



Full wwPDB EM Validation Report ⓘ

Jul 6, 2024 – 06:18 PM EDT

PDB ID : 8UGR
EMDB ID : EMD-42233
Title : In-situ structure of typeX supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-06
Resolution : 6.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

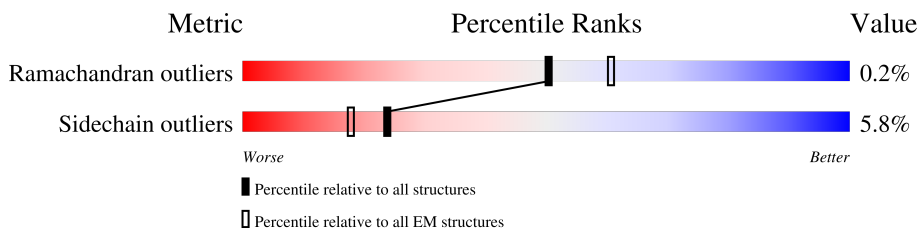
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 6.50 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	<div> <div>7%</div> <div>91%</div> <div>9%</div> </div>
1	5A	115	<div> <div>17%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	1B	258	<div> <div>53%</div> <div>6%</div> <div>40%</div> </div>
2	5B	258	<div> <div>55%</div> <div>5%</div> <div>40%</div> </div>
3	1C	264	<div> <div>76%</div> <div>.</div> <div>21%</div> </div>
3	5C	264	<div> <div>7%</div> <div>75%</div> <div>.</div> <div>21%</div> </div>
4	1D	476	<div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
4	5D	476	<div> <div>6%</div> <div>86%</div> <div>.</div> <div>10%</div> </div>
5	1E	249	<div> <div>10%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
5	5E	249	
6	1F	464	
6	5F	464	
7	1G	727	
7	5G	727	
8	1H	318	
8	5H	318	
9	1I	239	
9	5I	239	
10	1J	175	
10	5J	175	
11	1K	98	
11	5K	98	
12	1L	606	
12	5L	606	
13	1M	459	
13	5M	459	
14	1N	347	
14	5N	347	
15	1O	357	
15	5O	357	
16	1P	377	
16	5P	377	
17	1Q	175	
17	5Q	175	










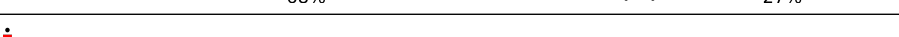
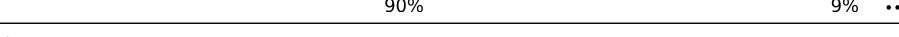
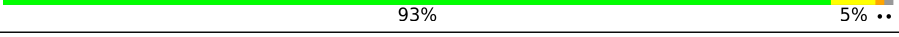



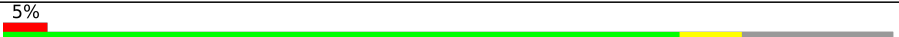
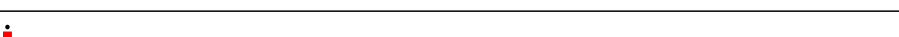

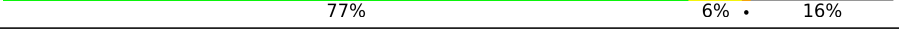
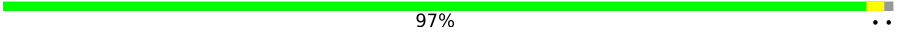
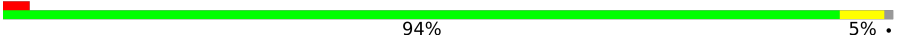




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Mol	Chain	Length	Quality of chain
18	1R	123	
18	5R	123	
19	1S	99	
19	5S	99	
20	1T	156	
20	1U	156	
20	5T	156	
20	5U	156	
21	1V	116	
21	5V	116	
22	1W	128	
22	5W	128	
23	1X	172	
23	5X	172	
24	1Y	141	
24	5Y	141	
25	1Z	144	
25	5Z	144	
26	1a	70	
26	5a	70	
27	1b	84	
27	5b	84	
28	1c	76	
28	5c	76	
29	1d	122	

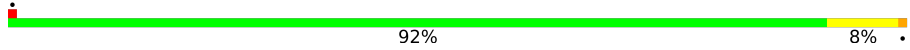
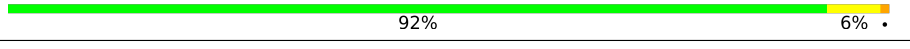
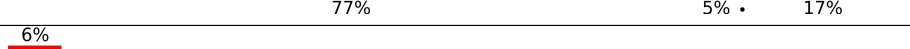
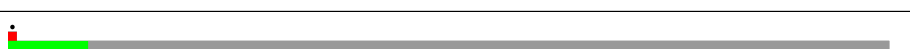



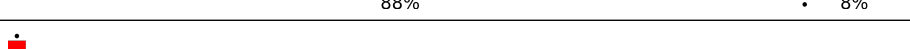



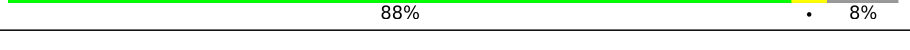
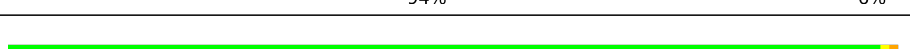
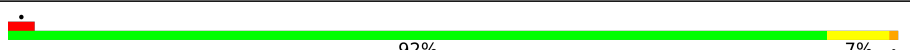
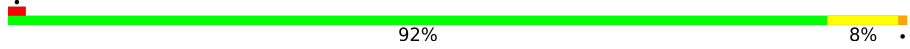

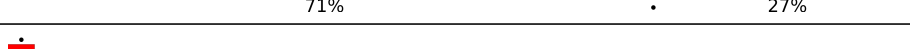







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Mol	Chain	Length	Quality of chain
29	5d	122	
30	1e	106	
30	5e	106	
31	1f	135	
31	5f	135	
32	1g	154	
32	5g	154	
33	1h	189	
33	5h	189	
34	1i	128	
34	5i	128	
35	1j	105	
35	5j	105	
36	1k	98	
36	5k	98	
37	1l	186	
37	5l	186	
38	1m	129	
38	5m	129	
39	1n	179	
39	5n	179	
40	1o	137	
40	5o	137	
41	1p	176	
41	5p	176	






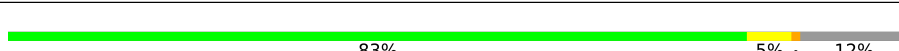
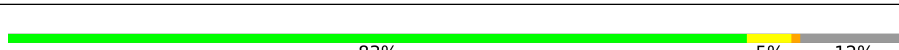

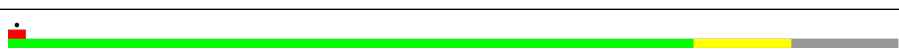

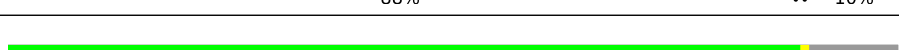
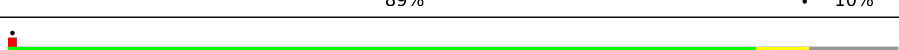

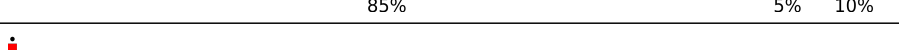
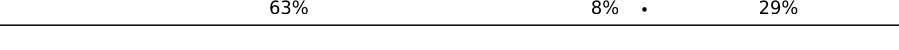
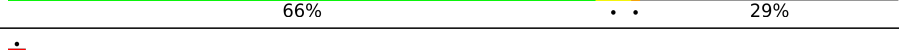





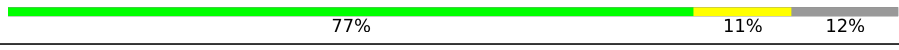
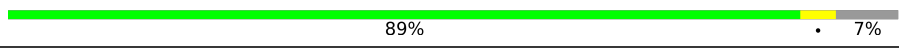


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Mol	Chain	Length	Quality of chain
42	1q	145	
42	5q	145	
43	1r	113	
43	5r	113	
44	1s	471	
44	5s	471	
45	3A	480	
45	3N	480	
45	6A	480	
45	6N	480	
46	3B	453	
46	3O	453	
46	6B	453	
46	6O	453	
47	3C	379	
47	3P	379	
47	6C	379	
47	6P	379	
48	3D	326	
48	3Q	326	
48	6D	326	
48	6Q	326	
49	3E	274	
49	3I	274	
49	3R	274	



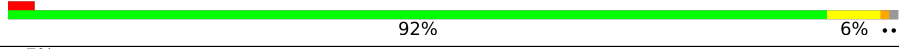

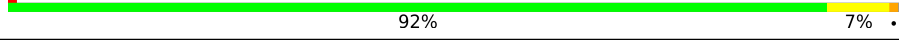
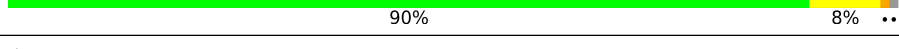
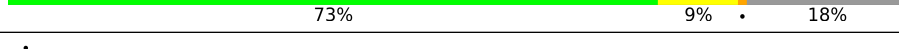
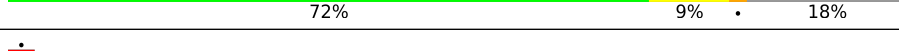
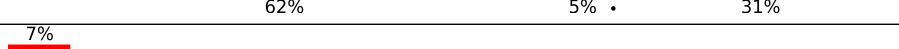
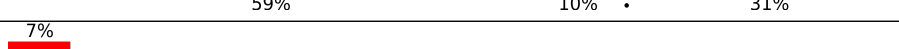
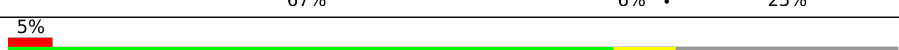

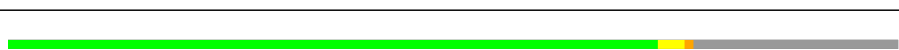

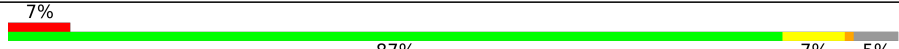





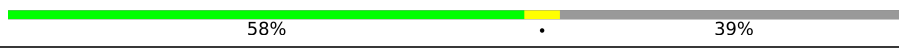
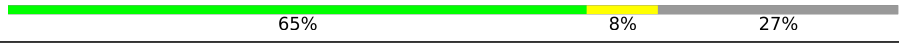



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Mol	Chain	Length	Quality of chain
49	3V	274	
49	6E	274	
49	6I	274	
49	6R	274	
49	6V	274	
50	3F	111	
50	3S	111	
50	6F	111	
50	6S	111	
51	3G	82	
51	3T	82	
51	6G	82	
51	6T	82	
52	3H	91	
52	3U	91	
52	6H	91	
52	6U	91	
53	3J	64	
53	3W	64	
53	6J	64	
53	6W	64	
54	3X	56	
54	3Y	56	
54	6X	56	
54	6Y	56	

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Mol	Chain	Length	Quality of chain
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	129	
60	8F	129	
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	
63	8I	75	
64	4J	80	
64	8J	80	
65	4K	80	
65	8K	80	
66	4L	63	
66	8L	63	
67	4M	70	

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Mol	Chain	Length	Quality of chain
67	8M	70	<div><div></div><div>53%</div><div>7%</div><div>39%</div></div>
68	4N	82	<div><div>5%</div><div></div><div>84%</div><div>16%</div></div>
68	8N	82	<div><div>7%</div><div></div><div>91%</div><div>9%</div></div>

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 234719 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		
1	5A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		
2	5B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		
3	5C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4
5C	104	GLN	ARG	conflict	UNP A0A286ZNN4
5C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		
4	5D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68
5D	0	GLY	GLU	conflict	UNP A0A8D0QM68

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		
5	5E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		
6	5F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		
7	5G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	5H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		
9	5I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		
10	5J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		
11	5K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		
12	5L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	5M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		
14	5N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		
15	5O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		
16	5P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		
17	5Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		
18	5R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		
19	5S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		
20	5T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	5U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		
21	5V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		
22	5W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		
23	5X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		
24	5Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		
25	5Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		
26	5a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		
27	5b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochond-

drial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		
28	5c	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		
29	5d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		
30	5e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		
31	5f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33

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Chain	Residue	Modelled	Actual	Comment	Reference
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33
5f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
5f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
5f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
5f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
5f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-67	THR	-	expression tag	UNP A0A8D1IZ33
5f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
5f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
5f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-57	ASN	-	expression tag	UNP A0A8D1IZ33

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Chain	Residue	Modelled	Actual	Comment	Reference
5f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
5f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
5f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		
32	5g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		
33	5h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		
34	5i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	5j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		
36	5k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		
37	5l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1m	128	Total	C	N	O		0	0
			1062	691	182	189			
38	5m	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		
39	5n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		
40	5o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1
5o	0	MYR	-	insertion	UNP F1SCH1

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		
41	5p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		
42	5q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		
43	5r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		
44	5s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		
45	6A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	6N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		
46	6B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	6O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		
47	6C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	6P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		
48	6D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	6Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		
49	6E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	6R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	6G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	6T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			454	295	81	78		
53	3W	56	Total	C	N	O	0	0
			454	295	81	78		
53	6J	56	Total	C	N	O	0	0
			454	295	81	78		
53	6W	56	Total	C	N	O	0	0
			454	295	81	78		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3J	60	ASN	LYS	conflict	UNP Q2EN79
3J	61	GLN	HIS	conflict	UNP Q2EN79
3J	62	GLY	LYS	conflict	UNP Q2EN79
3J	63	LYS	TYR	conflict	UNP Q2EN79
3W	56	ASN	LYS	conflict	UNP Q2EN79
3W	57	GLN	HIS	conflict	UNP Q2EN79
3W	58	GLY	LYS	conflict	UNP Q2EN79

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Chain	Residue	Modelled	Actual	Comment	Reference
3W	59	LYS	TYR	conflict	UNP Q2EN79
6J	60	ASN	LYS	conflict	UNP Q2EN79
6J	61	GLN	HIS	conflict	UNP Q2EN79
6J	62	GLY	LYS	conflict	UNP Q2EN79
6J	63	LYS	TYR	conflict	UNP Q2EN79
6W	56	ASN	LYS	conflict	UNP Q2EN79
6W	57	GLN	HIS	conflict	UNP Q2EN79
6W	58	GLY	LYS	conflict	UNP Q2EN79
6W	59	LYS	TYR	conflict	UNP Q2EN79

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
54	6X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	6Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	514	Total	C	N	O	S	0	0
			4025	2693	624	676	32		
55	8A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		
56	8B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		
57	8C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		
58	8D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		
59	8E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		
60	8F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		
61	8G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
62	8H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		
63	8I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		
64	8J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		
65	8K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		
66	8L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

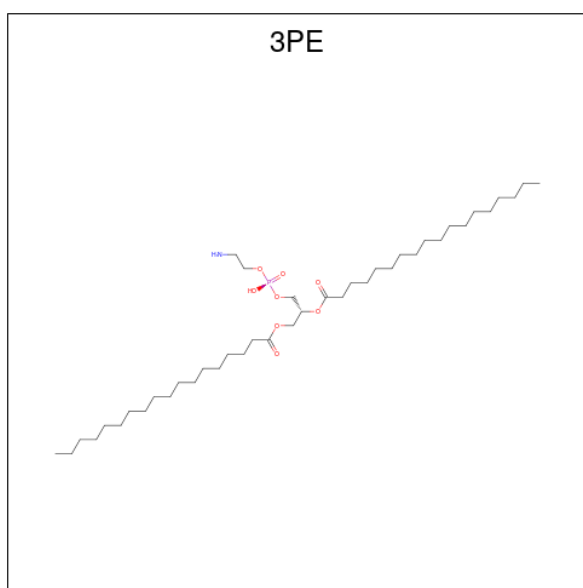
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		
67	8M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUF44.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		
68	8N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1K	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			51	41	1	8	1	

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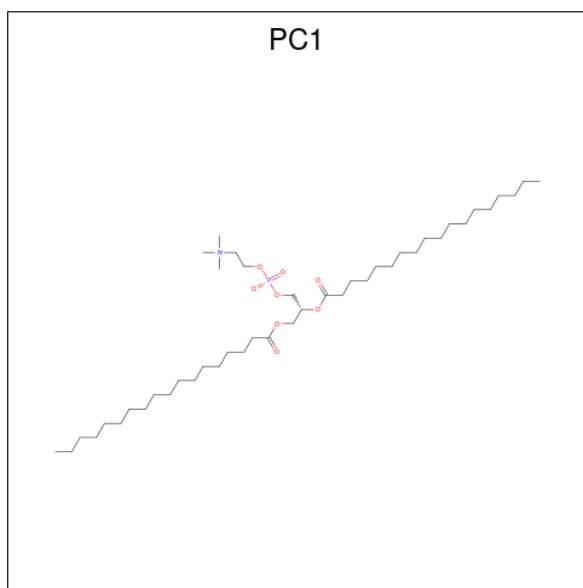
Mol	Chain	Residues	Atoms					AltConf
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	1P	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1d	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1j	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1m	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	5A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	5K	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	5L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	5L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	5M	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	5M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	5M	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	5M	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	5M	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	5P	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			31	21	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	5Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	5d	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	5j	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	5m	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	

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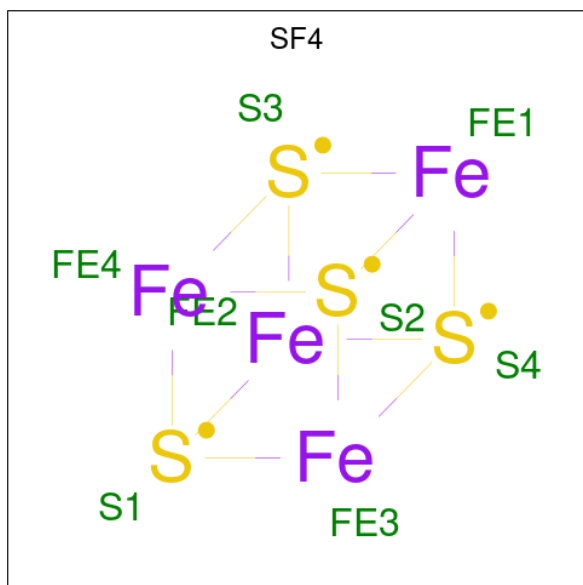
Mol	Chain	Residues	Atoms					AltConf
70	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	5A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	5A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	5B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	5B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	5H	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	5H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	5I	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	5M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	5P	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	5Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	5Y	1	Total	C	N	O	P	0
			46	36	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
70	5d	1	Total	C	N	O	P	0
			39	29	1	8	1	
70	5h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	5q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 71 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



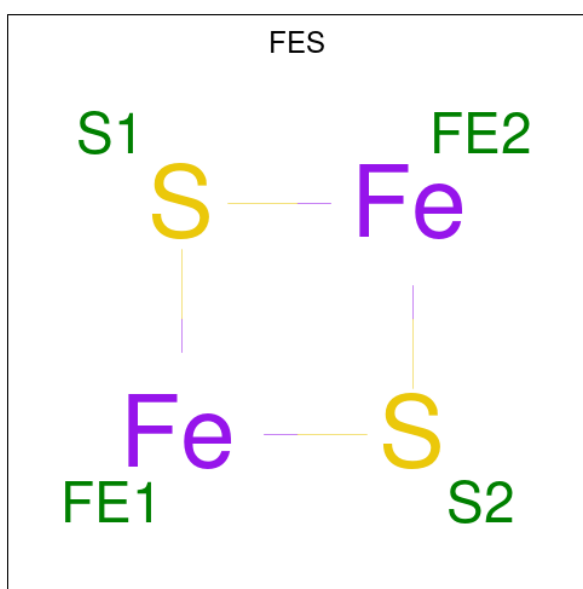
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	5B	1	Total	Fe	S	0
			8	4	4	
71	5F	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
71	5G	1	Total	Fe	S	0
			8	4	4	
71	5G	1	Total	Fe	S	0
			8	4	4	
71	5I	1	Total	Fe	S	0
			8	4	4	
71	5I	1	Total	Fe	S	0
			8	4	4	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



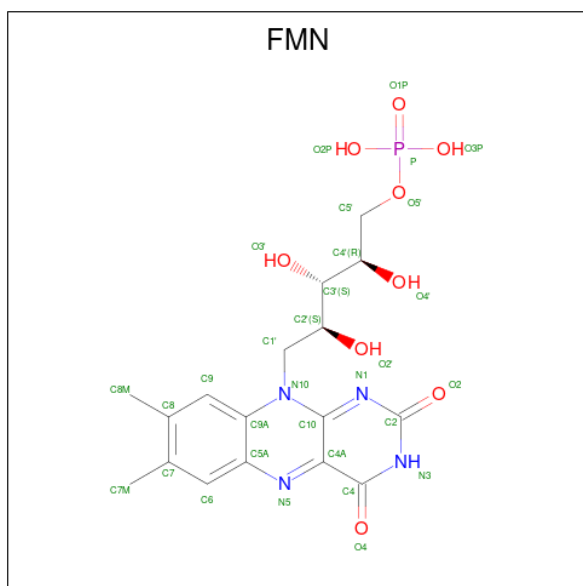
Mol	Chain	Residues	Atoms			AltConf
72	1E	1	Total	Fe	S	0
			4	2	2	
72	1G	1	Total	Fe	S	0
			4	2	2	
72	3E	1	Total	Fe	S	0
			4	2	2	
72	3R	1	Total	Fe	S	0
			4	2	2	
72	5E	1	Total	Fe	S	0
			4	2	2	
72	5G	1	Total	Fe	S	0
			4	2	2	
72	6E	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
72	6R	1	Total	Fe	S	0
			4	2	2	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

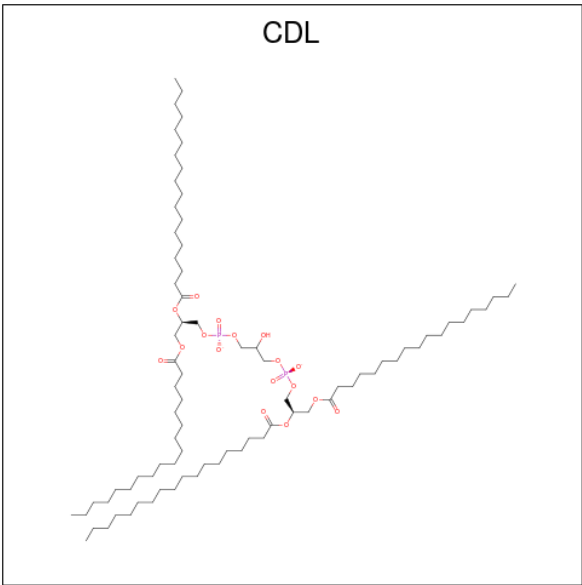


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	
73	5F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
74	1G	1	Total	K	0
			1	1	
74	5G	1	Total	K	0
			1	1	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



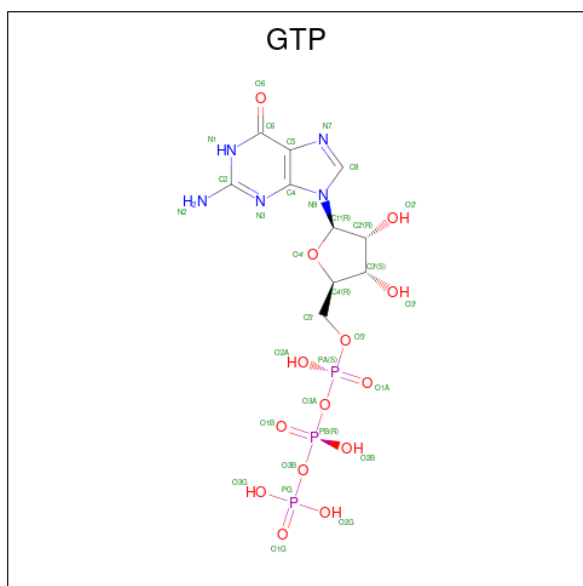
Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1a	1	Total	C	O	P	0
			61	42	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1h	1	Total	C	O	P	0
			80	61	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	4D	1	Total	C	O	P	0
			100	81	17	2	
75	5H	1	Total	C	O	P	0
			51	32	17	2	
75	5L	1	Total	C	O	P	0
			76	57	17	2	
75	5N	1	Total	C	O	P	0
			62	43	17	2	
75	5a	1	Total	C	O	P	0
			61	42	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	5d	1	Total	C	O	P	0
			86	67	17	2	
75	5d	1	Total	C	O	P	0
			65	46	17	2	
75	5h	1	Total	C	O	P	0
			80	61	17	2	
75	8A	1	Total	C	O	P	0
			100	81	17	2	
75	8C	1	Total	C	O	P	0
			100	81	17	2	
75	8D	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	
76	5O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 77 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

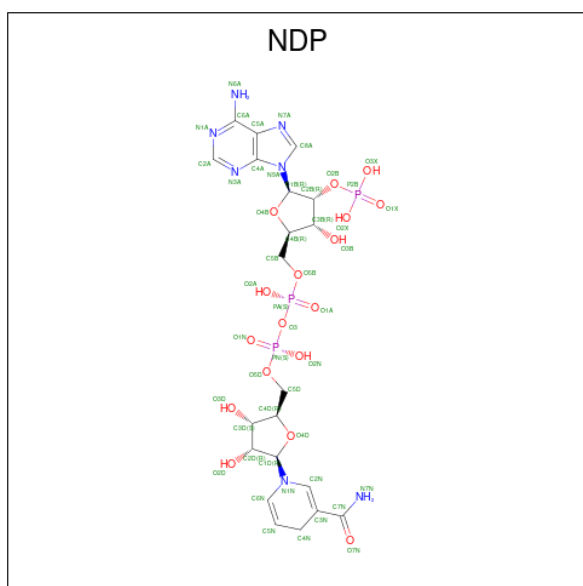
Mol	Chain	Residues	Atoms		AltConf
77	1O	1	Total	Mg	0
			1	1	

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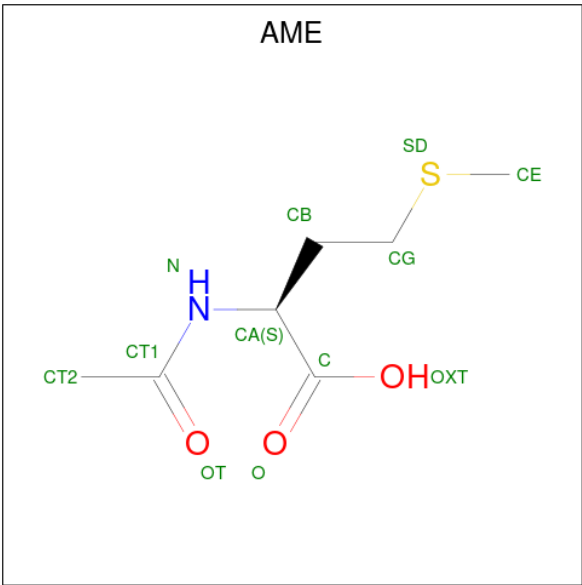
Mol	Chain	Residues	Atoms		AltConf
77	4A	1	Total	Mg	0
			1	1	
77	5O	1	Total	Mg	0
			1	1	
77	8A	1	Total	Mg	0
			1	1	

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



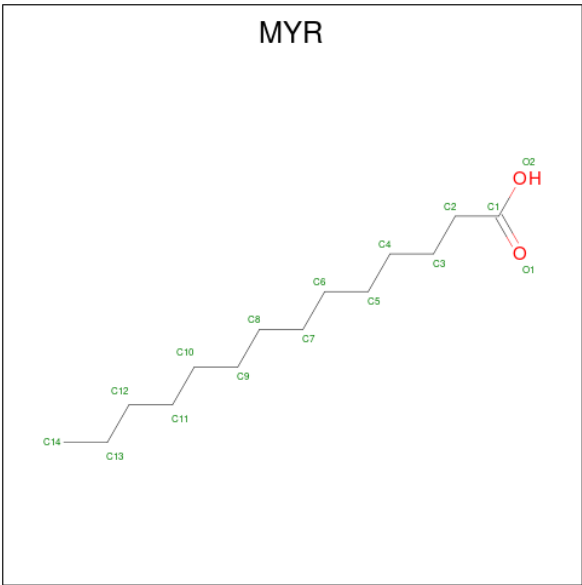
- # EHZ
-
- The chemical structure of EHZ (Ergosterol) is shown. It features a long hydrocarbon side chain (C18-C27) attached to a steroid nucleus. The side chain is composed of a long alkyl chain (C18-C27) and a terminal hydroxyl group (OH). The steroid nucleus is a four-ring system (A, B, C, D) with a ketone group at C3 and a hydroxyl group at C14. The side chain is attached to the D-ring at C17. The terminal hydroxyl group is shown in red. The structure is labeled with atom numbers (C18-C27, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O8

- Molecule 81 is N-ACETYLMETHIONINE (three-letter code: AME) (formula: $\text{C}_7\text{H}_{13}\text{NO}_3\text{S}$).



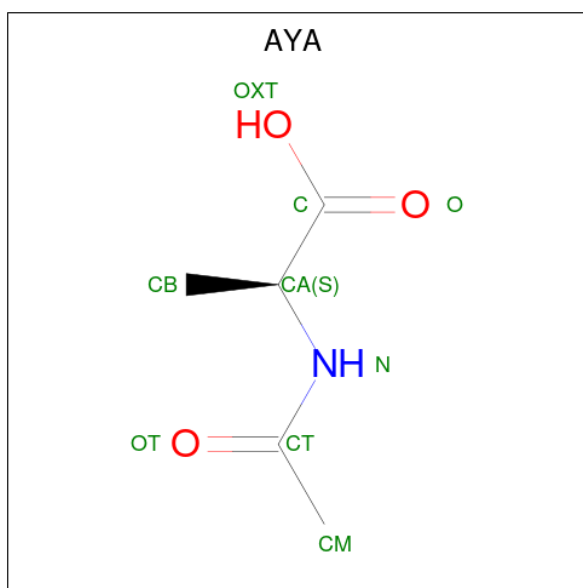
Mol	Chain	Residues	Atoms					AltConf
81	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	
81	5N	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 82 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



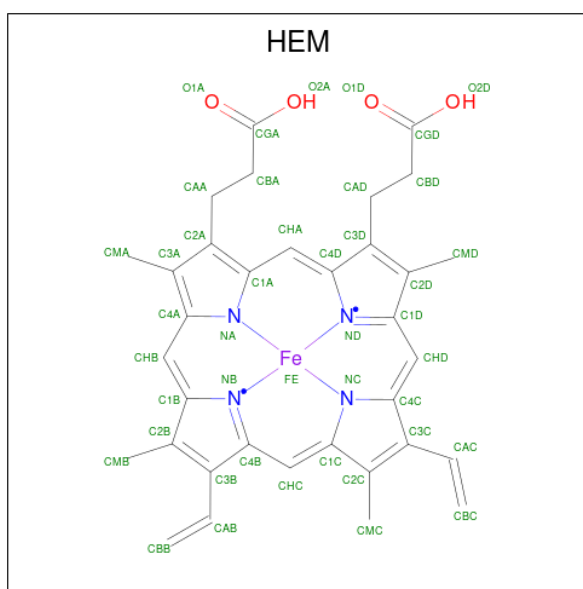
Mol	Chain	Residues	Atoms			AltConf
82	1l	1	Total	C	O	0
			15	14	1	
82	5l	1	Total	C	O	0
			15	14	1	

- Molecule 83 is N-ACETYLALANINE (three-letter code: AYA) (formula: $C_5H_9NO_3$).



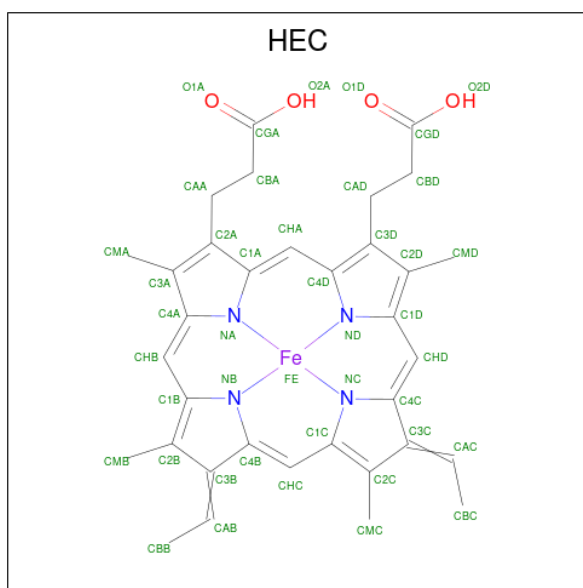
Mol	Chain	Residues	Atoms				AltConf
83	1q	1	Total	C	N	O	0
			8	5	1	2	
83	5q	1	Total	C	N	O	0
			8	5	1	2	

- Molecule 84 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



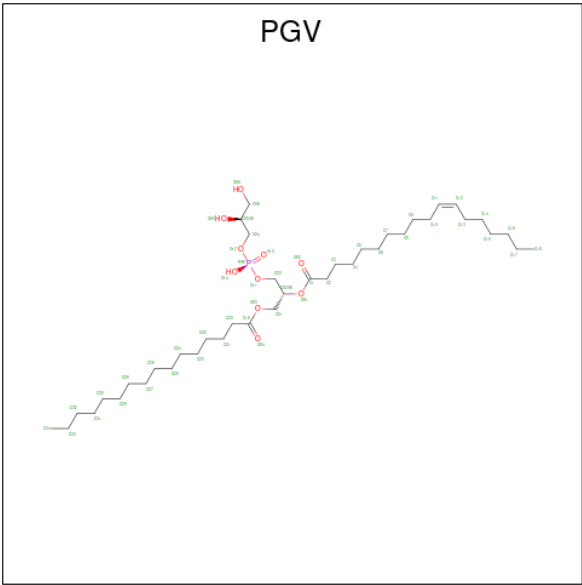
Mol	Chain	Residues	Atoms					AltConf
84	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	6C	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	6C	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	6P	1	Total 43	C 34	Fe 1	N 4	O 4	0
84	6P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 85 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					AltConf
85	3D	1	Total 42	C 34	Fe 1	N 4	O 3	0
85	3Q	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	6D	1	Total 42	C 34	Fe 1	N 4	O 3	0
85	6Q	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 86 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



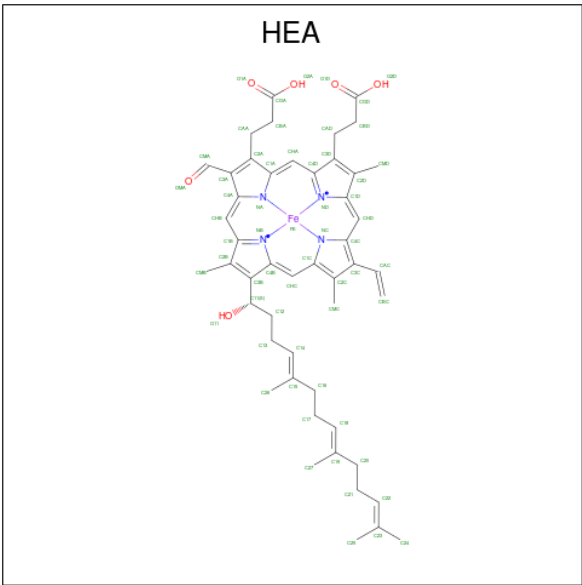
Mol	Chain	Residues	Atoms				AltConf
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4B	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4G	1	Total	C	O	P	0
			51	40	10	1	
86	4J	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
86	4K	1	Total	C	O	P	0
			51	40	10	1	
86	4L	1	Total	C	O	P	0
			51	40	10	1	
86	5i	1	Total	C	O	P	0
			51	40	10	1	
86	8A	1	Total	C	O	P	0
			51	40	10	1	
86	8A	1	Total	C	O	P	0
			51	40	10	1	
86	8A	1	Total	C	O	P	0
			51	40	10	1	
86	8A	1	Total	C	O	P	0
			51	40	10	1	
86	8B	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8D	1	Total	C	O	P	0
			51	40	10	1	
86	8G	1	Total	C	O	P	0
			51	40	10	1	
86	8J	1	Total	C	O	P	0
			51	40	10	1	
86	8K	1	Total	C	O	P	0
			51	40	10	1	
86	8L	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 87 is HEME-A (three-letter code: HEA) (formula: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms					AltConf
87	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
87	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
87	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0
87	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0

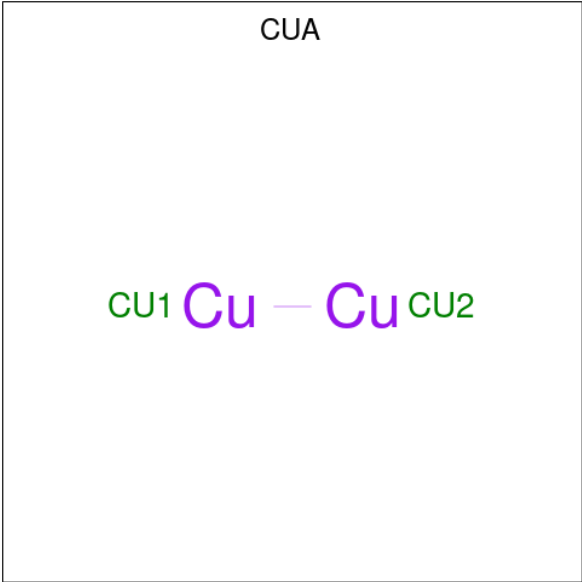
- Molecule 88 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
88	4A	1	Total	Cu	0
			1	1	
88	8A	1	Total	Cu	0
			1	1	

- Molecule 89 is SODIUM ION (three-letter code: NA) (formula: Na).

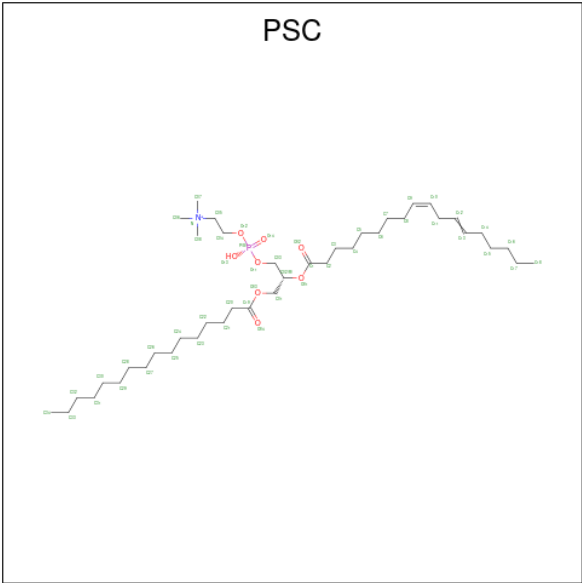
Mol	Chain	Residues	Atoms		AltConf
89	4A	1	Total	Na	0
			1	1	
89	8A	1	Total	Na	0
			1	1	

- Molecule 90 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
90	4B	1	Total	Cu	0
			2	2	
90	8B	1	Total	Cu	0
			2	2	

- Molecule 91 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



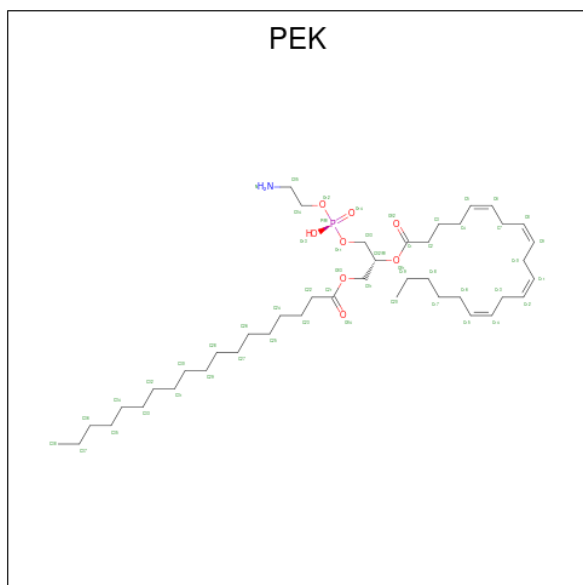
Mol	Chain	Residues	Atoms					AltConf
91	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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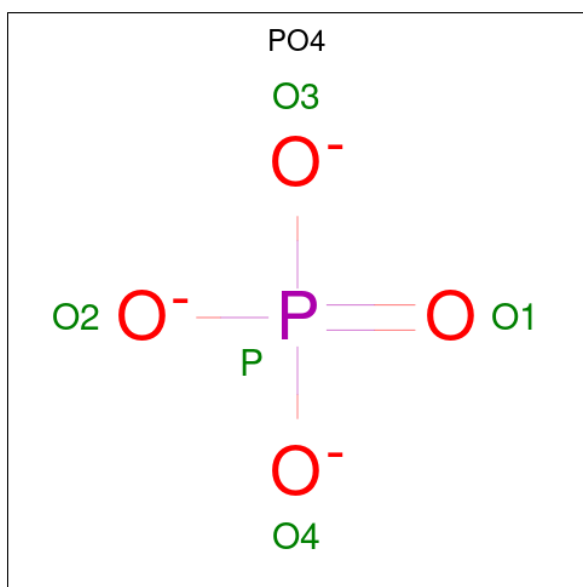
Mol	Chain	Residues	Atoms					AltConf
91	8A	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 92 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
92	4C	1	Total	C	N	O	P	0
			53	43	1	8	1	
92	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
92	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	
92	8G	1	Total	C	N	O	P	0
			53	43	1	8	1	

- Molecule 93 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

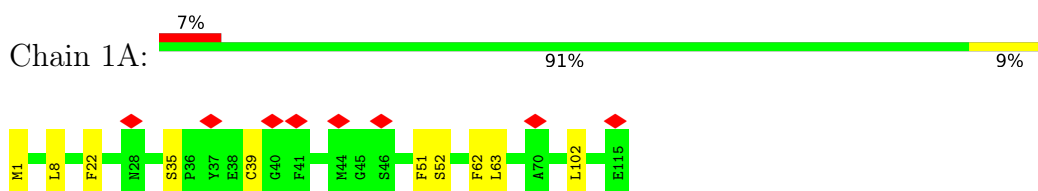


Mol	Chain	Residues	Atoms			AltConf
93	4H	1	Total	O	P	0
			5	4	1	
93	8H	1	Total	O	P	0
			5	4	1	

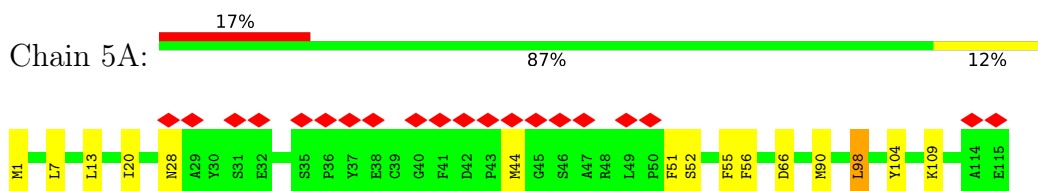
3 Residue-property plots [i](#)

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

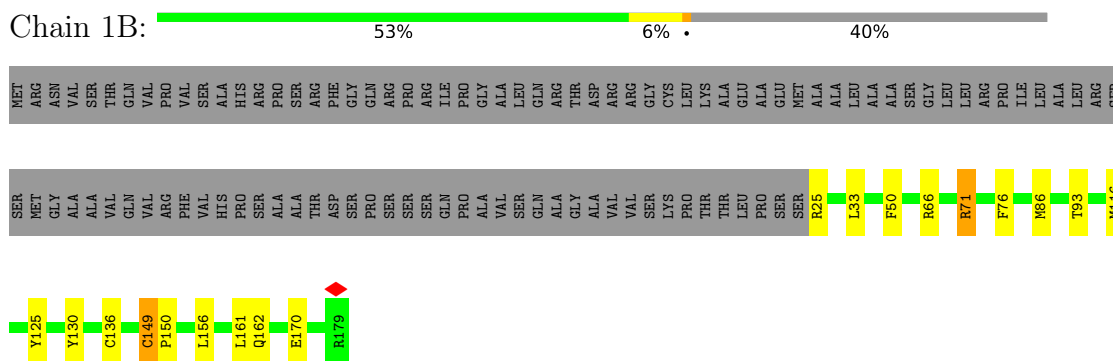
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



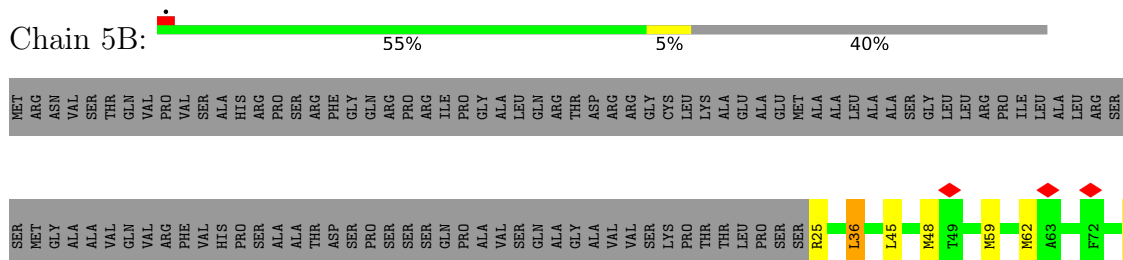
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

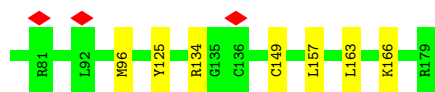


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

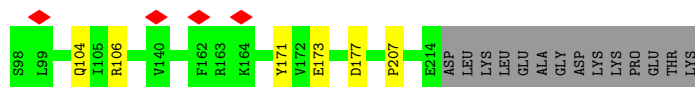
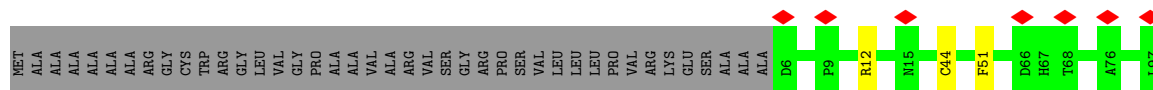
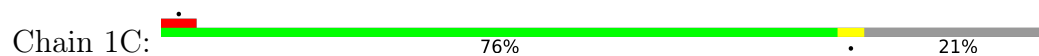


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

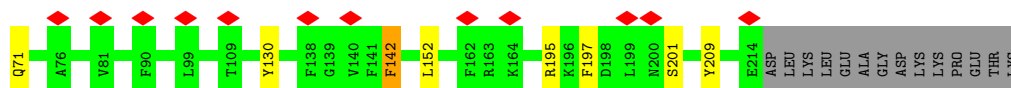
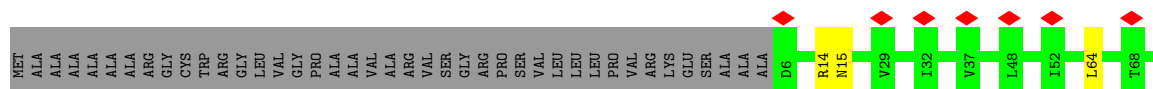
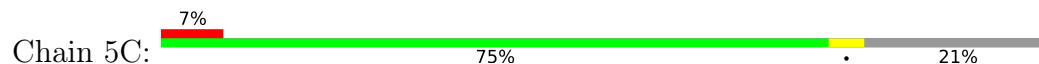




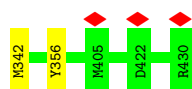
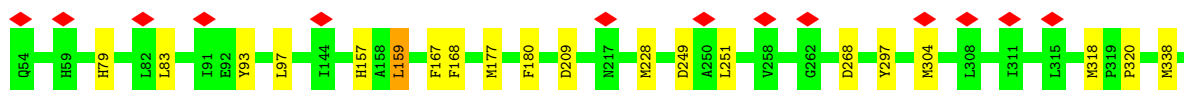
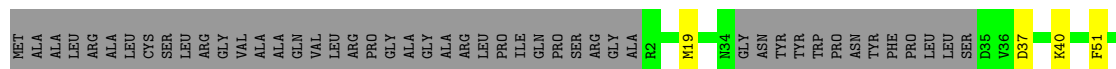
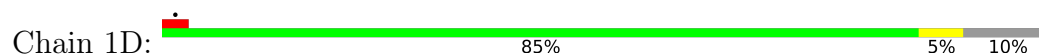
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



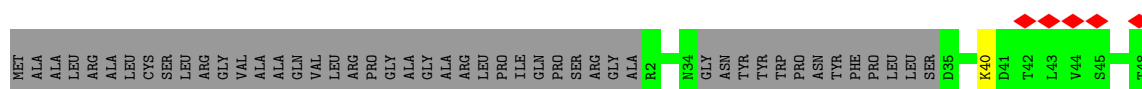
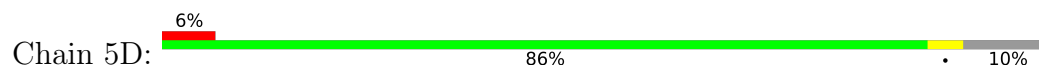
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

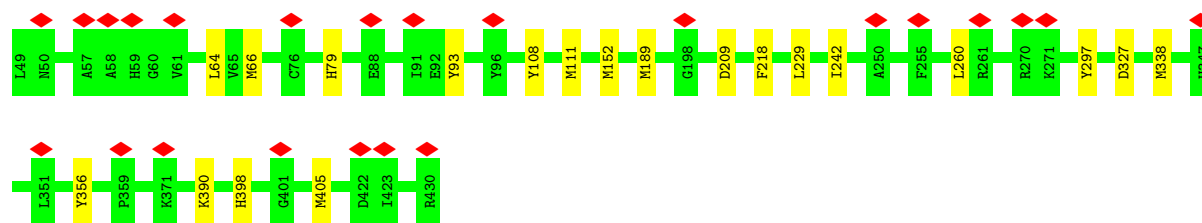


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

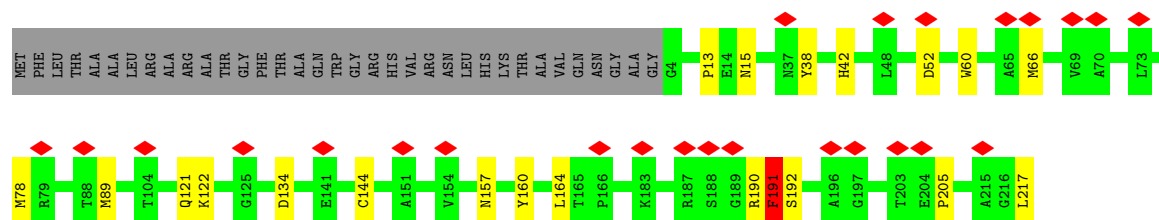
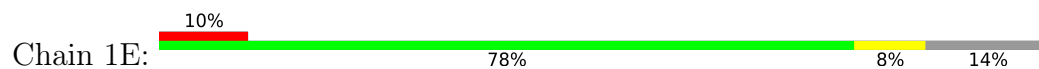


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

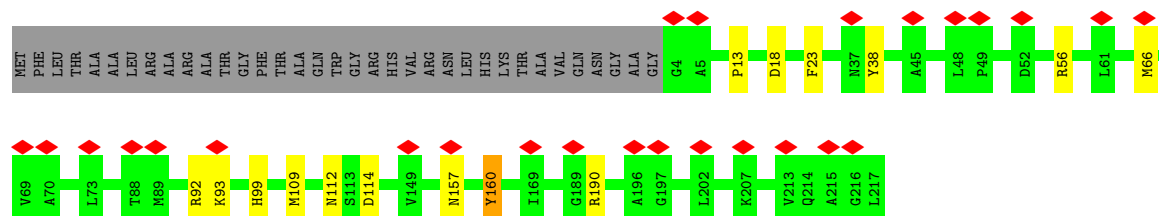
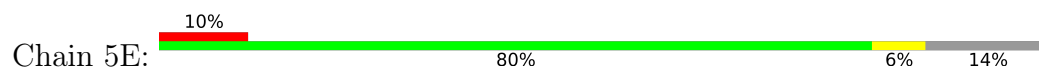




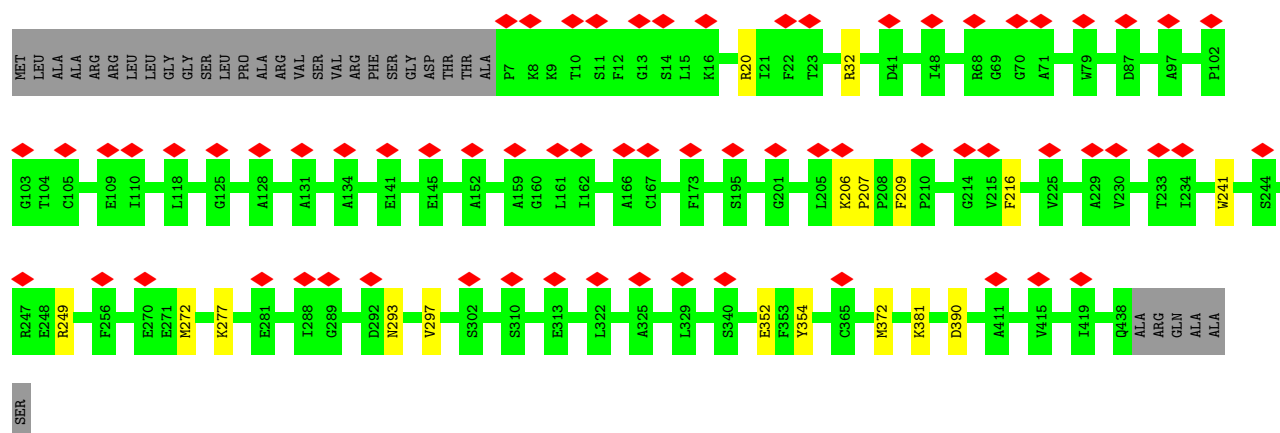
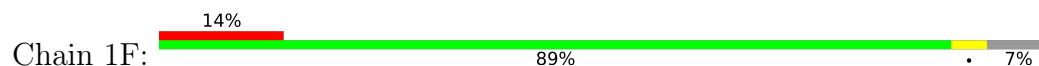
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



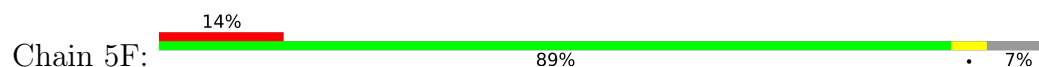
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

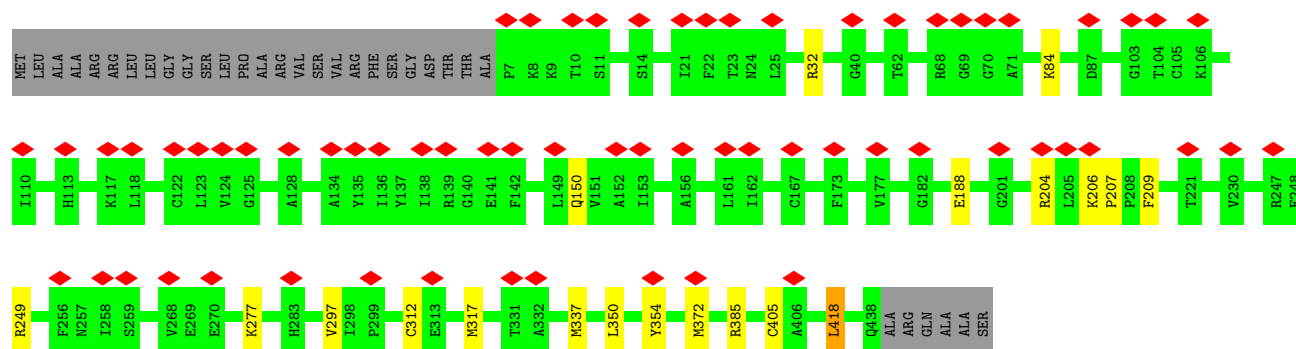


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



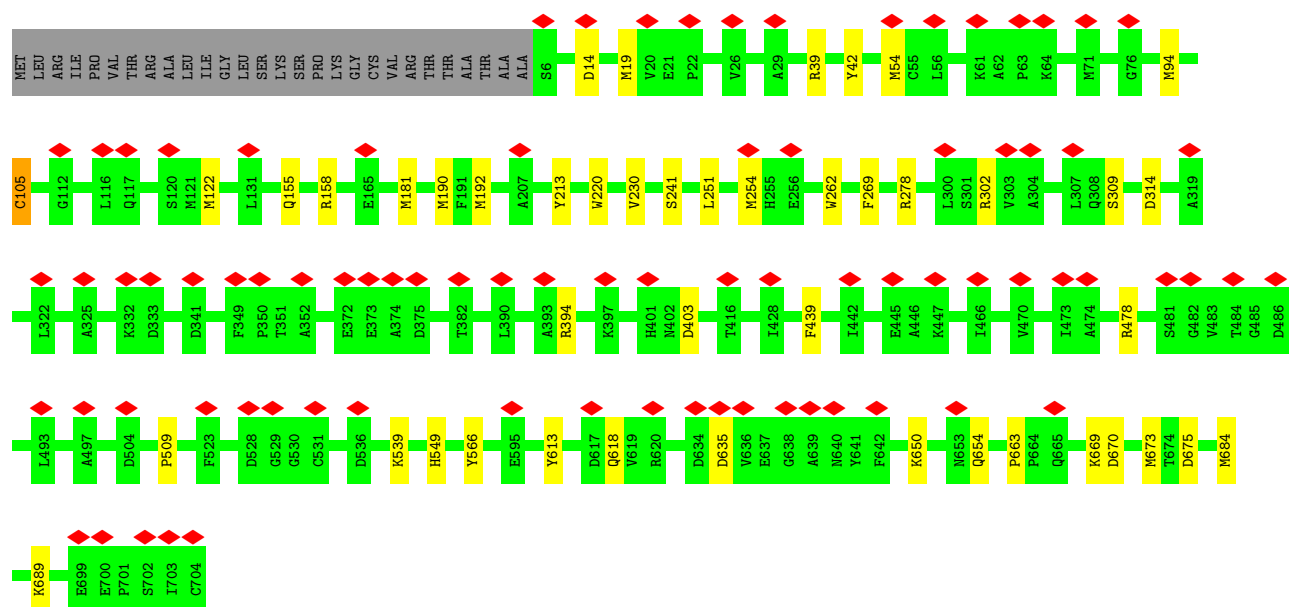
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





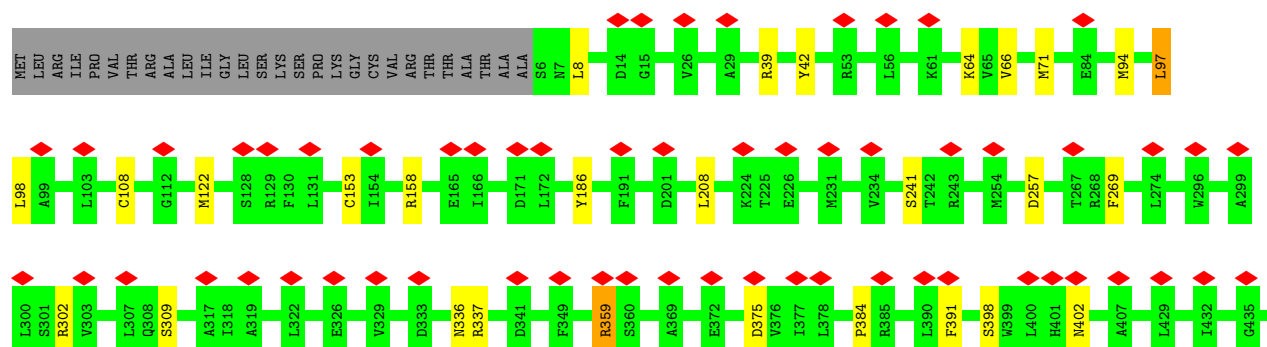
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

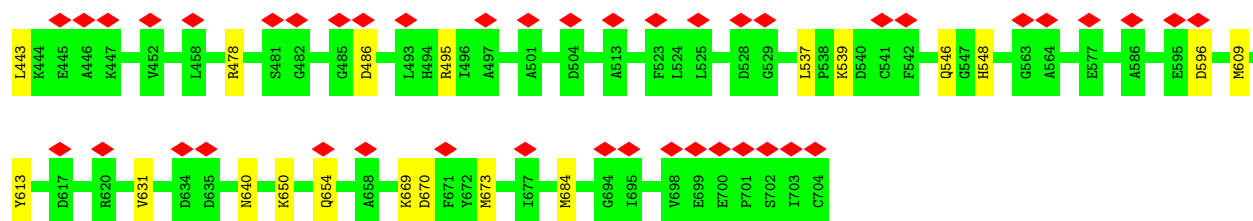
Chain 1G: 11% 90% 6% .



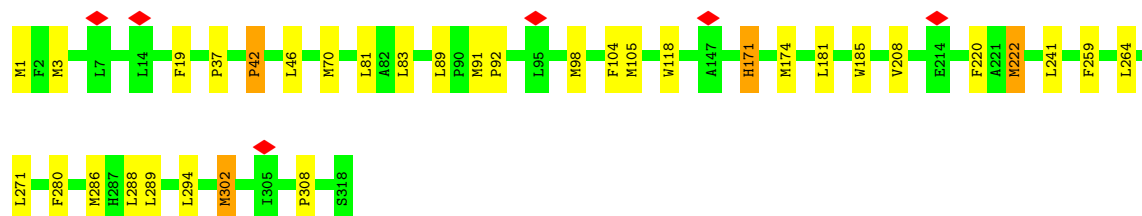
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 5G: 14% 90% 6% .

