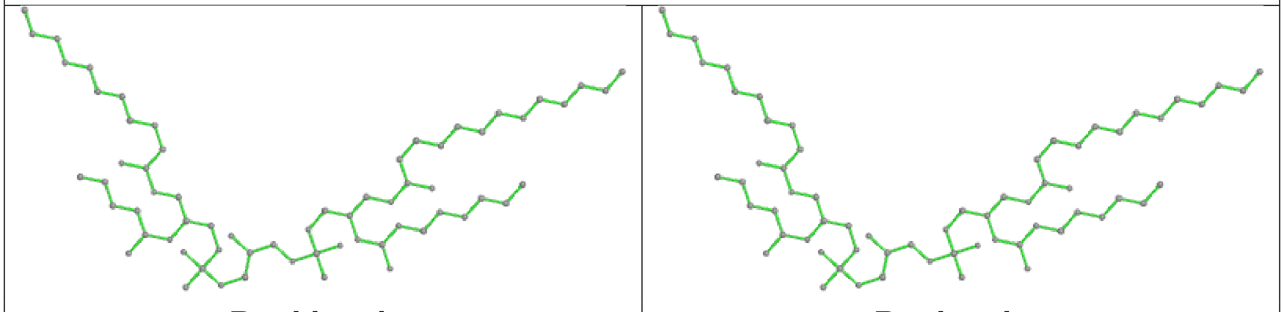


Bond lengths Bond angles

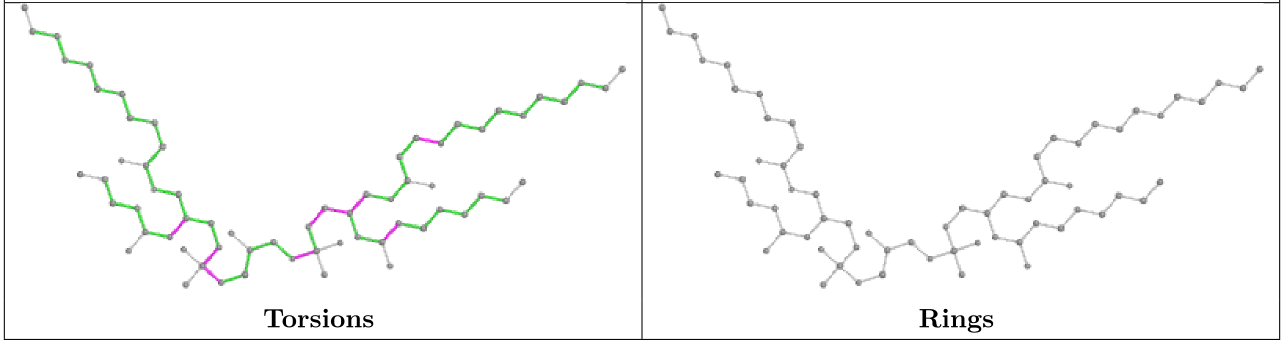


Torsions Rings

Ligand CDL Y7 501

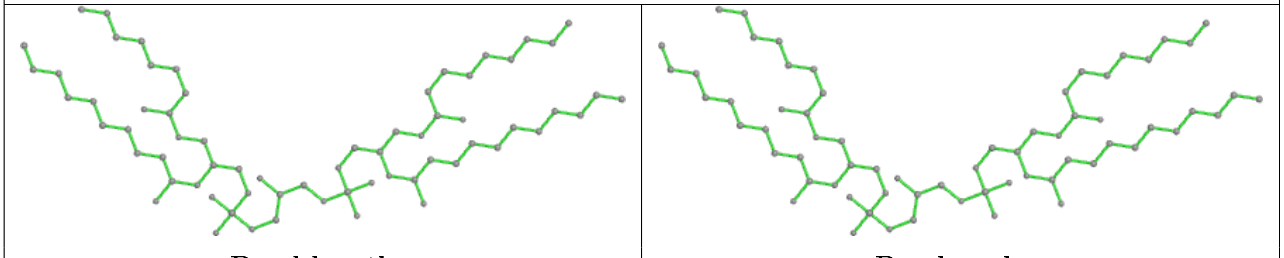


Bond lengths Bond angles



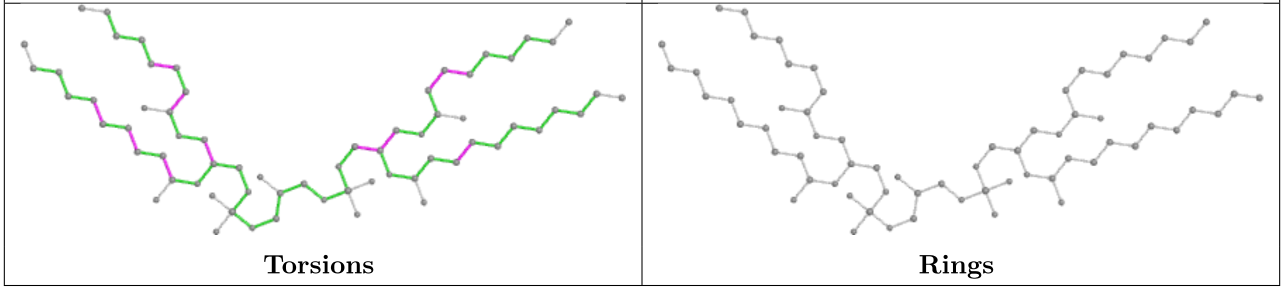
Torsions Rings

Ligand CDL m1 403



Bond lengths

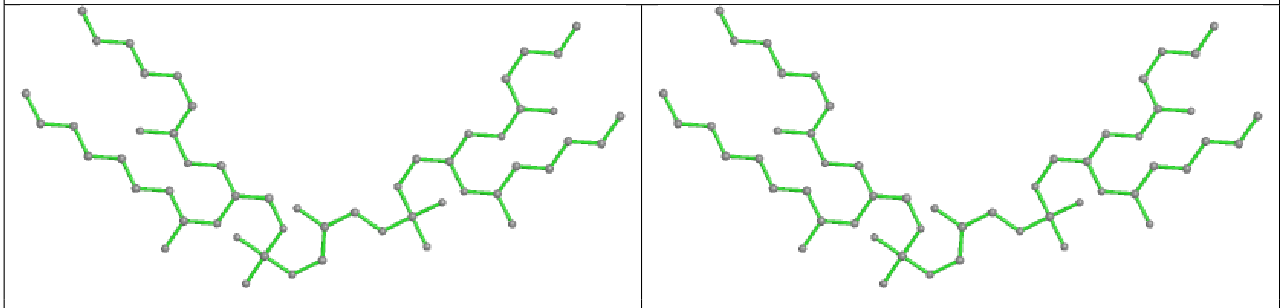
Bond angles



Torsions

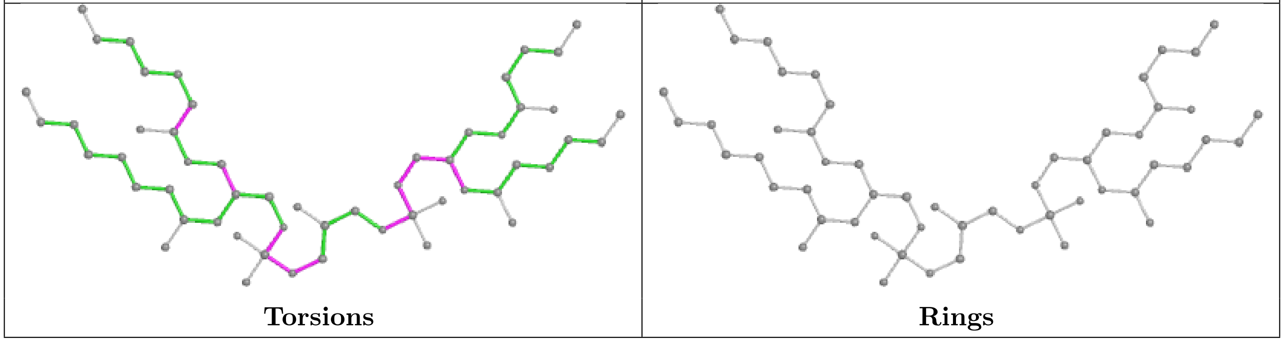
Rings

Ligand CDL m2 401



Bond lengths

Bond angles



Torsions

Rings

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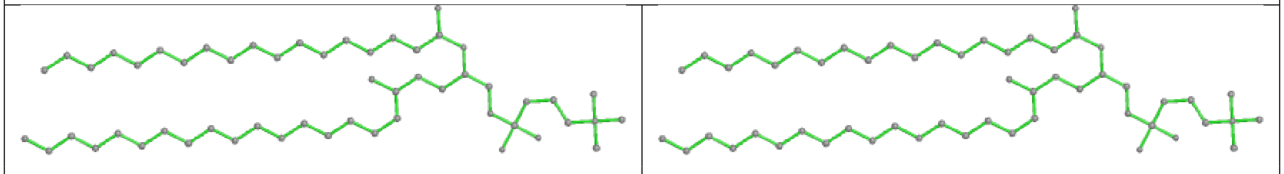
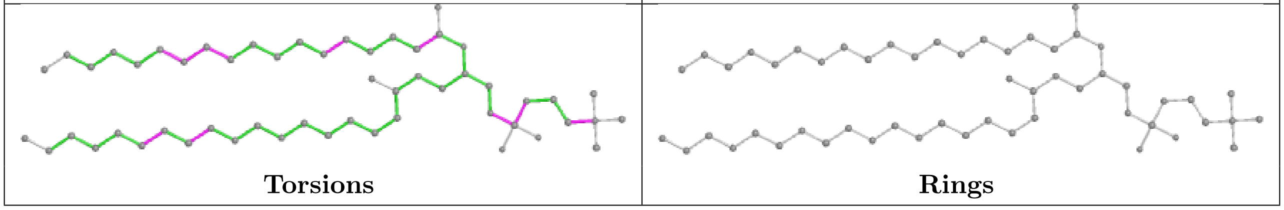


Bond lengths

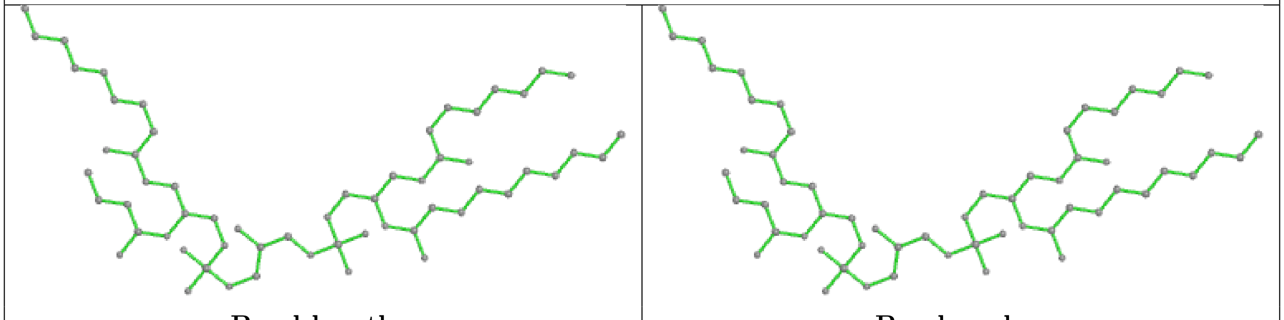
Bond angles



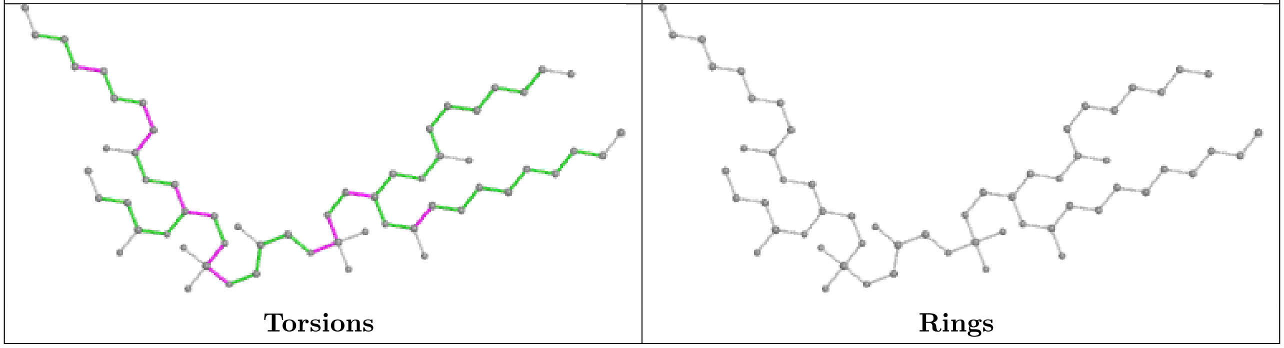
Torsions

Rings

Ligand CDL c1 706

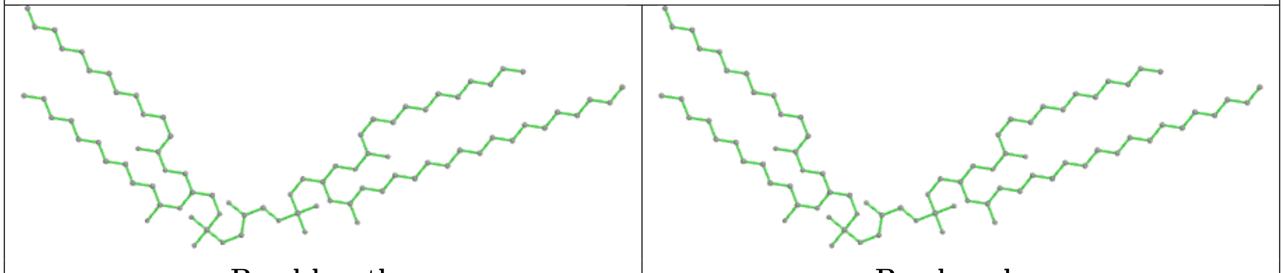


Bond lengths **Bond angles**

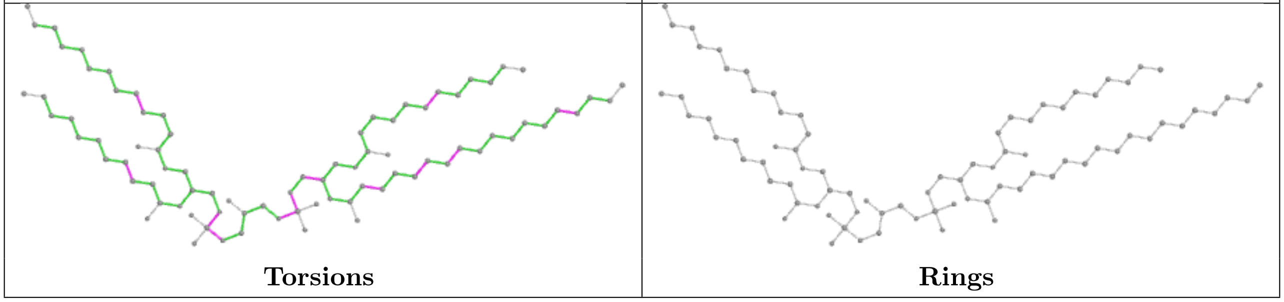


Torsions **Rings**

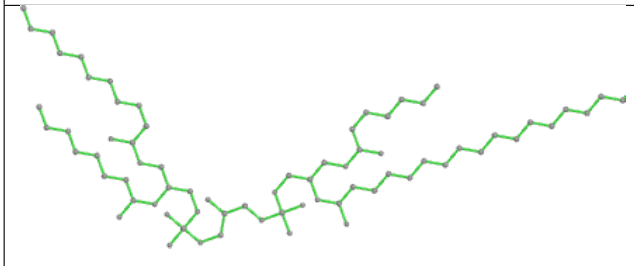
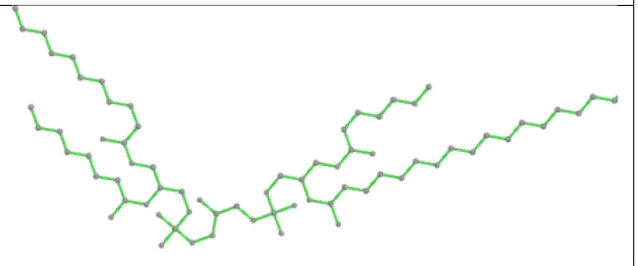
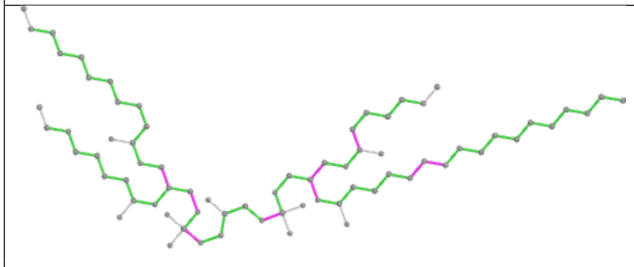
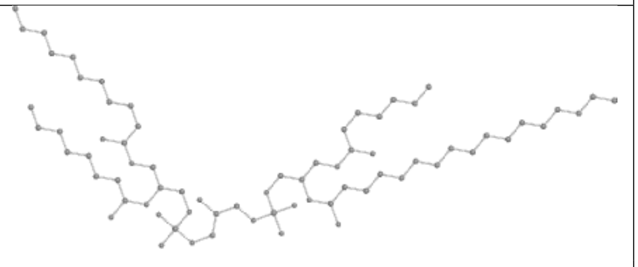
Ligand CDL U 201



Bond lengths **Bond angles**



Torsions **Rings**

Ligand CDL E 402	
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

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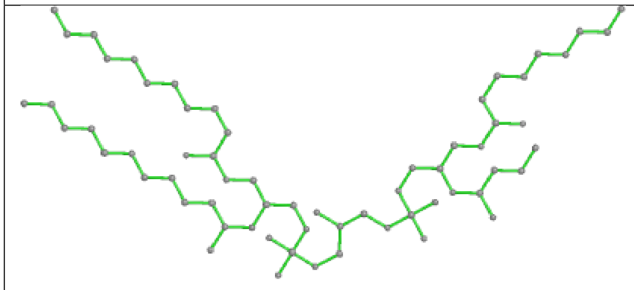
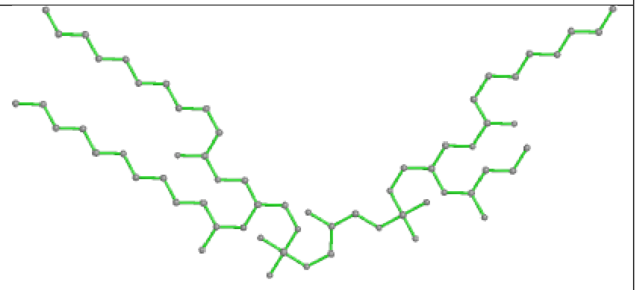
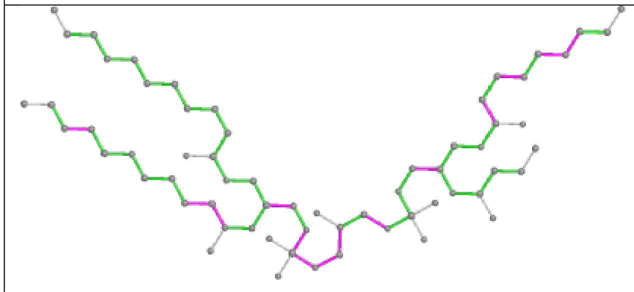
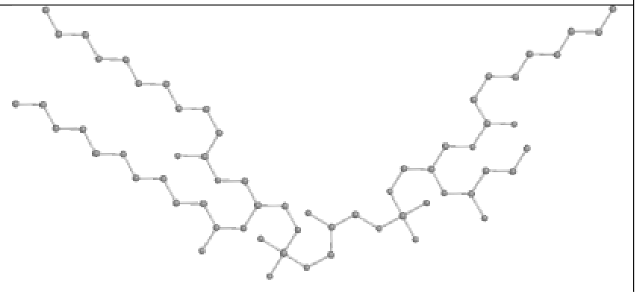
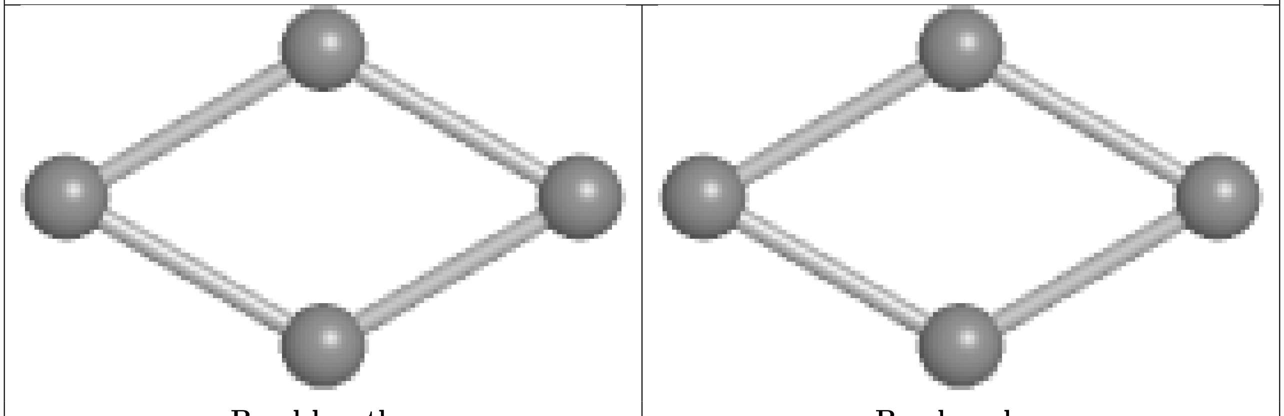
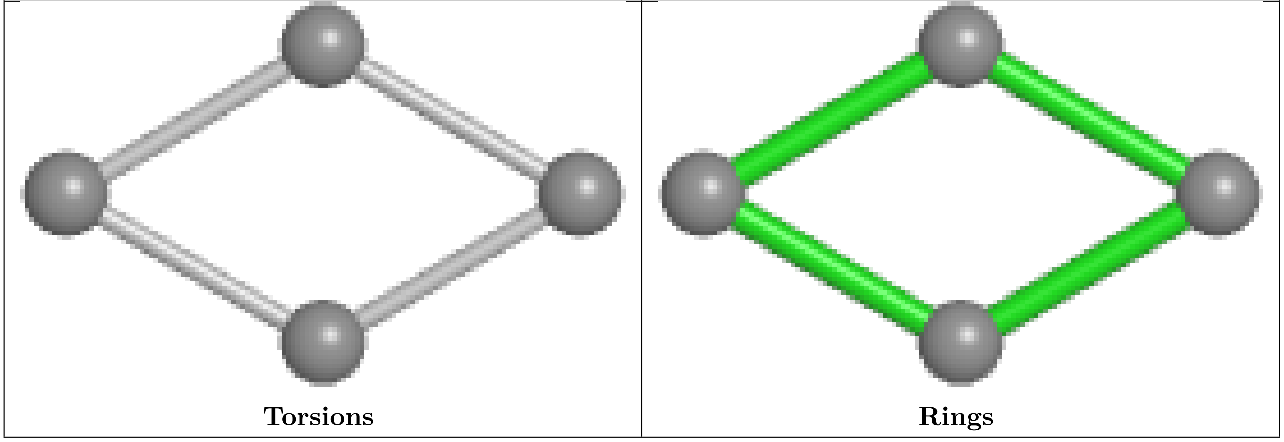
 **Bond lengths**	 **Bond angles**
 **Torsions**	 **Rings**