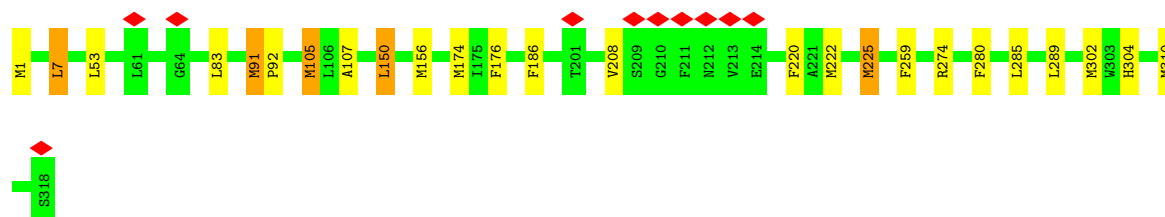




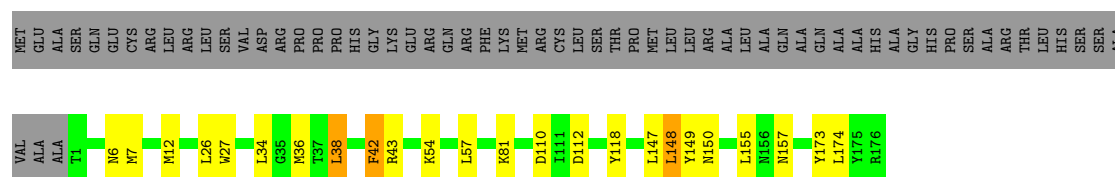
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



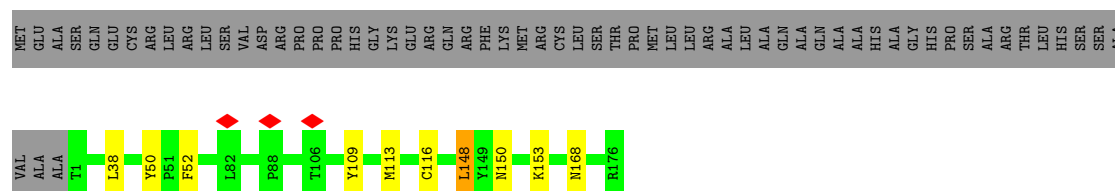
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

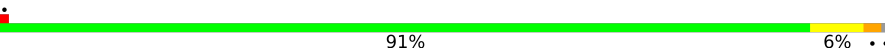


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:  91% 8%




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 5J:  91% 6%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:  87% 10%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 5K:  90% 10%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L:  93% 6%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 5L:  93% 7%



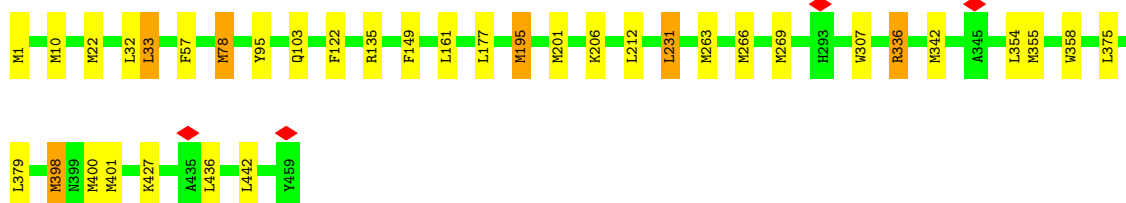
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:  96%



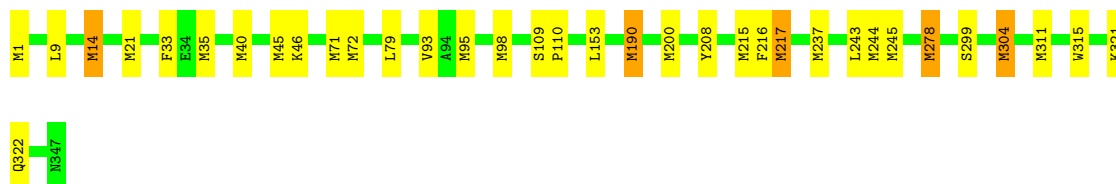
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 5M:  92%



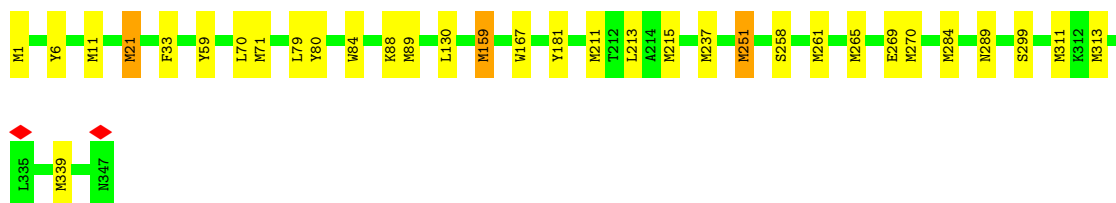
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:  90%




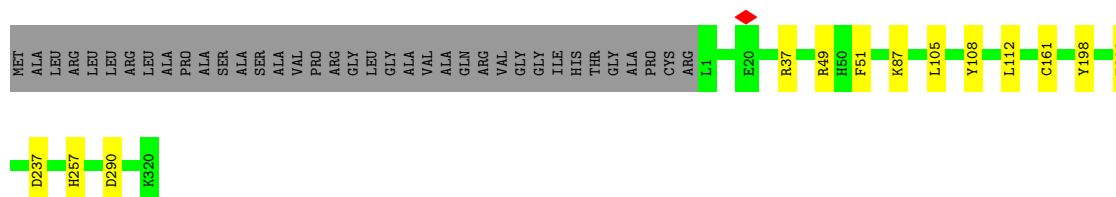
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 5N:  90%




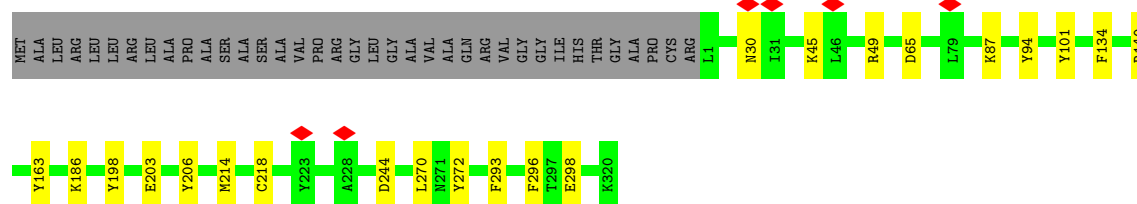
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 10:  86%




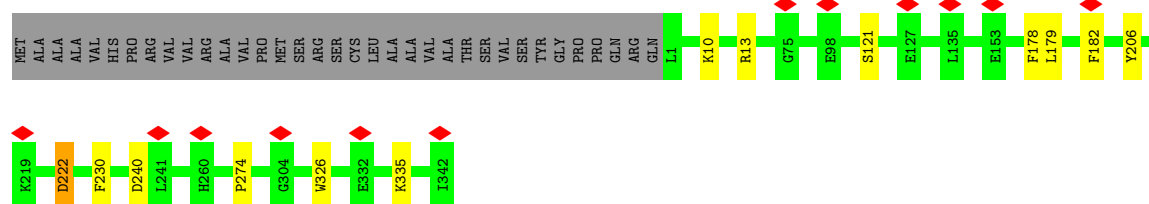
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 5O: 




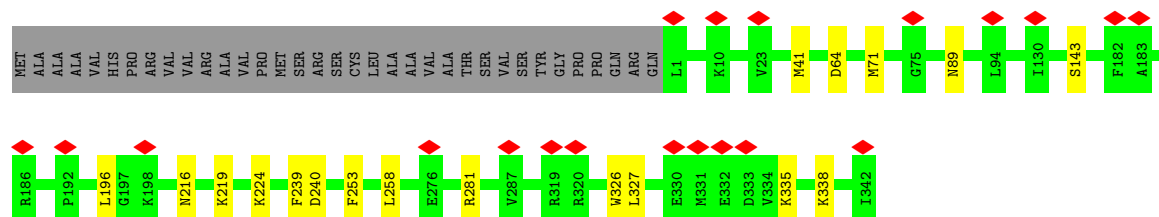
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P: 




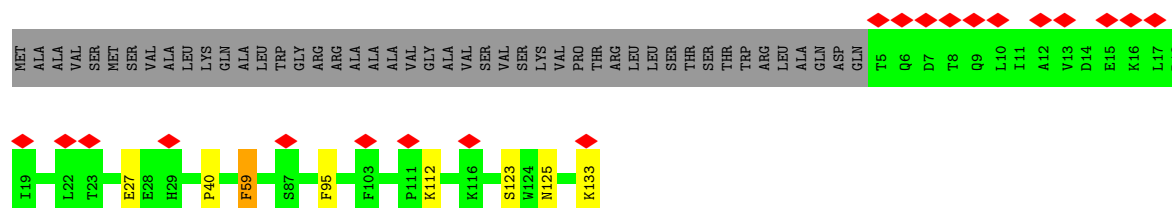
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 5P: 



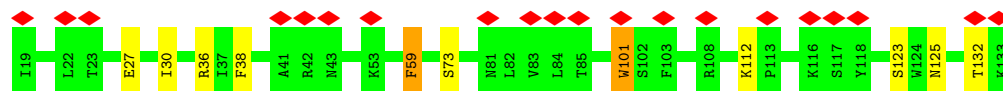
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q: 

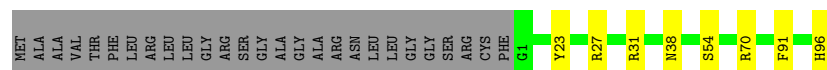


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

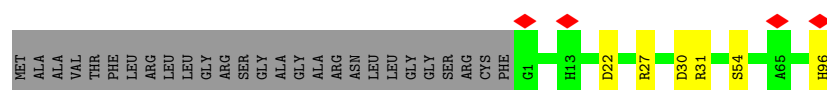
Chain 5Q: 



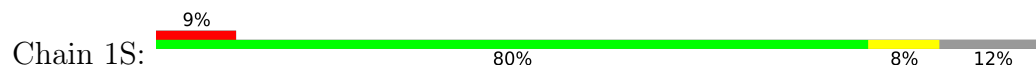
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



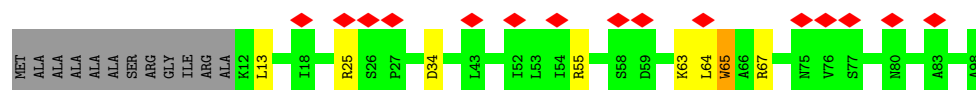
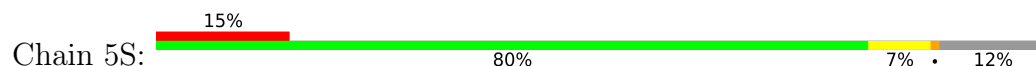
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

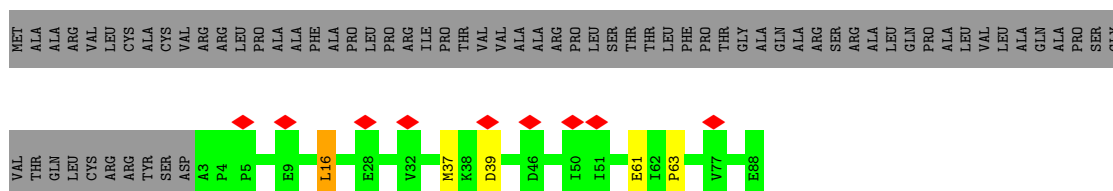


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

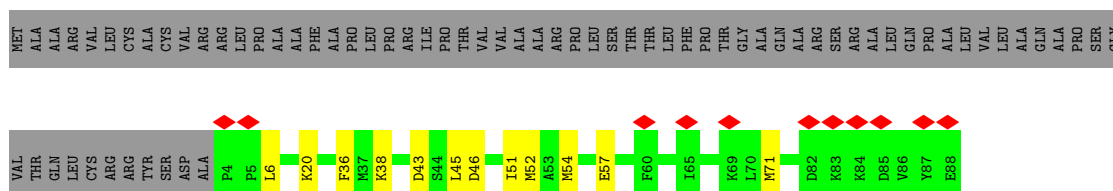


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

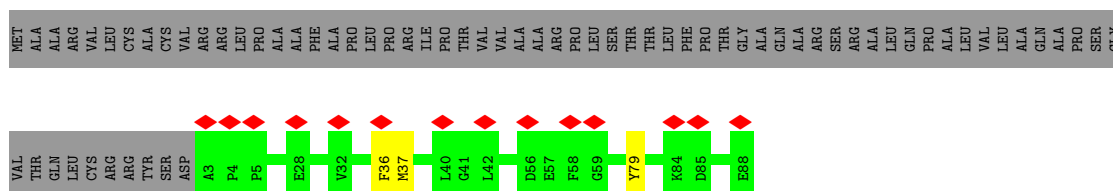




- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



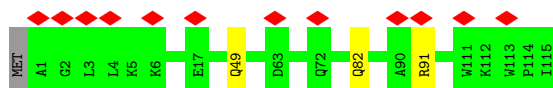
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



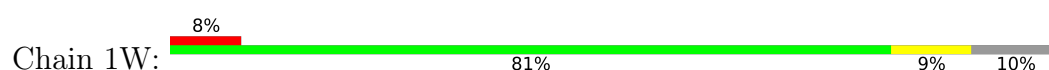
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



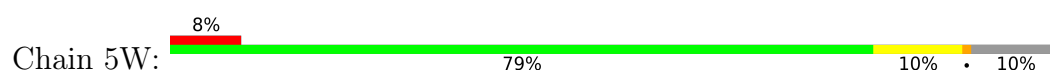
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



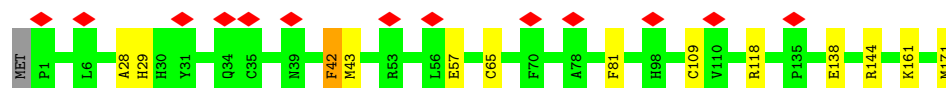
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



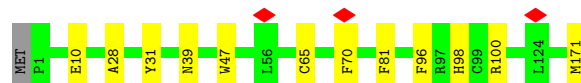
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



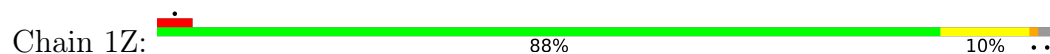
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



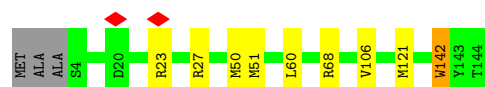
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



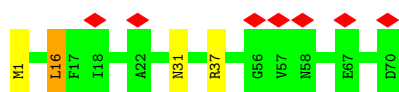
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



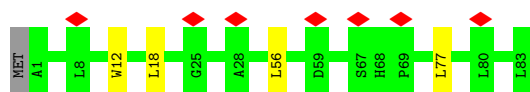
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



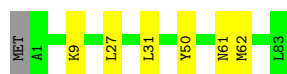
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



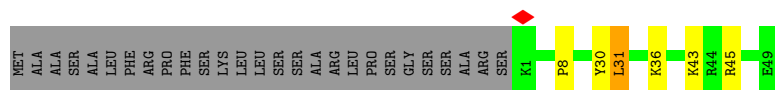
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



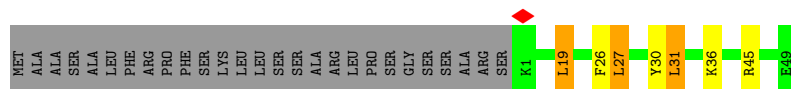
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2





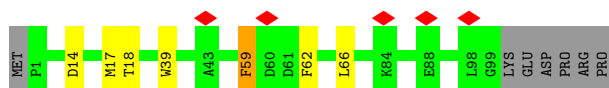
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 5d: 88% 9% ..



- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e: 5% 87% 6% • 7%



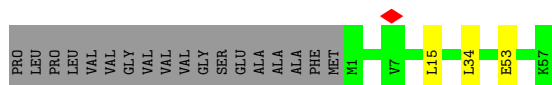
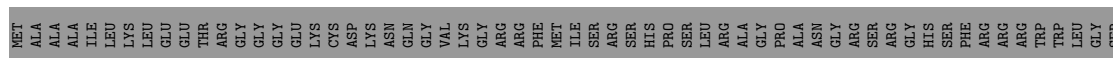
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 5e: 84% 8% • 7%



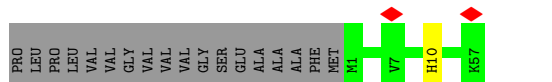
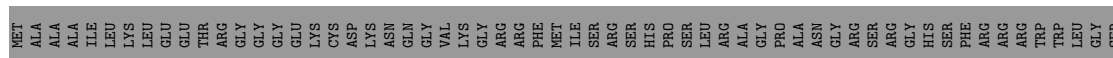
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f: 40% • 58%



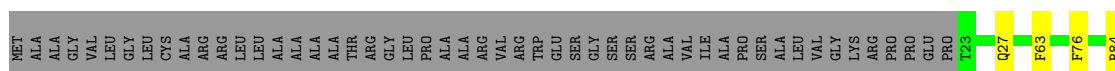
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 5f: 41% • 58%

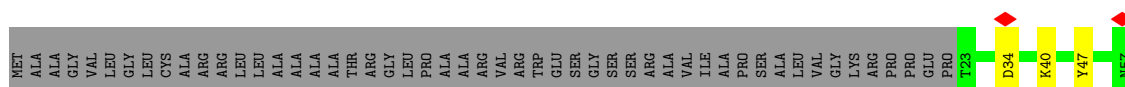


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

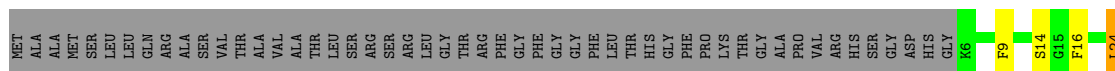
Chain 1g: 62% • 35%



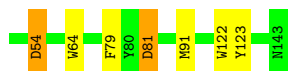
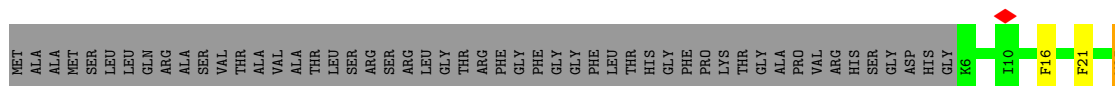
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



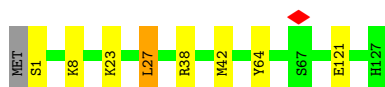
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



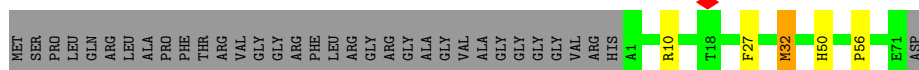
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



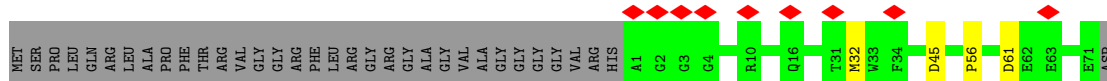
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



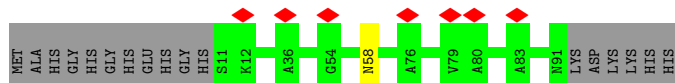
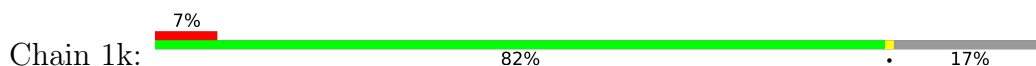
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



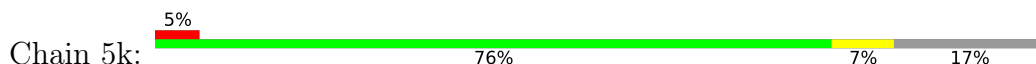
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



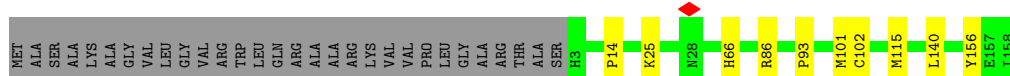
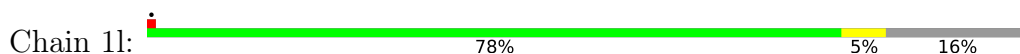
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



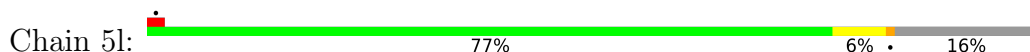
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

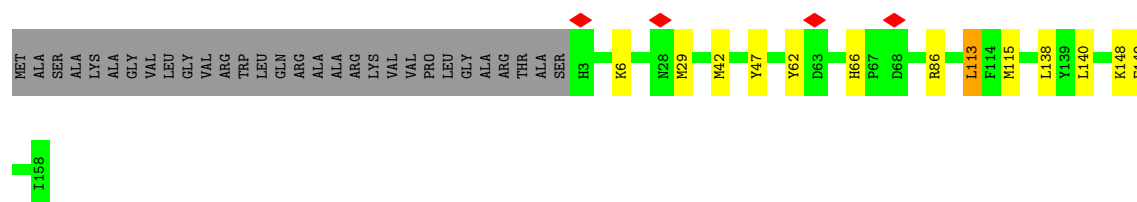


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





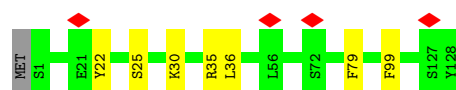
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 97%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 5m: 94%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n: 91%



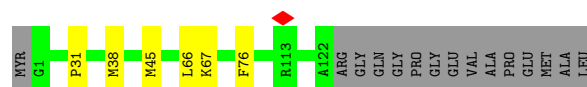
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 5n: 88%



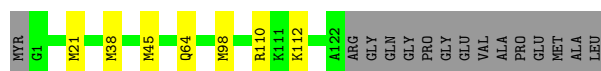
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o: 85%



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 5o: 84%



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



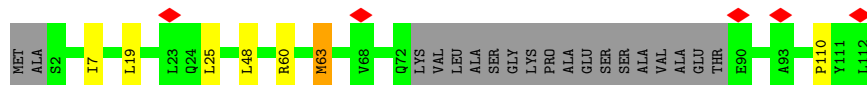
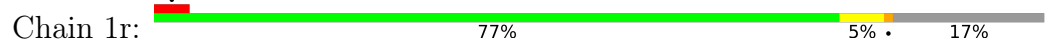
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



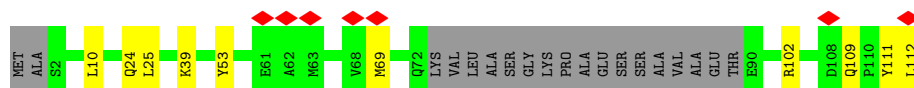
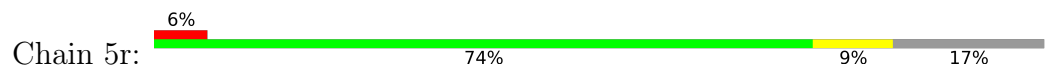
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

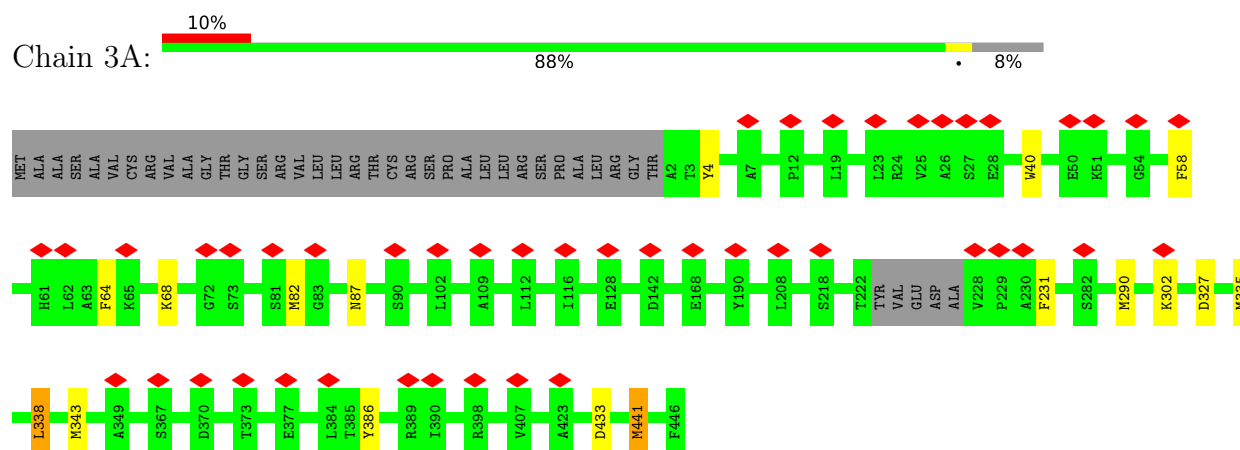


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

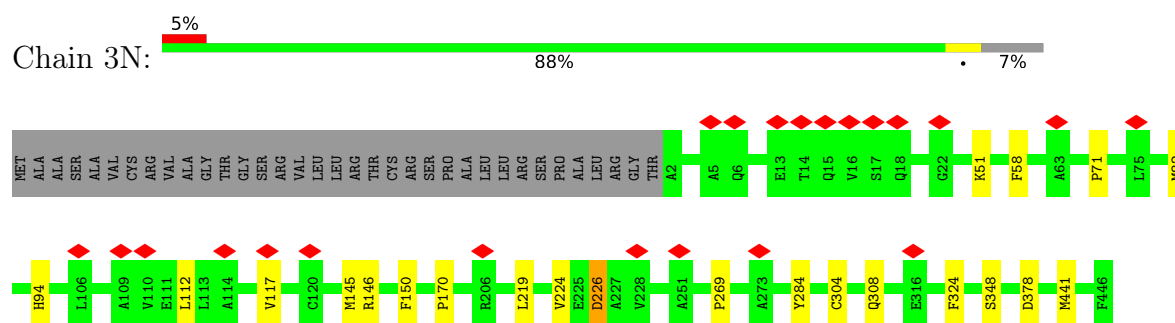
[illegible]

- [illegible]

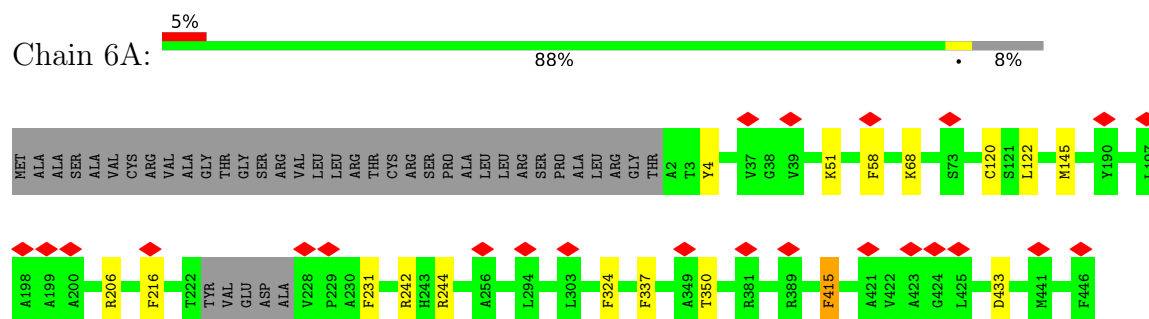
- 



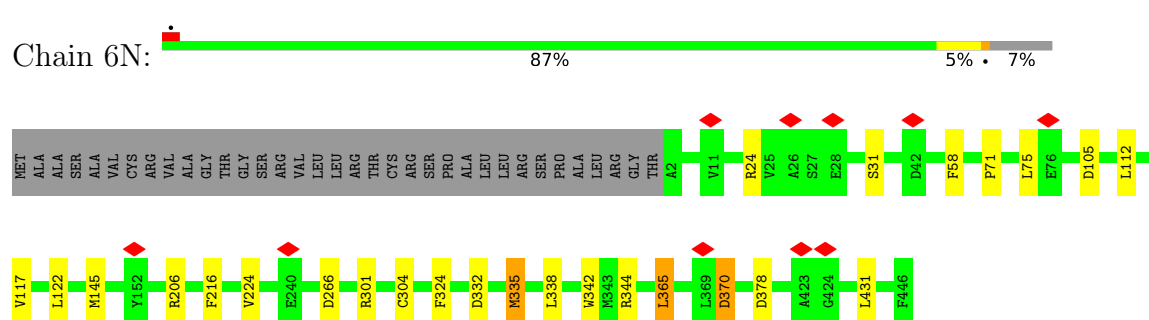
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



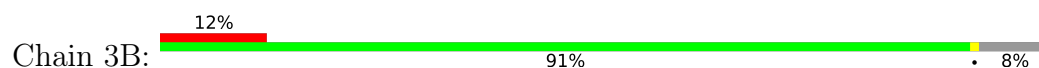
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

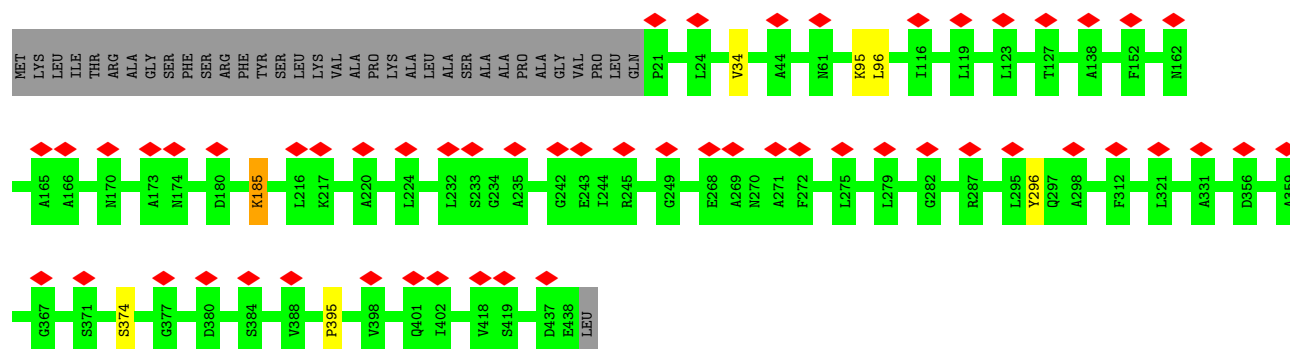


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

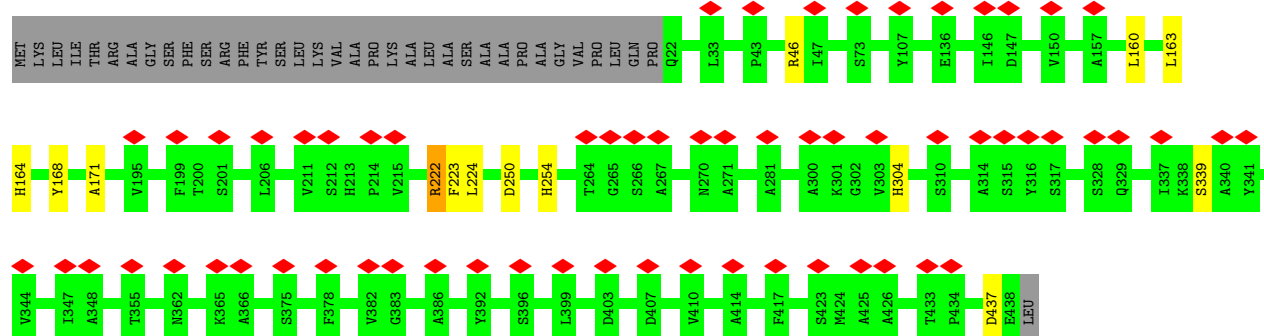


- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

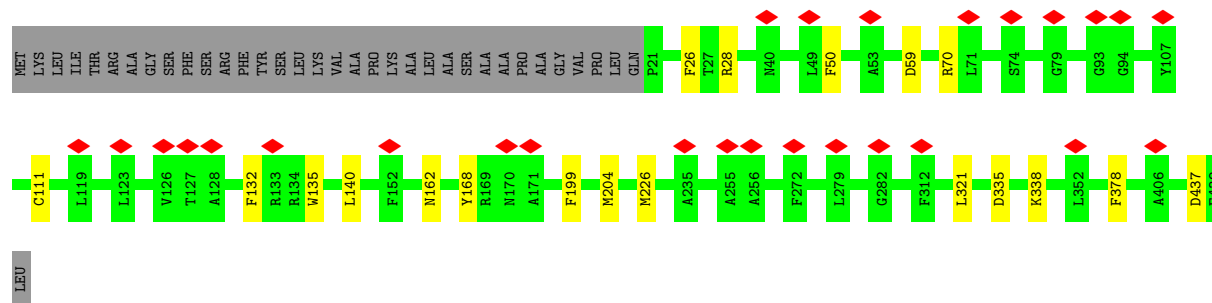
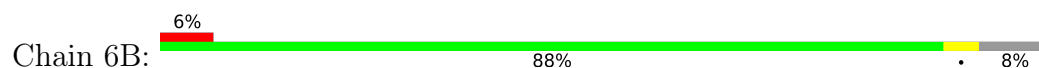




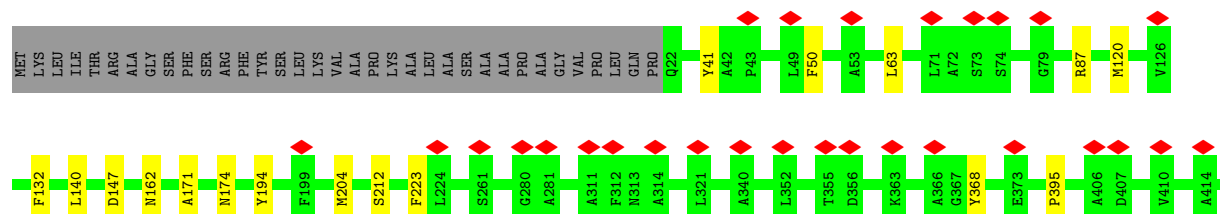
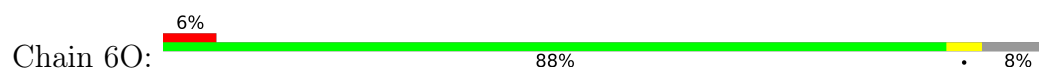
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

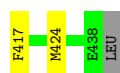


- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial





- Molecule 47: Cytochrome b

Chain 3C:  94% 6%



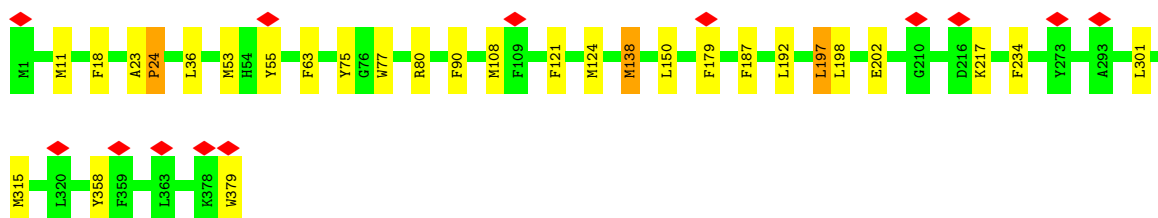
- Molecule 47: Cytochrome b

Chain 3P:  98% ..



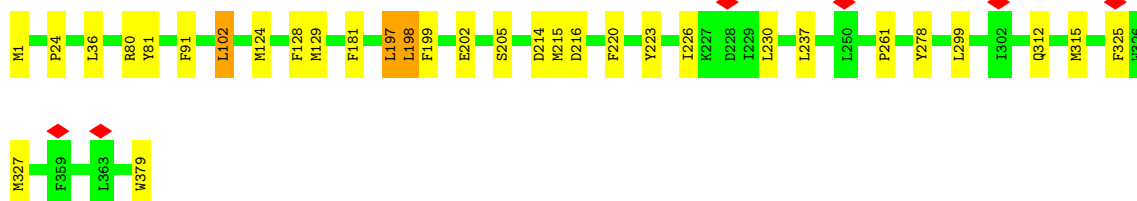
- Molecule 47: Cytochrome b

Chain 6C:  92% 7% .



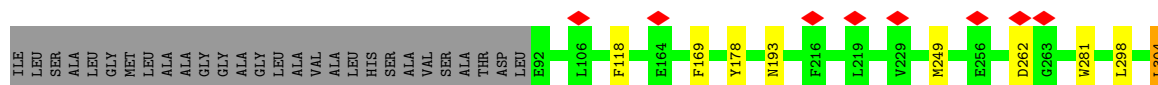
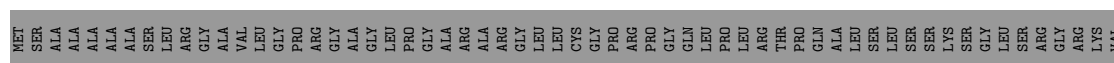
- Molecule 47: Cytochrome b

Chain 6P:  92% 8% .



- Molecule 48: Cytochrome c1

Chain 3D:  70% 27%





• Molecule 48: Cytochrome c1



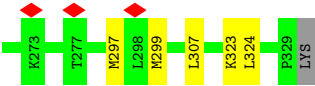
MET	SER	ALA	ALA	ALA	ALA	ALA	SER	LEU	GLY	ARG	GLY	ALA	VAL	LEU	GLY	PRO	ALA	ARG	GLY	ALA	GLY	GLY	LEU	ALA	GLY	LEU	GLY	LEU	ARG	ALA	ALA	ARG	GLY	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ILE	LEU	SER	ALA	ALA	LEU	LEU	GLY	MET	LEU	ALA	ALA	GLY	GLY	VAL	GLY	LEU	ALA	VAL	GLY	ALA	LEU	HIS	SER	LEU	ALA	VAL	SER	ALA	THR	D2	L5	S42	C55	E99	F128	F149	F171	F189	M204	M211	F240	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----	-----	-----	------	------	------	------	------	------	------	-----

• Molecule 48: Cytochrome c1



MET	SER	ALA	ALA	ALA	ALA	ALA	SER	LEU	GLY	ARG	GLY	ALA	VAL	LEU	GLY	PRO	ALA	ARG	GLY	ALA	GLY	GLY	SER	LEU	ALA	VAL	SER	ALA	THR	ASP	E92	E92	W100	K122	M131	L176	F179	N193	R206	G210	Y214	V215	F216	F237	M249	L258	P265	M268	S269
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



• Molecule 48: Cytochrome c1



MET	SER	ALA	ALA	ALA	ALA	ALA	SER	LEU	GLY	ARG	GLY	ALA	VAL	LEU	GLY	PRO	ALA	ARG	GLY	ALA	GLY	GLY	SER	LEU	ALA	VAL	SER	ALA	THR	D2	L3	E4	S13	L21	P22	H23	F30	L109	Y115	A119	F128	F153	F189	H200	M210	M211	M212	L216	K223
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------

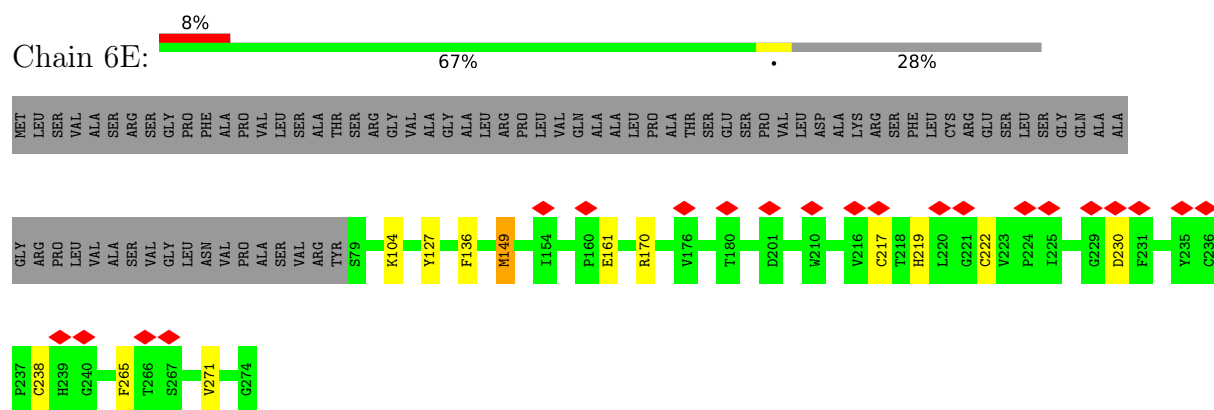


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

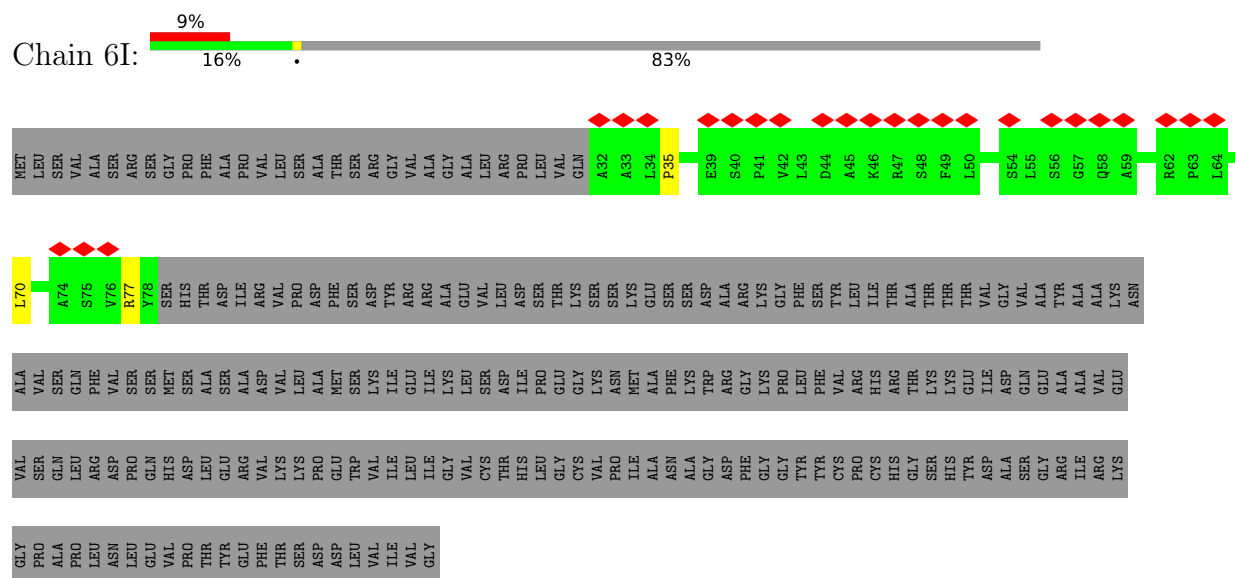


MET	LEU	VAL	VAL	SER	ARG	SER	GLY	PRO	PHE	ASN	VAL	PRO	VAL	SER	THR	ALA	SER	ARG	GLY	VAL	ALA	GLY	GLY	LEU	ARG	PRO	LEU	VAL	GLN	ALA	ALA	LEU	PRO	PRO	ALA	THR	SER	GLU	PRO	VAL	LEU	ASP	ALA	LYS	ARG	SER	PHE	LEU	CYS	ARG	SER	GLU	LEU	SER	GLY	GLN	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

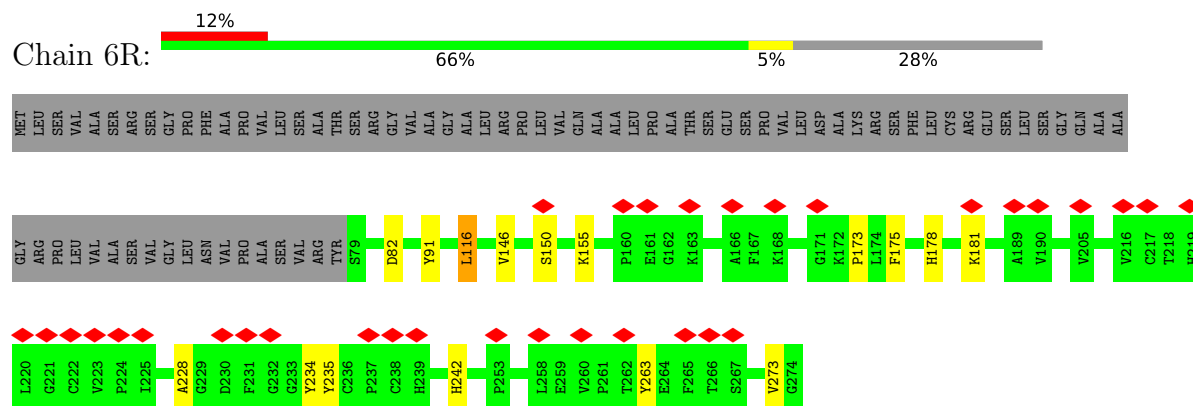
GLY	ARG	PRO	LEU	VAL	ALA	SER	VAL	GLY	LEU	ASN	VAL	PRO	ALA	VAL	SER	THR	ALA	SER	ARG	L116	F136	M149	M165	V176	K181	S193	R196	V216	C217	G229	H242	F264	F265	T266	S267	V271	G274
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

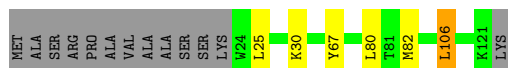
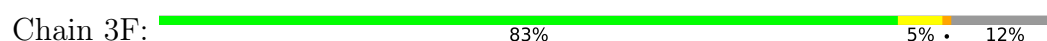


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

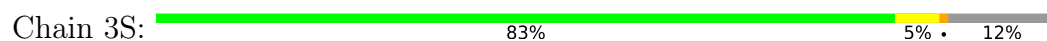




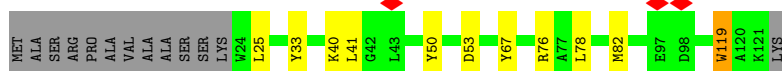
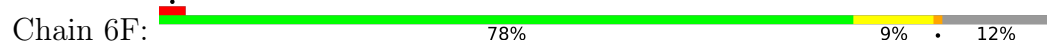
- Molecule 50: Cytochrome b-c1 complex subunit 7



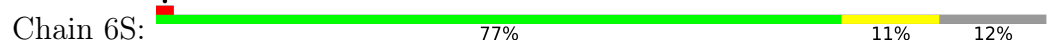
- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 50: Cytochrome b-c1 complex subunit 7

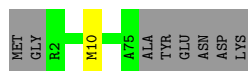


- Molecule 51: Cytochrome b-c1 complex subunit 8



- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T:  89% 10%




- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 6G:  84% 6% 10%



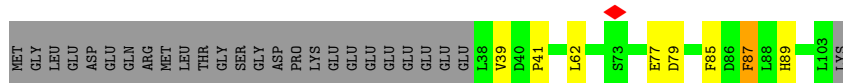
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 6T:  85% 5% 10%



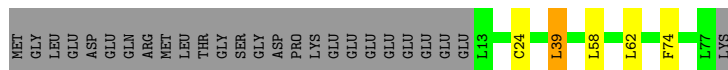
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H:  63% 8% 29%



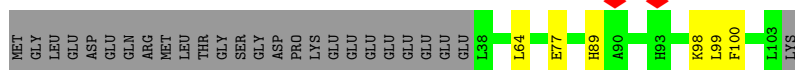
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U:  66% 29%



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 6H:  65% 7% 29%



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 6U:  64% 7% 29%



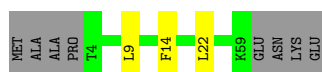
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J: 83% 12%



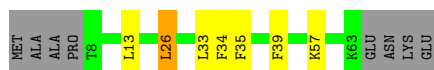
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W: 83% 5% 12%



- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 6J: 77% 9% 12%



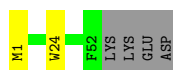
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 6W: 77% 11% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X: 89% 7%



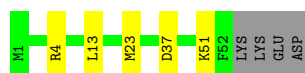
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y: 82% 9% 9%



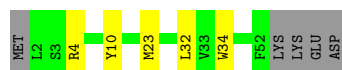
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 6X: 84% 9% 7%



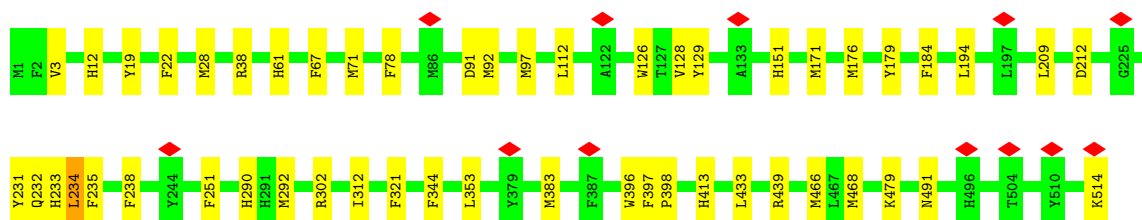
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 6Y: 82% 9% 9%



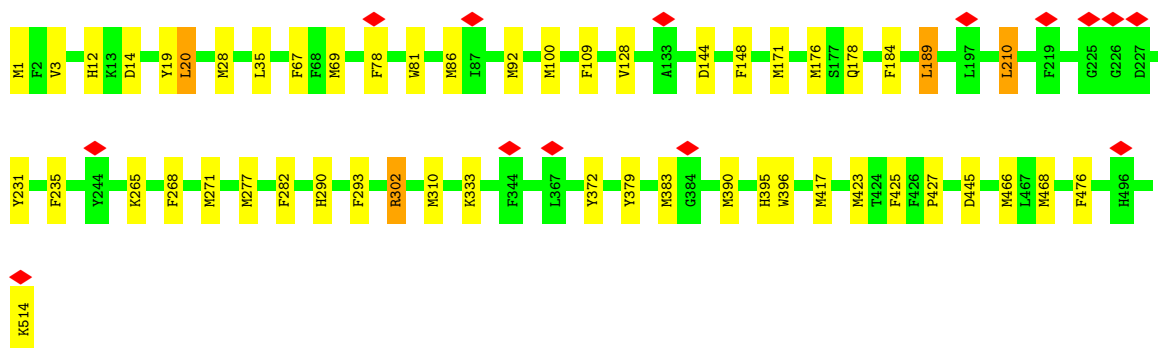
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A: 90% 10%



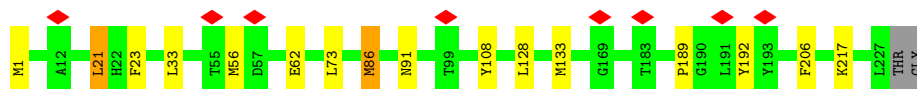
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 8A: 90% 9%



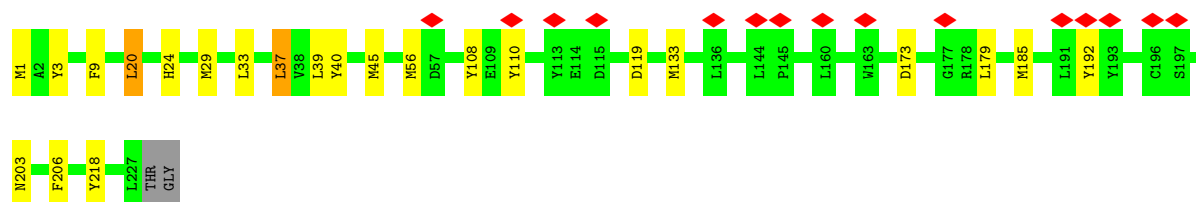
- Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 92% 6%



- Molecule 56: Cytochrome c oxidase subunit 2

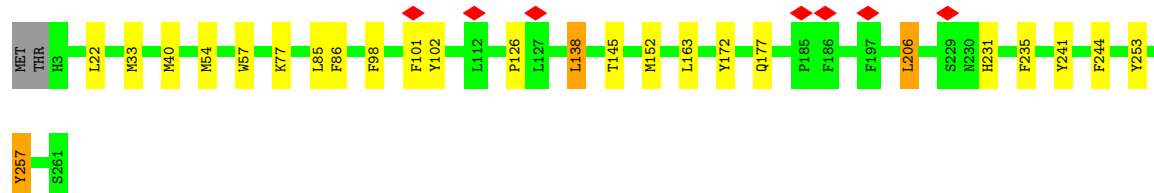
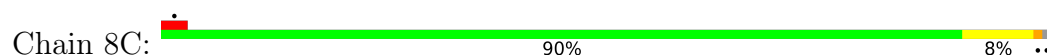
Chain 8B: 7% 89% 9%



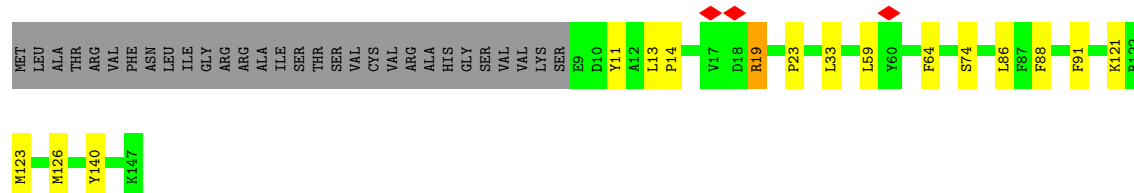
- Molecule 57: Cytochrome c oxidase subunit 3



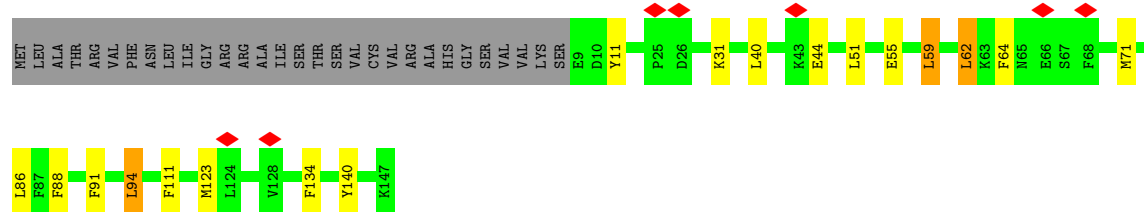
- Molecule 57: Cytochrome c oxidase subunit 3



- Molecule 58: Cytochrome c oxidase subunit 4

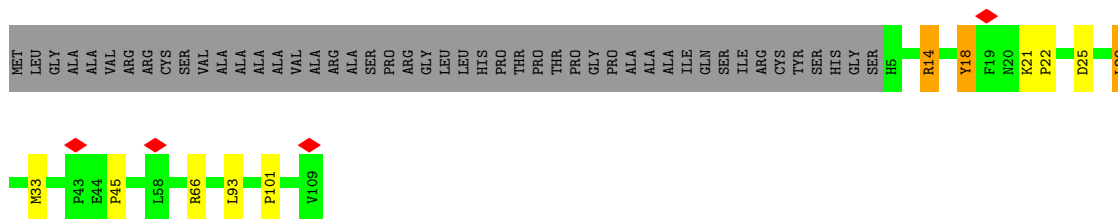


- Molecule 58: Cytochrome c oxidase subunit 4

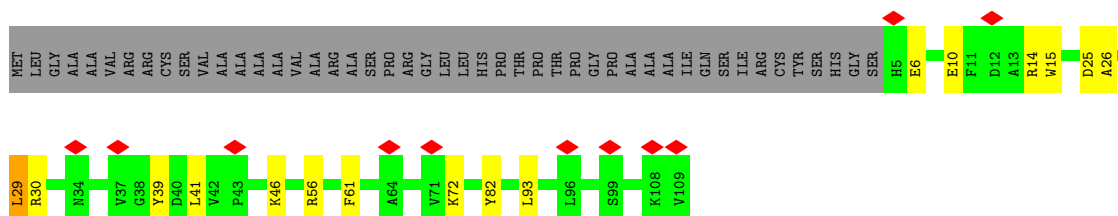


- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

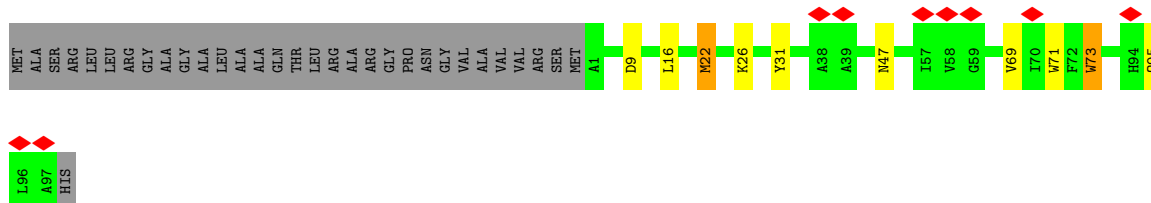




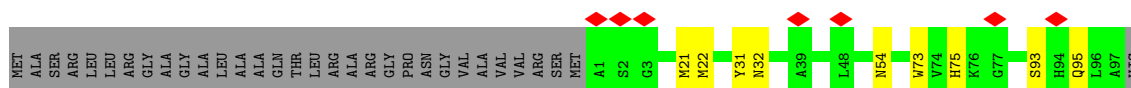
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



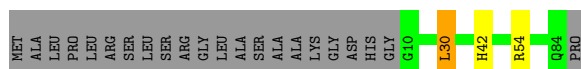
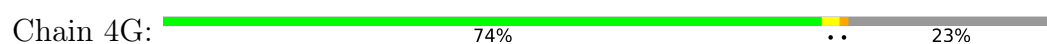
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



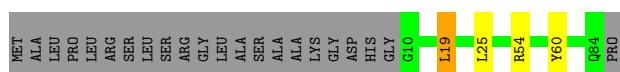
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



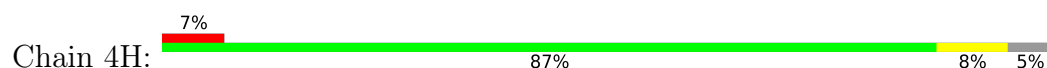
- Molecule 61: Cytochrome c oxidase subunit 6A2



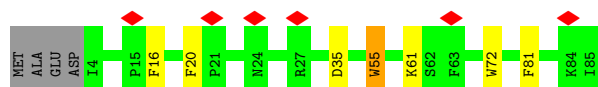
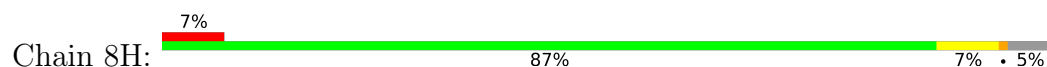
- Molecule 61: Cytochrome c oxidase subunit 6A2



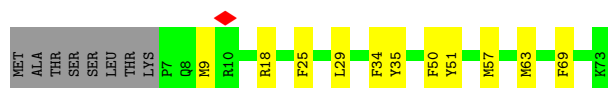
- Molecule 62: Cytochrome c oxidase subunit 6B1



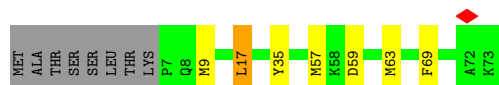
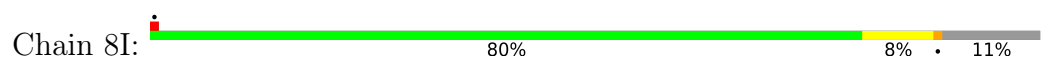
- Molecule 62: Cytochrome c oxidase subunit 6B1



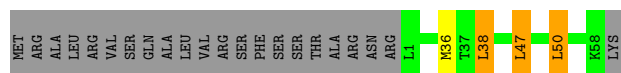
- Molecule 63: Cytochrome c oxidase subunit 6C



- Molecule 63: Cytochrome c oxidase subunit 6C



- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

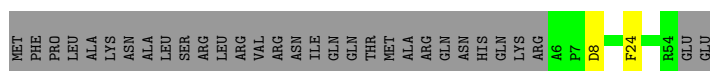


- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

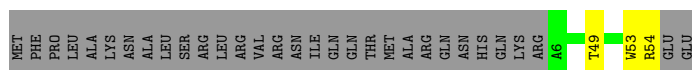


- Molecule 65: Cytochrome c oxidase subunit 7B

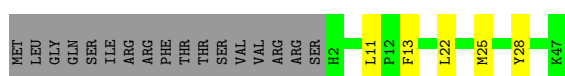




- Molecule 65: Cytochrome c oxidase subunit 7B



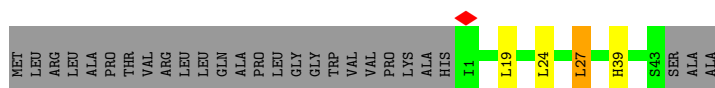
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



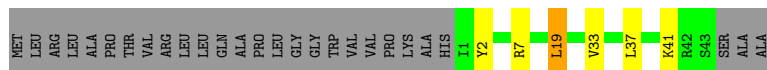
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



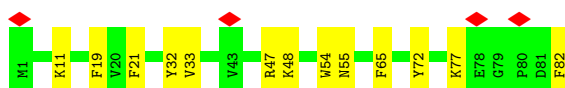
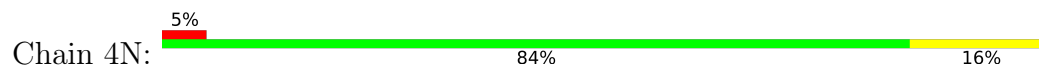
- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 67: Cytochrome c oxidase subunit 8

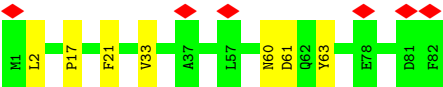


- Molecule 68: Cytochrome c oxidase subunit NDUF4A



- Molecule 68: Cytochrome c oxidase subunit NDUF4A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.533	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	798.72, 798.72, 798.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, FES, MYR, PGV, FMN, CUA, GTP, AME, SF4, NDP, 3PE, SAC, PSC, HEC, K, ZN, HEM, EHZ, CDL, PC1, NA, HEA, FME, PEK, CU, PO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.51	1/930 (0.1%)	0.79	1/1271 (0.1%)
1	5A	0.56	0/930	0.87	5/1271 (0.4%)
2	1B	0.56	2/1273 (0.2%)	0.89	4/1722 (0.2%)
2	5B	0.46	0/1273	0.91	10/1722 (0.6%)
3	1C	0.46	1/1791 (0.1%)	0.69	1/2439 (0.0%)
3	5C	0.61	6/1791 (0.3%)	0.71	3/2439 (0.1%)
4	1D	0.41	1/3545 (0.0%)	0.72	10/4806 (0.2%)
4	5D	0.35	0/3545	0.68	5/4806 (0.1%)
5	1E	0.44	2/1698 (0.1%)	0.67	5/2311 (0.2%)
5	5E	0.49	2/1698 (0.1%)	0.70	4/2311 (0.2%)
6	1F	0.33	0/3401	0.60	1/4595 (0.0%)
6	5F	0.30	0/3401	0.59	4/4595 (0.1%)
7	1G	0.38	2/5451 (0.0%)	0.67	9/7387 (0.1%)
7	5G	0.54	6/5451 (0.1%)	0.83	16/7387 (0.2%)
8	1H	1.08	11/2566 (0.4%)	1.23	28/3509 (0.8%)
8	5H	0.41	0/2566	0.76	11/3509 (0.3%)
9	1I	0.65	4/1443 (0.3%)	0.87	9/1952 (0.5%)
9	5I	0.47	0/1443	0.69	2/1952 (0.1%)
10	1J	0.57	2/1364 (0.1%)	0.84	5/1850 (0.3%)
10	5J	0.43	0/1364	0.72	4/1850 (0.2%)
11	1K	0.68	1/751 (0.1%)	1.34	11/1018 (1.1%)
11	5K	0.39	0/751	0.79	0/1018
12	1L	0.40	1/4939 (0.0%)	0.68	13/6718 (0.2%)
12	5L	0.43	2/4939 (0.0%)	0.80	25/6718 (0.4%)
13	1M	0.34	0/3713	0.68	5/5063 (0.1%)
13	5M	0.39	1/3713 (0.0%)	0.80	13/5063 (0.3%)
14	1N	0.50	2/2765 (0.1%)	0.87	15/3758 (0.4%)
14	5N	0.52	3/2765 (0.1%)	0.88	13/3758 (0.3%)
15	1O	0.31	0/2650	0.57	2/3588 (0.1%)
15	5O	0.42	3/2650 (0.1%)	0.64	2/3588 (0.1%)
16	1P	0.36	1/2828 (0.0%)	0.60	1/3834 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	5P	0.36	1/2828 (0.0%)	0.61	3/3834 (0.1%)
17	1Q	0.62	4/1070 (0.4%)	0.71	1/1446 (0.1%)
17	5Q	0.79	8/1070 (0.7%)	0.77	2/1446 (0.1%)
18	1R	0.31	0/755	0.61	1/1018 (0.1%)
18	5R	0.33	0/755	0.64	1/1018 (0.1%)
19	1S	0.44	0/711	0.81	1/956 (0.1%)
19	5S	0.55	1/711 (0.1%)	0.83	6/956 (0.6%)
20	1T	0.62	2/701 (0.3%)	0.84	4/946 (0.4%)
20	1U	0.46	1/706 (0.1%)	0.80	4/954 (0.4%)
20	5T	0.34	0/701	0.68	1/946 (0.1%)
20	5U	0.62	3/706 (0.4%)	0.71	0/954
21	1V	0.32	0/946	0.65	2/1281 (0.2%)
21	5V	0.29	0/946	0.56	0/1281
22	1W	0.34	0/995	0.75	2/1340 (0.1%)
22	5W	0.49	0/995	0.87	4/1340 (0.3%)
23	1X	0.45	3/1436 (0.2%)	0.59	0/1938
23	5X	0.53	3/1436 (0.2%)	0.61	0/1938
24	1Y	0.33	0/1037	0.74	6/1404 (0.4%)
24	5Y	0.32	0/1037	1.06	8/1404 (0.6%)
25	1Z	0.60	5/1199 (0.4%)	0.78	4/1617 (0.2%)
25	5Z	0.56	1/1199 (0.1%)	0.80	2/1617 (0.1%)
26	1a	0.41	0/577	0.78	2/777 (0.3%)
26	5a	0.37	0/577	0.65	1/777 (0.1%)
27	1b	0.34	0/664	0.62	1/912 (0.1%)
27	5b	0.31	0/664	0.67	2/912 (0.2%)
28	1c	0.68	1/430 (0.2%)	0.86	2/581 (0.3%)
28	5c	0.29	0/430	0.71	3/581 (0.5%)
29	1d	0.45	1/1016 (0.1%)	0.66	0/1374
29	5d	0.55	2/1016 (0.2%)	0.73	3/1374 (0.2%)
30	1e	0.60	2/836 (0.2%)	0.97	6/1118 (0.5%)
30	5e	0.58	3/836 (0.4%)	0.72	1/1118 (0.1%)
31	1f	0.25	0/499	0.65	2/673 (0.3%)
31	5f	0.29	0/499	0.65	0/673
32	1g	0.58	2/858 (0.2%)	0.70	0/1165
32	5g	0.51	1/858 (0.1%)	0.82	2/1165 (0.2%)
33	1h	0.45	1/1184 (0.1%)	0.74	2/1603 (0.1%)
33	5h	0.48	2/1184 (0.2%)	0.73	3/1603 (0.2%)
34	1i	0.49	2/1131 (0.2%)	0.79	4/1541 (0.3%)
34	5i	0.45	1/1131 (0.1%)	0.76	4/1541 (0.3%)
35	1j	0.42	0/627	0.70	2/858 (0.2%)
35	5j	0.33	0/627	0.64	1/858 (0.1%)
36	1k	0.32	0/668	0.54	0/903
36	5k	0.83	3/668 (0.4%)	0.85	3/903 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	1l	0.37	0/1365	0.71	5/1867 (0.3%)
37	5l	0.39	0/1365	0.68	3/1867 (0.2%)
38	1m	0.35	0/1092	0.62	1/1481 (0.1%)
38	5m	0.35	0/1092	0.69	1/1481 (0.1%)
39	1n	0.37	1/1549 (0.1%)	0.67	1/2098 (0.0%)
39	5n	0.61	6/1549 (0.4%)	0.79	4/2098 (0.2%)
40	1o	0.31	0/1069	0.69	2/1430 (0.1%)
40	5o	0.38	0/1069	0.71	1/1430 (0.1%)
41	1p	0.32	0/1481	0.56	0/1997
41	5p	0.38	0/1481	0.68	1/1997 (0.1%)
42	1q	0.55	3/1253 (0.2%)	0.77	3/1704 (0.2%)
42	5q	0.82	9/1253 (0.7%)	0.72	6/1704 (0.4%)
43	1r	0.37	0/777	0.85	5/1051 (0.5%)
43	5r	0.45	0/777	0.75	2/1051 (0.2%)
44	1s	1.04	5/394 (1.3%)	0.82	1/533 (0.2%)
44	5s	0.29	0/394	0.61	0/533
45	3A	0.37	2/3481 (0.1%)	0.62	5/4722 (0.1%)
45	3N	0.57	5/3496 (0.1%)	0.78	8/4723 (0.2%)
45	6A	0.37	0/3481	0.63	2/4722 (0.0%)
45	6N	0.34	0/3496	0.67	7/4723 (0.1%)
46	3B	0.36	2/3190 (0.1%)	0.61	2/4317 (0.0%)
46	3O	0.30	0/3175	0.59	3/4292 (0.1%)
46	6B	0.37	1/3190 (0.0%)	0.62	2/4317 (0.0%)
46	6O	0.33	0/3175	0.62	3/4292 (0.1%)
47	3C	0.41	2/3123 (0.1%)	0.70	9/4269 (0.2%)
47	3P	0.29	0/3122	0.59	4/4269 (0.1%)
47	6C	0.80	6/3123 (0.2%)	0.92	11/4269 (0.3%)
47	6P	0.59	3/3122 (0.1%)	0.92	23/4269 (0.5%)
48	3D	0.38	0/1946	0.69	3/2641 (0.1%)
48	3Q	0.32	0/1962	0.59	2/2663 (0.1%)
48	6D	0.39	0/1946	0.76	7/2641 (0.3%)
48	6Q	0.52	2/1962 (0.1%)	0.86	8/2663 (0.3%)
49	3E	0.31	0/1551	0.61	1/2098 (0.0%)
49	3I	0.64	1/342 (0.3%)	0.78	2/465 (0.4%)
49	3R	0.33	0/1551	0.60	0/2098
49	3V	0.28	0/225	0.62	0/303
49	6E	0.53	3/1551 (0.2%)	0.70	2/2098 (0.1%)
49	6I	0.48	1/342 (0.3%)	0.73	0/465
49	6R	0.60	4/1551 (0.3%)	0.82	4/2098 (0.2%)
49	6V	0.26	0/225	0.68	0/303
50	3F	0.35	0/888	0.71	3/1193 (0.3%)
50	3S	0.28	0/888	0.67	3/1193 (0.3%)
50	6F	0.55	1/888 (0.1%)	0.81	5/1193 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
50	6S	0.50	1/888 (0.1%)	0.87	5/1193 (0.4%)
51	3G	0.37	0/649	0.74	1/878 (0.1%)
51	3T	0.34	0/649	0.61	1/878 (0.1%)
51	6G	0.40	0/649	0.78	1/878 (0.1%)
51	6T	0.40	0/649	0.73	0/878
52	3H	1.11	8/539 (1.5%)	1.23	10/724 (1.4%)
52	3U	0.29	0/539	0.70	3/724 (0.4%)
52	6H	0.34	0/539	0.81	3/724 (0.4%)
52	6U	0.50	0/539	0.85	4/724 (0.6%)
53	3J	0.36	0/464	0.69	2/625 (0.3%)
53	3W	0.53	0/464	0.73	2/625 (0.3%)
53	6J	0.41	0/464	0.82	2/625 (0.3%)
53	6W	0.44	0/464	0.83	4/625 (0.6%)
54	3X	0.27	0/445	0.55	0/608
54	3Y	0.37	0/437	0.71	1/598 (0.2%)
54	6X	0.41	0/445	0.79	3/608 (0.5%)
54	6Y	0.59	1/437 (0.2%)	0.76	2/598 (0.3%)
55	4A	0.51	3/4156 (0.1%)	0.82	13/5679 (0.2%)
55	8A	0.56	6/4156 (0.1%)	0.96	12/5679 (0.2%)
56	4B	0.50	1/1865 (0.1%)	0.79	6/2544 (0.2%)
56	8B	0.43	0/1865	0.83	9/2544 (0.4%)
57	4C	0.55	2/2179 (0.1%)	0.66	3/2981 (0.1%)
57	8C	0.56	2/2179 (0.1%)	0.77	3/2981 (0.1%)
58	4D	0.53	0/1197	0.89	7/1617 (0.4%)
58	8D	0.61	3/1197 (0.3%)	0.86	6/1617 (0.4%)
59	4E	0.63	2/871 (0.2%)	0.97	6/1182 (0.5%)
59	8E	0.56	2/871 (0.2%)	0.93	4/1182 (0.3%)
60	4F	0.65	3/749 (0.4%)	0.76	2/1016 (0.2%)
60	8F	0.31	0/749	0.69	0/1016
61	4G	0.28	0/644	0.60	1/881 (0.1%)
61	8G	0.41	0/644	0.68	2/881 (0.2%)
62	4H	0.83	4/708 (0.6%)	0.86	5/956 (0.5%)
62	8H	0.63	1/708 (0.1%)	0.78	1/956 (0.1%)
63	4I	0.47	0/563	0.98	2/748 (0.3%)
63	8I	0.48	0/563	0.92	3/748 (0.4%)
64	4J	0.31	0/466	0.71	3/631 (0.5%)
64	8J	0.67	1/466 (0.2%)	0.94	5/631 (0.8%)
65	4K	0.29	0/396	0.50	0/543
65	8K	0.31	0/396	0.49	0/543
66	4L	0.49	0/394	0.73	1/528 (0.2%)
66	8L	0.63	0/394	1.07	7/528 (1.3%)
67	4M	0.46	0/349	0.80	3/477 (0.6%)
67	8M	0.45	0/349	0.83	3/477 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	4N	0.41	0/680	0.65	0/921
68	8N	0.46	0/680	0.66	1/921 (0.1%)
All	All	0.48	204/232954 (0.1%)	0.75	640/315994 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1B	0	2
3	1C	0	1
5	1E	0	1
6	1F	0	1
6	5F	0	1
7	5G	0	1
8	1H	0	2
8	5H	0	1
10	1J	0	1
11	5K	0	1
12	1L	0	1
12	5L	0	1
13	5M	0	1
16	1P	0	1
18	5R	0	1
23	5X	0	1
24	1Y	0	1
25	5Z	0	1
26	1a	0	1
33	1h	0	1
38	5m	0	1
39	1n	0	1
43	5r	0	1
45	3N	0	1
45	6A	0	1
45	6N	0	1
47	6C	0	2
48	6D	0	1
49	6E	0	1
52	6H	0	1
59	4E	0	1
59	8E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
68	4N	0	1
All	All	0	36

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1H	308	PRO	CG-CD	-30.86	0.48	1.50
47	6C	24	PRO	CB-CG	28.68	2.93	1.50
7	5G	384	PRO	CG-CD	-24.08	0.71	1.50
47	6C	24	PRO	CG-CD	-22.70	0.75	1.50
8	1H	42	PRO	CG-CD	-21.25	0.80	1.50
45	3N	170	PRO	CG-CD	-20.00	0.84	1.50
47	6P	24	PRO	CG-CD	-19.10	0.87	1.50
8	1H	42	PRO	CB-CG	18.68	2.43	1.50
42	5q	144	TYR	CD1-CE1	-14.51	1.17	1.39
45	3N	269	PRO	CG-CD	-13.77	1.05	1.50
44	1s	38	TYR	CD1-CE1	-13.63	1.19	1.39
42	5q	55	PHE	CB-CG	-12.38	1.30	1.51
36	5k	50	TRP	CB-CG	-11.55	1.29	1.50
8	1H	104	PHE	CE1-CZ	-11.41	1.15	1.37
64	8J	39	CYS	CB-SG	-11.14	1.63	1.82
49	6R	173	PRO	CG-CD	-10.88	1.14	1.50
52	3H	41	PRO	CG-CD	-10.86	1.14	1.50
3	5C	142	PHE	CD1-CE1	-10.77	1.17	1.39
23	5X	96	PHE	CD1-CE1	-10.71	1.17	1.39
49	3I	35	PRO	N-CD	-10.60	1.33	1.47
20	1T	75	GLU	CG-CD	-10.42	1.36	1.51
49	6E	238	CYS	CB-SG	10.24	1.99	1.82
52	3H	87	PHE	CD2-CE2	-10.21	1.18	1.39
62	4H	81	PHE	CD1-CE1	-10.20	1.18	1.39
8	1H	308	PRO	CB-CG	10.12	2.00	1.50
17	5Q	59	PHE	CD1-CE1	-9.74	1.19	1.39
45	3N	170	PRO	N-CD	9.56	1.61	1.47
25	1Z	53	TRP	CB-CG	-9.53	1.33	1.50
33	1h	124	GLN	C-N	-9.53	1.12	1.34
39	5n	114	TYR	CD2-CE2	-9.51	1.25	1.39
11	1K	38	LEU	CG-CD2	-9.33	1.17	1.51
14	5N	167	TRP	CE3-CZ3	-9.27	1.22	1.38
55	8A	476	PHE	CD1-CE1	-9.08	1.21	1.39
12	1L	556	ILE	CB-CG2	-8.99	1.25	1.52
39	5n	114	TYR	CG-CD2	-8.94	1.27	1.39
36	5k	21	TRP	CE3-CZ3	-8.94	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	4F	73	TRP	CB-CG	-8.93	1.34	1.50
9	1I	27	TRP	CE3-CZ3	-8.91	1.23	1.38
45	3N	269	PRO	N-CD	8.90	1.60	1.47
20	1T	75	GLU	CB-CG	-8.74	1.35	1.52
25	1Z	53	TRP	CE2-CZ2	-8.74	1.24	1.39
7	5G	359	ARG	CG-CD	-8.66	1.30	1.51
52	3H	87	PHE	CB-CG	-8.65	1.36	1.51
57	4C	242	TRP	CE3-CZ3	-8.57	1.23	1.38
52	3H	87	PHE	CG-CD2	-8.48	1.26	1.38
17	1Q	59	PHE	CD2-CE2	-8.38	1.22	1.39
32	1g	27	GLN	CB-CG	-8.36	1.29	1.52
2	1B	149	CYS	CB-SG	-8.32	1.68	1.82
52	3H	41	PRO	CB-CG	8.19	1.90	1.50
42	5q	144	TYR	CE1-CZ	-8.10	1.28	1.38
42	1q	49	TYR	CD1-CE1	-8.09	1.27	1.39
57	4C	248	VAL	CB-CG2	-8.05	1.35	1.52
14	1N	93	VAL	CB-CG2	-7.93	1.36	1.52
3	5C	130	TYR	CG-CD2	-7.89	1.28	1.39
62	4H	81	PHE	CE2-CZ	-7.87	1.22	1.37
30	5e	35	PHE	CD2-CE2	-7.85	1.23	1.39
52	3H	87	PHE	CE1-CZ	-7.84	1.22	1.37
14	5N	167	TRP	CB-CG	-7.83	1.36	1.50
28	1c	43	LYS	CD-CE	-7.79	1.31	1.51
49	6R	234	TYR	CD1-CE1	-7.78	1.27	1.39
62	4H	81	PHE	CG-CD1	-7.73	1.27	1.38
56	4B	189	PRO	CG-CD	-7.67	1.25	1.50
42	5q	55	PHE	CD2-CE2	-7.67	1.24	1.39
29	5d	73	TYR	CD2-CE2	7.65	1.50	1.39
17	5Q	59	PHE	CE2-CZ	-7.53	1.23	1.37
55	4A	466	MET	CB-CG	-7.51	1.27	1.51
14	5N	167	TRP	CE2-CZ2	-7.50	1.26	1.39
5	5E	160	TYR	CD1-CE1	-7.45	1.28	1.39
42	5q	55	PHE	CG-CD1	-7.34	1.27	1.38
3	5C	130	TYR	CD2-CE2	-7.30	1.28	1.39
49	6E	222	CYS	CB-SG	-7.17	1.70	1.82
7	5G	66	VAL	CB-CG1	7.14	1.67	1.52
7	5G	384	PRO	N-CD	7.13	1.57	1.47
50	6F	119	TRP	CE3-CZ3	-7.12	1.26	1.38
23	1X	42	PHE	CE2-CZ	-7.12	1.23	1.37
13	5M	354	LEU	CG-CD2	-7.12	1.25	1.51
54	6Y	34	TRP	CB-CG	-7.11	1.37	1.50
17	1Q	59	PHE	CB-CG	-7.05	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1U	63	PRO	CG-CD	-7.05	1.27	1.50
23	1X	42	PHE	CE1-CZ	-7.03	1.24	1.37
7	5G	122	MET	CB-CG	-7.01	1.28	1.51
8	1H	308	PRO	N-CD	7.00	1.57	1.47
7	5G	122	MET	CG-SD	-7.00	1.62	1.81
17	5Q	132	THR	CB-CG2	-6.93	1.29	1.52
30	5e	35	PHE	CB-CG	-6.90	1.39	1.51
49	6R	146	VAL	CB-CG1	-6.87	1.38	1.52
23	5X	96	PHE	CD2-CE2	-6.87	1.25	1.39
44	1s	38	TYR	CE1-CZ	-6.86	1.29	1.38
7	1G	230	VAL	CB-CG2	-6.85	1.38	1.52
30	1e	59	PHE	CD1-CE1	-6.85	1.25	1.39
34	1i	79	TRP	CG-CD1	-6.82	1.27	1.36
17	1Q	59	PHE	CG-CD2	-6.79	1.28	1.38
47	6C	23	ALA	C-N	-6.79	1.21	1.34
42	5q	55	PHE	CG-CD2	-6.78	1.28	1.38
42	5q	55	PHE	CD1-CE1	-6.75	1.25	1.39
47	3C	93	CYS	CB-SG	-6.75	1.70	1.82
8	1H	37	PRO	CG-CD	-6.75	1.28	1.50
42	5q	144	TYR	CD2-CE2	-6.73	1.29	1.39
52	3H	87	PHE	CD1-CE1	-6.67	1.25	1.39
44	1s	38	TYR	CZ-OH	-6.67	1.26	1.37
16	5P	239	PHE	CD1-CE1	-6.66	1.25	1.39
23	5X	96	PHE	CE1-CZ	-6.66	1.24	1.37
47	3C	326	TRP	CB-CG	-6.66	1.38	1.50
49	6I	35	PRO	N-CD	6.65	1.57	1.47
50	6S	97	VAL	CB-CG1	-6.64	1.39	1.52
3	1C	173	GLU	CG-CD	-6.57	1.42	1.51
12	5L	183	VAL	CB-CG2	-6.55	1.39	1.52
59	4E	18	TYR	CD2-CE2	-6.52	1.29	1.39
9	1I	27	TRP	CE2-CZ2	-6.46	1.28	1.39
60	4F	69	VAL	CB-CG1	-6.45	1.39	1.52
60	4F	73	TRP	CE3-CZ3	-6.44	1.27	1.38
17	1Q	59	PHE	CE1-CZ	-6.42	1.25	1.37
49	6E	217	CYS	CB-SG	-6.40	1.71	1.82
17	5Q	59	PHE	CD2-CE2	-6.37	1.26	1.39
57	8C	57	TRP	CE3-CZ3	-6.37	1.27	1.38
44	1s	38	TYR	CG-CD1	-6.35	1.30	1.39
59	4E	66	ARG	CG-CD	-6.34	1.36	1.51
45	3N	170	PRO	CB-CG	6.34	1.81	1.50
39	1n	162	LEU	CG-CD2	-6.26	1.28	1.51
17	5Q	59	PHE	CG-CD1	-6.25	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1g	27	GLN	CG-CD	-6.24	1.36	1.51
8	1H	104	PHE	CD1-CE1	-6.21	1.26	1.39
45	3A	4	TYR	CD2-CE2	-6.21	1.30	1.39
5	5E	160	TYR	CD2-CE2	-6.13	1.30	1.39
62	4H	81	PHE	CB-CG	-6.12	1.41	1.51
57	8C	257	TYR	CE1-CZ	-6.12	1.30	1.38
39	5n	117	TYR	CD1-CE1	-6.10	1.30	1.39
36	5k	21	TRP	CE2-CZ2	-6.09	1.29	1.39
30	5e	35	PHE	CG-CD2	-6.07	1.29	1.38
62	8H	55	TRP	CE3-CZ3	-6.06	1.28	1.38
9	1I	42	PHE	CD2-CE2	-6.06	1.27	1.39
42	1q	49	TYR	CG-CD1	-6.04	1.31	1.39
47	6P	24	PRO	N-CD	6.02	1.56	1.47
20	5U	79	TYR	CD2-CE2	-5.98	1.30	1.39
55	8A	476	PHE	CE2-CZ	-5.96	1.26	1.37
46	6B	168	TYR	CD1-CE1	-5.93	1.30	1.39
5	1E	42	HIS	CA-CB	-5.91	1.41	1.53
59	8E	10	GLU	CG-CD	-5.91	1.43	1.51
14	1N	315	TRP	CB-CG	-5.91	1.39	1.50
58	8D	55	GLU	CG-CD	-5.89	1.43	1.51
19	5S	65	TRP	CB-CG	-5.88	1.39	1.50
32	5g	88	TRP	CB-CG	-5.88	1.39	1.50
16	1P	10	LYS	CE-NZ	-5.85	1.34	1.49
23	1X	42	PHE	CG-CD1	-5.85	1.29	1.38
58	8D	51	LEU	CG-CD2	-5.81	1.30	1.51
55	8A	476	PHE	CD2-CE2	-5.79	1.27	1.39
3	5C	142	PHE	CE2-CZ	-5.77	1.26	1.37
39	5n	114	TYR	CE2-CZ	-5.76	1.31	1.38
45	3A	4	TYR	CD1-CE1	-5.75	1.30	1.39
10	1J	65	LEU	CG-CD1	-5.74	1.30	1.51
15	5O	198	TYR	CD2-CE2	-5.74	1.30	1.39
12	5L	240	PRO	CG-CD	-5.72	1.31	1.50
46	3B	185	LYS	CD-CE	-5.72	1.36	1.51
15	5O	198	TYR	CD1-CE1	-5.71	1.30	1.39
20	5U	79	TYR	CE1-CZ	-5.71	1.31	1.38
44	1s	38	TYR	CB-CG	-5.70	1.43	1.51
8	1H	104	PHE	CG-CD2	-5.70	1.30	1.38
47	6C	202	GLU	CG-CD	-5.70	1.43	1.51
9	1I	149	TYR	CD1-CE1	-5.68	1.30	1.39
17	5Q	101	TRP	CE3-CZ3	-5.67	1.28	1.38
8	1H	104	PHE	CD2-CE2	-5.66	1.27	1.39
3	5C	142	PHE	CD2-CE2	-5.60	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1G	105	CYS	CB-SG	-5.58	1.72	1.81
58	8D	51	LEU	CG-CD1	-5.57	1.31	1.51
17	5Q	101	TRP	CB-CG	-5.57	1.40	1.50
29	5d	77	LYS	CB-CG	-5.55	1.37	1.52
55	4A	232	GLN	CG-CD	-5.54	1.38	1.51
30	1e	14	ASP	CB-CG	-5.54	1.40	1.51
47	6C	24	PRO	CA-C	5.54	1.64	1.52
47	6C	23	ALA	C-O	-5.52	1.12	1.23
15	5O	270	LEU	CG-CD1	-5.48	1.31	1.51
52	3H	41	PRO	N-CD	5.44	1.55	1.47
46	3B	296	TYR	CD1-CE1	-5.42	1.31	1.39
5	1E	60	TRP	CB-CG	-5.39	1.40	1.50
1	1A	62	PHE	CB-CG	-5.37	1.42	1.51
34	5i	23	LYS	CD-CE	-5.32	1.38	1.51
3	5C	142	PHE	CG-CD1	-5.32	1.30	1.38
47	6P	202	GLU	CD-OE2	-5.30	1.19	1.25
25	1Z	53	TRP	CE3-CZ3	-5.30	1.29	1.38
33	5h	21	PHE	CD1-CE1	-5.28	1.28	1.39
25	1Z	53	TRP	CZ2-CH2	-5.27	1.27	1.37
42	1q	49	TYR	CE1-CZ	-5.26	1.31	1.38
4	1D	51	PHE	CD1-CE1	-5.26	1.28	1.39
59	8E	61	PHE	CD2-CE2	-5.26	1.28	1.39
34	1i	83	TYR	CD1-CE1	-5.25	1.31	1.39
10	1J	54	LEU	CG-CD1	-5.24	1.32	1.51
42	5q	55	PHE	CE1-CZ	-5.24	1.27	1.37
55	8A	171	MET	CB-CG	-5.24	1.34	1.51
25	5Z	142	TRP	CE3-CZ3	-5.20	1.29	1.38
39	5n	114	TYR	CB-CG	-5.20	1.43	1.51
2	1B	71	ARG	CG-CD	-5.19	1.39	1.51
48	6Q	223	LYS	CE-NZ	-5.18	1.36	1.49
48	6Q	223	LYS	CG-CD	-5.13	1.34	1.52
55	4A	466	MET	CG-SD	-5.11	1.67	1.81
8	1H	42	PRO	CA-CB	-5.11	1.43	1.53
33	5h	21	PHE	CD2-CE2	-5.10	1.29	1.39
49	6R	234	TYR	CD2-CE2	-5.07	1.31	1.39
20	5U	79	TYR	CD1-CE1	-5.05	1.31	1.39
55	8A	476	PHE	CB-CG	-5.04	1.42	1.51
55	8A	293	PHE	CD1-CE1	-5.04	1.29	1.39
29	1d	119	VAL	CB-CG2	-5.03	1.42	1.52
17	5Q	59	PHE	CE1-CZ	-5.01	1.27	1.37
25	1Z	53	TRP	CG-CD2	-5.00	1.35	1.43
39	5n	117	TYR	CE2-CZ	-5.00	1.32	1.38

All (640) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	6C	24	PRO	CB-CG-CD	-27.30	0.03	106.50
7	5G	384	PRO	N-CD-CG	-23.64	67.74	103.20
8	1H	42	PRO	CA-CB-CG	-23.19	59.94	104.00
8	1H	308	PRO	N-CD-CG	-21.88	70.38	103.20
55	8A	100	MET	CG-SD-CE	-21.54	65.73	100.20
55	8A	277	MET	CG-SD-CE	-20.88	66.79	100.20
8	1H	42	PRO	N-CD-CG	-20.50	72.44	103.20
45	3N	269	PRO	CA-N-CD	-20.43	82.90	111.50
24	5Y	114	CYS	CA-CB-SG	20.18	150.32	114.00
55	8A	171	MET	CG-SD-CE	-19.96	68.27	100.20
24	5Y	94	CYS	CA-CB-SG	19.72	149.50	114.00
7	5G	71	MET	CG-SD-CE	-18.29	70.94	100.20
47	3C	327	MET	CG-SD-CE	-18.28	70.95	100.20
47	6C	53	MET	CG-SD-CE	-18.19	71.10	100.20
55	4A	383	MET	CG-SD-CE	-17.65	71.96	100.20
47	6P	24	PRO	N-CD-CG	-16.97	77.75	103.20
34	1i	22	LEU	CB-CG-CD1	-16.57	82.83	111.00
7	5G	122	MET	CG-SD-CE	-15.73	75.03	100.20
11	1K	55	LEU	CA-CB-CG	15.65	151.29	115.30
45	3N	170	PRO	CA-N-CD	-15.39	89.95	111.50
7	5G	631	VAL	CG1-CB-CG2	-15.29	86.44	110.90
52	3H	41	PRO	CA-N-CD	-15.15	90.29	111.50
57	8C	22	LEU	CB-CG-CD1	-14.89	85.69	111.00
63	4I	9	MET	CG-SD-CE	-14.83	76.47	100.20
13	5M	32	LEU	CA-CB-CG	14.26	148.10	115.30
7	5G	384	PRO	CA-CB-CG	-14.09	77.23	104.00
48	6Q	223	LYS	CD-CE-NZ	-14.07	79.34	111.70
47	6C	24	PRO	CA-CB-CG	-13.98	77.44	104.00
8	1H	42	PRO	CB-CG-CD	-13.94	52.15	106.50
49	6R	173	PRO	N-CD-CG	-13.79	82.51	103.20
39	5n	114	TYR	CZ-CE2-CD2	13.72	132.15	119.80
22	5W	88	MET	CG-SD-CE	-13.58	78.48	100.20
11	1K	55	LEU	CB-CG-CD2	-13.46	88.12	111.00
30	1e	14	ASP	CB-CG-OD2	-13.31	106.32	118.30
45	3N	269	PRO	N-CD-CG	-13.30	83.25	103.20
55	8A	271	MET	CG-SD-CE	-13.14	79.18	100.20
55	8A	466	MET	CG-SD-CE	-13.05	79.33	100.20
11	1K	36	MET	CG-SD-CE	-13.03	79.35	100.20
20	1T	54	MET	CG-SD-CE	-12.91	79.54	100.20
45	3N	170	PRO	N-CD-CG	-12.67	84.19	103.20
56	8B	29	MET	CA-CB-CG	12.59	134.71	113.30
12	5L	573	MET	CA-CB-CG	12.56	134.66	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1I	34	LEU	CA-CB-CG	12.54	144.15	115.30
55	4A	466	MET	CG-SD-CE	-12.54	80.14	100.20
48	6Q	211	MET	CG-SD-CE	-12.47	80.24	100.20
8	1H	308	PRO	CA-CB-CG	-12.22	80.78	104.00
59	4E	45	PRO	CA-N-CD	-12.17	94.46	111.50
42	1q	49	TYR	CD1-CE1-CZ	12.05	130.65	119.80
12	1L	532	ILE	CA-CB-CG1	-12.00	88.20	111.00
47	6P	24	PRO	CA-CB-CG	-11.98	81.24	104.00
8	1H	37	PRO	CA-N-CD	-11.91	94.82	111.50
30	1e	17	MET	CG-SD-CE	11.88	119.22	100.20
45	3N	170	PRO	CA-CB-CG	-11.84	81.50	104.00
12	5L	150	MET	CB-CG-SD	-11.82	76.94	112.40
47	6P	237	LEU	CA-CB-CG	11.65	142.09	115.30
8	1H	42	PRO	CA-N-CD	-11.63	95.22	111.50
55	8A	100	MET	CA-CB-CG	11.57	132.98	113.30
48	3D	249	MET	CG-SD-CE	-11.51	81.79	100.20
12	5L	240	PRO	CA-N-CD	-11.38	95.57	111.50
5	5E	66	MET	CG-SD-CE	-11.26	82.18	100.20
58	4D	23	PRO	CA-N-CD	-11.20	95.82	111.50
20	1U	63	PRO	N-CD-CG	-11.19	86.41	103.20
25	5Z	60	LEU	CB-CG-CD2	11.15	129.96	111.00
10	1J	74	MET	CG-SD-CE	-11.08	82.47	100.20
12	5L	53	MET	CG-SD-CE	-10.89	82.78	100.20
45	3N	269	PRO	CA-CB-CG	-10.75	83.57	104.00
8	1H	222	MET	CG-SD-CE	-10.69	83.09	100.20
11	1K	6	MET	CG-SD-CE	10.56	117.10	100.20
43	1r	7	ILE	CG1-CB-CG2	10.52	134.53	111.40
35	1j	56	PRO	CA-N-CD	-10.46	96.86	111.50
8	1H	42	PRO	N-CA-CB	-10.41	90.80	103.30
52	6H	77	GLU	C-N-CA	10.34	147.56	121.70
47	6P	24	PRO	CA-N-CD	-10.32	97.06	111.50
12	5L	366	MET	CG-SD-CE	-10.24	83.81	100.20
49	6R	173	PRO	CA-N-CD	-10.18	97.25	111.50
55	8A	210	LEU	CA-CB-CG	10.09	138.50	115.30
14	1N	71	MET	CG-SD-CE	10.06	116.29	100.20
3	5C	130	TYR	CZ-CE2-CD2	10.05	128.84	119.80
27	1b	77	LEU	CB-CG-CD2	-10.04	93.93	111.00
43	1r	110	PRO	CA-N-CD	-9.94	97.58	111.50
55	4A	97	MET	CG-SD-CE	-9.87	84.41	100.20
66	8L	44	LEU	CB-CG-CD1	-9.84	94.28	111.00
3	1C	207	PRO	CA-N-CD	-9.77	97.83	111.50
55	8A	427	PRO	CA-N-CD	-9.74	97.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	5i	27	LEU	CB-CG-CD2	-9.71	94.49	111.00
45	6N	338	LEU	CA-CB-CG	9.71	137.63	115.30
52	3H	77	GLU	C-N-CA	9.64	145.81	121.70
49	6R	173	PRO	CA-CB-CG	-9.52	85.91	104.00
55	4A	466	MET	CA-CB-CG	-9.51	97.13	113.30
8	1H	308	PRO	CA-N-CD	-9.40	98.34	111.50
14	5N	311	MET	CG-SD-CE	-9.39	85.18	100.20
13	1M	231	LEU	CA-CB-CG	9.36	136.83	115.30
47	6P	261	PRO	CA-N-CD	-9.35	98.41	111.50
10	1J	171	ILE	CG1-CB-CG2	-9.29	90.96	111.40
19	1S	90	LEU	CB-CG-CD2	-9.29	95.21	111.00
7	5G	384	PRO	CB-CG-CD	9.23	142.51	106.50
48	6D	249	MET	CB-CG-SD	-9.21	84.77	112.40
13	1M	325	MET	CA-CB-CG	9.18	128.91	113.30
48	6Q	216	LEU	CA-CB-CG	9.09	136.21	115.30
47	6P	237	LEU	CB-CG-CD2	9.07	126.41	111.00
4	1D	320	PRO	CA-N-CD	-9.03	98.86	111.50
56	4B	86	MET	CG-SD-CE	9.01	114.62	100.20
37	1l	93	PRO	CA-N-CD	-8.98	98.93	111.50
22	1W	104	MET	CG-SD-CE	8.96	114.54	100.20
14	1N	153	LEU	CA-CB-CG	8.96	135.91	115.30
47	6P	1	MET	CA-CB-CG	8.91	128.45	113.30
8	5H	225	MET	CG-SD-CE	8.79	114.27	100.20
56	8B	39	LEU	CA-CB-CG	8.74	135.40	115.30
47	6P	315	MET	CB-CG-SD	8.71	138.54	112.40
25	1Z	120	MET	CB-CG-SD	-8.71	86.28	112.40
13	1M	310	MET	CG-SD-CE	-8.67	86.33	100.20
24	1Y	126	MET	CA-CB-CG	-8.63	98.63	113.30
20	1T	75	GLU	OE1-CD-OE2	8.62	133.64	123.30
25	1Z	120	MET	CG-SD-CE	-8.60	86.45	100.20
42	5q	144	TYR	CE1-CZ-OH	-8.57	96.97	120.10
14	5N	261	MET	CB-CG-SD	-8.53	86.80	112.40
14	5N	258	SER	C-N-CA	-8.50	104.45	122.30
63	4I	63	MET	CG-SD-CE	-8.43	86.72	100.20
30	1e	14	ASP	CB-CG-OD1	8.40	125.86	118.30
47	3P	366	MET	CA-CB-CG	8.40	127.58	113.30
22	5W	82	LEU	CA-CB-CG	8.38	134.58	115.30
37	1l	14	PRO	CA-N-CD	-8.37	99.78	111.50
56	8B	29	MET	CG-SD-CE	8.37	113.60	100.20
63	8I	9	MET	CA-CB-CG	8.33	127.47	113.30
5	5E	66	MET	CB-CG-SD	-8.31	87.47	112.40
12	1L	571	MET	CG-SD-CE	-8.23	87.04	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1N	217	MET	CG-SD-CE	-8.23	87.03	100.20
58	8D	94	LEU	CA-CB-CG	8.20	134.16	115.30
56	4B	133	MET	CG-SD-CE	-8.18	87.12	100.20
57	4C	248	VAL	CG1-CB-CG2	-8.17	97.82	110.90
14	1N	72	MET	CA-CB-CG	-8.17	99.41	113.30
52	3H	62	LEU	CB-CG-CD1	-8.14	97.16	111.00
56	4B	33	LEU	CB-CG-CD2	8.14	124.85	111.00
12	5L	338	MET	CG-SD-CE	-8.14	87.18	100.20
7	5G	537	LEU	CA-CB-CG	8.13	133.99	115.30
7	5G	384	PRO	CA-N-CD	-8.11	100.14	111.50
47	3C	324	LEU	CB-CG-CD1	8.07	124.72	111.00
10	1J	54	LEU	CB-CG-CD1	-8.05	97.31	111.00
53	6J	26	LEU	CA-CB-CG	8.03	133.78	115.30
28	1c	8	PRO	CA-N-CD	-8.03	100.26	111.50
64	8J	47	LEU	CA-CB-CG	8.00	133.70	115.30
62	4H	81	PHE	CD1-CE1-CZ	7.99	129.69	120.10
8	1H	302	MET	CG-SD-CE	-7.99	87.42	100.20
7	1G	509	PRO	N-CD-CG	-7.93	91.31	103.20
57	8C	206	LEU	CA-CB-CG	7.93	133.53	115.30
44	1s	38	TYR	CZ-CE2-CD2	-7.91	112.68	119.80
42	1q	38	LEU	CB-CG-CD2	-7.83	97.68	111.00
47	3C	237	LEU	CA-CB-CG	7.83	133.31	115.30
7	5G	8	LEU	CA-CB-CG	7.82	133.30	115.30
13	5M	442	LEU	CA-CB-CG	7.82	133.28	115.30
48	3Q	211	MET	CA-CB-CG	7.80	126.56	113.30
5	5E	109	MET	CG-SD-CE	7.73	112.57	100.20
26	1a	16	LEU	CA-CB-CG	7.71	133.03	115.30
4	1D	251	LEU	CA-CB-CG	7.69	132.99	115.30
30	1e	18	THR	CA-CB-CG2	-7.69	101.64	112.40
47	6C	108	MET	CG-SD-CE	-7.64	87.97	100.20
59	8E	41	LEU	CB-CG-CD1	-7.63	98.03	111.00
8	1H	271	LEU	CB-CG-CD2	-7.62	98.05	111.00
47	6C	36	LEU	CB-CG-CD2	7.62	123.94	111.00
7	1G	663	PRO	CA-N-CD	-7.61	100.84	111.50
55	8A	189	LEU	CA-CB-CG	7.61	132.80	115.30
48	6Q	211	MET	CA-CB-CG	7.61	126.23	113.30
7	5G	98	LEU	CA-CB-CG	7.60	132.78	115.30
8	5H	302	MET	CG-SD-CE	-7.60	88.05	100.20
1	5A	98	LEU	CA-CB-CG	7.59	132.77	115.30
54	6Y	23	MET	CG-SD-CE	-7.59	88.05	100.20
53	3W	9	LEU	CA-CB-CG	7.51	132.58	115.30
55	8A	20	LEU	CA-CB-CG	7.50	132.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5M	33	LEU	CA-CB-CG	7.50	132.55	115.30
47	6C	138	MET	CG-SD-CE	-7.47	88.25	100.20
17	5Q	30	ILE	CG1-CB-CG2	-7.46	94.99	111.40
55	4A	433	LEU	CA-CB-CG	7.45	132.43	115.30
48	3D	304	LEU	CA-CB-CG	7.44	132.42	115.30
12	1L	499	MET	CA-CB-CG	7.44	125.94	113.30
34	5i	27	LEU	CB-CG-CD1	-7.43	98.37	111.00
59	8E	26	ALA	CB-CA-C	7.43	121.24	110.10
37	1l	101	MET	CG-SD-CE	-7.42	88.32	100.20
47	3C	327	MET	CB-CG-SD	7.42	134.66	112.40
7	5G	359	ARG	CD-NE-CZ	-7.42	113.22	123.60
13	5M	32	LEU	CB-CG-CD1	7.41	123.59	111.00
13	5M	231	LEU	CA-CB-CG	7.39	132.31	115.30
50	6S	70	MET	CG-SD-CE	-7.36	88.42	100.20
7	5G	122	MET	CA-CB-CG	-7.36	100.79	113.30
17	5Q	132	THR	CA-CB-CG2	-7.36	102.10	112.40
56	8B	45	MET	CG-SD-CE	-7.31	88.50	100.20
46	6B	59	ASP	CB-CG-OD1	-7.31	111.72	118.30
11	1K	36	MET	CA-CB-CG	7.30	125.71	113.30
52	3H	41	PRO	N-CD-CG	-7.30	92.25	103.20
43	5r	25	LEU	CB-CG-CD2	7.28	123.38	111.00
12	5L	88	MET	CB-CG-SD	7.27	134.21	112.40
59	8E	29	LEU	CA-CB-CG	7.26	132.00	115.30
19	5S	13	LEU	CA-CB-CG	7.23	131.94	115.30
50	3S	94	LEU	CA-CB-CG	7.22	131.90	115.30
42	5q	144	TYR	OH-CZ-CE2	7.18	139.48	120.10
67	4M	19	LEU	CA-CB-CG	7.17	131.80	115.30
9	1I	38	LEU	CA-CB-CG	7.17	131.79	115.30
55	4A	398	PRO	CA-N-CD	-7.16	101.47	111.50
15	1O	105	LEU	CA-CB-CG	7.15	131.74	115.30
14	5N	21	MET	CA-CB-CG	7.14	125.44	113.30
4	5D	242	ILE	C-N-CA	-7.14	107.31	122.30
20	1U	63	PRO	CA-CB-CG	-7.12	90.47	104.00
47	3C	327	MET	CA-CB-CG	7.12	125.40	113.30
12	5L	94	LEU	CB-CG-CD2	-7.12	98.91	111.00
8	1H	181	LEU	CB-CG-CD2	-7.11	98.92	111.00
25	5Z	106	VAL	CG1-CB-CG2	-7.11	99.53	110.90
29	5d	73	TYR	CD1-CE1-CZ	7.10	126.19	119.80
24	1Y	126	MET	CG-SD-CE	-7.10	88.84	100.20
46	3B	185	LYS	CD-CE-NZ	7.09	128.00	111.70
7	1G	181	MET	CA-CB-CG	7.09	125.35	113.30
33	1h	141	PRO	CA-N-CD	-7.08	101.59	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3E	116	LEU	CA-CB-CG	7.08	131.57	115.30
37	1I	102	CYS	CA-CB-SG	7.07	126.73	114.00
47	6P	198	LEU	CA-CB-CG	7.06	131.54	115.30
58	4D	86	LEU	CA-CB-CG	7.06	131.53	115.30
6	5F	418	LEU	CB-CG-CD2	7.04	122.97	111.00
49	6R	116	LEU	CA-CB-CG	7.03	131.47	115.30
52	3H	39	VAL	C-N-CA	7.02	139.25	121.70
66	4L	25	MET	CG-SD-CE	7.01	111.42	100.20
10	5J	98	MET	CA-CB-CG	6.99	125.19	113.30
20	1U	63	PRO	CA-N-CD	-6.99	101.71	111.50
21	1V	57	MET	CG-SD-CE	-6.96	89.06	100.20
24	5Y	119	LEU	CA-CB-CG	6.96	131.30	115.30
4	1D	177	MET	CG-SD-CE	6.95	111.32	100.20
67	8M	33	VAL	CG1-CB-CG2	-6.95	99.78	110.90
14	1N	243	LEU	CB-CG-CD1	-6.94	99.20	111.00
12	5L	570	GLN	C-N-CA	-6.93	104.39	121.70
4	5D	64	LEU	CA-CB-CG	6.91	131.18	115.30
14	1N	9	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	5A	20	ILE	CG1-CB-CG2	-6.90	96.21	111.40
56	8B	179	LEU	CA-CB-CG	6.90	131.17	115.30
27	5b	31	LEU	CA-CB-CG	6.88	131.14	115.30
12	1L	482	MET	CG-SD-CE	-6.88	89.19	100.20
56	8B	20	LEU	CA-CB-CG	6.88	131.11	115.30
49	3I	35	PRO	CA-N-CD	6.87	121.32	111.70
2	5B	163	LEU	CB-CG-CD2	6.87	122.67	111.00
50	6S	63	LYS	CA-CB-CG	6.85	128.48	113.40
64	4J	47	LEU	CA-CB-CG	6.85	131.04	115.30
24	5Y	33	LEU	CA-CB-CG	6.85	131.04	115.30
14	5N	251	MET	CG-SD-CE	6.84	111.14	100.20
4	5D	405	MET	CG-SD-CE	6.83	111.13	100.20
47	6P	230	LEU	CA-CB-CG	6.82	130.99	115.30
52	6U	15	ASP	CB-CG-OD1	6.81	124.43	118.30
29	5d	77	LYS	CD-CE-NZ	6.80	127.34	111.70
64	8J	50	LEU	CA-CB-CG	6.79	130.91	115.30
45	3A	290	MET	CG-SD-CE	6.77	111.03	100.20
41	5p	19	PRO	CA-N-CD	-6.76	102.03	111.50
2	1B	150	PRO	CA-N-CD	-6.76	102.04	111.50
45	3A	290	MET	CA-CB-CG	6.75	124.77	113.30
11	1K	75	LEU	CA-CB-CG	6.74	130.81	115.30
49	6E	149	MET	CG-SD-CE	6.74	110.98	100.20
53	6W	36	ASP	CB-CG-OD1	-6.74	112.23	118.30
34	5i	23	LYS	CD-CE-NZ	-6.74	96.20	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1N	72	MET	CG-SD-CE	-6.71	89.47	100.20
13	5M	195	MET	CA-CB-CG	6.71	124.70	113.30
13	1M	208	PRO	CA-N-CD	-6.70	102.11	111.50
47	6C	23	ALA	O-C-N	-6.67	108.42	121.10
46	3O	160	LEU	CB-CG-CD1	-6.66	99.68	111.00
13	5M	354	LEU	CD1-CG-CD2	-6.64	90.58	110.50
14	1N	45	MET	CA-CB-CG	6.64	124.58	113.30
5	1E	217	LEU	CB-CG-CD1	-6.62	99.75	111.00
8	1H	98	MET	CB-CG-SD	-6.61	92.57	112.40
21	1V	87	LEU	CA-CB-CG	6.61	130.50	115.30
14	5N	79	LEU	CA-CB-CG	6.58	130.45	115.30
37	5I	138	LEU	CA-CB-CG	6.57	130.42	115.30
48	6D	307	LEU	CB-CG-CD2	6.57	122.17	111.00
64	8J	39	CYS	N-CA-CB	-6.56	98.78	110.60
32	5g	58	MET	CB-CG-SD	6.54	132.03	112.40
2	5B	149	CYS	CA-CB-SG	-6.54	102.22	114.00
18	5R	30	ASP	CB-CG-OD1	6.54	124.18	118.30
7	1G	54	MET	CG-SD-CE	-6.54	89.74	100.20
55	4A	28	MET	CG-SD-CE	-6.53	89.75	100.20
66	8L	22	LEU	CB-CG-CD2	6.53	122.10	111.00
19	5S	64	LEU	CA-CB-CG	6.51	130.27	115.30
46	3O	163	LEU	CA-CB-CG	6.50	130.25	115.30
37	5I	115	MET	CG-SD-CE	-6.50	89.80	100.20
56	8B	37	LEU	CA-CB-CG	6.50	130.24	115.30
48	6Q	223	LYS	CG-CD-CE	-6.49	92.43	111.90
34	1i	22	LEU	CA-CB-CG	6.48	130.21	115.30
13	1M	371	PRO	CA-N-CD	-6.48	102.43	111.50
8	1H	89	LEU	CB-CG-CD1	-6.47	99.99	111.00
8	5H	222	MET	CG-SD-CE	-6.47	89.84	100.20
67	4M	24	LEU	CA-CB-CG	6.46	130.16	115.30
14	1N	200	MET	CG-SD-CE	-6.45	89.89	100.20
66	8L	21	LEU	CD1-CG-CD2	-6.44	91.19	110.50
47	6P	24	PRO	C-N-CA	-6.41	105.67	121.70
48	6D	297	MET	CG-SD-CE	6.40	110.45	100.20
10	1J	65	LEU	CA-CB-CG	6.40	130.03	115.30
45	3A	338	LEU	CB-CG-CD1	-6.39	100.13	111.00
12	1L	169	LEU	CA-CB-CG	6.39	130.00	115.30
52	3H	41	PRO	N-CA-CB	-6.38	95.58	102.60
62	4H	27	ARG	CG-CD-NE	-6.38	98.40	111.80
1	5A	7	LEU	CA-CB-CG	6.37	129.96	115.30
5	1E	191	PHE	CB-CG-CD2	-6.37	116.34	120.80
14	5N	89	MET	CG-SD-CE	-6.37	90.01	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1N	304	MET	CG-SD-CE	6.37	110.39	100.20
48	6Q	212	MET	CA-CB-CG	-6.37	102.48	113.30
6	5F	350	LEU	CA-CB-CG	6.35	129.91	115.30
53	3J	33	LEU	CA-CB-CG	6.35	129.91	115.30
52	3H	62	LEU	CA-CB-CG	6.35	129.90	115.30
60	4F	22	MET	CA-CB-CG	6.34	124.08	113.30
19	5S	13	LEU	CB-CG-CD1	-6.34	100.23	111.00
46	6B	59	ASP	CB-CG-OD2	6.34	124.00	118.30
4	1D	304	MET	CG-SD-CE	6.33	110.34	100.20
66	8L	44	LEU	CA-CB-CG	6.33	129.85	115.30
9	1I	57	LEU	CA-CB-CG	6.32	129.85	115.30
48	6D	268	MET	CG-SD-CE	-6.32	90.09	100.20
48	6D	175	LEU	CB-CG-CD1	-6.31	100.27	111.00
8	1H	98	MET	CG-SD-CE	6.30	110.28	100.20
11	1K	63	LEU	CA-CB-CG	6.30	129.79	115.30
35	5j	56	PRO	CA-N-CD	-6.30	102.68	111.50
39	5n	113	MET	CA-CB-CG	6.30	124.00	113.30
39	5n	162	LEU	CA-CB-CG	6.30	129.78	115.30
36	5k	42	ASP	CB-CG-OD1	6.29	123.96	118.30
52	3U	62	LEU	CB-CG-CD1	-6.29	100.31	111.00
15	5O	298	GLU	OE1-CD-OE2	-6.28	115.76	123.30
45	3N	441	MET	CA-CB-CG	6.26	123.95	113.30
61	8G	25	LEU	CB-CG-CD1	-6.26	100.36	111.00
28	1c	31	LEU	CA-CB-CG	6.25	129.69	115.30
63	8I	17	LEU	CA-CB-CG	6.25	129.68	115.30
8	1H	294	LEU	CA-CB-CG	6.25	129.67	115.30
52	3U	58	LEU	CA-CB-CG	6.24	129.66	115.30
3	5C	152	LEU	CB-CG-CD1	-6.23	100.41	111.00
25	1Z	51	MET	CA-CB-CG	6.23	123.89	113.30
59	4E	29	LEU	CA-CB-CG	6.22	129.60	115.30
24	1Y	119	LEU	CA-CB-CG	6.20	129.57	115.30
31	1f	34	LEU	CA-CB-CG	6.20	129.57	115.30
47	6P	315	MET	CG-SD-CE	6.20	110.12	100.20
4	1D	268	ASP	CB-CG-OD1	6.20	123.88	118.30
2	5B	163	LEU	CA-CB-CG	6.20	129.55	115.30
12	5L	573	MET	CB-CG-SD	6.18	130.95	112.40
8	1H	70	MET	CA-CB-CG	6.18	123.81	113.30
8	1H	286	MET	CB-CG-SD	6.17	130.92	112.40
12	5L	101	MET	CG-SD-CE	6.17	110.07	100.20
24	1Y	117	MET	CB-CG-SD	6.16	130.89	112.40
26	5a	66	LEU	CA-CB-CG	6.16	129.47	115.30
13	5M	78	MET	CG-SD-CE	6.16	110.05	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	8B	33	LEU	CA-CB-CG	6.16	129.46	115.30
12	1L	341	MET	CG-SD-CE	-6.15	90.36	100.20
24	5Y	123	LEU	CA-CB-CG	6.15	129.44	115.30
45	3A	441	MET	CG-SD-CE	-6.14	90.37	100.20
45	6N	365	LEU	CA-CB-CG	6.14	129.41	115.30
13	5M	398	MET	CA-CB-CG	6.12	123.71	113.30
45	6N	370	ASP	CB-CG-OD2	6.12	123.81	118.30
7	1G	509	PRO	CA-N-CD	-6.12	102.94	111.50
11	1K	38	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	1A	8	LEU	CA-CB-CG	6.10	129.34	115.30
51	3G	59	LEU	CA-CB-CG	6.10	129.33	115.30
15	5O	214	MET	CA-CB-CG	6.10	123.67	113.30
12	5L	577	VAL	CA-CB-CG2	-6.10	101.75	110.90
4	5D	229	LEU	CA-CB-CG	-6.09	101.28	115.30
33	5h	54	ASP	CB-CG-OD1	6.08	123.78	118.30
4	1D	251	LEU	CB-CG-CD1	6.07	121.32	111.00
8	1H	37	PRO	N-CD-CG	-6.06	94.11	103.20
9	1I	36	MET	CB-CG-SD	6.06	130.59	112.40
12	5L	240	PRO	N-CD-CG	-6.05	94.13	103.20
47	6C	198	LEU	CB-CG-CD2	6.05	121.29	111.00
36	5k	28	LEU	CB-CG-CD1	-6.04	100.73	111.00
40	1o	31	PRO	CA-N-CD	-6.04	103.05	111.50
58	4D	14	PRO	CA-N-CD	-6.04	103.05	111.50
14	1N	190	MET	CA-CB-CG	6.03	123.55	113.30
11	1K	33	LEU	CA-CB-CG	6.02	129.15	115.30
47	6P	197	LEU	CA-CB-CG	6.01	129.13	115.30
16	5P	327	LEU	CA-CB-CG	6.01	129.12	115.30
49	3I	35	PRO	N-CA-CB	-5.98	96.02	102.60
58	8D	62	LEU	CA-CB-CG	5.98	129.05	115.30
52	6U	18	THR	CA-CB-CG2	5.97	120.77	112.40
4	5D	66	MET	CA-CB-CG	5.97	123.45	113.30
13	5M	401	MET	CA-CB-CG	5.96	123.43	113.30
27	5b	27	LEU	CA-CB-CG	5.96	129.01	115.30
45	6A	415	PHE	CB-CG-CD2	-5.96	116.63	120.80
46	6O	395	PRO	CA-N-CD	-5.96	103.16	111.50
2	5B	96	MET	CB-CG-SD	-5.95	94.54	112.40
47	6P	237	LEU	CD1-CG-CD2	-5.95	92.64	110.50
66	8L	22	LEU	CB-CG-CD1	5.95	121.11	111.00
64	4J	38	LEU	CA-CB-CG	5.95	128.97	115.30
8	5H	285	LEU	CA-CB-CG	5.94	128.97	115.30
47	6P	1	MET	N-CA-C	-5.94	94.96	111.00
7	5G	257	ASP	CB-CG-OD1	5.94	123.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1r	63	MET	CA-CB-CG	5.93	123.39	113.30
48	3D	298	LEU	CA-CB-CG	5.93	128.95	115.30
12	1L	338	MET	CG-SD-CE	-5.92	90.72	100.20
58	8D	40	LEU	CB-CG-CD2	-5.92	100.93	111.00
12	1L	154	LEU	CB-CG-CD2	-5.90	100.98	111.00
42	5q	55	PHE	CD1-CE1-CZ	-5.89	113.03	120.10
57	4C	138	LEU	CA-CB-CG	5.88	128.83	115.30
48	6Q	211	MET	N-CA-CB	5.88	121.18	110.60
47	6P	1	MET	CB-CG-SD	-5.88	94.78	112.40
12	1L	48	LEU	CA-CB-CG	5.87	128.80	115.30
63	8I	63	MET	CG-SD-CE	5.86	109.57	100.20
24	1Y	126	MET	CB-CG-SD	-5.86	94.84	112.40
7	5G	97	LEU	CA-CB-CG	5.85	128.75	115.30
37	5l	113	LEU	CA-CB-CG	5.85	128.75	115.30
8	1H	104	PHE	CG-CD2-CE2	-5.85	114.37	120.80
6	5F	350	LEU	CB-CG-CD2	5.85	120.94	111.00
29	5d	62	LEU	CA-CB-CG	5.85	128.75	115.30
47	6C	192	LEU	CA-CB-CG	5.85	128.75	115.30
5	5E	92	ARG	CG-CD-NE	-5.84	99.54	111.80
58	4D	59	LEU	CA-CB-CG	5.83	128.72	115.30
48	6D	131	MET	CA-CB-CG	5.83	123.22	113.30
48	6Q	109	LEU	CA-CB-CG	5.83	128.71	115.30
20	1T	76	ILE	CG1-CB-CG2	5.83	124.23	111.40
4	1D	159	LEU	CA-CB-CG	5.83	128.70	115.30
61	8G	19	LEU	CA-CB-CG	5.82	128.69	115.30
19	5S	63	LYS	CB-CG-CD	5.82	126.73	111.60
47	3C	197	LEU	CA-CB-CG	5.82	128.68	115.30
12	5L	150	MET	CG-SD-CE	-5.81	90.90	100.20
47	6C	11	MET	CG-SD-CE	-5.81	90.90	100.20
68	8N	17	PRO	CA-N-CD	-5.81	103.36	111.50
52	6H	99	LEU	CA-CB-CG	5.80	128.65	115.30
56	8B	33	LEU	CB-CG-CD2	5.80	120.86	111.00
9	5I	38	LEU	CB-CG-CD2	-5.79	101.16	111.00
54	6X	13	LEU	CA-CB-CG	5.79	128.62	115.30
17	1Q	40	PRO	CA-N-CD	-5.78	103.40	111.50
46	3B	34	VAL	CG1-CB-CG2	-5.78	101.66	110.90
12	5L	229	LEU	CB-CG-CD1	-5.78	101.18	111.00
24	5Y	114	CYS	N-CA-CB	5.78	121.00	110.60
36	5k	50	TRP	CA-CB-CG	5.78	124.67	113.70
7	5G	359	ARG	CG-CD-NE	-5.77	99.68	111.80
42	5q	7	LEU	CA-CB-CG	5.76	128.55	115.30
54	6X	51	LYS	CD-CE-NZ	-5.76	98.46	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	4H	13	THR	CA-CB-CG2	-5.75	104.34	112.40
12	5L	129	MET	CG-SD-CE	5.75	109.40	100.20
13	5M	375	LEU	CB-CG-CD2	5.75	120.78	111.00
45	6N	431	LEU	CB-CG-CD2	5.75	120.77	111.00
12	1L	488	MET	CA-CB-CG	5.74	123.05	113.30
53	6W	36	ASP	CB-CG-OD2	5.73	123.46	118.30
47	6C	197	LEU	CA-CB-CG	5.72	128.46	115.30
31	1f	15	LEU	CA-CB-CG	5.72	128.45	115.30
45	6A	122	LEU	CA-CB-CG	5.72	128.46	115.30
15	1O	112	LEU	CA-CB-CG	5.71	128.44	115.30
2	1B	149	CYS	CA-CB-SG	5.71	124.27	114.00
52	3H	41	PRO	CA-CB-CG	-5.71	93.16	104.00
62	4H	81	PHE	CG-CD1-CE1	-5.71	114.52	120.80
8	1H	308	PRO	N-CA-CB	-5.71	96.32	102.60
55	8A	35	LEU	CA-CB-CG	5.70	128.42	115.30
38	1m	5	TYR	C-N-CA	-5.70	107.46	121.70
52	6U	39	LEU	CA-CB-CG	5.70	128.40	115.30
53	3J	26	LEU	CA-CB-CG	5.69	128.38	115.30
26	1a	1	MET	CB-CG-SD	5.69	129.46	112.40
62	4H	81	PHE	CB-CG-CD1	-5.69	116.82	120.80
54	3Y	48	ILE	CG1-CB-CG2	-5.68	98.89	111.40
37	1l	115	MET	CA-CB-CG	5.68	122.96	113.30
24	1Y	71	LEU	CA-CB-CG	5.68	128.36	115.30
47	3C	294	LEU	CA-CB-CG	5.68	128.36	115.30
38	5m	36	LEU	CB-CG-CD2	5.68	120.65	111.00
8	5H	53	LEU	CA-CB-CG	5.67	128.35	115.30
6	5F	337	MET	CA-CB-CG	5.67	122.94	113.30
7	1G	251	LEU	CA-CB-CG	5.66	128.32	115.30
47	6P	102	LEU	CA-CB-CG	5.66	128.32	115.30
16	1P	222	ASP	CB-CG-OD1	5.66	123.39	118.30
5	1E	164	LEU	CB-CG-CD2	-5.65	101.40	111.00
12	1L	592	LEU	CA-CB-CG	5.65	128.29	115.30
53	6W	22	LEU	CA-CB-CG	5.64	128.26	115.30
64	4J	50	LEU	CA-CB-CG	5.63	128.26	115.30
2	1B	161	LEU	CB-CG-CD2	5.63	120.57	111.00
67	8M	19	LEU	CA-CB-CG	5.63	128.24	115.30
53	6J	33	LEU	CA-CB-CG	5.62	128.22	115.30
43	1r	25	LEU	CB-CG-CD1	-5.61	101.46	111.00
46	3O	222	ARG	C-N-CA	-5.61	107.66	121.70
7	1G	94	MET	CA-CB-CG	5.61	122.84	113.30
55	4A	234	LEU	CA-CB-CG	5.60	128.18	115.30
14	1N	217	MET	CB-CG-SD	-5.60	95.61	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1K	10	MET	CG-SD-CE	-5.59	91.26	100.20
53	6W	13	LEU	CA-CB-CG	5.59	128.15	115.30
35	1j	32	MET	CA-CB-CG	5.58	122.79	113.30
12	5L	229	LEU	CA-CB-CG	5.58	128.14	115.30
48	6D	324	LEU	CA-CB-CG	5.58	128.14	115.30
47	6P	129	MET	CB-CG-SD	-5.58	95.67	112.40
45	6N	370	ASP	CB-CG-OD1	-5.57	113.28	118.30
61	4G	30	LEU	CA-CB-CG	5.57	128.11	115.30
16	5P	41	MET	CA-CB-CG	5.57	122.77	113.30
50	6F	82	MET	CB-CG-SD	-5.57	95.70	112.40
47	6P	216	ASP	CB-CG-OD1	5.57	123.31	118.30
51	3T	10	MET	CG-SD-CE	-5.56	91.31	100.20
50	3S	50	LEU	CA-CB-CG	5.56	128.08	115.30
8	1H	81	LEU	CA-CB-CG	5.55	128.08	115.30
50	6F	78	LEU	CA-CB-CG	5.55	128.06	115.30
45	3N	219	LEU	CA-CB-CG	-5.54	102.55	115.30
47	3P	124	MET	CA-CB-CG	5.54	122.73	113.30
47	6P	215	MET	N-CA-CB	-5.53	100.64	110.60
30	5e	60	ASP	CB-CG-OD1	-5.51	113.34	118.30
59	4E	22	PRO	CA-N-CD	-5.51	103.79	111.50
50	6F	53	ASP	CB-CG-OD1	5.51	123.26	118.30
5	1E	205	PRO	CA-N-CD	-5.50	103.79	111.50
30	1e	39	TRP	CA-CB-CG	-5.50	103.25	113.70
18	1R	27	ARG	CG-CD-NE	-5.50	100.26	111.80
55	4A	71	MET	CB-CG-SD	5.50	128.89	112.40
20	1T	75	GLU	CG-CD-OE1	-5.49	107.31	118.30
52	3U	39	LEU	CA-CB-CG	5.49	127.94	115.30
56	4B	21	LEU	CA-CB-CG	5.49	127.93	115.30
53	3W	22	LEU	CA-CB-CG	5.49	127.93	115.30
60	4F	69	VAL	CA-CB-CG1	-5.49	102.66	110.90
7	1G	192	MET	CG-SD-CE	5.49	108.98	100.20
34	1i	22	LEU	CB-CG-CD2	5.48	120.32	111.00
12	5L	380	LEU	CA-CB-CG	5.48	127.90	115.30
8	1H	288	LEU	CA-CB-CG	5.47	127.89	115.30
14	5N	251	MET	CA-CB-CG	5.47	122.61	113.30
52	6U	66	ASP	CB-CG-OD2	5.47	123.23	118.30
52	3H	79	ASP	CB-CG-OD1	5.47	123.22	118.30
64	8J	31	LEU	CA-CB-CG	5.46	127.87	115.30
9	1I	174	LEU	CA-CB-CG	5.46	127.86	115.30
14	1N	14	MET	CA-CB-CG	5.46	122.58	113.30
50	3F	82	MET	CG-SD-CE	-5.45	91.48	100.20
55	4A	312	ILE	CG1-CB-CG2	-5.45	99.42	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1H	46	LEU	CA-CB-CG	5.44	127.82	115.30
9	1I	148	LEU	CA-CB-CG	5.44	127.82	115.30
47	6P	327	MET	CA-CB-CG	5.43	122.52	113.30
57	8C	138	LEU	CA-CB-CG	5.43	127.78	115.30
8	1H	264	LEU	CB-CG-CD1	-5.42	101.78	111.00
47	3P	236	MET	CA-CB-CG	5.42	122.52	113.30
28	5c	27	LEU	CA-CB-CG	5.42	127.77	115.30
58	4D	123	MET	CG-SD-CE	5.42	108.87	100.20
2	1B	33	LEU	CB-CG-CD2	5.42	120.21	111.00
8	5H	105	MET	CB-CG-SD	5.42	128.65	112.40
2	5B	62	MET	CG-SD-CE	-5.42	91.54	100.20
7	5G	71	MET	CA-CB-CG	-5.42	104.09	113.30
47	3P	197	LEU	CA-CB-CG	5.41	127.75	115.30
8	5H	289	LEU	CB-CG-CD2	5.41	120.20	111.00
24	5Y	5	LEU	CA-CB-CG	5.41	127.74	115.30
10	5J	161	LEU	CA-CB-CG	5.41	127.73	115.30
6	1F	390	ASP	CB-CG-OD1	5.40	123.16	118.30
58	8D	44	GLU	CG-CD-OE2	-5.39	107.51	118.30
1	5A	66	ASP	CB-CG-OD1	5.39	123.15	118.30
13	5M	436	LEU	CA-CB-CG	5.39	127.70	115.30
14	5N	71	MET	CG-SD-CE	5.39	108.83	100.20
22	5W	90	LEU	CD1-CG-CD2	-5.39	94.33	110.50
50	6S	70	MET	CB-CG-SD	-5.39	96.23	112.40
8	1H	174	MET	CB-CG-SD	-5.39	96.24	112.40
54	6X	37	ASP	CB-CG-OD1	5.39	123.15	118.30
59	8E	25	ASP	CB-CG-OD1	5.37	123.14	118.30
54	6Y	32	LEU	CA-CB-CG	5.36	127.63	115.30
8	5H	174	MET	CB-CG-SD	-5.36	96.33	112.40
24	5Y	94	CYS	N-CA-CB	5.35	120.23	110.60
58	8D	59	LEU	CA-CB-CG	5.35	127.60	115.30
57	4C	252	LEU	CA-CB-CG	5.34	127.59	115.30
59	4E	101	PRO	CA-N-CD	-5.34	104.02	111.50
19	5S	55	ARG	C-N-CA	5.34	135.05	121.70
28	5c	31	LEU	CA-CB-CG	5.33	127.57	115.30
32	5g	96	LEU	CA-CB-CG	5.33	127.56	115.30
40	5o	98	MET	CA-CB-CG	5.33	122.36	113.30
3	5C	64	LEU	CA-CB-CG	5.33	127.56	115.30
66	8L	21	LEU	CB-CG-CD2	5.33	120.05	111.00
12	5L	179	ASP	CB-CG-OD1	-5.32	113.51	118.30
14	5N	313	MET	CA-CB-CG	5.32	122.33	113.30
58	8D	51	LEU	CD1-CG-CD2	-5.32	94.55	110.50
59	4E	21	LYS	CA-CB-CG	5.31	125.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1I	26	LEU	CA-CB-CG	5.30	127.50	115.30
45	3A	338	LEU	CA-CB-CG	5.30	127.50	115.30
50	3F	106	LEU	CA-CB-CG	5.30	127.49	115.30
58	4D	59	LEU	CB-CG-CD2	5.30	120.01	111.00
49	6E	149	MET	CA-CB-CG	5.29	122.30	113.30
55	8A	302	ARG	CD-NE-CZ	-5.29	116.19	123.60
2	5B	96	MET	CG-SD-CE	-5.29	91.73	100.20
50	6F	78	LEU	CB-CG-CD1	-5.29	102.01	111.00
12	1L	7	LEU	CA-CB-CG	5.29	127.46	115.30
8	5H	7	LEU	CA-CB-CG	5.29	127.46	115.30
12	5L	153	LEU	CA-CB-CG	5.28	127.45	115.30
2	5B	45	LEU	CA-CB-CG	5.27	127.42	115.30
43	5r	25	LEU	CA-CB-CG	5.27	127.41	115.30
10	5J	169	MET	CG-SD-CE	5.26	108.62	100.20
52	6H	64	LEU	CA-CB-CG	5.26	127.39	115.30
42	5q	55	PHE	CZ-CE2-CD2	-5.26	113.79	120.10
55	4A	194	LEU	CA-CB-CG	5.24	127.36	115.30
20	1U	16	LEU	CA-CB-CG	5.24	127.35	115.30
56	4B	73	LEU	CA-CB-CG	5.24	127.34	115.30
5	1E	52	ASP	CB-CG-OD1	5.23	123.01	118.30
46	6O	147	ASP	CB-CG-OD1	5.23	123.01	118.30
16	5P	258	LEU	CA-CB-CG	5.23	127.33	115.30
42	1q	133	LYS	CD-CE-NZ	5.22	123.72	111.70
39	5n	117	TYR	CA-CB-CG	5.22	123.33	113.40
8	1H	289	LEU	CB-CG-CD1	-5.22	102.12	111.00
52	3H	41	PRO	CB-CG-CD	-5.22	86.14	106.50
19	5S	55	ARG	NE-CZ-NH1	5.22	122.91	120.30
55	4A	209	LEU	CA-CB-CG	5.21	127.30	115.30
67	8M	37	LEU	CB-CG-CD2	5.21	119.86	111.00
22	1W	88	MET	CG-SD-CE	-5.21	91.87	100.20
50	3F	80	LEU	CA-CB-CG	5.21	127.27	115.30
64	8J	38	LEU	CA-CB-CG	5.20	127.27	115.30
39	1n	43	MET	CG-SD-CE	5.20	108.52	100.20
33	1h	24	LEU	CA-CB-CG	5.20	127.26	115.30
9	5I	148	LEU	CA-CB-CG	5.20	127.26	115.30
9	1I	81	LYS	CD-CE-NZ	5.20	123.65	111.70
59	4E	66	ARG	CG-CD-NE	-5.19	100.90	111.80
55	4A	209	LEU	CB-CG-CD1	5.18	119.81	111.00
42	5q	55	PHE	CB-CA-C	-5.18	100.04	110.40
8	5H	107	ALA	CB-CA-C	5.18	117.87	110.10
51	6G	9	LEU	CB-CG-CD2	-5.17	102.21	111.00
4	1D	83	LEU	CA-CB-CG	5.17	127.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5L	530	PRO	CA-N-CD	-5.17	104.27	111.50
22	5W	90	LEU	CB-CG-CD2	-5.16	102.23	111.00
14	1N	278	MET	CA-CB-CG	5.16	122.07	113.30
13	5M	379	LEU	CA-CB-CG	5.15	127.16	115.30
45	6N	122	LEU	CA-CB-CG	5.15	127.15	115.30
40	1o	66	LEU	CA-CB-CG	5.14	127.13	115.30
47	6P	36	LEU	CB-CG-CD2	5.14	119.74	111.00
12	5L	314	MET	CG-SD-CE	-5.14	91.97	100.20
4	1D	228	MET	CG-SD-CE	-5.14	91.98	100.20
47	3C	327	MET	N-CA-CB	5.13	119.84	110.60
12	5L	366	MET	CB-CG-SD	5.13	127.79	112.40
47	6P	226	ILE	CG1-CB-CG2	-5.12	100.13	111.40
50	6S	67	ASP	CB-CG-OD1	5.12	122.91	118.30
2	5B	36	LEU	CB-CG-CD2	5.12	119.70	111.00
11	1K	73	LEU	CA-CB-CG	-5.11	103.54	115.30
14	5N	70	LEU	CA-CB-CG	5.11	127.05	115.30
33	5h	81	ASP	CB-CG-OD1	5.11	122.90	118.30
14	5N	159	MET	CA-CB-CG	5.11	121.98	113.30
45	6N	335	MET	CA-CB-CG	5.11	121.98	113.30
9	1I	7	MET	CG-SD-CE	-5.10	92.04	100.20
14	5N	130	LEU	CB-CG-CD2	5.10	119.67	111.00
28	5c	19	LEU	CA-CB-CG	5.09	127.00	115.30
56	4B	128	LEU	CB-CG-CD2	-5.08	102.36	111.00
12	1L	599	MET	CA-CB-CG	5.08	121.94	113.30
30	1e	66	LEU	CA-CB-CG	5.08	126.98	115.30
67	4M	27	LEU	CA-CB-CG	5.08	126.98	115.30
10	5J	103	MET	CA-CB-CG	5.08	121.93	113.30
1	5A	13	LEU	CA-CB-CG	5.08	126.97	115.30
10	1J	103	MET	CA-CB-CG	5.07	121.93	113.30
14	1N	79	LEU	CA-CB-CG	5.07	126.96	115.30
2	5B	36	LEU	CA-CB-CG	5.07	126.96	115.30
50	6F	50	TYR	CA-CB-CG	-5.07	103.77	113.40
50	6S	45	GLU	CA-CB-CG	5.07	124.55	113.40
20	5T	51	ILE	C-N-CA	-5.06	109.04	121.70
25	1Z	71	LEU	CB-CG-CD2	5.06	119.60	111.00
2	5B	157	LEU	CB-CG-CD2	-5.06	102.40	111.00
4	1D	342	MET	CA-CB-CG	5.06	121.90	113.30
62	8H	35	ASP	CB-CG-OD1	5.05	122.85	118.30
46	6O	87	ARG	CA-CB-CG	5.05	124.51	113.40
7	1G	663	PRO	N-CD-CG	-5.04	95.64	103.20
34	1i	9	LEU	CA-CB-CG	5.03	126.87	115.30
12	5L	94	LEU	CA-CB-CG	5.03	126.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5h	25	MET	CA-CB-CG	5.03	121.85	113.30
47	3C	93	CYS	CA-CB-SG	-5.03	104.95	114.00
50	3S	90	LEU	CA-CB-CG	5.03	126.86	115.30
12	5L	216	LEU	CA-CB-CG	5.02	126.85	115.30
43	1r	63	MET	CG-SD-CE	5.02	108.23	100.20
48	3Q	5	LEU	CB-CG-CD2	-5.02	102.47	111.00
58	4D	19	ARG	NE-CZ-NH2	-5.02	117.79	120.30
8	5H	150	LEU	CA-CB-CG	5.01	126.83	115.30
34	5i	27	LEU	CD1-CG-CD2	5.01	125.53	110.50
66	8L	21	LEU	CB-CG-CD1	-5.00	102.50	111.00

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	71	ARG	Sidechain
2	1B	93	THR	Peptide
3	1C	106	ARG	Sidechain
5	1E	191	PHE	Sidechain
6	1F	206	LYS	Peptide
8	1H	171	HIS	Sidechain
8	1H	91	MET	Peptide
10	1J	126	VAL	Peptide
12	1L	61	MET	Peptide
16	1P	179	LEU	Peptide
24	1Y	139	LYS	Peptide
26	1a	16	LEU	Peptide
33	1h	69	HIS	Peptide
39	1n	55	ASP	Peptide
45	3N	226	ASP	Peptide
59	4E	14	ARG	Sidechain
68	4N	48	LYS	Peptide
6	5F	206	LYS	Peptide
7	5G	359	ARG	Sidechain
8	5H	91	MET	Peptide
11	5K	2	PRO	Peptide
12	5L	176	ARG	Sidechain
13	5M	336	ARG	Sidechain
18	5R	31	ARG	Sidechain
23	5X	100	ARG	Sidechain
25	5Z	23	ARG	Sidechain
38	5m	35	ARG	Sidechain