Ligand FES fs 201

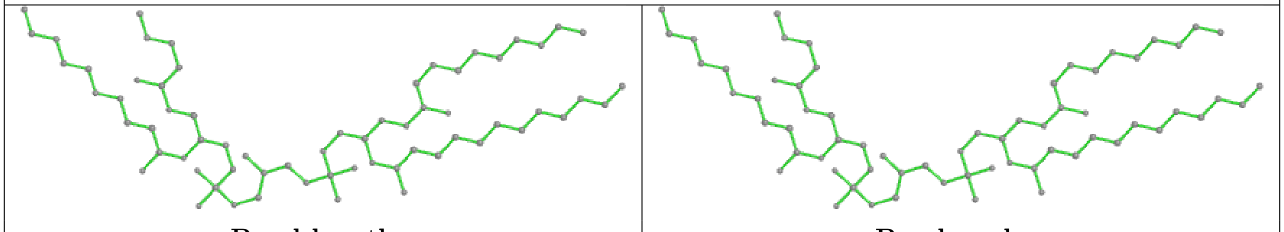


Bond lengths Bond angles

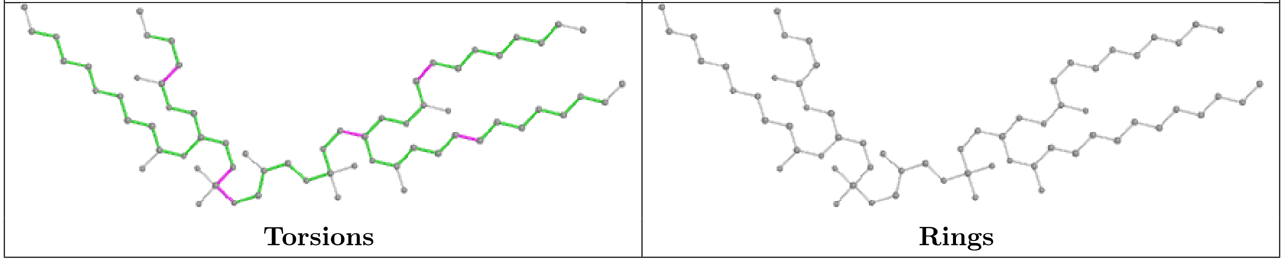


Torsions Rings

Ligand CDL c1 707

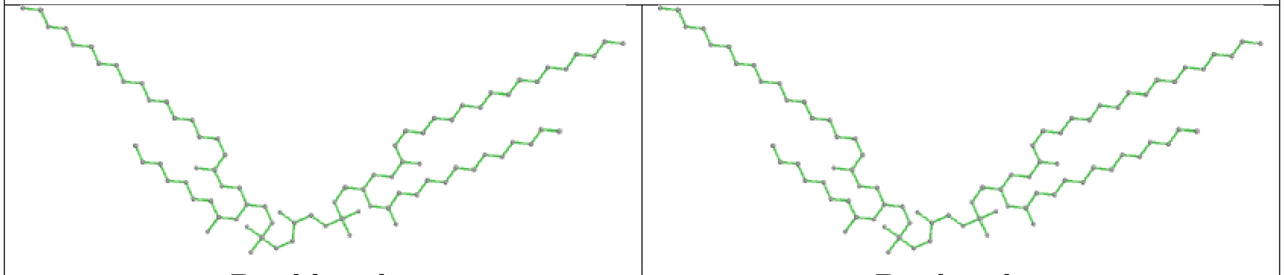


Bond lengths Bond angles



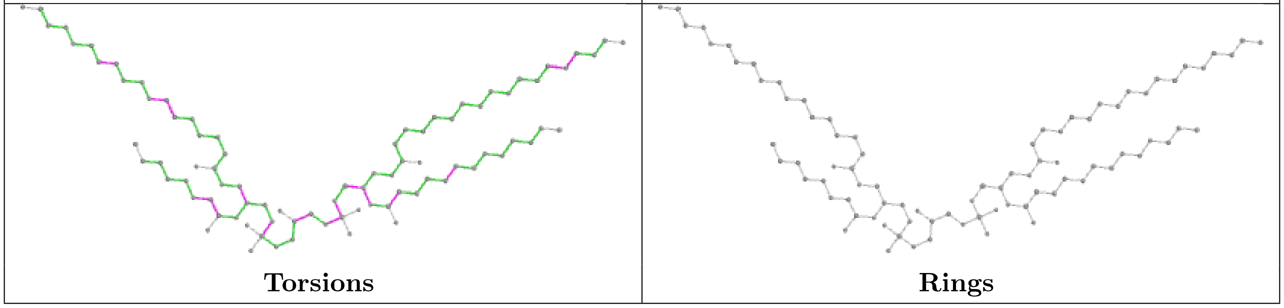
Torsions Rings

Ligand CDL 7C 301



Bond lengths

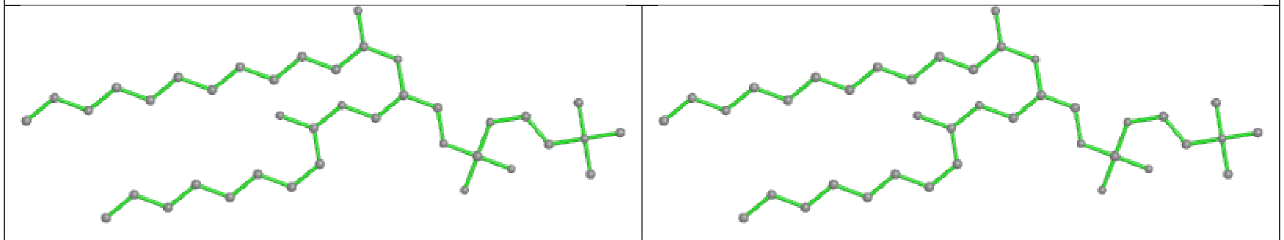
Bond angles



Torsions

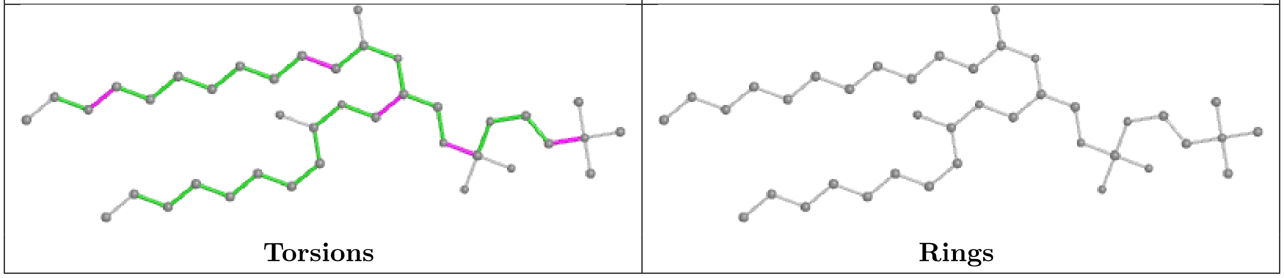
Rings

Ligand PC1 C3 602



Bond lengths

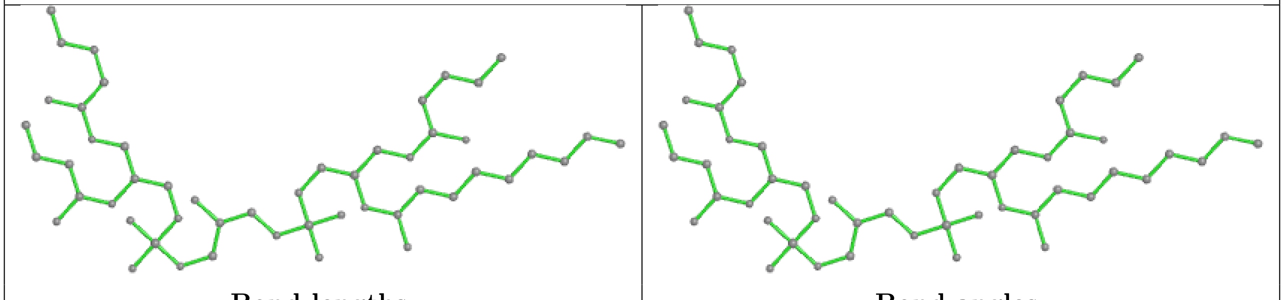
Bond angles



Torsions

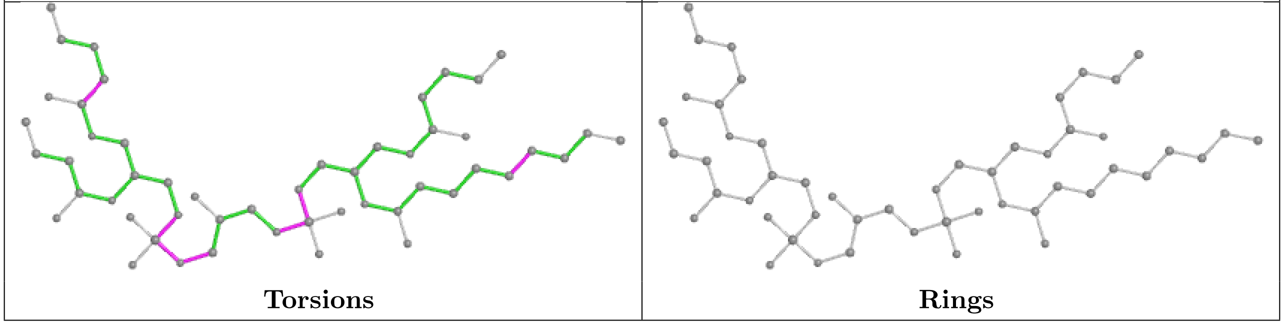
Rings

Ligand CDL M3 402



Bond lengths

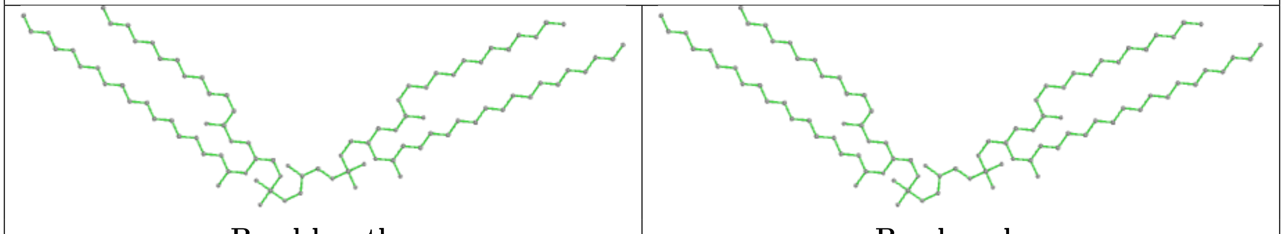
Bond angles



Torsions

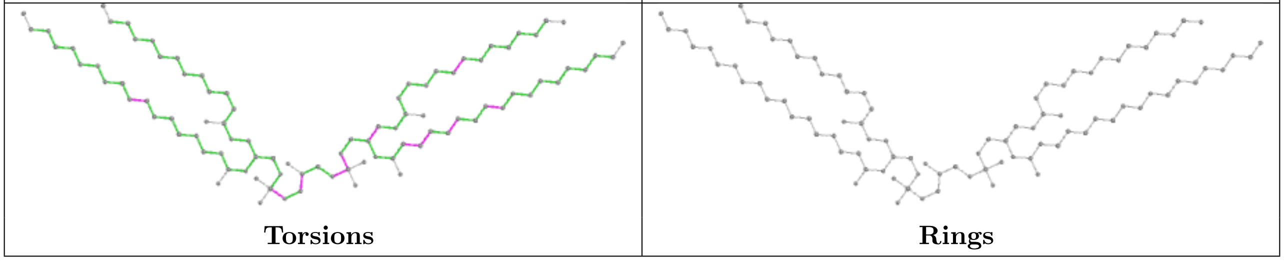
Rings

Ligand CDL v 201



Bond lengths

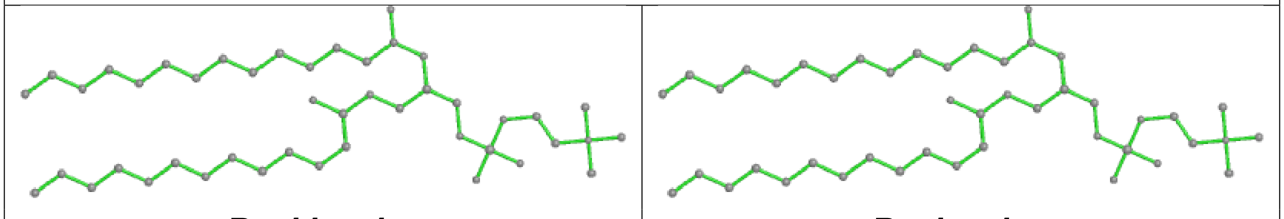
Bond angles



Torsions

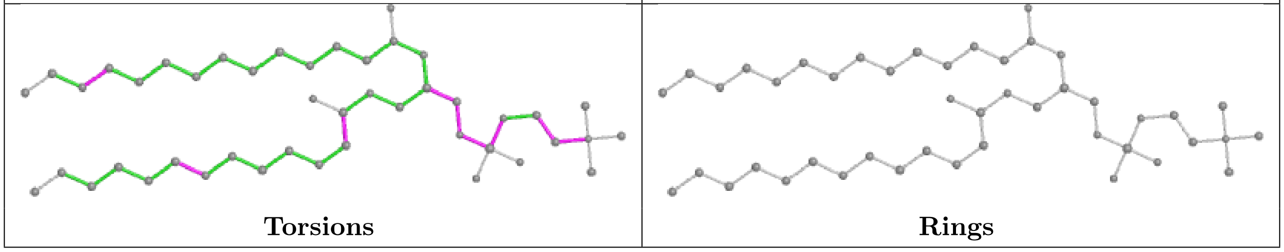
Rings

Ligand PC1 a 501



Bond lengths

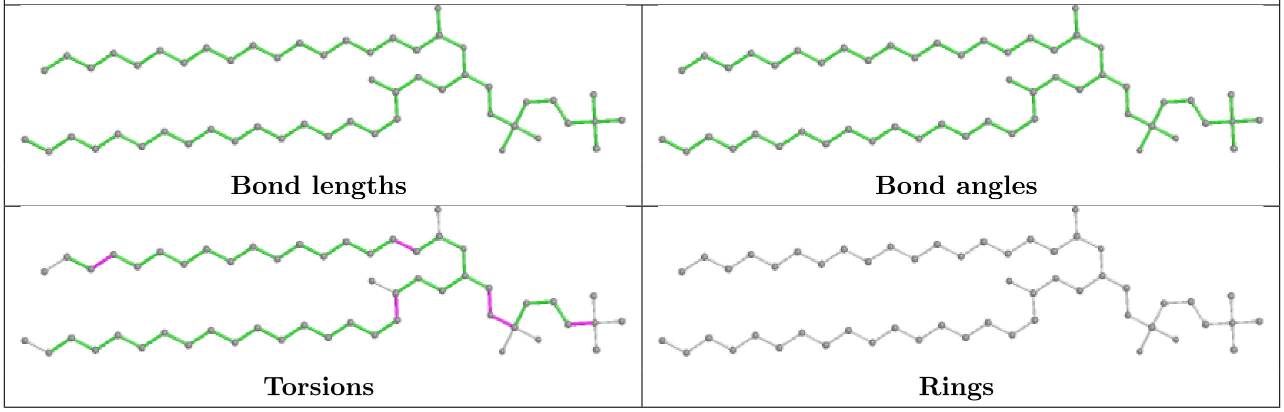
Bond angles



Torsions

Rings

Ligand PC1 m2 406



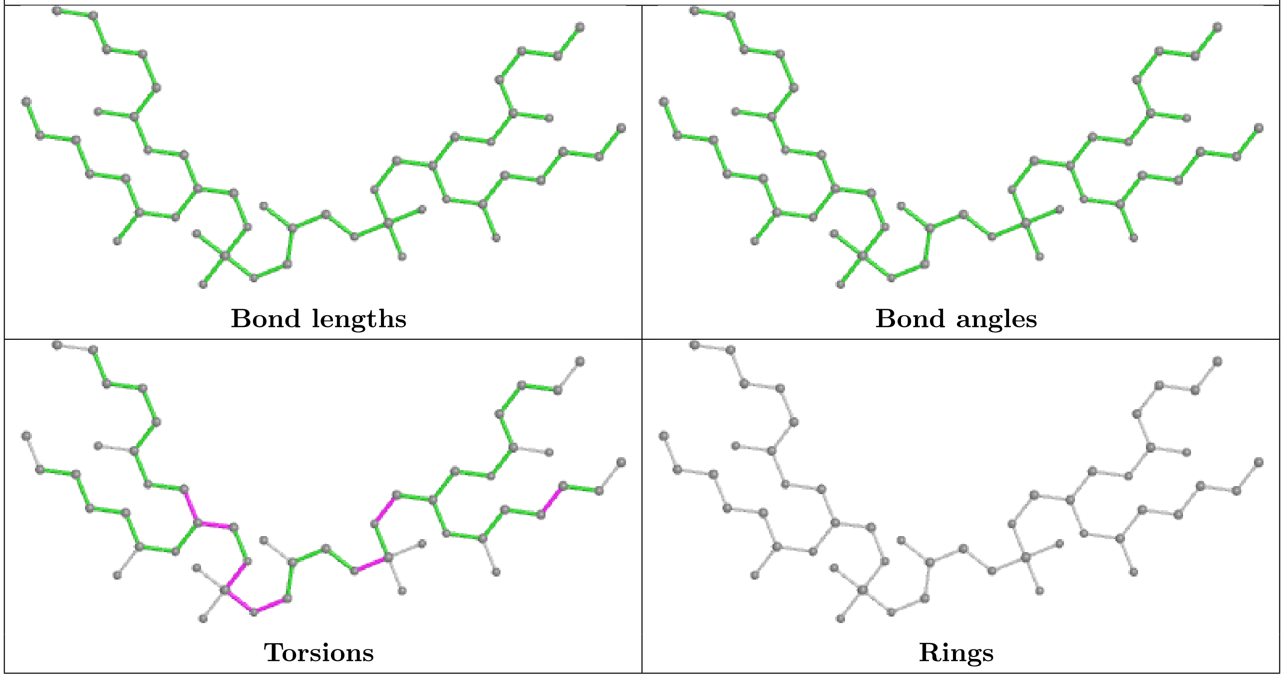
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL 7c 302



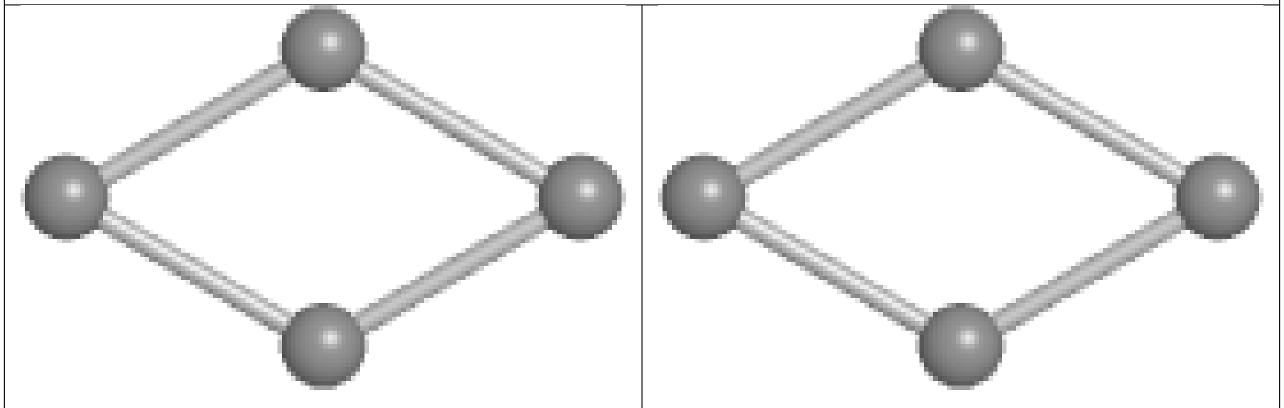
Bond lengths

Bond angles

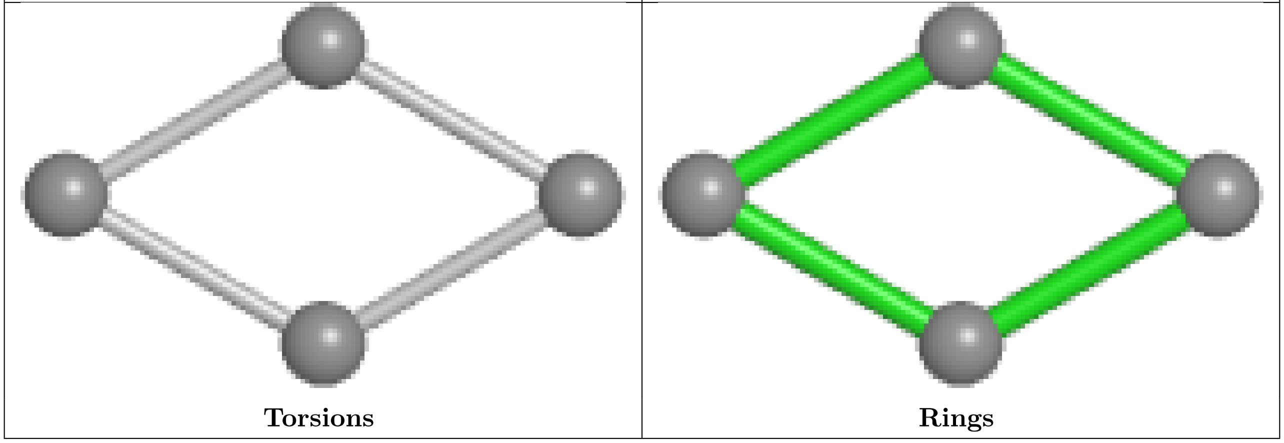
Torsions

Rings

Ligand FES fs 202

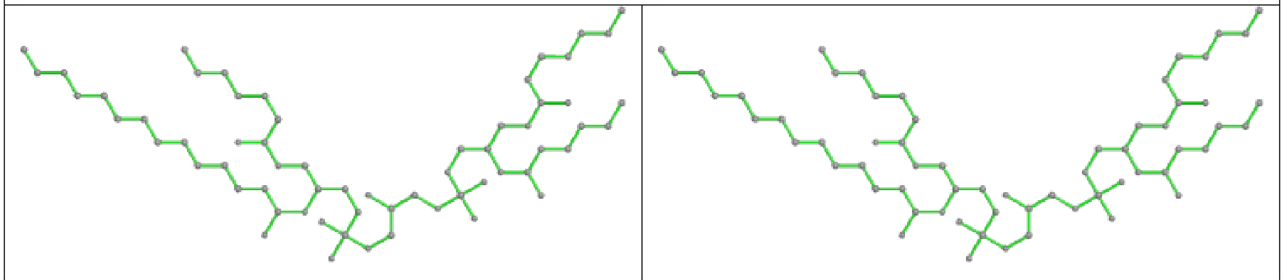


Bond lengths | Bond angles

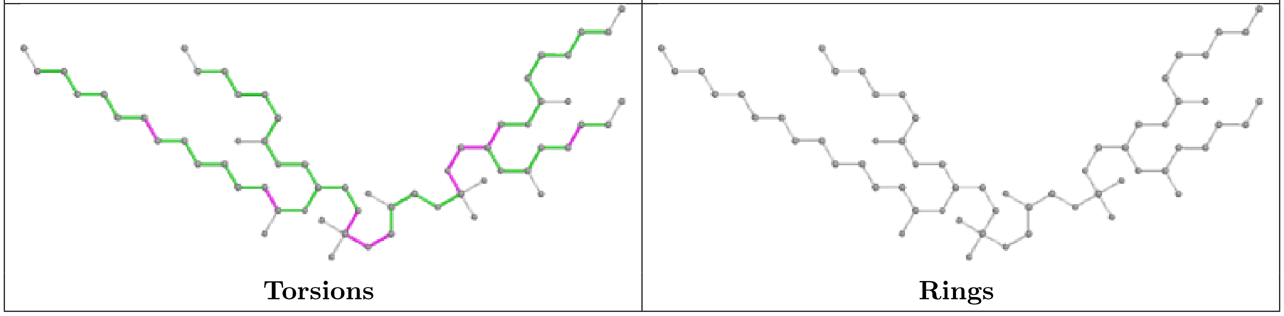


Torsions | Rings

Ligand CDL b 501

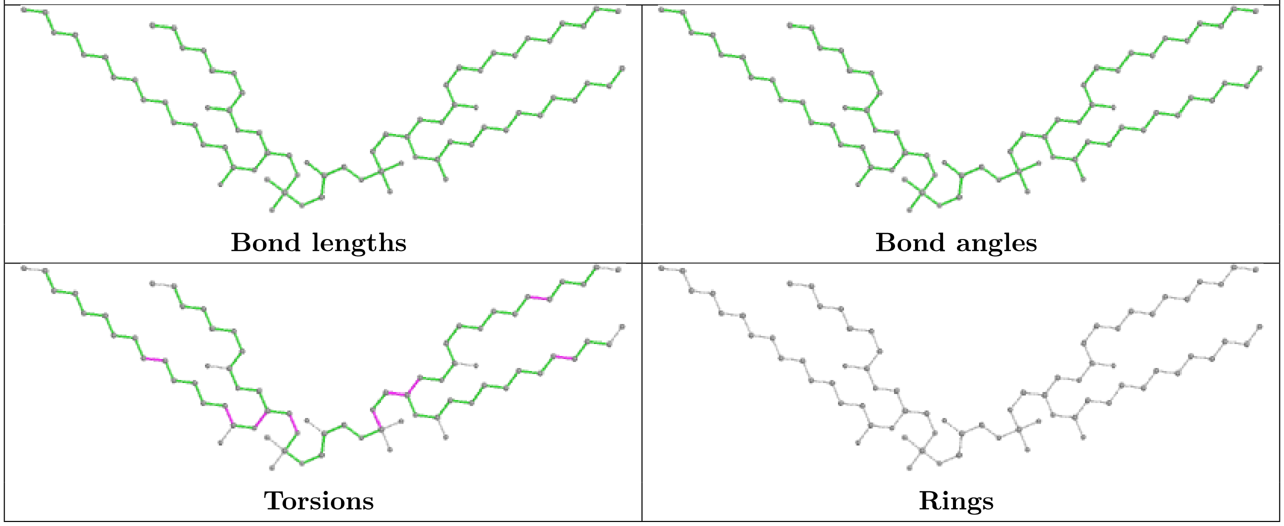


Bond lengths | Bond angles



Torsions | Rings

Ligand CDL t 202



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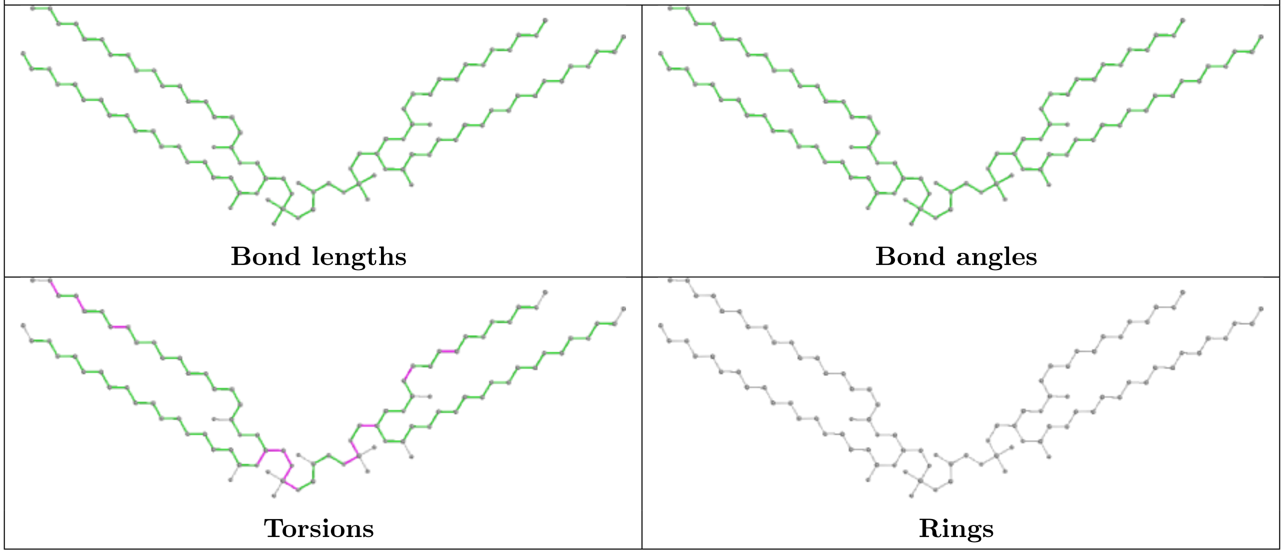

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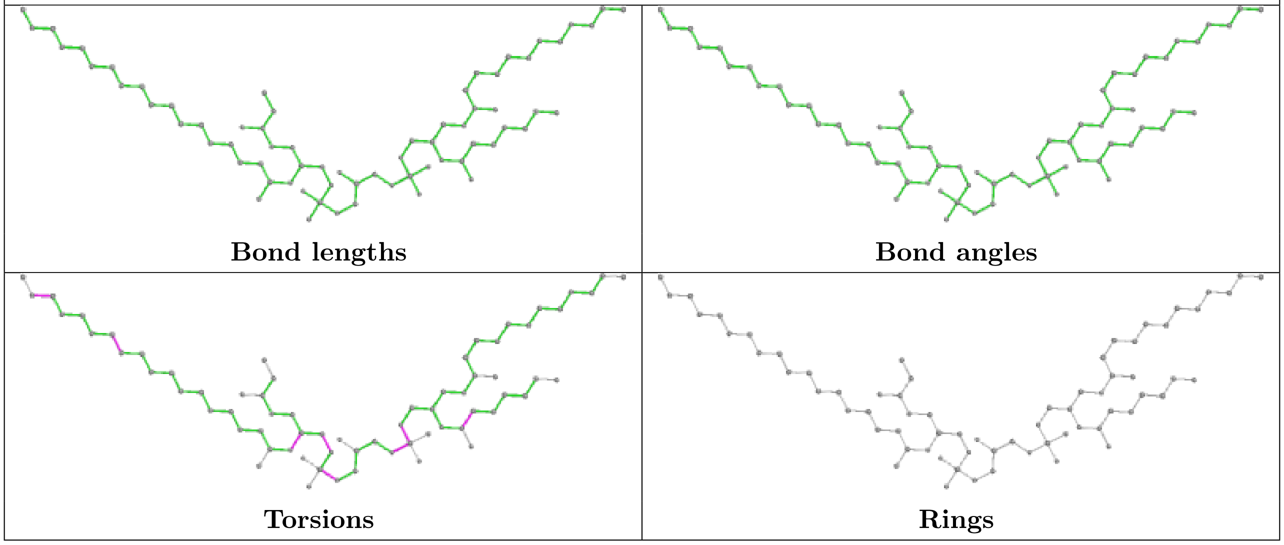

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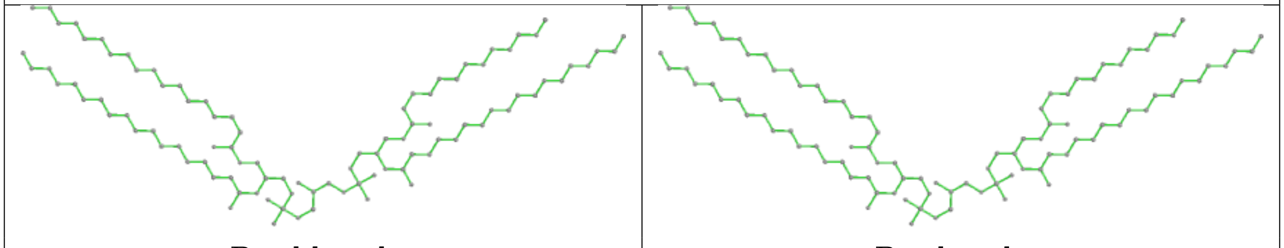
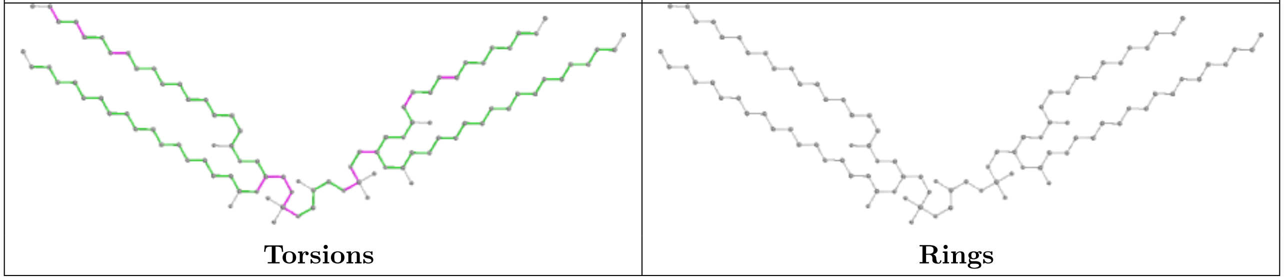
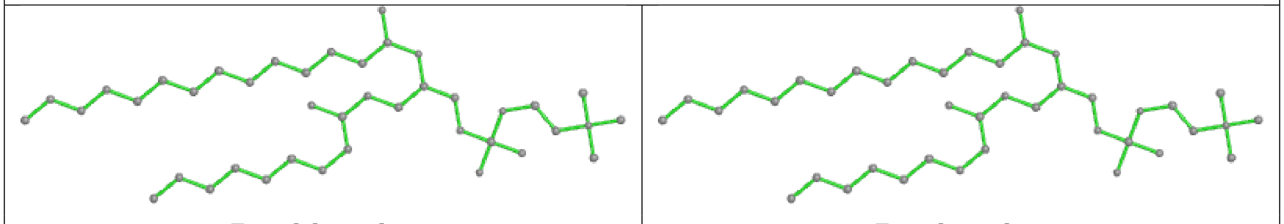


Bond lengths **Bond angles**

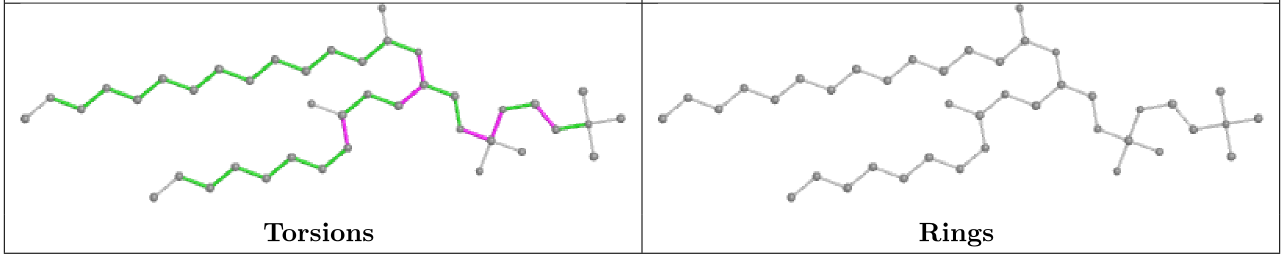


Torsions **Rings**

Ligand PC1 A 502

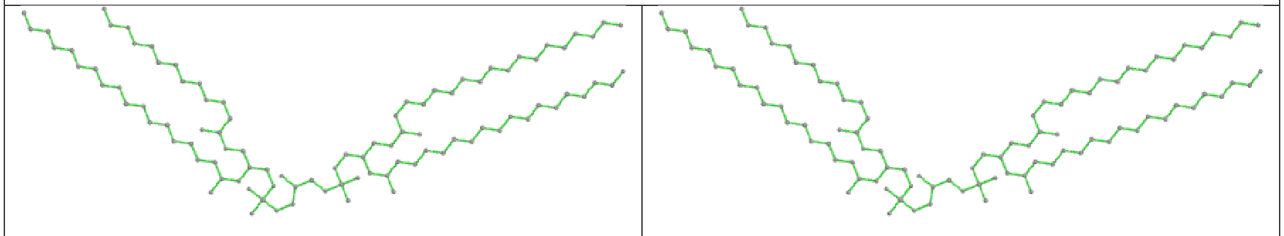


Bond lengths **Bond angles**

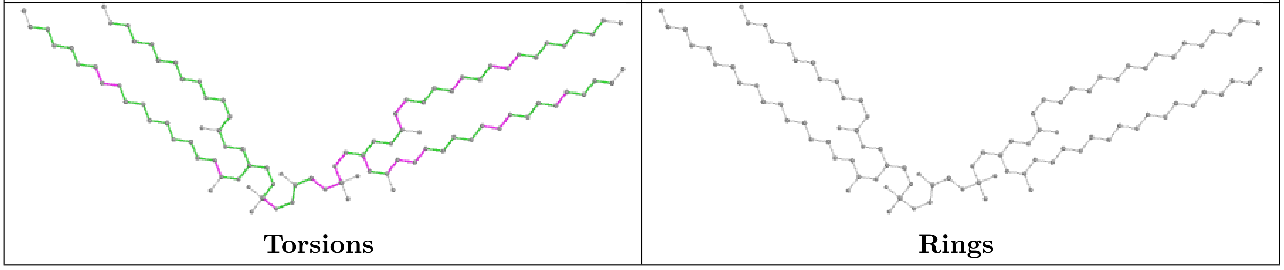


Torsions **Rings**

Ligand CDL M1 401

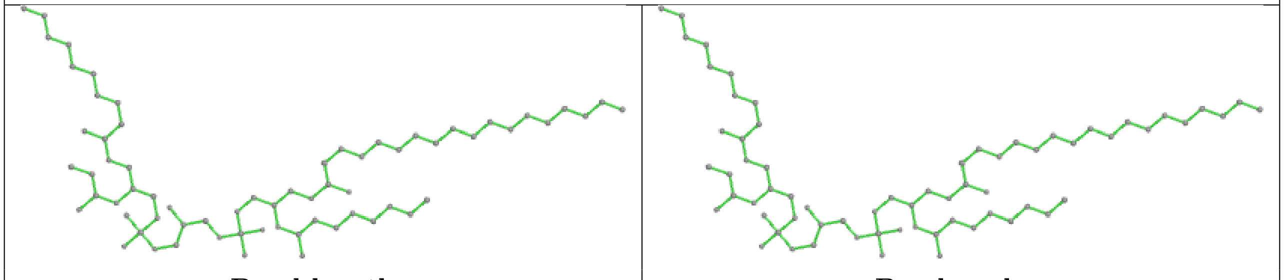


Bond lengths **Bond angles**



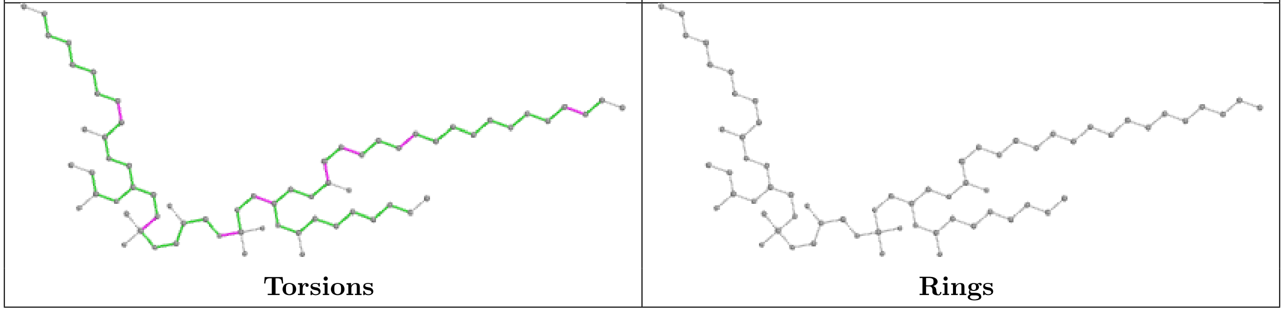
Torsions **Rings**

Ligand CDL 5b 703



Bond lengths

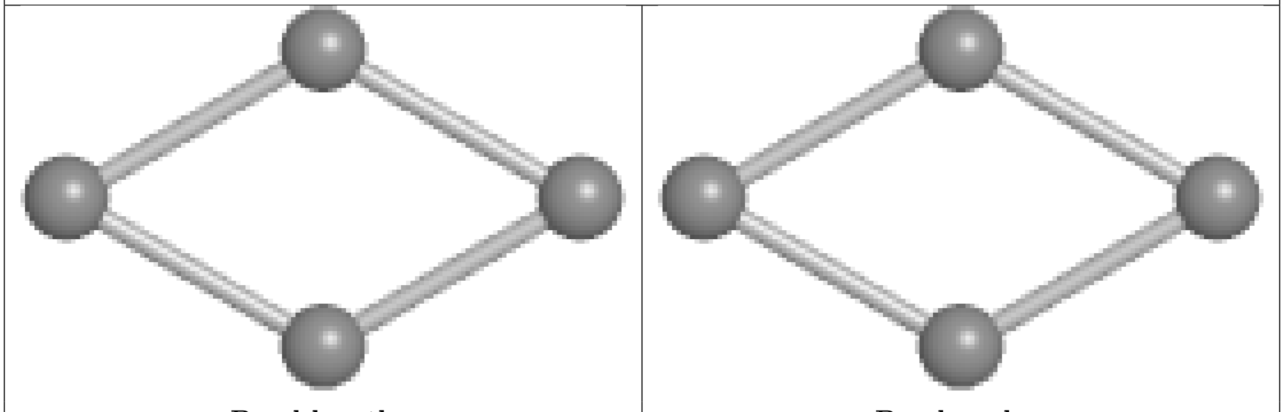
Bond angles



Torsions

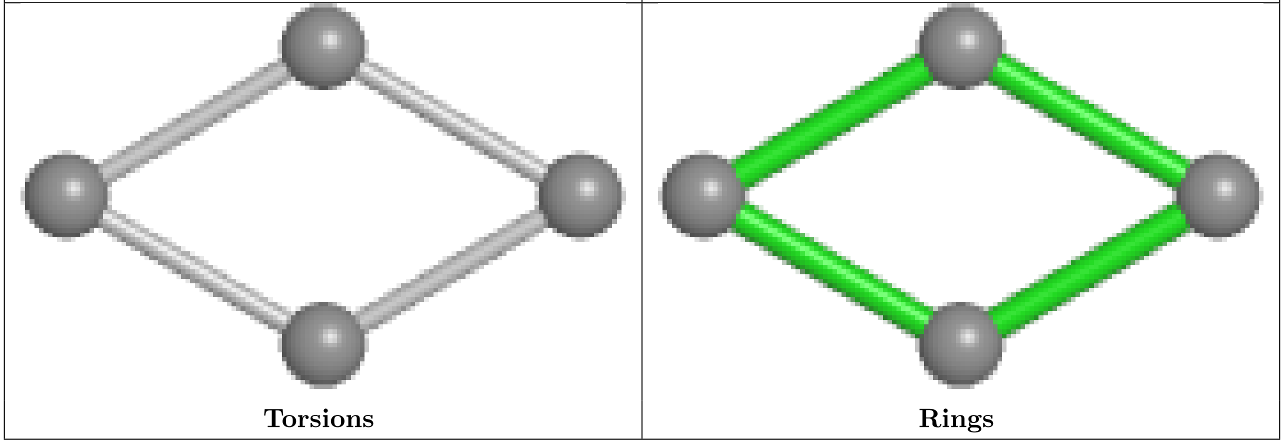
Rings

Ligand FES FS 202



Bond lengths

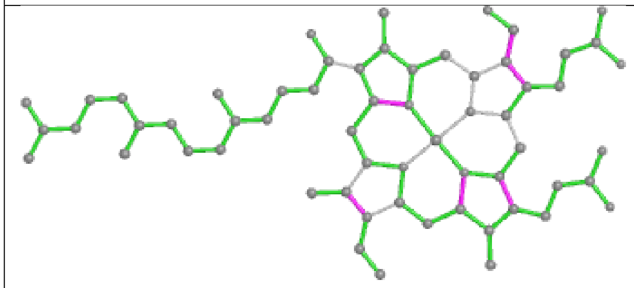
Bond angles

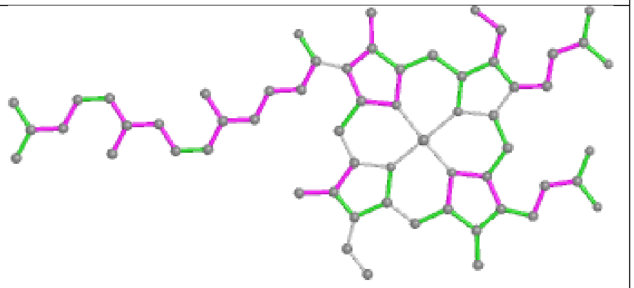


Torsions

Rings

Ligand HEA C1 701


Bond lengths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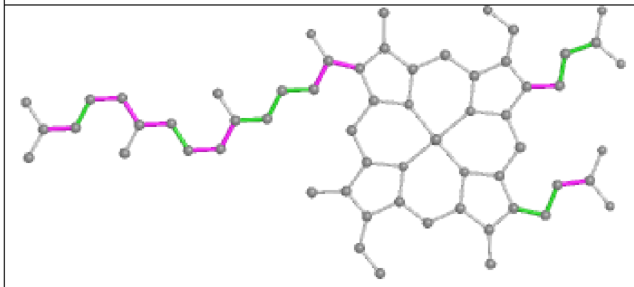
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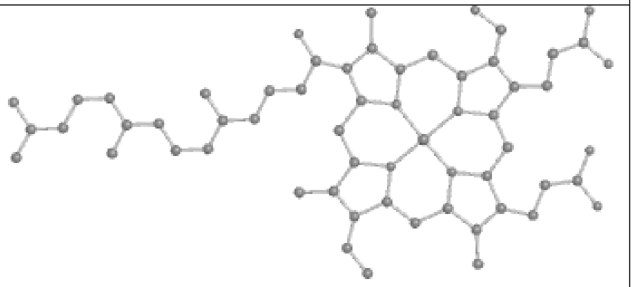
Rings