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Mol	Chain	Res	Type	Group
43	5r	24	GLN	Peptide
45	6A	415	PHE	Sidechain
47	6C	24	PRO	Mainchain
47	6C	80	ARG	Sidechain
48	6D	323	LYS	Peptide
49	6E	219	HIS	Sidechain
52	6H	98	LYS	Peptide
45	6N	301	ARG	Sidechain
59	8E	56	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	100 (88%)	11 (10%)	2 (2%)	8	40
1	5A	113/115 (98%)	106 (94%)	5 (4%)	2 (2%)	8	40
2	1B	153/258 (59%)	140 (92%)	13 (8%)	0	100	100
2	5B	153/258 (59%)	141 (92%)	12 (8%)	0	100	100
3	1C	207/264 (78%)	187 (90%)	20 (10%)	0	100	100
3	5C	207/264 (78%)	197 (95%)	10 (5%)	0	100	100
4	1D	427/476 (90%)	398 (93%)	29 (7%)	0	100	100
4	5D	427/476 (90%)	400 (94%)	27 (6%)	0	100	100
5	1E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	29	69
5	5E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	29	69
6	1F	430/464 (93%)	401 (93%)	26 (6%)	3 (1%)	22	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5F	430/464 (93%)	404 (94%)	23 (5%)	3 (1%)	22	63
7	1G	697/727 (96%)	657 (94%)	38 (6%)	2 (0%)	41	76
7	5G	697/727 (96%)	661 (95%)	34 (5%)	2 (0%)	41	76
8	1H	316/318 (99%)	289 (92%)	25 (8%)	2 (1%)	25	66
8	5H	316/318 (99%)	290 (92%)	24 (8%)	2 (1%)	25	66
9	1I	174/239 (73%)	163 (94%)	11 (6%)	0	100	100
9	5I	174/239 (73%)	164 (94%)	10 (6%)	0	100	100
10	1J	172/175 (98%)	159 (92%)	12 (7%)	1 (1%)	25	66
10	5J	172/175 (98%)	155 (90%)	16 (9%)	1 (1%)	25	66
11	1K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
11	5K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	545 (90%)	57 (9%)	2 (0%)	41	76
12	5L	604/606 (100%)	559 (92%)	44 (7%)	1 (0%)	47	81
13	1M	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
13	5M	457/459 (100%)	436 (95%)	21 (5%)	0	100	100
14	1N	345/347 (99%)	322 (93%)	21 (6%)	2 (1%)	25	66
14	5N	345/347 (99%)	315 (91%)	30 (9%)	0	100	100
15	1O	318/357 (89%)	301 (95%)	17 (5%)	0	100	100
15	5O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	321 (94%)	19 (6%)	0	100	100
16	5P	340/377 (90%)	317 (93%)	22 (6%)	1 (0%)	41	76
17	1Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
17	5Q	127/175 (73%)	116 (91%)	11 (9%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
18	5R	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
19	1S	85/99 (86%)	76 (89%)	9 (11%)	0	100	100
19	5S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	1T	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
20	1U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
20	5T	83/156 (53%)	78 (94%)	5 (6%)	0	100	100
20	5U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1V	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
21	5V	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
22	5W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	66
23	5X	169/172 (98%)	160 (95%)	8 (5%)	1 (1%)	25	66
24	1Y	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
24	5Y	137/141 (97%)	130 (95%)	7 (5%)	0	100	100
25	1Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
25	5Z	139/144 (96%)	131 (94%)	8 (6%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
26	5a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
27	5b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
28	5c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	1d	117/122 (96%)	111 (95%)	6 (5%)	0	100	100
29	5d	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
30	5e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
31	5f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	84 (86%)	14 (14%)	0	100	100
32	5g	98/154 (64%)	86 (88%)	12 (12%)	0	100	100
33	1h	136/189 (72%)	127 (93%)	9 (7%)	0	100	100
33	5h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	1i	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	19	60
34	5i	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	64 (93%)	5 (7%)	0	100	100
35	5j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	139 (90%)	15 (10%)	0	100	100
37	5l	154/186 (83%)	138 (90%)	16 (10%)	0	100	100
38	1m	126/129 (98%)	118 (94%)	8 (6%)	0	100	100
38	5m	126/129 (98%)	116 (92%)	10 (8%)	0	100	100
39	1n	170/179 (95%)	160 (94%)	10 (6%)	0	100	100
39	5n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	25	66
40	1o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
40	5o	120/137 (88%)	110 (92%)	10 (8%)	0	100	100
41	1p	171/176 (97%)	169 (99%)	2 (1%)	0	100	100
41	5p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
42	5q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
43	1r	90/113 (80%)	83 (92%)	7 (8%)	0	100	100
43	5r	90/113 (80%)	84 (93%)	6 (7%)	0	100	100
44	1s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
44	5s	43/471 (9%)	40 (93%)	3 (7%)	0	100	100
45	3A	436/480 (91%)	424 (97%)	11 (2%)	1 (0%)	47	81
45	3N	444/480 (92%)	424 (96%)	18 (4%)	2 (0%)	29	69
45	6A	436/480 (91%)	426 (98%)	8 (2%)	2 (0%)	29	69
45	6N	444/480 (92%)	430 (97%)	12 (3%)	2 (0%)	29	69
46	3B	414/453 (91%)	396 (96%)	18 (4%)	0	100	100
46	3O	413/453 (91%)	404 (98%)	8 (2%)	1 (0%)	47	81
46	6B	414/453 (91%)	401 (97%)	13 (3%)	0	100	100
46	6O	413/453 (91%)	403 (98%)	9 (2%)	1 (0%)	47	81
47	3C	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
47	3P	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
47	6C	377/379 (100%)	355 (94%)	22 (6%)	0	100	100
47	6P	377/379 (100%)	364 (97%)	13 (3%)	0	100	100
48	3D	235/326 (72%)	227 (97%)	8 (3%)	0	100	100
48	3Q	237/326 (73%)	230 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	6D	235/326 (72%)	226 (96%)	9 (4%)	0	100	100
48	6Q	237/326 (73%)	225 (95%)	12 (5%)	0	100	100
49	3E	194/274 (71%)	170 (88%)	22 (11%)	2 (1%)	15	54
49	3I	45/274 (16%)	42 (93%)	3 (7%)	0	100	100
49	3R	194/274 (71%)	170 (88%)	20 (10%)	4 (2%)	7	36
49	3V	29/274 (11%)	29 (100%)	0	0	100	100
49	6E	194/274 (71%)	175 (90%)	18 (9%)	1 (0%)	29	69
49	6I	45/274 (16%)	42 (93%)	3 (7%)	0	100	100
49	6R	194/274 (71%)	172 (89%)	18 (9%)	4 (2%)	7	36
49	6V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	96 (100%)	0	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	6F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	6S	96/111 (86%)	94 (98%)	2 (2%)	0	100	100
51	3G	72/82 (88%)	66 (92%)	6 (8%)	0	100	100
51	3T	72/82 (88%)	69 (96%)	3 (4%)	0	100	100
51	6G	72/82 (88%)	68 (94%)	4 (6%)	0	100	100
51	6T	72/82 (88%)	67 (93%)	5 (7%)	0	100	100
52	3H	63/91 (69%)	60 (95%)	3 (5%)	0	100	100
52	3U	63/91 (69%)	63 (100%)	0	0	100	100
52	6H	63/91 (69%)	60 (95%)	3 (5%)	0	100	100
52	6U	63/91 (69%)	61 (97%)	2 (3%)	0	100	100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	8	38
53	3W	54/64 (84%)	52 (96%)	2 (4%)	0	100	100
53	6J	54/64 (84%)	53 (98%)	0	1 (2%)	8	38
53	6W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
54	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	3Y	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
54	6X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	6Y	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
55	4A	512/514 (100%)	480 (94%)	30 (6%)	2 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	8A	512/514 (100%)	481 (94%)	29 (6%)	2 (0%)	34	72
56	4B	225/229 (98%)	209 (93%)	16 (7%)	0	100	100
56	8B	225/229 (98%)	207 (92%)	18 (8%)	0	100	100
57	4C	257/261 (98%)	241 (94%)	16 (6%)	0	100	100
57	8C	257/261 (98%)	240 (93%)	17 (7%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
58	8D	137/169 (81%)	122 (89%)	15 (11%)	0	100	100
59	4E	103/152 (68%)	100 (97%)	3 (3%)	0	100	100
59	8E	103/152 (68%)	97 (94%)	6 (6%)	0	100	100
60	4F	95/129 (74%)	91 (96%)	3 (3%)	1 (1%)	14	52
60	8F	95/129 (74%)	91 (96%)	3 (3%)	1 (1%)	14	52
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	67 (92%)	6 (8%)	0	100	100
62	4H	80/86 (93%)	73 (91%)	7 (9%)	0	100	100
62	8H	80/86 (93%)	71 (89%)	9 (11%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
63	8I	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
65	8K	47/80 (59%)	43 (92%)	4 (8%)	0	100	100
66	4L	44/63 (70%)	39 (89%)	5 (11%)	0	100	100
66	8L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
67	4M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
67	8M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
68	4N	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	48
68	8N	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	48
All	All	28146/34018 (83%)	26515 (94%)	1569 (6%)	62 (0%)	50	81

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	39	CYS

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Mol	Chain	Res	Type
8	1H	92	PRO
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	VAL
53	3J	57	LYS
45	3N	224	VAL
49	3R	150	SER
10	5J	66	VAL
23	5X	28	ALA
49	6E	271	VAL
45	6N	224	VAL
68	8N	33	VAL
6	1F	297	VAL
8	1H	208	VAL
49	3R	181	LYS
49	3R	273	VAL
68	4N	33	VAL
12	5L	2	ASN
53	6J	57	LYS
49	6R	150	SER
49	6R	228	ALA
49	6R	273	VAL
5	1E	157	ASN
6	1F	249	ARG
14	1N	46	LYS
14	1N	110	PRO
46	3O	171	ALA
49	3R	228	ALA
1	5A	109	LYS
5	5E	157	ASN
6	5F	297	VAL
8	5H	208	VAL
49	6R	181	LYS
1	1A	52	SER
7	1G	155	GLN
60	4F	95	GLN
1	5A	52	SER
6	5F	249	ARG
60	8F	95	GLN
7	1G	654	GLN
12	1L	2	ASN
34	1i	75	LEU

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Mol	Chain	Res	Type
45	3A	231	PHE
55	4A	3	VAL
6	5F	207	PRO
45	6A	231	PHE
46	6O	171	ALA
6	1F	207	PRO
12	1L	72	GLN
49	3E	196	ARG
7	5G	186	TYR
7	5G	654	GLN
16	5P	64	ASP
39	5n	31	VAL
45	6A	350	THR
55	8A	3	VAL
45	6N	71	PRO
45	3N	71	PRO
55	4A	128	VAL
8	5H	92	PRO
55	8A	128	VAL

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	
1	1A	99/99 (100%)	94 (95%)	5 (5%)	24	49
1	5A	99/99 (100%)	91 (92%)	8 (8%)	11	35
2	1B	131/212 (62%)	118 (90%)	13 (10%)	8	26
2	5B	131/212 (62%)	123 (94%)	8 (6%)	18	44
3	1C	190/227 (84%)	184 (97%)	6 (3%)	39	61
3	5C	190/227 (84%)	182 (96%)	8 (4%)	30	54
4	1D	371/405 (92%)	354 (95%)	17 (5%)	27	52
4	5D	371/405 (92%)	355 (96%)	16 (4%)	29	53
5	1E	183/207 (88%)	169 (92%)	14 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5E	183/207 (88%)	172 (94%)	11 (6%)	19	44
6	1F	346/368 (94%)	334 (96%)	12 (4%)	36	59
6	5F	346/368 (94%)	332 (96%)	14 (4%)	31	55
7	1G	588/610 (96%)	553 (94%)	35 (6%)	19	44
7	5G	588/610 (96%)	553 (94%)	35 (6%)	19	44
8	1H	274/274 (100%)	260 (95%)	14 (5%)	24	49
8	5H	274/274 (100%)	259 (94%)	15 (6%)	21	47
9	1I	151/201 (75%)	136 (90%)	15 (10%)	8	26
9	5I	151/201 (75%)	142 (94%)	9 (6%)	19	44
10	1J	140/141 (99%)	133 (95%)	7 (5%)	24	49
10	5J	140/141 (99%)	127 (91%)	13 (9%)	9	29
11	1K	84/84 (100%)	78 (93%)	6 (7%)	14	39
11	5K	84/84 (100%)	76 (90%)	8 (10%)	8	28
12	1L	539/539 (100%)	515 (96%)	24 (4%)	27	52
12	5L	539/539 (100%)	518 (96%)	21 (4%)	32	56
13	1M	408/408 (100%)	395 (97%)	13 (3%)	39	61
13	5M	408/408 (100%)	380 (93%)	28 (7%)	15	40
14	1N	310/310 (100%)	288 (93%)	22 (7%)	14	39
14	5N	310/310 (100%)	288 (93%)	22 (7%)	14	39
15	1O	283/307 (92%)	272 (96%)	11 (4%)	32	56
15	5O	283/307 (92%)	265 (94%)	18 (6%)	17	42
16	1P	296/323 (92%)	285 (96%)	11 (4%)	34	58
16	5P	296/323 (92%)	283 (96%)	13 (4%)	28	53
17	1Q	117/152 (77%)	110 (94%)	7 (6%)	19	44
17	5Q	117/152 (77%)	108 (92%)	9 (8%)	13	37
18	1R	79/97 (81%)	72 (91%)	7 (9%)	9	30
18	5R	79/97 (81%)	75 (95%)	4 (5%)	24	49
19	1S	77/82 (94%)	70 (91%)	7 (9%)	9	30
19	5S	77/82 (94%)	73 (95%)	4 (5%)	23	48
20	1T	79/133 (59%)	71 (90%)	8 (10%)	7	25
20	1U	79/133 (59%)	75 (95%)	4 (5%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	5T	79/133 (59%)	68 (86%)	11 (14%)	3	17
20	5U	79/133 (59%)	77 (98%)	2 (2%)	47	68
21	1V	100/101 (99%)	97 (97%)	3 (3%)	41	63
21	5V	100/101 (99%)	97 (97%)	3 (3%)	41	63
22	1W	107/112 (96%)	98 (92%)	9 (8%)	11	34
22	5W	107/112 (96%)	95 (89%)	12 (11%)	6	22
23	1X	153/154 (99%)	141 (92%)	12 (8%)	12	36
23	5X	153/154 (99%)	144 (94%)	9 (6%)	19	45
24	1Y	101/102 (99%)	93 (92%)	8 (8%)	12	36
24	5Y	101/102 (99%)	88 (87%)	13 (13%)	4	18
25	1Z	123/124 (99%)	111 (90%)	12 (10%)	8	27
25	5Z	123/124 (99%)	117 (95%)	6 (5%)	25	50
26	1a	58/58 (100%)	56 (97%)	2 (3%)	37	60
26	5a	58/58 (100%)	52 (90%)	6 (10%)	7	25
27	1b	69/70 (99%)	66 (96%)	3 (4%)	29	53
27	5b	69/70 (99%)	65 (94%)	4 (6%)	20	45
28	1c	45/66 (68%)	41 (91%)	4 (9%)	9	30
28	5c	45/66 (68%)	38 (84%)	7 (16%)	2	14
29	1d	106/109 (97%)	98 (92%)	8 (8%)	13	38
29	5d	106/109 (97%)	96 (91%)	10 (9%)	8	28
30	1e	87/94 (93%)	85 (98%)	2 (2%)	50	70
30	5e	87/94 (93%)	78 (90%)	9 (10%)	7	25
31	1f	54/113 (48%)	53 (98%)	1 (2%)	57	75
31	5f	54/113 (48%)	53 (98%)	1 (2%)	57	75
32	1g	92/129 (71%)	89 (97%)	3 (3%)	38	61
32	5g	92/129 (71%)	82 (89%)	10 (11%)	6	23
33	1h	121/158 (77%)	109 (90%)	12 (10%)	8	26
33	5h	121/158 (77%)	112 (93%)	9 (7%)	13	38
34	1i	119/120 (99%)	112 (94%)	7 (6%)	19	45
34	5i	119/120 (99%)	113 (95%)	6 (5%)	24	49
35	1j	62/84 (74%)	58 (94%)	4 (6%)	17	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	5j	62/84 (74%)	59 (95%)	3 (5%)	25	51
36	1k	63/76 (83%)	62 (98%)	1 (2%)	62	79
36	5k	63/76 (83%)	60 (95%)	3 (5%)	25	51
37	1l	141/161 (88%)	136 (96%)	5 (4%)	36	59
37	5l	141/161 (88%)	130 (92%)	11 (8%)	12	36
38	1m	113/114 (99%)	111 (98%)	2 (2%)	59	77
38	5m	113/114 (99%)	108 (96%)	5 (4%)	28	53
39	1n	156/160 (98%)	148 (95%)	8 (5%)	24	49
39	5n	156/160 (98%)	147 (94%)	9 (6%)	20	45
40	1o	110/119 (92%)	106 (96%)	4 (4%)	35	59
40	5o	110/119 (92%)	104 (94%)	6 (6%)	21	47
41	1p	154/156 (99%)	144 (94%)	10 (6%)	17	42
41	5p	154/156 (99%)	146 (95%)	8 (5%)	23	48
42	1q	131/131 (100%)	121 (92%)	10 (8%)	13	37
42	5q	131/131 (100%)	121 (92%)	10 (8%)	13	37
43	1r	85/98 (87%)	81 (95%)	4 (5%)	26	51
43	5r	85/98 (87%)	77 (91%)	8 (9%)	8	28
44	1s	44/351 (12%)	43 (98%)	1 (2%)	50	70
44	5s	44/351 (12%)	42 (96%)	2 (4%)	27	52
45	3A	367/397 (92%)	353 (96%)	14 (4%)	33	57
45	3N	372/397 (94%)	356 (96%)	16 (4%)	29	53
45	6A	367/397 (92%)	354 (96%)	13 (4%)	36	59
45	6N	372/397 (94%)	352 (95%)	20 (5%)	22	47
46	3B	328/355 (92%)	323 (98%)	5 (2%)	65	80
46	3O	327/355 (92%)	316 (97%)	11 (3%)	37	60
46	6B	328/355 (92%)	311 (95%)	17 (5%)	23	48
46	6O	327/355 (92%)	312 (95%)	15 (5%)	27	52
47	3C	332/332 (100%)	316 (95%)	16 (5%)	25	51
47	3P	332/332 (100%)	324 (98%)	8 (2%)	49	69
47	6C	332/332 (100%)	313 (94%)	19 (6%)	20	45
47	6P	332/332 (100%)	313 (94%)	19 (6%)	20	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	3D	202/259 (78%)	194 (96%)	8 (4%)	31	55
48	3Q	204/259 (79%)	197 (97%)	7 (3%)	37	60
48	6D	202/259 (78%)	194 (96%)	8 (4%)	31	55
48	6Q	204/259 (79%)	193 (95%)	11 (5%)	22	47
49	3E	166/225 (74%)	160 (96%)	6 (4%)	35	59
49	3I	36/225 (16%)	35 (97%)	1 (3%)	43	65
49	3R	166/225 (74%)	158 (95%)	8 (5%)	25	51
49	3V	24/225 (11%)	23 (96%)	1 (4%)	30	54
49	6E	166/225 (74%)	158 (95%)	8 (5%)	25	51
49	6I	36/225 (16%)	34 (94%)	2 (6%)	21	46
49	6R	166/225 (74%)	157 (95%)	9 (5%)	22	47
49	6V	24/225 (11%)	24 (100%)	0	100	100
50	3F	90/99 (91%)	86 (96%)	4 (4%)	28	53
50	3S	90/99 (91%)	86 (96%)	4 (4%)	28	53
50	6F	90/99 (91%)	83 (92%)	7 (8%)	12	36
50	6S	90/99 (91%)	83 (92%)	7 (8%)	12	36
51	3G	67/73 (92%)	65 (97%)	2 (3%)	41	63
51	3T	67/73 (92%)	67 (100%)	0	100	100
51	6G	67/73 (92%)	63 (94%)	4 (6%)	19	44
51	6T	67/73 (92%)	63 (94%)	4 (6%)	19	44
52	3H	62/85 (73%)	59 (95%)	3 (5%)	25	51
52	3U	62/85 (73%)	59 (95%)	3 (5%)	25	51
52	6H	62/85 (73%)	60 (97%)	2 (3%)	39	61
52	6U	62/85 (73%)	58 (94%)	4 (6%)	17	42
53	3J	45/51 (88%)	44 (98%)	1 (2%)	52	71
53	3W	45/51 (88%)	44 (98%)	1 (2%)	52	71
53	6J	45/51 (88%)	40 (89%)	5 (11%)	6	22
53	6W	45/51 (88%)	41 (91%)	4 (9%)	9	30
54	3X	42/46 (91%)	40 (95%)	2 (5%)	25	51
54	3Y	41/46 (89%)	37 (90%)	4 (10%)	8	27
54	6X	42/46 (91%)	40 (95%)	2 (5%)	25	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	6Y	41/46 (89%)	39 (95%)	2 (5%)	25	50
55	4A	424/424 (100%)	386 (91%)	38 (9%)	9	30
55	8A	424/424 (100%)	384 (91%)	40 (9%)	8	28
56	4B	210/211 (100%)	200 (95%)	10 (5%)	25	51
56	8B	210/211 (100%)	193 (92%)	17 (8%)	11	35
57	4C	223/225 (99%)	205 (92%)	18 (8%)	11	35
57	8C	223/225 (99%)	200 (90%)	23 (10%)	7	25
58	4D	124/149 (83%)	113 (91%)	11 (9%)	9	30
58	8D	124/149 (83%)	110 (89%)	14 (11%)	6	21
59	4E	92/124 (74%)	86 (94%)	6 (6%)	17	42
59	8E	92/124 (74%)	82 (89%)	10 (11%)	6	23
60	4F	80/101 (79%)	72 (90%)	8 (10%)	7	26
60	8F	80/101 (79%)	72 (90%)	8 (10%)	7	26
61	4G	65/80 (81%)	62 (95%)	3 (5%)	27	52
61	8G	65/80 (81%)	62 (95%)	3 (5%)	27	52
62	4H	73/76 (96%)	69 (94%)	4 (6%)	21	47
62	8H	73/76 (96%)	67 (92%)	6 (8%)	11	34
63	4I	54/61 (88%)	45 (83%)	9 (17%)	2	12
63	8I	54/61 (88%)	49 (91%)	5 (9%)	9	29
64	4J	49/68 (72%)	45 (92%)	4 (8%)	11	34
64	8J	49/68 (72%)	43 (88%)	6 (12%)	5	20
65	4K	38/66 (58%)	36 (95%)	2 (5%)	22	47
65	8K	38/66 (58%)	35 (92%)	3 (8%)	12	36
66	4L	39/55 (71%)	35 (90%)	4 (10%)	7	25
66	8L	39/55 (71%)	33 (85%)	6 (15%)	2	14
67	4M	37/57 (65%)	35 (95%)	2 (5%)	22	47
67	8M	37/57 (65%)	33 (89%)	4 (11%)	6	23
68	4N	70/70 (100%)	59 (84%)	11 (16%)	2	14
68	8N	70/70 (100%)	65 (93%)	5 (7%)	14	39
All	All	24526/28666 (86%)	23099 (94%)	1427 (6%)	24	45

All (1427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	22	PHE
1	1A	35	SER
1	1A	51	PHE
1	1A	63	LEU
1	1A	102	LEU
2	1B	25	ARG
2	1B	50	PHE
2	1B	66	ARG
2	1B	76	PHE
2	1B	86	MET
2	1B	116	MET
2	1B	125	TYR
2	1B	130	TYR
2	1B	136	CYS
2	1B	149	CYS
2	1B	156	LEU
2	1B	162	GLN
2	1B	170	GLU
3	1C	12	ARG
3	1C	44	CYS
3	1C	51	PHE
3	1C	104	GLN
3	1C	171	TYR
3	1C	177	ASP
4	1D	19	MET
4	1D	37	ASP
4	1D	40	LYS
4	1D	79	HIS
4	1D	93	TYR
4	1D	97	LEU
4	1D	157	HIS
4	1D	159	LEU
4	1D	167	PHE
4	1D	168	PHE
4	1D	180	PHE
4	1D	209	ASP
4	1D	249	ASP
4	1D	297	TYR
4	1D	318	MET
4	1D	338	MET
4	1D	356	TYR
5	1E	13	PRO
5	1E	15	ASN

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Mol	Chain	Res	Type
5	1E	38	TYR
5	1E	66	MET
5	1E	78	MET
5	1E	89	MET
5	1E	121	GLN
5	1E	122	LYS
5	1E	134	ASP
5	1E	144	CYS
5	1E	160	TYR
5	1E	190	ARG
5	1E	191	PHE
5	1E	192	SER
6	1F	20	ARG
6	1F	32	ARG
6	1F	209	PHE
6	1F	216	PHE
6	1F	241	TRP
6	1F	272	MET
6	1F	277	LYS
6	1F	293	ASN
6	1F	352	GLU
6	1F	354	TYR
6	1F	372	MET
6	1F	381	LYS
7	1G	14	ASP
7	1G	19	MET
7	1G	39	ARG
7	1G	42	TYR
7	1G	105	CYS
7	1G	122	MET
7	1G	158	ARG
7	1G	190	MET
7	1G	213	TYR
7	1G	220	TRP
7	1G	241	SER
7	1G	254	MET
7	1G	262	TRP
7	1G	269	PHE
7	1G	278	ARG
7	1G	302	ARG
7	1G	309	SER
7	1G	314	ASP

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Mol	Chain	Res	Type
7	1G	394	ARG
7	1G	403	ASP
7	1G	439	PHE
7	1G	478	ARG
7	1G	539	LYS
7	1G	549	HIS
7	1G	566	TYR
7	1G	613	TYR
7	1G	618	GLN
7	1G	635	ASP
7	1G	650	LYS
7	1G	669	LYS
7	1G	670	ASP
7	1G	673	MET
7	1G	675	ASP
7	1G	684	MET
7	1G	689	LYS
8	1H	3	MET
8	1H	19	PHE
8	1H	42	PRO
8	1H	83	LEU
8	1H	105	MET
8	1H	118	TRP
8	1H	171	HIS
8	1H	185	TRP
8	1H	220	PHE
8	1H	222	MET
8	1H	241	LEU
8	1H	259	PHE
8	1H	280	PHE
8	1H	302	MET
9	1I	6	ASN
9	1I	12	MET
9	1I	38	LEU
9	1I	42	PHE
9	1I	43	ARG
9	1I	54	LYS
9	1I	110	ASP
9	1I	112	ASP
9	1I	118	TYR
9	1I	147	LEU
9	1I	148	LEU

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Mol	Chain	Res	Type
9	1I	150	ASN
9	1I	155	LEU
9	1I	157	ASN
9	1I	173	TYR
10	1J	41	CYS
10	1J	64	MET
10	1J	78	MET
10	1J	122	LEU
10	1J	128	TYR
10	1J	161	LEU
10	1J	169	MET
11	1K	10	MET
11	1K	12	PHE
11	1K	26	LEU
11	1K	37	MET
11	1K	63	LEU
11	1K	75	LEU
12	1L	25	ASN
12	1L	84	TYR
12	1L	89	PHE
12	1L	113	PHE
12	1L	169	LEU
12	1L	186	MET
12	1L	211	MET
12	1L	232	TRP
12	1L	262	ARG
12	1L	271	LYS
12	1L	340	PHE
12	1L	393	ASP
12	1L	422	TYR
12	1L	437	PHE
12	1L	470	ASN
12	1L	485	TYR
12	1L	510	TYR
12	1L	541	ASN
12	1L	571	MET
12	1L	572	LYS
12	1L	573	MET
12	1L	596	MET
12	1L	602	PHE
12	1L	604	TYR
13	1M	14	MET

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Mol	Chain	Res	Type
13	1M	57	PHE
13	1M	78	MET
13	1M	135	ARG
13	1M	183	SER
13	1M	231	LEU
13	1M	304	GLN
13	1M	307	TRP
13	1M	328	CYS
13	1M	342	MET
13	1M	378	GLU
13	1M	408	LEU
13	1M	427	LYS
14	1N	14	MET
14	1N	21	MET
14	1N	33	PHE
14	1N	35	MET
14	1N	40	MET
14	1N	95	MET
14	1N	98	MET
14	1N	109	SER
14	1N	190	MET
14	1N	208	TYR
14	1N	215	MET
14	1N	216	PHE
14	1N	217	MET
14	1N	237	MET
14	1N	244	MET
14	1N	245	MET
14	1N	278	MET
14	1N	299	SER
14	1N	304	MET
14	1N	311	MET
14	1N	321	LYS
14	1N	322	GLN
15	1O	37	ARG
15	1O	49	ARG
15	1O	51	PHE
15	1O	87	LYS
15	1O	108	TYR
15	1O	161	CYS
15	1O	198	TYR
15	1O	203	GLU

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Mol	Chain	Res	Type
15	1O	237	ASP
15	1O	257	HIS
15	1O	290	ASP
16	1P	13	ARG
16	1P	121	SER
16	1P	178	PHE
16	1P	182	PHE
16	1P	206	TYR
16	1P	222	ASP
16	1P	230	PHE
16	1P	240	ASP
16	1P	274	PRO
16	1P	326	TRP
16	1P	335	LYS
17	1Q	27	GLU
17	1Q	59	PHE
17	1Q	95	PHE
17	1Q	112	LYS
17	1Q	123	SER
17	1Q	125	ASN
17	1Q	133	LYS
18	1R	23	TYR
18	1R	31	ARG
18	1R	38	ASN
18	1R	54	SER
18	1R	70	ARG
18	1R	91	PHE
18	1R	96	HIS
19	1S	25	ARG
19	1S	34	ASP
19	1S	40	TYR
19	1S	44	LYS
19	1S	63	LYS
19	1S	67	ARG
19	1S	68	TYR
20	1T	6	LEU
20	1T	20	LYS
20	1T	29	LYS
20	1T	38	LYS
20	1T	46	ASP
20	1T	55	GLU
20	1T	57	GLU

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Mol	Chain	Res	Type
20	1T	88	GLU
20	1U	16	LEU
20	1U	37	MET
20	1U	39	ASP
20	1U	61	GLU
21	1V	27	TYR
21	1V	57	MET
21	1V	99	TRP
22	1W	18	LYS
22	1W	25	MET
22	1W	30	ARG
22	1W	50	PHE
22	1W	53	ASP
22	1W	68	MET
22	1W	106	PHE
22	1W	107	PHE
22	1W	118	PHE
23	1X	29	HIS
23	1X	42	PHE
23	1X	43	MET
23	1X	57	GLU
23	1X	65	CYS
23	1X	81	PHE
23	1X	109	CYS
23	1X	118	ARG
23	1X	138	GLU
23	1X	144	ARG
23	1X	161	LYS
23	1X	171	MET
24	1Y	8	TYR
24	1Y	9	SER
24	1Y	19	ARG
24	1Y	94	CYS
24	1Y	114	CYS
24	1Y	119	LEU
24	1Y	132	TRP
24	1Y	135	PHE
25	1Z	10	MET
25	1Z	20	ASP
25	1Z	23	ARG
25	1Z	28	ARG
25	1Z	31	SER

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Mol	Chain	Res	Type
25	1Z	51	MET
25	1Z	72	MET
25	1Z	74	LEU
25	1Z	98	MET
25	1Z	103	ASP
25	1Z	121	MET
25	1Z	142	TRP
26	1a	31	ASN
26	1a	37	ARG
27	1b	12	TRP
27	1b	18	LEU
27	1b	56	LEU
28	1c	30	TYR
28	1c	31	LEU
28	1c	36	LYS
28	1c	45	ARG
29	1d	2	MET
29	1d	19	ARG
29	1d	34	MET
29	1d	39	TYR
29	1d	63	LEU
29	1d	68	PHE
29	1d	82	MET
29	1d	83	TYR
30	1e	59	PHE
30	1e	62	PHE
31	1f	53	GLU
32	1g	63	PHE
32	1g	76	PHE
32	1g	84	ARG
33	1h	9	PHE
33	1h	14	SER
33	1h	16	PHE
33	1h	24	LEU
33	1h	25	MET
33	1h	26	ARG
33	1h	44	ASN
33	1h	67	PHE
33	1h	79	PHE
33	1h	91	MET
33	1h	107	GLU
33	1h	134	ASP

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Mol	Chain	Res	Type
34	1i	34	LEU
34	1i	45	PHE
34	1i	65	ARG
34	1i	83	TYR
34	1i	119	MET
34	1i	125	GLN
34	1i	126	HIS
35	1j	10	ARG
35	1j	27	PHE
35	1j	32	MET
35	1j	50	HIS
36	1k	58	ASN
37	1l	25	LYS
37	1l	66	HIS
37	1l	86	ARG
37	1l	140	LEU
37	1l	156	TYR
38	1m	46	TYR
38	1m	52	ASP
39	1n	25	HIS
39	1n	36	TYR
39	1n	52	ASN
39	1n	55	ASP
39	1n	61	GLN
39	1n	89	SER
39	1n	137	LYS
39	1n	176	ARG
40	1o	38	MET
40	1o	45	MET
40	1o	67	LYS
40	1o	76	PHE
41	1p	50	PHE
41	1p	59	ARG
41	1p	62	TYR
41	1p	64	HIS
41	1p	85	PHE
41	1p	95	TYR
41	1p	121	ARG
41	1p	138	PHE
41	1p	161	ARG
41	1p	162	MET
42	1q	1	MET

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Mol	Chain	Res	Type
42	1q	49	TYR
42	1q	53	LYS
42	1q	55	PHE
42	1q	58	ARG
42	1q	81	MET
42	1q	127	TYR
42	1q	132	LYS
42	1q	135	GLN
42	1q	145	LYS
43	1r	19	LEU
43	1r	48	LEU
43	1r	60	ARG
43	1r	63	MET
44	1s	51	PHE
45	3A	40	TRP
45	3A	58	PHE
45	3A	64	PHE
45	3A	68	LYS
45	3A	82	MET
45	3A	87	ASN
45	3A	302	LYS
45	3A	327	ASP
45	3A	335	MET
45	3A	338	LEU
45	3A	343	MET
45	3A	386	TYR
45	3A	433	ASP
45	3A	441	MET
46	3B	95	LYS
46	3B	96	LEU
46	3B	185	LYS
46	3B	374	SER
46	3B	395	PRO
47	3C	6	LYS
47	3C	80	ARG
47	3C	90	PHE
47	3C	91	PHE
47	3C	108	MET
47	3C	179	PHE
47	3C	183	PHE
47	3C	199	PHE
47	3C	235	MET

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Mol	Chain	Res	Type
47	3C	273	TYR
47	3C	294	LEU
47	3C	320	LEU
47	3C	325	PHE
47	3C	358	TYR
47	3C	373	GLU
47	3C	379	TRP
48	3D	118	PHE
48	3D	169	PHE
48	3D	178	TYR
48	3D	193	ASN
48	3D	262	ASP
48	3D	281	TRP
48	3D	304	LEU
48	3D	307	LEU
49	3E	136	PHE
49	3E	149	MET
49	3E	165	MET
49	3E	181	LYS
49	3E	217	CYS
49	3E	242	HIS
50	3F	25	LEU
50	3F	30	LYS
50	3F	67	TYR
50	3F	106	LEU
51	3G	12	MET
51	3G	59	LEU
52	3H	85	PHE
52	3H	87	PHE
52	3H	89	HIS
49	3I	78	TYR
53	3J	26	LEU
45	3N	51	LYS
45	3N	58	PHE
45	3N	82	MET
45	3N	94	HIS
45	3N	112	LEU
45	3N	117	VAL
45	3N	145	MET
45	3N	146	ARG
45	3N	150	PHE
45	3N	226	ASP

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Mol	Chain	Res	Type
45	3N	284	TYR
45	3N	304	CYS
45	3N	308	GLN
45	3N	324	PHE
45	3N	348	SER
45	3N	378	ASP
46	3O	46	ARG
46	3O	164	HIS
46	3O	168	TYR
46	3O	222	ARG
46	3O	223	PHE
46	3O	224	LEU
46	3O	250	ASP
46	3O	254	HIS
46	3O	304	HIS
46	3O	339	SER
46	3O	437	ASP
47	3P	12	LYS
47	3P	124	MET
47	3P	178	PHE
47	3P	197	LEU
47	3P	236	MET
47	3P	345	HIS
47	3P	366	MET
47	3P	379	TRP
48	3Q	42	SER
48	3Q	55	CYS
48	3Q	128	PHE
48	3Q	149	PHE
48	3Q	171	PHE
48	3Q	189	PHE
48	3Q	204	MET
49	3R	82	ASP
49	3R	149	MET
49	3R	155	LYS
49	3R	169	TRP
49	3R	178	HIS
49	3R	180	THR
49	3R	235	TYR
49	3R	257	ASN
50	3S	42	ASP
50	3S	55	TYR

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Mol	Chain	Res	Type
50	3S	70	MET
50	3S	94	LEU
52	3U	24	CYS
52	3U	39	LEU
52	3U	74	PHE
49	3V	67	SER
53	3W	14	PHE
54	3X	1	MET
54	3X	24	TRP
54	3Y	10	TYR
54	3Y	15	ARG
54	3Y	47	TYR
54	3Y	51	LYS
55	4A	12	HIS
55	4A	19	TYR
55	4A	22	PHE
55	4A	38	ARG
55	4A	61	HIS
55	4A	67	PHE
55	4A	78	PHE
55	4A	91	ASP
55	4A	92	MET
55	4A	112	LEU
55	4A	126	TRP
55	4A	129	TYR
55	4A	151	HIS
55	4A	171	MET
55	4A	176	MET
55	4A	179	TYR
55	4A	184	PHE
55	4A	212	ASP
55	4A	231	TYR
55	4A	233	HIS
55	4A	234	LEU
55	4A	235	PHE
55	4A	238	PHE
55	4A	251	PHE
55	4A	290	HIS
55	4A	292	MET
55	4A	302	ARG
55	4A	321	PHE
55	4A	344	PHE

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Mol	Chain	Res	Type
55	4A	353	LEU
55	4A	396	TRP
55	4A	397	PHE
55	4A	413	HIS
55	4A	439	ARG
55	4A	468	MET
55	4A	479	LYS
55	4A	491	ASN
55	4A	514	LYS
56	4B	21	LEU
56	4B	23	PHE
56	4B	56	MET
56	4B	62	GLU
56	4B	86	MET
56	4B	91	ASN
56	4B	108	TYR
56	4B	192	TYR
56	4B	206	PHE
56	4B	217	LYS
57	4C	10	MET
57	4C	81	TYR
57	4C	93	PHE
57	4C	97	PHE
57	4C	99	TRP
57	4C	101	PHE
57	4C	133	ASN
57	4C	138	LEU
57	4C	152	MET
57	4C	193	TYR
57	4C	197	PHE
57	4C	203	PHE
57	4C	214	PHE
57	4C	242	TRP
57	4C	244	PHE
57	4C	251	PHE
57	4C	253	TYR
57	4C	257	TYR
58	4D	11	TYR
58	4D	13	LEU
58	4D	19	ARG
58	4D	33	LEU
58	4D	64	PHE

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Mol	Chain	Res	Type
58	4D	74	SER
58	4D	88	PHE
58	4D	91	PHE
58	4D	121	LYS
58	4D	126	MET
58	4D	140	TYR
59	4E	14	ARG
59	4E	18	TYR
59	4E	25	ASP
59	4E	29	LEU
59	4E	33	MET
59	4E	93	LEU
60	4F	9	ASP
60	4F	16	LEU
60	4F	22	MET
60	4F	26	LYS
60	4F	31	TYR
60	4F	47	ASN
60	4F	71	TRP
60	4F	73	TRP
61	4G	30	LEU
61	4G	42	HIS
61	4G	54	ARG
62	4H	20	PHE
62	4H	36	PHE
62	4H	46	LYS
62	4H	60	TYR
63	4I	18	ARG
63	4I	25	PHE
63	4I	29	LEU
63	4I	34	PHE
63	4I	35	TYR
63	4I	50	PHE
63	4I	51	TYR
63	4I	57	MET
63	4I	69	PHE
64	4J	36	MET
64	4J	38	LEU
64	4J	47	LEU
64	4J	50	LEU
65	4K	8	ASP
65	4K	24	PHE

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Mol	Chain	Res	Type
66	4L	11	LEU
66	4L	13	PHE
66	4L	22	LEU
66	4L	28	TYR
67	4M	27	LEU
67	4M	39	HIS
68	4N	11	LYS
68	4N	19	PHE
68	4N	21	PHE
68	4N	32	TYR
68	4N	47	ARG
68	4N	54	TRP
68	4N	55	ASN
68	4N	65	PHE
68	4N	72	TYR
68	4N	77	LYS
68	4N	82	PHE
1	5A	28	ASN
1	5A	44	MET
1	5A	51	PHE
1	5A	55	PHE
1	5A	56	PHE
1	5A	90	MET
1	5A	98	LEU
1	5A	104	TYR
2	5B	25	ARG
2	5B	36	LEU
2	5B	48	MET
2	5B	59	MET
2	5B	76	PHE
2	5B	125	TYR
2	5B	134	ARG
2	5B	166	LYS
3	5C	14	ARG
3	5C	15	ASN
3	5C	71	GLN
3	5C	142	PHE
3	5C	195	ARG
3	5C	197	PHE
3	5C	201	SER
3	5C	209	TYR
4	5D	40	LYS

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Mol	Chain	Res	Type
4	5D	79	HIS
4	5D	93	TYR
4	5D	108	TYR
4	5D	111	MET
4	5D	152	MET
4	5D	189	MET
4	5D	209	ASP
4	5D	218	PHE
4	5D	260	LEU
4	5D	297	TYR
4	5D	327	ASP
4	5D	338	MET
4	5D	356	TYR
4	5D	390	LYS
4	5D	398	HIS
5	5E	13	PRO
5	5E	18	ASP
5	5E	23	PHE
5	5E	38	TYR
5	5E	56	ARG
5	5E	93	LYS
5	5E	99	HIS
5	5E	112	ASN
5	5E	114	ASP
5	5E	160	TYR
5	5E	190	ARG
6	5F	32	ARG
6	5F	84	LYS
6	5F	150	GLN
6	5F	188	GLU
6	5F	204	ARG
6	5F	209	PHE
6	5F	277	LYS
6	5F	312	CYS
6	5F	317	MET
6	5F	354	TYR
6	5F	372	MET
6	5F	385	ARG
6	5F	405	CYS
6	5F	418	LEU
7	5G	39	ARG
7	5G	42	TYR

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Mol	Chain	Res	Type
7	5G	64	LYS
7	5G	94	MET
7	5G	97	LEU
7	5G	108	CYS
7	5G	153	CYS
7	5G	158	ARG
7	5G	208	LEU
7	5G	241	SER
7	5G	269	PHE
7	5G	302	ARG
7	5G	309	SER
7	5G	336	ASN
7	5G	337	ARG
7	5G	375	ASP
7	5G	391	PHE
7	5G	398	SER
7	5G	402	ASN
7	5G	443	LEU
7	5G	478	ARG
7	5G	486	ASP
7	5G	495	ARG
7	5G	539	LYS
7	5G	546	GLN
7	5G	548	HIS
7	5G	596	ASP
7	5G	609	MET
7	5G	613	TYR
7	5G	640	ASN
7	5G	650	LYS
7	5G	669	LYS
7	5G	670	ASP
7	5G	673	MET
7	5G	684	MET
8	5H	7	LEU
8	5H	83	LEU
8	5H	91	MET
8	5H	105	MET
8	5H	150	LEU
8	5H	156	MET
8	5H	176	PHE
8	5H	186	PHE
8	5H	220	PHE

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Mol	Chain	Res	Type
8	5H	225	MET
8	5H	259	PHE
8	5H	274	ARG
8	5H	280	PHE
8	5H	304	HIS
8	5H	310	MET
9	5I	50	TYR
9	5I	52	PHE
9	5I	109	TYR
9	5I	113	MET
9	5I	116	CYS
9	5I	148	LEU
9	5I	150	ASN
9	5I	153	LYS
9	5I	168	ASN
10	5J	3	MET
10	5J	20	PHE
10	5J	33	LEU
10	5J	60	TYR
10	5J	64	MET
10	5J	68	PHE
10	5J	78	MET
10	5J	79	TYR
10	5J	98	MET
10	5J	99	MET
10	5J	103	MET
10	5J	161	LEU
10	5J	169	MET
11	5K	5	TYR
11	5K	21	MET
11	5K	27	MET
11	5K	37	MET
11	5K	58	MET
11	5K	66	PHE
11	5K	73	LEU
11	5K	75	LEU
12	5L	20	MET
12	5L	35	TYR
12	5L	108	MET
12	5L	165	ASN
12	5L	263	PHE
12	5L	264	TYR

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Mol	Chain	Res	Type
12	5L	271	LYS
12	5L	334	PHE
12	5L	336	LYS
12	5L	340	PHE
12	5L	392	LYS
12	5L	393	ASP
12	5L	403	TYR
12	5L	470	ASN
12	5L	475	MET
12	5L	488	MET
12	5L	498	PHE
12	5L	541	ASN
12	5L	571	MET
12	5L	589	LEU
12	5L	602	PHE
13	5M	10	MET
13	5M	22	MET
13	5M	33	LEU
13	5M	57	PHE
13	5M	78	MET
13	5M	95	TYR
13	5M	103	GLN
13	5M	122	PHE
13	5M	135	ARG
13	5M	149	PHE
13	5M	161	LEU
13	5M	177	LEU
13	5M	195	MET
13	5M	201	MET
13	5M	206	LYS
13	5M	212	LEU
13	5M	231	LEU
13	5M	263	MET
13	5M	266	MET
13	5M	269	MET
13	5M	307	TRP
13	5M	336	ARG
13	5M	342	MET
13	5M	355	MET
13	5M	358	TRP
13	5M	398	MET
13	5M	400	MET

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Mol	Chain	Res	Type
13	5M	427	LYS
14	5N	6	TYR
14	5N	11	MET
14	5N	21	MET
14	5N	33	PHE
14	5N	59	TYR
14	5N	80	TYR
14	5N	84	TRP
14	5N	88	LYS
14	5N	159	MET
14	5N	181	TYR
14	5N	211	MET
14	5N	213	LEU
14	5N	215	MET
14	5N	237	MET
14	5N	251	MET
14	5N	265	MET
14	5N	269	GLU
14	5N	270	MET
14	5N	284	MET
14	5N	289	ASN
14	5N	299	SER
14	5N	339	MET
15	5O	30	ASN
15	5O	45	LYS
15	5O	49	ARG
15	5O	65	ASP
15	5O	87	LYS
15	5O	94	TYR
15	5O	101	TYR
15	5O	134	PHE
15	5O	140	ARG
15	5O	163	TYR
15	5O	186	LYS
15	5O	203	GLU
15	5O	206	TYR
15	5O	218	CYS
15	5O	244	ASP
15	5O	272	TYR
15	5O	293	PHE
15	5O	296	PHE
16	5P	71	MET

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Mol	Chain	Res	Type
16	5P	89	ASN
16	5P	143	SER
16	5P	196	LEU
16	5P	216	ASN
16	5P	219	LYS
16	5P	224	LYS
16	5P	240	ASP
16	5P	253	PHE
16	5P	281	ARG
16	5P	326	TRP
16	5P	335	LYS
16	5P	338	LYS
17	5Q	27	GLU
17	5Q	36	ARG
17	5Q	38	PHE
17	5Q	59	PHE
17	5Q	73	SER
17	5Q	101	TRP
17	5Q	112	LYS
17	5Q	123	SER
17	5Q	125	ASN
18	5R	22	ASP
18	5R	27	ARG
18	5R	54	SER
18	5R	96	HIS
19	5S	25	ARG
19	5S	34	ASP
19	5S	65	TRP
19	5S	67	ARG
20	5T	6	LEU
20	5T	20	LYS
20	5T	36	PHE
20	5T	38	LYS
20	5T	43	ASP
20	5T	45	LEU
20	5T	46	ASP
20	5T	52	MET
20	5T	54	MET
20	5T	57	GLU
20	5T	71	MET
20	5U	36	PHE
20	5U	37	MET

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Mol	Chain	Res	Type
21	5V	49	GLN
21	5V	82	GLN
21	5V	91	ARG
22	5W	23	ARG
22	5W	24	ASP
22	5W	45	ASN
22	5W	57	LYS
22	5W	62	LYS
22	5W	68	MET
22	5W	69	LYS
22	5W	85	LYS
22	5W	87	LYS
22	5W	88	MET
22	5W	95	ASN
22	5W	106	PHE
23	5X	10	GLU
23	5X	31	TYR
23	5X	39	ASN
23	5X	47	TRP
23	5X	65	CYS
23	5X	70	PHE
23	5X	81	PHE
23	5X	98	HIS
23	5X	171	MET
24	5Y	2	LYS
24	5Y	5	LEU
24	5Y	9	SER
24	5Y	19	ARG
24	5Y	33	LEU
24	5Y	39	SER
24	5Y	94	CYS
24	5Y	106	SER
24	5Y	114	CYS
24	5Y	116	TYR
24	5Y	119	LEU
24	5Y	123	LEU
24	5Y	132	TRP
25	5Z	27	ARG
25	5Z	50	MET
25	5Z	51	MET
25	5Z	68	ARG
25	5Z	121	MET

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Mol	Chain	Res	Type
25	5Z	142	TRP
26	5a	16	LEU
26	5a	25	HIS
26	5a	36	LYS
26	5a	41	PHE
26	5a	48	MET
26	5a	50	ARG
27	5b	9	LYS
27	5b	50	TYR
27	5b	61	ASN
27	5b	62	MET
28	5c	19	LEU
28	5c	26	PHE
28	5c	27	LEU
28	5c	30	TYR
28	5c	31	LEU
28	5c	36	LYS
28	5c	45	ARG
29	5d	13	PHE
29	5d	28	ASP
29	5d	36	PHE
29	5d	51	ARG
29	5d	62	LEU
29	5d	70	PHE
29	5d	74	TYR
29	5d	90	MET
29	5d	91	PHE
29	5d	105	ASP
30	5e	2	PHE
30	5e	8	ARG
30	5e	15	ARG
30	5e	17	MET
30	5e	35	PHE
30	5e	59	PHE
30	5e	72	MET
30	5e	84	LYS
30	5e	98	LEU
31	5f	10	HIS
32	5g	34	ASP
32	5g	40	LYS
32	5g	47	TYR
32	5g	64	PHE

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Mol	Chain	Res	Type
32	5g	76	PHE
32	5g	83	TYR
32	5g	85	MET
32	5g	95	ARG
32	5g	96	LEU
32	5g	105	LEU
33	5h	16	PHE
33	5h	25	MET
33	5h	54	ASP
33	5h	64	TRP
33	5h	79	PHE
33	5h	81	ASP
33	5h	91	MET
33	5h	122	TRP
33	5h	123	TYR
34	5i	8	LYS
34	5i	27	LEU
34	5i	38	ARG
34	5i	42	MET
34	5i	64	TYR
34	5i	121	GLU
35	5j	32	MET
35	5j	45	ASP
35	5j	61	ASP
36	5k	47	ASN
36	5k	52	TYR
36	5k	66	LEU
37	5l	6	LYS
37	5l	29	MET
37	5l	42	MET
37	5l	47	TYR
37	5l	62	TYR
37	5l	66	HIS
37	5l	86	ARG
37	5l	113	LEU
37	5l	140	LEU
37	5l	148	LYS
37	5l	149	GLU
38	5m	22	TYR
38	5m	25	SER
38	5m	30	LYS
38	5m	79	PHE

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Mol	Chain	Res	Type
38	5m	99	PHE
39	5n	16	LEU
39	5n	20	LYS
39	5n	32	HIS
39	5n	38	TYR
39	5n	50	HIS
39	5n	79	TYR
39	5n	123	GLN
39	5n	158	LYS
39	5n	176	ARG
40	5o	21	MET
40	5o	38	MET
40	5o	45	MET
40	5o	64	GLN
40	5o	110	ARG
40	5o	112	LYS
41	5p	64	HIS
41	5p	84	MET
41	5p	85	PHE
41	5p	95	TYR
41	5p	121	ARG
41	5p	123	ASN
41	5p	131	PHE
41	5p	138	PHE
42	5q	1	MET
42	5q	7	LEU
42	5q	31	ASN
42	5q	47	LYS
42	5q	52	ASN
42	5q	107	LYS
42	5q	115	PHE
42	5q	127	TYR
42	5q	144	TYR
42	5q	145	LYS
43	5r	10	LEU
43	5r	39	LYS
43	5r	53	TYR
43	5r	69	MET
43	5r	102	ARG
43	5r	109	GLN
43	5r	111	TYR
43	5r	112	LEU

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Mol	Chain	Res	Type
44	5s	33	PHE
44	5s	61	PHE
45	6A	4	TYR
45	6A	51	LYS
45	6A	58	PHE
45	6A	68	LYS
45	6A	120	CYS
45	6A	145	MET
45	6A	206	ARG
45	6A	216	PHE
45	6A	242	ARG
45	6A	244	ARG
45	6A	324	PHE
45	6A	337	PHE
45	6A	433	ASP
46	6B	26	PHE
46	6B	28	ARG
46	6B	50	PHE
46	6B	70	ARG
46	6B	111	CYS
46	6B	132	PHE
46	6B	135	TRP
46	6B	140	LEU
46	6B	162	ASN
46	6B	199	PHE
46	6B	204	MET
46	6B	226	MET
46	6B	321	LEU
46	6B	335	ASP
46	6B	338	LYS
46	6B	378	PHE
46	6B	437	ASP
47	6C	18	PHE
47	6C	55	TYR
47	6C	63	PHE
47	6C	75	TYR
47	6C	77	TRP
47	6C	90	PHE
47	6C	121	PHE
47	6C	124	MET
47	6C	138	MET
47	6C	150	LEU

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Mol	Chain	Res	Type
47	6C	179	PHE
47	6C	187	PHE
47	6C	197	LEU
47	6C	217	LYS
47	6C	234	PHE
47	6C	301	LEU
47	6C	315	MET
47	6C	358	TYR
47	6C	379	TRP
48	6D	100	TRP
48	6D	122	LYS
48	6D	179	PHE
48	6D	193	ASN
48	6D	214	TYR
48	6D	216	PHE
48	6D	268	MET
48	6D	299	MET
49	6E	104	LYS
49	6E	127	TYR
49	6E	136	PHE
49	6E	149	MET
49	6E	161	GLU
49	6E	170	ARG
49	6E	230	ASP
49	6E	265	PHE
50	6F	25	LEU
50	6F	33	TYR
50	6F	40	LYS
50	6F	41	LEU
50	6F	67	TYR
50	6F	76	ARG
50	6F	119	TRP
51	6G	11	ARG
51	6G	12	MET
51	6G	34	LYS
51	6G	54	PHE
52	6H	89	HIS
52	6H	100	PHE
49	6I	70	LEU
49	6I	77	ARG
53	6J	13	LEU
53	6J	26	LEU

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Mol	Chain	Res	Type
53	6J	34	PHE
53	6J	35	PHE
53	6J	39	PHE
45	6N	24	ARG
45	6N	31	SER
45	6N	58	PHE
45	6N	75	LEU
45	6N	105	ASP
45	6N	112	LEU
45	6N	117	VAL
45	6N	145	MET
45	6N	206	ARG
45	6N	216	PHE
45	6N	266	ASP
45	6N	304	CYS
45	6N	324	PHE
45	6N	332	ASP
45	6N	335	MET
45	6N	342	TRP
45	6N	344	ARG
45	6N	365	LEU
45	6N	370	ASP
45	6N	378	ASP
46	6O	41	TYR
46	6O	50	PHE
46	6O	63	LEU
46	6O	120	MET
46	6O	132	PHE
46	6O	140	LEU
46	6O	162	ASN
46	6O	174	ASN
46	6O	194	TYR
46	6O	204	MET
46	6O	212	SER
46	6O	223	PHE
46	6O	368	TYR
46	6O	417	PHE
46	6O	424	MET
47	6P	80	ARG
47	6P	81	TYR
47	6P	91	PHE
47	6P	102	LEU

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Mol	Chain	Res	Type
47	6P	124	MET
47	6P	128	PHE
47	6P	181	PHE
47	6P	197	LEU
47	6P	198	LEU
47	6P	199	PHE
47	6P	205	SER
47	6P	214	ASP
47	6P	220	PHE
47	6P	223	TYR
47	6P	278	TYR
47	6P	299	LEU
47	6P	312	GLN
47	6P	325	PHE
47	6P	379	TRP
48	6Q	13	SER
48	6Q	21	LEU
48	6Q	23	HIS
48	6Q	30	PHE
48	6Q	115	TYR
48	6Q	128	PHE
48	6Q	153	PHE
48	6Q	189	PHE
48	6Q	200	HIS
48	6Q	210	MET
48	6Q	216	LEU
49	6R	82	ASP
49	6R	91	TYR
49	6R	116	LEU
49	6R	155	LYS
49	6R	175	PHE
49	6R	178	HIS
49	6R	235	TYR
49	6R	242	HIS
49	6R	263	TYR
50	6S	29	LEU
50	6S	40	ASP
50	6S	48	ARG
50	6S	91	GLU
50	6S	95	LYS
50	6S	101	ARG
50	6S	107	TRP

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Mol	Chain	Res	Type
51	6T	10	MET
51	6T	16	TYR
51	6T	30	PHE
51	6T	71	ARG
52	6U	15	ASP
52	6U	62	LEU
52	6U	68	CYS
52	6U	74	PHE
53	6W	14	PHE
53	6W	20	PHE
53	6W	35	PHE
53	6W	53	LYS
54	6X	4	ARG
54	6X	23	MET
54	6Y	4	ARG
54	6Y	10	TYR
55	8A	12	HIS
55	8A	14	ASP
55	8A	19	TYR
55	8A	20	LEU
55	8A	28	MET
55	8A	67	PHE
55	8A	69	MET
55	8A	78	PHE
55	8A	81	TRP
55	8A	86	MET
55	8A	92	MET
55	8A	109	PHE
55	8A	144	ASP
55	8A	148	PHE
55	8A	176	MET
55	8A	178	GLN
55	8A	184	PHE
55	8A	189	LEU
55	8A	210	LEU
55	8A	231	TYR
55	8A	235	PHE
55	8A	265	LYS
55	8A	268	PHE
55	8A	282	PHE
55	8A	290	HIS
55	8A	302	ARG

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Mol	Chain	Res	Type
55	8A	310	MET
55	8A	333	LYS
55	8A	372	TYR
55	8A	379	TYR
55	8A	383	MET
55	8A	390	MET
55	8A	395	HIS
55	8A	396	TRP
55	8A	417	MET
55	8A	423	MET
55	8A	425	PHE
55	8A	445	ASP
55	8A	468	MET
55	8A	514	LYS
56	8B	3	TYR
56	8B	9	PHE
56	8B	20	LEU
56	8B	24	HIS
56	8B	37	LEU
56	8B	40	TYR
56	8B	56	MET
56	8B	108	TYR
56	8B	110	TYR
56	8B	119	ASP
56	8B	133	MET
56	8B	173	ASP
56	8B	185	MET
56	8B	192	TYR
56	8B	203	ASN
56	8B	206	PHE
56	8B	218	TYR
57	8C	33	MET
57	8C	40	MET
57	8C	54	MET
57	8C	77	LYS
57	8C	85	LEU
57	8C	86	PHE
57	8C	98	PHE
57	8C	101	PHE
57	8C	102	TYR
57	8C	126	PRO
57	8C	138	LEU

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Mol	Chain	Res	Type
57	8C	145	THR
57	8C	152	MET
57	8C	163	LEU
57	8C	172	TYR
57	8C	177	GLN
57	8C	206	LEU
57	8C	231	HIS
57	8C	235	PHE
57	8C	241	TYR
57	8C	244	PHE
57	8C	253	TYR
57	8C	257	TYR
58	8D	11	TYR
58	8D	31	LYS
58	8D	59	LEU
58	8D	62	LEU
58	8D	64	PHE
58	8D	71	MET
58	8D	86	LEU
58	8D	88	PHE
58	8D	91	PHE
58	8D	94	LEU
58	8D	111	PHE
58	8D	123	MET
58	8D	134	PHE
58	8D	140	TYR
59	8E	6	GLU
59	8E	14	ARG
59	8E	15	TRP
59	8E	29	LEU
59	8E	30	ARG
59	8E	39	TYR
59	8E	46	LYS
59	8E	72	LYS
59	8E	82	TYR
59	8E	93	LEU
60	8F	21	MET
60	8F	22	MET
60	8F	31	TYR
60	8F	32	ASN
60	8F	54	ASN
60	8F	73	TRP

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Mol	Chain	Res	Type
60	8F	75	HIS
60	8F	93	SER
61	8G	19	LEU
61	8G	54	ARG
61	8G	60	TYR
62	8H	16	PHE
62	8H	20	PHE
62	8H	55	TRP
62	8H	61	LYS
62	8H	72	TRP
62	8H	81	PHE
63	8I	17	LEU
63	8I	35	TYR
63	8I	57	MET
63	8I	59	ASP
63	8I	69	PHE
64	8J	10	LYS
64	8J	36	MET
64	8J	38	LEU
64	8J	40	LEU
64	8J	47	LEU
64	8J	50	LEU
65	8K	49	THR
65	8K	53	TRP
65	8K	54	ARG
66	8L	13	PHE
66	8L	29	PHE
66	8L	33	PHE
66	8L	37	PHE
66	8L	38	PHE
66	8L	47	LYS
67	8M	2	TYR
67	8M	7	ARG
67	8M	19	LEU
67	8M	41	LYS
68	8N	2	LEU
68	8N	21	PHE
68	8N	60	ASN
68	8N	61	ASP
68	8N	63	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	10	ASN
2	1B	127	HIS
3	1C	88	ASN
3	1C	211	GLN
5	1E	16	ASN
5	1E	55	GLN
5	1E	91	ASN
5	1E	159	ASN
6	1F	29	HIS
6	1F	150	GLN
6	1F	200	GLN
6	1F	250	ASN
6	1F	264	HIS
6	1F	326	GLN
6	1F	373	ASN
6	1F	438	GLN
7	1G	101	HIS
7	1G	182	GLN
8	1H	47	GLN
9	1I	49	ASN
9	1I	150	ASN
10	1J	86	ASN
11	1K	7	ASN
12	1L	23	ASN
12	1L	194	ASN
12	1L	206	ASN
12	1L	505	ASN
12	1L	524	ASN
13	1M	213	HIS
13	1M	220	HIS
13	1M	415	GLN
15	1O	153	ASN
15	1O	309	ASN
16	1P	44	GLN
16	1P	131	HIS
16	1P	136	ASN
16	1P	306	GLN
17	1Q	44	ASN
21	1V	110	GLN
22	1W	58	GLN
22	1W	102	HIS
23	1X	30	HIS
23	1X	150	ASN

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Mol	Chain	Res	Type
24	1Y	128	GLN
25	1Z	76	GLN
26	1a	31	ASN
29	1d	79	GLN
30	1e	20	GLN
33	1h	124	GLN
33	1h	143	ASN
34	1i	73	HIS
34	1i	88	HIS
35	1j	42	HIS
39	1n	11	HIS
39	1n	52	ASN
39	1n	74	GLN
39	1n	123	GLN
40	1o	46	ASN
41	1p	22	GLN
41	1p	106	GLN
41	1p	123	ASN
42	1q	91	HIS
42	1q	135	GLN
43	1r	12	ASN
43	1r	20	GLN
43	1r	35	GLN
44	1s	65	GLN
45	3A	126	GLN
45	3A	136	GLN
45	3A	139	GLN
45	3A	159	GLN
45	3A	339	GLN
45	3A	435	ASN
46	3B	190	GLN
47	3C	32	ASN
47	3C	196	HIS
45	3N	9	GLN
45	3N	274	ASN
48	3Q	105	ASN
49	3R	186	GLN
49	3R	239	HIS
49	3R	257	ASN
51	3T	12	HIS
55	4A	61	HIS
55	4A	80	ASN

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Mol	Chain	Res	Type
55	4A	290	HIS
55	4A	328	HIS
55	4A	406	ASN
55	4A	413	HIS
55	4A	428	GLN
57	4C	9	HIS
57	4C	177	GLN
60	4F	47	ASN
62	4H	32	ASN
66	4L	43	GLN
68	4N	4	GLN
68	4N	55	ASN
1	5A	10	ASN
2	5B	162	GLN
3	5C	71	GLN
3	5C	144	ASN
4	5D	50	ASN
4	5D	135	GLN
4	5D	150	HIS
4	5D	398	HIS
5	5E	16	ASN
6	5F	144	ASN
6	5F	250	ASN
6	5F	373	ASN
7	5G	16	GLN
7	5G	101	HIS
7	5G	182	GLN
7	5G	255	HIS
7	5G	259	ASN
7	5G	581	GLN
10	5J	86	ASN
11	5K	50	ASN
11	5K	57	ASN
12	5L	23	ASN
12	5L	135	ASN
12	5L	194	ASN
12	5L	199	GLN
12	5L	248	HIS
12	5L	296	ASN
13	5M	48	ASN
14	5N	144	GLN
14	5N	221	HIS

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Mol	Chain	Res	Type
14	5N	235	ASN
15	5O	151	HIS
15	5O	288	GLN
16	5P	180	ASN
17	5Q	29	HIS
19	5S	61	GLN
20	5U	47	GLN
23	5X	30	HIS
23	5X	39	ASN
29	5d	46	ASN
29	5d	59	HIS
29	5d	79	GLN
33	5h	69	HIS
33	5h	143	ASN
38	5m	51	ASN
39	5n	11	HIS
39	5n	13	GLN
39	5n	61	GLN
39	5n	77	GLN
39	5n	168	HIS
42	5q	54	GLN
43	5r	12	ASN
43	5r	35	GLN
43	5r	46	HIS
44	5s	65	GLN
44	5s	75	HIS
45	6A	363	ASN
45	6A	435	ASN
46	6B	143	GLN
46	6B	162	ASN
47	6C	26	ASN
47	6C	32	ASN
47	6C	196	HIS
47	6C	312	GLN
48	6D	193	ASN
50	6F	34	ASN
51	6G	14	HIS
52	6H	48	GLN
52	6H	93	HIS
45	6N	6	GLN
45	6N	9	GLN
45	6N	85	HIS

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Mol	Chain	Res	Type
45	6N	141	ASN
45	6N	308	GLN
45	6N	430	GLN
47	6P	374	ASN
48	6Q	105	ASN
48	6Q	156	GLN
49	6R	199	GLN
49	6R	219	HIS
53	6W	47	ASN
55	8A	52	GLN
55	8A	232	GLN
55	8A	428	GLN
56	8B	24	HIS
57	8C	6	HIS
57	8C	12	ASN
57	8C	68	GLN
57	8C	231	HIS
58	8D	76	ASN
59	8E	5	HIS
59	8E	78	HIS
60	8F	88	HIS
62	8H	23	GLN
62	8H	25	GLN
66	8L	42	HIS
67	8M	15	GLN
68	8N	50	ASN
68	8N	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	$\# Z > 2$
13	FME	1M	1	13	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
1	FME	1A	1	1	8,9,10	0.52	0	7,9,11	1.09	1 (14%)
13	FME	5M	1	13	8,9,10	0.52	0	7,9,11	1.04	1 (14%)
34	SAC	5i	1	34	7,8,9	0.54	0	8,9,11	0.86	1 (12%)
11	FME	1K	1	11	8,9,10	0.51	0	7,9,11	1.21	1 (14%)
12	FME	5L	1	12	8,9,10	0.51	0	7,9,11	0.95	1 (14%)
14	FME	5N	1	14	8,9,10	0.52	0	7,9,11	0.99	1 (14%)
34	SAC	1i	1	34	7,8,9	0.54	0	8,9,11	0.89	1 (12%)
8	FME	5H	1	8	8,9,10	0.52	0	7,9,11	1.08	1 (14%)
1	FME	5A	1	1	8,9,10	0.53	0	7,9,11	2.61	3 (42%)
12	FME	1L	1	12	8,9,10	0.51	0	7,9,11	0.88	1 (14%)
8	FME	1H	1	8	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
11	FME	5K	1	11	8,9,10	0.47	0	7,9,11	1.25	1 (14%)
56	FME	8B	1	56	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
55	FME	8A	1	55	8,9,10	0.52	0	7,9,11	1.38	2 (28%)
56	FME	4B	1	56	8,9,10	0.53	0	7,9,11	0.84	1 (14%)
55	FME	4A	1	55	6,7,10	0.55	0	5,5,11	0.64	0
14	FME	1N	1	14	8,9,10	0.51	0	7,9,11	1.05	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	1M	1	13	-	2/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
13	FME	5M	1	13	-	0/7/9/11	-
34	SAC	5i	1	34	-	0/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
12	FME	5L	1	12	-	0/7/9/11	-
14	FME	5N	1	14	-	2/7/9/11	-
34	SAC	1i	1	34	-	0/7/8/10	-
8	FME	5H	1	8	-	1/7/9/11	-
1	FME	5A	1	1	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	1L	1	12	-	0/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
11	FME	5K	1	11	-	0/7/9/11	-
56	FME	8B	1	56	-	1/7/9/11	-
55	FME	8A	1	55	-	3/7/9/11	-
56	FME	4B	1	56	-	1/7/9/11	-
55	FME	4A	1	55	-	2/3/4/11	-
14	FME	1N	1	14	-	1/7/9/11	-

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5A	1	FME	CA-N-CN	4.68	130.02	122.82
1	5A	1	FME	O-C-CA	-3.64	115.24	124.78
1	5A	1	FME	C-CA-N	3.37	115.81	109.73
11	5K	1	FME	O-C-CA	-3.17	116.47	124.78
11	1K	1	FME	O-C-CA	-2.74	117.59	124.78
8	1H	1	FME	O-C-CA	-2.58	118.01	124.78
8	5H	1	FME	O-C-CA	-2.58	118.03	124.78
13	1M	1	FME	O-C-CA	-2.52	118.17	124.78
1	1A	1	FME	O-C-CA	-2.51	118.21	124.78
56	8B	1	FME	O-C-CA	-2.50	118.23	124.78
13	5M	1	FME	O-C-CA	-2.49	118.26	124.78
14	1N	1	FME	O-C-CA	-2.47	118.30	124.78
55	8A	1	FME	O-C-CA	-2.45	118.37	124.78
14	5N	1	FME	O-C-CA	-2.42	118.43	124.78
34	1i	1	SAC	O-C-CA	-2.36	118.59	124.78
12	5L	1	FME	O-C-CA	-2.35	118.62	124.78
34	5i	1	SAC	O-C-CA	-2.30	118.75	124.78
55	8A	1	FME	CA-N-CN	2.28	126.33	122.82
12	1L	1	FME	O-C-CA	-2.17	119.10	124.78
56	4B	1	FME	O-C-CA	-2.16	119.12	124.78

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	CB-CA-N-CN
8	1H	1	FME	O1-CN-N-CA
11	1K	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
13	1M	1	FME	O-C-CA-CB
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
8	5H	1	FME	O1-CN-N-CA
14	5N	1	FME	O1-CN-N-CA
56	8B	1	FME	O1-CN-N-CA
55	8A	1	FME	CA-CB-CG-SD
14	5N	1	FME	CB-CG-SD-CE
55	4A	1	FME	CA-CB-CG-SD
55	8A	1	FME	C-CA-CB-CG
1	5A	1	FME	CB-CG-SD-CE
13	1M	1	FME	C-CA-CB-CG
55	4A	1	FME	C-CA-CB-CG
55	8A	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 14 are monoatomic - leaving 176 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	$\# Z > 2$
75	CDL	1a	201	-	60,60,99	0.34	0	66,72,111	0.43	0
86	PGV	4A	602	-	50,50,50	0.33	0	53,56,56	1.00	2 (3%)
70	PC1	5q	201	-	48,48,53	0.27	0	54,56,61	0.33	0
75	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.43	1 (0%)
75	CDL	8A	605	-	99,99,99	0.26	0	105,111,111	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	1d	202	-	48,48,50	0.26	0	51,53,55	0.35	0
75	CDL	1X	201	-	85,85,99	0.28	0	91,97,111	0.38	0
82	MYR	1l	201	-	14,14,15	0.34	0	13,13,15	0.39	0
86	PGV	4C	303	-	50,50,50	0.28	0	53,56,56	0.31	0
69	3PE	1A	201	-	46,46,50	0.27	0	49,51,55	0.35	0
75	CDL	1N	401	-	61,61,99	0.31	0	67,73,111	0.65	1 (1%)
75	CDL	5d	201	-	85,85,99	0.31	0	91,97,111	0.54	1 (1%)
69	3PE	5M	906	-	49,49,50	0.26	0	52,54,55	0.31	0
69	3PE	5Y	203	-	39,39,50	0.31	0	42,44,55	0.49	0
75	CDL	5N	401	-	61,61,99	0.31	0	67,73,111	0.61	1 (1%)
80	EHZ	1n	201	-	29,36,37	0.15	0	35,44,47	1.08	1 (2%)
84	HEM	3P	502	47	41,50,50	1.35	6 (14%)	45,82,82	1.74	7 (15%)
92	PEK	8G	102	-	52,52,52	0.27	0	55,57,57	0.41	0
70	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.34	0
69	3PE	1j	101	-	43,43,50	0.28	0	46,48,55	0.42	0
69	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.33	0
69	3PE	5M	903	-	47,47,50	0.27	0	50,52,55	0.35	0
72	FES	6E	301	49	0,4,4	-	-	-		
70	PC1	5M	905	-	43,43,53	0.30	0	49,51,61	0.37	0
70	PC1	5H	403	-	47,47,53	0.29	0	53,55,61	0.37	0
72	FES	3R	301	49	0,4,4	-	-	-		
86	PGV	5i	201	34	50,50,50	0.28	0	53,56,56	0.36	0
69	3PE	5P	403	-	34,34,50	0.32	0	37,39,55	0.43	0
70	PC1	5H	402	-	53,53,53	0.26	0	59,61,61	0.35	0
70	PC1	5B	203	-	47,47,53	0.28	0	53,55,61	0.41	0
70	PC1	5h	202	-	46,46,53	0.28	0	52,54,61	0.30	0
73	FMN	5F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
72	FES	1G	803	7	0,4,4	-	-	-		
72	FES	1E	301	5	0,4,4	-	-	-		
84	HEM	6C	502	-	41,50,50	1.34	7 (17%)	45,82,82	1.72	6 (13%)
72	FES	5E	301	5	0,4,4	-	-	-		
84	HEM	6C	501	47	41,50,50	1.34	6 (14%)	45,82,82	1.87	8 (17%)
71	SF4	5B	201	2	0,12,12	-	-	-		
70	PC1	5B	202	-	45,45,53	0.28	0	51,53,61	0.37	0
75	CDL	4D	201	-	99,99,99	0.26	0	105,111,111	0.41	0
70	PC1	1M	504	-	43,43,53	0.36	0	49,51,61	0.42	0
70	PC1	1B	203	-	47,47,53	0.28	0	53,55,61	0.39	0
86	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.74	1 (1%)
75	CDL	1h	202	-	79,79,99	0.30	0	85,91,111	0.46	0
71	SF4	1I	203	9	0,12,12	-	-	-		
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	1Y	203	-	32,32,50	0.32	0	35,37,55	0.50	0
75	CDL	5a	201	-	60,60,99	0.33	0	66,72,111	0.42	0
75	CDL	5d	204	-	64,64,99	0.32	0	70,76,111	0.47	0
69	3PE	1Y	204	-	26,26,50	0.35	0	29,31,55	0.54	0
92	PEK	4C	308	-	52,52,52	0.26	0	55,57,57	0.38	0
76	GTP	5O	401	77	26,34,34	0.95	2 (7%)	32,54,54	0.82	1 (3%)
86	PGV	8A	604	-	50,50,50	0.28	0	53,56,56	0.41	0
69	3PE	1d	201	-	47,47,50	0.27	0	50,52,55	0.33	0
86	PGV	4C	305	-	50,50,50	0.29	0	53,56,56	0.47	1 (1%)
69	3PE	5Y	204	-	29,29,50	0.34	0	32,34,55	0.75	1 (3%)
86	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
73	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.70	1 (2%)
70	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.38	0
85	HEC	3D	501	48	31,49,50	2.45	12 (38%)	22,80,82	2.24	4 (18%)
87	HEA	8A	606	55	57,67,67	2.23	20 (35%)	61,103,103	2.35	26 (42%)
69	3PE	5d	202	-	48,48,50	0.26	0	51,53,55	0.35	0
86	PGV	8C	306	-	50,50,50	0.29	0	53,56,56	0.35	0
71	SF4	1I	202	9	0,12,12	-	-	-	-	-
71	SF4	5I	202	9	0,12,12	-	-	-	-	-
69	3PE	1K	101	-	43,43,50	0.28	0	46,48,55	0.33	0
69	3PE	5M	904	-	50,50,50	0.27	0	53,55,55	0.48	0
71	SF4	1G	802	7	0,12,12	-	-	-	-	-
86	PGV	8B	301	56	50,50,50	0.27	0	53,56,56	0.41	0
86	PGV	8D	202	-	50,50,50	0.30	0	53,56,56	0.40	0
69	3PE	1m	201	-	40,40,50	0.28	0	43,45,55	0.38	0
93	PO4	8H	101	-	4,4,4	0.92	0	6,6,6	0.43	0
75	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.58	0
86	PGV	8C	302	-	50,50,50	0.28	0	53,56,56	0.30	0
90	CUA	4B	303	56	0,1,1	-	-	-	-	-
86	PGV	8A	601	-	50,50,50	0.28	0	53,56,56	0.42	0
86	PGV	8A	602	-	50,50,50	0.28	0	53,56,56	0.34	0
86	PGV	8C	301	-	50,50,50	0.29	0	53,56,56	0.65	1 (1%)
69	3PE	5L	701	-	45,45,50	0.28	0	48,50,55	0.32	0
87	HEA	8A	607	55	57,67,67	2.02	16 (28%)	61,103,103	2.55	26 (42%)
78	NDP	5P	402	-	45,52,52	0.61	0	53,80,80	0.76	2 (3%)
75	CDL	5L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
70	PC1	5Y	201	-	34,34,53	0.32	0	40,42,61	0.54	1 (2%)
70	PC1	1A	202	-	34,34,53	0.33	0	40,42,61	0.41	0
84	HEM	6P	502	47	41,50,50	1.35	7 (17%)	45,82,82	1.76	7 (15%)
69	3PE	1M	505	-	49,49,50	0.27	0	52,54,55	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	HEC	3Q	501	-	32,50,50	2.44	12 (37%)	24,82,82	2.27	4 (16%)
69	3PE	1M	501	-	44,44,50	0.28	0	47,49,55	0.37	0
70	PC1	1d	203	-	38,38,53	0.30	0	44,46,61	0.46	0
71	SF4	5F	502	6	0,12,12	-	-	-		
84	HEM	6P	501	47	41,50,50	1.36	6 (14%)	45,82,82	1.83	8 (17%)
69	3PE	1M	503	-	50,50,50	0.28	0	53,55,55	0.43	0
75	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.39	0
69	3PE	1P	403	-	34,34,50	0.32	0	37,39,55	0.43	0
70	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.36	0
86	PGV	4G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
86	PGV	4K	101	-	50,50,50	0.29	0	53,56,56	0.33	0
91	PSC	4B	304	-	51,51,51	0.29	0	57,59,59	0.45	1 (1%)
71	SF4	1G	801	7	0,12,12	-	-	-		
69	3PE	1L	704	-	48,48,50	0.27	0	51,53,55	0.37	0
69	3PE	5L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
70	PC1	5d	203	-	38,38,53	0.30	0	44,46,61	0.46	0
69	3PE	1Y	202	-	29,29,50	0.34	0	32,34,55	0.82	1 (3%)
71	SF4	5G	801	7	0,12,12	-	-	-		
71	SF4	5I	201	9	0,12,12	-	-	-		
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
80	EHZ	1T	101	20	29,36,37	0.17	0	35,44,47	1.04	1 (2%)
91	PSC	8A	611	-	51,51,51	0.31	0	57,59,59	0.54	1 (1%)
90	CUA	8B	302	56	0,1,1	-	-	-		
86	PGV	4L	101	-	50,50,50	0.28	0	53,56,56	0.42	0
69	3PE	5m	201	-	40,40,50	0.28	0	43,45,55	0.38	0
84	HEM	3C	502	-	41,50,50	1.35	6 (14%)	45,82,82	1.77	8 (17%)
80	EHZ	5n	201	-	29,36,37	0.14	0	35,44,47	1.02	1 (2%)
81	AME	5N	402	-	9,10,11	0.49	0	9,11,13	1.01	1 (11%)
69	3PE	5A	201	-	46,46,50	0.27	0	49,51,55	0.40	0
80	EHZ	5T	101	20	29,36,37	0.17	0	35,44,47	1.24	1 (2%)
81	AME	1h	201	-	9,10,11	0.49	0	9,11,13	0.95	1 (11%)
69	3PE	1Y	201	-	39,39,50	0.31	0	42,44,55	0.49	0
83	AYA	5q	202	-	6,7,8	0.65	0	5,8,10	0.40	0
70	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.45	0
70	PC1	1q	201	-	48,48,53	0.27	0	54,56,61	0.39	0
70	PC1	1M	502	-	34,34,53	0.33	0	40,42,61	0.63	1 (2%)
75	CDL	5h	201	-	79,79,99	0.30	0	85,91,111	0.40	0
70	PC1	1I	201	-	53,53,53	0.32	0	59,61,61	0.81	3 (5%)
82	MYR	5I	201	-	14,14,15	0.34	0	13,13,15	0.38	0
86	PGV	8J	101	-	50,50,50	0.27	0	53,56,56	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	5Y	205	-	32,32,50	0.33	0	35,37,55	0.56	0
69	3PE	5j	101	-	43,43,50	0.29	0	46,48,55	0.49	1 (2%)
75	CDL	8C	305	-	99,99,99	0.39	1 (1%)	105,111,111	0.56	0
86	PGV	8G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
69	3PE	5K	101	-	43,43,50	0.29	0	46,48,55	0.35	0
71	SF4	1B	201	2	0,12,12	-	-	-	-	-
84	HEM	3C	501	47	41,50,50	1.33	7 (17%)	45,82,82	1.83	9 (20%)
75	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.30	0
69	3PE	1L	705	-	30,30,50	0.33	0	33,35,55	0.55	0
86	PGV	4A	601	-	50,50,50	0.29	0	53,56,56	0.42	0
78	NDP	1P	402	-	45,52,52	0.60	0	53,80,80	0.79	2 (3%)
86	PGV	4C	301	-	50,50,50	0.29	0	53,56,56	0.32	0
76	GTP	1O	401	77	26,34,34	0.95	2 (7%)	32,54,54	0.80	0
75	CDL	1d	204	-	64,64,99	0.31	0	70,76,111	0.43	0
86	PGV	8L	101	-	50,50,50	0.28	0	53,56,56	0.37	0
85	HEC	6Q	501	48	32,50,50	2.50	12 (37%)	24,82,82	2.29	4 (16%)
84	HEM	3P	501	47	41,50,50	1.34	5 (12%)	45,82,82	1.91	11 (24%)
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
71	SF4	5G	802	7	0,12,12	-	-	-	-	-
69	3PE	5Y	206	-	26,26,50	0.34	0	29,31,55	0.53	0
69	3PE	5Y	202	-	30,30,50	0.33	0	33,35,55	0.50	0
70	PC1	1L	706	-	45,45,53	0.29	0	51,53,61	0.31	0
70	PC1	5I	203	-	43,43,53	0.29	0	49,51,61	0.32	0
72	FES	6R	301	49	0,4,4	-	-	-	-	-
87	HEA	4A	604	55	57,67,67	2.24	21 (36%)	61,103,103	2.38	24 (39%)
92	PEK	8C	307	-	51,51,52	0.29	0	54,56,57	0.68	2 (3%)
92	PEK	4C	309	-	51,51,52	0.27	0	54,56,57	0.43	0
70	PC1	1H	402	-	47,47,53	0.42	0	53,55,61	1.17	5 (9%)
70	PC1	5A	203	-	34,34,53	0.32	0	40,42,61	0.38	0
86	PGV	4C	304	-	50,50,50	0.29	0	53,56,56	0.52	0
86	PGV	8C	304	-	50,50,50	0.30	0	53,56,56	0.45	0
72	FES	3E	301	49	0,4,4	-	-	-	-	-
72	FES	5G	803	7	0,4,4	-	-	-	-	-
86	PGV	8A	603	-	50,50,50	0.28	0	53,56,56	0.35	0
69	3PE	5M	901	-	48,48,50	0.27	0	51,53,55	0.38	0
86	PGV	4C	307	-	50,50,50	0.28	0	53,56,56	0.35	0
87	HEA	4A	605	55	57,67,67	2.06	18 (31%)	61,103,103	2.50	26 (42%)
70	PC1	5Y	207	-	45,45,53	0.28	0	51,53,61	0.31	0
70	PC1	1B	202	-	45,45,53	0.27	0	51,53,61	0.36	0
86	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	AYA	1q	202	-	6,7,8	0.64	0	5,8,10	0.41	0
86	PGV	4A	603	-	50,50,50	0.29	0	53,56,56	0.37	0
86	PGV	4B	301	56	50,50,50	0.29	0	53,56,56	0.44	1 (1%)
86	PGV	4J	101	-	50,50,50	0.29	0	53,56,56	0.40	0
75	CDL	5H	401	-	50,50,99	0.36	0	56,62,111	0.58	0
69	3PE	5M	902	-	44,44,50	0.29	0	47,49,55	0.37	0
93	PO4	4H	101	-	4,4,4	0.93	0	6,6,6	0.42	0
70	PC1	1P	401	-	32,32,53	0.34	0	38,40,61	0.37	0
71	SF4	1F	502	6	0,12,12	-	-	-	-	-
85	HEC	6D	501	48	31,49,50	2.49	12 (38%)	22,80,82	2.34	5 (22%)

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
75	CDL	1a	201	-	-	10/71/71/110	-
86	PGV	4A	602	-	-	9/55/55/55	-
71	SF4	1F	502	6	-	-	0/6/5/5
70	PC1	5q	201	-	-	4/52/52/57	-
75	CDL	4C	306	-	-	25/110/110/110	-
75	CDL	8A	605	-	-	15/110/110/110	-
69	3PE	1d	202	-	-	11/52/52/54	-
75	CDL	1X	201	-	-	20/96/96/110	-
82	MYR	1l	201	-	-	1/11/12/13	-
86	PGV	4C	303	-	-	10/55/55/55	-
69	3PE	1A	201	-	-	8/50/50/54	-
75	CDL	1N	401	-	-	17/71/71/110	-
75	CDL	5d	201	-	-	22/96/96/110	-
69	3PE	5M	906	-	-	7/53/53/54	-
69	3PE	5Y	203	-	-	12/43/43/54	-
75	CDL	5N	401	-	-	18/71/71/110	-
80	EHZ	1n	201	-	-	5/42/44/45	-
84	HEM	3P	502	47	-	6/12/54/54	-
92	PEK	8G	102	-	-	5/56/56/56	-
70	PC1	1I	204	-	-	5/47/47/57	-
69	3PE	1j	101	-	-	5/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1L	701	-	-	5/49/49/54	-
69	3PE	5M	903	-	-	18/51/51/54	-
72	FES	6E	301	49	-	-	0/1/1/1
70	PC1	5M	905	-	-	13/47/47/57	-
70	PC1	5H	403	-	-	8/51/51/57	-
86	PGV	5i	201	34	-	4/55/55/55	-
72	FES	3R	301	49	-	-	0/1/1/1
69	3PE	5P	403	-	-	8/38/38/54	-
70	PC1	5H	402	-	-	9/57/57/57	-
70	PC1	5B	203	-	-	11/51/51/57	-
70	PC1	5h	202	-	-	14/50/50/57	-
73	FMN	5F	501	-	-	7/18/18/18	0/3/3/3
72	FES	1G	803	7	-	-	0/1/1/1
72	FES	1E	301	5	-	-	0/1/1/1
84	HEM	6C	502	-	-	4/12/54/54	-
84	HEM	6C	501	47	-	5/12/54/54	-
72	FES	5E	301	5	-	-	0/1/1/1
71	SF4	5B	201	2	-	-	0/6/5/5
70	PC1	5B	202	-	-	4/49/49/57	-
75	CDL	4D	201	-	-	24/110/110/110	-
70	PC1	1M	504	-	-	17/47/47/57	-
70	PC1	1B	203	-	-	10/51/51/57	-
86	PGV	4C	302	-	-	13/55/55/55	-
75	CDL	1h	202	-	-	23/90/90/110	-
71	SF4	1I	203	9	-	-	0/6/5/5
70	PC1	1h	203	-	-	13/50/50/57	-
69	3PE	1Y	203	-	-	6/36/36/54	-
75	CDL	5a	201	-	-	9/71/71/110	-
75	CDL	5d	204	-	-	21/75/75/110	-
69	3PE	1Y	204	-	-	7/30/30/54	-
92	PEK	4C	308	-	-	8/56/56/56	-
76	GTP	5O	401	77	-	4/18/38/38	0/3/3/3
86	PGV	8A	604	-	-	3/55/55/55	-
69	3PE	1d	201	-	-	16/51/51/54	-
86	PGV	4C	305	-	-	7/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	5Y	204	-	-	12/33/33/54	-
86	PGV	8K	101	-	-	13/55/55/55	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
70	PC1	5P	401	-	-	4/36/36/57	-
85	HEC	3D	501	48	-	3/8/53/54	-
87	HEA	8A	606	55	-	12/32/76/76	-
69	3PE	5d	202	-	-	8/52/52/54	-
86	PGV	8C	306	-	-	3/55/55/55	-
71	SF4	1I	202	9	-	-	0/6/5/5
69	3PE	1K	101	-	-	11/47/47/54	-
71	SF4	5I	202	9	-	-	0/6/5/5
69	3PE	5M	904	-	-	12/54/54/54	-
86	PGV	8B	301	56	-	6/55/55/55	-
71	SF4	1G	802	7	-	-	0/6/5/5
86	PGV	8D	202	-	-	15/55/55/55	-
69	3PE	1m	201	-	-	12/44/44/54	-
75	CDL	1H	401	-	-	10/61/61/110	-
86	PGV	8C	302	-	-	10/55/55/55	-
86	PGV	8A	601	-	-	18/55/55/55	-
86	PGV	8A	602	-	-	6/55/55/55	-
86	PGV	8C	301	-	-	12/55/55/55	-
69	3PE	5L	701	-	-	7/49/49/54	-
87	HEA	8A	607	55	-	4/32/76/76	-
78	NDP	5P	402	-	-	5/30/77/77	0/5/5/5
75	CDL	5L	702	-	-	19/86/86/110	-
70	PC1	5Y	201	-	-	10/38/38/57	-
70	PC1	1A	202	-	-	5/38/38/57	-
84	HEM	6P	502	47	-	6/12/54/54	-
69	3PE	1M	505	-	-	9/53/53/54	-
85	HEC	3Q	501	-	-	2/10/54/54	-
69	3PE	1M	501	-	-	9/48/48/54	-
70	PC1	1d	203	-	-	10/42/42/57	-
71	SF4	5F	502	6	-	-	0/6/5/5
84	HEM	6P	501	47	-	6/12/54/54	-
69	3PE	1M	503	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	8D	201	-	-	21/110/110/110	-
69	3PE	1P	403	-	-	7/38/38/54	-
70	PC1	1J	201	-	-	4/38/38/57	-
86	PGV	4G	101	-	-	10/55/55/55	-
86	PGV	4K	101	-	-	11/55/55/55	-
91	PSC	4B	304	-	-	18/55/55/55	-
71	SF4	1G	801	7	-	-	0/6/5/5
69	3PE	1L	704	-	-	12/52/52/54	-
69	3PE	5L	703	-	-	6/48/48/54	-
70	PC1	5d	203	-	-	8/42/42/57	-
69	3PE	1Y	202	-	-	13/33/33/54	-
71	SF4	5G	801	7	-	-	0/6/5/5
75	CDL	1L	702	-	-	24/86/86/110	-
80	EHZ	1T	101	20	-	10/42/44/45	-
91	PSC	8A	611	-	-	23/55/55/55	-
71	SF4	5I	201	9	-	-	0/6/5/5
86	PGV	4L	101	-	-	14/55/55/55	-
69	3PE	5m	201	-	-	14/44/44/54	-
84	HEM	3C	502	-	-	4/12/54/54	-
80	EHZ	5n	201	-	-	4/42/44/45	-
81	AME	5N	402	-	-	0/9/10/12	-
69	3PE	5A	201	-	-	8/50/50/54	-
80	EHZ	5T	101	20	-	9/42/44/45	-
81	AME	1h	201	-	-	1/9/10/12	-
69	3PE	1Y	201	-	-	12/43/43/54	-
83	AYA	5q	202	-	-	0/4/6/8	-
70	PC1	5A	202	-	-	12/38/38/57	-
70	PC1	1q	201	-	-	4/52/52/57	-
70	PC1	1M	502	-	-	10/38/38/57	-
75	CDL	5h	201	-	-	22/90/90/110	-
70	PC1	1I	201	-	-	9/57/57/57	-
82	MYR	5l	201	-	-	0/11/12/13	-
86	PGV	8J	101	-	-	7/55/55/55	-
69	3PE	5Y	205	-	-	5/36/36/54	-
69	3PE	5j	101	-	-	8/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	8C	305	-	-	23/110/110/110	-
86	PGV	8G	101	-	-	9/55/55/55	-
69	3PE	5K	101	-	-	10/47/47/54	-
84	HEM	3C	501	47	-	5/12/54/54	-
71	SF4	1B	201	2	-	-	0/6/5/5
75	CDL	4B	302	-	-	20/110/110/110	-
69	3PE	1L	705	-	-	10/34/34/54	-
86	PGV	4A	601	-	-	17/55/55/55	-
78	NDP	1P	402	-	-	6/30/77/77	0/5/5/5
86	PGV	4C	301	-	-	6/55/55/55	-
76	GTP	1O	401	77	-	5/18/38/38	0/3/3/3
75	CDL	1d	204	-	-	16/75/75/110	-
86	PGV	8L	101	-	-	7/55/55/55	-
85	HEC	6Q	501	48	-	2/10/54/54	-
84	HEM	3P	501	47	-	7/12/54/54	-
69	3PE	1L	703	-	-	8/48/48/54	-
69	3PE	5Y	206	-	-	7/30/30/54	-
69	3PE	5Y	202	-	-	12/34/34/54	-
70	PC1	1L	706	-	-	9/49/49/57	-
70	PC1	5I	203	-	-	6/47/47/57	-
71	SF4	5G	802	7	-	-	0/6/5/5
72	FES	6R	301	49	-	-	0/1/1/1
87	HEA	4A	604	55	-	10/32/76/76	-
92	PEK	8C	307	-	-	5/55/55/56	-
92	PEK	4C	309	-	-	3/55/55/56	-
70	PC1	1H	402	-	-	6/51/51/57	-
70	PC1	5A	203	-	-	4/38/38/57	-
86	PGV	8C	304	-	-	6/55/55/55	-
72	FES	3E	301	49	-	-	0/1/1/1
72	FES	5G	803	7	-	-	0/1/1/1
86	PGV	8A	603	-	-	8/55/55/55	-
69	3PE	5M	901	-	-	13/52/52/54	-
86	PGV	4C	307	-	-	7/55/55/55	-
87	HEA	4A	605	55	-	5/32/76/76	-
70	PC1	5Y	207	-	-	8/49/49/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	1B	202	-	-	3/49/49/57	-
86	PGV	8C	303	-	-	10/55/55/55	-
83	AYA	1q	202	-	-	0/4/6/8	-
86	PGV	4A	603	-	-	8/55/55/55	-
86	PGV	4B	301	56	-	7/55/55/55	-
86	PGV	4J	101	-	-	9/55/55/55	-
75	CDL	5H	401	-	-	8/61/61/110	-
69	3PE	5M	902	-	-	11/48/48/54	-
70	PC1	1P	401	-	-	3/36/36/57	-
86	PGV	4C	304	-	-	14/55/55/55	-
85	HEC	6D	501	48	-	4/8/53/54	-

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	6Q	501	HEC	C2B-C3B	7.45	1.48	1.40
85	6Q	501	HEC	C3C-C2C	7.23	1.48	1.40
85	3Q	501	HEC	C2B-C3B	7.12	1.48	1.40
85	6D	501	HEC	C2B-C3B	7.08	1.48	1.40
85	3Q	501	HEC	C3C-C2C	7.03	1.48	1.40
85	6D	501	HEC	C3C-C2C	7.03	1.48	1.40
85	3D	501	HEC	C3C-C2C	6.99	1.48	1.40
85	3D	501	HEC	C2B-C3B	6.93	1.48	1.40
87	8A	606	HEA	C3A-C2A	6.25	1.49	1.40
87	4A	604	HEA	C3B-C2B	6.09	1.48	1.34
87	8A	606	HEA	C3B-C2B	6.09	1.48	1.34
87	4A	604	HEA	C3A-C2A	5.91	1.48	1.40
87	4A	605	HEA	C3B-C2B	5.55	1.47	1.34
87	8A	607	HEA	C3B-C2B	5.48	1.47	1.34
87	8A	606	HEA	C3D-C2D	5.40	1.48	1.36
87	4A	604	HEA	C3D-C2D	5.29	1.48	1.36
87	8A	606	HEA	CHD-C1D	5.25	1.48	1.35
87	4A	604	HEA	CHD-C1D	5.08	1.48	1.35
87	4A	605	HEA	C3D-C2D	5.07	1.47	1.36
87	4A	604	HEA	C3C-C2C	5.03	1.47	1.40
87	4A	604	HEA	CHC-C4B	5.01	1.47	1.35
87	8A	607	HEA	C3A-C2A	4.89	1.47	1.40
87	4A	605	HEA	C3C-C2C	4.82	1.47	1.40
87	8A	607	HEA	C3D-C2D	4.80	1.46	1.36
87	8A	606	HEA	C3C-C2C	4.79	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4A	605	HEA	CHD-C1D	4.78	1.47	1.35
87	4A	605	HEA	C3A-C2A	4.69	1.46	1.40
87	8A	607	HEA	CHD-C1D	4.65	1.46	1.35
87	8A	606	HEA	CHC-C4B	4.42	1.46	1.35
87	8A	607	HEA	CHC-C4B	4.36	1.46	1.35
87	8A	607	HEA	C3C-C2C	4.36	1.46	1.40
87	4A	605	HEA	CHC-C4B	4.22	1.45	1.35
84	3C	502	HEM	C4D-ND	-3.65	1.34	1.40
84	3C	502	HEM	C1B-NB	-3.61	1.34	1.40
84	3P	502	HEM	C1B-NB	-3.60	1.34	1.40
84	6P	502	HEM	C1B-NB	-3.60	1.34	1.40
84	6P	502	HEM	C4D-ND	-3.58	1.34	1.40
84	6C	502	HEM	C1B-NB	-3.58	1.34	1.40
84	3P	501	HEM	C1B-NB	-3.54	1.34	1.40
84	6P	501	HEM	C1B-NB	-3.54	1.34	1.40
85	6D	501	HEC	C3C-C4C	3.52	1.49	1.43
84	3P	502	HEM	C4D-ND	-3.51	1.34	1.40
85	6Q	501	HEC	C2A-C3A	3.48	1.48	1.37
84	6C	502	HEM	C4D-ND	-3.47	1.34	1.40
84	6P	501	HEM	C4D-ND	-3.46	1.34	1.40
85	6Q	501	HEC	C3D-C2D	3.44	1.47	1.37
85	3Q	501	HEC	C2A-C3A	3.43	1.47	1.37
85	3D	501	HEC	C2A-C3A	3.41	1.47	1.37
84	3C	501	HEM	C4D-ND	-3.39	1.34	1.40
85	3Q	501	HEC	C3D-C2D	3.39	1.47	1.37
84	6C	501	HEM	C1B-NB	-3.39	1.34	1.40
87	8A	606	HEA	C1D-ND	-3.38	1.34	1.40
84	3C	501	HEM	C1B-NB	-3.38	1.34	1.40
84	6C	501	HEM	C4D-ND	-3.37	1.34	1.40
85	6D	501	HEC	C2A-C3A	3.37	1.47	1.37
87	4A	604	HEA	C4B-NB	-3.37	1.34	1.40
85	3D	501	HEC	C3C-C4C	3.34	1.49	1.43
87	8A	606	HEA	C4B-NB	-3.30	1.34	1.40
85	6D	501	HEC	C3D-C2D	3.26	1.47	1.37
84	3P	501	HEM	C4D-ND	-3.23	1.34	1.40
85	6D	501	HEC	C4B-C3B	3.20	1.48	1.43
85	3D	501	HEC	C4B-C3B	3.14	1.48	1.43
87	4A	604	HEA	C1D-ND	-3.14	1.34	1.40
87	4A	605	HEA	C4B-NB	-3.13	1.34	1.40
85	3Q	501	HEC	C3C-C4C	3.12	1.48	1.43
85	3D	501	HEC	C3D-C2D	3.06	1.46	1.37
87	4A	605	HEA	C2A-C1A	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4A	605	HEA	C1D-ND	-3.05	1.35	1.40
85	6D	501	HEC	C1D-CHD	3.03	1.49	1.41
87	8A	607	HEA	C4B-NB	-3.03	1.35	1.40
87	8A	607	HEA	FE-NB	2.96	2.11	1.96
87	8A	607	HEA	FE-ND	2.95	2.11	1.96
87	4A	604	HEA	C4B-C3B	2.91	1.49	1.44
87	8A	607	HEA	C1D-ND	-2.88	1.35	1.40
87	4A	605	HEA	FE-NB	2.87	2.11	1.96
85	6D	501	HEC	C2A-C1A	2.87	1.49	1.42
85	6Q	501	HEC	C3C-C4C	2.87	1.48	1.43
85	3Q	501	HEC	C2A-C1A	2.86	1.49	1.42
87	8A	607	HEA	C2A-C1A	2.84	1.49	1.42
85	3Q	501	HEC	C3A-C4A	2.84	1.49	1.42
84	3C	501	HEM	FE-NB	2.83	2.10	1.96
85	6Q	501	HEC	C3A-C4A	2.83	1.49	1.42
87	4A	605	HEA	FE-ND	2.81	2.10	1.96
85	6Q	501	HEC	C4B-C3B	2.81	1.48	1.43
84	3P	501	HEM	FE-NB	2.80	2.10	1.96
84	6P	501	HEM	FE-NB	2.79	2.10	1.96
85	3D	501	HEC	C3A-C4A	2.77	1.48	1.42
85	3D	501	HEC	C2A-C1A	2.76	1.48	1.42
84	6C	501	HEM	FE-NB	2.76	2.10	1.96
85	6D	501	HEC	C3A-C4A	2.71	1.48	1.42
85	3D	501	HEC	C1D-CHD	2.71	1.48	1.41
87	8A	606	HEA	C2A-C1A	2.70	1.48	1.42
85	3Q	501	HEC	C1D-CHD	2.70	1.48	1.41
84	3C	502	HEM	FE-NB	2.70	2.10	1.96
84	6P	502	HEM	FE-NB	2.70	2.10	1.96
84	6C	502	HEM	FE-NB	2.69	2.10	1.96
84	3P	502	HEM	FE-NB	2.69	2.10	1.96
85	6Q	501	HEC	C2A-C1A	2.66	1.48	1.42
87	4A	604	HEA	C2A-C1A	2.65	1.48	1.42
85	6Q	501	HEC	C1B-CHB	2.65	1.48	1.41
87	8A	607	HEA	C4B-C3B	2.59	1.49	1.44
87	8A	606	HEA	FE-NB	2.57	2.09	1.96
76	1O	401	GTP	C5-C6	-2.57	1.42	1.47
76	5O	401	GTP	C5-C6	-2.57	1.42	1.47
85	3Q	501	HEC	C4B-C3B	2.57	1.47	1.43
85	6Q	501	HEC	C1D-CHD	2.56	1.48	1.41
87	8A	606	HEA	FE-ND	2.55	2.09	1.96
87	8A	606	HEA	C4C-CHD	2.53	1.48	1.41
87	4A	604	HEA	FE-ND	2.53	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	6Q	501	HEC	C1C-CHC	2.51	1.48	1.41
85	3Q	501	HEC	C1B-CHB	2.50	1.48	1.41
87	8A	606	HEA	CHB-C1B	2.50	1.48	1.41
85	6D	501	HEC	C4D-CHA	2.49	1.47	1.41
85	6Q	501	HEC	C4D-CHA	2.49	1.47	1.41
87	4A	604	HEA	CHB-C1B	2.48	1.48	1.41
85	3Q	501	HEC	C4D-CHA	2.47	1.47	1.41
87	8A	606	HEA	C4D-C3D	2.47	1.49	1.45
85	6D	501	HEC	C1C-CHC	2.47	1.47	1.41
84	6C	501	HEM	C1D-ND	-2.46	1.33	1.38
85	3Q	501	HEC	C1C-CHC	2.45	1.47	1.41
87	4A	604	HEA	FE-NB	2.42	2.08	1.96
87	8A	606	HEA	C1B-C2B	2.42	1.49	1.44
85	3D	501	HEC	C4D-CHA	2.41	1.47	1.41
87	4A	604	HEA	C4C-CHD	2.38	1.47	1.41
87	8A	606	HEA	C1B-NB	-2.37	1.33	1.38
87	4A	604	HEA	C1C-CHC	2.36	1.47	1.41
84	3P	501	HEM	C1D-ND	-2.33	1.34	1.38
87	4A	605	HEA	C4B-C3B	2.33	1.48	1.44
87	4A	604	HEA	C1B-C2B	2.33	1.49	1.44
85	3D	501	HEC	C1C-CHC	2.33	1.47	1.41
85	6D	501	HEC	C1B-CHB	2.31	1.47	1.41
87	8A	606	HEA	C1D-C2D	2.29	1.49	1.44
85	3D	501	HEC	C1B-CHB	2.27	1.47	1.41
87	4A	604	HEA	C4D-C3D	2.27	1.48	1.45
84	3P	502	HEM	C1D-ND	-2.26	1.34	1.38
87	4A	604	HEA	C1B-NB	-2.26	1.34	1.38
84	6P	502	HEM	C1D-ND	-2.26	1.34	1.38
87	4A	604	HEA	CHA-C4D	2.25	1.47	1.41
84	6P	501	HEM	C1D-ND	-2.24	1.34	1.38
87	4A	605	HEA	C4C-CHD	2.22	1.47	1.41
87	8A	607	HEA	C1D-C2D	2.21	1.48	1.44
87	8A	606	HEA	C1C-CHC	2.20	1.47	1.41
87	4A	604	HEA	C1D-C2D	2.19	1.48	1.44
87	8A	607	HEA	C4C-CHD	2.17	1.47	1.41
87	8A	607	HEA	C1B-C2B	2.16	1.48	1.44
84	6C	502	HEM	C1D-ND	-2.14	1.34	1.38
87	4A	605	HEA	C1B-NB	-2.13	1.34	1.38
84	6P	502	HEM	FE-ND	-2.13	1.86	1.96
87	8A	606	HEA	C4B-C3B	2.12	1.48	1.44
84	3C	501	HEM	C1D-ND	-2.12	1.34	1.38
84	6C	501	HEM	FE-ND	-2.11	1.86	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	8C	305	CDL	C72-C71	-2.11	1.44	1.52
87	4A	605	HEA	CHA-C4D	2.11	1.47	1.41
84	3P	502	HEM	FE-ND	-2.11	1.86	1.96
87	4A	605	HEA	C1B-C2B	2.10	1.48	1.44
84	3C	502	HEM	FE-ND	-2.09	1.86	1.96
84	3P	501	HEM	FE-ND	-2.08	1.86	1.96
84	6P	501	HEM	C4B-NB	-2.07	1.34	1.38
84	6C	502	HEM	C4B-NB	-2.07	1.34	1.38
84	6C	501	HEM	C4B-NB	-2.07	1.34	1.38
76	5O	401	GTP	C8-N7	-2.07	1.31	1.35
84	6C	502	HEM	FE-ND	-2.06	1.86	1.96
87	8A	606	HEA	CHA-C4D	2.06	1.47	1.41
87	4A	605	HEA	C4D-C3D	2.06	1.48	1.45
84	3P	502	HEM	C4B-NB	-2.06	1.34	1.38
87	4A	605	HEA	C1D-C2D	2.06	1.48	1.44
84	3C	502	HEM	C1D-ND	-2.05	1.34	1.38
84	3C	501	HEM	C4B-NB	-2.05	1.34	1.38
76	1O	401	GTP	C8-N7	-2.05	1.31	1.35
87	4A	604	HEA	C4D-ND	-2.05	1.34	1.38
84	6P	502	HEM	CHB-C1B	2.03	1.40	1.35
84	6P	502	HEM	C4B-NB	-2.03	1.34	1.38
84	3C	502	HEM	C4B-NB	-2.03	1.34	1.38
84	3C	501	HEM	CHB-C1B	2.03	1.40	1.35
84	6C	502	HEM	CHB-C1B	2.02	1.40	1.35
84	6P	501	HEM	FE-ND	-2.02	1.86	1.96
84	3C	501	HEM	FE-ND	-2.02	1.86	1.96
87	8A	607	HEA	C4D-ND	-2.01	1.34	1.38

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	607	HEA	C3D-C4D-ND	6.91	117.05	110.36
87	4A	604	HEA	C4D-CHA-C1A	-6.65	113.78	122.56
80	5T	101	EHZ	C10-S1-C9	6.61	122.46	101.87
86	4A	602	PGV	O01-C1-C2	6.33	125.14	111.50
85	6D	501	HEC	CMC-C2C-C3C	6.24	133.16	125.82
85	6Q	501	HEC	C1D-C2D-C3D	-6.24	102.66	107.00
87	4A	605	HEA	C3B-C4B-NB	6.14	117.12	109.84
85	3D	501	HEC	CMC-C2C-C3C	5.95	132.82	125.82
80	1n	201	EHZ	C10-S1-C9	5.86	120.12	101.87
87	4A	605	HEA	C3D-C4D-ND	5.85	116.03	110.36
87	8A	607	HEA	C3B-C4B-NB	5.83	116.75	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	1H	402	PC1	O21-C21-C22	-5.78	99.04	111.50
85	3Q	501	HEC	C1D-C2D-C3D	-5.76	102.99	107.00
87	8A	607	HEA	C2B-C1B-NB	5.74	116.76	109.88
80	5n	201	EHZ	C10-S1-C9	5.68	119.57	101.87
87	4A	604	HEA	CHA-C4D-ND	-5.65	118.30	124.43
87	4A	605	HEA	C2B-C1B-NB	5.62	116.62	109.88
85	3Q	501	HEC	CMC-C2C-C3C	5.55	132.35	125.82
85	6D	501	HEC	CMB-C2B-C3B	5.55	132.35	125.82
87	8A	606	HEA	C3B-C4B-NB	5.47	116.32	109.84
87	8A	607	HEA	C2D-C1D-ND	5.38	116.21	109.84
80	1T	101	EHZ	C10-S1-C9	5.36	118.55	101.87
87	8A	606	HEA	CHA-C4D-ND	-5.31	118.66	124.43
85	3D	501	HEC	CMB-C2B-C3B	5.31	132.06	125.82
84	3P	501	HEM	CHD-C1D-ND	5.24	130.13	124.43
84	6C	501	HEM	CHC-C4B-NB	5.24	130.12	124.43
84	3C	501	HEM	CHC-C4B-NB	5.17	130.04	124.43
87	4A	605	HEA	C2D-C1D-ND	5.14	115.93	109.84
84	6C	501	HEM	CHD-C1D-ND	5.13	130.00	124.43
87	4A	605	HEA	CMC-C2C-C3C	5.05	134.12	124.68
84	3P	501	HEM	CHC-C4B-NB	5.02	129.88	124.43
87	8A	606	HEA	CHB-C1B-NB	-4.84	119.18	124.43
87	8A	606	HEA	C3D-C4D-ND	4.83	115.03	110.36
85	6Q	501	HEC	CMB-C2B-C3B	4.81	131.47	125.82
84	6P	502	HEM	CHC-C4B-NB	4.80	129.64	124.43
84	6P	501	HEM	CHC-C4B-NB	4.78	129.62	124.43
85	3Q	501	HEC	CMB-C2B-C3B	4.77	131.43	125.82
84	3P	502	HEM	CHC-C4B-NB	4.72	129.56	124.43
84	3C	502	HEM	CHC-C4B-NB	4.68	129.52	124.43
84	6C	502	HEM	C1B-NB-C4B	4.67	109.90	105.07
87	8A	606	HEA	C4D-CHA-C1A	-4.67	116.40	122.56
87	4A	604	HEA	C3D-C4D-ND	4.65	114.86	110.36
85	6Q	501	HEC	CMC-C2C-C3C	4.62	131.25	125.82
84	6P	502	HEM	C1B-NB-C4B	4.54	109.76	105.07
84	3C	502	HEM	C1B-NB-C4B	4.41	109.63	105.07
84	3P	502	HEM	C1B-NB-C4B	4.38	109.60	105.07
84	6C	502	HEM	CHC-C4B-NB	4.38	129.19	124.43
84	6P	501	HEM	CHD-C1D-ND	4.37	129.18	124.43
85	6D	501	HEC	C1D-C2D-C3D	-4.32	103.99	107.00
84	3C	501	HEM	CHD-C1D-ND	4.29	129.09	124.43
87	8A	607	HEA	CHA-C4D-ND	-4.23	119.83	124.43
87	4A	605	HEA	C1D-C2D-C3D	-4.22	102.52	106.96
87	8A	607	HEA	C1D-C2D-C3D	-4.21	102.53	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	604	HEA	C3B-C4B-NB	4.19	114.80	109.84
87	8A	607	HEA	C13-C12-C11	-4.11	108.17	114.35
85	3D	501	HEC	C1D-C2D-C3D	-4.11	104.14	107.00
87	8A	606	HEA	C2D-C1D-ND	4.09	114.69	109.84
84	6P	501	HEM	C1B-NB-C4B	4.04	109.25	105.07
87	4A	604	HEA	C2D-C1D-ND	4.02	114.60	109.84
84	3C	501	HEM	C1B-NB-C4B	4.00	109.20	105.07
84	6P	502	HEM	CHD-C1D-ND	3.99	128.77	124.43
87	4A	605	HEA	CHA-C4D-ND	-3.99	120.10	124.43
84	3P	502	HEM	CHD-C1D-ND	3.95	128.72	124.43
87	4A	604	HEA	CHC-C4B-NB	-3.90	119.56	124.38
87	4A	605	HEA	C13-C12-C11	-3.89	108.50	114.35
87	4A	604	HEA	C1D-C2D-C3D	-3.84	102.92	106.96
87	4A	604	HEA	CHB-C1B-NB	-3.81	120.30	124.43
87	4A	604	HEA	C2B-C1B-NB	3.79	114.43	109.88
87	8A	606	HEA	C4B-C3B-C2B	-3.79	100.93	107.41
75	1N	401	CDL	OB6-CB5-C51	3.79	118.06	111.09
84	6C	501	HEM	C1B-NB-C4B	3.75	108.95	105.07
87	8A	607	HEA	C1B-C2B-C3B	-3.75	102.32	106.80
87	8A	607	HEA	C3C-C4C-NC	3.73	114.03	109.21
86	4C	302	PGV	O01-C1-C2	3.72	119.51	111.50
70	1I	201	PC1	O21-C2-C3	3.69	121.76	108.40
87	8A	607	HEA	CMC-C2C-C3C	3.67	131.55	124.68
84	3C	502	HEM	CHA-C4D-ND	3.66	128.90	124.38
84	3P	501	HEM	CHD-C1D-C2D	-3.64	119.29	124.98
84	6C	501	HEM	CHA-C4D-ND	3.61	128.84	124.38
87	8A	606	HEA	C1D-C2D-C3D	-3.60	103.17	106.96
84	3P	501	HEM	C1B-NB-C4B	3.60	108.79	105.07
84	3C	502	HEM	CHD-C1D-ND	3.59	128.33	124.43
87	4A	605	HEA	C1B-C2B-C3B	-3.58	102.52	106.80
84	6C	502	HEM	CHD-C1D-ND	3.54	128.27	124.43
84	3C	501	HEM	CHA-C4D-ND	3.51	128.71	124.38
87	4A	605	HEA	C3C-C4C-NC	3.50	113.74	109.21
84	3P	501	HEM	CHB-C1B-NB	3.48	128.68	124.38
75	5N	401	CDL	OB6-CB5-C51	3.47	117.48	111.09
87	8A	606	HEA	CAD-C3D-C4D	3.45	130.69	124.66
70	1I	201	PC1	O21-C21-C22	3.42	118.87	111.50
85	6Q	501	HEC	CBD-CAD-C3D	-3.41	106.81	112.62
87	4A	605	HEA	C4B-C3B-C2B	-3.38	101.63	107.41
87	8A	607	HEA	C4D-C3D-C2D	-3.36	102.00	106.90
87	4A	605	HEA	CHB-C1B-NB	-3.31	120.84	124.43
84	6P	501	HEM	CHB-C1B-NB	3.28	128.44	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	607	HEA	CHB-C1B-NB	-3.28	120.87	124.43
86	8C	301	PGV	O01-C1-C2	3.27	118.56	111.50
87	8A	606	HEA	C2B-C1B-NB	3.27	113.80	109.88
87	4A	604	HEA	C26-C15-C16	3.24	120.72	115.27
87	8A	606	HEA	C4D-C3D-C2D	-3.24	102.18	106.90
69	1Y	202	3PE	O21-C21-C22	3.23	118.46	111.50
84	6C	501	HEM	CHB-C1B-NB	3.22	128.36	124.38
84	3P	502	HEM	CHA-C4D-ND	3.21	128.34	124.38
87	4A	604	HEA	C13-C14-C15	-3.20	119.94	127.66
84	3C	501	HEM	CHB-C1B-NB	3.20	128.34	124.38
84	6P	502	HEM	CHA-C4D-ND	3.20	128.33	124.38
84	3P	501	HEM	CHA-C4D-ND	3.20	128.33	124.38
87	8A	607	HEA	C13-C14-C15	-3.16	120.05	127.66
87	8A	607	HEA	C4B-C3B-C2B	-3.14	102.05	107.41
84	6C	502	HEM	CHA-C4D-ND	3.12	128.24	124.38
87	4A	604	HEA	CAD-C3D-C4D	3.12	130.11	124.66
87	8A	606	HEA	CMC-C2C-C3C	3.12	130.52	124.68
84	6C	502	HEM	C4D-ND-C1D	3.11	108.29	105.07
87	4A	605	HEA	C4D-C3D-C2D	-3.11	102.37	106.90
84	6P	502	HEM	CHB-C1B-NB	3.11	128.22	124.38
87	4A	604	HEA	C4B-C3B-C2B	-3.10	102.12	107.41
87	8A	607	HEA	C26-C15-C16	3.07	120.43	115.27
70	1H	402	PC1	O22-C21-C22	3.06	135.68	123.73
84	6P	501	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
87	4A	604	HEA	C1B-C2B-C3B	-3.05	103.16	106.80
84	6P	501	HEM	CHA-C4D-ND	3.04	128.14	124.38
87	8A	606	HEA	C13-C14-C15	-3.02	120.40	127.66
84	3C	502	HEM	CHB-C1B-NB	3.01	128.10	124.38
87	4A	604	HEA	C17-C18-C19	-3.00	120.44	127.66
78	5P	402	NDP	O4D-C1D-C2D	-2.96	100.18	106.64
87	8A	606	HEA	CHC-C4B-NB	-2.96	120.72	124.38
87	4A	604	HEA	C4D-C3D-C2D	-2.95	102.59	106.90
84	6C	501	HEM	CHD-C1D-C2D	-2.94	120.38	124.98
87	4A	605	HEA	C13-C14-C15	-2.94	120.58	127.66
81	5N	402	AME	O-C-CA	-2.94	117.08	124.78
84	3P	502	HEM	C4D-ND-C1D	2.91	108.08	105.07
84	3P	502	HEM	CHB-C1B-NB	2.91	127.97	124.38
87	4A	604	HEA	CMC-C2C-C3C	2.90	130.11	124.68
78	1P	402	NDP	O4D-C1D-C2D	-2.89	100.35	106.64
87	4A	605	HEA	C4B-NB-C1B	-2.88	102.10	105.07
87	8A	607	HEA	C4B-NB-C1B	-2.86	102.12	105.07
84	6C	502	HEM	CHB-C1B-NB	2.86	127.92	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	605	HEA	C27-C19-C20	2.85	120.06	115.27
91	8A	611	PSC	O01-C1-C2	2.84	117.62	111.50
87	4A	604	HEA	CAD-CBD-CGD	-2.83	107.52	113.60
85	3Q	501	HEC	CBD-CAD-C3D	-2.80	107.84	112.62
69	5Y	204	3PE	O21-C21-C22	2.80	117.53	111.50
84	6P	502	HEM	C4D-ND-C1D	2.80	107.96	105.07
84	6P	501	HEM	CBA-CAA-C2A	-2.78	107.88	112.62
84	3C	502	HEM	C4D-ND-C1D	2.77	107.93	105.07
87	8A	607	HEA	C1D-ND-C4D	-2.77	102.22	105.07
81	1h	201	AME	O-C-CA	-2.73	117.63	124.78
87	8A	606	HEA	C17-C18-C19	-2.73	121.09	127.66
87	8A	606	HEA	CHD-C1D-ND	-2.70	121.05	124.38
75	5d	201	CDL	CA6-CA4-CA3	2.69	118.15	111.79
84	3P	501	HEM	CBA-CAA-C2A	-2.67	108.06	112.62
84	6P	501	HEM	CAD-CBD-CGD	-2.67	107.85	113.60
87	8A	607	HEA	CMB-C2B-C1B	2.64	129.06	125.04
70	1H	402	PC1	C3-C2-C1	2.64	118.03	111.79
84	3C	501	HEM	CHD-C1D-C2D	-2.63	120.88	124.98
87	4A	604	HEA	C3C-C4C-NC	2.61	112.58	109.21
87	8A	606	HEA	C26-C15-C16	2.59	119.63	115.27
87	8A	607	HEA	CMD-C2D-C1D	2.57	128.95	125.04
87	4A	605	HEA	C4D-CHA-C1A	-2.54	119.21	122.56
87	8A	607	HEA	CAD-C3D-C4D	2.52	129.06	124.66
85	6D	501	HEC	CAA-CBA-CGA	-2.46	106.86	113.76
87	8A	607	HEA	C27-C19-C20	2.46	119.41	115.27
87	8A	606	HEA	C25-C23-C24	2.44	119.99	114.60
87	4A	605	HEA	C26-C15-C16	2.42	119.34	115.27
84	3C	501	HEM	CBA-CAA-C2A	-2.40	108.53	112.62
84	6C	501	HEM	C4D-ND-C1D	2.40	107.55	105.07
87	4A	605	HEA	C25-C23-C24	2.39	119.89	114.60
87	4A	604	HEA	CBA-CAA-C2A	-2.38	108.59	112.60
87	8A	607	HEA	C17-C18-C19	-2.37	121.96	127.66
87	4A	604	HEA	CMB-C2B-C1B	2.37	128.64	125.04
84	3P	501	HEM	CAD-CBD-CGD	-2.36	108.53	113.60
87	8A	607	HEA	C25-C23-C24	2.35	119.80	114.60
87	4A	604	HEA	C25-C23-C24	2.35	119.80	114.60
85	3D	501	HEC	CMA-C3A-C2A	2.34	129.35	124.94
85	6D	501	HEC	CMA-C3A-C2A	2.33	129.34	124.94
84	6C	501	HEM	CHA-C4D-C3D	-2.33	120.95	125.33
87	8A	606	HEA	OMA-CMA-C3A	-2.32	119.85	124.91
87	4A	604	HEA	CMD-C2D-C1D	2.32	128.57	125.04
84	3C	501	HEM	C4D-ND-C1D	2.30	107.45	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	8C	307	PEK	O01-C1-C2	2.29	116.44	111.50
87	8A	606	HEA	C13-C12-C11	-2.29	110.91	114.35
70	1H	402	PC1	O21-C2-C1	-2.29	100.11	108.40
70	1M	502	PC1	O21-C21-C22	2.29	116.43	111.50
87	8A	606	HEA	CMD-C2D-C1D	2.28	128.52	125.04
87	8A	606	HEA	C1B-C2B-C3B	-2.28	104.07	106.80
87	8A	606	HEA	CMB-C2B-C1B	2.28	128.52	125.04
86	4A	602	PGV	O02-C1-C2	-2.27	114.87	123.73
78	1P	402	NDP	C5A-C6A-N6A	2.27	123.80	120.35
84	3C	502	HEM	CHA-C4D-C3D	-2.26	121.08	125.33
84	6P	502	HEM	CHD-C1D-C2D	-2.26	121.45	124.98
87	4A	605	HEA	CAA-CBA-CGA	-2.25	107.44	113.76
78	5P	402	NDP	C5A-C6A-N6A	2.25	123.77	120.35
70	1H	402	PC1	O21-C2-C3	-2.24	100.30	108.40
87	8A	606	HEA	C27-C19-C20	2.24	119.03	115.27
87	8A	607	HEA	C21-C22-C23	-2.23	120.13	127.75
84	3P	501	HEM	C4D-ND-C1D	2.20	107.35	105.07
92	8C	307	PEK	O11-P-O14	-2.20	100.47	109.07
84	3P	502	HEM	CHD-C1D-C2D	-2.18	121.57	124.98
87	8A	607	HEA	CAD-CBD-CGD	-2.18	108.91	113.60
84	3C	501	HEM	CHA-C4D-C3D	-2.17	121.25	125.33
87	8A	606	HEA	C3C-C4C-NC	2.16	112.00	109.21
87	4A	605	HEA	CHD-C1D-C2D	-2.14	120.79	126.72
87	8A	607	HEA	CHD-C1D-C2D	-2.14	120.80	126.72
86	4G	101	PGV	O01-C1-C2	2.14	116.11	111.50
86	4C	305	PGV	O01-C1-C2	2.13	116.10	111.50
69	5j	101	3PE	O21-C21-C22	2.13	116.09	111.50
86	8G	101	PGV	O01-C1-C2	2.12	116.08	111.50
87	4A	605	HEA	CMB-C2B-C1B	2.12	128.27	125.04
87	4A	604	HEA	C21-C22-C23	-2.12	120.52	127.75
73	1F	501	FMN	C4-N3-C2	-2.09	121.77	125.64
87	4A	605	HEA	CAD-C3D-C4D	2.07	128.27	124.66
86	4B	301	PGV	O01-C02-C03	2.07	115.88	108.40
76	5O	401	GTP	O6-C6-C5	2.06	128.40	124.37
84	3P	501	HEM	CHB-C1B-C2B	-2.06	121.02	126.72
87	4A	605	HEA	C21-C22-C23	-2.06	120.71	127.75
84	3C	502	HEM	CAD-CBD-CGD	-2.06	109.18	113.60
91	4B	304	PSC	O01-C1-C2	2.05	115.91	111.50
87	4A	605	HEA	C17-C18-C19	-2.04	122.74	127.66
75	4C	306	CDL	OB6-CB5-C51	2.03	115.87	111.50
70	5Y	201	PC1	O21-C21-C22	2.03	115.87	111.50
84	3P	501	HEM	CMA-C3A-C4A	-2.02	125.36	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	605	HEA	CHC-C4B-NB	-2.02	121.89	124.38
70	1I	201	PC1	O21-C2-C1	-2.01	101.12	108.40
73	5F	501	FMN	C4-N3-C2	-2.01	121.94	125.64
87	8A	606	HEA	C21-C22-C23	-2.01	120.89	127.75

There are no chirality outliers.