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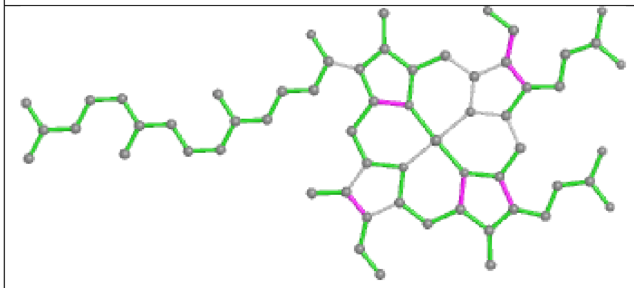
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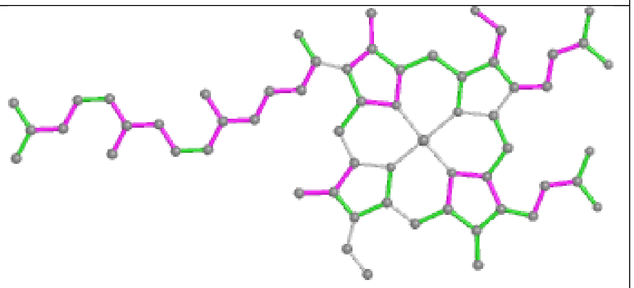
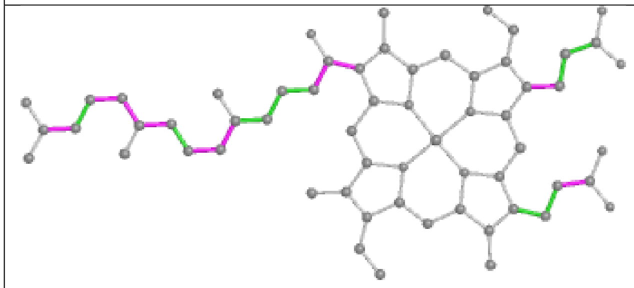

Bond angles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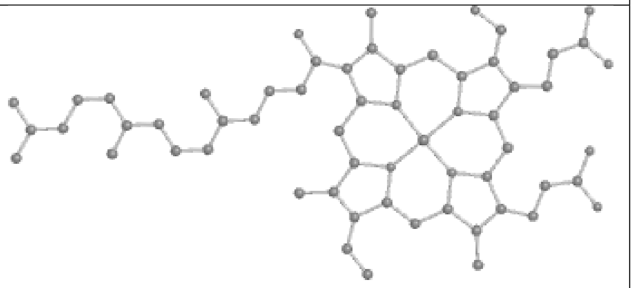
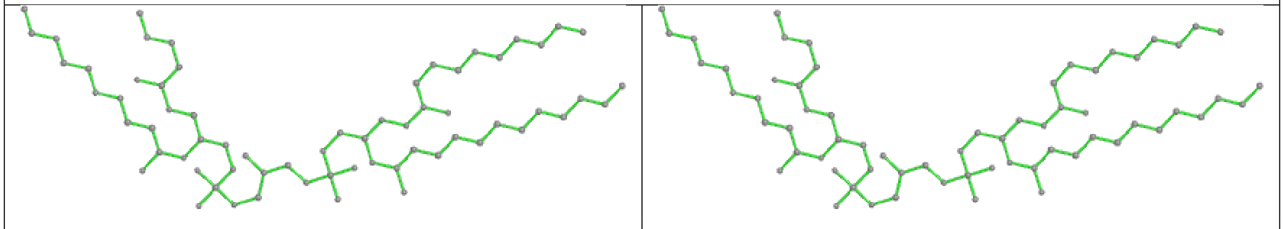
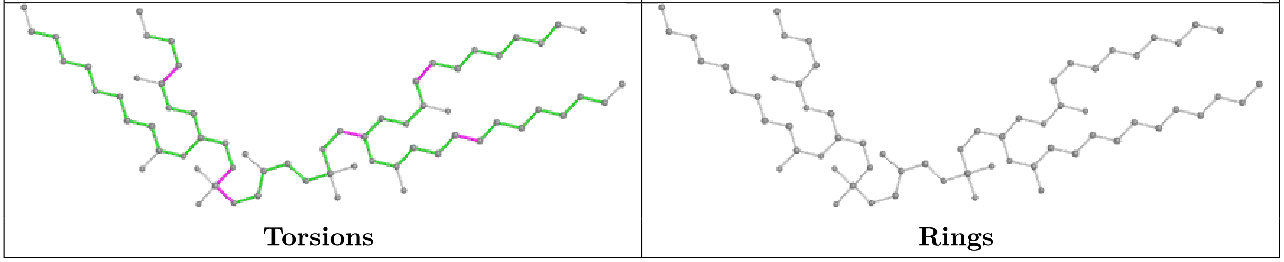

Rings

Ligand CDL C1 707

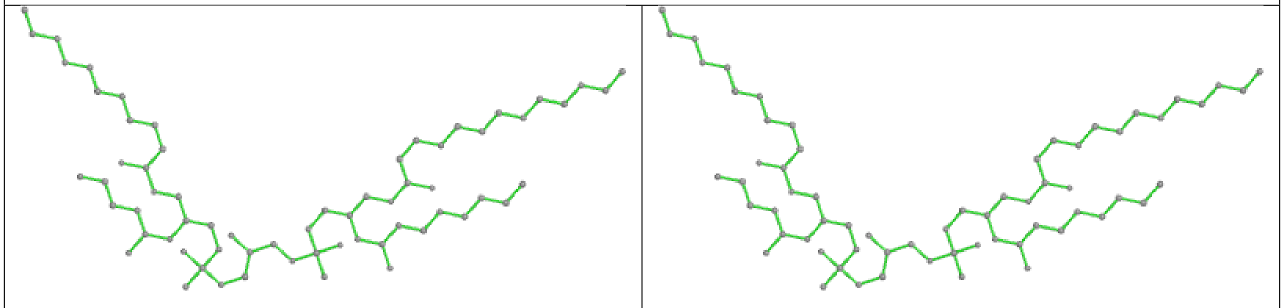


Bond lengths **Bond angles**

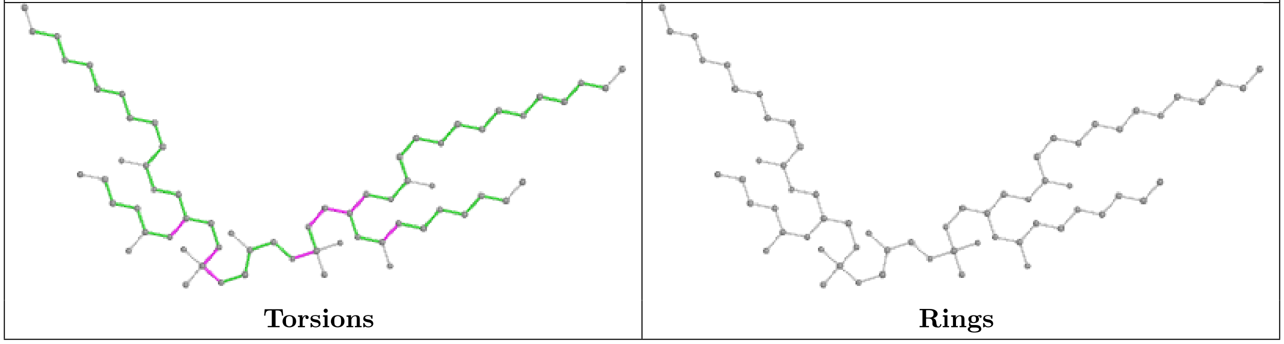


Torsions **Rings**

Ligand CDL y7 501

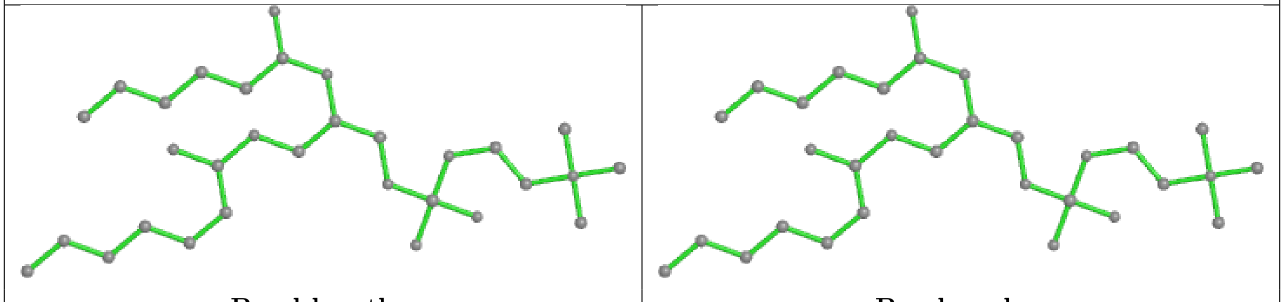


Bond lengths **Bond angles**

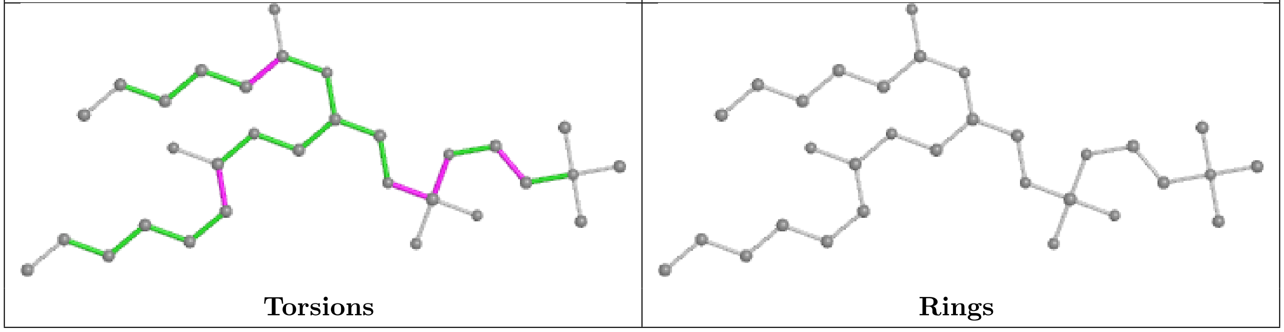


Torsions **Rings**

Ligand PC1 c3 603

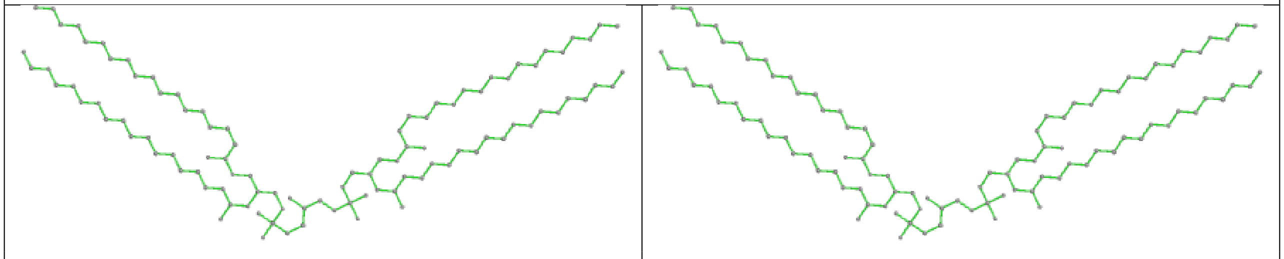


Bond lengths Bond angles

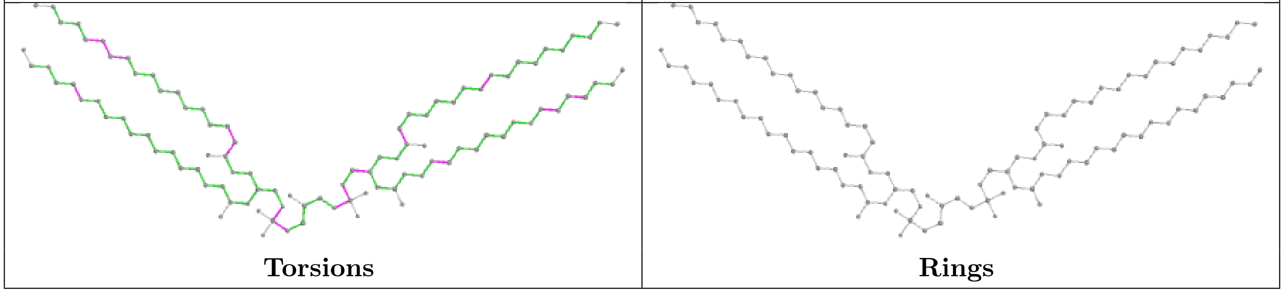


Torsions Rings

Ligand CDL 7a 202

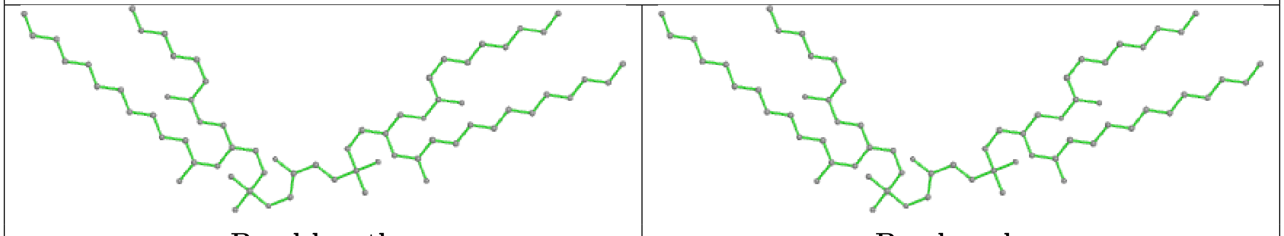


Bond lengths Bond angles



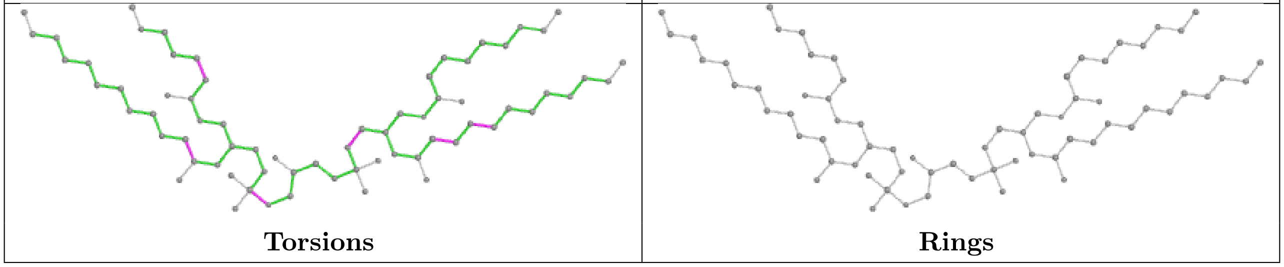
Torsions Rings

Ligand CDL c3 604



Bond lengths

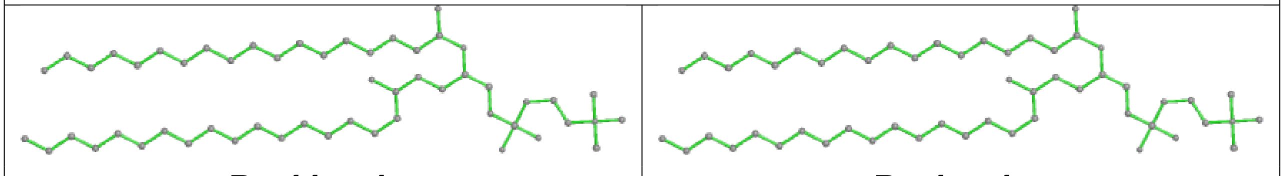
Bond angles



Torsions

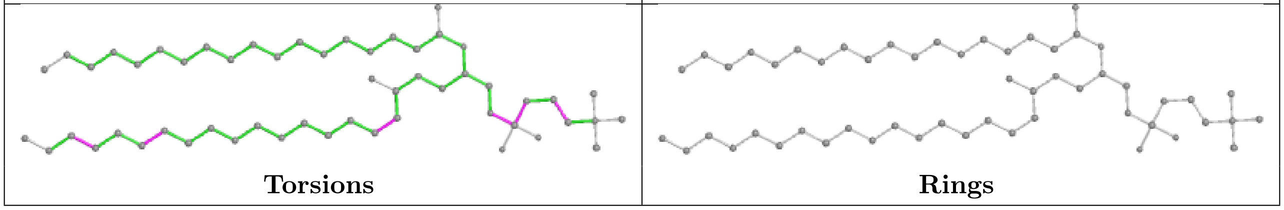
Rings

Ligand PC1 v 202



Bond lengths

Bond angles



Torsions

Rings

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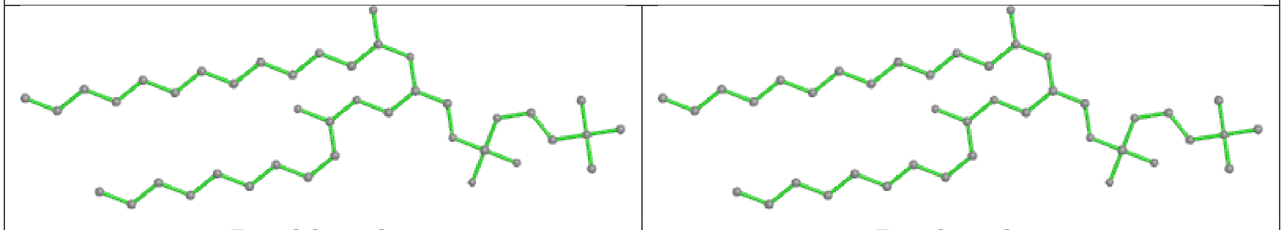
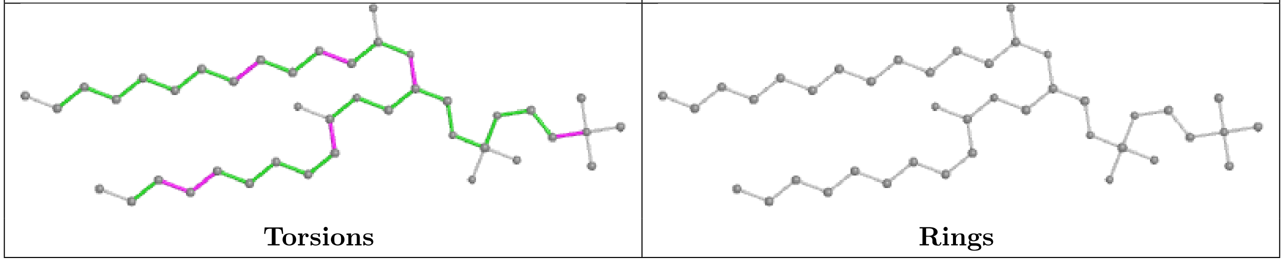


Bond lengths

Bond angles



Torsions

Rings

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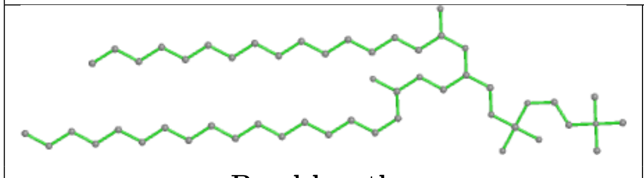

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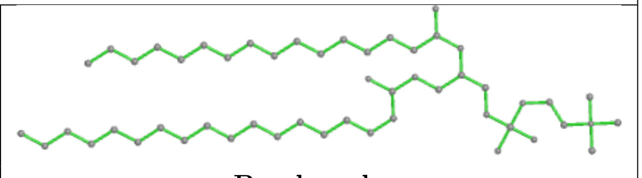
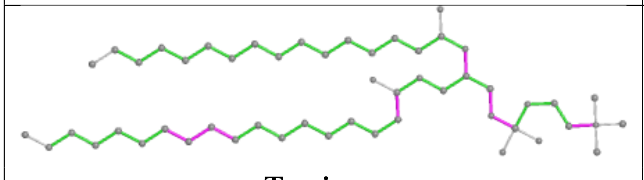


Bond angles



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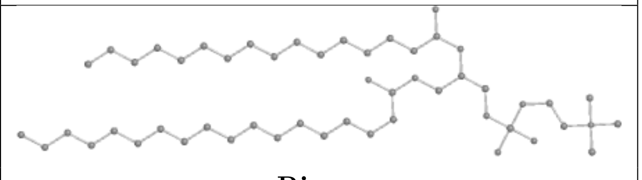
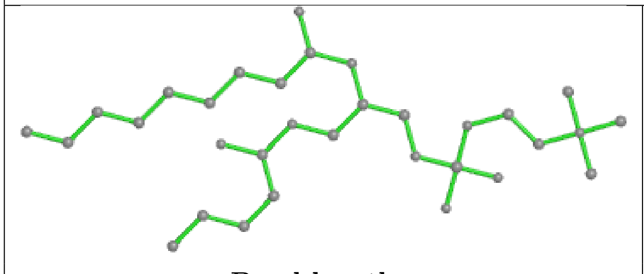


Rings

Ligand PC1 n 301



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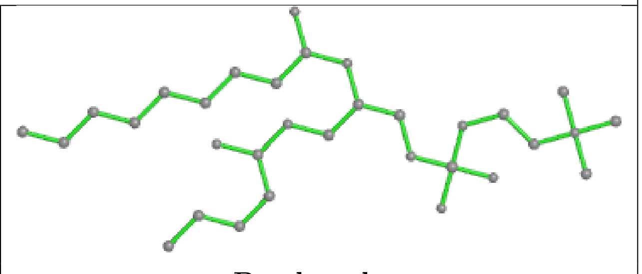
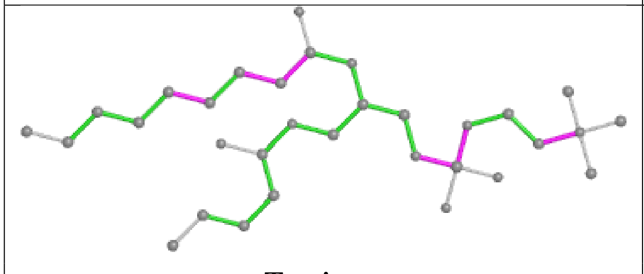


Bond angles



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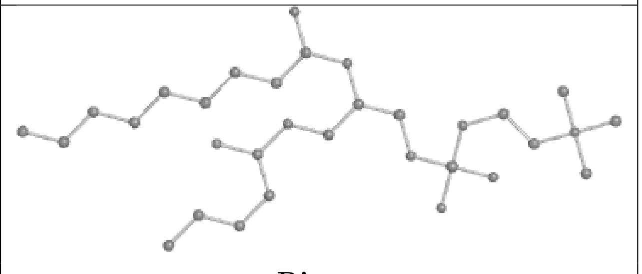
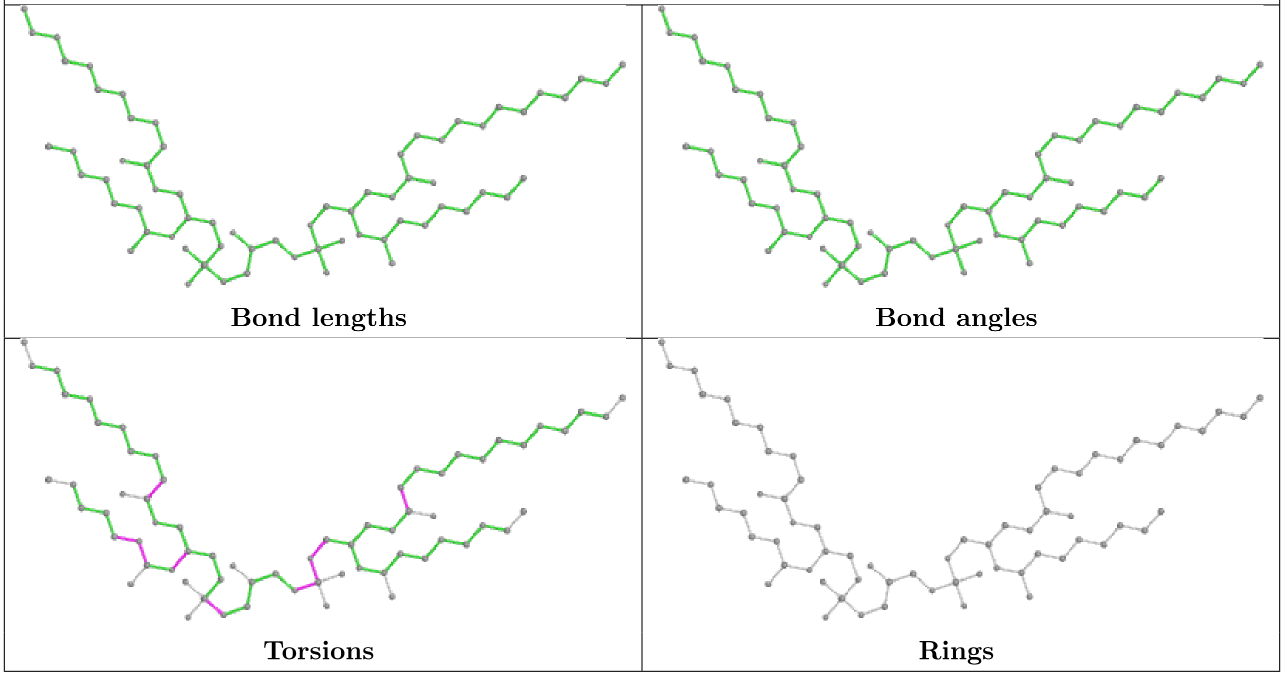


Rings

Ligand CDL 7A 201



Bond lengths

Bond angles

Torsions

Rings

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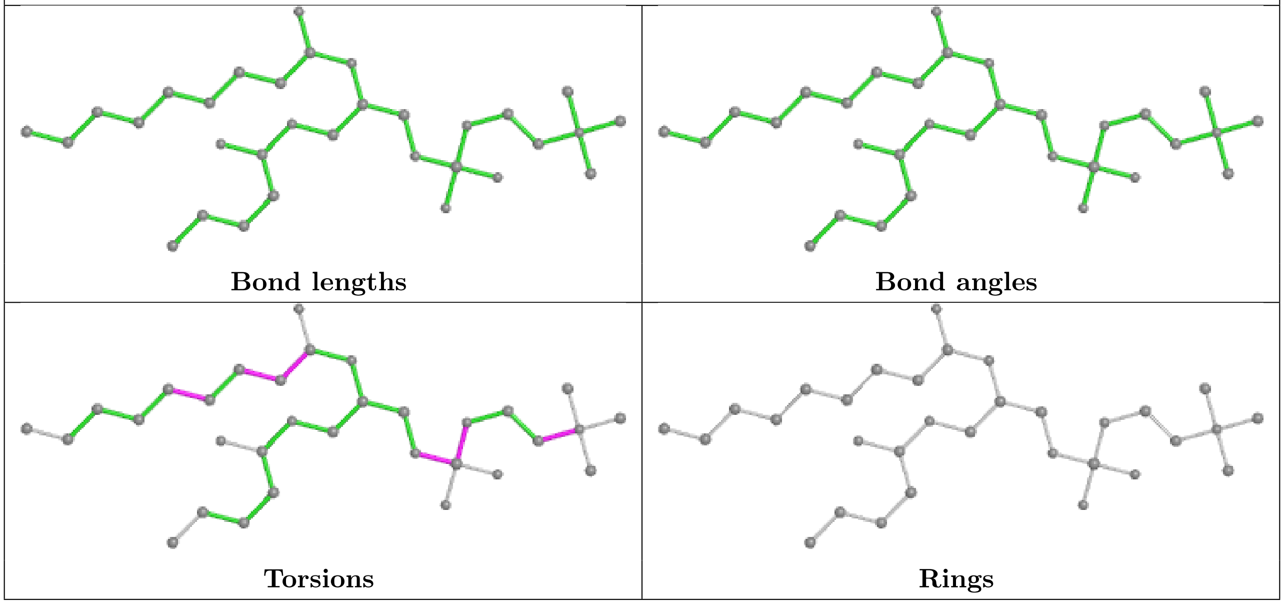


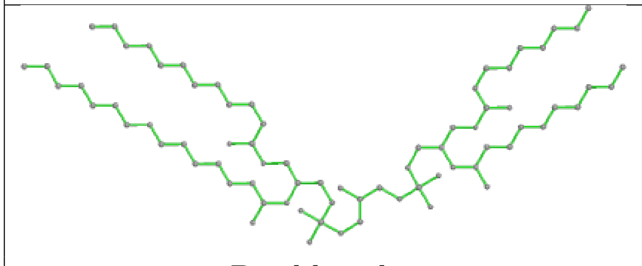
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL M2 404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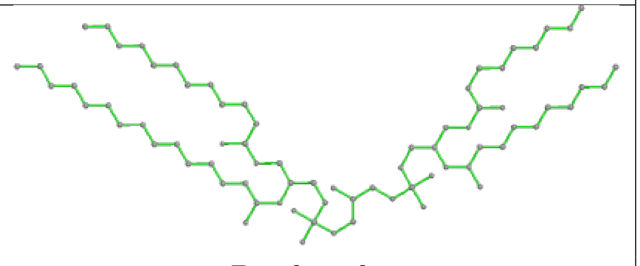
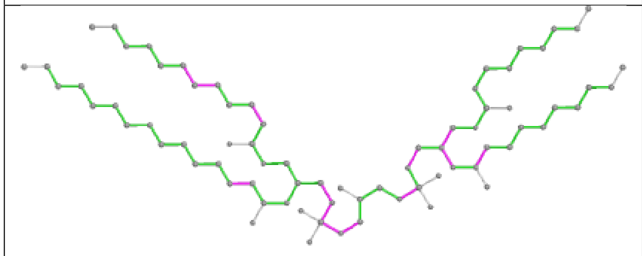

Bond angles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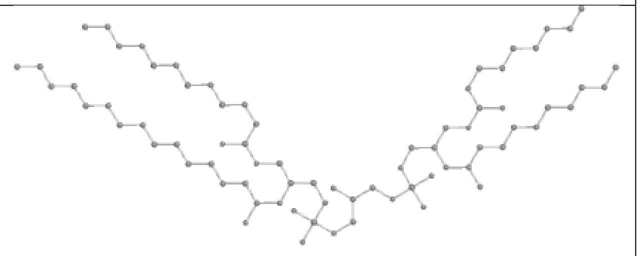
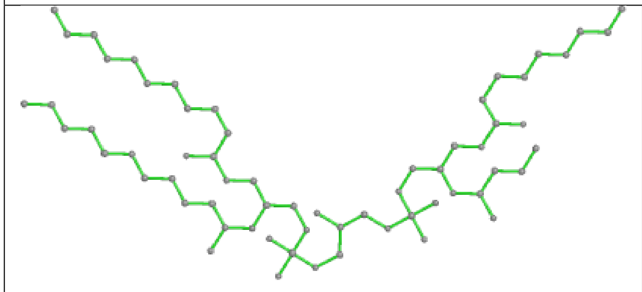

Rings

Ligand CDL m3 403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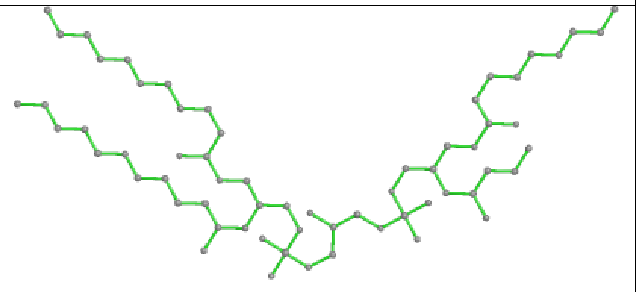
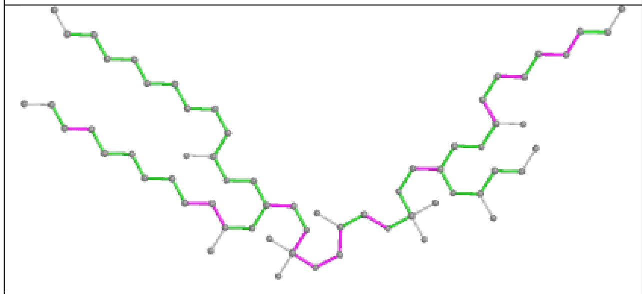