All (1424) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O12
69	1K	101	3PE	C1-O11-P-O14
69	1L	701	3PE	O32-C31-O31-C3
69	1L	701	3PE	C32-C31-O31-C3
69	1L	704	3PE	C1-O11-P-O12
69	1L	704	3PE	C1-O11-P-O13
69	1L	704	3PE	C1-O11-P-O14
69	1L	705	3PE	C2-C1-O11-P
69	1M	503	3PE	C2-C1-O11-P
69	1M	505	3PE	C1-O11-P-O14
69	1P	403	3PE	C1-O11-P-O12
69	1P	403	3PE	C1-O11-P-O14
69	1Y	201	3PE	C1-O11-P-O13
69	1Y	201	3PE	C1-O11-P-O14
69	1Y	201	3PE	C2-C1-O11-P
69	1Y	201	3PE	O22-C21-O21-C2
69	1Y	201	3PE	C22-C21-O21-C2
69	1Y	202	3PE	O22-C21-O21-C2
69	1Y	202	3PE	C22-C21-O21-C2
69	1Y	204	3PE	C11-O13-P-O14
69	1d	201	3PE	C1-O11-P-O12
69	1d	201	3PE	C2-C1-O11-P
69	1d	201	3PE	O32-C31-O31-C3
69	1d	201	3PE	C32-C31-O31-C3
69	1j	101	3PE	O22-C21-O21-C2
69	1j	101	3PE	C22-C21-O21-C2
69	1m	201	3PE	O32-C31-O31-C3
69	1m	201	3PE	C32-C31-O31-C3
69	5A	201	3PE	C11-O13-P-O12
69	5K	101	3PE	C1-O11-P-O14
69	5K	101	3PE	C12-C11-O13-P
69	5L	701	3PE	O32-C31-O31-C3
69	5L	701	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	5L	703	3PE	C2-C1-O11-P
69	5M	901	3PE	C1-O11-P-O12
69	5M	901	3PE	C1-O11-P-O13
69	5M	901	3PE	C1-O11-P-O14
69	5M	902	3PE	C11-O13-P-O11
69	5M	902	3PE	C11-O13-P-O14
69	5M	903	3PE	C1-O11-P-O12
69	5M	903	3PE	C2-C1-O11-P
69	5M	903	3PE	O32-C31-O31-C3
69	5M	903	3PE	C32-C31-O31-C3
69	5M	904	3PE	C2-C1-O11-P
69	5M	906	3PE	C1-O11-P-O14
69	5P	403	3PE	C1-O11-P-O12
69	5Y	202	3PE	C11-O13-P-O14
69	5Y	202	3PE	C2-C1-O11-P
69	5Y	203	3PE	C1-O11-P-O13
69	5Y	203	3PE	C1-O11-P-O14
69	5Y	203	3PE	C2-C1-O11-P
69	5Y	203	3PE	O22-C21-O21-C2
69	5Y	203	3PE	C22-C21-O21-C2
69	5Y	204	3PE	O22-C21-O21-C2
69	5Y	204	3PE	C22-C21-O21-C2
69	5Y	206	3PE	C11-O13-P-O14
69	5j	101	3PE	C11-O13-P-O14
69	5j	101	3PE	C12-C11-O13-P
69	5j	101	3PE	O22-C21-O21-C2
69	5j	101	3PE	C22-C21-O21-C2
69	5m	201	3PE	O32-C31-O31-C3
69	5m	201	3PE	C32-C31-O31-C3
70	1B	203	PC1	O22-C21-O21-C2
70	1B	203	PC1	C22-C21-O21-C2
70	1M	502	PC1	C11-O13-P-O14
70	1M	502	PC1	O22-C21-O21-C2
70	1M	502	PC1	C22-C21-O21-C2
70	1M	504	PC1	C11-O13-P-O12
70	1M	504	PC1	C11-O13-P-O14
70	1M	504	PC1	C11-O13-P-O11
70	1d	203	PC1	O22-C21-O21-C2
70	1d	203	PC1	C22-C21-O21-C2
70	1h	203	PC1	O32-C31-O31-C3
70	1h	203	PC1	C32-C31-O31-C3
70	5A	202	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
70	5A	202	PC1	C1-O11-P-O14
70	5A	202	PC1	C1-O11-P-O13
70	5B	203	PC1	O22-C21-O21-C2
70	5B	203	PC1	C22-C21-O21-C2
70	5H	403	PC1	C1-O11-P-O14
70	5M	905	PC1	C1-O11-P-O12
70	5M	905	PC1	C1-O11-P-O14
70	5Y	201	PC1	O22-C21-O21-C2
70	5Y	201	PC1	C22-C21-O21-C2
70	5d	203	PC1	O22-C21-O21-C2
70	5d	203	PC1	C22-C21-O21-C2
70	5h	202	PC1	C2-C1-O11-P
70	5h	202	PC1	O32-C31-O31-C3
70	5h	202	PC1	C32-C31-O31-C3
73	5F	501	FMN	C2'-C3'-C4'-C5'
73	5F	501	FMN	O3'-C3'-C4'-C5'
75	1H	401	CDL	CA3-OA5-PA1-OA4
75	1H	401	CDL	CA4-CA3-OA5-PA1
75	1H	401	CDL	OB7-CB5-OB6-CB4
75	1H	401	CDL	C51-CB5-OB6-CB4
75	1L	702	CDL	CA2-OA2-PA1-OA5
75	1L	702	CDL	OA6-CA4-CA6-OA8
75	1L	702	CDL	CB2-OB2-PB2-OB3
75	1N	401	CDL	OA6-CA4-CA6-OA8
75	1N	401	CDL	CB3-OB5-PB2-OB3
75	1X	201	CDL	C1-CA2-OA2-PA1
75	1X	201	CDL	CA2-OA2-PA1-OA5
75	1X	201	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CA2-OA2-PA1-OA4
75	1h	202	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	CB3-OB5-PB2-OB2
75	1h	202	CDL	OB7-CB5-OB6-CB4
75	1h	202	CDL	C51-CB5-OB6-CB4
75	1h	202	CDL	OB9-CB7-OB8-CB6
75	1h	202	CDL	C71-CB7-OB8-CB6
75	4B	302	CDL	OA9-CA7-OA8-CA6
75	4B	302	CDL	C31-CA7-OA8-CA6
75	4B	302	CDL	CB3-OB5-PB2-OB3
75	4C	306	CDL	C1-CA2-OA2-PA1
75	4C	306	CDL	OB7-CB5-OB6-CB4
75	4C	306	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	4C	306	CDL	OB9-CB7-OB8-CB6
75	4C	306	CDL	C71-CB7-OB8-CB6
75	4D	201	CDL	O1-C1-CB2-OB2
75	4D	201	CDL	C1-CA2-OA2-PA1
75	4D	201	CDL	CA3-OA5-PA1-OA3
75	4D	201	CDL	CB3-OB5-PB2-OB3
75	4D	201	CDL	OB7-CB5-OB6-CB4
75	4D	201	CDL	C51-CB5-OB6-CB4
75	4D	201	CDL	OB9-CB7-OB8-CB6
75	4D	201	CDL	C71-CB7-OB8-CB6
75	5H	401	CDL	CA2-C1-CB2-OB2
75	5H	401	CDL	CA4-CA3-OA5-PA1
75	5H	401	CDL	OB7-CB5-OB6-CB4
75	5H	401	CDL	C51-CB5-OB6-CB4
75	5L	702	CDL	CA2-OA2-PA1-OA5
75	5L	702	CDL	OA6-CA4-CA6-OA8
75	5L	702	CDL	CB3-OB5-PB2-OB4
75	5N	401	CDL	C1-CA2-OA2-PA1
75	5N	401	CDL	OA6-CA4-CA6-OA8
75	5N	401	CDL	CB3-OB5-PB2-OB3
75	5d	201	CDL	C1-CA2-OA2-PA1
75	5d	201	CDL	CA2-OA2-PA1-OA5
75	5d	201	CDL	C1-CB2-OB2-PB2
75	5h	201	CDL	O1-C1-CA2-OA2
75	5h	201	CDL	CB3-OB5-PB2-OB3
75	5h	201	CDL	OB7-CB5-OB6-CB4
75	5h	201	CDL	C51-CB5-OB6-CB4
75	5h	201	CDL	OB9-CB7-OB8-CB6
75	5h	201	CDL	C71-CB7-OB8-CB6
75	8A	605	CDL	OA9-CA7-OA8-CA6
75	8A	605	CDL	C31-CA7-OA8-CA6
75	8A	605	CDL	CB3-OB5-PB2-OB3
75	8C	305	CDL	C1-CA2-OA2-PA1
75	8C	305	CDL	OB7-CB5-OB6-CB4
75	8C	305	CDL	C51-CB5-OB6-CB4
75	8C	305	CDL	OB9-CB7-OB8-CB6
75	8C	305	CDL	C71-CB7-OB8-CB6
75	8D	201	CDL	C1-CA2-OA2-PA1
75	8D	201	CDL	CA3-OA5-PA1-OA3
75	8D	201	CDL	CB3-OB5-PB2-OB2
75	8D	201	CDL	CB3-OB5-PB2-OB3
75	8D	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	8D	201	CDL	C51-CB5-OB6-CB4
75	8D	201	CDL	OB9-CB7-OB8-CB6
75	8D	201	CDL	C71-CB7-OB8-CB6
76	5O	401	GTP	PB-O3A-PA-O5'
78	1P	402	NDP	O4D-C1D-N1N-C6N
80	1T	101	EHZ	C7-C8-C9-S1
80	1T	101	EHZ	N2-C15-C16-O5
80	1n	201	EHZ	C7-C8-C9-O2
80	5T	101	EHZ	N2-C15-C16-O5
84	3C	501	HEM	C2B-C3B-CAB-CBB
84	3C	501	HEM	C4B-C3B-CAB-CBB
84	3C	502	HEM	C2B-C3B-CAB-CBB
84	3C	502	HEM	C4B-C3B-CAB-CBB
84	3P	501	HEM	C2B-C3B-CAB-CBB
84	3P	501	HEM	C4B-C3B-CAB-CBB
84	3P	502	HEM	C2B-C3B-CAB-CBB
84	3P	502	HEM	C4B-C3B-CAB-CBB
84	6C	501	HEM	C2B-C3B-CAB-CBB
84	6C	501	HEM	C4B-C3B-CAB-CBB
84	6P	501	HEM	C2B-C3B-CAB-CBB
84	6P	501	HEM	C4B-C3B-CAB-CBB
84	6P	502	HEM	C2B-C3B-CAB-CBB
84	6P	502	HEM	C4B-C3B-CAB-CBB
86	4A	601	PGV	O04-C19-O03-C01
86	4A	601	PGV	C20-C19-O03-C01
86	4A	603	PGV	C03-O11-P-O12
86	4C	302	PGV	O02-C1-O01-C02
86	4C	302	PGV	C2-C1-O01-C02
86	4C	303	PGV	C03-O11-P-O12
86	4C	303	PGV	O04-C19-O03-C01
86	4C	303	PGV	C20-C19-O03-C01
86	4C	304	PGV	C03-O11-P-O12
86	4C	304	PGV	C03-O11-P-O13
86	4C	304	PGV	C03-O11-P-O14
86	4C	304	PGV	C02-C03-O11-P
86	4C	305	PGV	C03-O11-P-O12
86	4C	305	PGV	O02-C1-O01-C02
86	4C	305	PGV	C2-C1-O01-C02
86	4G	101	PGV	O02-C1-O01-C02
86	4G	101	PGV	C2-C1-O01-C02
86	4G	101	PGV	O04-C19-O03-C01
86	4G	101	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
86	4K	101	PGV	C03-O11-P-O12
86	4K	101	PGV	O04-C19-O03-C01
86	4K	101	PGV	C20-C19-O03-C01
86	8A	601	PGV	O04-C19-O03-C01
86	8A	601	PGV	C20-C19-O03-C01
86	8A	603	PGV	C04-O12-P-O14
86	8A	603	PGV	C02-C03-O11-P
86	8C	301	PGV	O02-C1-O01-C02
86	8C	301	PGV	C2-C1-O01-C02
86	8C	302	PGV	C03-O11-P-O12
86	8C	302	PGV	O04-C19-O03-C01
86	8C	302	PGV	C20-C19-O03-C01
86	8C	304	PGV	O02-C1-O01-C02
86	8C	304	PGV	C2-C1-O01-C02
86	8G	101	PGV	O02-C1-O01-C02
86	8G	101	PGV	C2-C1-O01-C02
86	8G	101	PGV	O04-C19-O03-C01
86	8G	101	PGV	C20-C19-O03-C01
86	8K	101	PGV	C03-O11-P-O14
86	8K	101	PGV	O04-C19-O03-C01
86	8K	101	PGV	C20-C19-O03-C01
87	4A	604	HEA	C3B-C11-C12-C13
87	4A	604	HEA	O11-C11-C12-C13
87	4A	604	HEA	C11-C12-C13-C14
87	8A	606	HEA	C3B-C11-C12-C13
87	8A	606	HEA	O11-C11-C12-C13
87	8A	607	HEA	C2A-CAA-CBA-CGA
91	4B	304	PSC	C03-O11-P-O12
91	4B	304	PSC	C02-C03-O11-P
91	4B	304	PSC	O02-C1-O01-C02
91	4B	304	PSC	C2-C1-O01-C02
91	8A	611	PSC	C03-O11-P-O12
91	8A	611	PSC	C02-C03-O11-P
91	8A	611	PSC	O02-C1-O01-C02
91	8A	611	PSC	C2-C1-O01-C02
80	1T	101	EHZ	C13-C12-N1-C11
80	5T	101	EHZ	C13-C12-N1-C11
75	4C	306	CDL	O1-C1-CA2-OA2
75	8C	305	CDL	O1-C1-CA2-OA2
75	8D	201	CDL	O1-C1-CB2-OB2
75	1N	401	CDL	C51-CB5-OB6-CB4
75	5N	401	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	1N	401	CDL	OB7-CB5-OB6-CB4
75	5N	401	CDL	OB7-CB5-OB6-CB4
73	5F	501	FMN	O3'-C3'-C4'-O4'
78	1P	402	NDP	O4D-C4D-C5D-O5D
78	1P	402	NDP	C3D-C4D-C5D-O5D
78	5P	402	NDP	O4D-C4D-C5D-O5D
78	5P	402	NDP	C3D-C4D-C5D-O5D
73	5F	501	FMN	C2'-C3'-C4'-O4'
86	8D	202	PGV	C14-C15-C16-C17
70	1h	203	PC1	C2-C1-O11-P
70	5Y	207	PC1	C2-C1-O11-P
75	1N	401	CDL	C1-CA2-OA2-PA1
86	4A	603	PGV	C02-C03-O11-P
86	4C	305	PGV	C02-C03-O11-P
75	8C	305	CDL	C75-C76-C77-C78
80	1T	101	EHZ	O3-C12-N1-C11
80	5T	101	EHZ	O3-C12-N1-C11
75	4D	201	CDL	CA2-C1-CB2-OB2
75	5h	201	CDL	CB2-C1-CA2-OA2
75	8C	305	CDL	CB2-C1-CA2-OA2
78	5P	402	NDP	O4D-C1D-N1N-C6N
86	8C	303	PGV	C5-C6-C7-C8
75	1L	702	CDL	O1-C1-CB2-OB2
75	5d	204	CDL	O1-C1-CA2-OA2
75	5h	201	CDL	O1-C1-CB2-OB2
69	5d	202	3PE	C31-C32-C33-C34
75	1L	702	CDL	CA7-C31-C32-C33
69	1K	101	3PE	C32-C33-C34-C35
86	4J	101	PGV	C21-C22-C23-C24
69	1d	202	3PE	C31-C32-C33-C34
70	5H	403	PC1	C21-C22-C23-C24
87	4A	605	HEA	C2A-CAA-CBA-CGA
70	5I	203	PC1	C31-C32-C33-C34
75	5L	702	CDL	CA7-C31-C32-C33
69	5m	201	3PE	C31-C32-C33-C34
70	1q	201	PC1	C31-C32-C33-C34
75	1X	201	CDL	CA7-C31-C32-C33
75	1d	204	CDL	CA5-C11-C12-C13
75	5d	201	CDL	CA7-C31-C32-C33
86	8C	303	PGV	C1-C2-C3-C4
70	1M	504	PC1	C23-C24-C25-C26
70	1L	706	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
69	1m	201	3PE	C31-C32-C33-C34
70	1I	201	PC1	C31-C32-C33-C34
70	5q	201	PC1	C31-C32-C33-C34
69	1L	704	3PE	C32-C33-C34-C35
80	5T	101	EHZ	C2-C3-C4-C5
87	4A	604	HEA	C19-C20-C21-C22
69	1M	503	3PE	C31-C32-C33-C34
69	1M	505	3PE	C21-C22-C23-C24
70	5H	403	PC1	C31-C32-C33-C34
69	5K	101	3PE	C32-C33-C34-C35
69	1K	101	3PE	C1-O11-P-O13
69	1L	705	3PE	C1-O11-P-O13
69	1P	403	3PE	C1-O11-P-O13
69	5K	101	3PE	C1-O11-P-O13
69	5M	903	3PE	C1-O11-P-O13
69	5Y	202	3PE	C1-O11-P-O13
69	5j	101	3PE	C1-O11-P-O13
70	1I	204	PC1	C1-O11-P-O13
70	1M	502	PC1	C11-O13-P-O11
70	1M	504	PC1	C1-O11-P-O13
70	5H	403	PC1	C1-O11-P-O13
70	5I	203	PC1	C1-O11-P-O13
70	5M	905	PC1	C1-O11-P-O13
70	5Y	201	PC1	C11-O13-P-O11
75	1L	702	CDL	CB3-OB5-PB2-OB2
75	1h	202	CDL	CA2-OA2-PA1-OA5
75	1h	202	CDL	CB2-OB2-PB2-OB5
75	4B	302	CDL	CA3-OA5-PA1-OA2
75	5h	201	CDL	CB3-OB5-PB2-OB2
86	8A	603	PGV	C04-O12-P-O11
86	8K	101	PGV	C03-O11-P-O12
75	4C	306	CDL	C75-C76-C77-C78
69	5M	904	3PE	C31-C32-C33-C34
69	1L	703	3PE	C39-C3A-C3B-C3C
69	5M	901	3PE	C33-C34-C35-C36
69	5d	202	3PE	C35-C36-C37-C38
86	4L	101	PGV	C22-C23-C24-C25
69	5Y	204	3PE	C23-C24-C25-C26
75	8C	305	CDL	C79-C80-C81-C82
87	8A	606	HEA	C2D-C3D-CAD-CBD
69	1Y	202	3PE	C23-C24-C25-C26
75	5a	201	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
86	4A	602	PGV	C3-C4-C5-C6
86	4C	303	PGV	C5-C6-C7-C8
70	5M	905	PC1	C21-C22-C23-C24
69	1L	703	3PE	C2-C1-O11-P
73	1F	501	FMN	C4'-C5'-O5'-P
86	8C	301	PGV	C05-C04-O12-P
69	5L	703	3PE	C39-C3A-C3B-C3C
75	1d	204	CDL	O1-C1-CA2-OA2
75	5H	401	CDL	O1-C1-CB2-OB2
84	3P	501	HEM	C3D-CAD-CBD-CGD
69	5M	906	3PE	C2B-C2C-C2D-C2E
69	5P	403	3PE	C23-C24-C25-C26
69	5M	902	3PE	C26-C27-C28-C29
69	5Y	204	3PE	C22-C23-C24-C25
75	8A	605	CDL	C59-C60-C61-C62
86	8L	101	PGV	C14-C15-C16-C17
69	1M	501	3PE	C26-C27-C28-C29
86	4C	302	PGV	C7-C8-C9-C10
86	8C	301	PGV	C27-C28-C29-C30
91	8A	611	PSC	C19-C20-C21-C22
75	5d	204	CDL	C71-C72-C73-C74
86	8C	302	PGV	C5-C6-C7-C8
70	5B	203	PC1	C28-C29-C2A-C2B
86	4C	302	PGV	C27-C28-C29-C30
86	8A	604	PGV	C22-C23-C24-C25
70	1H	402	PC1	C31-C32-C33-C34
69	1d	202	3PE	C3C-C3D-C3E-C3F
86	4C	302	PGV	C26-C27-C28-C29
86	4C	307	PGV	C7-C8-C9-C10
75	4C	306	CDL	C36-C37-C38-C39
69	5Y	204	3PE	C25-C26-C27-C28
86	5i	201	PGV	C30-C31-C32-C33
91	8A	611	PSC	C25-C26-C27-C28
69	1M	501	3PE	C1-C2-C3-O31
75	1a	201	CDL	C16-C17-C18-C19
75	8D	201	CDL	C71-C72-C73-C74
87	8A	606	HEA	C4D-C3D-CAD-CBD
86	8K	101	PGV	C1-C2-C3-C4
75	8C	305	CDL	C74-C75-C76-C77
86	4L	101	PGV	C6-C7-C8-C9
69	1M	503	3PE	C38-C39-C3A-C3B
86	4B	301	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
86	8C	301	PGV	C26-C27-C28-C29
70	1M	504	PC1	C2C-C2D-C2E-C2F
75	1L	702	CDL	CA2-C1-CB2-OB2
75	4C	306	CDL	CB2-C1-CA2-OA2
69	1M	501	3PE	C21-C22-C23-C24
86	4L	101	PGV	C21-C22-C23-C24
69	5d	202	3PE	C3C-C3D-C3E-C3F
86	5i	201	PGV	C22-C23-C24-C25
91	4B	304	PSC	C25-C26-C27-C28
75	4B	302	CDL	C59-C60-C61-C62
69	5M	903	3PE	C3B-C3C-C3D-C3E
69	1Y	201	3PE	C31-C32-C33-C34
69	1d	201	3PE	C3B-C3C-C3D-C3E
86	4B	301	PGV	C24-C25-C26-C27
69	5d	202	3PE	C28-C29-C2A-C2B
75	1h	202	CDL	C60-C61-C62-C63
70	1I	204	PC1	C31-C32-C33-C34
91	8A	611	PSC	C1-C2-C3-C4
69	1d	201	3PE	C22-C23-C24-C25
69	5M	903	3PE	C22-C23-C24-C25
84	6C	502	HEM	C2B-C3B-CAB-CBB
69	5M	904	3PE	C35-C36-C37-C38
75	1d	204	CDL	CA7-C31-C32-C33
69	5Y	203	3PE	C22-C23-C24-C25
70	1L	706	PC1	C23-C24-C25-C26
69	1A	201	3PE	C36-C37-C38-C39
75	8C	305	CDL	C36-C37-C38-C39
86	8C	303	PGV	C4-C5-C6-C7
86	4C	304	PGV	O03-C01-C02-O01
75	5h	201	CDL	C60-C61-C62-C63
86	8L	101	PGV	C21-C22-C23-C24
86	8D	202	PGV	C12-C13-C14-C15
69	5M	906	3PE	C21-C22-C23-C24
70	5B	203	PC1	C35-C36-C37-C38
75	4D	201	CDL	C71-C72-C73-C74
70	5I	203	PC1	C37-C38-C39-C3A
73	5F	501	FMN	O2'-C2'-C3'-C4'
69	1d	201	3PE	C1-O11-P-O13
75	1H	401	CDL	CA3-OA5-PA1-OA2
75	8A	605	CDL	CB3-OB5-PB2-OB2
70	1I	204	PC1	C37-C38-C39-C3A
75	1L	702	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
69	1L	704	3PE	C2-C1-O11-P
73	5F	501	FMN	C4'-C5'-O5'-P
86	8C	304	PGV	C02-C03-O11-P
86	8K	101	PGV	C02-C03-O11-P
75	1d	204	CDL	OA5-CA3-CA4-CA6
91	8A	611	PSC	C15-C16-C17-C18
70	1J	201	PC1	C21-C22-C23-C24
70	1h	203	PC1	C32-C33-C34-C35
75	5L	702	CDL	C57-C58-C59-C60
70	1B	203	PC1	C35-C36-C37-C38
75	5L	702	CDL	C11-C12-C13-C14
75	1d	204	CDL	C71-C72-C73-C74
75	4B	302	CDL	C38-C39-C40-C41
86	8C	301	PGV	C7-C8-C9-C10
86	8J	101	PGV	C21-C22-C23-C24
80	1T	101	EHZ	C21-C22-C23-C24
86	8C	301	PGV	C3-C4-C5-C6
69	1L	704	3PE	C2E-C2F-C2G-C2H
69	1Y	202	3PE	C1-C2-C3-O31
69	1d	202	3PE	C28-C29-C2A-C2B
69	5L	703	3PE	C1-C2-C3-O31
70	5B	203	PC1	C1-C2-C3-O31
70	5M	905	PC1	C23-C24-C25-C26
75	1L	702	CDL	CA3-CA4-CA6-OA8
75	1N	401	CDL	CA3-CA4-CA6-OA8
75	1N	401	CDL	CB3-CB4-CB6-OB8
75	5L	702	CDL	CA3-CA4-CA6-OA8
75	5N	401	CDL	C12-C13-C14-C15
86	8D	202	PGV	C3-C4-C5-C6
86	8J	101	PGV	O03-C01-C02-C03
92	4C	309	PEK	O03-C01-C02-C03
69	1Y	202	3PE	C25-C26-C27-C28
70	5Y	207	PC1	C23-C24-C25-C26
75	4C	306	CDL	C59-C60-C61-C62
92	8G	102	PEK	C21-C22-C23-C24
86	8K	101	PGV	C3-C4-C5-C6
80	1T	101	EHZ	O4-C15-C16-O5
80	5T	101	EHZ	O4-C15-C16-O5
87	4A	604	HEA	C15-C16-C17-C18
69	5M	901	3PE	C2E-C2F-C2G-C2H
69	5Y	205	3PE	C33-C34-C35-C36
75	1X	201	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
86	4K	101	PGV	C22-C23-C24-C25
75	1N	401	CDL	C12-C13-C14-C15
80	5T	101	EHZ	C21-C22-C23-C24
86	8B	301	PGV	C2-C3-C4-C5
86	4J	101	PGV	C19-C20-C21-C22
75	1L	702	CDL	C57-C58-C59-C60
75	1a	201	CDL	C52-C51-CB5-OB6
75	8C	305	CDL	C51-C52-C53-C54
75	1d	204	CDL	C72-C73-C74-C75
75	8D	201	CDL	C59-C60-C61-C62
86	4K	101	PGV	C2-C3-C4-C5
69	1Y	203	3PE	C33-C34-C35-C36
69	5M	901	3PE	C2-C1-O11-P
86	4C	302	PGV	C05-C04-O12-P
86	8C	306	PGV	C02-C03-O11-P
75	5N	401	CDL	C32-C31-CA7-OA8
86	8C	306	PGV	C5-C6-C7-C8
86	4L	101	PGV	C3-C4-C5-C6
84	3C	501	HEM	C3D-CAD-CBD-CGD
84	6C	501	HEM	C3D-CAD-CBD-CGD
69	5M	901	3PE	C32-C33-C34-C35
69	1A	201	3PE	O21-C21-C22-C23
92	4C	308	PEK	O03-C21-C22-C23
69	1L	703	3PE	O21-C2-C3-O31
69	1L	704	3PE	O21-C2-C3-O31
70	1M	504	PC1	O21-C2-C3-O31
70	5M	905	PC1	O21-C2-C3-O31
75	1d	204	CDL	OA6-CA4-CA6-OA8
75	5N	401	CDL	OB6-CB4-CB6-OB8
75	8A	605	CDL	OB6-CB4-CB6-OB8
92	4C	309	PEK	O03-C01-C02-O01
92	8C	307	PEK	O03-C01-C02-O01
75	8C	305	CDL	C59-C60-C61-C62
86	4L	101	PGV	C19-C20-C21-C22
69	5M	901	3PE	C3A-C3B-C3C-C3D
86	4C	304	PGV	C20-C21-C22-C23
75	4C	306	CDL	C11-C12-C13-C14
69	1d	201	3PE	C2D-C2E-C2F-C2G
69	1L	704	3PE	O11-C1-C2-C3
69	1M	503	3PE	O11-C1-C2-C3
69	1m	201	3PE	O11-C1-C2-C3
69	5m	201	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
70	5h	202	PC1	O11-C1-C2-C3
75	5d	204	CDL	OA5-CA3-CA4-CA6
75	8C	305	CDL	OB5-CB3-CB4-CB6
86	4A	602	PGV	C01-C02-C03-O11
69	5Y	203	3PE	C31-C32-C33-C34
70	5h	202	PC1	C32-C33-C34-C35
70	1H	402	PC1	C21-C22-C23-C24
75	5h	201	CDL	CB7-C71-C72-C73
86	8B	301	PGV	C1-C2-C3-C4
92	4C	308	PEK	C21-C22-C23-C24
70	1h	203	PC1	C2A-C2B-C2C-C2D
75	5a	201	CDL	C52-C51-CB5-OB6
69	5Y	204	3PE	C2-C1-O11-P
75	5h	201	CDL	CB4-CB3-OB5-PB2
86	4C	307	PGV	C02-C03-O11-P
86	4K	101	PGV	C02-C03-O11-P
86	4K	101	PGV	C05-C04-O12-P
86	8G	101	PGV	C02-C03-O11-P
86	8K	101	PGV	C05-C04-O12-P
69	1M	505	3PE	C2B-C2C-C2D-C2E
70	1B	202	PC1	C37-C38-C39-C3A
70	5M	905	PC1	C2A-C2B-C2C-C2D
75	1X	201	CDL	C61-C62-C63-C64
75	1h	202	CDL	C76-C77-C78-C79
75	5d	201	CDL	C61-C62-C63-C64
75	5d	201	CDL	C23-C24-C25-C26
86	8D	202	PGV	C20-C21-C22-C23
69	1L	703	3PE	C1-C2-C3-O31
69	1L	704	3PE	C1-C2-C3-O31
69	1L	705	3PE	C1-C2-C3-O31
69	1d	201	3PE	C1-C2-C3-O31
69	5M	903	3PE	C1-C2-C3-O31
69	5Y	202	3PE	C1-C2-C3-O31
69	5Y	204	3PE	C1-C2-C3-O31
70	1h	203	PC1	C1-C2-C3-O31
75	5N	401	CDL	CB3-CB4-CB6-OB8
75	8A	605	CDL	CB3-CB4-CB6-OB8
86	4C	304	PGV	O03-C01-C02-C03
86	4J	101	PGV	O03-C01-C02-C03
69	5A	201	3PE	O21-C21-C22-C23
86	4A	601	PGV	C14-C15-C16-C17
70	1M	504	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
75	4C	306	CDL	C79-C80-C81-C82
69	5j	101	3PE	C11-O13-P-O11
75	1L	702	CDL	CB2-OB2-PB2-OB5
91	4B	304	PSC	C9-C10-C11-C12
91	4B	304	PSC	C10-C11-C12-C13
91	8A	611	PSC	C9-C10-C11-C12
91	8A	611	PSC	C10-C11-C12-C13
92	4C	308	PEK	C5-C6-C7-C8
92	4C	308	PEK	C9-C10-C11-C12
92	8C	307	PEK	C11-C12-C13-C14
92	8G	102	PEK	C5-C6-C7-C8
92	8G	102	PEK	C9-C10-C11-C12
75	1X	201	CDL	C23-C24-C25-C26
69	1Y	201	3PE	O11-C1-C2-O21
70	5H	402	PC1	O11-C1-C2-O21
75	1L	702	CDL	OA5-CA3-CA4-OA6
75	1X	201	CDL	OB5-CB3-CB4-OB6
75	5d	201	CDL	OB5-CB3-CB4-OB6
91	8A	611	PSC	O01-C02-C03-O11
75	5h	201	CDL	C76-C77-C78-C79
69	5Y	204	3PE	O31-C31-C32-C33
70	1L	706	PC1	O31-C31-C32-C33
92	8G	102	PEK	O03-C21-C22-C23
70	5H	402	PC1	C2B-C2C-C2D-C2E
69	1L	705	3PE	O21-C2-C3-O31
69	1Y	202	3PE	O21-C2-C3-O31
69	5M	903	3PE	O21-C2-C3-O31
69	5Y	204	3PE	O21-C2-C3-O31
75	5d	204	CDL	OA6-CA4-CA6-OA8
86	8C	303	PGV	O03-C01-C02-O01
91	8A	611	PSC	C7-C8-C9-C10
69	1d	201	3PE	C34-C35-C36-C37
69	5Y	203	3PE	C27-C28-C29-C2A
70	5d	203	PC1	C37-C38-C39-C3A
86	4C	307	PGV	C26-C27-C28-C29
75	8D	201	CDL	CA2-C1-CB2-OB2
69	1Y	201	3PE	C22-C23-C24-C25
70	5H	402	PC1	C27-C28-C29-C2A
70	5Y	207	PC1	C33-C34-C35-C36
70	5h	202	PC1	C2A-C2B-C2C-C2D
75	1X	201	CDL	C36-C37-C38-C39
75	4D	201	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
75	4B	302	CDL	C31-C32-C33-C34
70	1M	504	PC1	C2-C1-O11-P
70	5M	905	PC1	C2-C1-O11-P
75	8A	605	CDL	C1-CA2-OA2-PA1
86	4G	101	PGV	C02-C03-O11-P
86	8C	303	PGV	C02-C03-O11-P
86	8A	601	PGV	C11-C10-C9-C8
86	4L	101	PGV	C14-C15-C16-C17
69	1Y	202	3PE	O31-C31-C32-C33
75	1X	201	CDL	C32-C31-CA7-OA8
80	5T	101	EHZ	C4-C5-C6-C7
69	1L	703	3PE	C33-C34-C35-C36
75	4B	302	CDL	C33-C34-C35-C36
75	1N	401	CDL	CA7-C31-C32-C33
69	1M	505	3PE	C23-C24-C25-C26
86	4C	301	PGV	C26-C27-C28-C29
70	5H	403	PC1	C39-C3A-C3B-C3C
75	5d	204	CDL	C42-C43-C44-C45
69	5M	901	3PE	O11-C1-C2-C3
69	5M	904	3PE	O11-C1-C2-C3
75	4C	306	CDL	OB5-CB3-CB4-CB6
75	8A	605	CDL	OA5-CA3-CA4-CA6
75	5d	201	CDL	C32-C31-CA7-OA8
75	8C	305	CDL	C11-C12-C13-C14
86	8A	602	PGV	C30-C31-C32-C33
69	1A	201	3PE	C31-C32-C33-C34
75	5d	201	CDL	C58-C59-C60-C61
86	4G	101	PGV	C7-C8-C9-C10
69	1Y	202	3PE	C22-C23-C24-C25
86	8A	601	PGV	C14-C15-C16-C17
69	1Y	202	3PE	C24-C25-C26-C27
86	8K	101	PGV	C22-C23-C24-C25
69	1M	505	3PE	C27-C28-C29-C2A
70	5q	201	PC1	C2A-C2B-C2C-C2D
75	1L	702	CDL	C33-C34-C35-C36
75	1d	204	CDL	C42-C43-C44-C45
69	1Y	202	3PE	C2-C1-O11-P
69	5M	902	3PE	C1-C2-C3-O31
70	1B	203	PC1	C1-C2-C3-O31
70	1I	201	PC1	C1-C2-C3-O31
70	5h	202	PC1	C1-C2-C3-O31
75	1d	204	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
75	1h	202	CDL	CA3-CA4-CA6-OA8
75	4B	302	CDL	CB3-CB4-CB6-OB8
75	5N	401	CDL	CA3-CA4-CA6-OA8
75	5d	204	CDL	CA3-CA4-CA6-OA8
86	4A	601	PGV	C02-C03-O11-P
86	4C	304	PGV	C05-C04-O12-P
69	1L	704	3PE	O11-C1-C2-O21
69	1m	201	3PE	O11-C1-C2-O21
69	5M	901	3PE	O11-C1-C2-O21
69	5M	902	3PE	O11-C1-C2-O21
69	5Y	203	3PE	O11-C1-C2-O21
69	5m	201	3PE	O11-C1-C2-O21
70	5A	202	PC1	O11-C1-C2-O21
75	1h	202	CDL	OB5-CB3-CB4-OB6
86	4A	601	PGV	O01-C02-C03-O11
86	8A	601	PGV	O01-C02-C03-O11
86	8C	302	PGV	O01-C02-C03-O11
91	4B	304	PSC	O01-C02-C03-O11
69	1K	101	3PE	O31-C31-C32-C33
84	6C	502	HEM	C4B-C3B-CAB-CBB
86	4B	301	PGV	C2-C3-C4-C5
75	5d	201	CDL	CB2-C1-CA2-OA2
80	1n	201	EHZ	O1-C7-C8-C9
70	1I	204	PC1	C24-C25-C26-C27
70	1M	504	PC1	C32-C33-C34-C35
69	5Y	202	3PE	O21-C2-C3-O31
75	1N	401	CDL	OB6-CB4-CB6-OB8
75	1h	202	CDL	OB6-CB4-CB6-OB8
86	4J	101	PGV	O03-C01-C02-O01
69	5M	904	3PE	C24-C25-C26-C27
86	8D	202	PGV	C7-C8-C9-C10
80	5T	101	EHZ	C1-C21-C22-C23
86	4L	101	PGV	C26-C27-C28-C29
86	8A	603	PGV	C25-C26-C27-C28
70	5M	905	PC1	C32-C33-C34-C35
76	1O	401	GTP	PA-O3A-PB-O1B
69	5K	101	3PE	O31-C31-C32-C33
75	5d	204	CDL	C72-C73-C74-C75
70	1L	706	PC1	C36-C37-C38-C39
81	1h	201	AME	C-CA-N-CT1
86	8A	601	PGV	C29-C30-C31-C32
69	1A	201	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	1M	503	3PE	C1-O11-P-O13
69	1Y	204	3PE	C11-O13-P-O11
69	5A	201	3PE	C11-O13-P-O11
69	5M	904	3PE	C1-O11-P-O13
69	5P	403	3PE	C1-O11-P-O13
69	5Y	202	3PE	C11-O13-P-O11
69	5Y	206	3PE	C11-O13-P-O11
70	5M	905	PC1	C11-O13-P-O11
75	1N	401	CDL	CB3-OB5-PB2-OB2
75	4C	306	CDL	CA3-OA5-PA1-OA2
75	5L	702	CDL	CB3-OB5-PB2-OB2
75	5N	401	CDL	CB3-OB5-PB2-OB2
75	5a	201	CDL	CB2-OB2-PB2-OB5
75	8C	305	CDL	CA3-OA5-PA1-OA2
86	4A	603	PGV	C04-O12-P-O11
86	8A	603	PGV	C03-O11-P-O12
86	8A	604	PGV	C04-O12-P-O11
86	8C	304	PGV	C03-O11-P-O12
69	5M	903	3PE	C34-C35-C36-C37
70	5h	202	PC1	C2B-C2C-C2D-C2E
75	5L	702	CDL	C33-C34-C35-C36
75	5h	201	CDL	C34-C35-C36-C37
69	5d	202	3PE	C2-C1-O11-P
70	1I	201	PC1	C2-C1-O11-P
70	5H	402	PC1	C2-C1-O11-P
75	1L	702	CDL	CA4-CA3-OA5-PA1
75	1d	204	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CB4-CB3-OB5-PB2
75	5d	204	CDL	C1-CA2-OA2-PA1
75	5d	204	CDL	C1-CB2-OB2-PB2
75	5h	201	CDL	C1-CB2-OB2-PB2
69	1A	201	3PE	C11-O13-P-O14
69	1K	101	3PE	C1-O11-P-O12
69	1L	705	3PE	C1-O11-P-O14
69	1d	201	3PE	C1-O11-P-O14
69	5A	201	3PE	C11-O13-P-O14
69	5K	101	3PE	C1-O11-P-O12
69	5M	903	3PE	C1-O11-P-O14
69	5P	403	3PE	C1-O11-P-O14
69	5Y	202	3PE	C1-O11-P-O14
69	5j	101	3PE	C1-O11-P-O14
70	1I	204	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
70	1M	502	PC1	C11-O13-P-O12
70	1M	504	PC1	C1-O11-P-O12
70	1M	504	PC1	C1-O11-P-O14
70	5H	403	PC1	C1-O11-P-O12
70	5I	203	PC1	C1-O11-P-O14
70	5Y	201	PC1	C11-O13-P-O12
70	5Y	201	PC1	C11-O13-P-O14
75	1H	401	CDL	CA3-OA5-PA1-OA3
75	1L	702	CDL	CA2-OA2-PA1-OA4
75	1L	702	CDL	CB3-OB5-PB2-OB3
75	1X	201	CDL	CA2-OA2-PA1-OA4
75	1h	202	CDL	CB3-OB5-PB2-OB4
75	4B	302	CDL	CA3-OA5-PA1-OA3
75	5L	702	CDL	CA2-OA2-PA1-OA4
75	5L	702	CDL	CB3-OB5-PB2-OB3
75	5d	201	CDL	CA2-OA2-PA1-OA4
75	5h	201	CDL	CB3-OB5-PB2-OB4
75	8A	605	CDL	CB3-OB5-PB2-OB4
86	4A	603	PGV	C03-O11-P-O14
86	4C	303	PGV	C03-O11-P-O14
86	4C	305	PGV	C03-O11-P-O14
86	4K	101	PGV	C03-O11-P-O14
86	8C	302	PGV	C03-O11-P-O14
86	8C	304	PGV	C03-O11-P-O14
91	4B	304	PSC	C03-O11-P-O13
91	8A	611	PSC	C03-O11-P-O13
69	5Y	202	3PE	O11-C1-C2-C3
70	1M	504	PC1	O11-C1-C2-C3
75	1h	202	CDL	OB5-CB3-CB4-CB6
75	4B	302	CDL	OA5-CA3-CA4-CA6
86	8D	202	PGV	C01-C02-C03-O11
75	5d	201	CDL	C55-C56-C57-C58
69	1K	101	3PE	C12-C11-O13-P
69	1L	701	3PE	C12-C11-O13-P
69	1M	503	3PE	C12-C11-O13-P
69	1Y	201	3PE	C12-C11-O13-P
69	1Y	203	3PE	C12-C11-O13-P
69	1Y	204	3PE	C12-C11-O13-P
69	1j	101	3PE	C12-C11-O13-P
69	5L	701	3PE	C12-C11-O13-P
69	5M	904	3PE	C12-C11-O13-P
69	5Y	203	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
69	5Y	206	3PE	C12-C11-O13-P
69	5m	201	3PE	C12-C11-O13-P
70	1A	202	PC1	C12-C11-O13-P
70	1B	203	PC1	C12-C11-O13-P
70	1J	201	PC1	C12-C11-O13-P
70	1P	401	PC1	C12-C11-O13-P
70	5B	203	PC1	C12-C11-O13-P
70	5P	401	PC1	C12-C11-O13-P
92	4C	308	PEK	C05-C04-O12-P
92	8C	307	PEK	C05-C04-O12-P
92	8G	102	PEK	C05-C04-O12-P
86	8C	301	PGV	C6-C7-C8-C9
86	8D	202	PGV	C15-C16-C17-C18
69	1M	503	3PE	C24-C25-C26-C27
69	5M	901	3PE	C38-C39-C3A-C3B
70	1H	402	PC1	C32-C31-O31-C3
75	1X	201	CDL	CB2-C1-CA2-OA2
75	5h	201	CDL	CA2-C1-CB2-OB2
69	1M	503	3PE	O11-C1-C2-O21
70	1M	504	PC1	O11-C1-C2-O21
75	1d	204	CDL	OA5-CA3-CA4-OA6
75	5d	204	CDL	OA5-CA3-CA4-OA6
75	8A	605	CDL	OA5-CA3-CA4-OA6
75	8C	305	CDL	OB5-CB3-CB4-OB6
86	4A	602	PGV	O01-C02-C03-O11
70	1A	202	PC1	C22-C23-C24-C25
86	8L	101	PGV	C11-C12-C13-C14
85	6D	501	HEC	C3D-CAD-CBD-CGD
69	5M	903	3PE	C24-C25-C26-C27
86	4A	601	PGV	C29-C30-C31-C32
80	1n	201	EHZ	C10-C11-N1-C12
75	1L	702	CDL	C58-C59-C60-C61
75	4D	201	CDL	C62-C63-C64-C65
70	1M	502	PC1	C11-C12-N-C15
75	5N	401	CDL	CA7-C31-C32-C33
70	1A	202	PC1	O13-C11-C12-N
70	1B	203	PC1	O13-C11-C12-N
70	1L	706	PC1	O13-C11-C12-N
70	1P	401	PC1	O13-C11-C12-N
70	1h	203	PC1	O13-C11-C12-N
70	5A	202	PC1	O13-C11-C12-N
70	5B	203	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
70	5P	401	PC1	O13-C11-C12-N
70	5Y	207	PC1	O13-C11-C12-N
70	5h	202	PC1	O13-C11-C12-N
75	1d	204	CDL	CA3-CA4-CA6-OA8
80	5n	201	EHZ	C16-C17-C20-O6
85	6D	501	HEC	C2D-C3D-CAD-CBD
69	1M	501	3PE	O21-C2-C3-O31
69	5L	703	3PE	O21-C2-C3-O31
75	4B	302	CDL	OB6-CB4-CB6-OB8
86	8J	101	PGV	O03-C01-C02-O01
86	8B	301	PGV	C27-C28-C29-C30
70	1B	203	PC1	C28-C29-C2A-C2B
70	5B	202	PC1	C37-C38-C39-C3A
69	5M	901	3PE	C23-C24-C25-C26
86	8A	601	PGV	C02-C03-O11-P
75	4C	306	CDL	C81-C82-C83-C84
75	5d	201	CDL	C35-C36-C37-C38
75	1N	401	CDL	C32-C31-CA7-OA8
70	1h	203	PC1	C2B-C2C-C2D-C2E
86	8A	602	PGV	C26-C27-C28-C29
75	4C	306	CDL	C51-C52-C53-C54
86	8B	301	PGV	C21-C22-C23-C24
70	5I	203	PC1	C24-C25-C26-C27
75	4C	306	CDL	C52-C53-C54-C55
86	8A	602	PGV	C2-C3-C4-C5
86	8A	602	PGV	C4-C5-C6-C7
75	1a	201	CDL	CA5-C11-C12-C13
69	5L	701	3PE	C28-C29-C2A-C2B
69	1m	201	3PE	O21-C21-C22-C23
70	1d	203	PC1	C38-C39-C3A-C3B
80	5n	201	EHZ	C19-C17-C20-O6
86	4J	101	PGV	C9-C10-C11-C12
69	5L	701	3PE	C33-C34-C35-C36
75	4C	306	CDL	C74-C75-C76-C77
86	4L	101	PGV	C20-C21-C22-C23
86	8A	602	PGV	C21-C22-C23-C24
69	5M	903	3PE	C3A-C3B-C3C-C3D
75	1X	201	CDL	C63-C64-C65-C66
75	4B	302	CDL	C32-C33-C34-C35
86	4C	307	PGV	C4-C5-C6-C7
86	5i	201	PGV	C1-C2-C3-C4
86	4A	603	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
75	1H	401	CDL	CA3-CA4-OA6-CA5
75	5H	401	CDL	CA3-CA4-OA6-CA5
70	5M	905	PC1	O11-C1-C2-C3
87	8A	606	HEA	C11-C12-C13-C14
69	5L	703	3PE	C33-C34-C35-C36
69	1M	501	3PE	C23-C24-C25-C26
69	5m	201	3PE	O21-C21-C22-C23
75	8C	305	CDL	C71-C72-C73-C74
75	8D	201	CDL	C62-C63-C64-C65
86	4A	601	PGV	C9-C10-C11-C12
86	4C	301	PGV	C11-C12-C13-C14
69	1d	202	3PE	C2-C1-O11-P
69	1Y	204	3PE	O11-C1-C2-O21
69	5M	904	3PE	O11-C1-C2-O21
70	1B	203	PC1	O11-C1-C2-O21
70	5M	905	PC1	O11-C1-C2-O21
70	5h	202	PC1	O11-C1-C2-O21
75	4B	302	CDL	OA5-CA3-CA4-OA6
86	4C	303	PGV	O01-C02-C03-O11
86	8D	202	PGV	O01-C02-C03-O11
91	4B	304	PSC	C2-C3-C4-C5
70	1M	502	PC1	C11-C12-N-C14
69	5L	703	3PE	C32-C33-C34-C35
75	5d	204	CDL	C32-C33-C34-C35
87	4A	605	HEA	C2D-C3D-CAD-CBD
69	5M	904	3PE	C37-C38-C39-C3A
75	1X	201	CDL	C55-C56-C57-C58
86	8C	302	PGV	C9-C10-C11-C12
86	8C	304	PGV	C9-C10-C11-C12
70	5H	403	PC1	O21-C21-C22-C23
69	1d	201	3PE	O21-C2-C3-O31
70	1B	203	PC1	O21-C2-C3-O31
70	5B	203	PC1	O21-C2-C3-O31
69	1L	701	3PE	C11-O13-P-O11
69	1L	705	3PE	C11-O13-P-O11
69	1M	501	3PE	C11-O13-P-O11
69	1M	503	3PE	C11-O13-P-O11
69	1M	505	3PE	C1-O11-P-O13
69	1M	505	3PE	C11-O13-P-O11
69	1Y	203	3PE	C1-O11-P-O13
69	1d	201	3PE	C11-O13-P-O11
69	1d	202	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	1j	101	3PE	C1-O11-P-O13
69	1j	101	3PE	C11-O13-P-O11
69	1m	201	3PE	C11-O13-P-O11
69	5L	701	3PE	C11-O13-P-O11
69	5M	903	3PE	C11-O13-P-O11
69	5M	904	3PE	C11-O13-P-O11
69	5M	906	3PE	C1-O11-P-O13
69	5M	906	3PE	C11-O13-P-O11
69	5Y	205	3PE	C1-O11-P-O13
69	5d	202	3PE	C11-O13-P-O11
69	5m	201	3PE	C11-O13-P-O11
70	1B	202	PC1	C11-O13-P-O11
70	1J	201	PC1	C1-O11-P-O13
70	1M	502	PC1	C1-O11-P-O13
70	1d	203	PC1	C1-O11-P-O13
70	1h	203	PC1	C11-O13-P-O11
70	1q	201	PC1	C1-O11-P-O13
70	5A	203	PC1	C1-O11-P-O13
70	5B	202	PC1	C11-O13-P-O11
70	5Y	201	PC1	C1-O11-P-O13
70	5d	203	PC1	C1-O11-P-O13
70	5h	202	PC1	C11-O13-P-O11
70	5q	201	PC1	C1-O11-P-O13
75	1N	401	CDL	CA3-OA5-PA1-OA2
75	1X	201	CDL	CB3-OB5-PB2-OB2
75	1a	201	CDL	CA3-OA5-PA1-OA2
75	1a	201	CDL	CB2-OB2-PB2-OB5
75	1d	204	CDL	CB2-OB2-PB2-OB5
75	4B	302	CDL	CB3-OB5-PB2-OB2
75	4C	306	CDL	CB2-OB2-PB2-OB5
75	4C	306	CDL	CB3-OB5-PB2-OB2
75	4D	201	CDL	CA3-OA5-PA1-OA2
75	4D	201	CDL	CB2-OB2-PB2-OB5
75	4D	201	CDL	CB3-OB5-PB2-OB2
75	5N	401	CDL	CA3-OA5-PA1-OA2
75	5a	201	CDL	CA3-OA5-PA1-OA2
75	5d	201	CDL	CB3-OB5-PB2-OB2
75	5d	204	CDL	CB2-OB2-PB2-OB5
75	5h	201	CDL	CA2-OA2-PA1-OA5
75	8A	605	CDL	CA3-OA5-PA1-OA2
75	8C	305	CDL	CB2-OB2-PB2-OB5
75	8C	305	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
75	8D	201	CDL	CA3-OA5-PA1-OA2
75	8D	201	CDL	CB2-OB2-PB2-OB5
86	4A	601	PGV	C04-O12-P-O11
86	4G	101	PGV	C04-O12-P-O11
86	4K	101	PGV	C04-O12-P-O11
86	4L	101	PGV	C03-O11-P-O12
86	4L	101	PGV	C04-O12-P-O11
86	5i	201	PGV	C04-O12-P-O11
86	8A	601	PGV	C04-O12-P-O11
86	8G	101	PGV	C04-O12-P-O11
86	8K	101	PGV	C04-O12-P-O11
86	8L	101	PGV	C03-O11-P-O12
86	8L	101	PGV	C04-O12-P-O11
70	1q	201	PC1	C2A-C2B-C2C-C2D
86	4C	302	PGV	C1-C2-C3-C4
70	1M	504	PC1	C1-C2-C3-O31
70	5H	402	PC1	C1-C2-C3-O31
70	5M	905	PC1	C1-C2-C3-O31
70	1H	402	PC1	C39-C3A-C3B-C3C
75	1L	702	CDL	C37-C38-C39-C40
86	8A	604	PGV	C30-C31-C32-C33
69	1d	201	3PE	C24-C25-C26-C27
87	4A	605	HEA	C4D-C3D-CAD-CBD
70	5Y	201	PC1	C11-C12-N-C15
69	5m	201	3PE	C23-C24-C25-C26
70	5I	203	PC1	C23-C24-C25-C26
69	5M	904	3PE	C34-C35-C36-C37
75	5L	702	CDL	CA4-CA3-OA5-PA1
86	8D	202	PGV	C05-C04-O12-P
86	8A	602	PGV	C11-C12-C13-C14
86	8A	603	PGV	C11-C12-C13-C14
86	8J	101	PGV	C9-C10-C11-C12
86	8K	101	PGV	C9-C10-C11-C12
84	3P	502	HEM	CAD-CBD-CGD-O1D
75	5L	702	CDL	C58-C59-C60-C61
75	5d	204	CDL	CB2-C1-CA2-OA2
75	5d	204	CDL	CA7-C31-C32-C33
86	4C	301	PGV	C11-C10-C9-C8
86	4A	602	PGV	C22-C23-C24-C25
86	4A	603	PGV	C11-C12-C13-C14
70	1B	202	PC1	C36-C37-C38-C39
69	5M	903	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
75	1X	201	CDL	C34-C35-C36-C37
70	1H	402	PC1	O21-C21-C22-C23
70	5H	402	PC1	C31-C32-C33-C34
70	5A	202	PC1	C22-C23-C24-C25
70	5B	202	PC1	C36-C37-C38-C39
86	8G	101	PGV	C7-C8-C9-C10
86	8A	601	PGV	C13-C14-C15-C16
80	1n	201	EHZ	O4-C15-C16-C17
86	4C	302	PGV	C11-C12-C13-C14
86	8C	301	PGV	C11-C12-C13-C14
69	5P	403	3PE	C36-C37-C38-C39
86	4G	101	PGV	C13-C14-C15-C16
75	1L	702	CDL	C38-C39-C40-C41
84	3P	501	HEM	CAA-CBA-CGA-O1A
70	5Y	207	PC1	O31-C31-C32-C33
69	1Y	201	3PE	C27-C28-C29-C2A
86	8A	601	PGV	C24-C25-C26-C27
69	1d	201	3PE	C2B-C2C-C2D-C2E
84	6C	502	HEM	CAA-CBA-CGA-O1A
84	6P	502	HEM	CAA-CBA-CGA-O1A
84	6P	502	HEM	CAD-CBD-CGD-O1D
69	5M	901	3PE	O21-C2-C3-O31
69	5M	902	3PE	O21-C2-C3-O31
86	4C	301	PGV	O03-C01-C02-O01
91	8A	611	PSC	O03-C01-C02-O01
75	5d	201	CDL	C31-C32-C33-C34
75	5d	204	CDL	CA4-CA3-OA5-PA1
84	3C	501	HEM	CAA-CBA-CGA-O1A
86	4C	305	PGV	C9-C10-C11-C12
86	8D	202	PGV	C9-C10-C11-C12
86	4B	301	PGV	C27-C28-C29-C30
84	3C	502	HEM	CAA-CBA-CGA-O1A
84	6P	501	HEM	CAD-CBD-CGD-O1D
70	5A	203	PC1	C21-C22-C23-C24
80	5n	201	EHZ	C10-C11-N1-C12
87	8A	607	HEA	C3D-CAD-CBD-CGD
84	3C	501	HEM	CAA-CBA-CGA-O2A
84	3P	502	HEM	CAA-CBA-CGA-O1A
84	6P	501	HEM	CAA-CBA-CGA-O2A
86	4C	304	PGV	C13-C14-C15-C16
92	8C	307	PEK	O03-C01-C02-C03
69	1P	403	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
75	5d	201	CDL	C63-C64-C65-C66
84	3P	501	HEM	CAA-CBA-CGA-O2A
87	8A	606	HEA	CAD-CBD-CGD-O1D
86	8L	101	PGV	C9-C10-C11-C12
70	1L	706	PC1	C25-C26-C27-C28
69	1M	505	3PE	C26-C27-C28-C29
84	6P	502	HEM	CAA-CBA-CGA-O2A
80	1T	101	EHZ	C1-C21-C22-C23
80	1T	101	EHZ	C7-C8-C9-O2
80	1n	201	EHZ	N2-C15-C16-C17
92	8C	307	PEK	C17-C18-C19-C20
75	1h	202	CDL	CB7-C71-C72-C73
70	5P	401	PC1	C24-C25-C26-C27
75	1h	202	CDL	C34-C35-C36-C37
84	3C	502	HEM	CAA-CBA-CGA-O2A
69	1M	503	3PE	C1-C2-O21-C21
69	1Y	203	3PE	C1-C2-O21-C21
87	8A	606	HEA	C27-C19-C20-C21
69	5A	201	3PE	C35-C36-C37-C38
70	1M	502	PC1	C11-C12-N-C13
86	4K	101	PGV	C9-C10-C11-C12
91	8A	611	PSC	C12-C13-C14-C15
91	8A	611	PSC	C4-C5-C6-C7
84	6C	501	HEM	CAA-CBA-CGA-O1A
84	6P	502	HEM	CAD-CBD-CGD-O2D
75	1h	202	CDL	C74-C75-C76-C77
86	4C	304	PGV	C23-C24-C25-C26
86	4A	602	PGV	C05-C04-O12-P
75	5L	702	CDL	C37-C38-C39-C40
69	1d	202	3PE	O11-C1-C2-O21
75	5h	201	CDL	OB5-CB3-CB4-OB6
75	4C	306	CDL	C18-C19-C20-C21
69	1L	705	3PE	O11-C1-C2-C3
70	1L	706	PC1	O11-C1-C2-C3
70	5A	202	PC1	O11-C1-C2-C3
70	5H	403	PC1	O11-C1-C2-C3
86	4L	101	PGV	C01-C02-C03-O11
86	8C	303	PGV	C9-C10-C11-C12
84	3P	502	HEM	CAA-CBA-CGA-O2A
84	6P	501	HEM	CAD-CBD-CGD-O2D
87	4A	605	HEA	CAD-CBD-CGD-O1D
69	5Y	202	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
69	5P	403	3PE	C37-C38-C39-C3A
86	8B	301	PGV	C24-C25-C26-C27
75	5N	401	CDL	O1-C1-CB2-OB2
84	3P	502	HEM	CAD-CBD-CGD-O2D
84	6P	501	HEM	CAA-CBA-CGA-O1A
75	4C	306	CDL	C38-C39-C40-C41
75	5L	702	CDL	C38-C39-C40-C41
80	1T	101	EHZ	C11-C10-S1-C9
80	5T	101	EHZ	C11-C10-S1-C9
70	1I	201	PC1	O21-C2-C3-O31
75	5a	201	CDL	OB6-CB4-CB6-OB8
75	8D	201	CDL	OA6-CA4-CA6-OA8
86	4A	601	PGV	O03-C01-C02-O01
92	4C	308	PEK	C17-C18-C19-C20
87	4A	605	HEA	CAD-CBD-CGD-O2D
69	1L	703	3PE	C32-C33-C34-C35
69	1L	704	3PE	C23-C24-C25-C26
69	5A	201	3PE	C32-C33-C34-C35
92	4C	308	PEK	O04-C21-C22-C23
69	1P	403	3PE	C37-C38-C39-C3A
86	8A	601	PGV	C21-C22-C23-C24
75	8A	605	CDL	C12-C11-CA5-OA6
92	4C	308	PEK	C22-C23-C24-C25
84	6C	501	HEM	CAA-CBA-CGA-O2A
86	4A	603	PGV	C26-C27-C28-C29
75	4D	201	CDL	C38-C39-C40-C41
84	6C	502	HEM	CAA-CBA-CGA-O2A
69	5M	903	3PE	C2B-C2C-C2D-C2E
86	8C	301	PGV	C9-C10-C11-C12
86	8C	303	PGV	C20-C21-C22-C23
76	5O	401	GTP	O4'-C4'-C5'-O5'
86	4C	302	PGV	C6-C7-C8-C9
87	8A	606	HEA	CAA-CBA-CGA-O1A
86	4C	302	PGV	C3-C4-C5-C6
87	4A	604	HEA	CAD-CBD-CGD-O2D
75	5d	201	CDL	C60-C61-C62-C63
86	8A	603	PGV	C6-C7-C8-C9
75	1a	201	CDL	C13-C14-C15-C16
86	8A	603	PGV	C2-C3-C4-C5
86	4C	304	PGV	C9-C10-C11-C12
86	8D	202	PGV	C11-C12-C13-C14
69	5Y	206	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
75	4C	306	CDL	OB5-CB3-CB4-OB6
86	4L	101	PGV	O01-C02-C03-O11
75	5a	201	CDL	CA5-C11-C12-C13
86	4C	304	PGV	C5-C6-C7-C8
75	1a	201	CDL	C52-C51-CB5-OB7
85	3D	501	HEC	CAA-CBA-CGA-O2A
76	1O	401	GTP	PB-O3A-PA-O5'
86	8C	302	PGV	C26-C27-C28-C29
69	1M	501	3PE	C3A-C3B-C3C-C3D
86	4C	305	PGV	C19-C20-C21-C22
86	8D	202	PGV	C25-C26-C27-C28
69	1Y	201	3PE	O11-C1-C2-C3
69	5Y	203	3PE	O11-C1-C2-C3
70	1B	203	PC1	O11-C1-C2-C3
70	1I	201	PC1	O11-C1-C2-C3
70	5H	402	PC1	O11-C1-C2-C3
75	1L	702	CDL	OA5-CA3-CA4-CA6
75	1X	201	CDL	OB5-CB3-CB4-CB6
75	5h	201	CDL	OB5-CB3-CB4-CB6
91	4B	304	PSC	C01-C02-C03-O11
91	8A	611	PSC	C01-C02-C03-O11
70	5B	202	PC1	C3D-C3E-C3F-C3G
86	8L	101	PGV	C3-C4-C5-C6
75	5N	401	CDL	C32-C31-CA7-OA9
73	5F	501	FMN	O2'-C2'-C3'-O3'
75	1N	401	CDL	C1-CB2-OB2-PB2
86	8J	101	PGV	C3-C4-C5-C6
70	1h	203	PC1	O21-C2-C3-O31
75	1a	201	CDL	OB6-CB4-CB6-OB8
75	1h	202	CDL	OA6-CA4-CA6-OA8
69	1K	101	3PE	C26-C27-C28-C29
69	5m	201	3PE	C2C-C2D-C2E-C2F
75	8C	305	CDL	C18-C19-C20-C21
69	1A	201	3PE	O22-C21-C22-C23
69	1L	703	3PE	C35-C36-C37-C38
75	4C	306	CDL	C22-C23-C24-C25
87	4A	604	HEA	CAD-CBD-CGD-O1D
87	8A	606	HEA	CAD-CBD-CGD-O2D
86	4C	307	PGV	C9-C10-C11-C12
75	4B	302	CDL	C56-C57-C58-C59
87	8A	606	HEA	C26-C15-C16-C17
87	8A	606	HEA	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
80	5n	201	EHZ	C18-C17-C20-O6
69	5A	201	3PE	C2A-C2B-C2C-C2D
86	4A	602	PGV	O01-C1-C2-C3
86	4A	601	PGV	C11-C10-C9-C8
86	4J	101	PGV	C6-C7-C8-C9
69	1L	704	3PE	C33-C34-C35-C36
69	1K	101	3PE	C24-C25-C26-C27
69	5Y	206	3PE	O21-C21-C22-C23
75	4B	302	CDL	C12-C11-CA5-OA6
86	4C	302	PGV	C9-C10-C11-C12
86	4C	303	PGV	C9-C10-C11-C12
86	4C	307	PGV	C11-C12-C13-C14
86	4K	101	PGV	C11-C12-C13-C14
86	8A	601	PGV	C9-C10-C11-C12
86	8C	306	PGV	C11-C12-C13-C14
86	8G	101	PGV	C9-C10-C11-C12
91	4B	304	PSC	C12-C13-C14-C15
85	3D	501	HEC	CAA-CBA-CGA-O1A
85	6Q	501	HEC	CAA-CBA-CGA-O2A
69	1L	705	3PE	C1-C2-O21-C21
69	5M	902	3PE	C1-C2-O21-C21
69	5M	904	3PE	C1-C2-O21-C21
69	5Y	205	3PE	C1-C2-O21-C21
69	5Y	206	3PE	C3-C2-O21-C21
86	4C	304	PGV	C01-C02-O01-C1
86	8C	303	PGV	C01-C02-O01-C1
85	3D	501	HEC	C3D-CAD-CBD-CGD
86	4A	601	PGV	O03-C19-C20-C21
86	4C	301	PGV	O03-C19-C20-C21
69	5K	101	3PE	C26-C27-C28-C29
75	1N	401	CDL	C39-C40-C41-C42
84	3P	501	HEM	CAD-CBD-CGD-O1D
85	3Q	501	HEC	CAA-CBA-CGA-O2A
75	1X	201	CDL	C60-C61-C62-C63
75	5d	204	CDL	C32-C31-CA7-OA8
70	1M	504	PC1	C28-C29-C2A-C2B
86	4B	301	PGV	C9-C10-C11-C12
86	8A	601	PGV	C11-C12-C13-C14
86	8K	101	PGV	C11-C12-C13-C14
69	1Y	202	3PE	C26-C27-C28-C29
86	4A	601	PGV	C24-C25-C26-C27
75	4C	306	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
70	1I	201	PC1	O11-C1-C2-O21
70	5B	203	PC1	O11-C1-C2-O21
75	1H	401	CDL	OB5-CB3-CB4-OB6
75	5H	401	CDL	OB5-CB3-CB4-OB6
69	1Y	204	3PE	O21-C21-C22-C23
86	8A	601	PGV	O03-C19-C20-C21
70	1L	706	PC1	O32-C31-C32-C33
75	8C	305	CDL	C52-C53-C54-C55
75	5N	401	CDL	C39-C40-C41-C42
86	8C	303	PGV	C13-C14-C15-C16
84	3P	501	HEM	CAD-CBD-CGD-O2D
86	4G	101	PGV	C9-C10-C11-C12
86	4C	303	PGV	C26-C27-C28-C29
85	3Q	501	HEC	CAA-CBA-CGA-O1A
85	6Q	501	HEC	CAA-CBA-CGA-O1A
69	5P	403	3PE	O21-C21-C22-C23
75	1a	201	CDL	C12-C11-CA5-OA6
69	5K	101	3PE	C24-C25-C26-C27
86	4J	101	PGV	C2-C3-C4-C5
70	5P	401	PC1	C33-C34-C35-C36
70	5B	203	PC1	O11-C1-C2-C3
75	5H	401	CDL	OB5-CB3-CB4-CB6
75	5d	201	CDL	OB5-CB3-CB4-CB6
86	4A	601	PGV	C01-C02-C03-O11
86	8A	601	PGV	C01-C02-C03-O11
70	1d	203	PC1	O21-C21-C22-C23
69	1Y	201	3PE	C34-C35-C36-C37
70	1P	401	PC1	C33-C34-C35-C36
70	5q	201	PC1	C32-C33-C34-C35
86	4B	301	PGV	C20-C21-C22-C23
87	8A	607	HEA	CAD-CBD-CGD-O2D
78	1P	402	NDP	C2B-O2B-P2B-O2X
87	4A	604	HEA	C4D-C3D-CAD-CBD
70	1I	201	PC1	C33-C34-C35-C36
69	1K	101	3PE	O32-C31-C32-C33
70	5d	203	PC1	O21-C21-C22-C23
80	1T	101	EHZ	C1-C2-C3-C4
86	8B	301	PGV	C22-C23-C24-C25
86	4L	101	PGV	C9-C10-C11-C12
69	1P	403	3PE	O21-C21-C22-C23
69	1d	202	3PE	C2-C3-O31-C31
86	4B	301	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
70	5Y	207	PC1	C24-C25-C26-C27
87	8A	606	HEA	CAA-CBA-CGA-O2A
86	8J	101	PGV	O03-C19-C20-C21
76	1O	401	GTP	PA-O3A-PB-O2B
76	5O	401	GTP	PA-O3A-PB-O1B
85	6D	501	HEC	CAA-CBA-CGA-O2A
75	5d	204	CDL	C32-C31-CA7-OA9
70	5H	402	PC1	C36-C37-C38-C39
70	5Y	201	PC1	C11-C12-N-C14
82	1l	201	MYR	C3-C4-C5-C6
70	1d	203	PC1	C37-C38-C39-C3A
87	4A	604	HEA	CAA-CBA-CGA-O1A
69	5K	101	3PE	O32-C31-C32-C33
86	4A	602	PGV	O02-C1-C2-C3
86	4J	101	PGV	C30-C31-C32-C33
69	1M	505	3PE	C33-C34-C35-C36
86	4C	304	PGV	C6-C7-C8-C9
69	1Y	204	3PE	O22-C21-C22-C23
75	1X	201	CDL	C32-C31-CA7-OA9
86	4A	602	PGV	C9-C10-C11-C12
86	4A	602	PGV	C11-C12-C13-C14
86	4A	601	PGV	C21-C22-C23-C24
86	4C	301	PGV	O04-C19-C20-C21
69	1d	202	3PE	C35-C36-C37-C38
69	5m	201	3PE	C29-C2A-C2B-C2C
75	5h	201	CDL	C74-C75-C76-C77
69	5j	101	3PE	C1-C2-C3-O31
91	8A	611	PSC	O03-C01-C02-C03
69	5M	902	3PE	C25-C26-C27-C28
69	1Y	203	3PE	C21-C22-C23-C24
86	8A	601	PGV	O04-C19-C20-C21
70	5Y	207	PC1	C22-C23-C24-C25
70	1d	203	PC1	C34-C35-C36-C37
75	1L	702	CDL	C52-C51-CB5-OB6
70	5Y	207	PC1	C25-C26-C27-C28
75	1L	702	CDL	C52-C51-CB5-OB7
86	8D	202	PGV	C27-C28-C29-C30
91	4B	304	PSC	C28-C29-C30-C31
75	4D	201	CDL	C37-C38-C39-C40
69	1K	101	3PE	C11-O13-P-O14
69	1L	701	3PE	C11-O13-P-O14
69	1L	705	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
69	1M	501	3PE	C11-O13-P-O14
69	1Y	203	3PE	C1-O11-P-O14
69	1m	201	3PE	C11-O13-P-O14
69	5K	101	3PE	C11-O13-P-O14
69	5L	701	3PE	C11-O13-P-O14
69	5Y	202	3PE	C1-O11-P-O12
69	5d	202	3PE	C11-O13-P-O14
69	5m	201	3PE	C11-O13-P-O14
70	1J	201	PC1	C1-O11-P-O14
70	1M	502	PC1	C1-O11-P-O14
70	1d	203	PC1	C1-O11-P-O14
70	1h	203	PC1	C11-O13-P-O14
70	5A	203	PC1	C1-O11-P-O14
70	5Y	201	PC1	C1-O11-P-O14
70	5Y	201	PC1	C11-C12-N-C13
70	5d	203	PC1	C1-O11-P-O14
70	5h	202	PC1	C11-O13-P-O14
75	1N	401	CDL	CA3-OA5-PA1-OA3
75	1X	201	CDL	CB2-OB2-PB2-OB3
75	1d	204	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	CB2-OB2-PB2-OB4
75	4B	302	CDL	CB3-OB5-PB2-OB4
75	4D	201	CDL	CB2-OB2-PB2-OB3
75	5N	401	CDL	CA3-OA5-PA1-OA3
75	5d	201	CDL	CB2-OB2-PB2-OB3
75	5d	204	CDL	CA3-OA5-PA1-OA3
75	5d	204	CDL	CB2-OB2-PB2-OB3
75	5d	204	CDL	CB3-OB5-PB2-OB3
75	5h	201	CDL	CA2-OA2-PA1-OA3
75	8D	201	CDL	CB2-OB2-PB2-OB3
76	1O	401	GTP	C5'-O5'-PA-O1A
76	5O	401	GTP	C5'-O5'-PA-O1A
78	1P	402	NDP	C2N-C3N-C7N-N7N
78	5P	402	NDP	C2N-C3N-C7N-N7N
86	4A	601	PGV	C04-O12-P-O13
86	4A	603	PGV	C04-O12-P-O14
86	4L	101	PGV	C03-O11-P-O13
86	8A	601	PGV	C04-O12-P-O13
86	8K	101	PGV	C04-O12-P-O13
91	4B	304	PSC	C04-O12-P-O14
91	8A	611	PSC	C04-O12-P-O14
76	1O	401	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
78	1P	402	NDP	O4B-C4B-C5B-O5B
78	5P	402	NDP	O4B-C4B-C5B-O5B
91	4B	304	PSC	C4-C5-C6-C7
91	8A	611	PSC	C24-C25-C26-C27
69	5Y	206	3PE	O22-C21-C22-C23
70	1d	203	PC1	O22-C21-C22-C23
75	5d	201	CDL	C32-C31-CA7-OA9
69	1d	202	3PE	O11-C1-C2-C3
69	5M	902	3PE	O11-C1-C2-C3
75	1H	401	CDL	OB5-CB3-CB4-CB6
86	8C	302	PGV	C01-C02-C03-O11
86	4A	601	PGV	C15-C16-C17-C18
87	8A	607	HEA	CAD-CBD-CGD-O1D
75	4B	302	CDL	C11-C12-C13-C14
70	5d	203	PC1	O22-C21-C22-C23
75	1a	201	CDL	C12-C11-CA5-OA7
86	4A	601	PGV	O04-C19-C20-C21
69	5M	903	3PE	O21-C21-C22-C23
70	1M	504	PC1	C31-C32-C33-C34
69	1d	201	3PE	C3A-C3B-C3C-C3D
91	4B	304	PSC	C27-C28-C29-C30
69	5M	906	3PE	C27-C28-C29-C2A
75	5d	201	CDL	C34-C35-C36-C37
69	1L	705	3PE	O31-C31-C32-C33
75	1L	702	CDL	C32-C31-CA7-OA8
75	8D	201	CDL	C32-C31-CA7-OA8
75	8D	201	CDL	C52-C51-CB5-OB6
69	5A	201	3PE	O22-C21-C22-C23
70	1I	201	PC1	C2-C3-O31-C31
75	5a	201	CDL	C52-C51-CB5-OB7
86	4J	101	PGV	C27-C28-C29-C30
70	1L	706	PC1	C3A-C3B-C3C-C3D
75	5N	401	CDL	C32-C33-C34-C35
75	8D	201	CDL	C38-C39-C40-C41
69	1M	501	3PE	C12-C11-O13-P
69	1Y	204	3PE	C3-C2-O21-C21
69	1m	201	3PE	C12-C11-O13-P
69	5M	902	3PE	C12-C11-O13-P
69	5Y	202	3PE	C1-C2-O21-C21
69	5Y	202	3PE	C3-C2-O21-C21
69	5Y	205	3PE	C12-C11-O13-P
69	5Y	205	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
70	5A	202	PC1	C12-C11-O13-P
70	5A	203	PC1	C12-C11-O13-P
75	1d	204	CDL	CA6-CA4-OA6-CA5
75	5d	204	CDL	CA6-CA4-OA6-CA5
92	4C	309	PEK	C05-C04-O12-P
70	1h	203	PC1	C23-C24-C25-C26
75	4D	201	CDL	C75-C76-C77-C78
86	4G	101	PGV	C27-C28-C29-C30
75	8A	605	CDL	C81-C82-C83-C84
86	8C	301	PGV	C5-C6-C7-C8
70	1q	201	PC1	C32-C33-C34-C35
86	4C	303	PGV	C6-C7-C8-C9
70	1A	202	PC1	O31-C31-C32-C33
70	5h	202	PC1	O31-C31-C32-C33
75	5a	201	CDL	C12-C11-CA5-OA6
86	8C	303	PGV	O01-C1-C2-C3
91	4B	304	PSC	O01-C1-C2-C3
75	4D	201	CDL	C42-C43-C44-C45
86	8J	101	PGV	C27-C28-C29-C30
69	1L	703	3PE	C29-C2A-C2B-C2C
70	1I	201	PC1	C2B-C2C-C2D-C2E
91	8A	611	PSC	C27-C28-C29-C30
69	1Y	202	3PE	O21-C21-C22-C23
70	1d	203	PC1	O31-C31-C32-C33
70	5A	202	PC1	O31-C31-C32-C33
75	1N	401	CDL	C12-C11-CA5-OA6
75	4B	302	CDL	C32-C31-CA7-OA8
75	4D	201	CDL	C32-C31-CA7-OA8
86	4C	302	PGV	O03-C19-C20-C21
75	1d	204	CDL	CB2-C1-CA2-OA2
69	1m	201	3PE	C23-C24-C25-C26
69	5M	906	3PE	C33-C34-C35-C36
86	8A	601	PGV	C15-C16-C17-C18
70	1H	402	PC1	O11-C1-C2-O21
73	1F	501	FMN	N10-C1'-C2'-O2'
69	1Y	202	3PE	O22-C21-C22-C23
75	5L	702	CDL	C52-C51-CB5-OB7
69	1d	202	3PE	C34-C35-C36-C37
75	8A	605	CDL	C56-C57-C58-C59
91	8A	611	PSC	C3-C4-C5-C6
69	1K	101	3PE	O21-C21-C22-C23
69	1d	202	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
69	1m	201	3PE	O31-C31-C32-C33
69	5M	903	3PE	O31-C31-C32-C33
69	5d	202	3PE	O31-C31-C32-C33
69	5m	201	3PE	O31-C31-C32-C33
70	1h	203	PC1	O31-C31-C32-C33
70	5A	202	PC1	O21-C21-C22-C23
70	5B	203	PC1	O21-C21-C22-C23
70	5d	203	PC1	O31-C31-C32-C33
75	1H	401	CDL	C52-C51-CB5-OB6
75	5L	702	CDL	C32-C31-CA7-OA8
75	5L	702	CDL	C52-C51-CB5-OB6
86	8D	202	PGV	O01-C1-C2-C3
86	8D	202	PGV	O03-C19-C20-C21
69	1A	201	3PE	C2B-C2C-C2D-C2E
75	8C	305	CDL	C13-C14-C15-C16
70	5A	202	PC1	C23-C24-C25-C26
69	5P	403	3PE	O22-C21-C22-C23
75	4D	201	CDL	C12-C11-CA5-OA6
75	4D	201	CDL	C52-C51-CB5-OB6
86	4C	307	PGV	O03-C19-C20-C21
86	8C	301	PGV	O03-C19-C20-C21
69	1P	403	3PE	O22-C21-C22-C23
69	5Y	204	3PE	O32-C31-C32-C33
70	5h	202	PC1	O32-C31-C32-C33
75	5L	702	CDL	C32-C31-CA7-OA9
75	8D	201	CDL	C32-C31-CA7-OA9
70	5H	402	PC1	C2A-C2B-C2C-C2D
69	5M	902	3PE	O31-C31-C32-C33
69	5Y	203	3PE	O31-C31-C32-C33
69	5Y	204	3PE	O21-C21-C22-C23
70	1A	202	PC1	O21-C21-C22-C23
86	4C	303	PGV	O03-C19-C20-C21
86	8C	302	PGV	O03-C19-C20-C21
91	8A	611	PSC	O01-C1-C2-C3
69	1m	201	3PE	O32-C31-C32-C33
70	5A	202	PC1	O32-C31-C32-C33
75	4D	201	CDL	C12-C11-CA5-OA7
85	6D	501	HEC	CAA-CBA-CGA-O1A
86	8G	101	PGV	C3-C4-C5-C6
86	4C	302	PGV	C19-C20-C21-C22
69	5Y	204	3PE	O22-C21-C22-C23
69	5m	201	3PE	O32-C31-C32-C33

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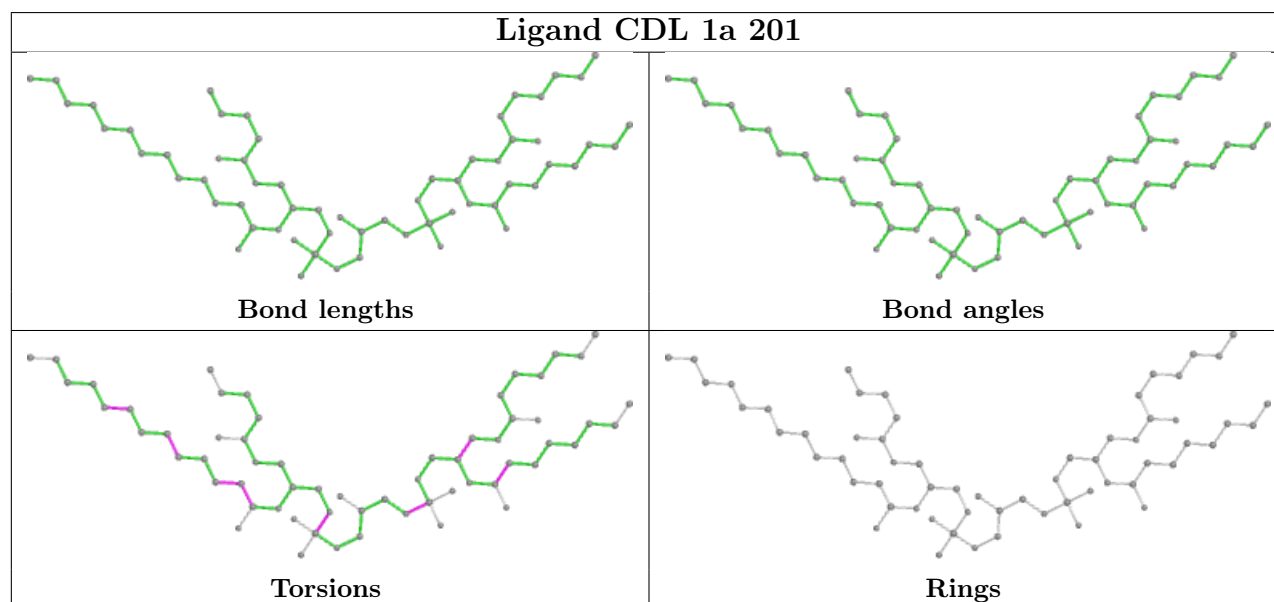
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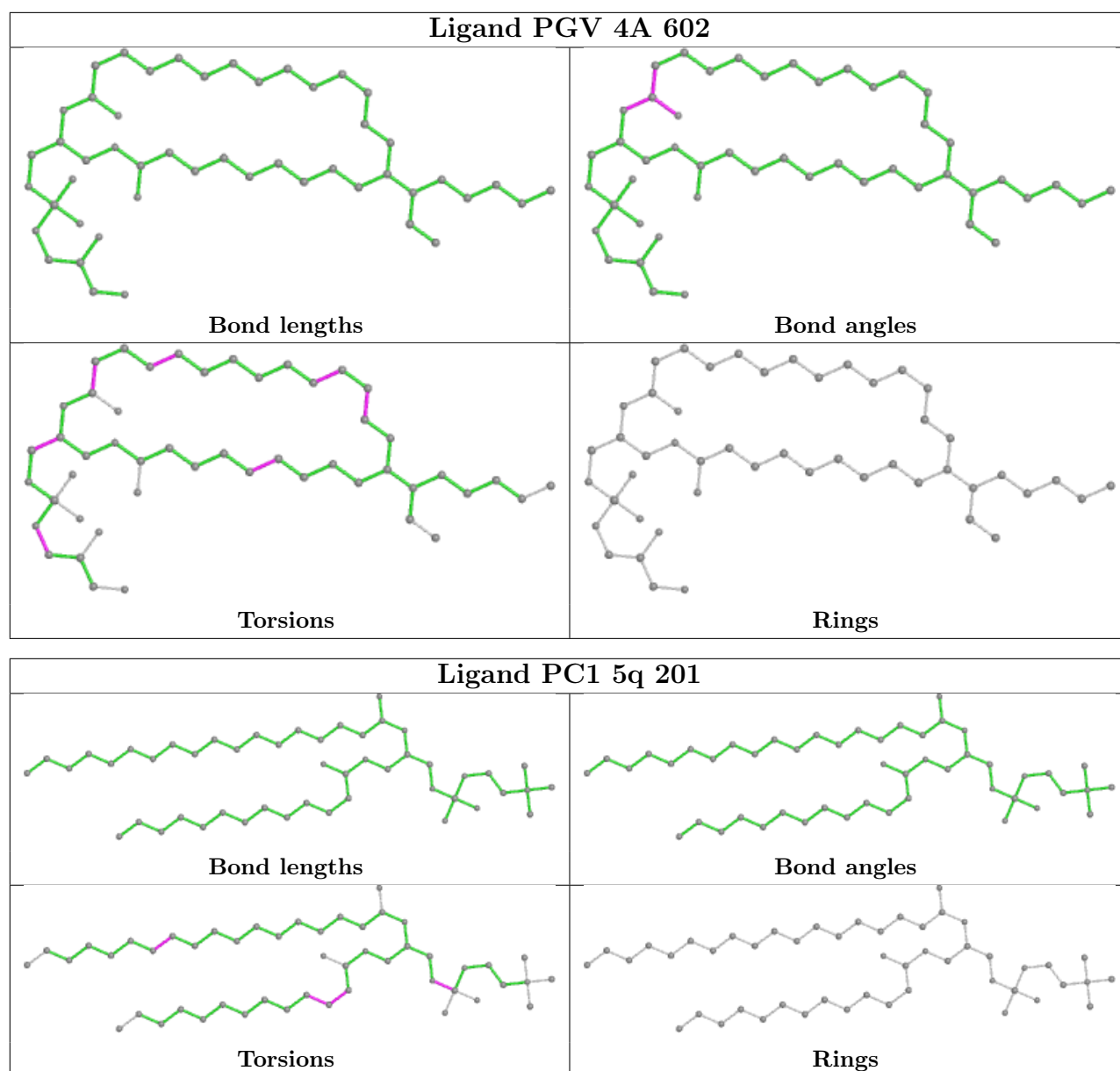
Mol	Chain	Res	Type	Atoms
75	1L	702	CDL	C32-C31-CA7-OA9
75	5a	201	CDL	C12-C11-CA5-OA7
75	5d	201	CDL	C14-C15-C16-C17
91	4B	304	PSC	O03-C19-C20-C21
87	4A	604	HEA	CAA-CBA-CGA-O2A

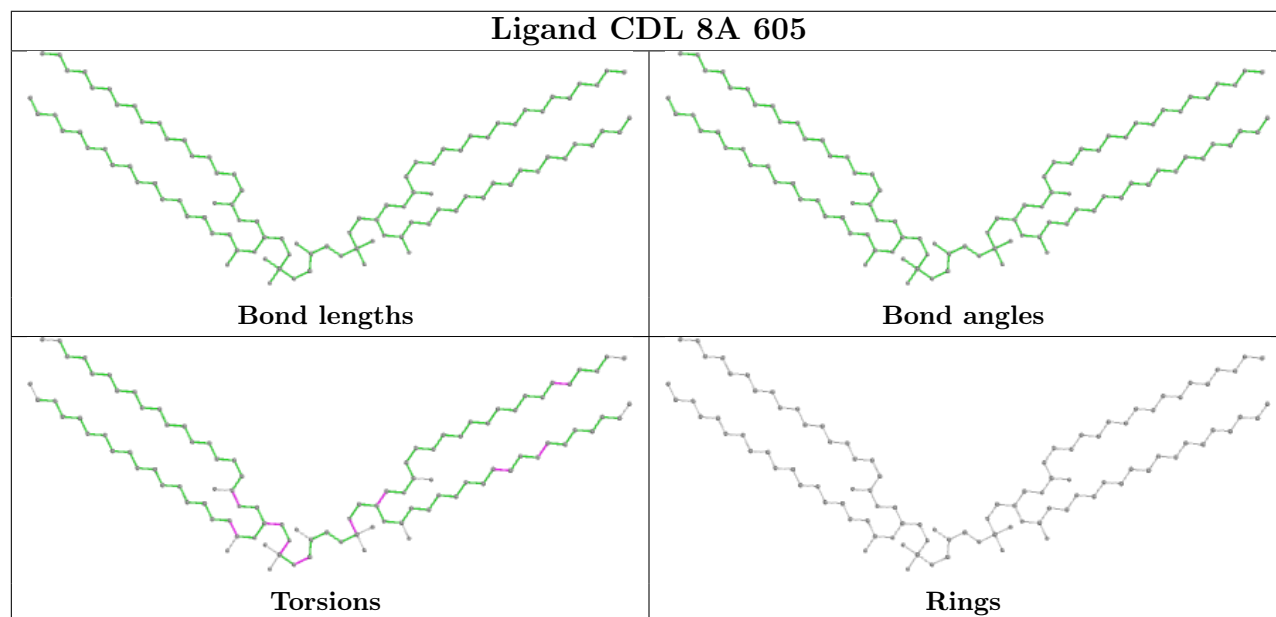
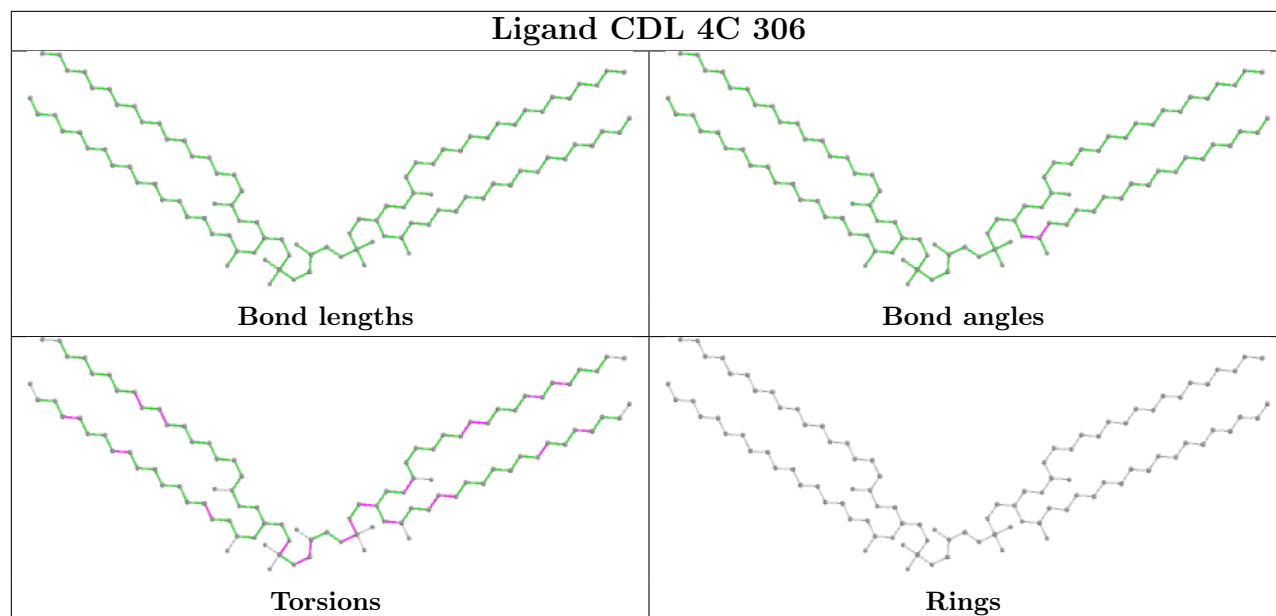
There are no ring outliers.

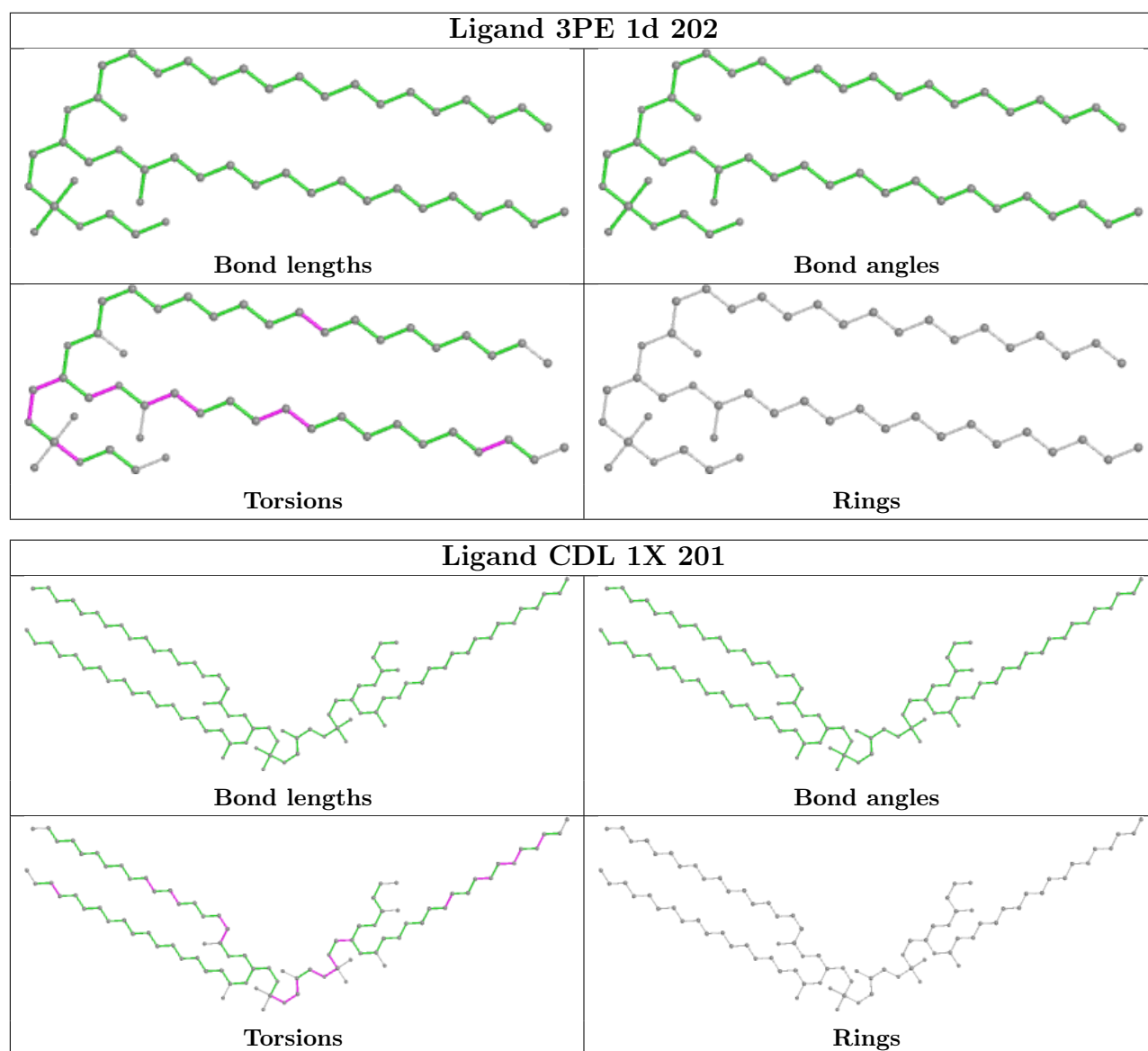
No monomer is involved in short contacts.

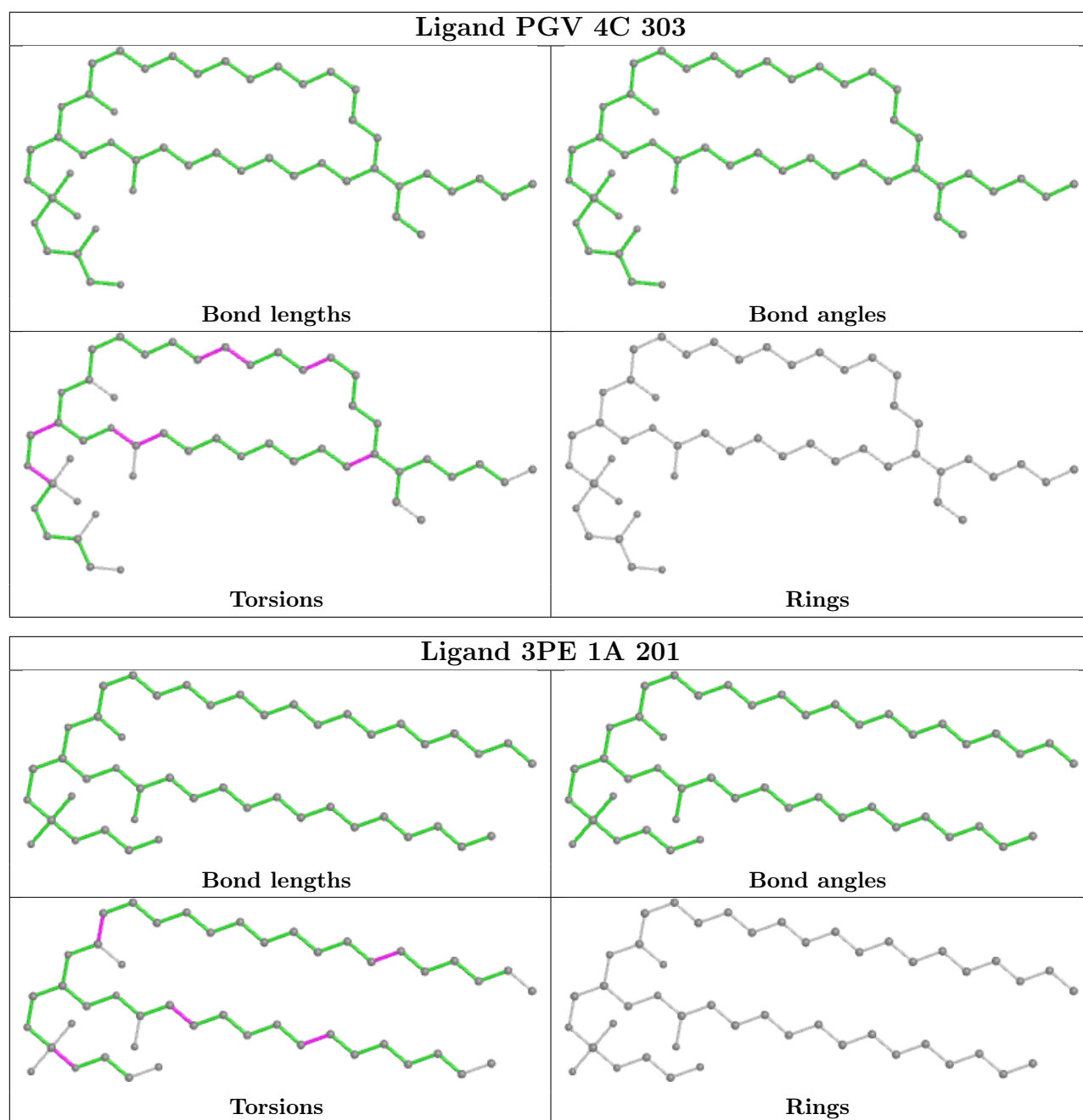
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

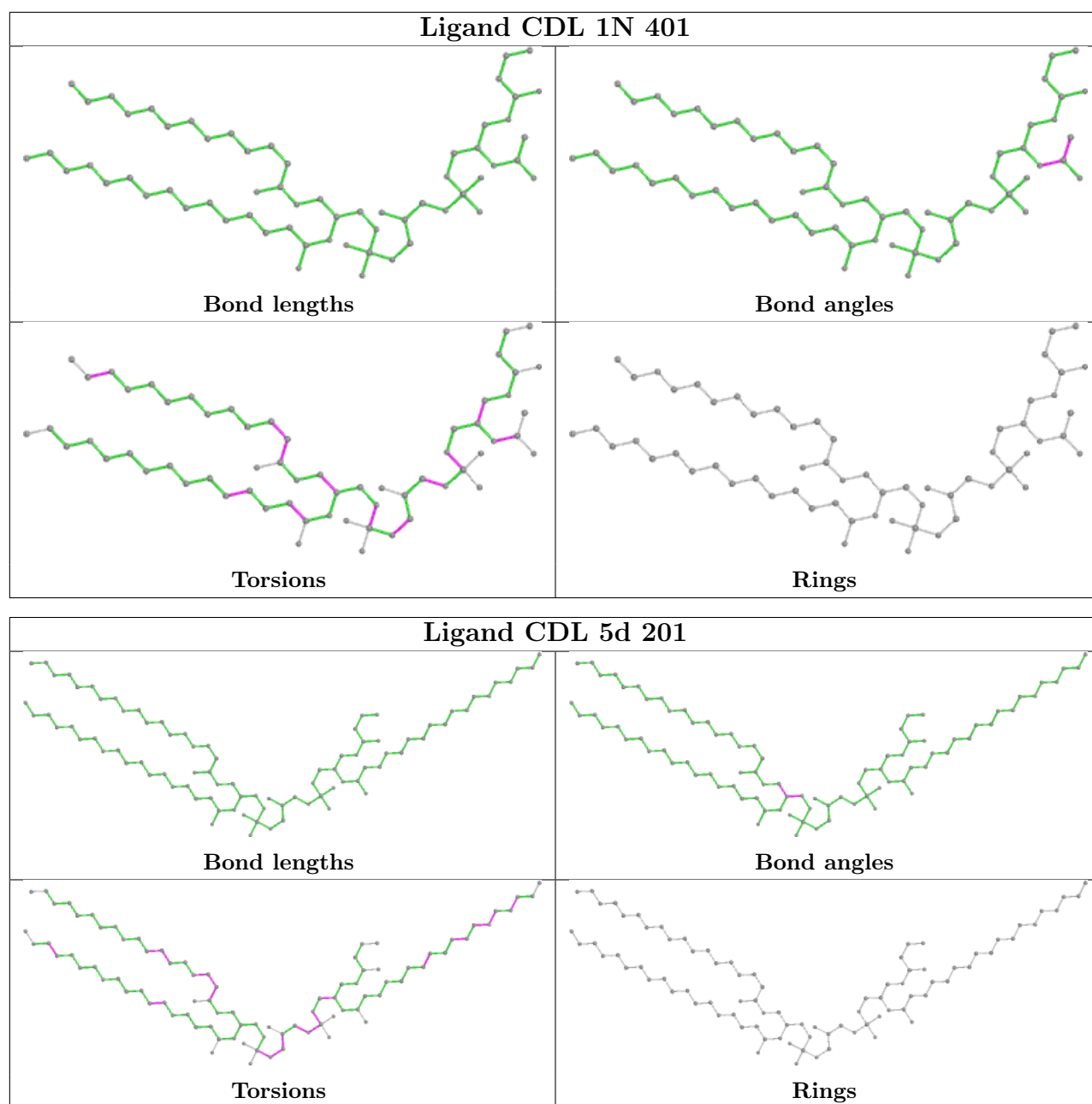


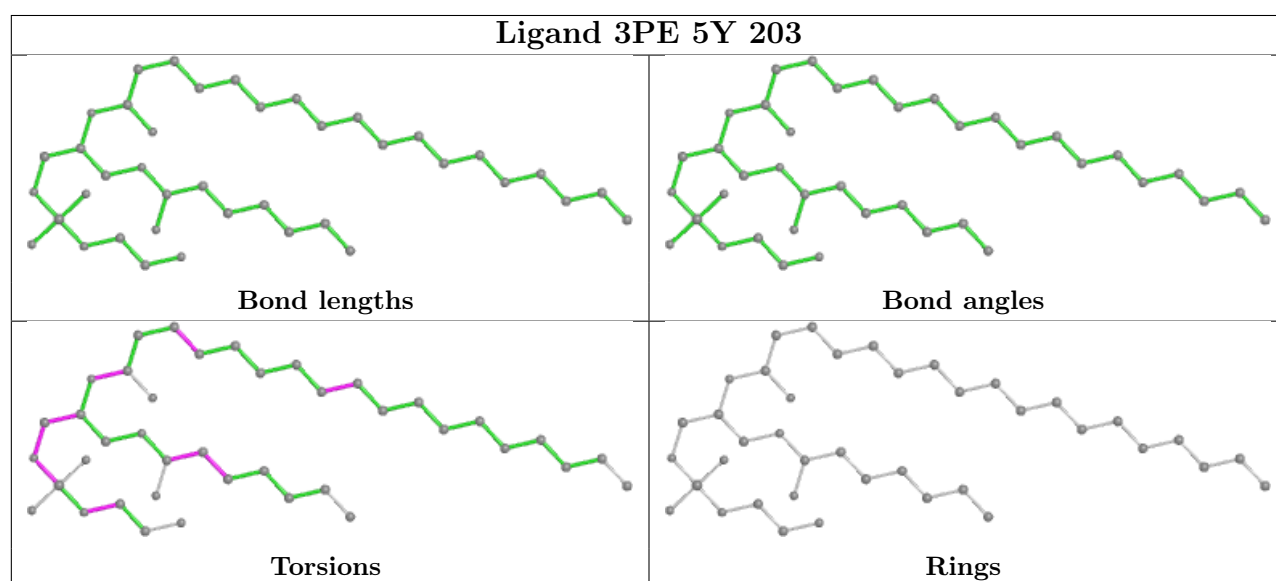
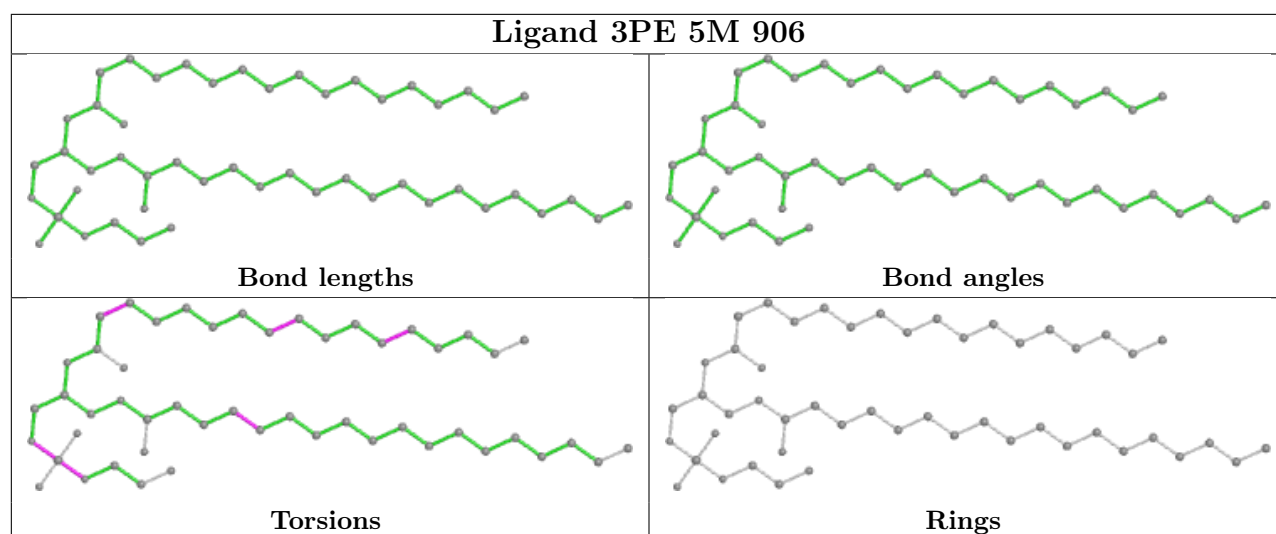


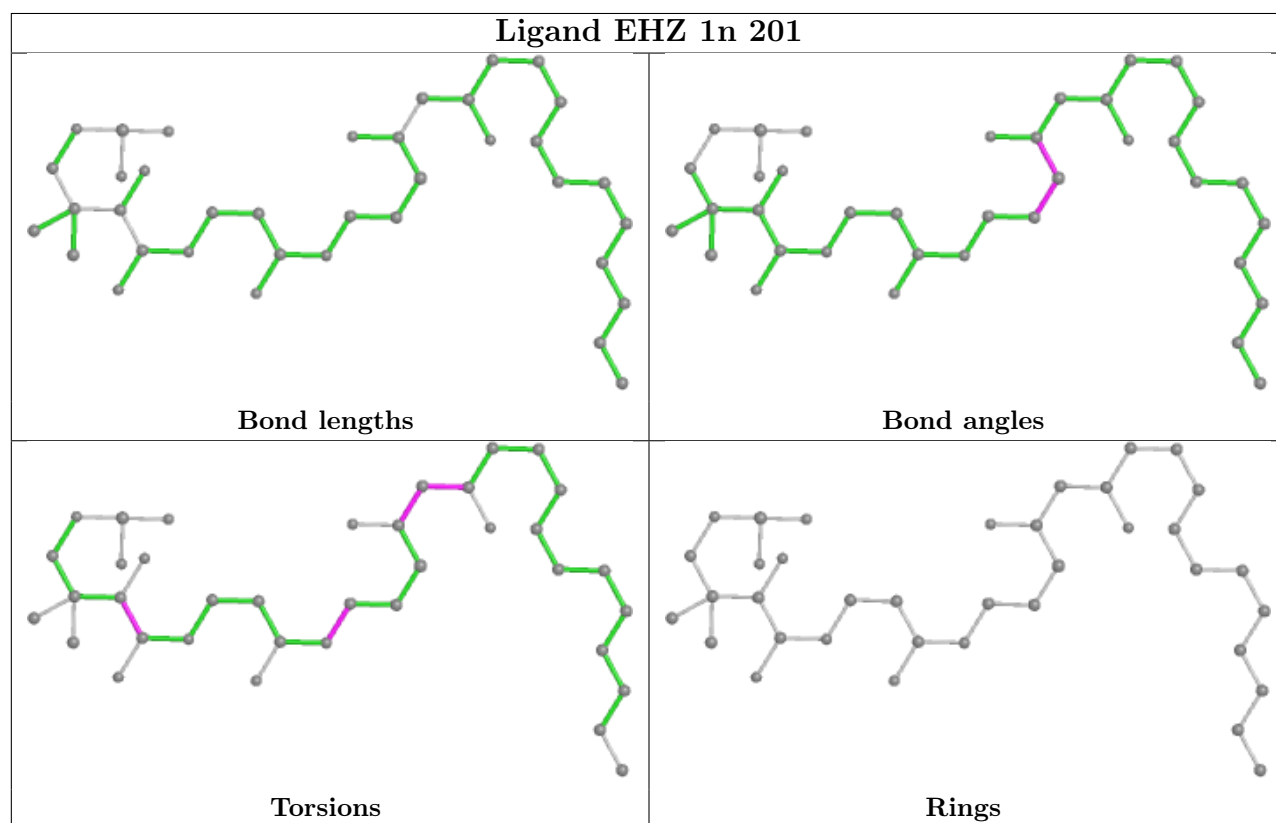
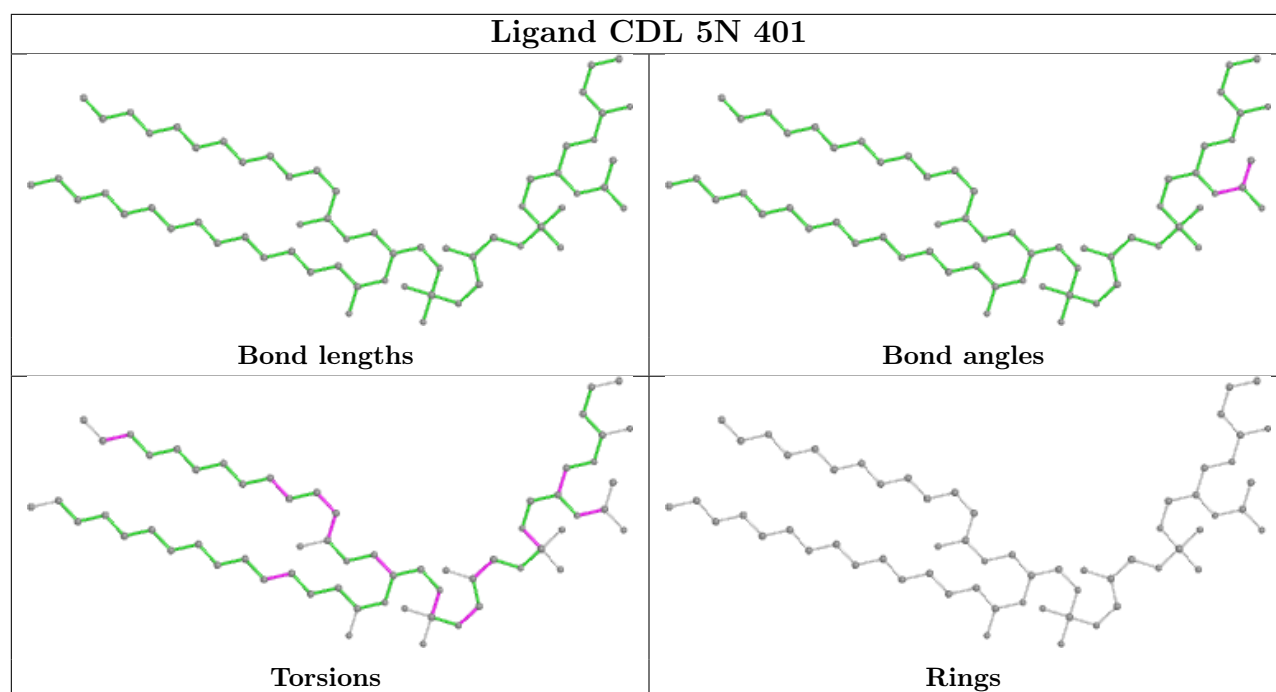


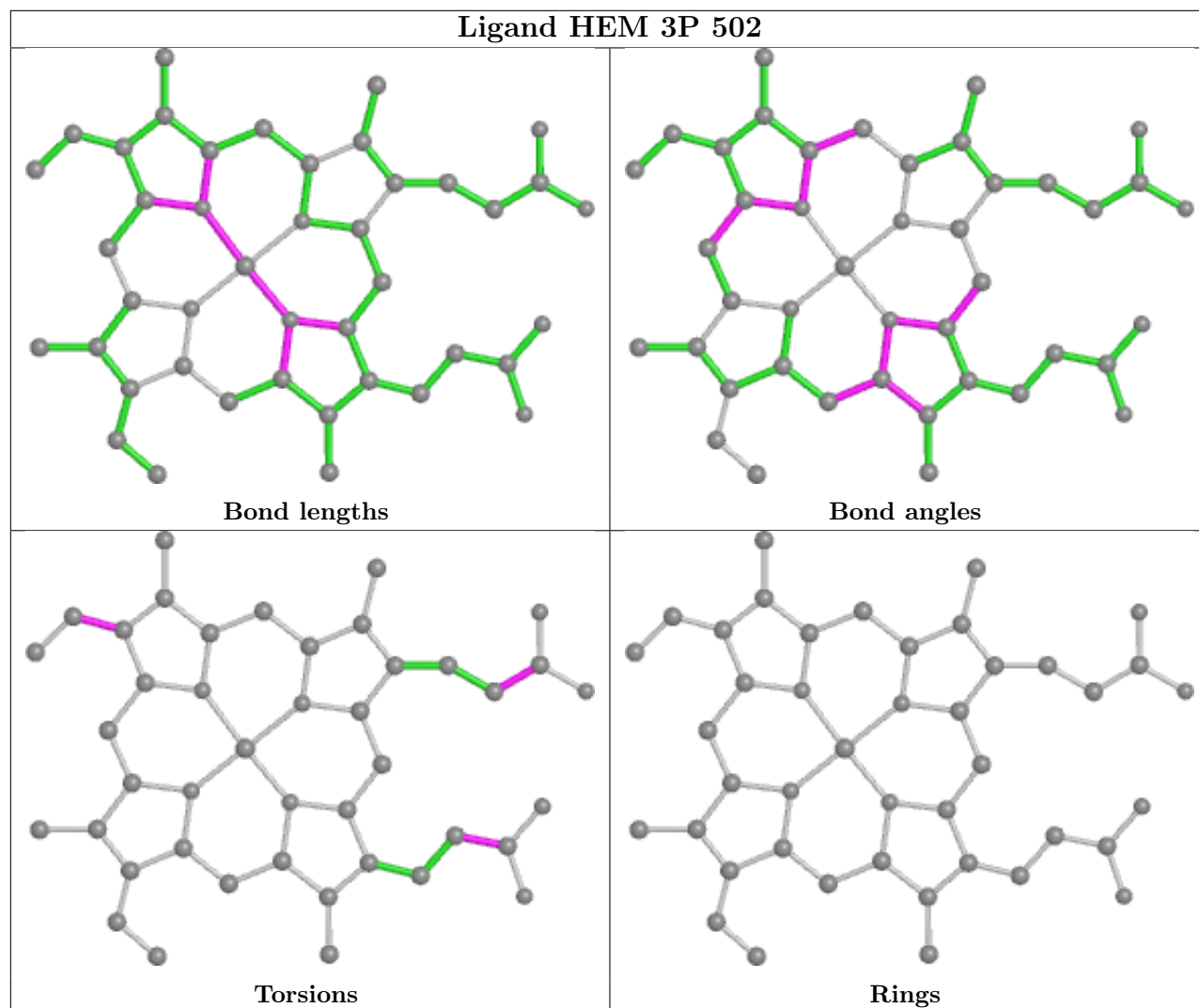


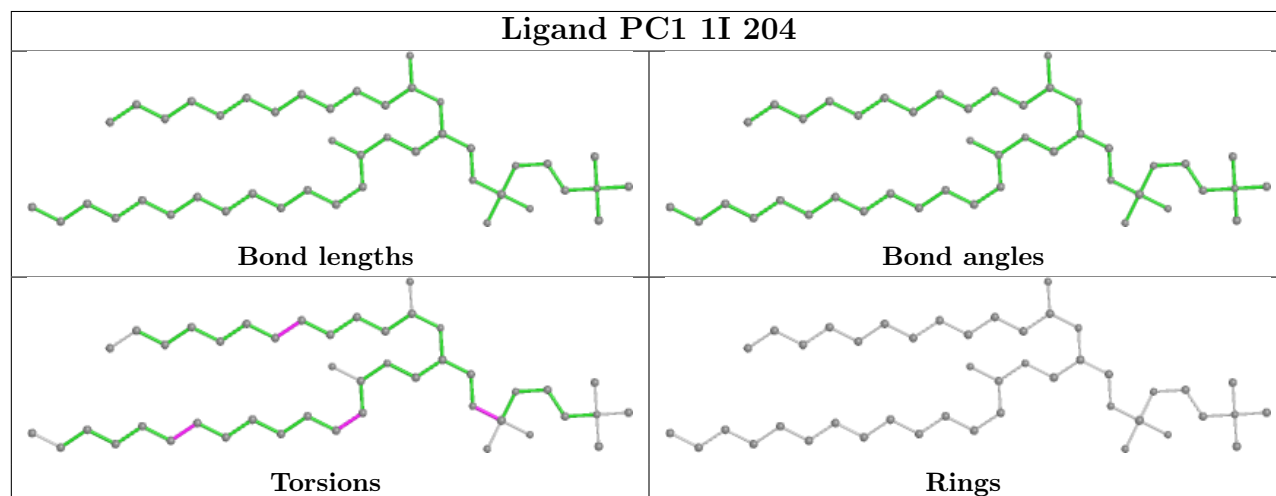
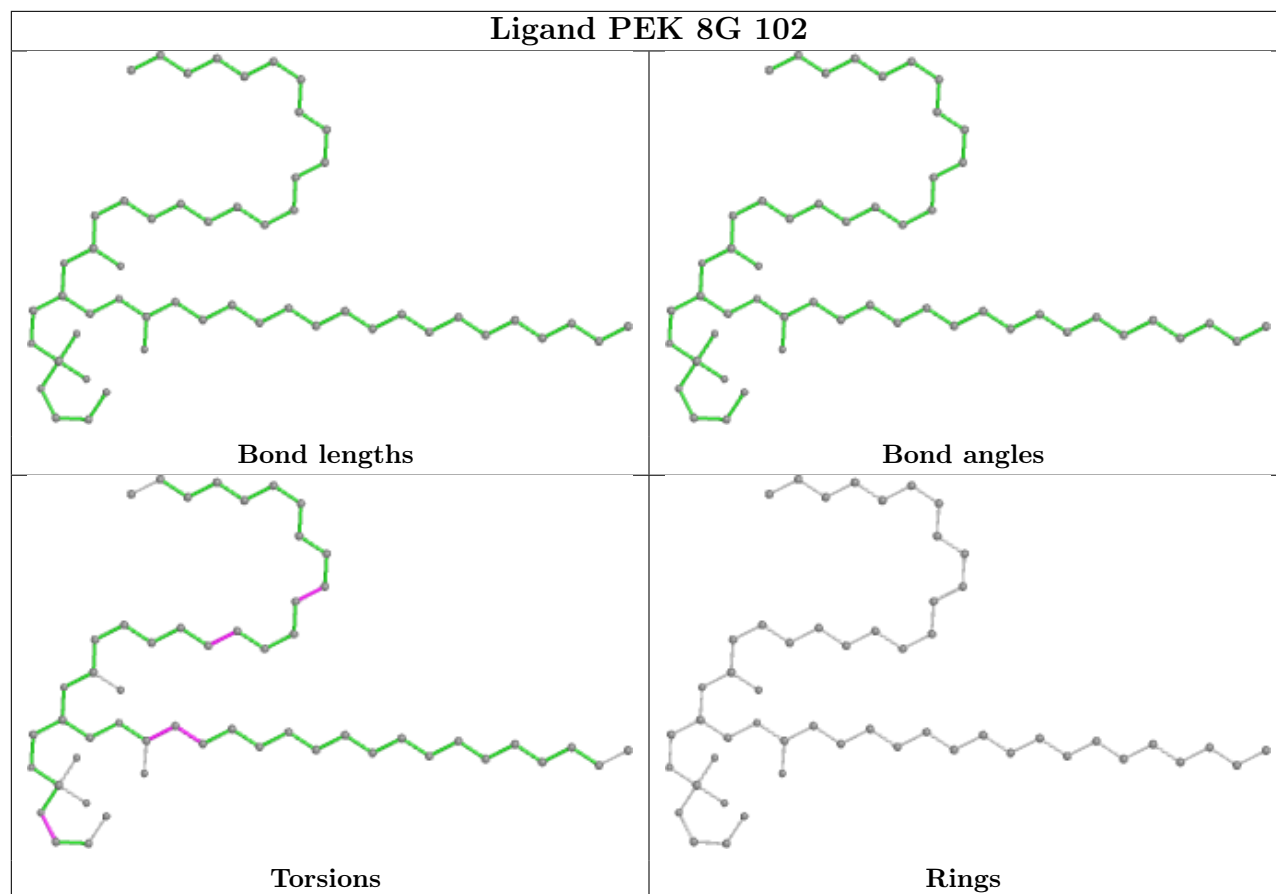


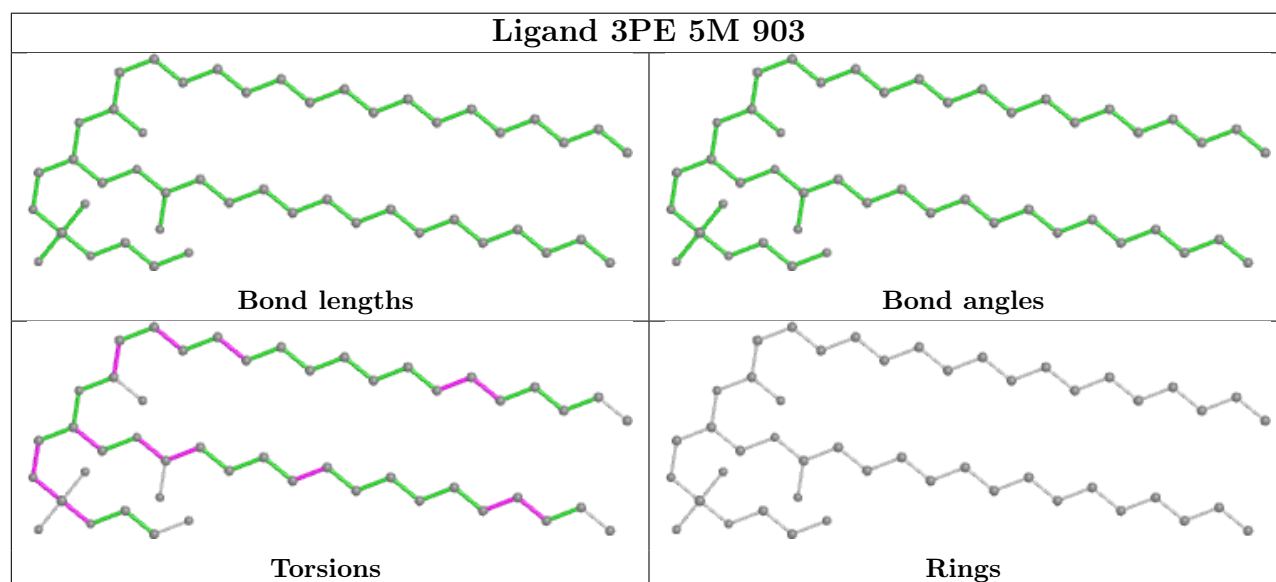
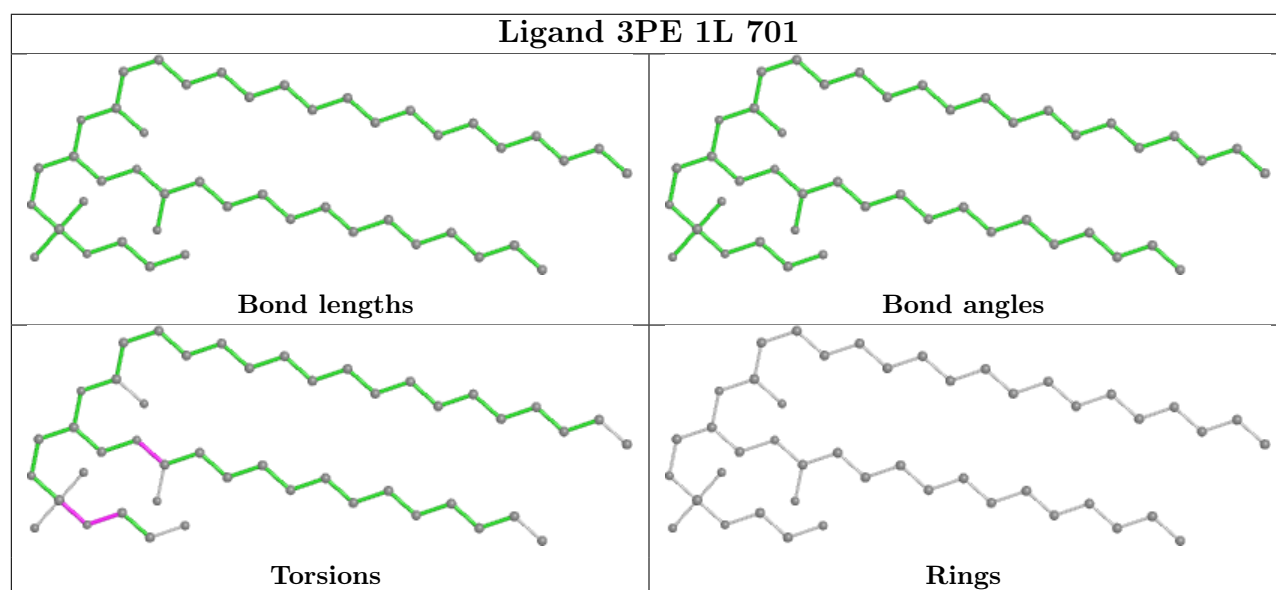
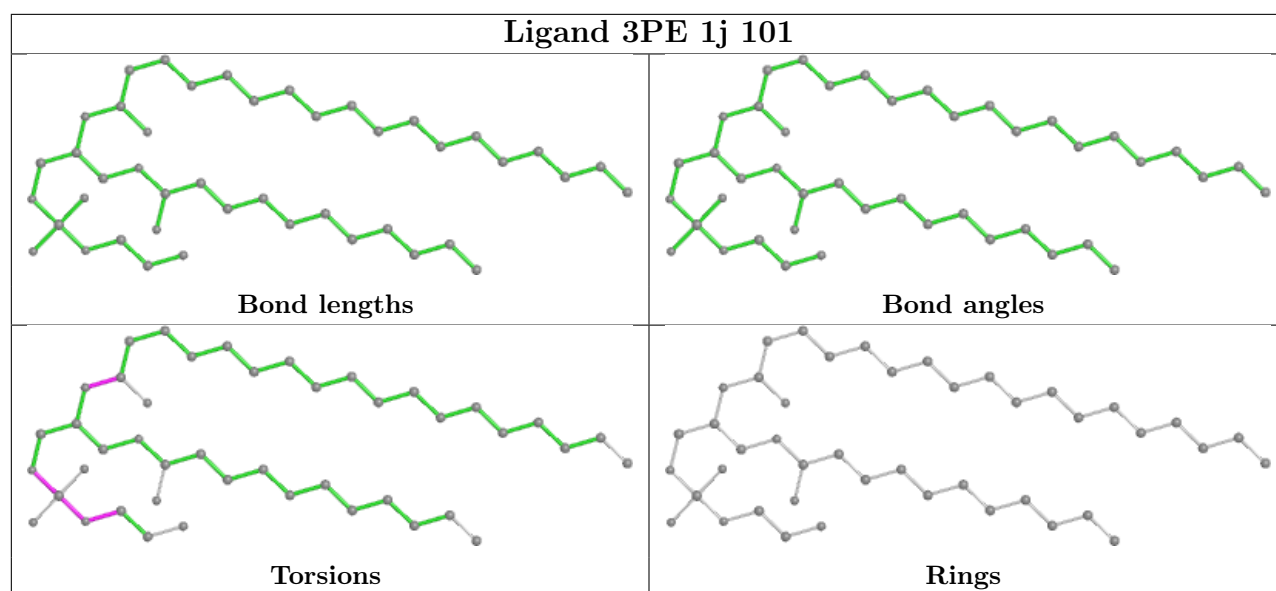


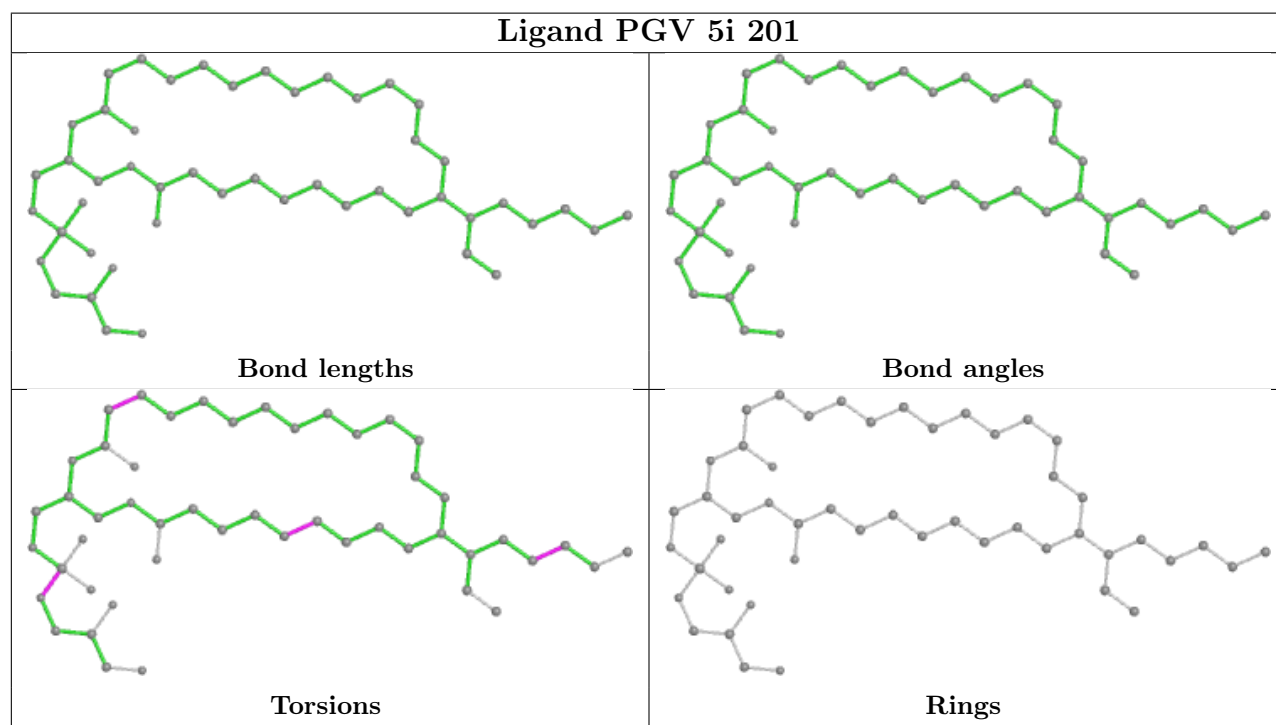
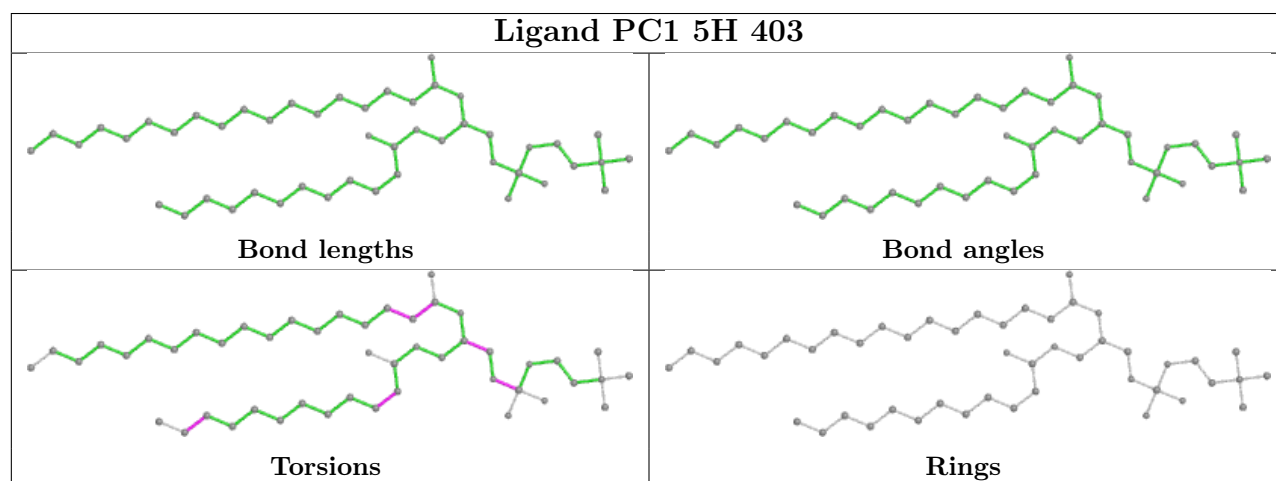
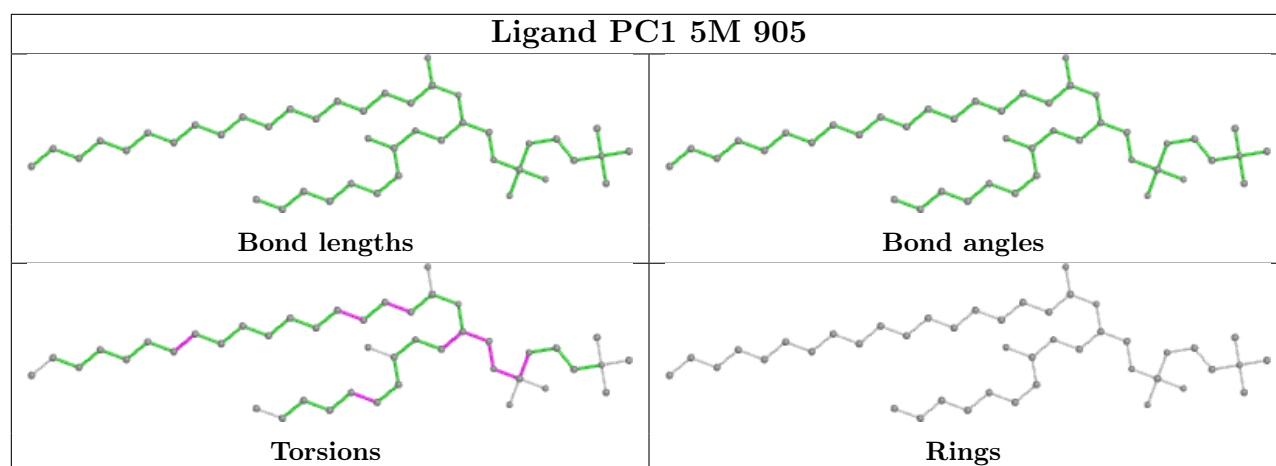


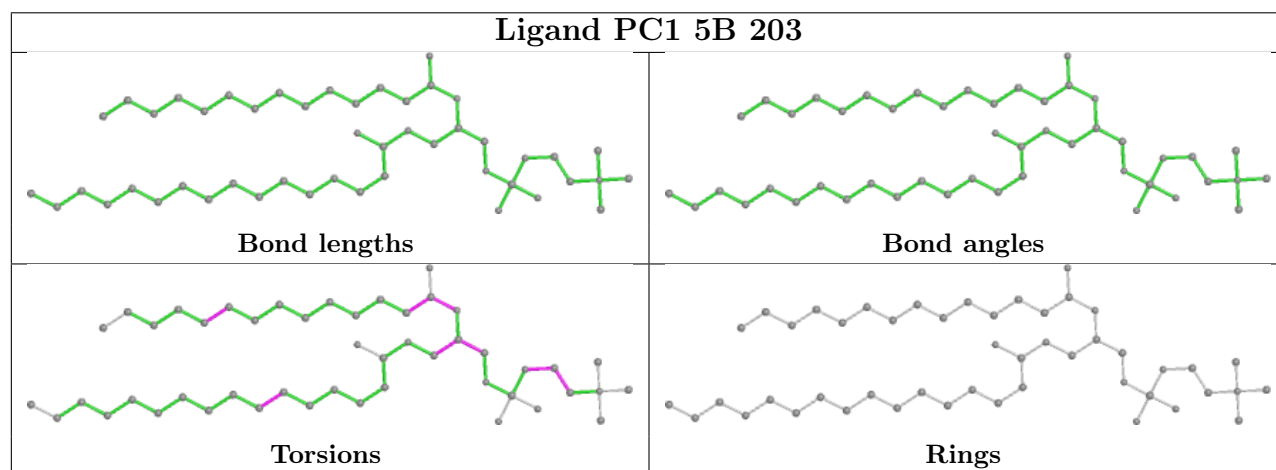
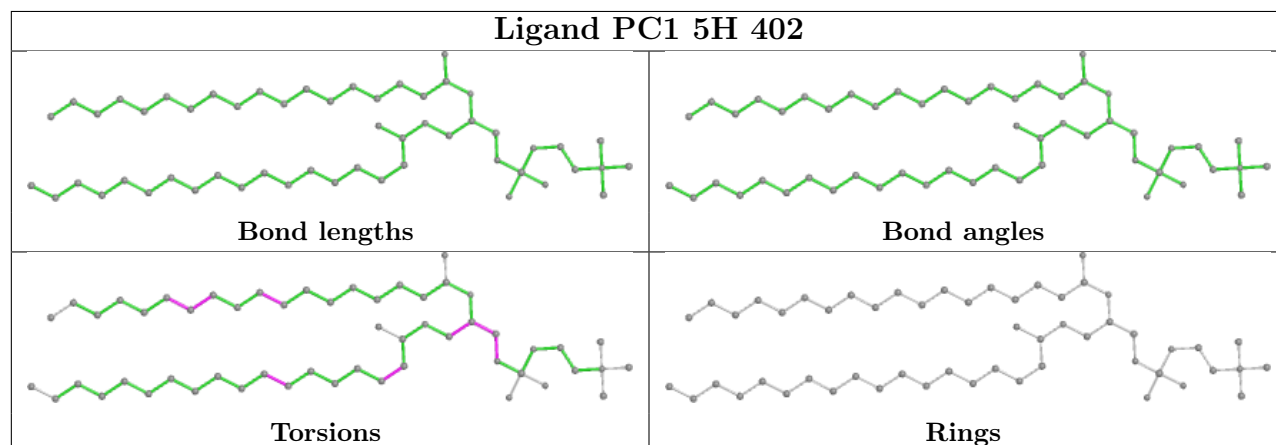
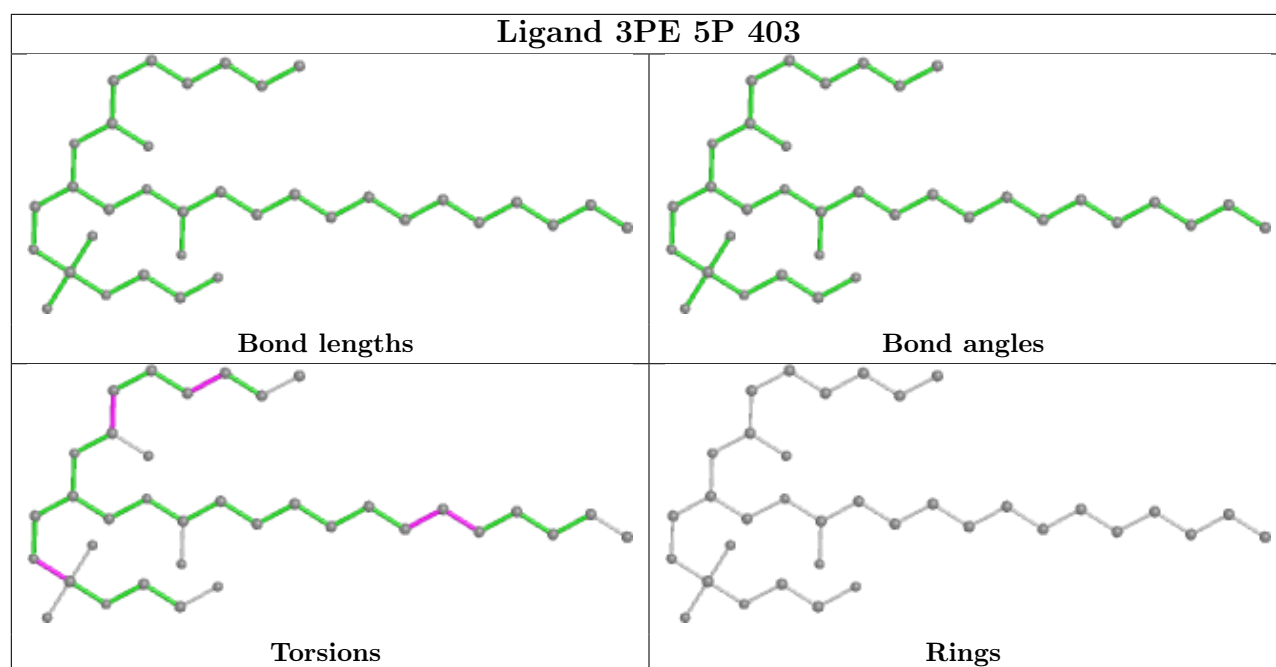