Bond angles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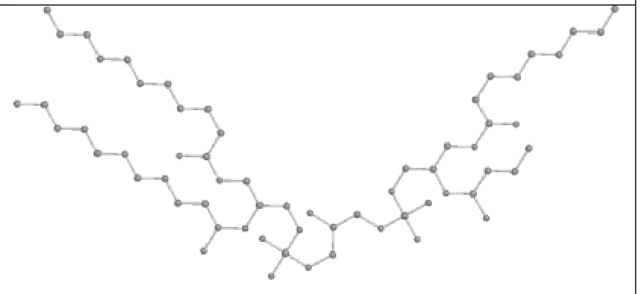
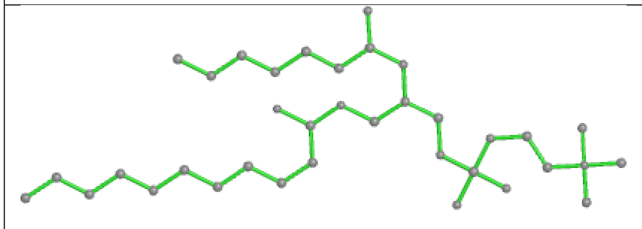

Rings

Ligand PC1 N 302



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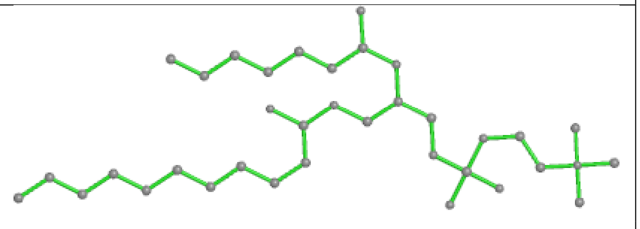
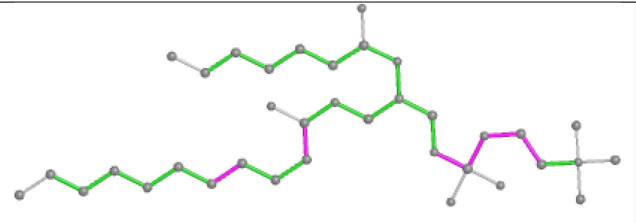


Bond angles



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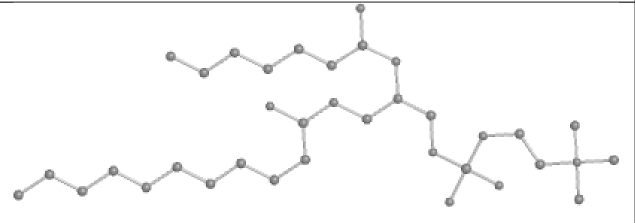
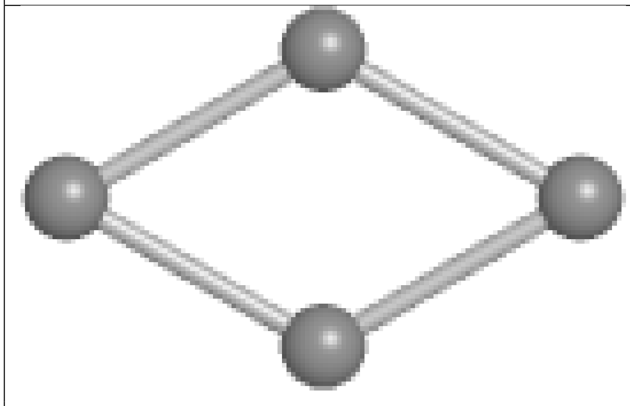


Rings

Ligand FES FS 201



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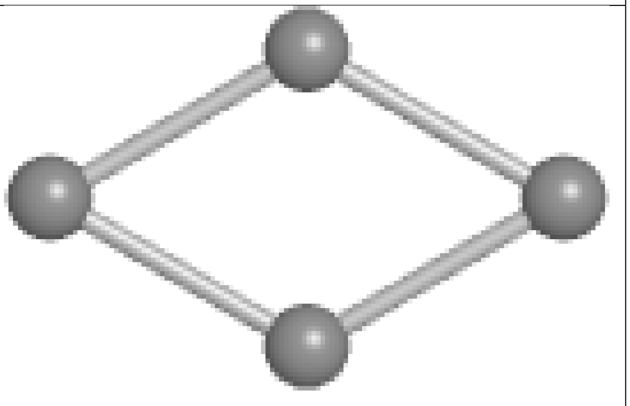
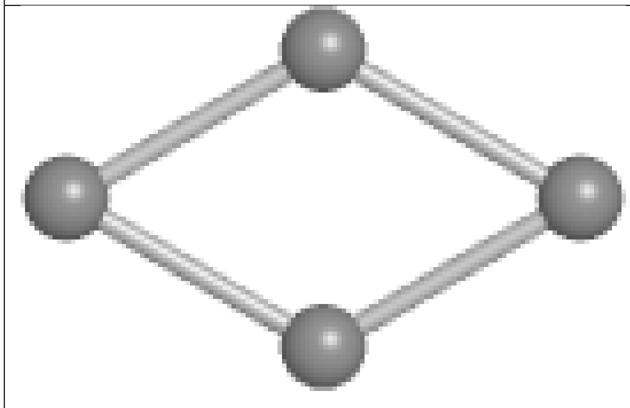


Bond angles



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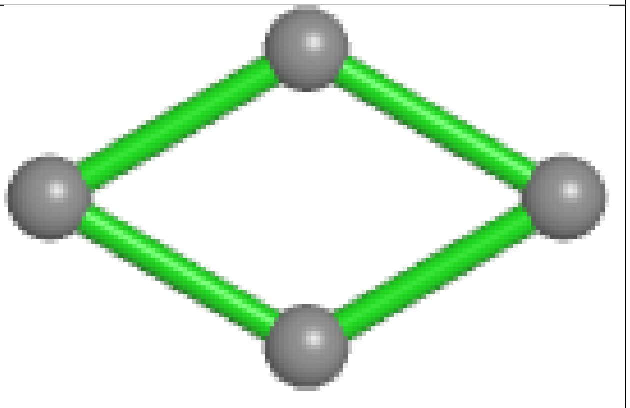
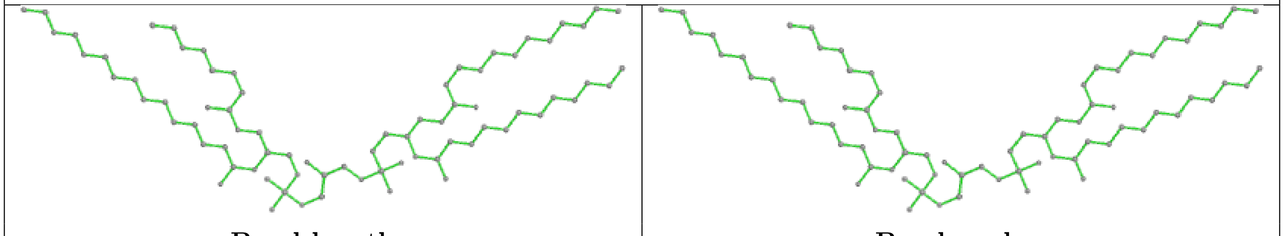


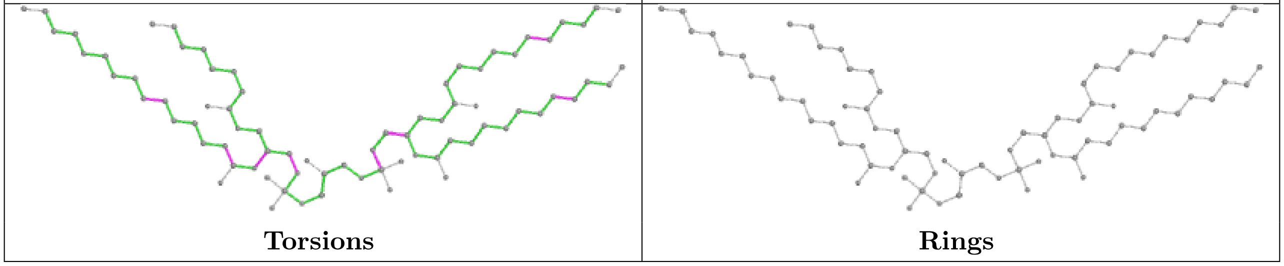
Rings

Ligand CDL T 202



Bond lengths

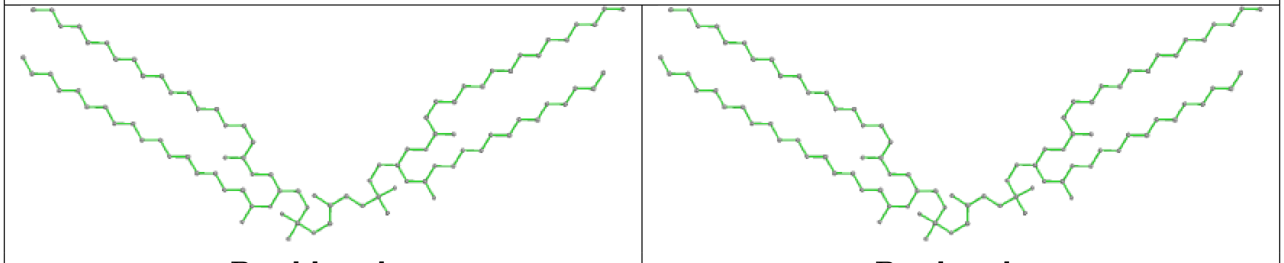
Bond angles



Torsions

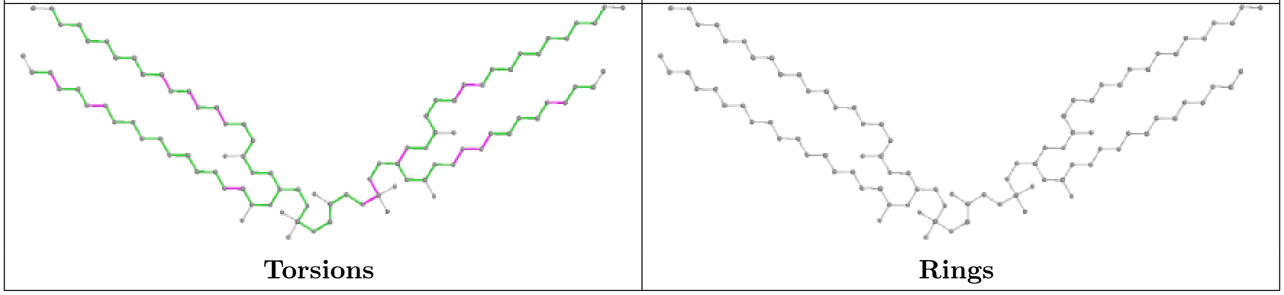
Rings

Ligand CDL m3 401



Bond lengths

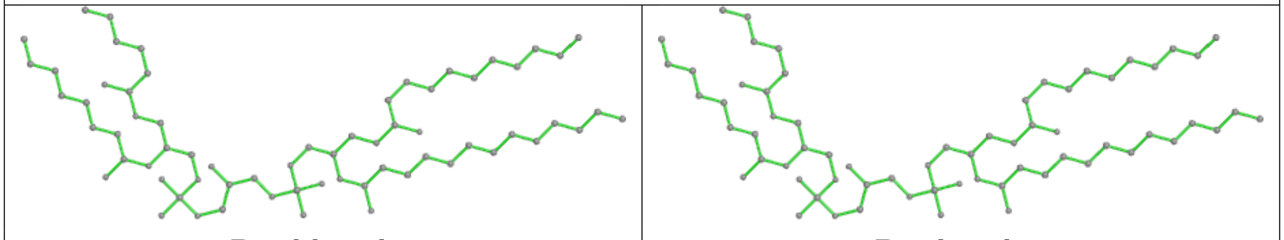
Bond angles



Torsions

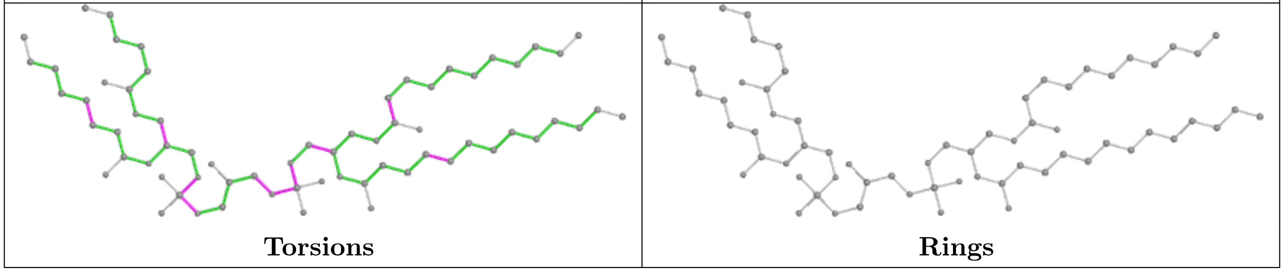
Rings

Ligand CDL m2 403



Bond lengths

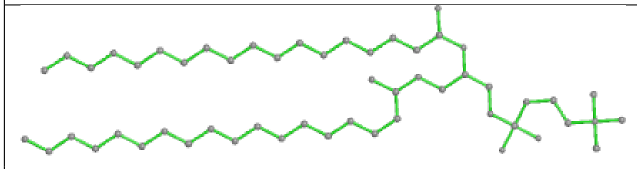
Bond angles



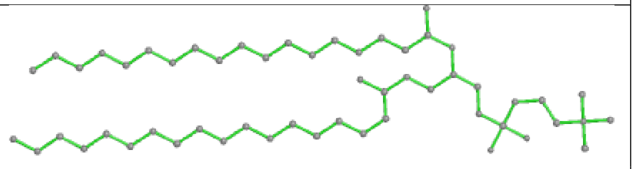
Torsions

Rings

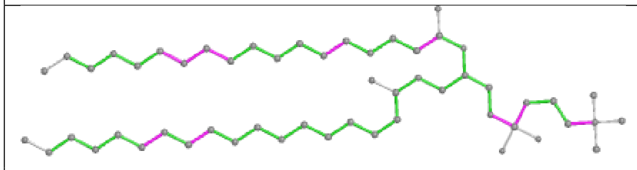
Ligand PC1 7C 302



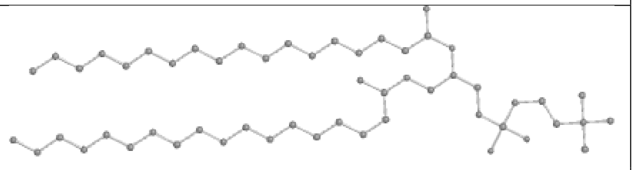
Bond lengths



Bond angles

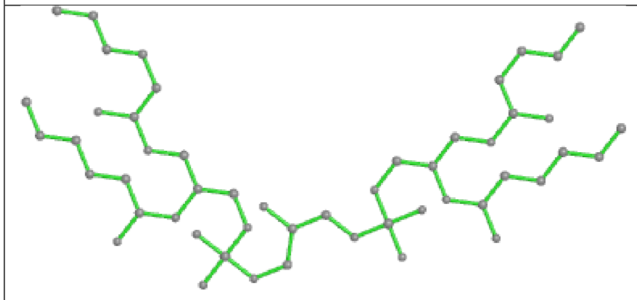


Torsions



Rings

Ligand CDL A 503



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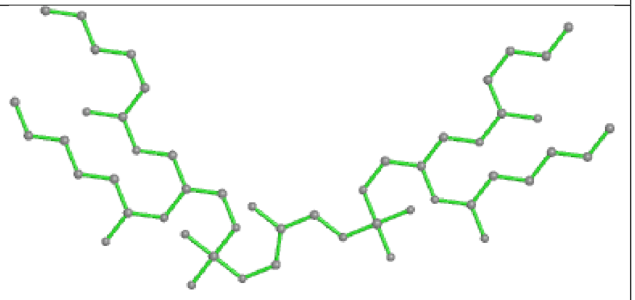
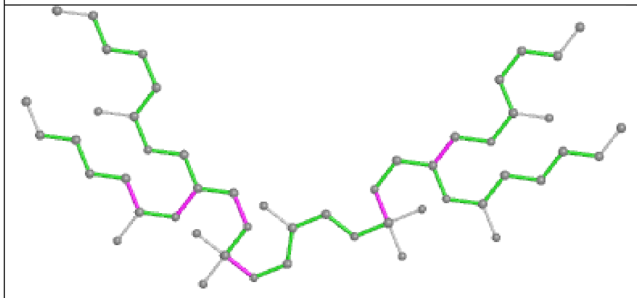
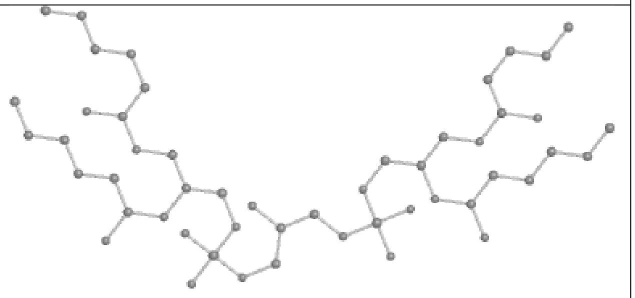


Bond angles

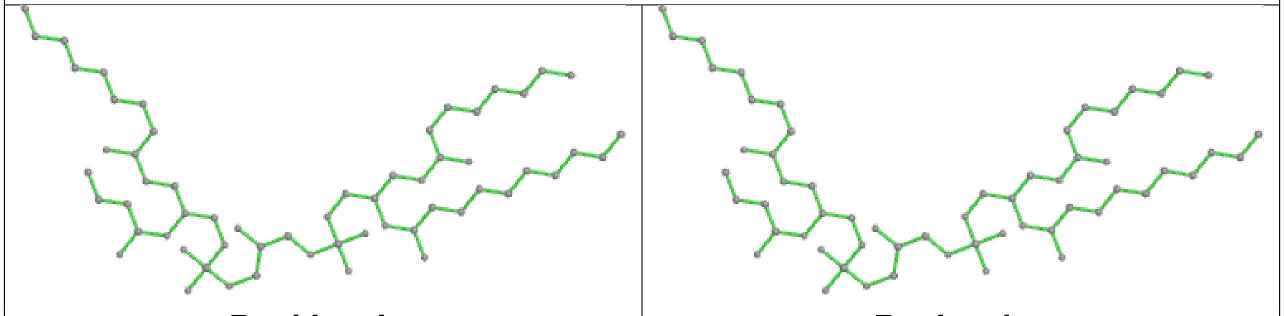


Torsions

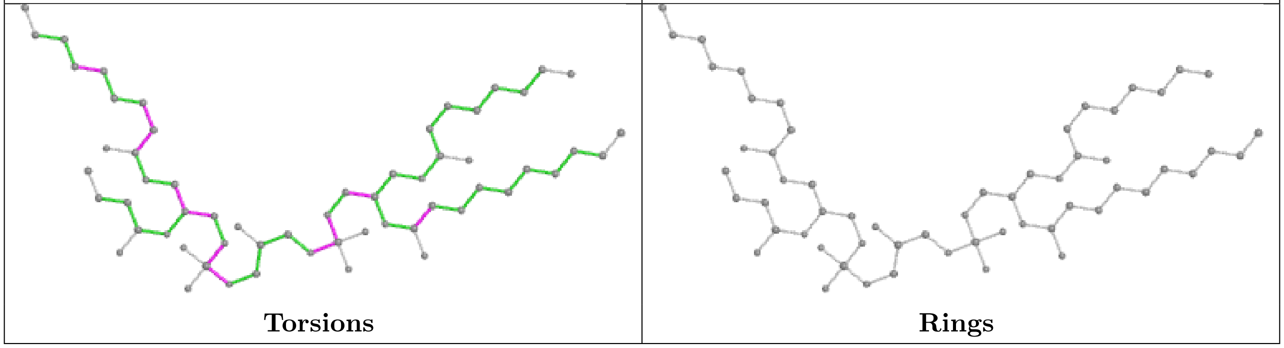


Rings

Ligand CDL C1 706

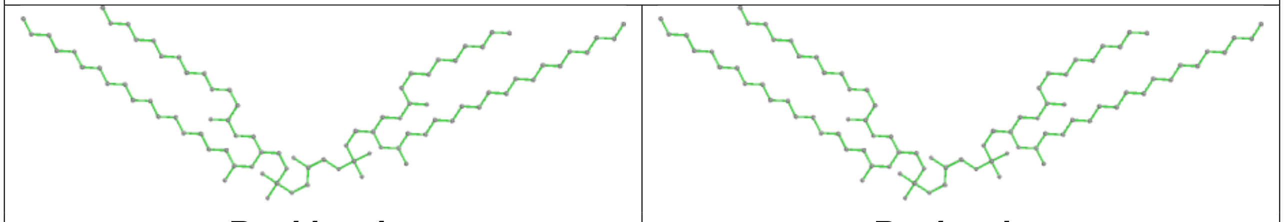


Bond lengths **Bond angles**

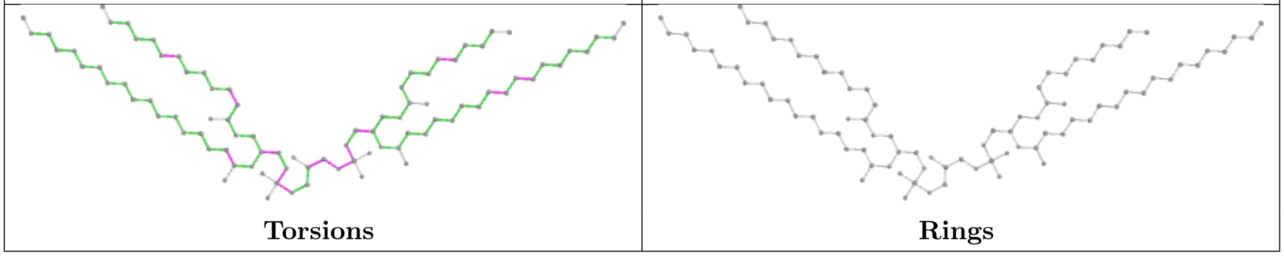


Torsions **Rings**

Ligand CDL 5B 702

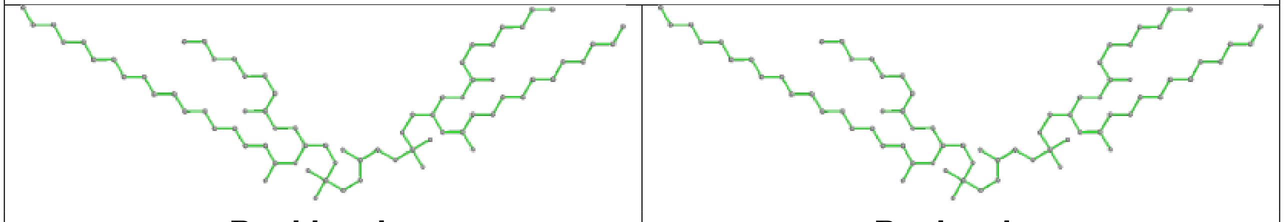


Bond lengths **Bond angles**

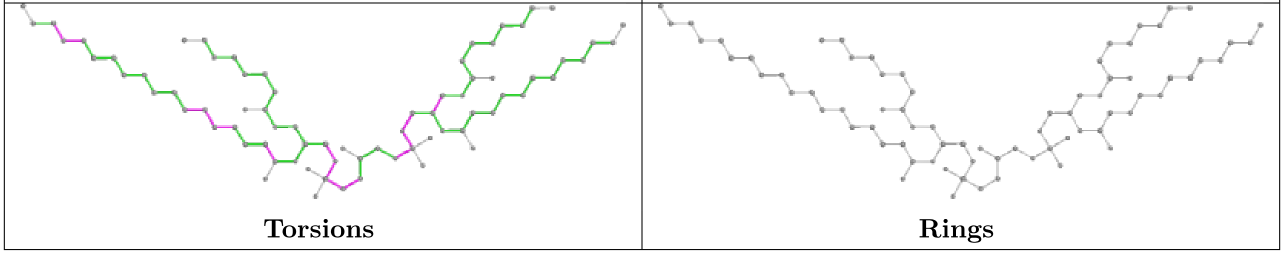


Torsions **Rings**

Ligand CDL L 301

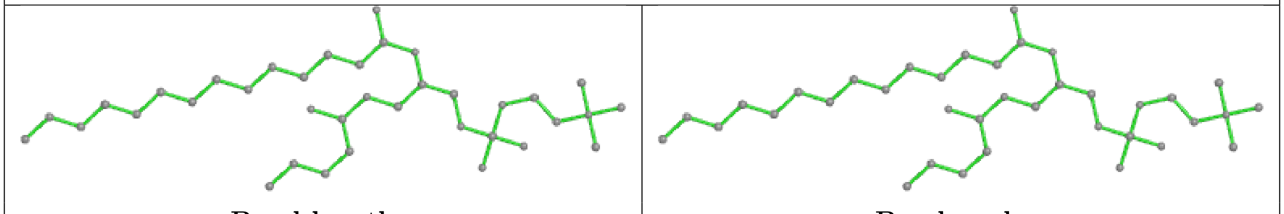


Bond lengths Bond angles

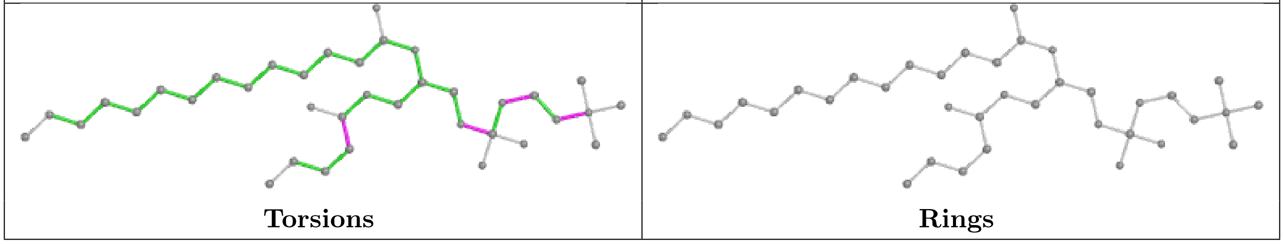


Torsions Rings

Ligand PC1 J 302

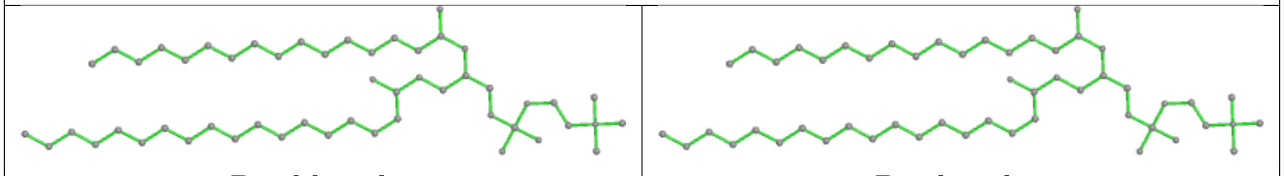


Bond lengths Bond angles

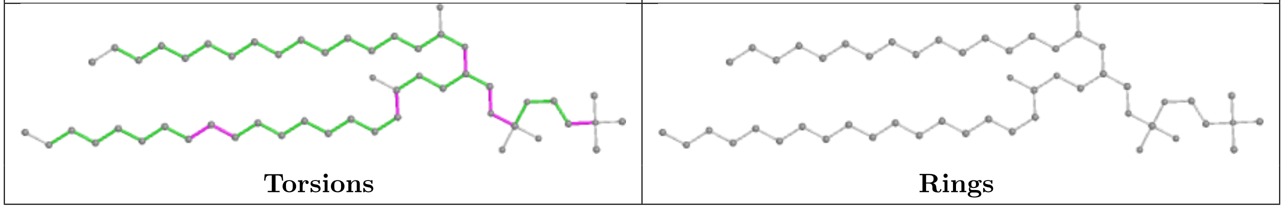


Torsions Rings

Ligand PC1 C3 601

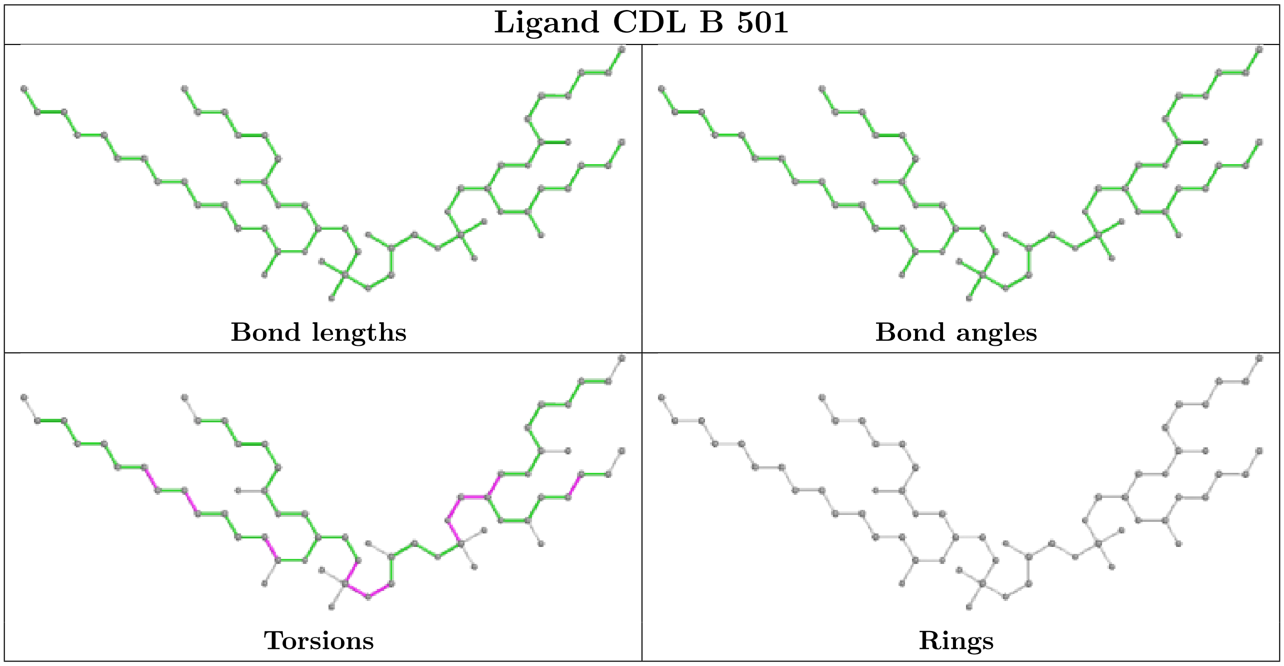


Bond lengths Bond angles



Torsions Rings

Ligand CDL B 501

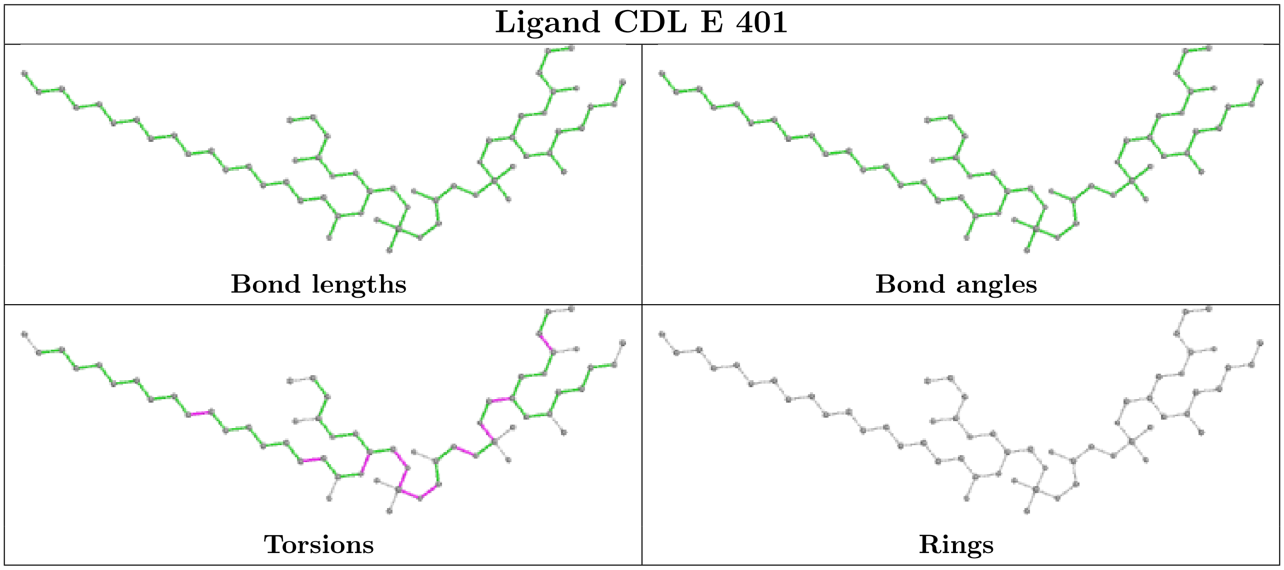

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL E 401

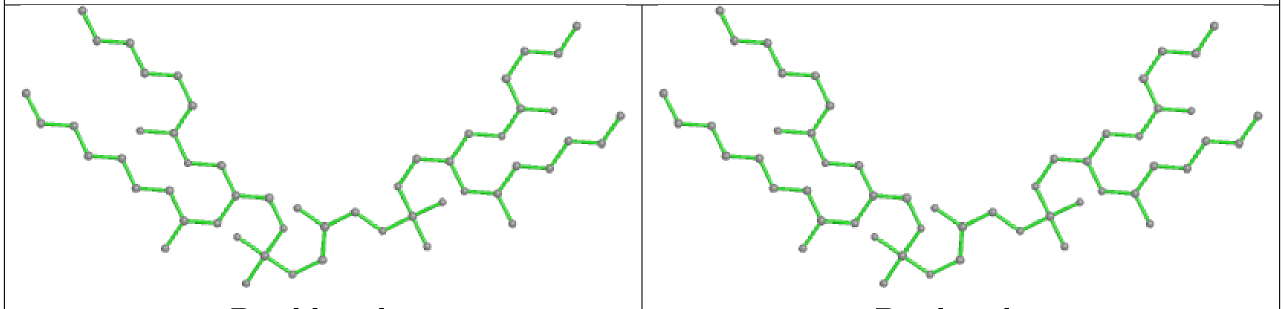

Bond lengths

Bond angles

Torsions

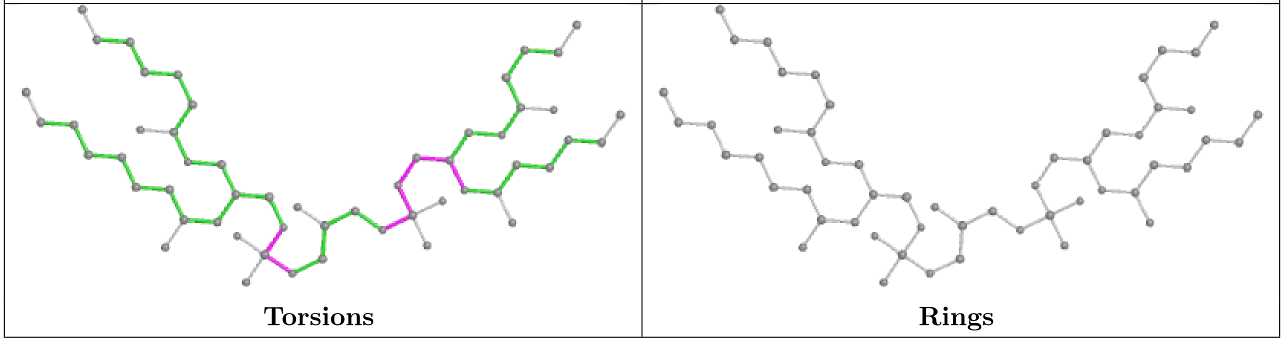
Rings

Ligand CDL M2 401



Bond lengths

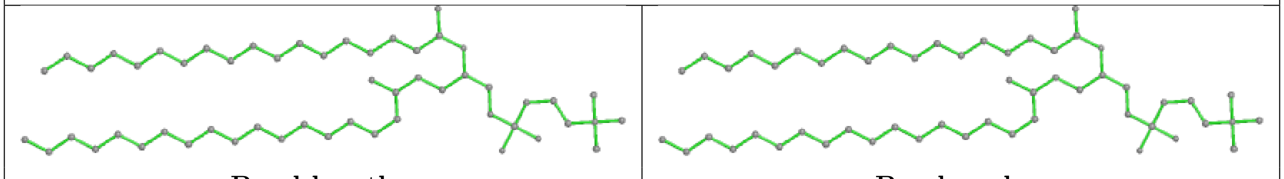
Bond angles



Torsions

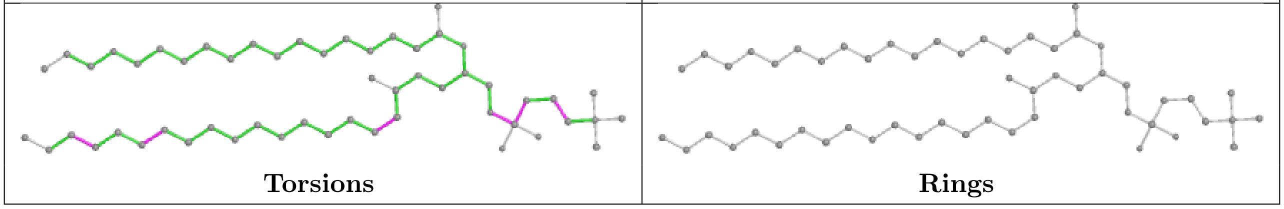
Rings

Ligand PC1 V 202



Bond lengths

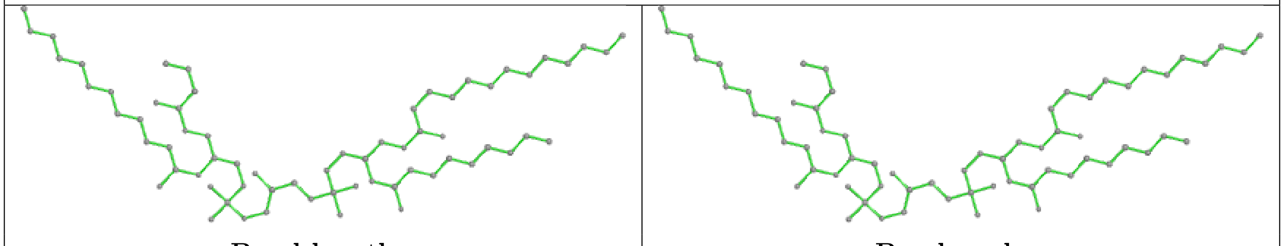
Bond angles



Torsions

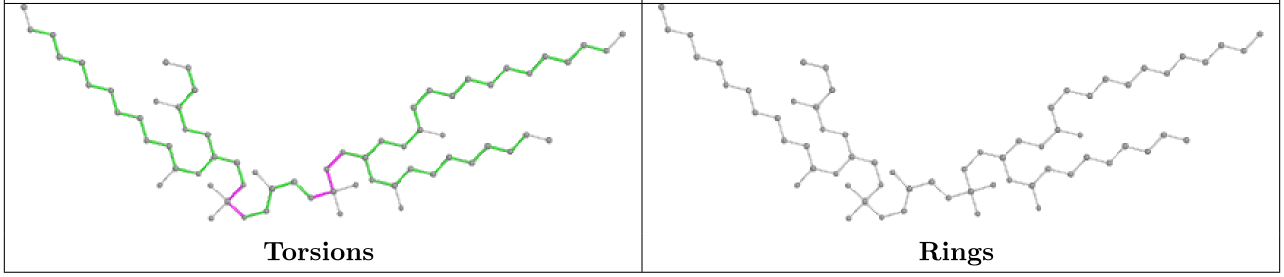
Rings

Ligand CDL m1 404



Bond lengths

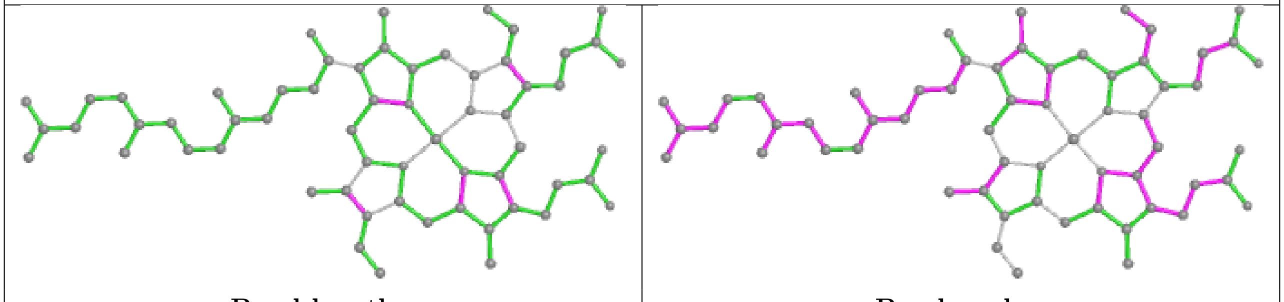
Bond angles



Torsions

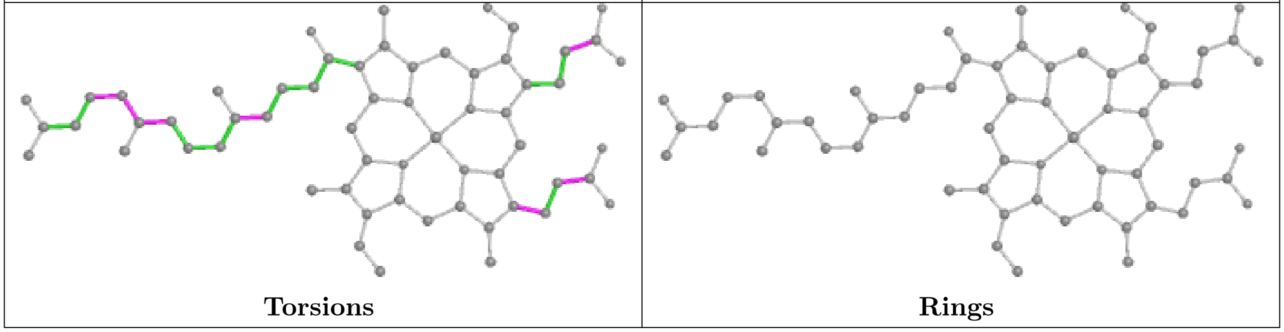
Rings

Ligand HEA C1 702



Bond lengths

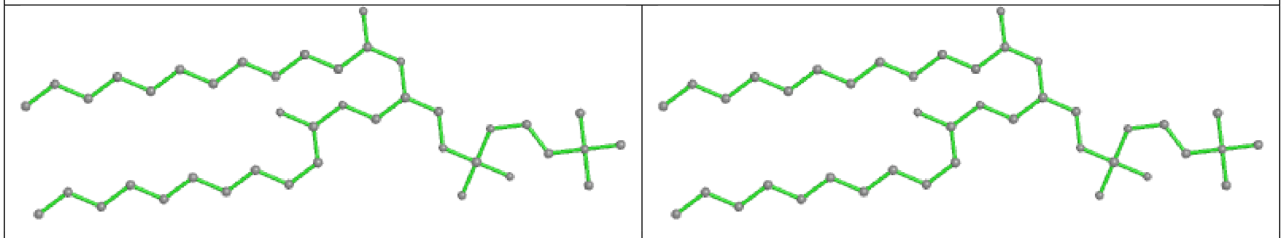
Bond angles



Torsions

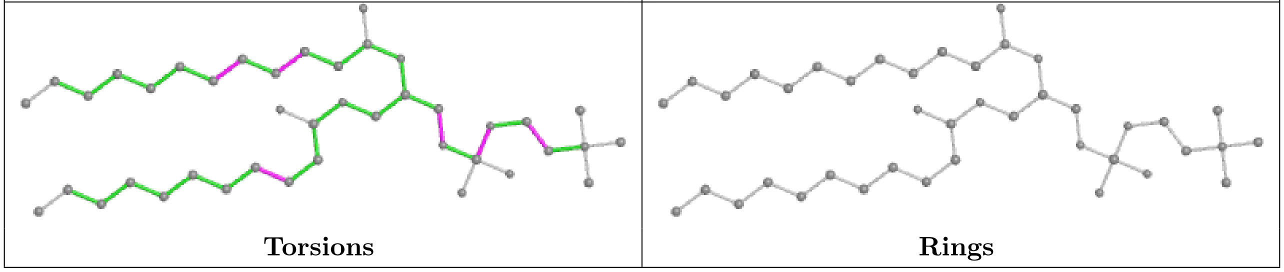
Rings

Ligand PC1 m2 405



Bond lengths

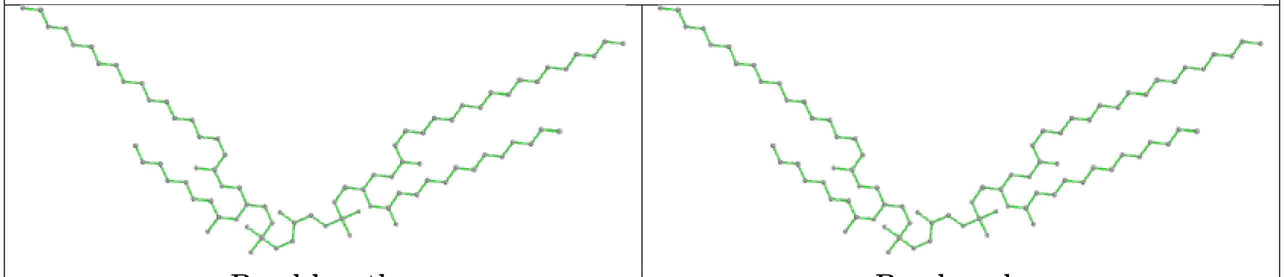
Bond angles



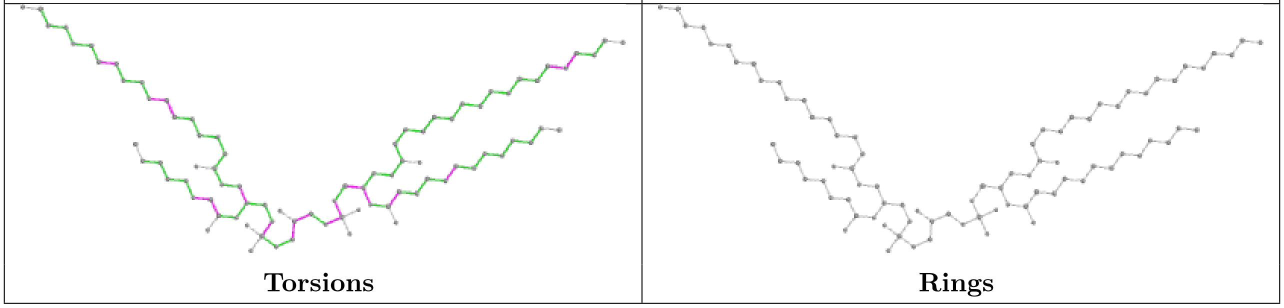
Torsions

Rings

Ligand CDL 7c 301

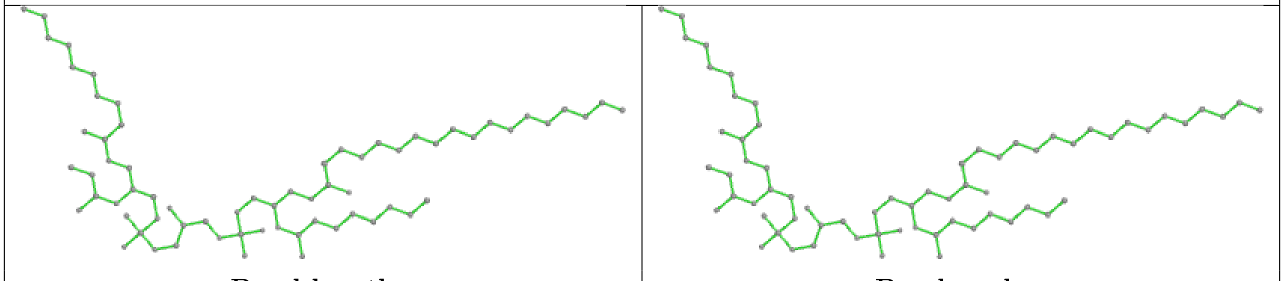


Bond lengths Bond angles

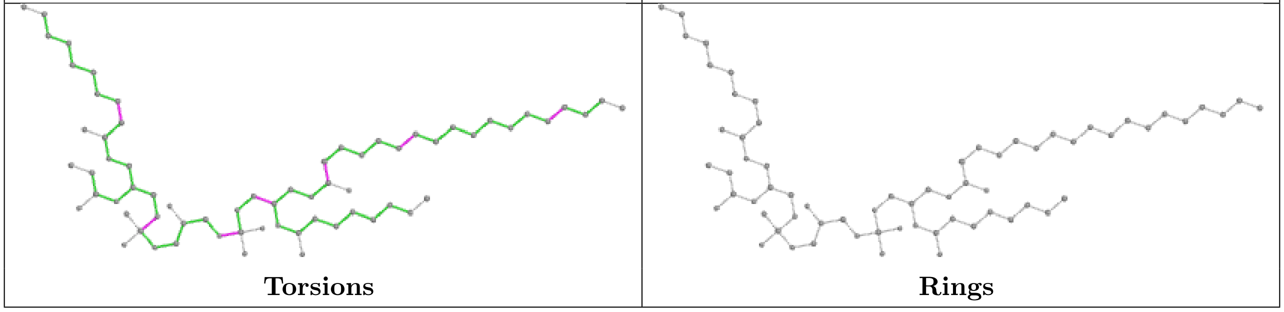


Torsions Rings

Ligand CDL 5B 704



Bond lengths Bond angles



Torsions Rings

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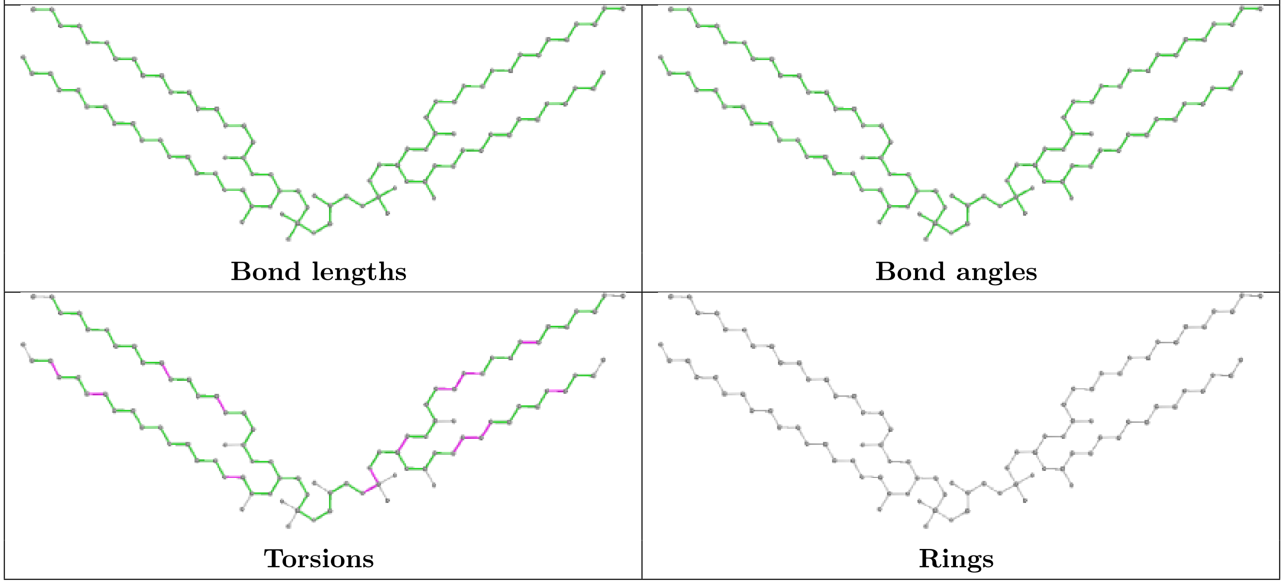

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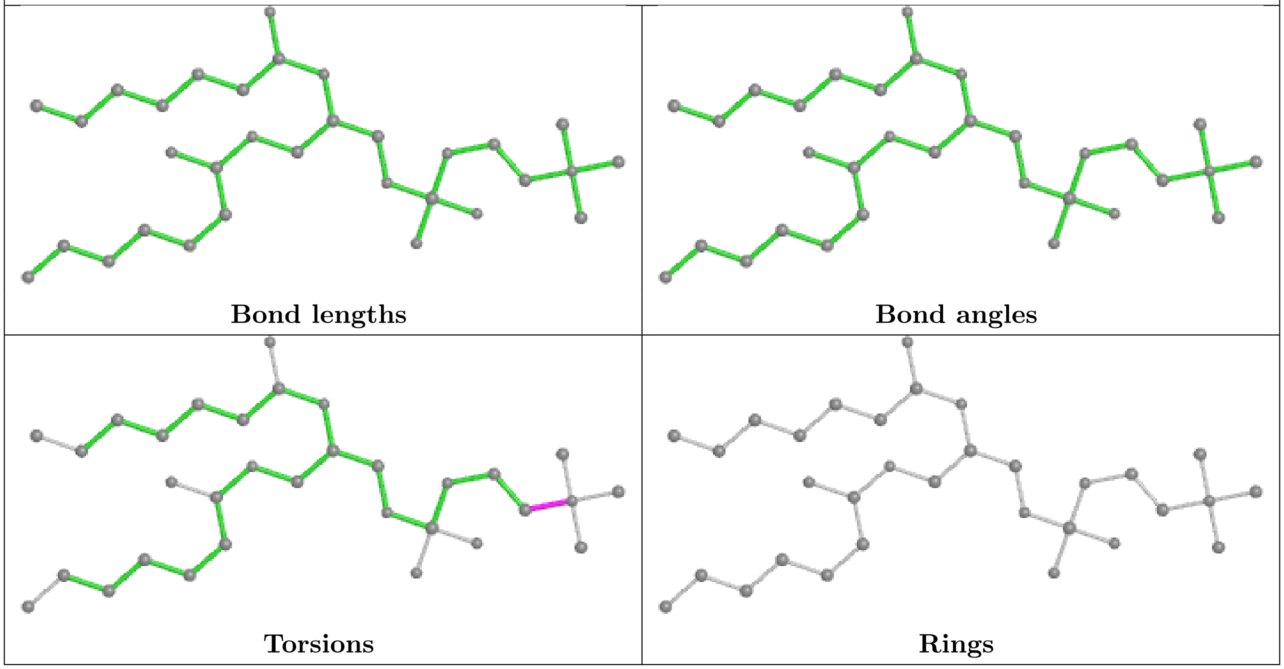

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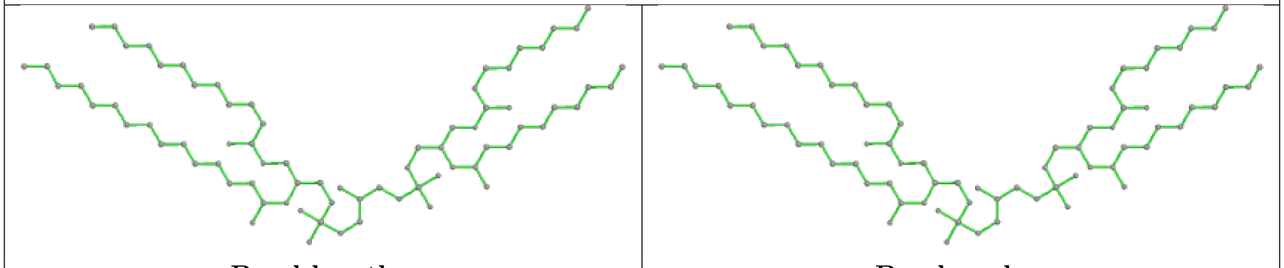
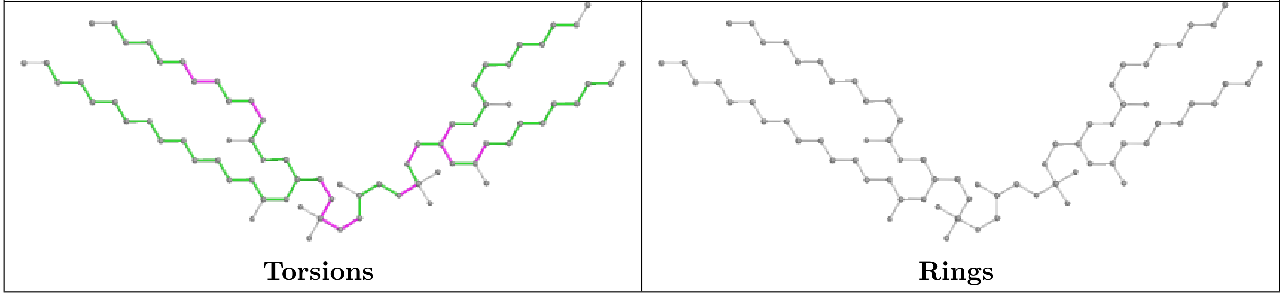


Bond lengths

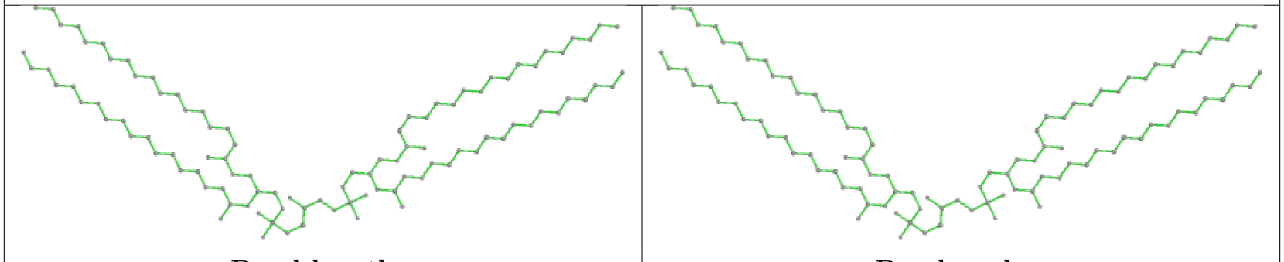
Bond angles



Torsions

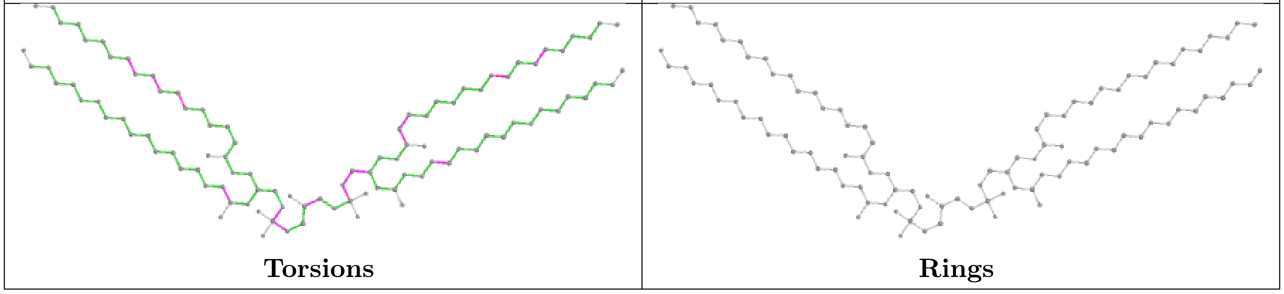
Rings

Ligand CDL f 401



Bond lengths

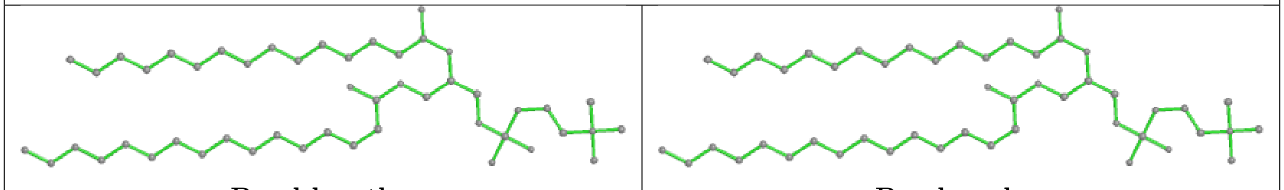
Bond angles



Torsions

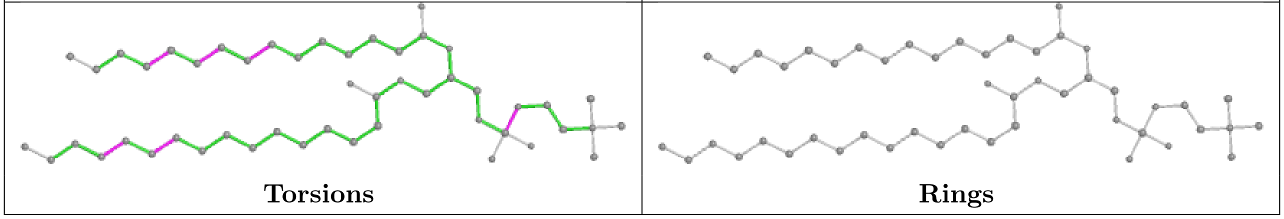
Rings

Ligand PC1 c1 705



Bond lengths

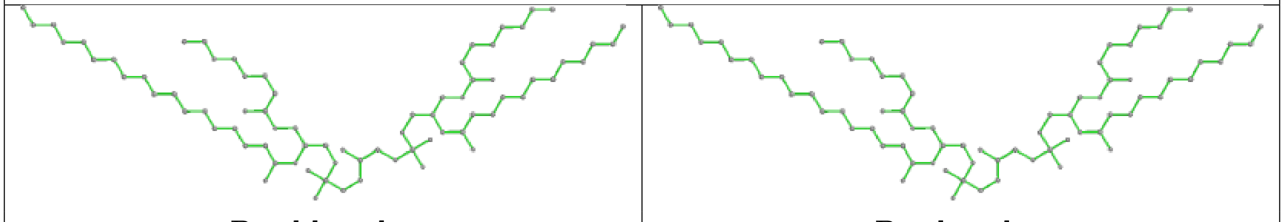
Bond angles



Torsions

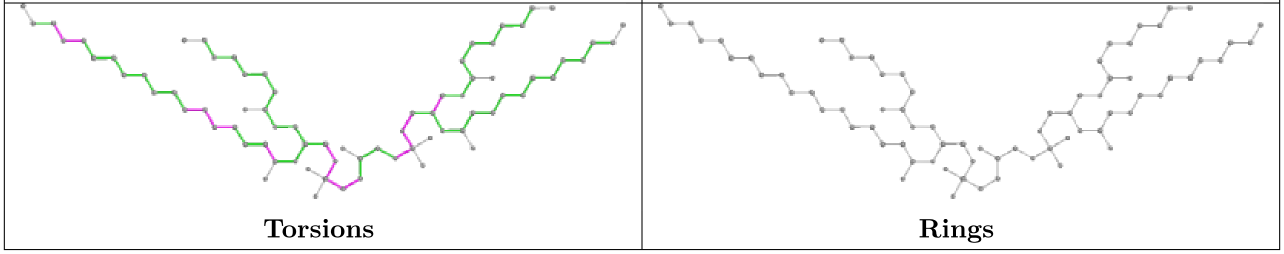
Rings

Ligand CDL l 301



Bond lengths

Bond angles



Torsions

Rings

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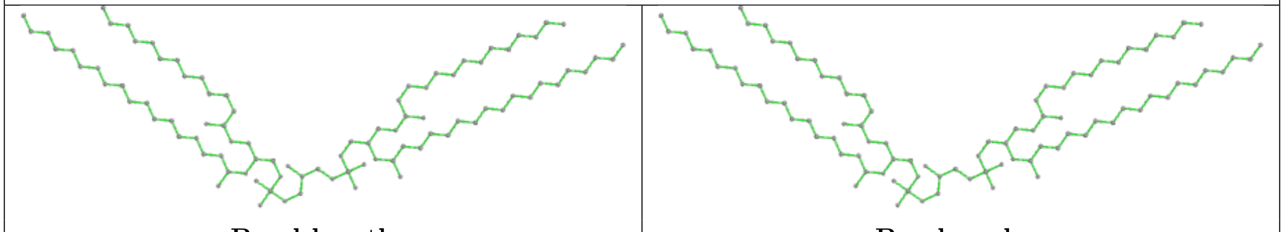
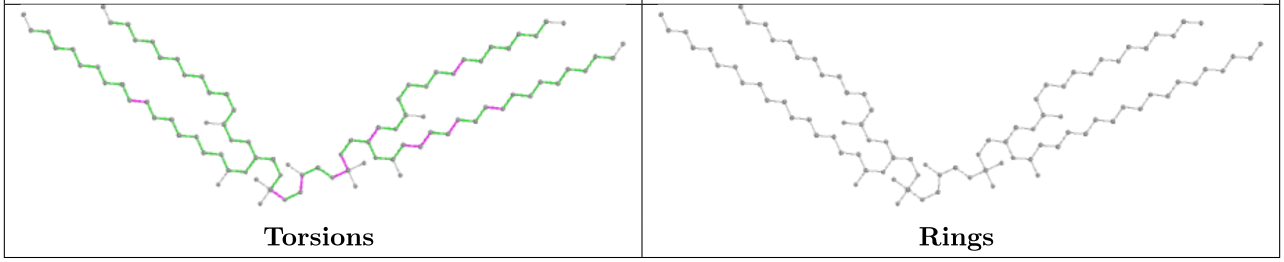


Bond lengths

Bond angles



Torsions

Rings

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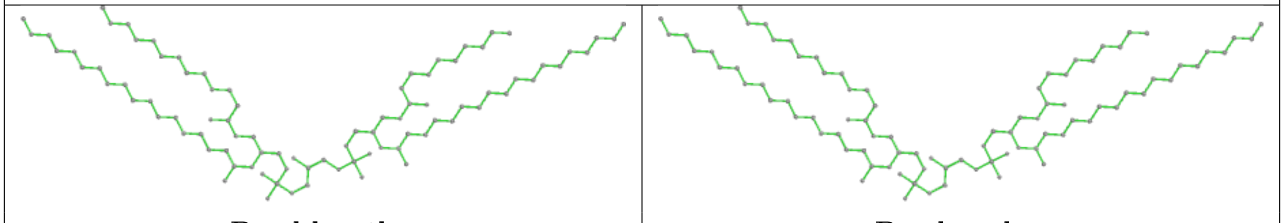
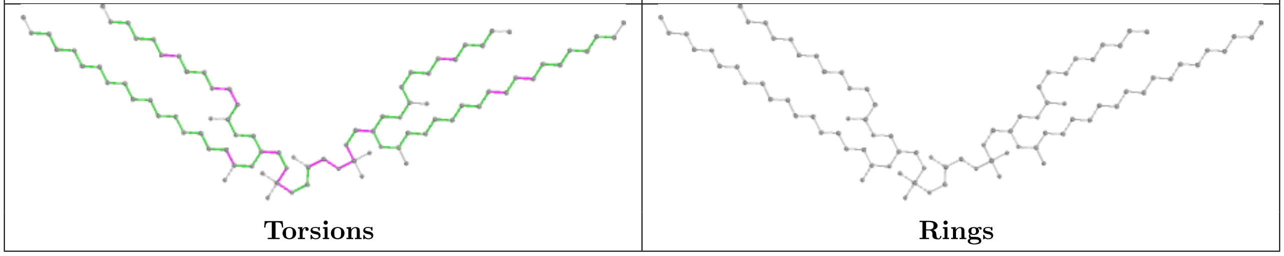


Bond lengths

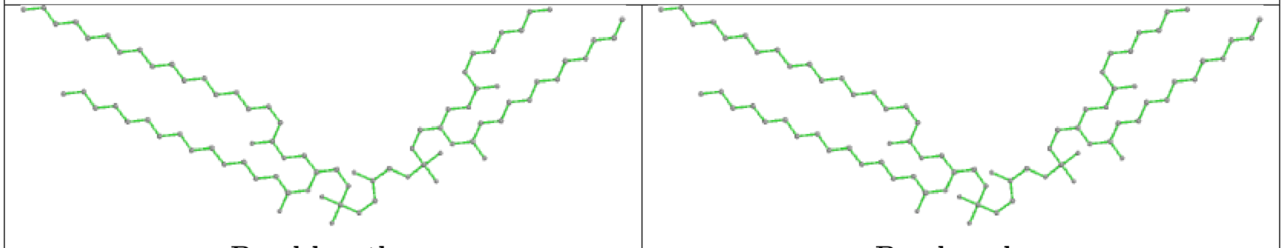
Bond angles



Torsions

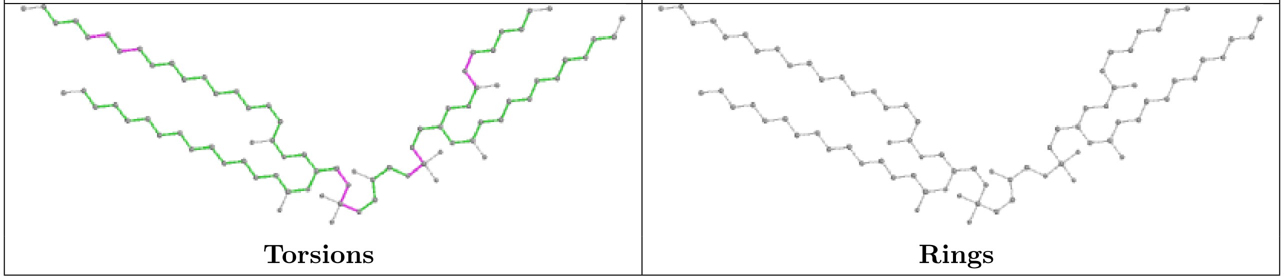
Rings

Ligand CDL y5 201



Bond lengths

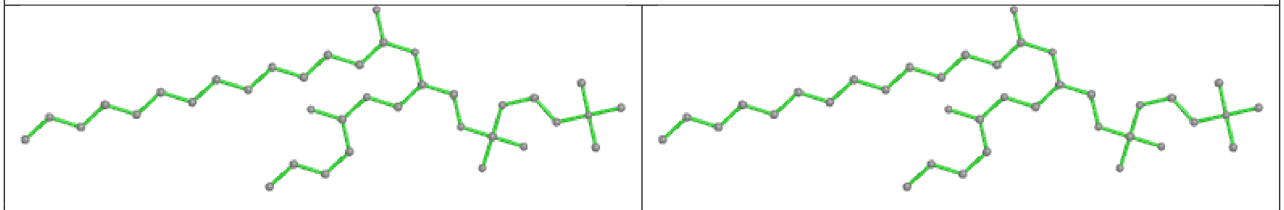
Bond angles



Torsions

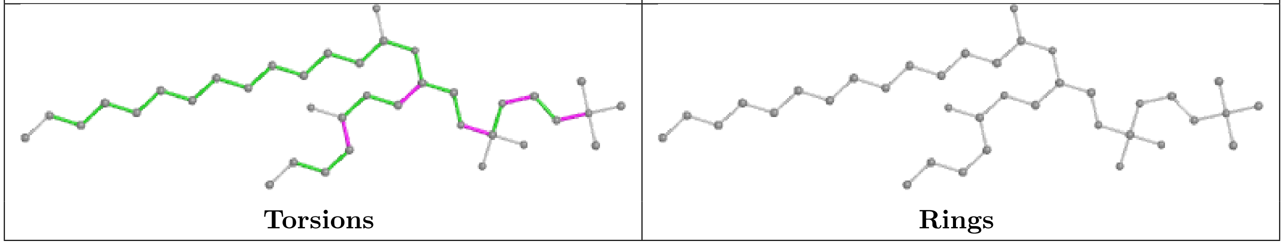
Rings

Ligand PC1 j 302



Bond lengths

Bond angles



Torsions

Rings

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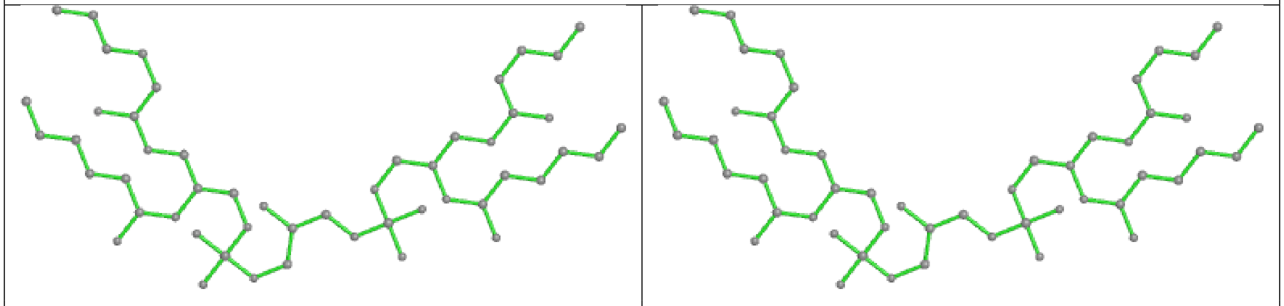
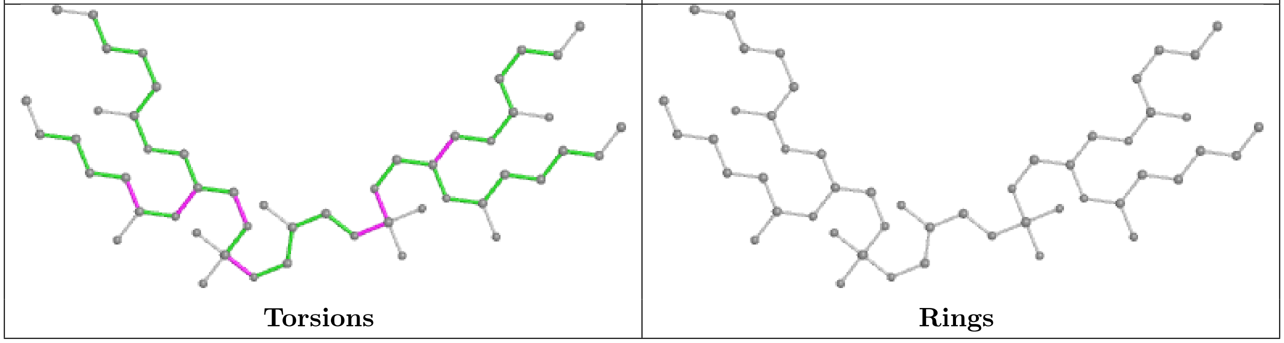


Bond lengths

Bond angles



Torsions

Rings

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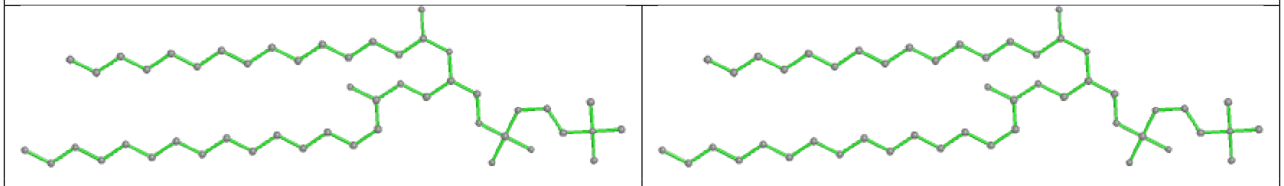
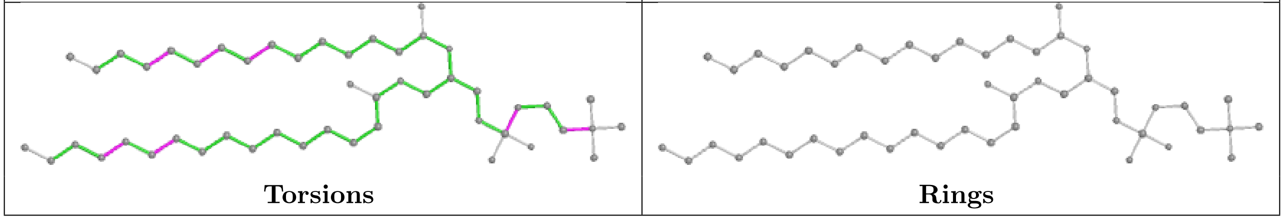


Bond lengths

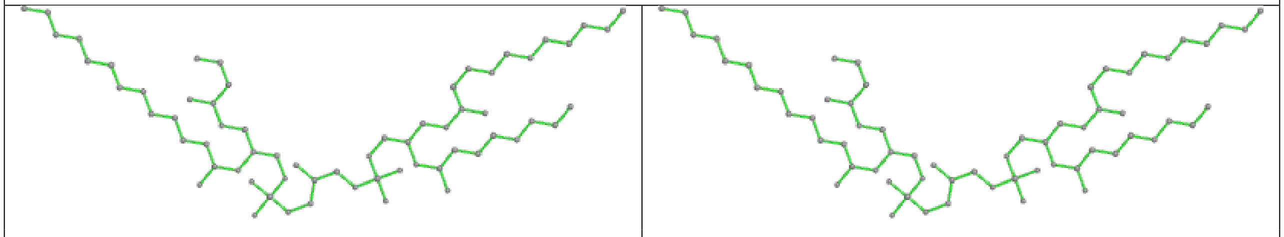
Bond angles



Torsions

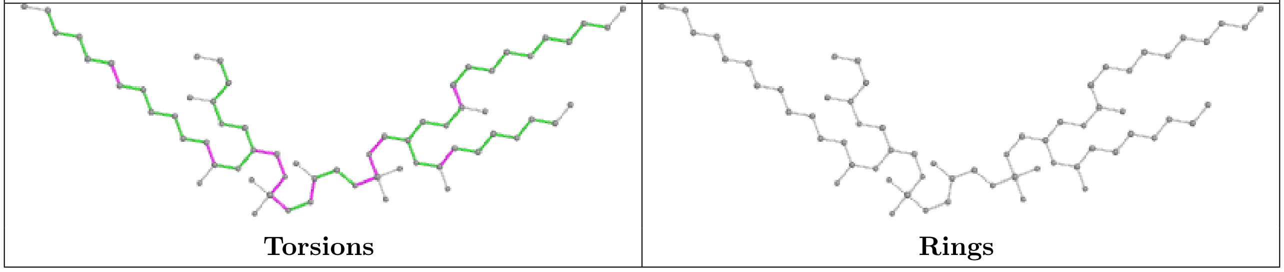
Rings

Ligand CDL Y0 101



Bond lengths

Bond angles



Torsions

Rings

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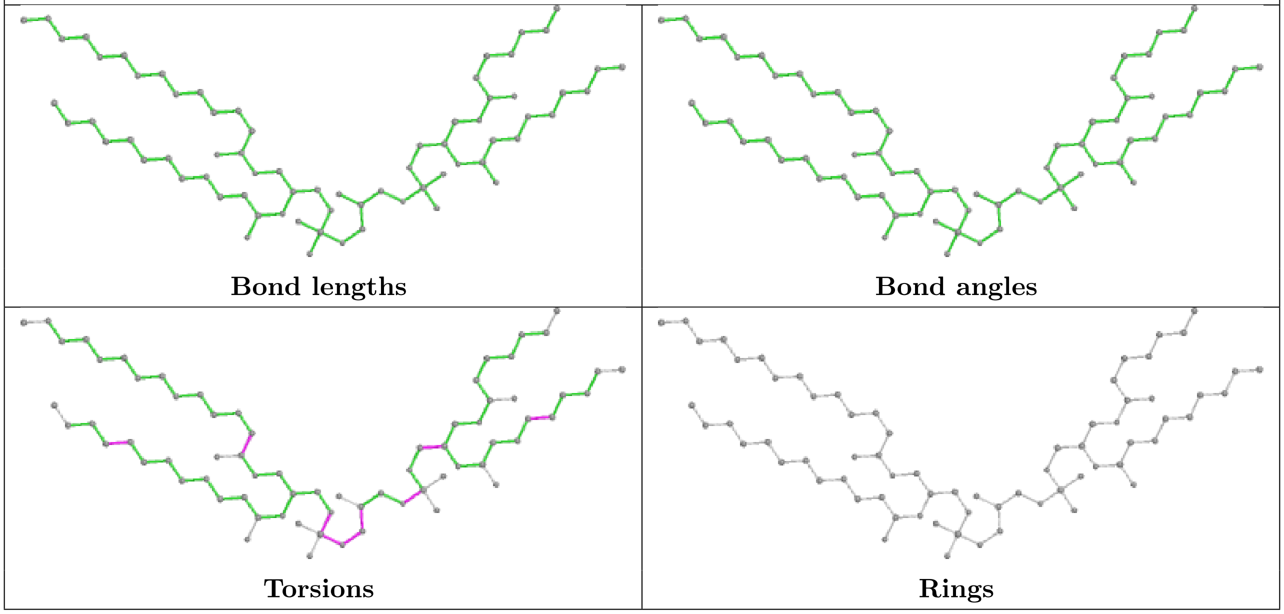


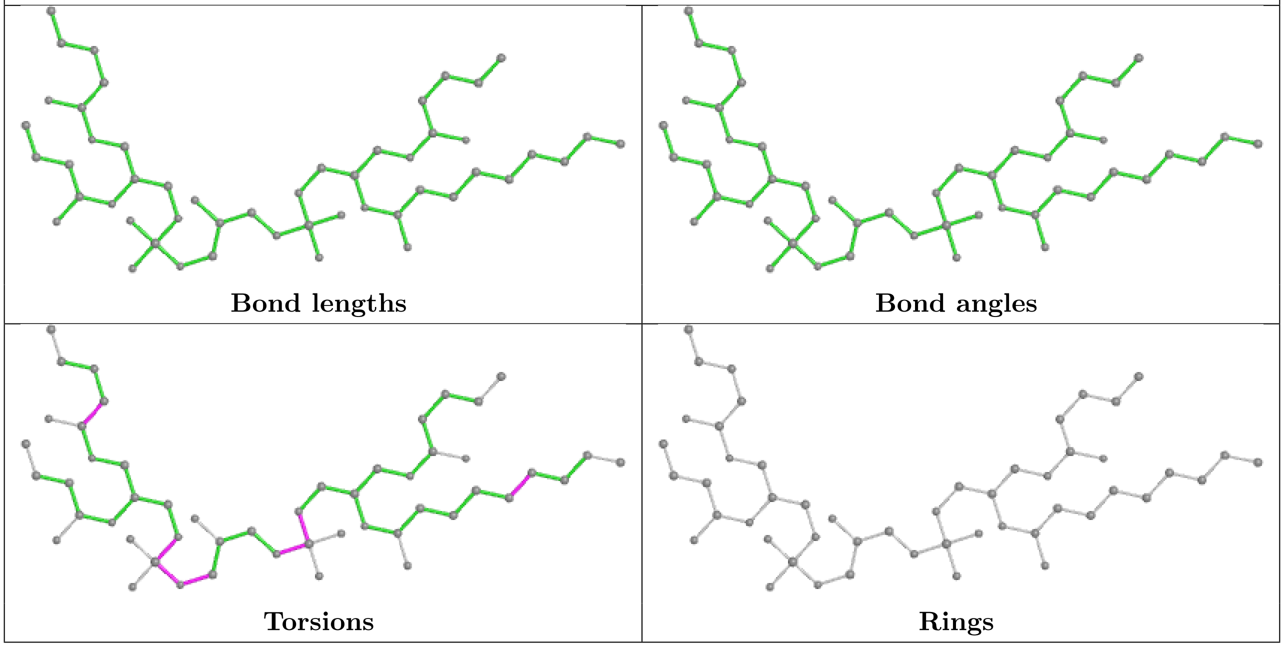
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL m3 402



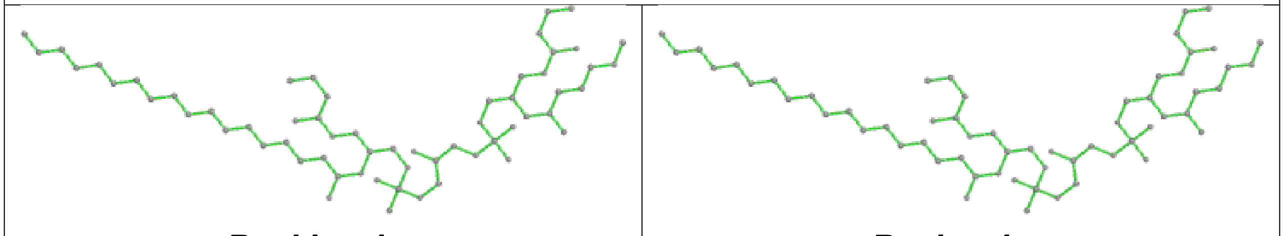
Bond lengths

Bond angles

Torsions

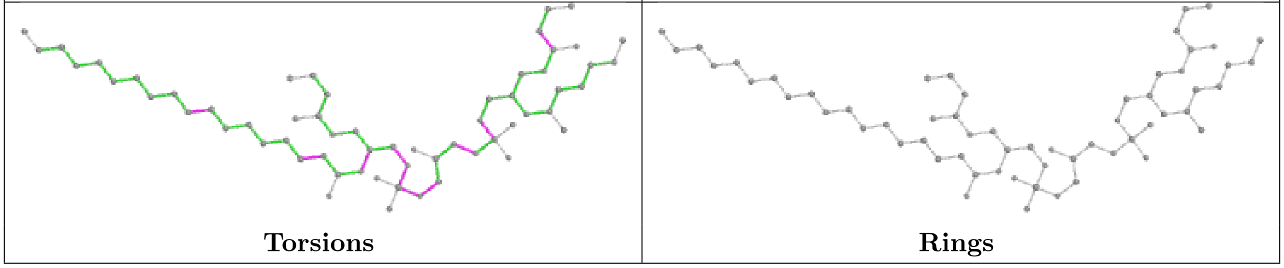
Rings

Ligand CDL e 401



Bond lengths

Bond angles



Torsions

Rings

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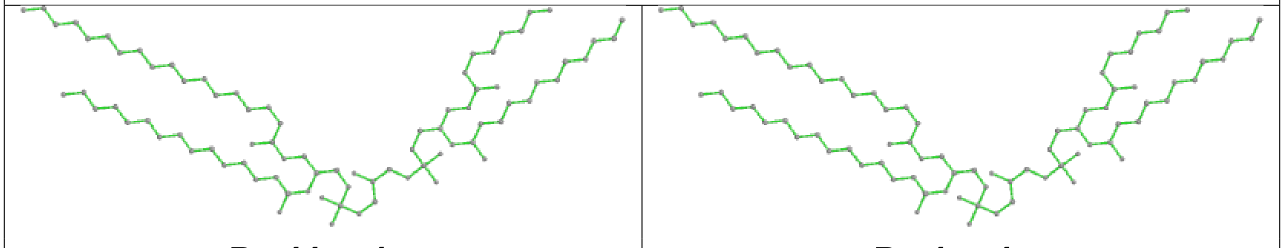

Bond lengths

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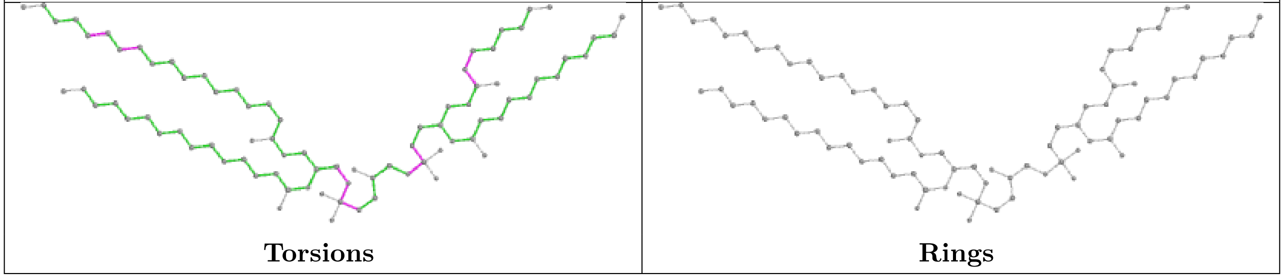
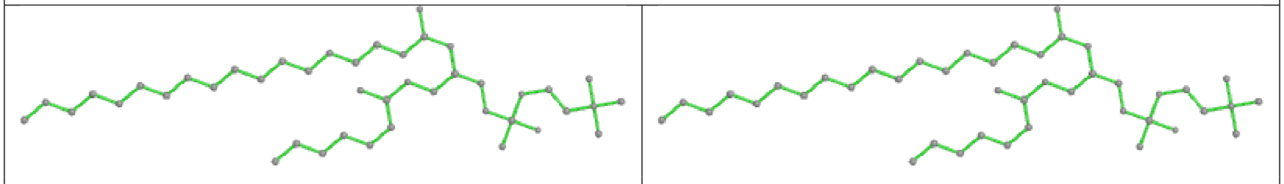


Torsions

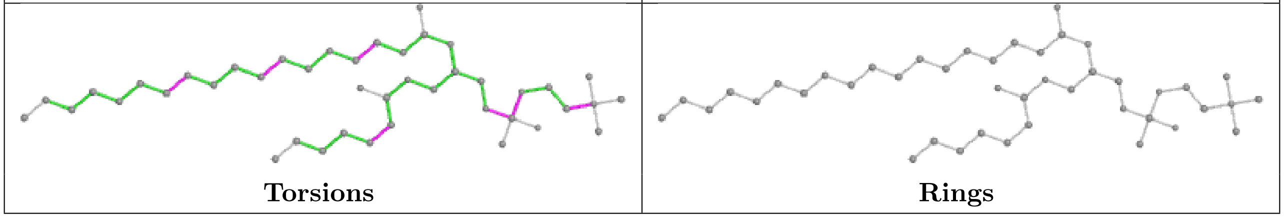
Rings

Ligand PC1 7c 303



Bond lengths

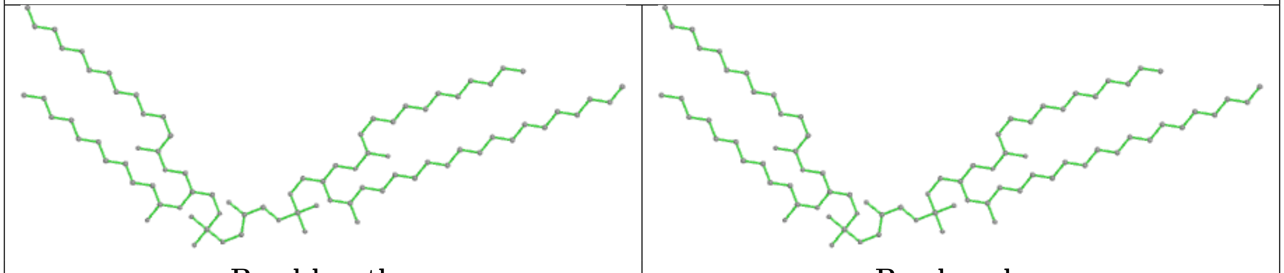
Bond angles

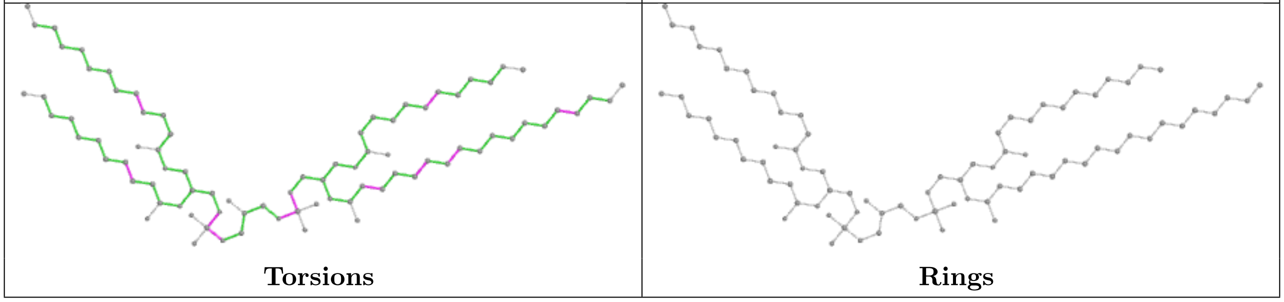


Torsions

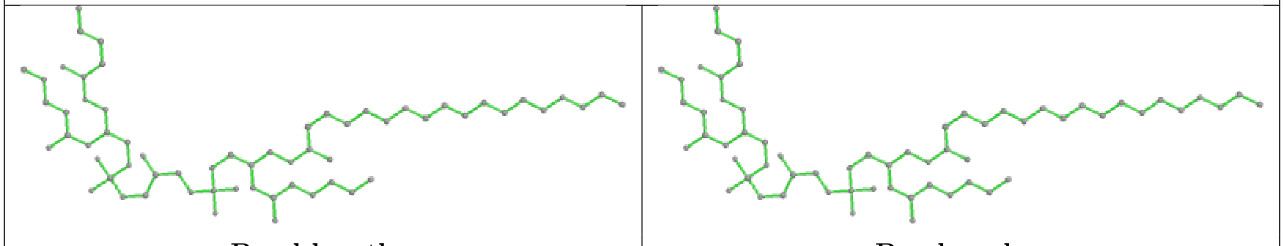
Rings

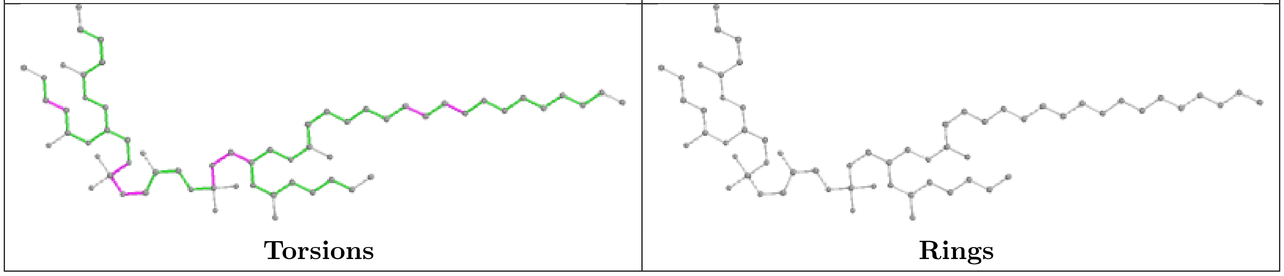
Ligand CDL u 201


Bond lengths Bond angles

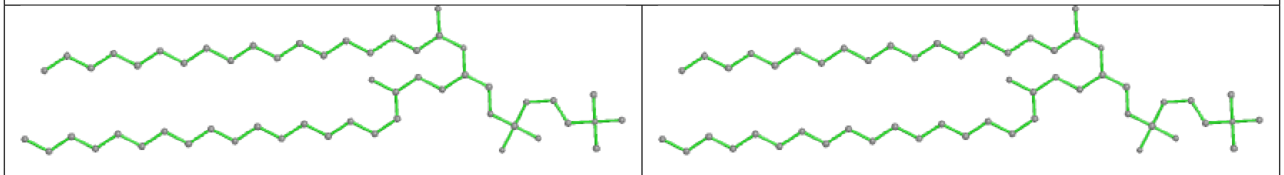

Torsions Rings

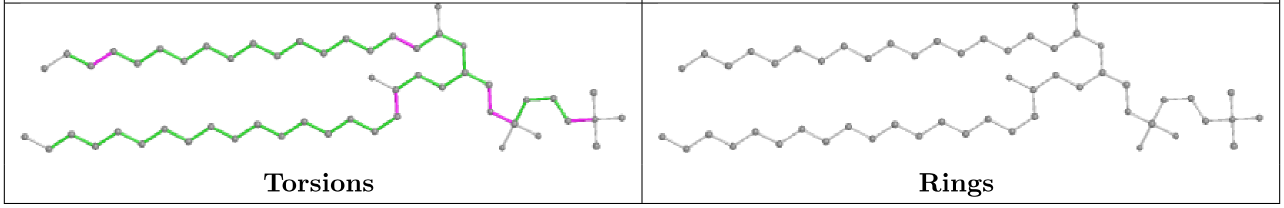
Ligand CDL 5B 703


Bond lengths Bond angles

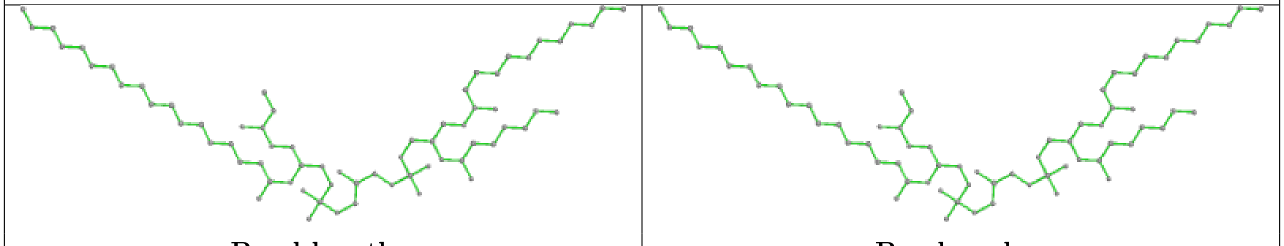

Torsions Rings

Ligand PC1 M2 406


Bond lengths Bond angles

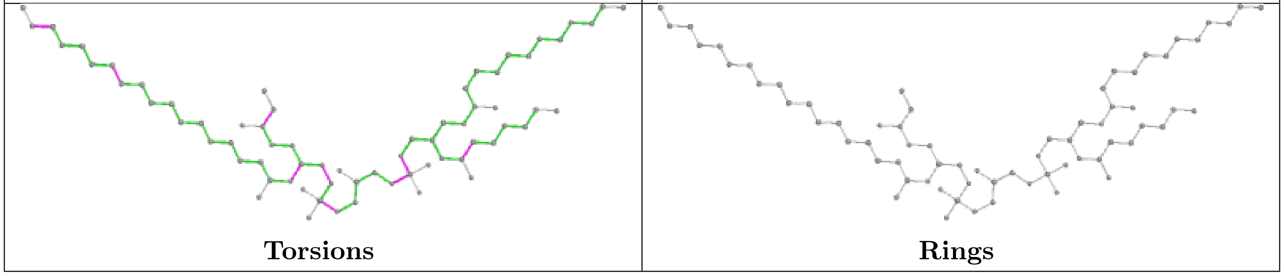

Torsions Rings

Ligand CDL T 201



Bond lengths

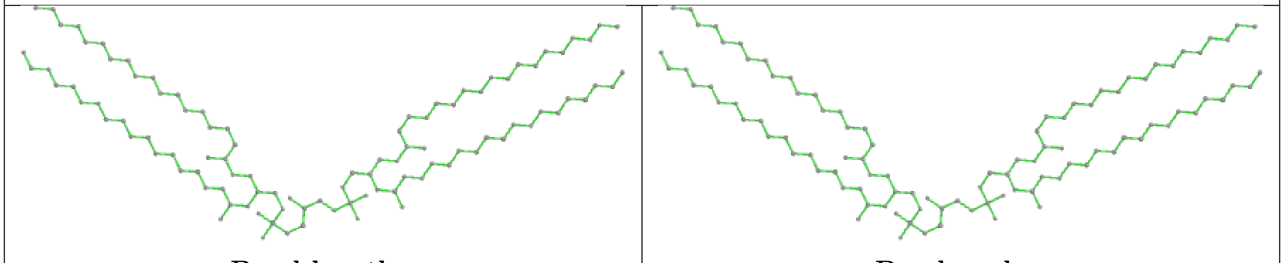
Bond angles



Torsions

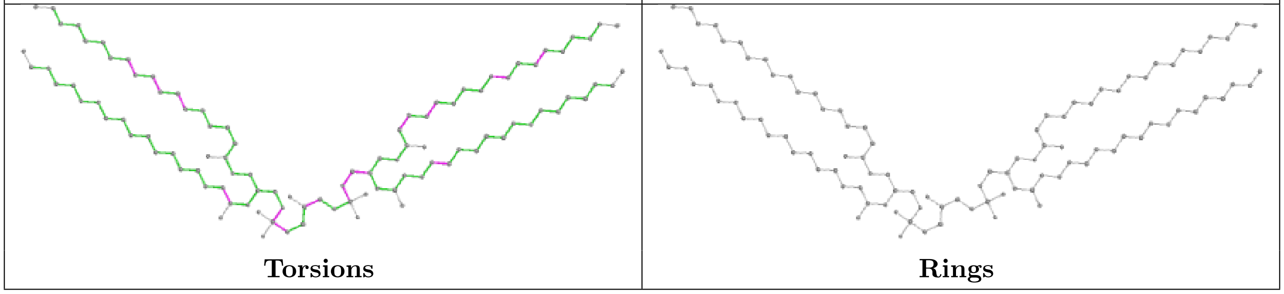
Rings

Ligand CDL F 401



Bond lengths

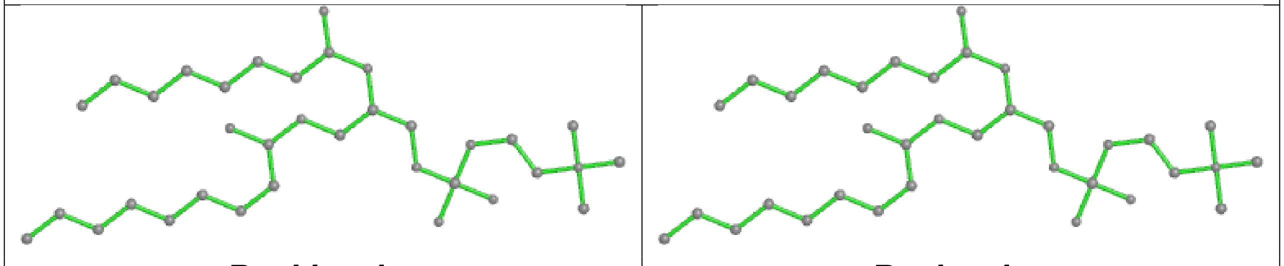
Bond angles



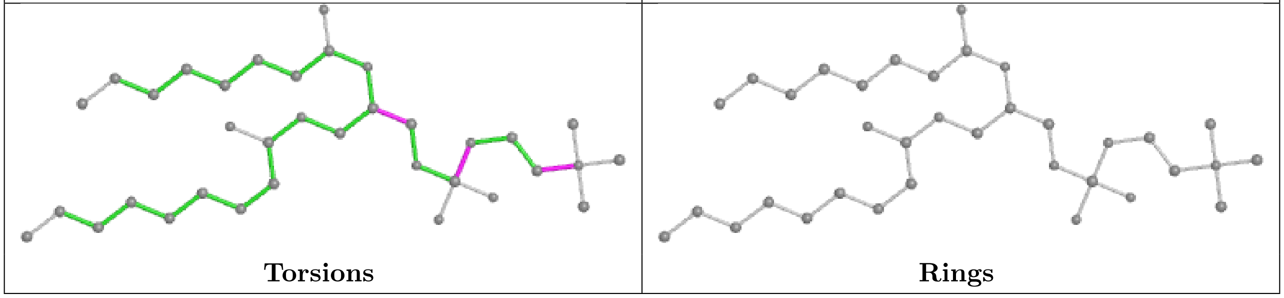
Torsions

Rings

Ligand PC1 M1 404

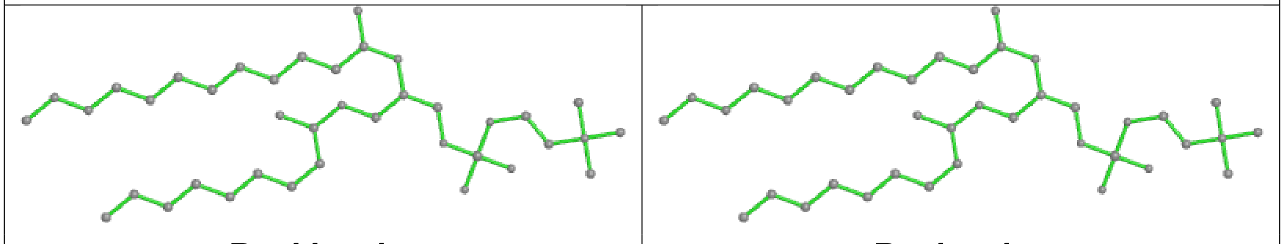


Bond lengths Bond angles

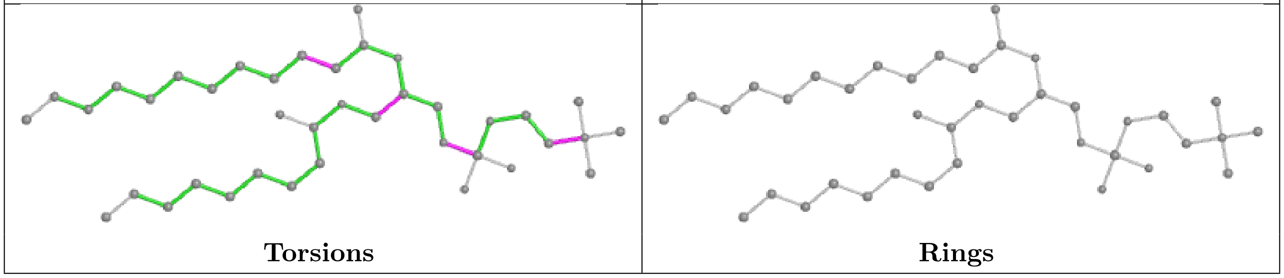


Torsions Rings

Ligand PC1 c3 602

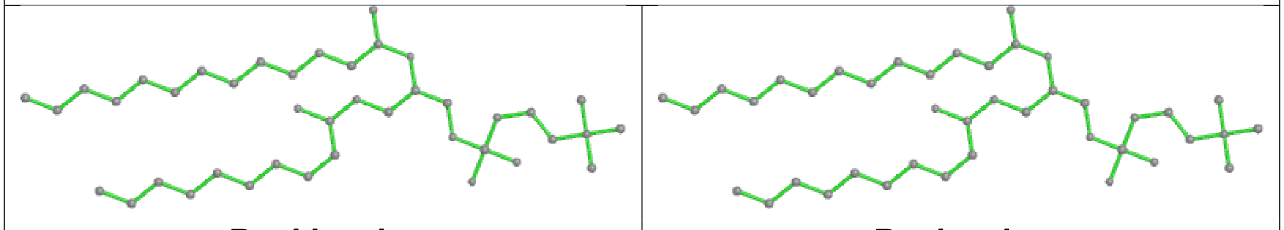


Bond lengths Bond angles

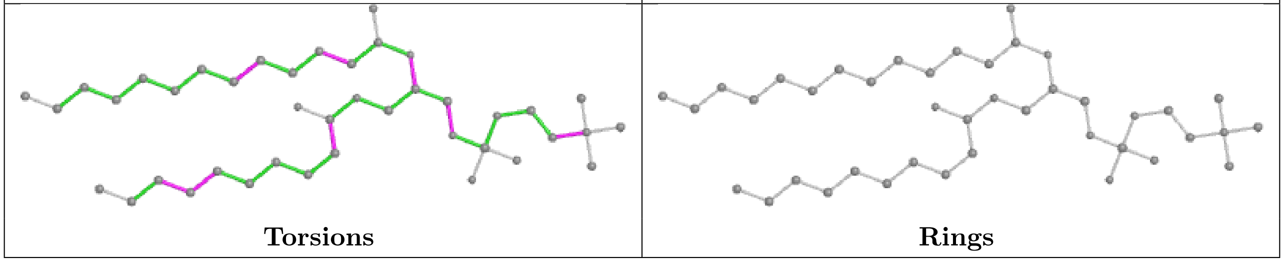


Torsions Rings

Ligand PC1 C3 605

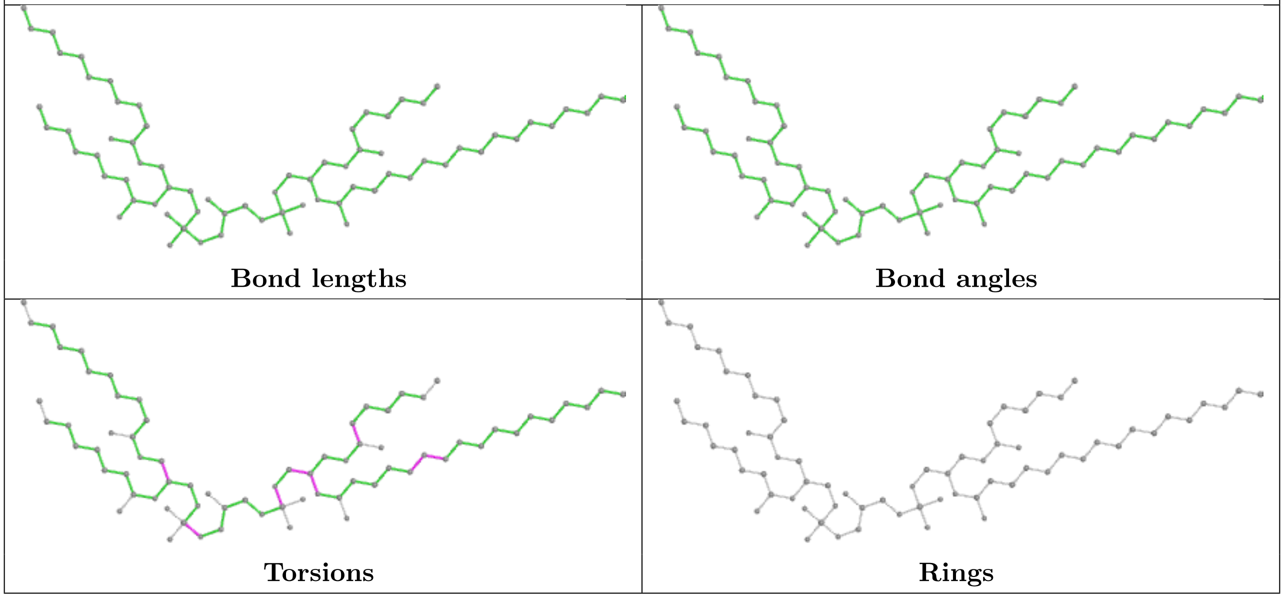


Bond lengths Bond angles



Torsions Rings

Ligand CDL e 402



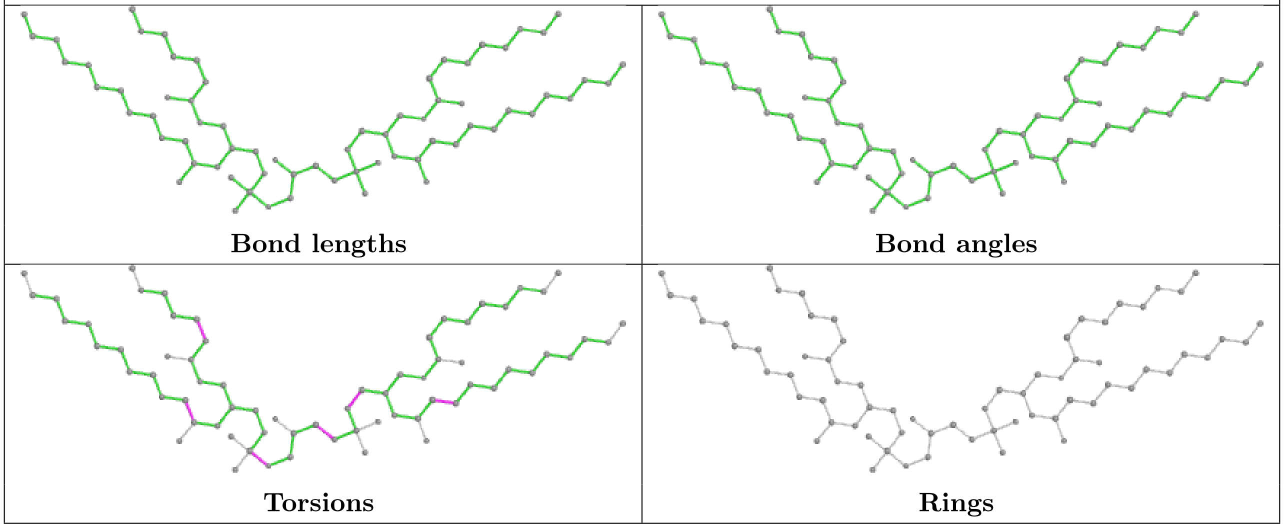
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL C3 604



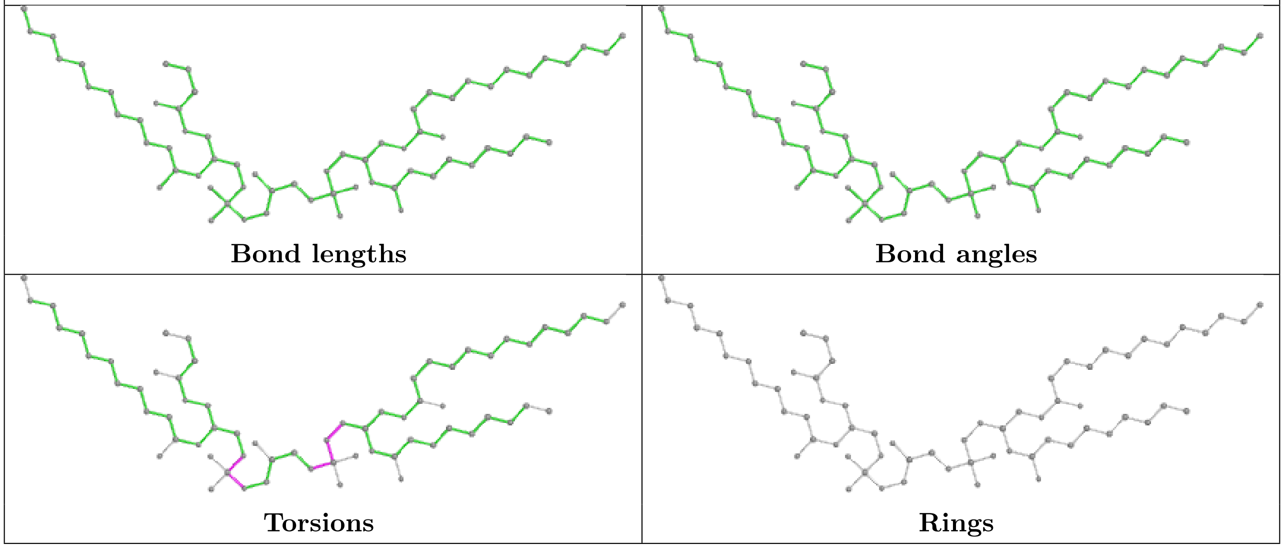
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL M1 403



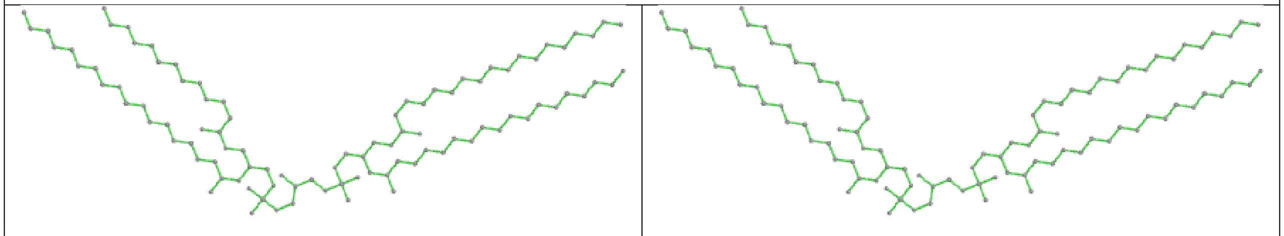
Bond lengths

Bond angles

Torsions

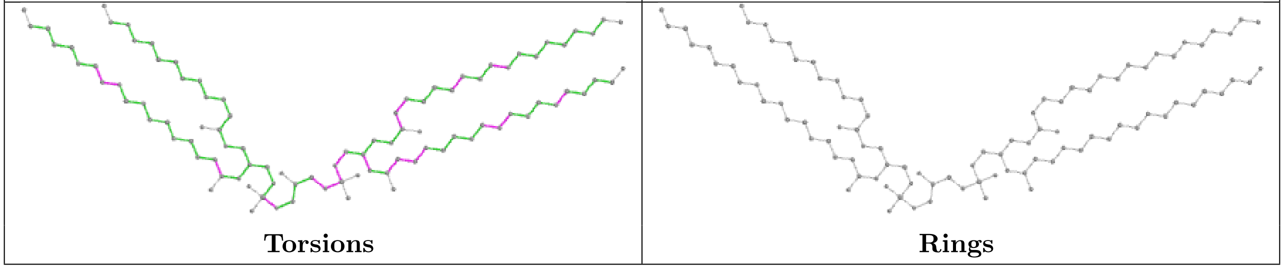
Rings

Ligand CDL m1 401



Bond lengths

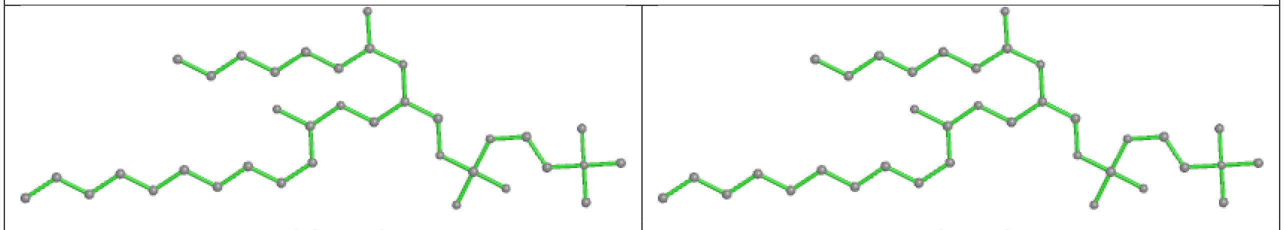
Bond angles



Torsions

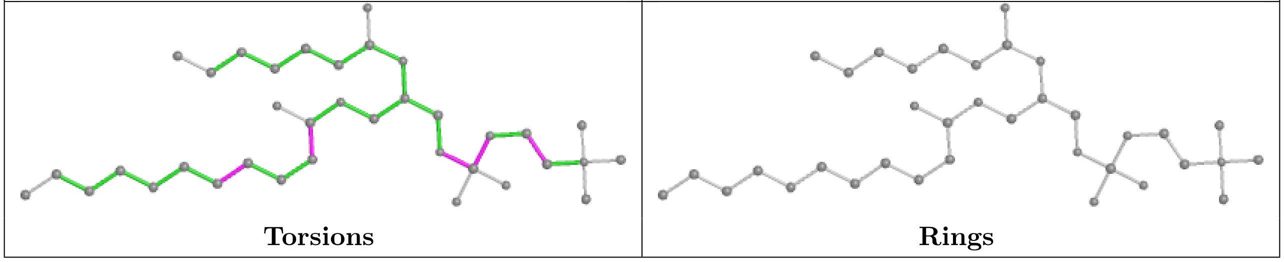
Rings

Ligand PC1 n 302



Bond lengths

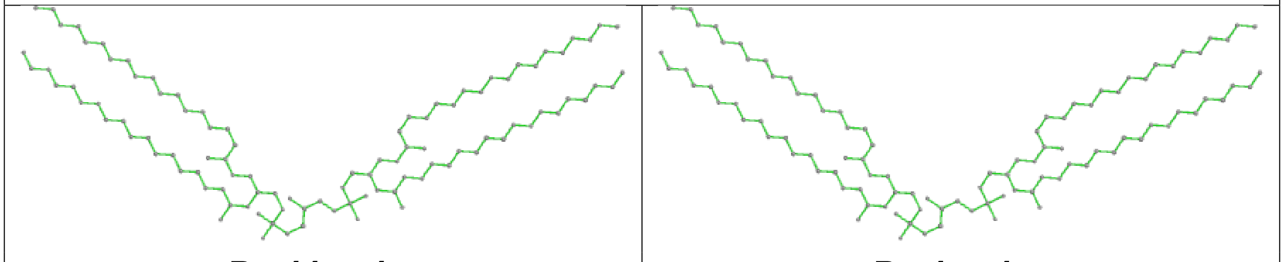
Bond angles



Torsions

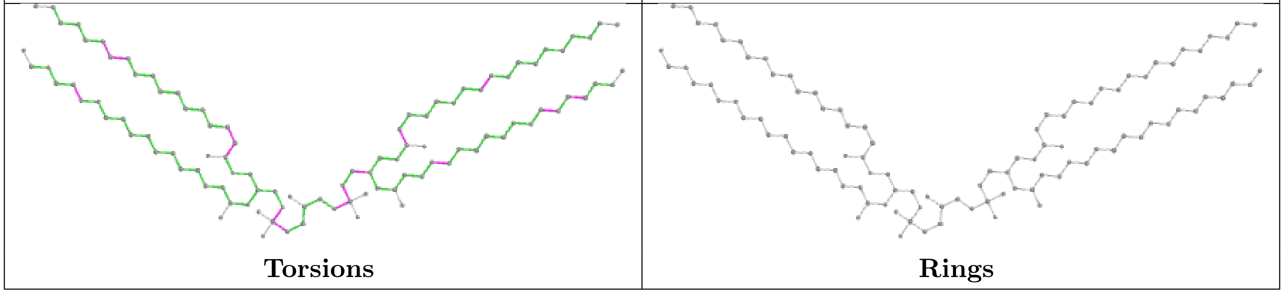
Rings

Ligand CDL 7A 202



Bond lengths

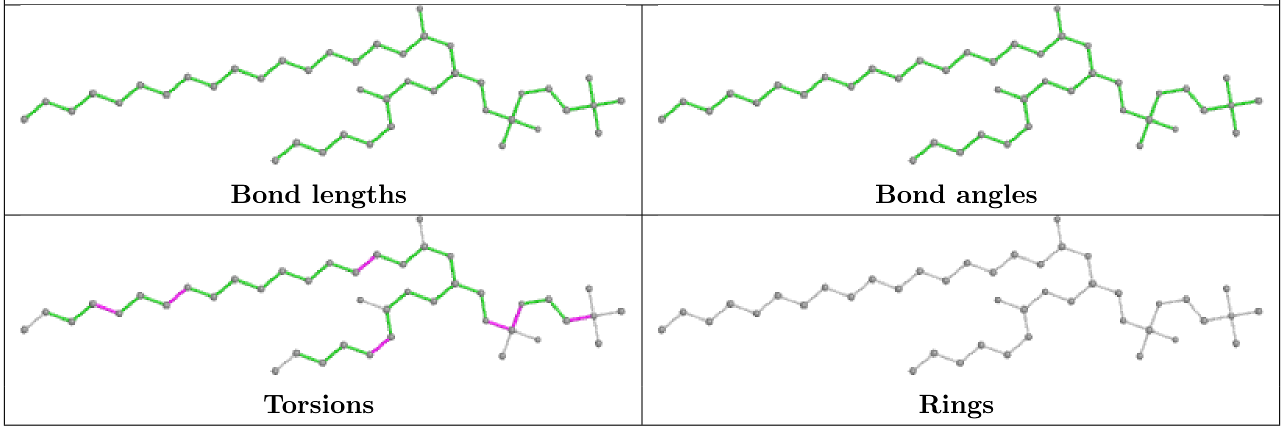
Bond angles



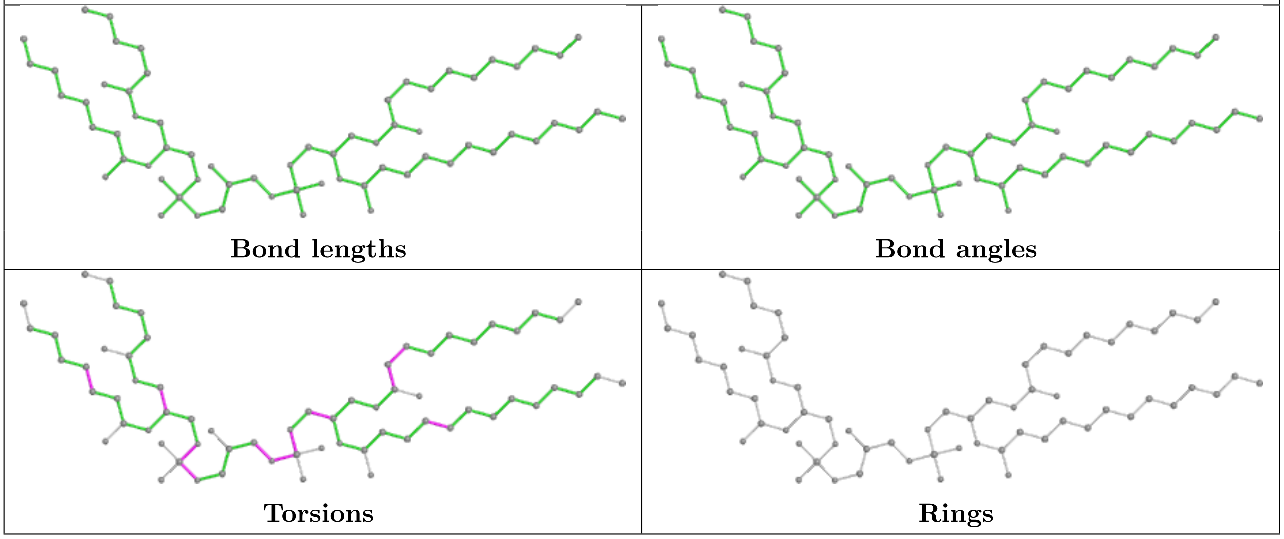
Torsions

Rings

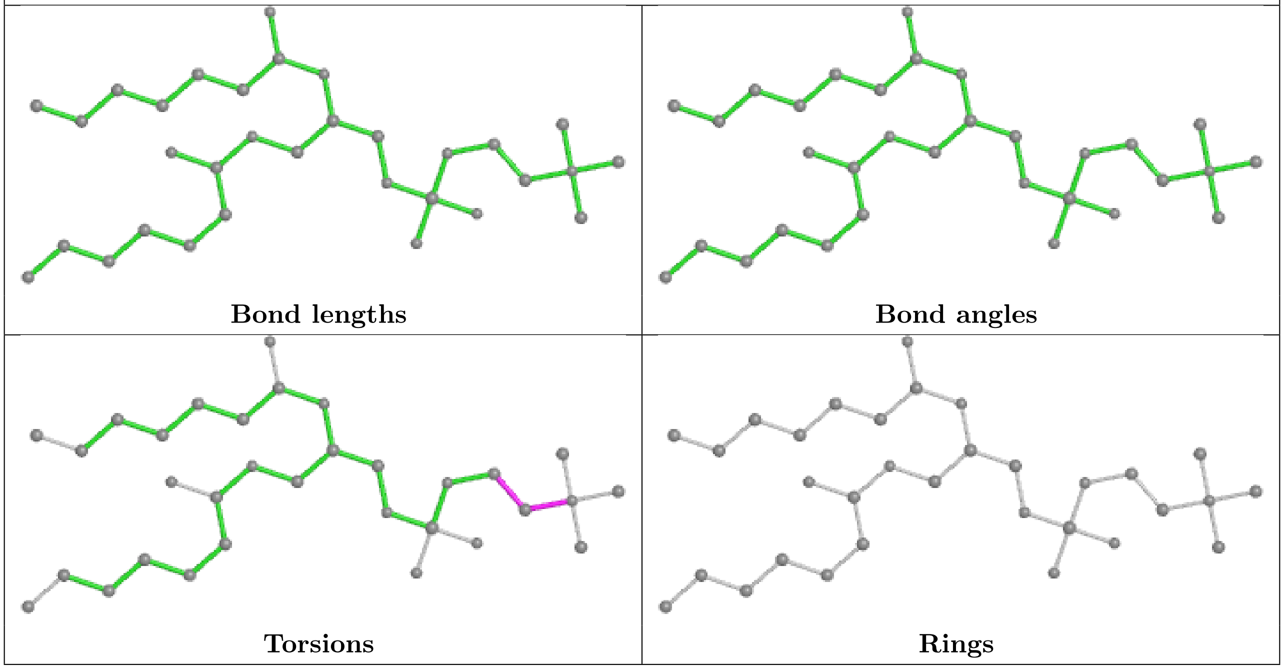
Ligand PC1 7C 304


Bond lengths
Bond angles
Torsions
Rings

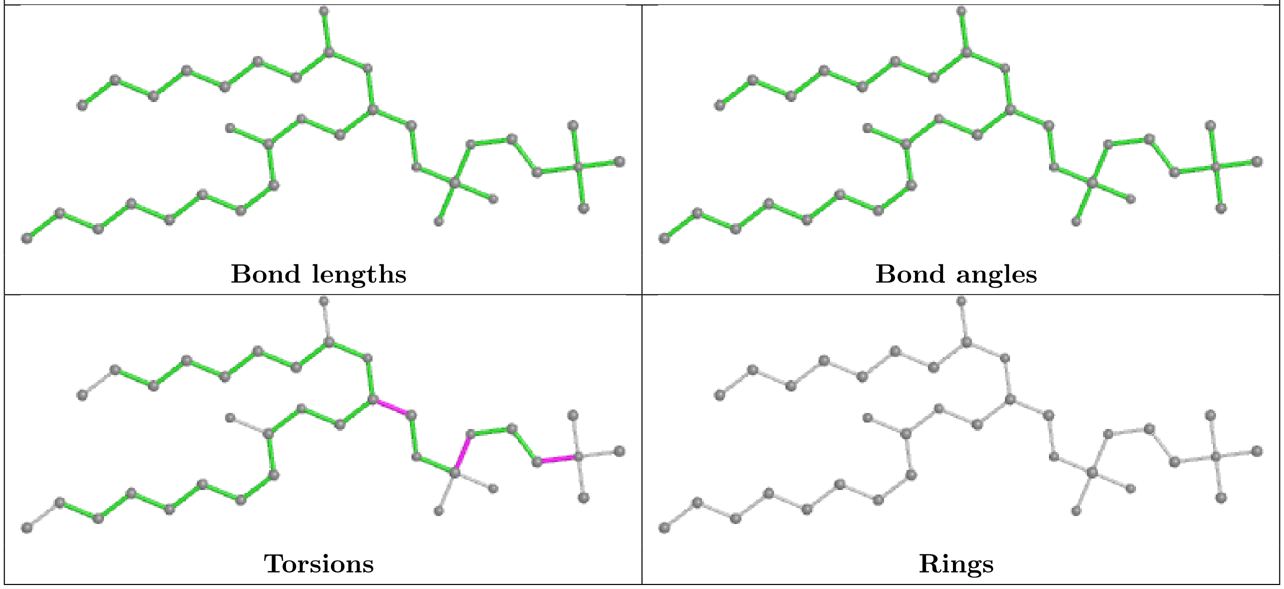
Ligand CDL M2 403


Bond lengths
Bond angles
Torsions
Rings

Ligand PC1 M2 402


Bond lengths
Bond angles
Torsions
Rings

Ligand PC1 m1 405



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

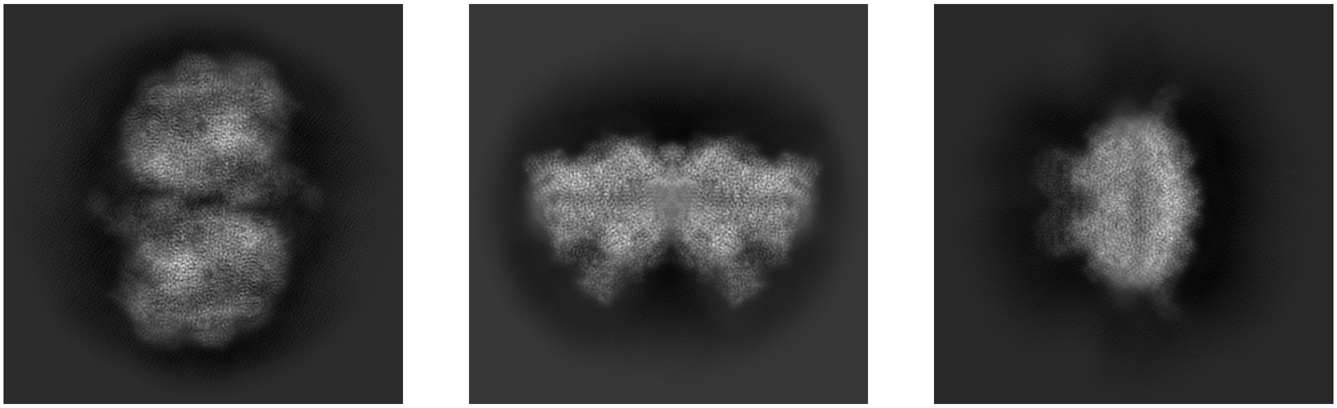
6 Map visualisation ⓘ

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.

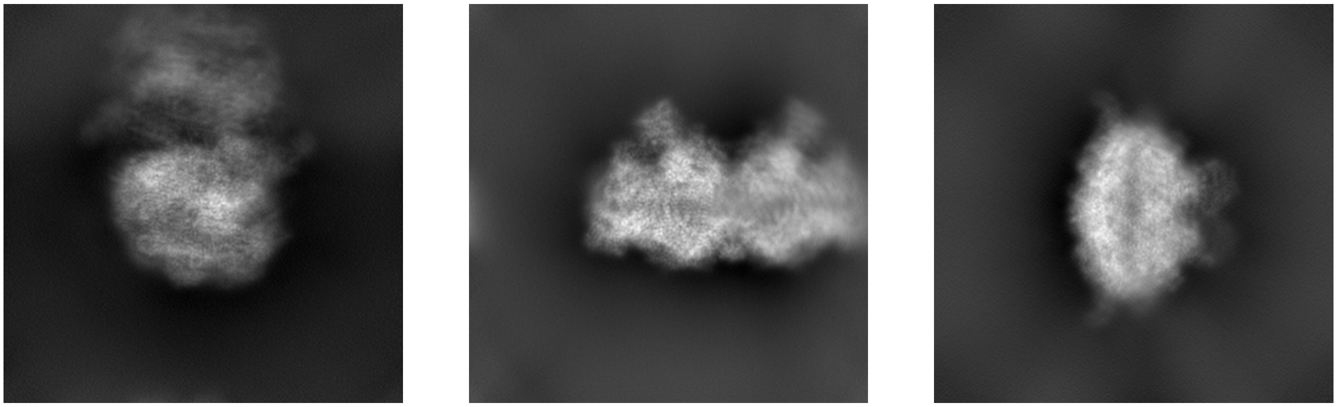
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

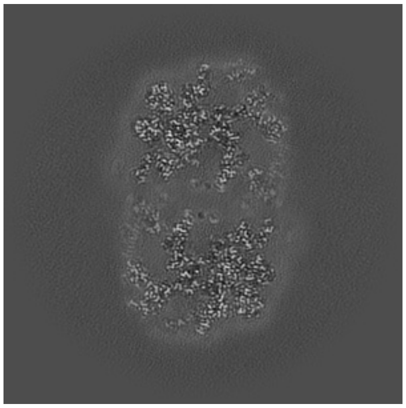


X Y Z

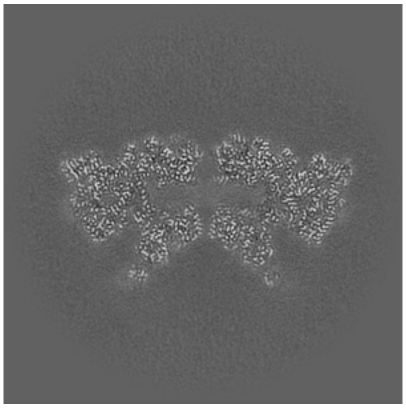
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

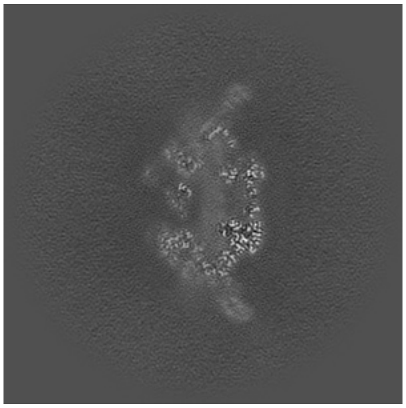
6.2.1 Primary map



X Index: 256

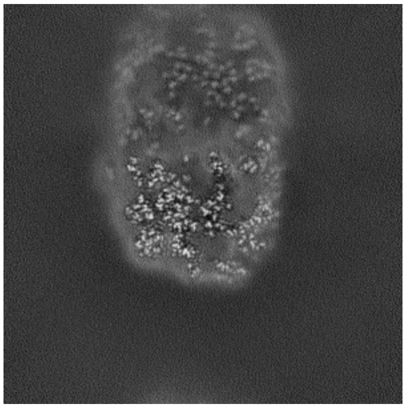


Y Index: 256

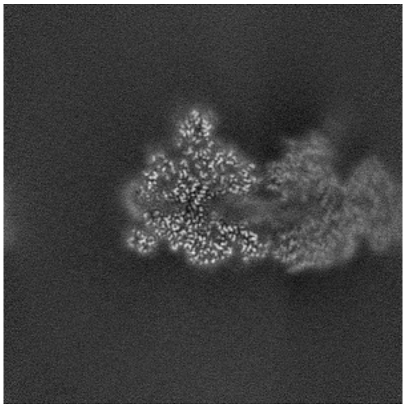


Z Index: 256

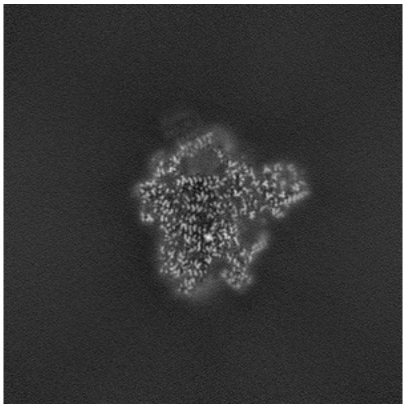
6.2.2 Raw map



X Index: 256



Y Index: 256

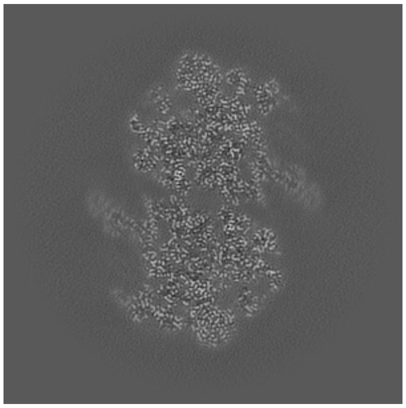


Z Index: 256

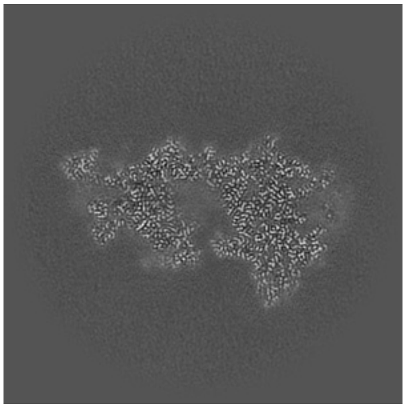
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

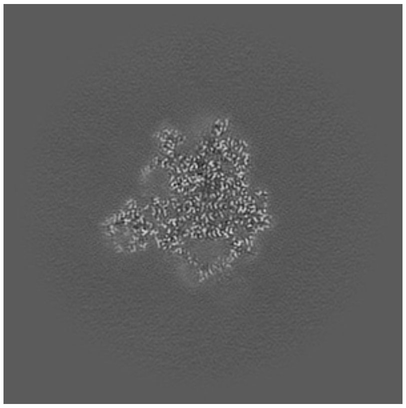
6.3.1 Primary map



X Index: 297

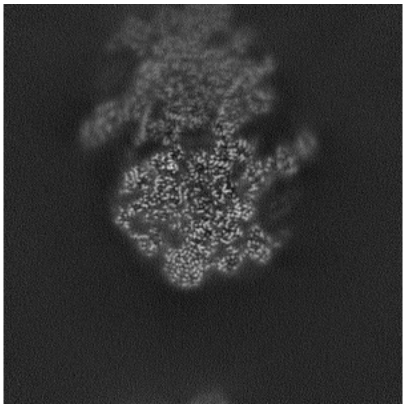


Y Index: 286

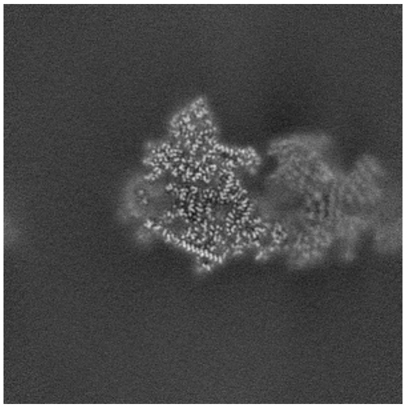


Z Index: 180

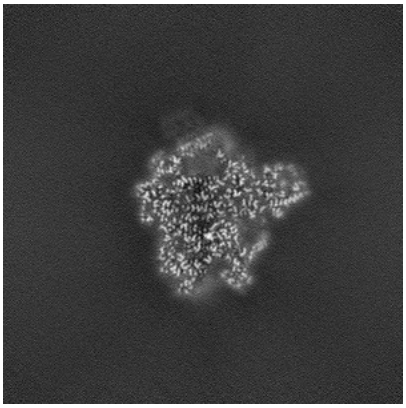
6.3.2 Raw map



X Index: 217



Y Index: 273

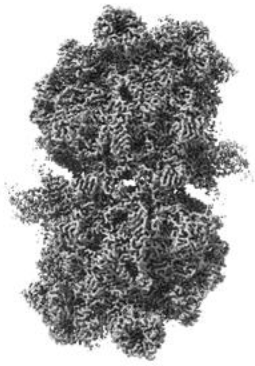


Z Index: 257

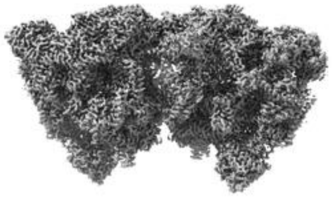
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X



Y

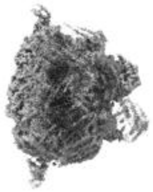
Z

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.

6.4.2 Raw map

X

Y



Z

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

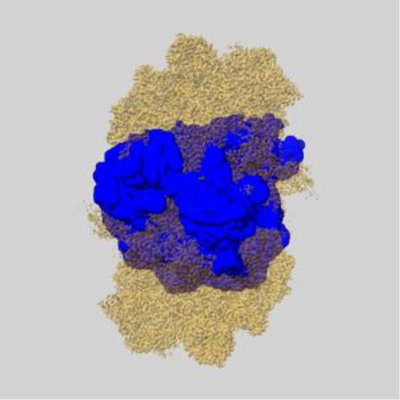
6.5 Mask visualisation

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

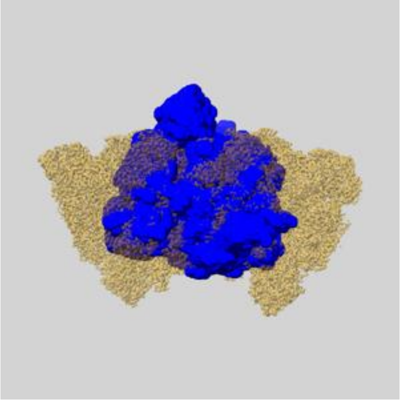
A mask typically either:

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

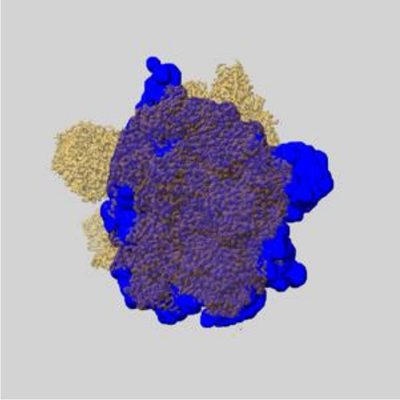
6.5.1 emd_32325_msk_1.map



X



Y

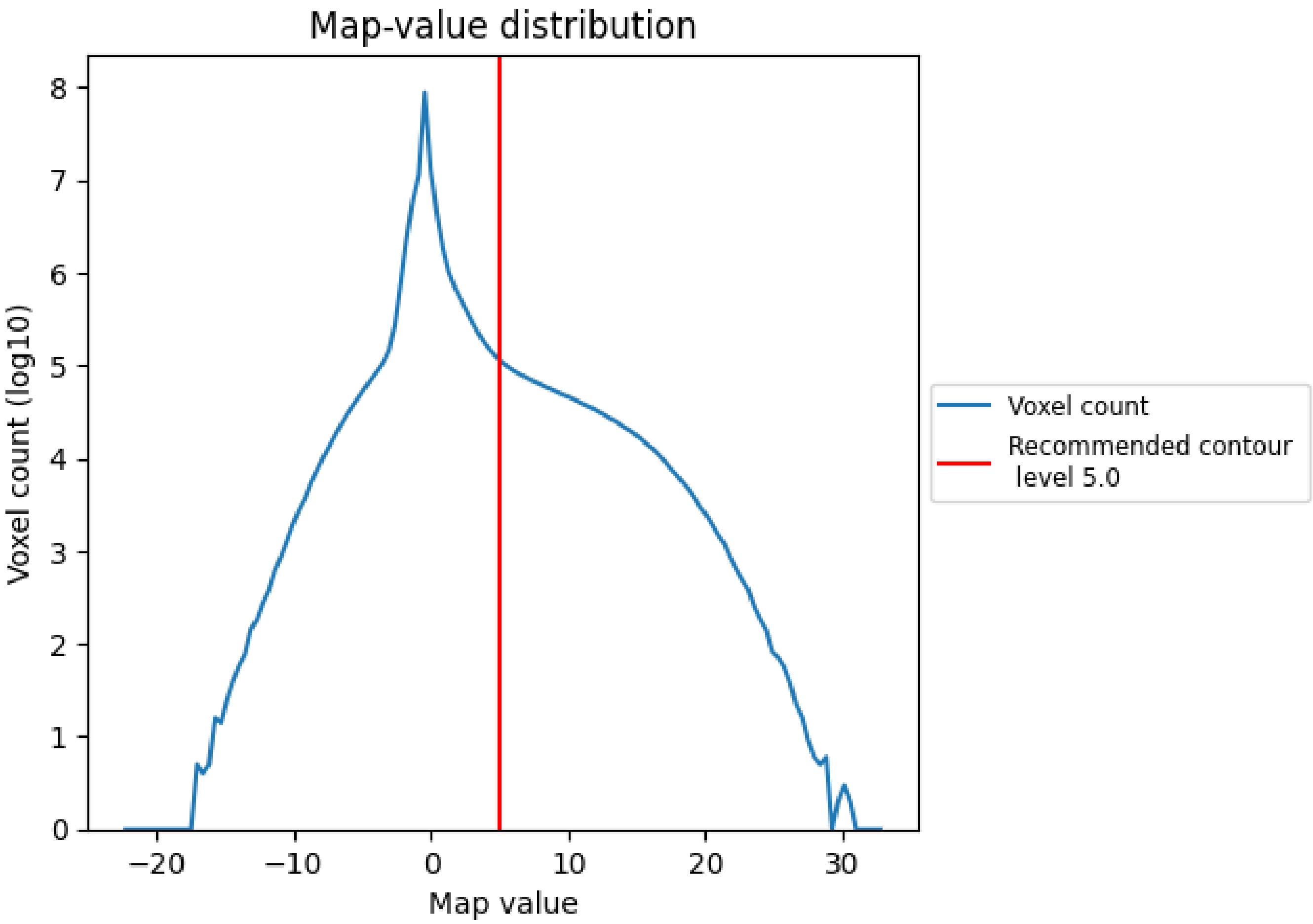


Z

7 Map analysis (i)

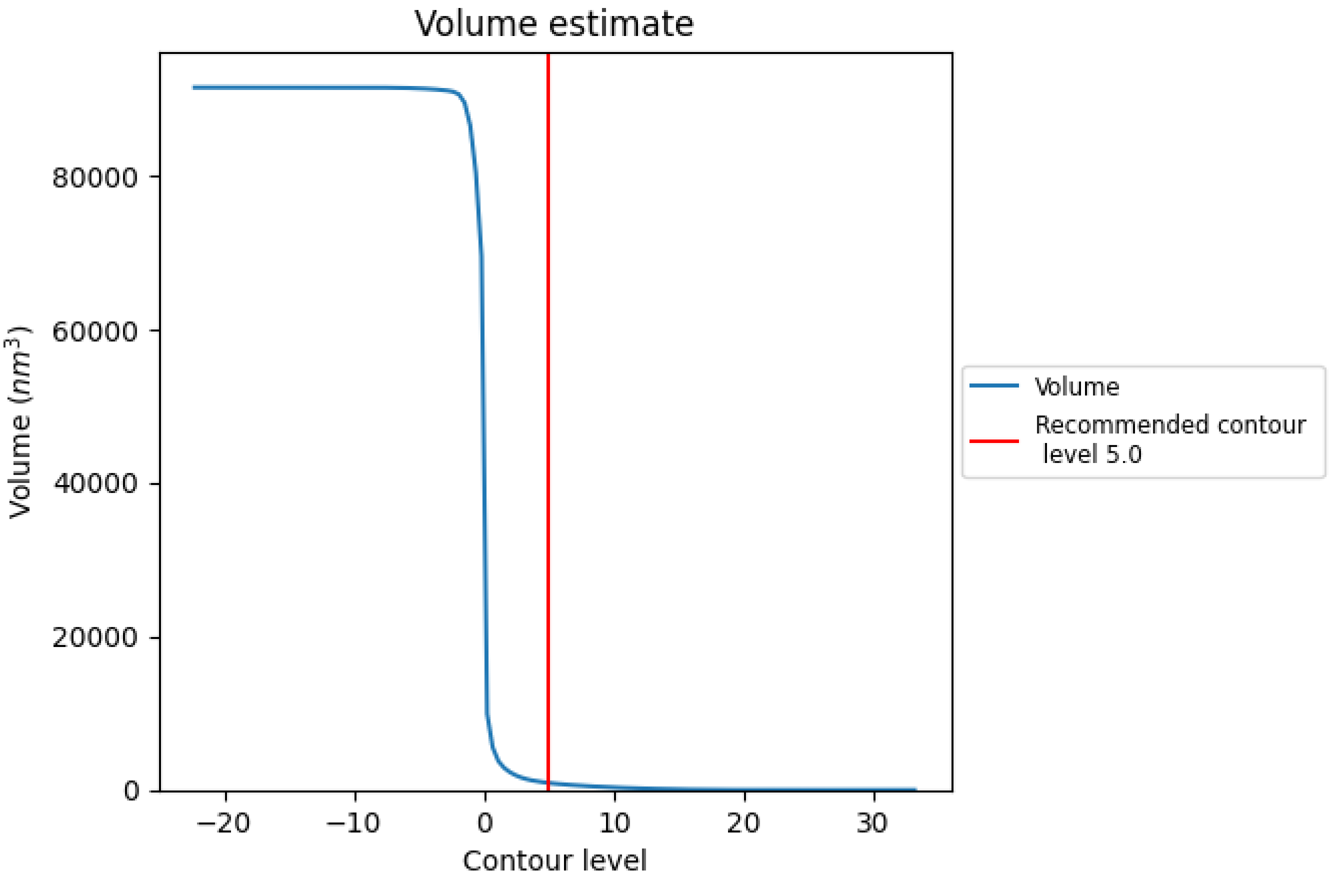
This section contains the results of statistical analysis of the map.

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.

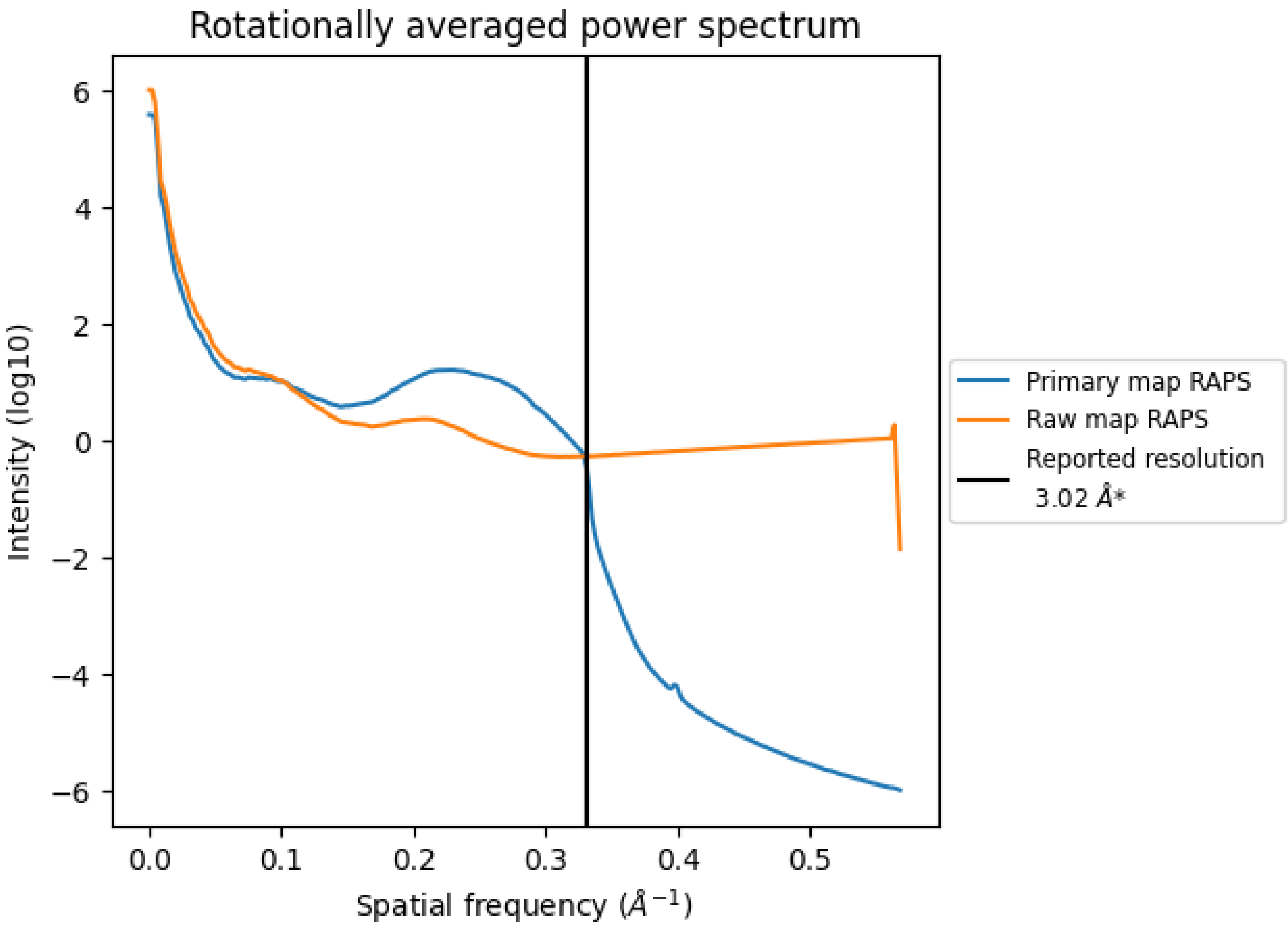
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 911 nm^3; 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 ⓘ

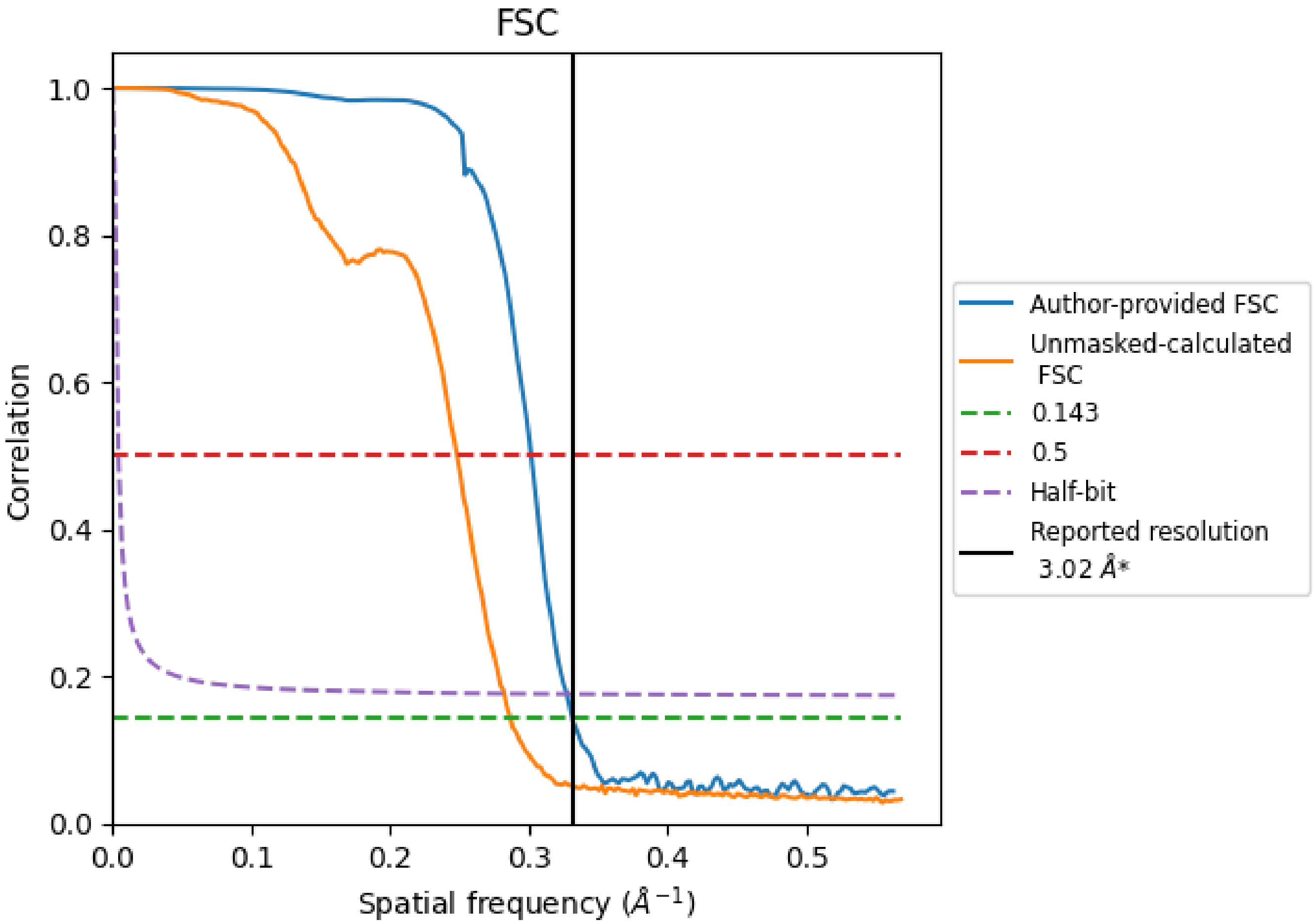


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.331 $Å^{-1}$

8.2 Resolution estimates ⓘ

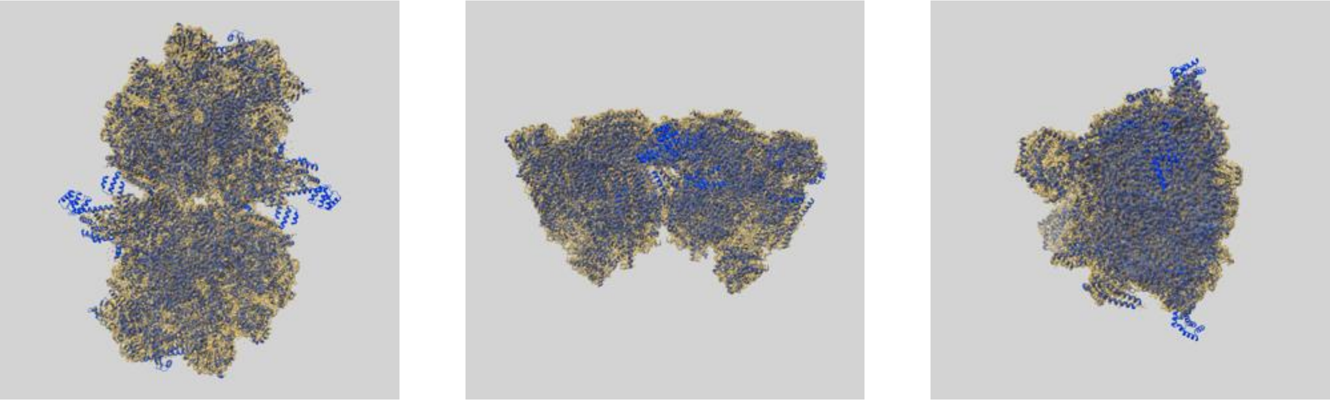
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.31	3.05
Unmasked-calculated*	3.49	4.03	3.54

*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)



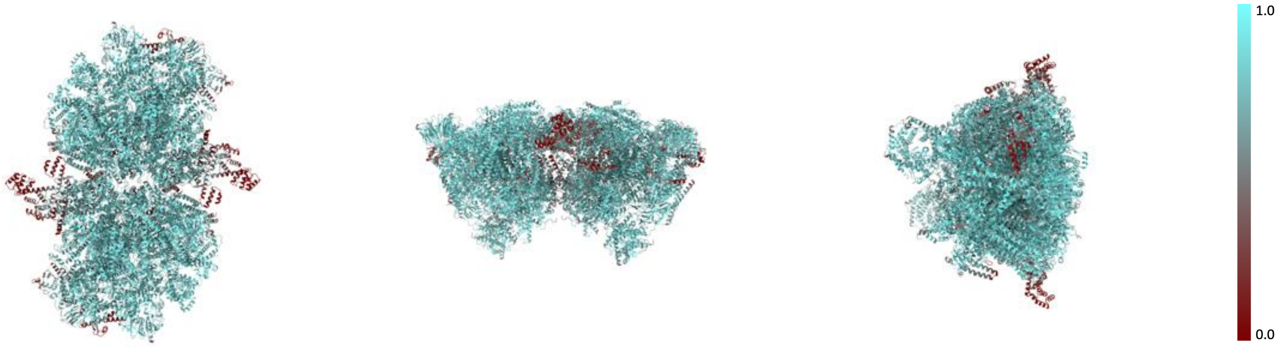
X Y Z

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 ⓘ

This section was not generated.

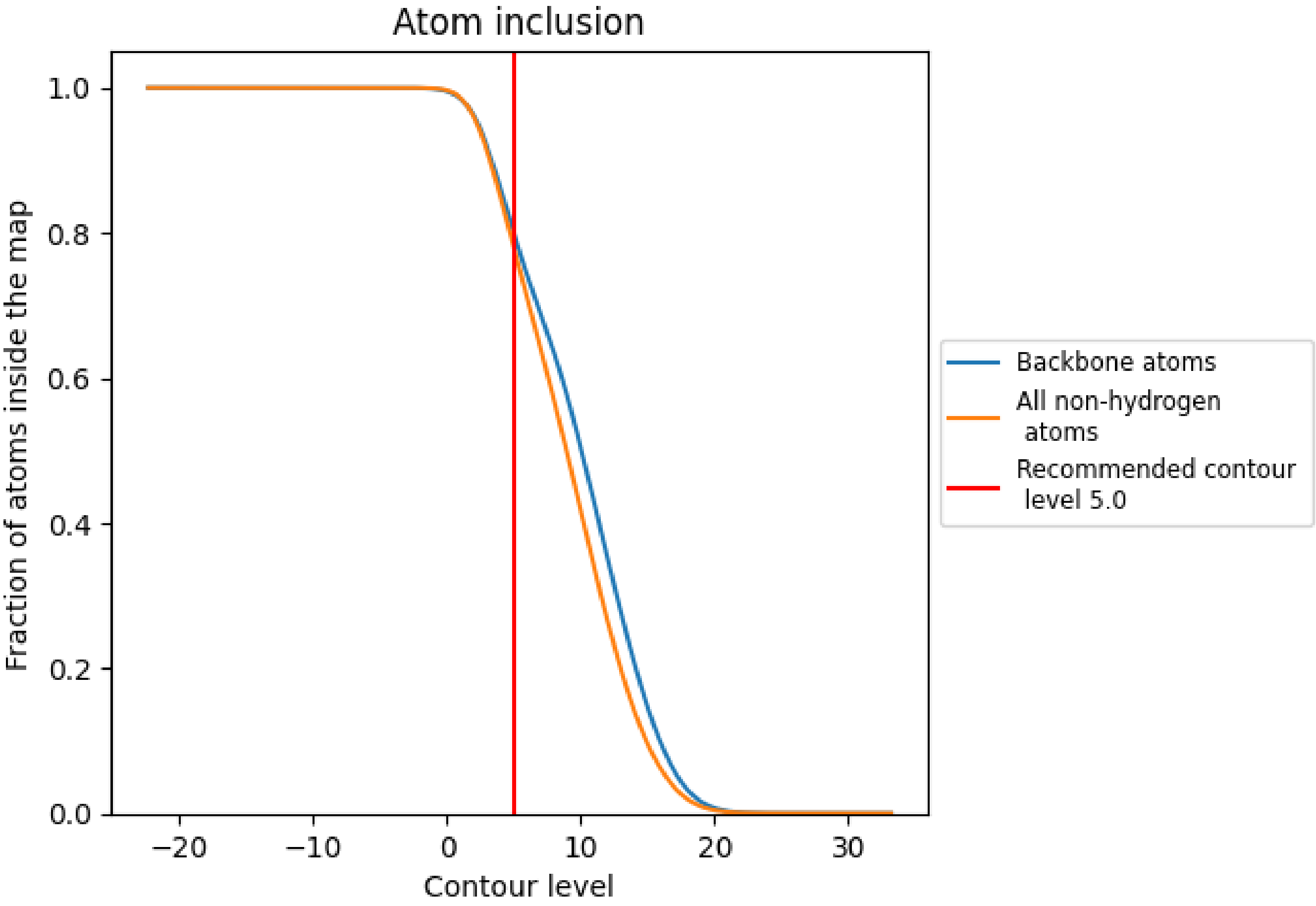
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.0).

9.4 Atom inclusion ⓘ



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 (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.7811
5B	0.8081
5b	0.8083
6A	0.8122
6B	0.8534
6C	0.8017
6L	0.8293
6a	0.8103
6b	0.8578
6c	0.8005
6l	0.8230
7A	0.8534
7C	0.8457
7L	0.8015
7a	0.8503
7c	0.8421
7l	0.8015
A	0.8400
AC	0.8350
B	0.5964
BP	0.8081
C	0.2691
C1	0.8484
C2	0.8258
C3	0.7672
D	0.7746
E	0.7784
F	0.8505
FS	0.8392
G	0.8751
H	0.7432
I	0.5909
J	0.8190
K	0.8383
L	0.7808

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
M	■ 0.7181
M1	■ 0.8403
M2	■ 0.8438
M3	■ 0.7891
N	■ 0.8297
O	■ 0.8084
P	■ 0.7948
Q	■ 0.8474
R	■ 0.6284
S	■ 0.4685
T	■ 0.7563
T1	■ 0.8120
T2	■ 0.7564
T3	■ 0.7430
T4	■ 0.8165
T5	■ 0.7708
T6	■ 0.7910
U	■ 0.8165
U1	■ 0.7551
U2	■ 0.1764
U3	■ 0.2824
U4	■ 0.1600
U5	■ 0.4153
U6	■ 0.4109
V	■ 0.8101
W	■ 0.7222
X	■ 0.8521
Y	■ 0.8764
Y0	■ 0.8455
Y5	■ 0.7015
Y7	■ 0.6184
Z	■ 0.5876
a	■ 0.8442
ac	■ 0.8325
b	■ 0.5999
bp	■ 0.8060
c	■ 0.2797
c1	■ 0.8498
c2	■ 0.8299
c3	■ 0.7678
d	■ 0.7737
e	■ 0.7799

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Chain	Atom inclusion
f	0.8554
fs	0.8412
g	0.8764
h	0.7448
i	0.5981
j	0.8190
k	0.8343
l	0.7790
m	0.7253
m1	0.8333
m2	0.8424
m3	0.7916
n	0.8297
o	0.8093
p	0.7898
q	0.8467
r	0.6347
s	0.4676
t	0.7563
t1	0.8177
t2	0.7683
t3	0.7384
t4	0.8101
t5	0.7787
t6	0.7874
u	0.8076
u1	0.7469
u2	0.1818
u3	0.2529
u4	0.1533
u5	0.4195
u6	0.4073
v	0.8086
w	0.7233
x	0.8561
y	0.8800
y0	0.8370
y5	0.7005
y7	0.6153
z	0.5940