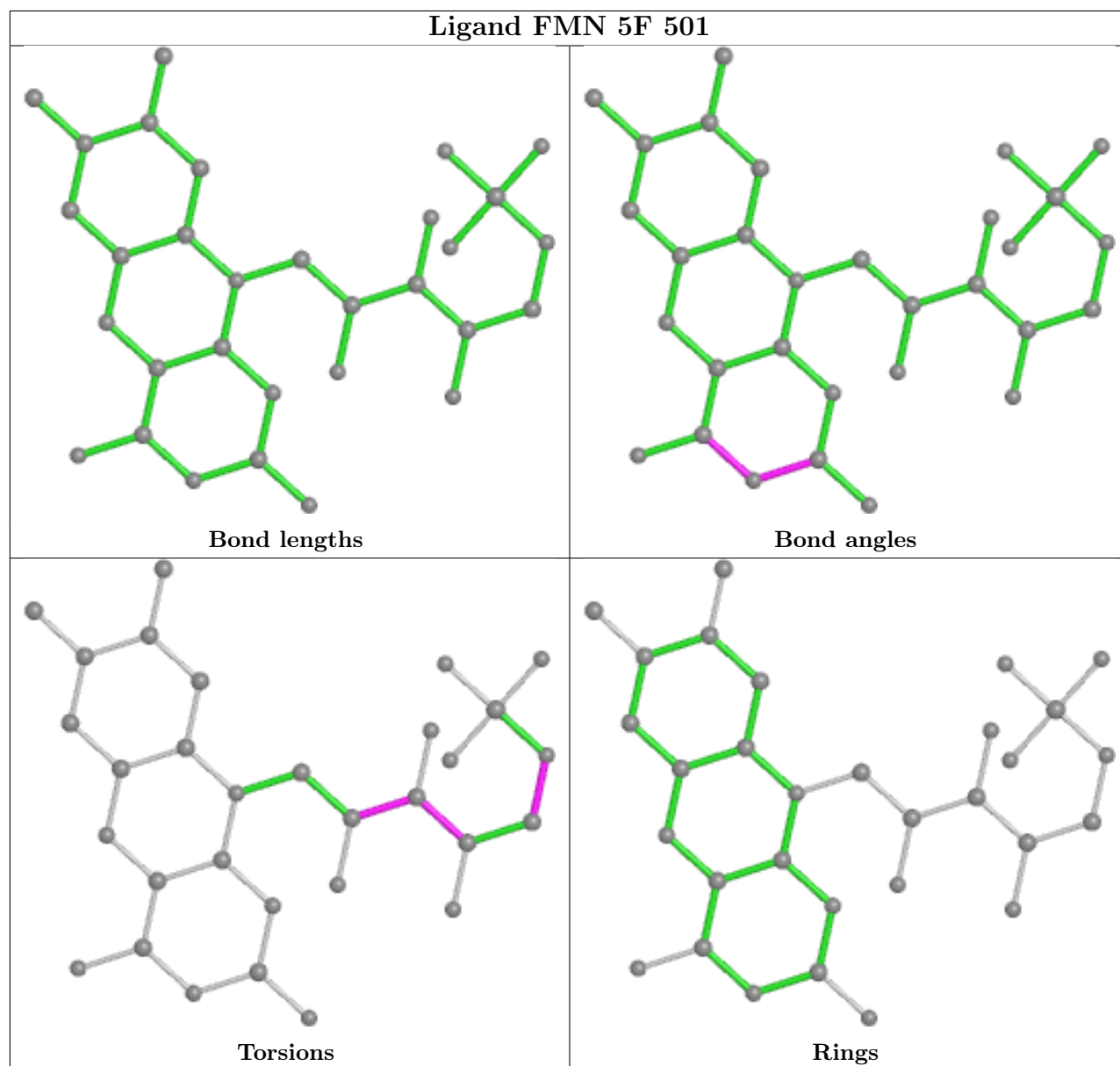
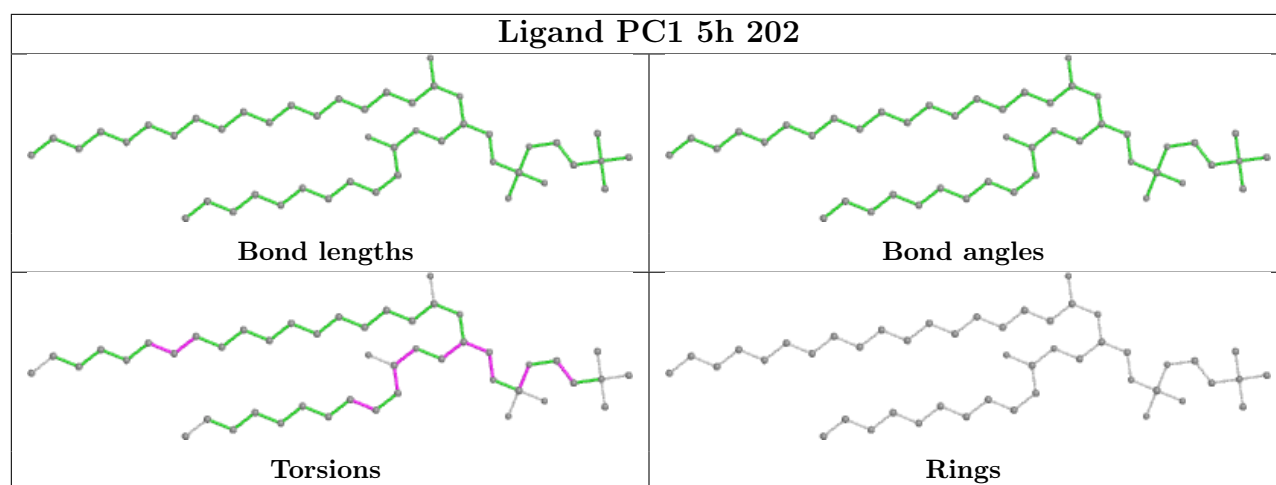


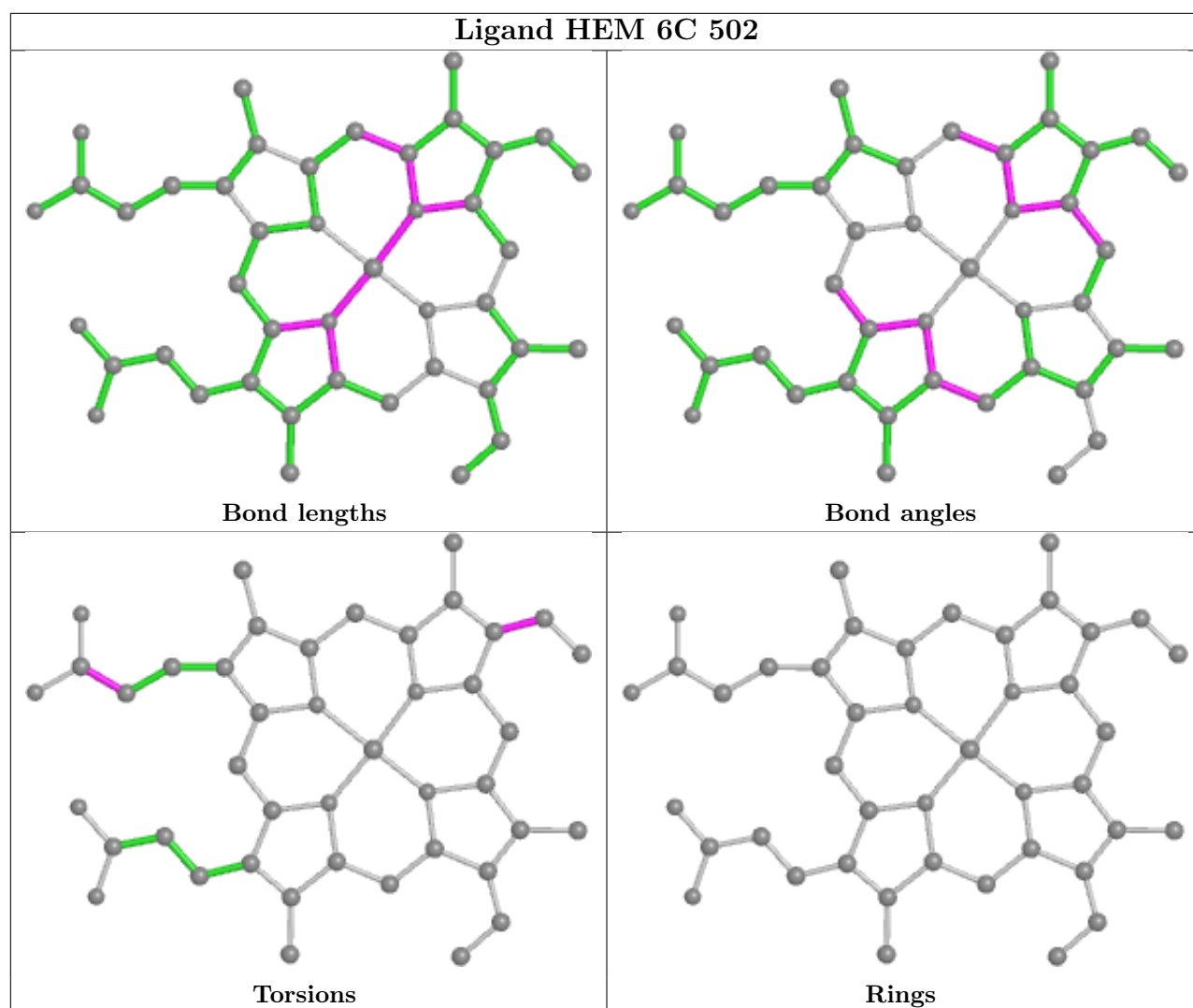




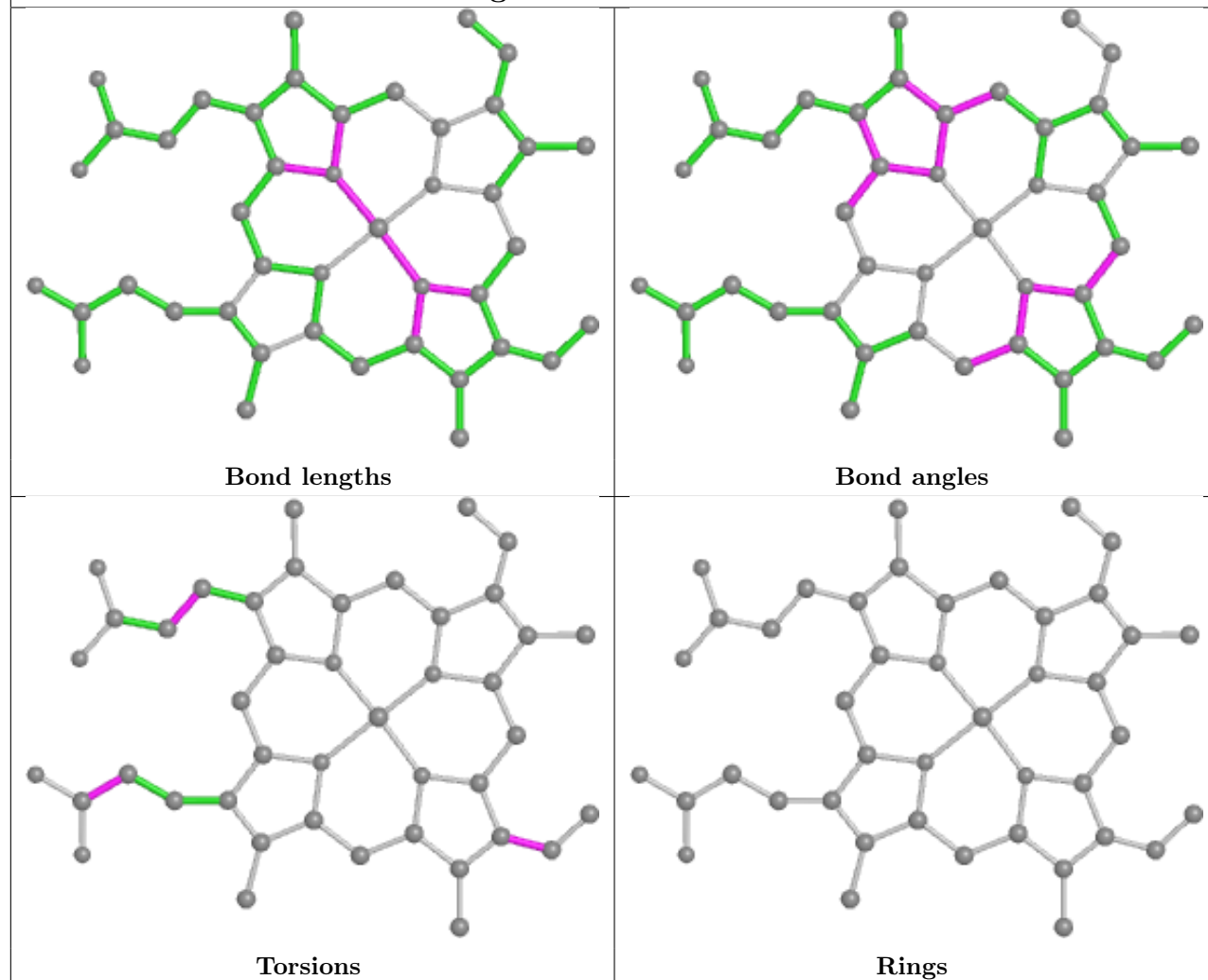




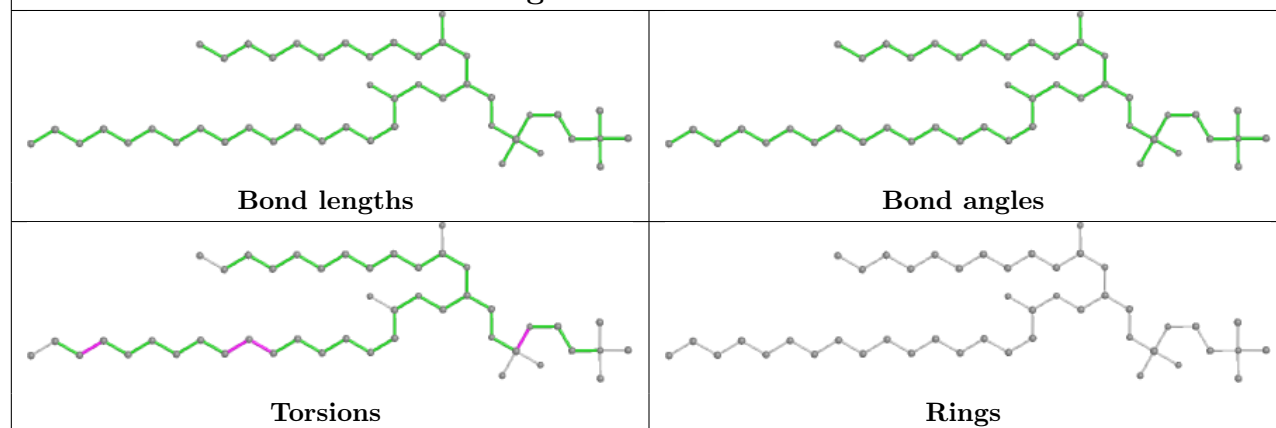


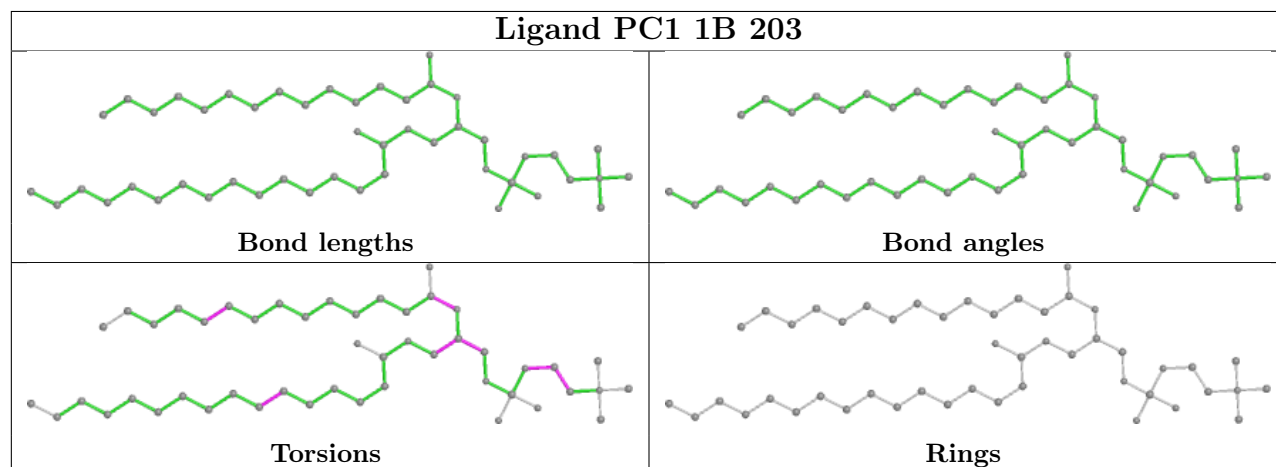
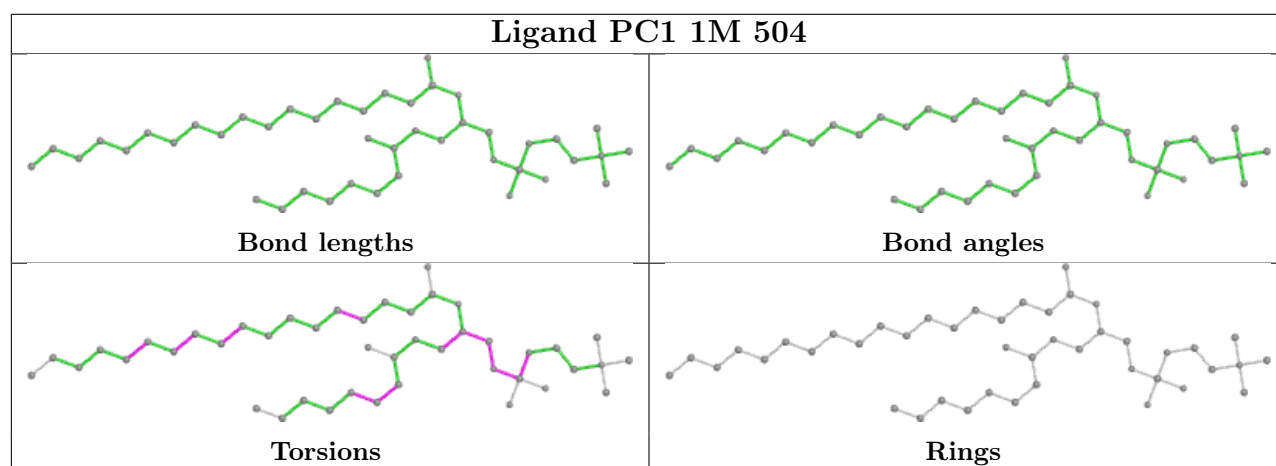
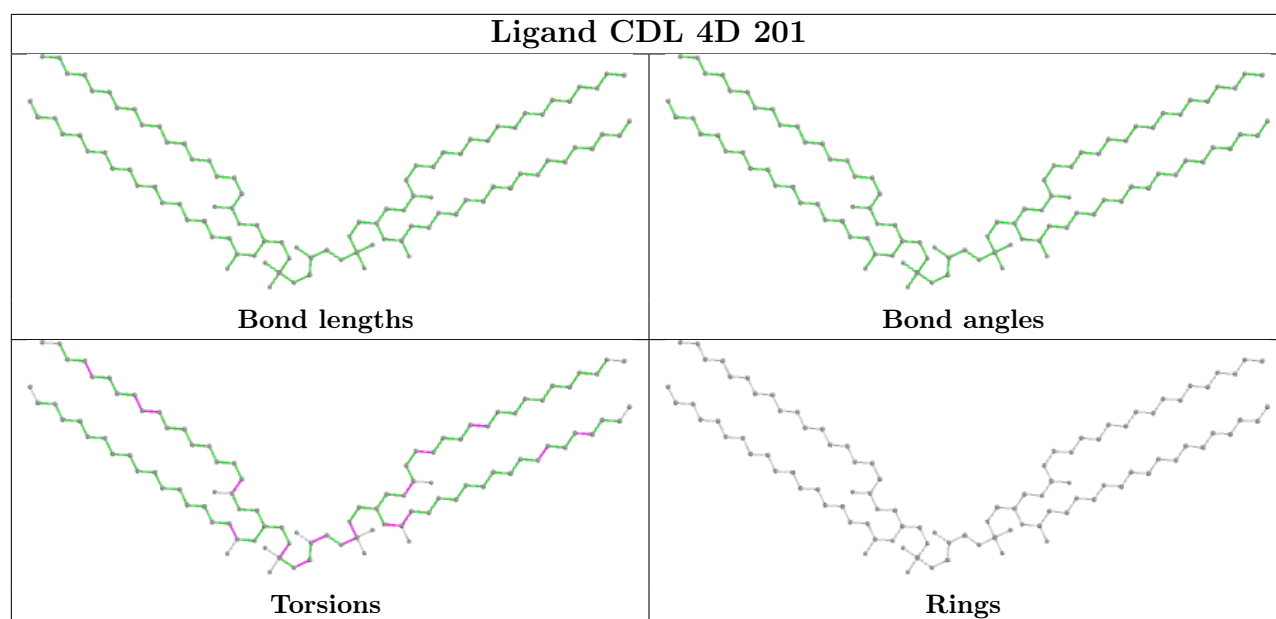


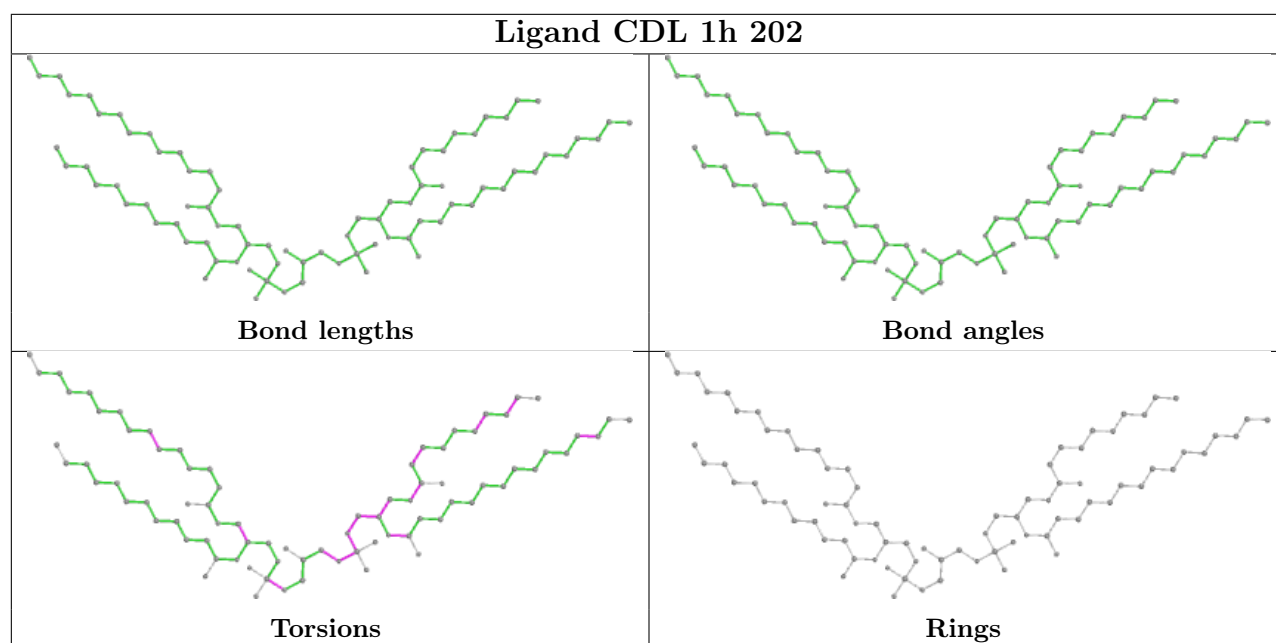
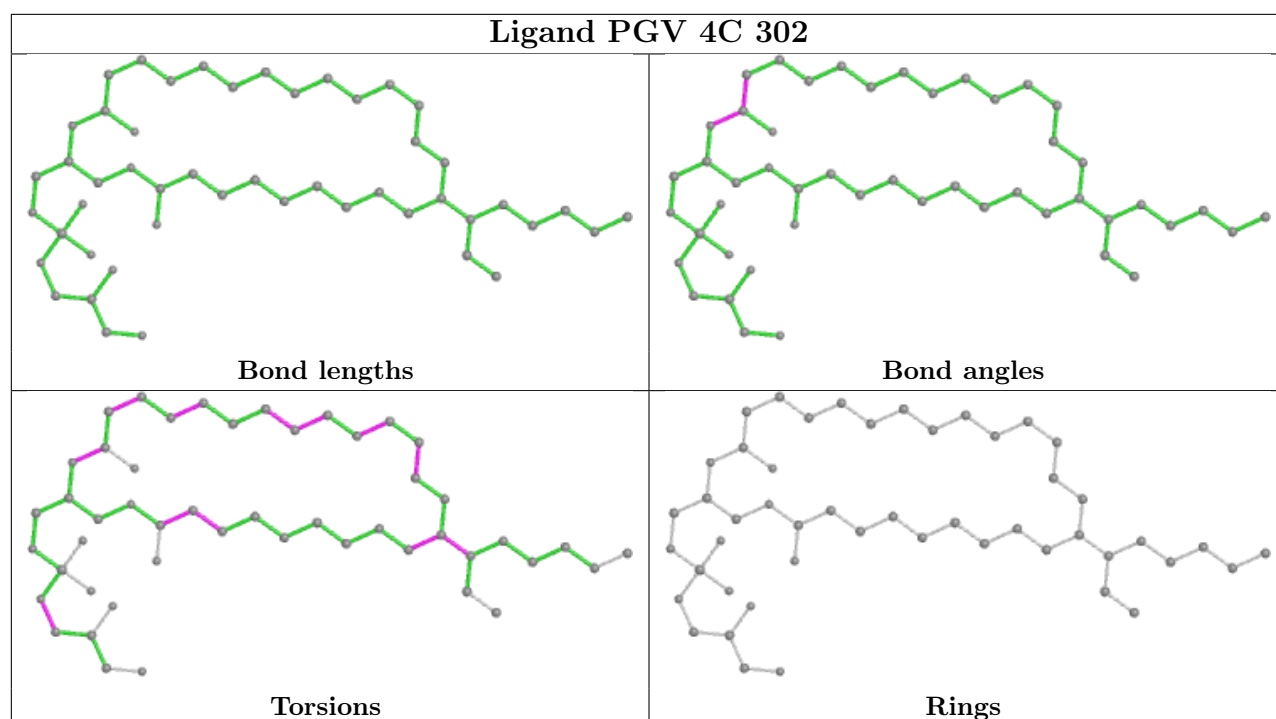
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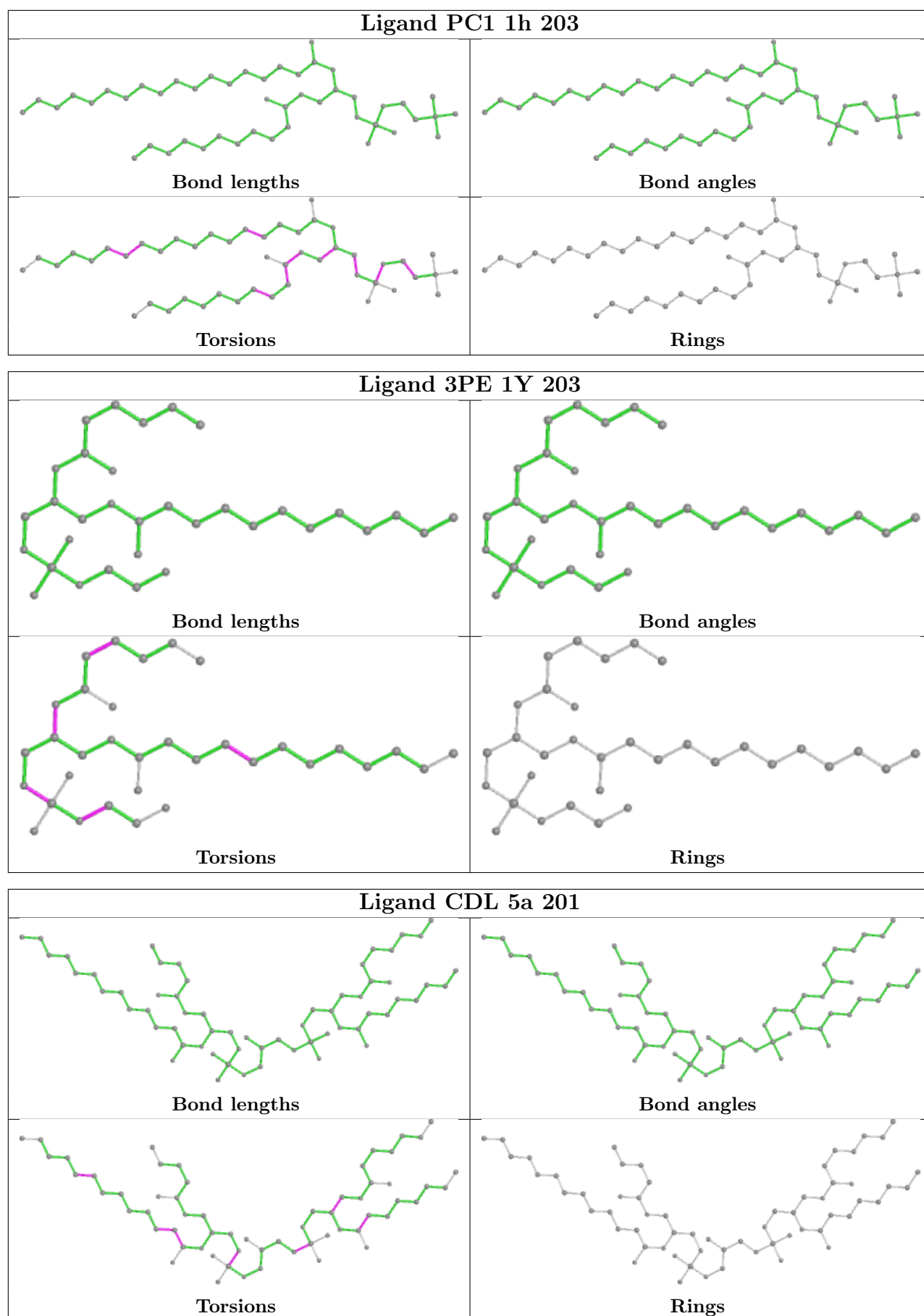


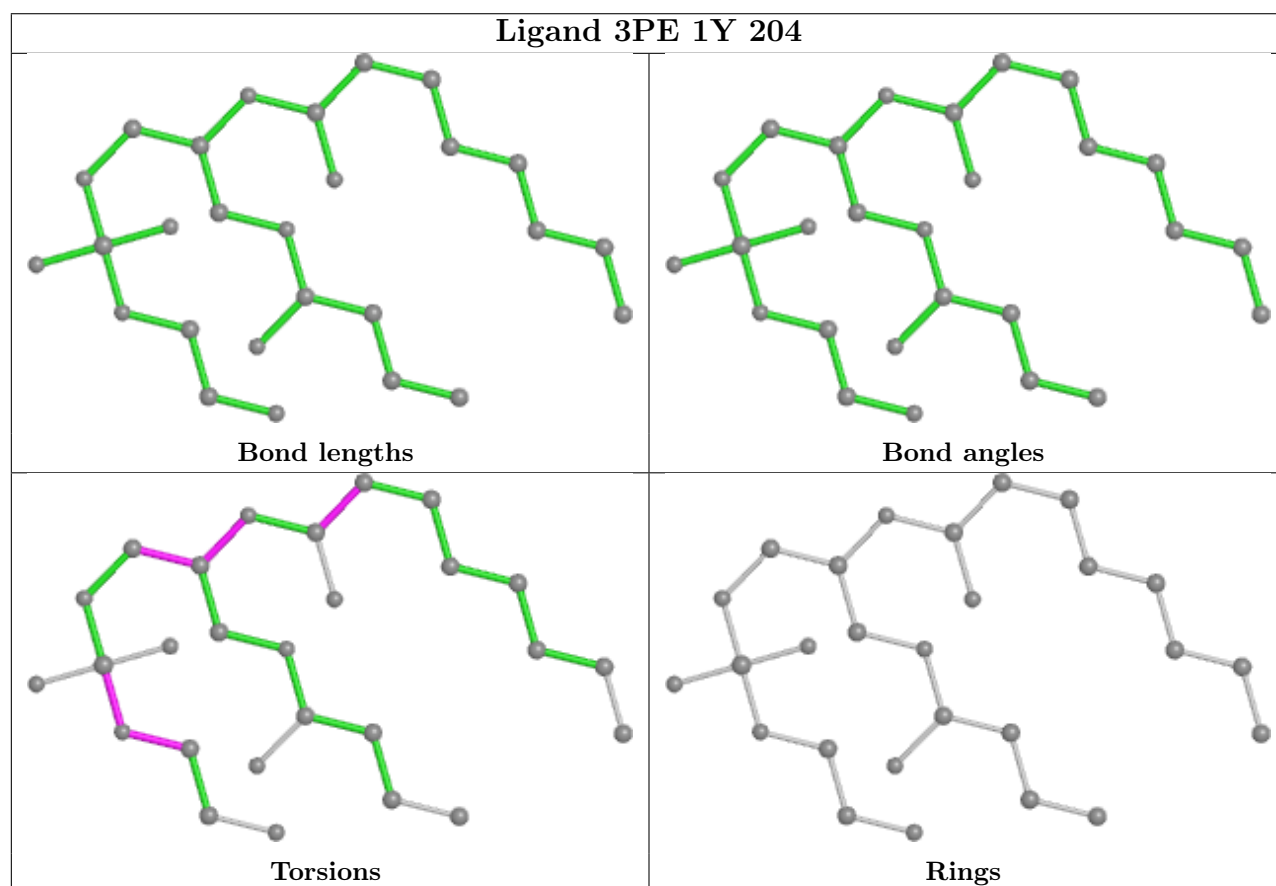
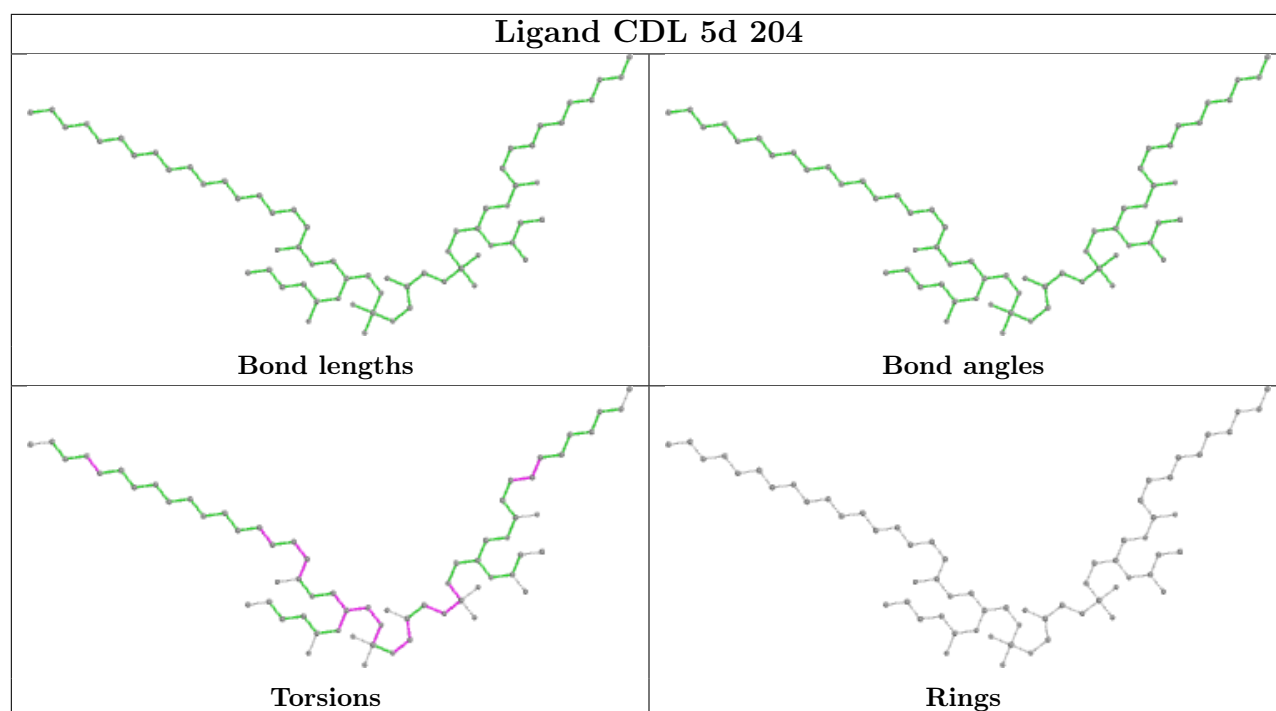
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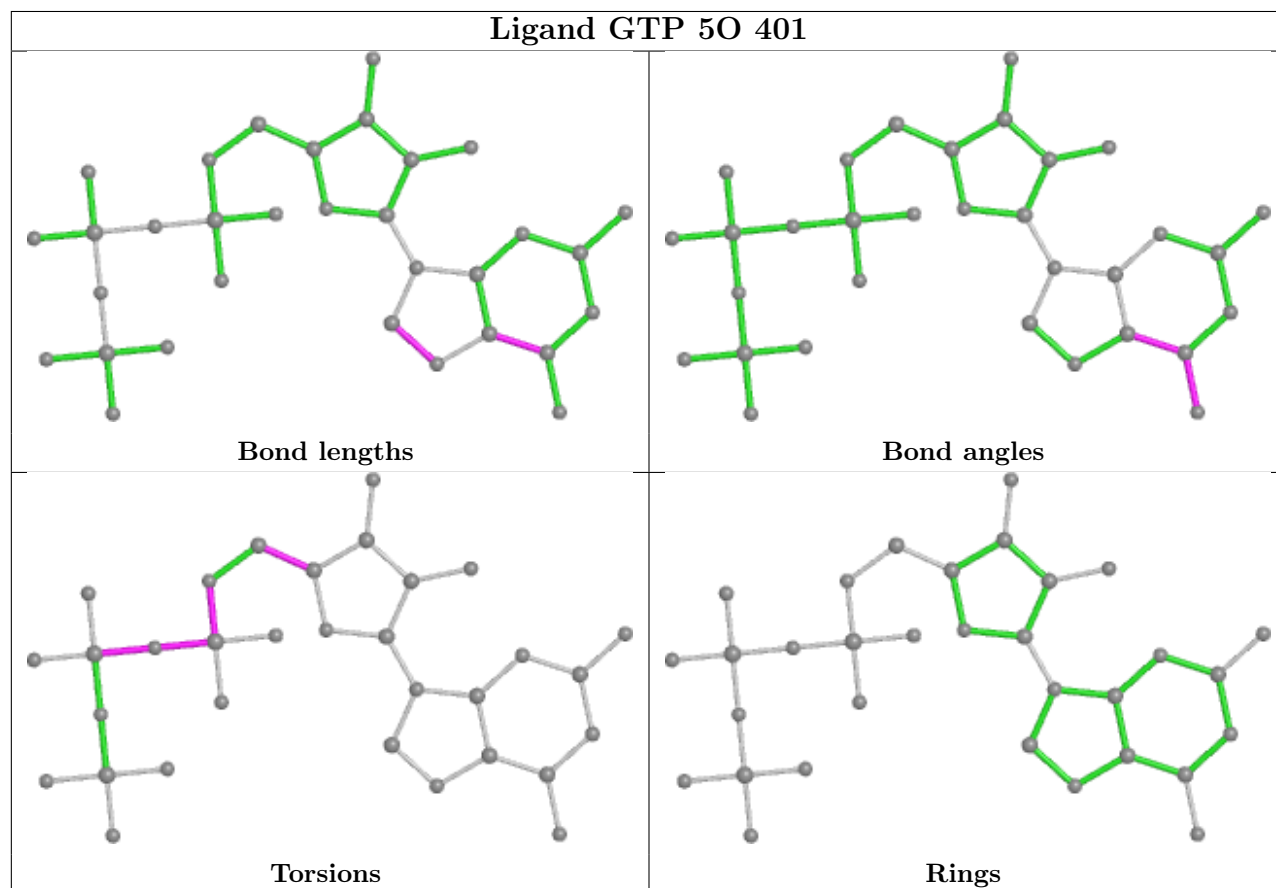
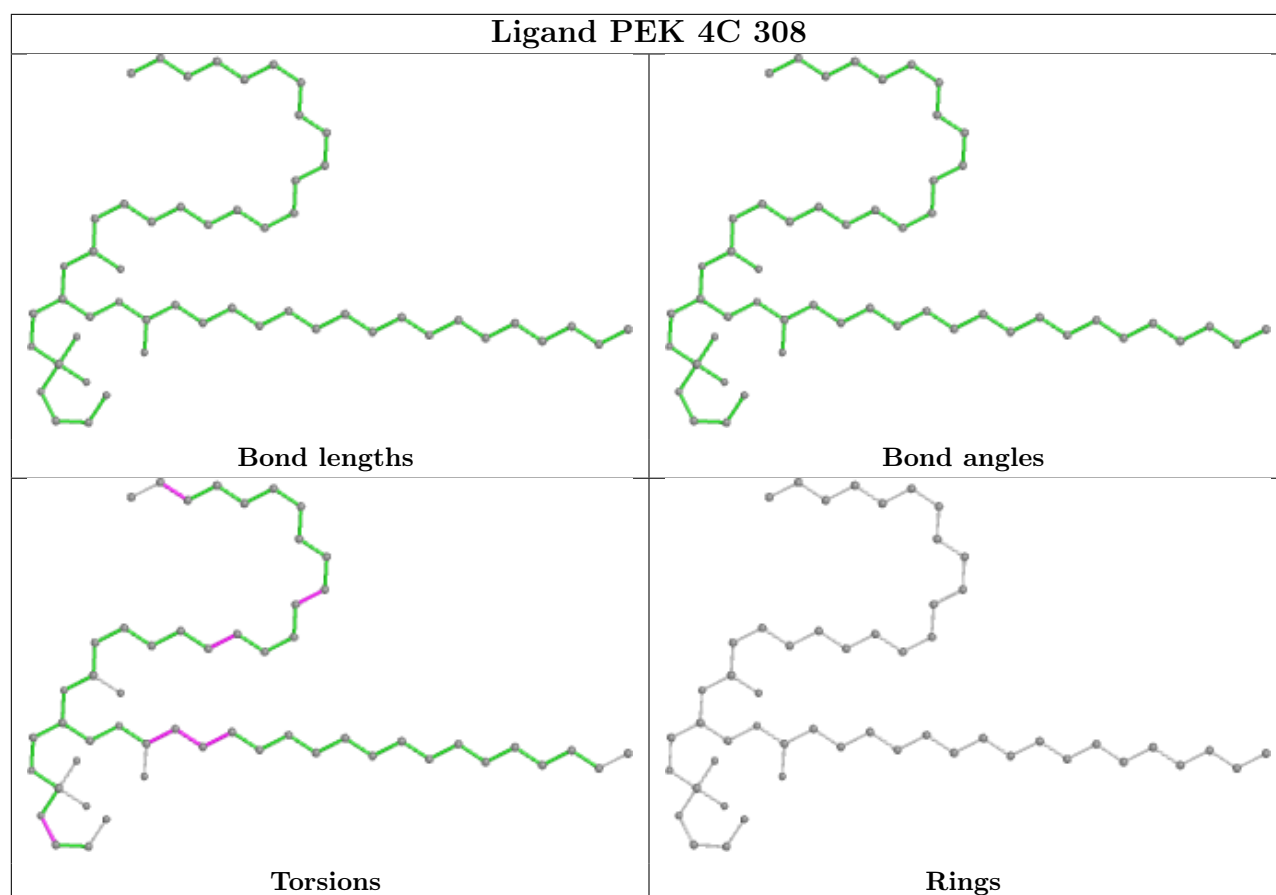


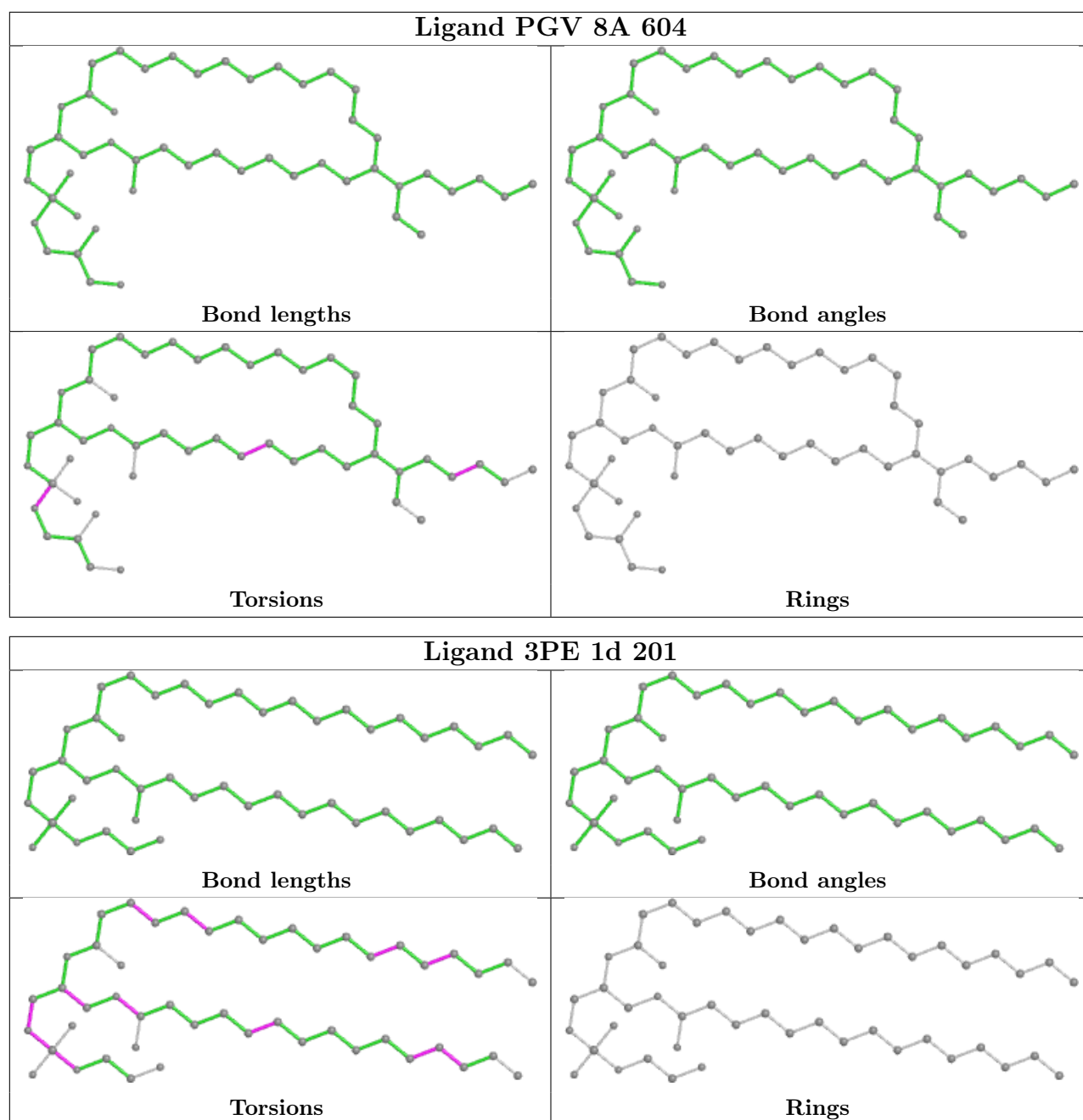


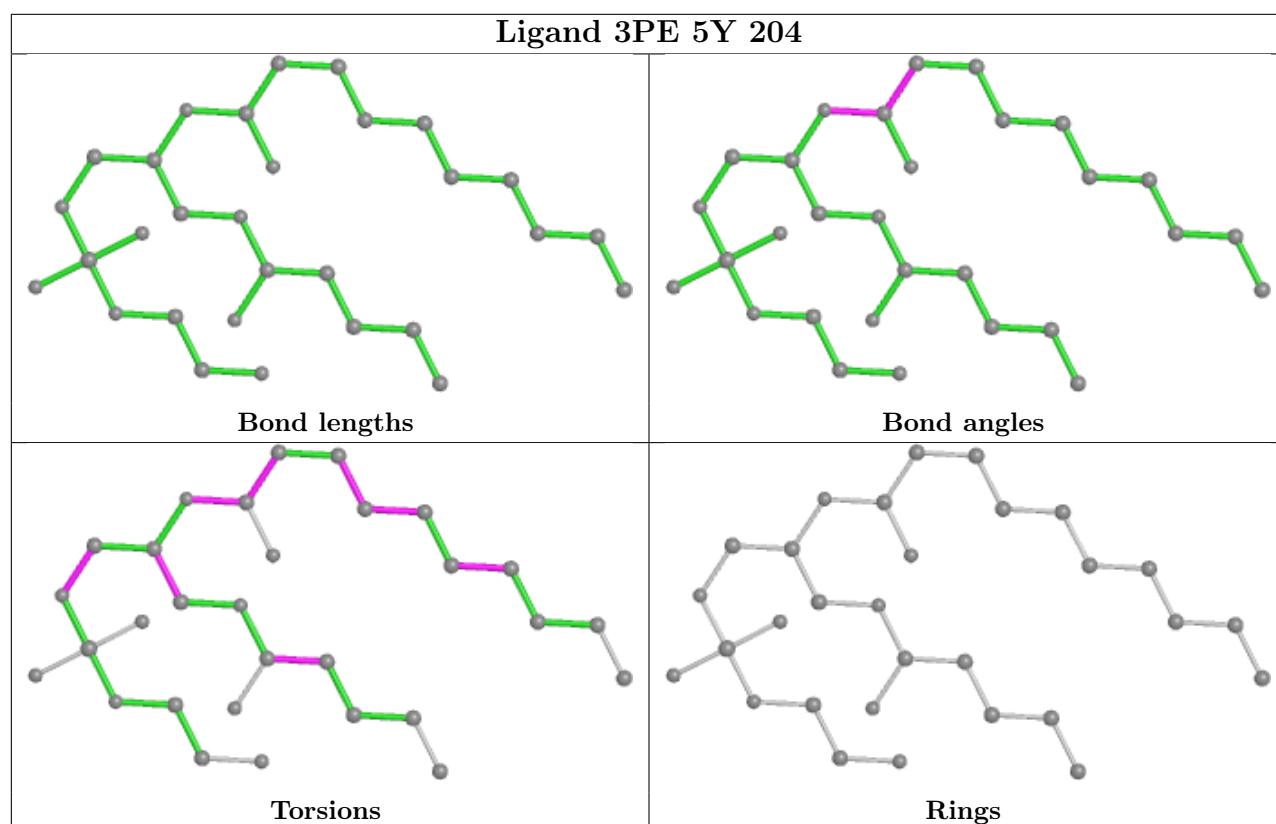
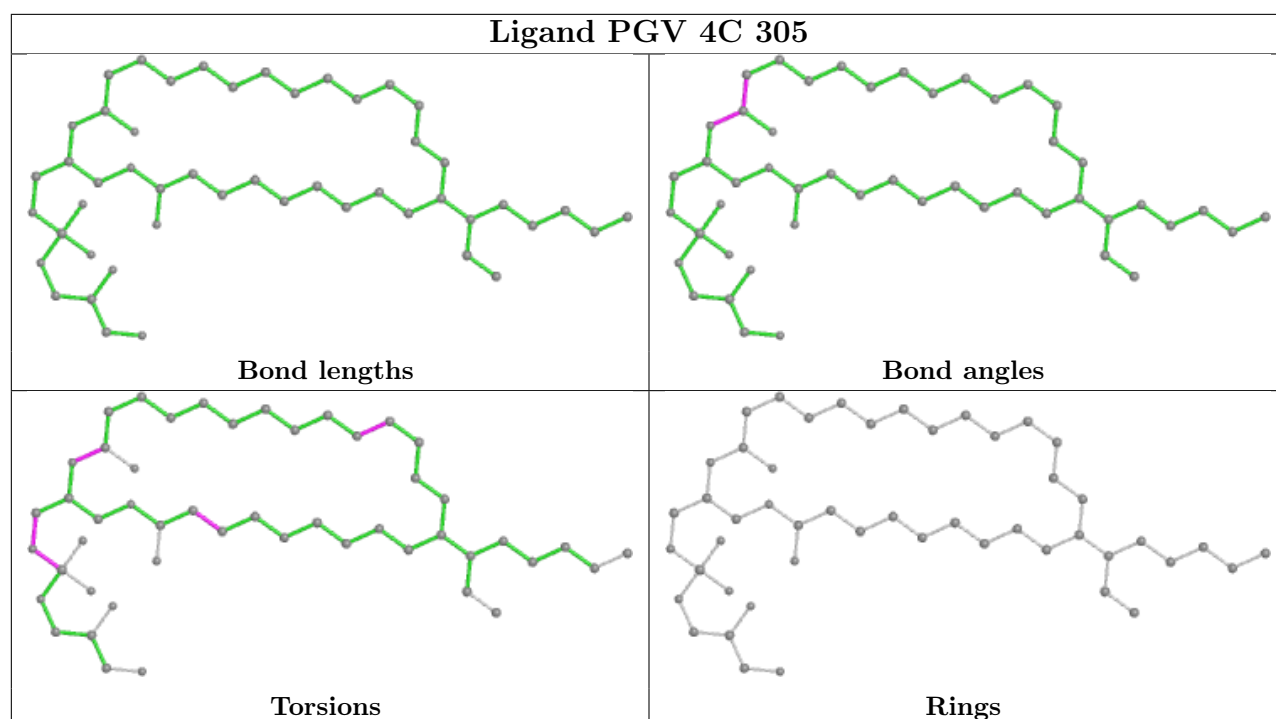


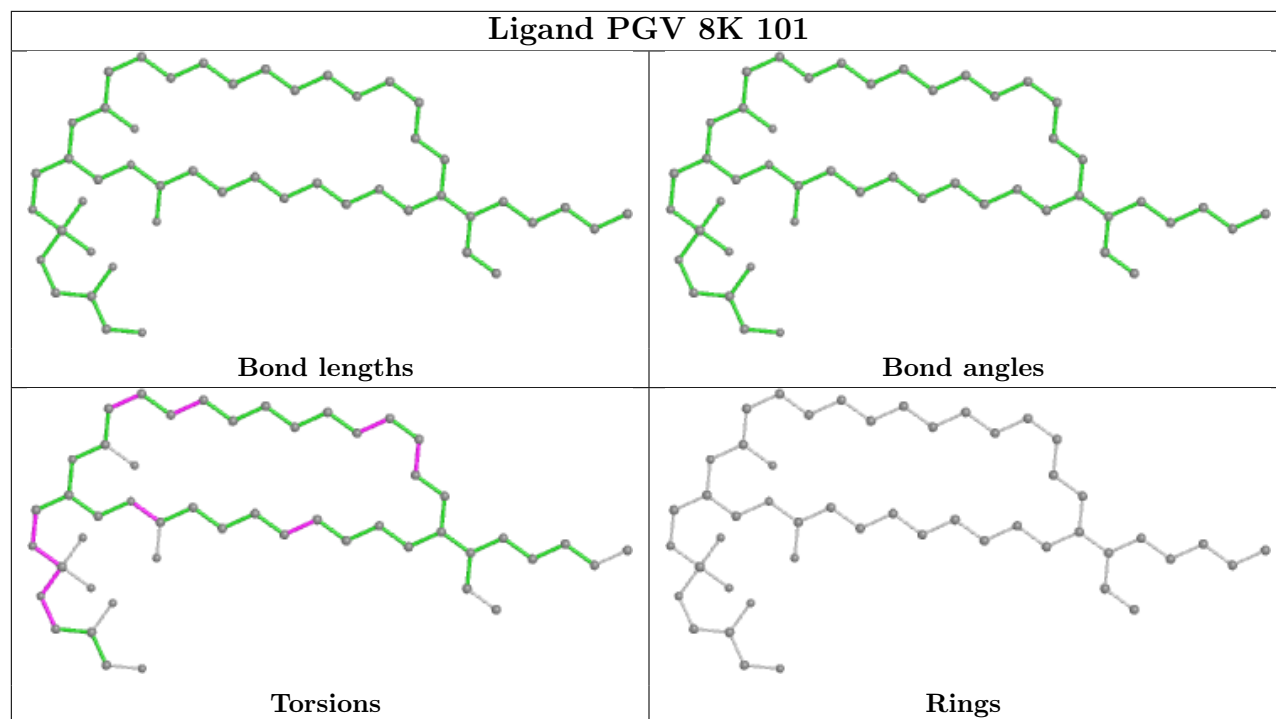




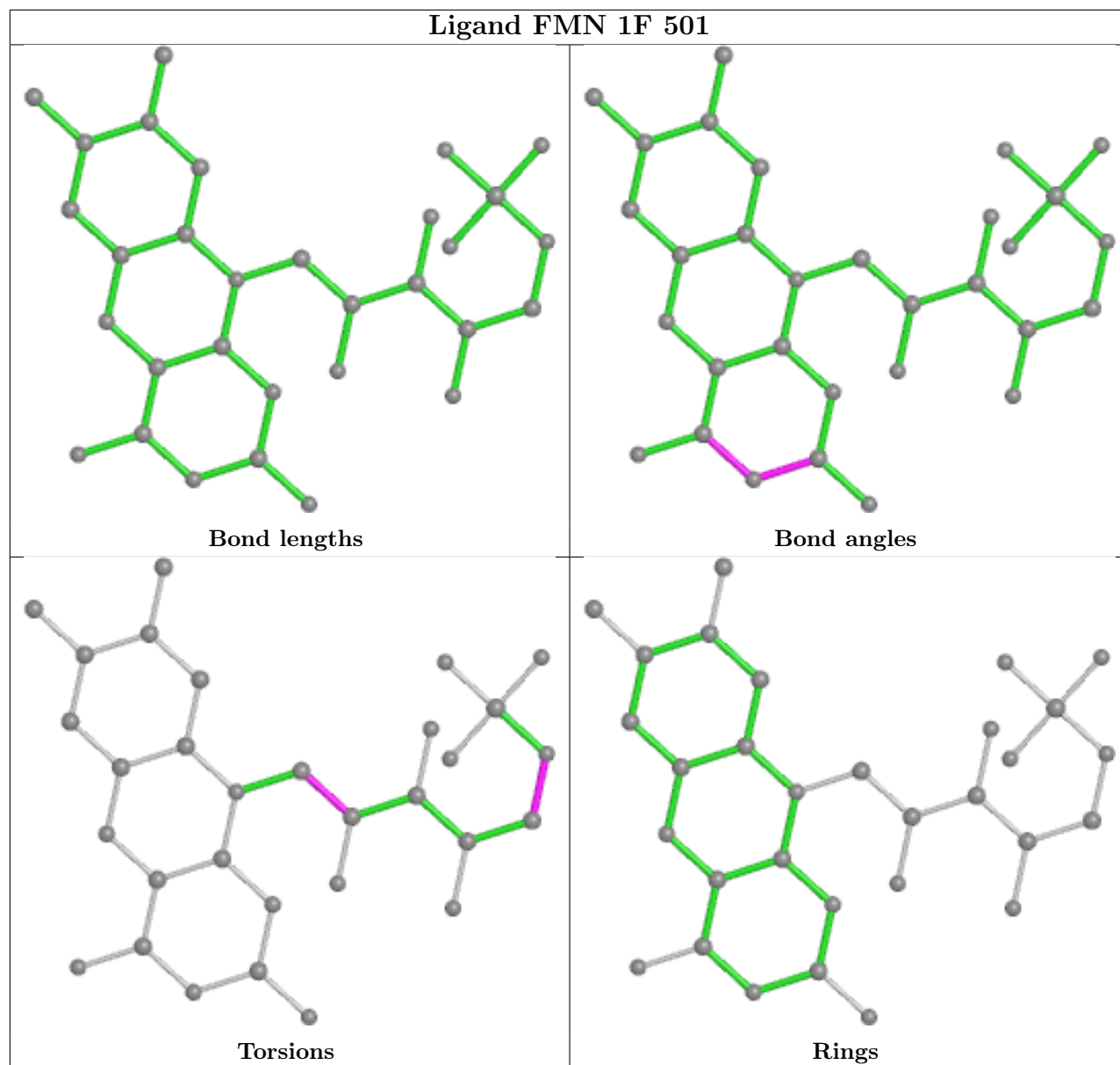


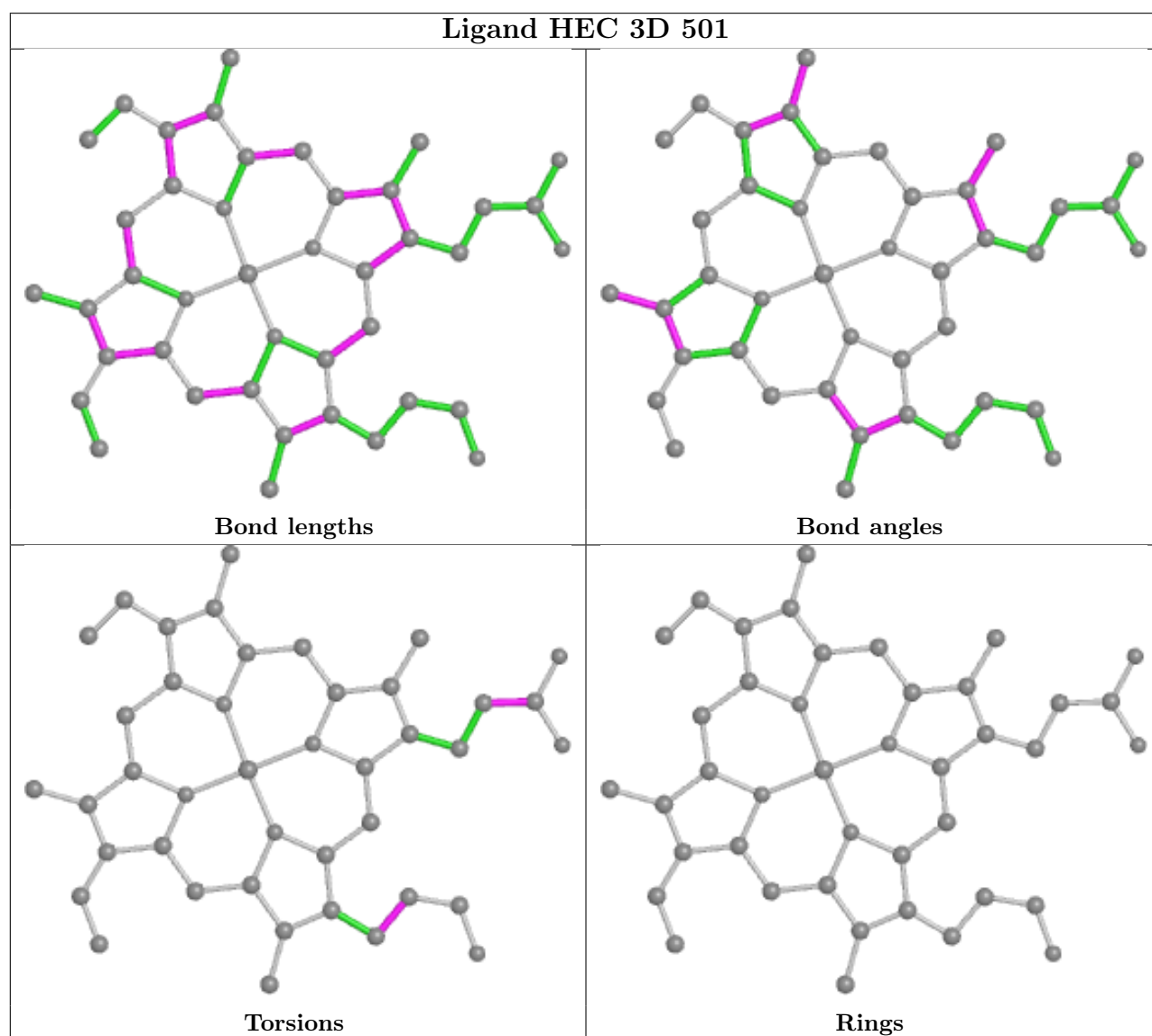
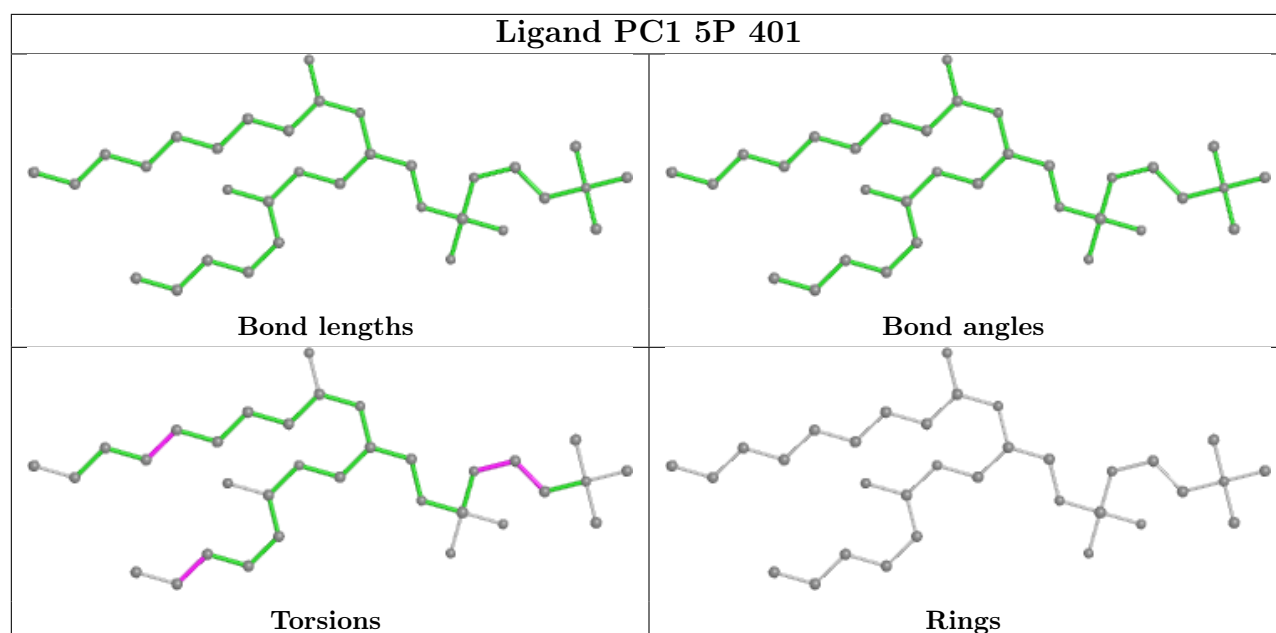


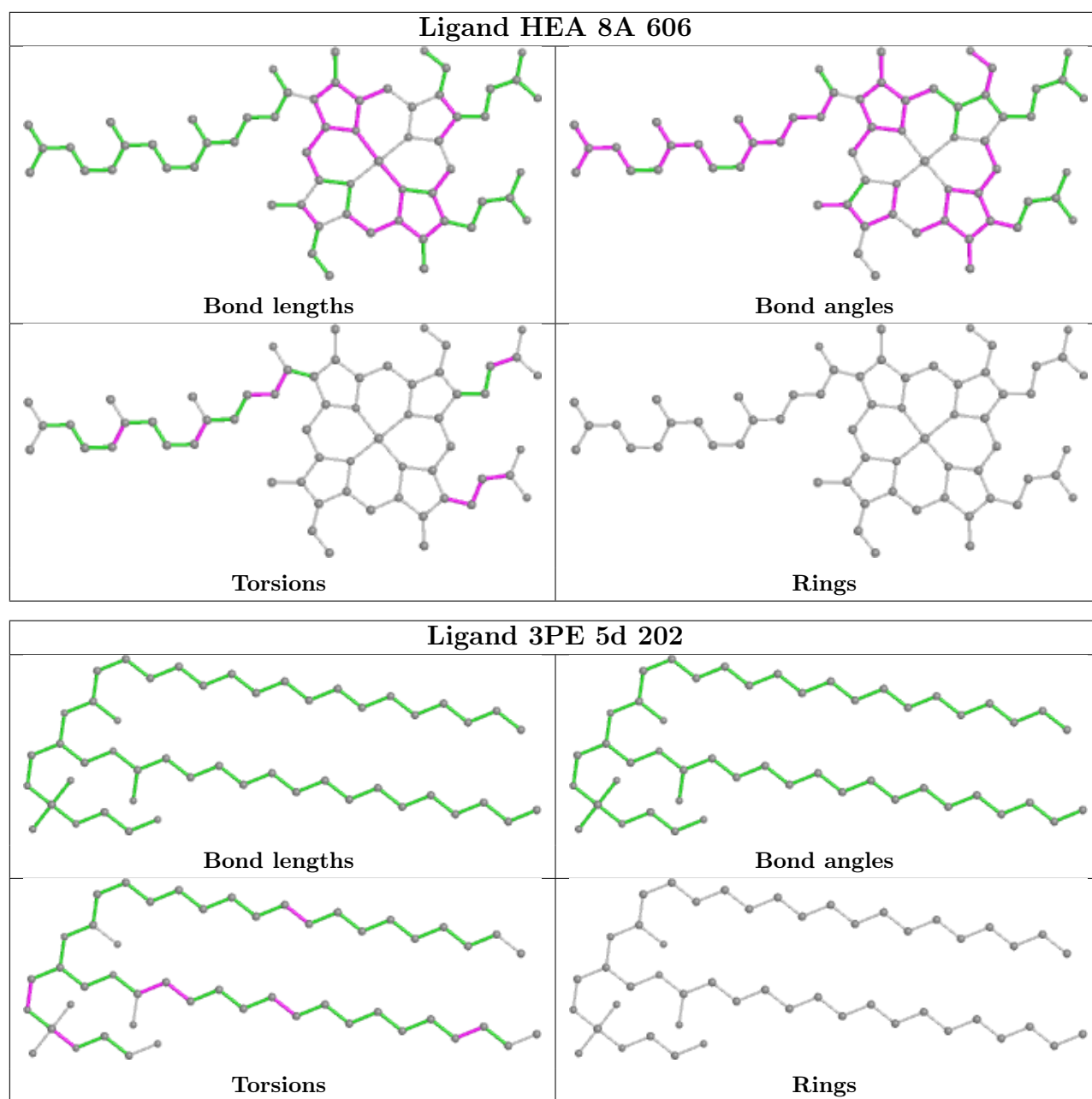


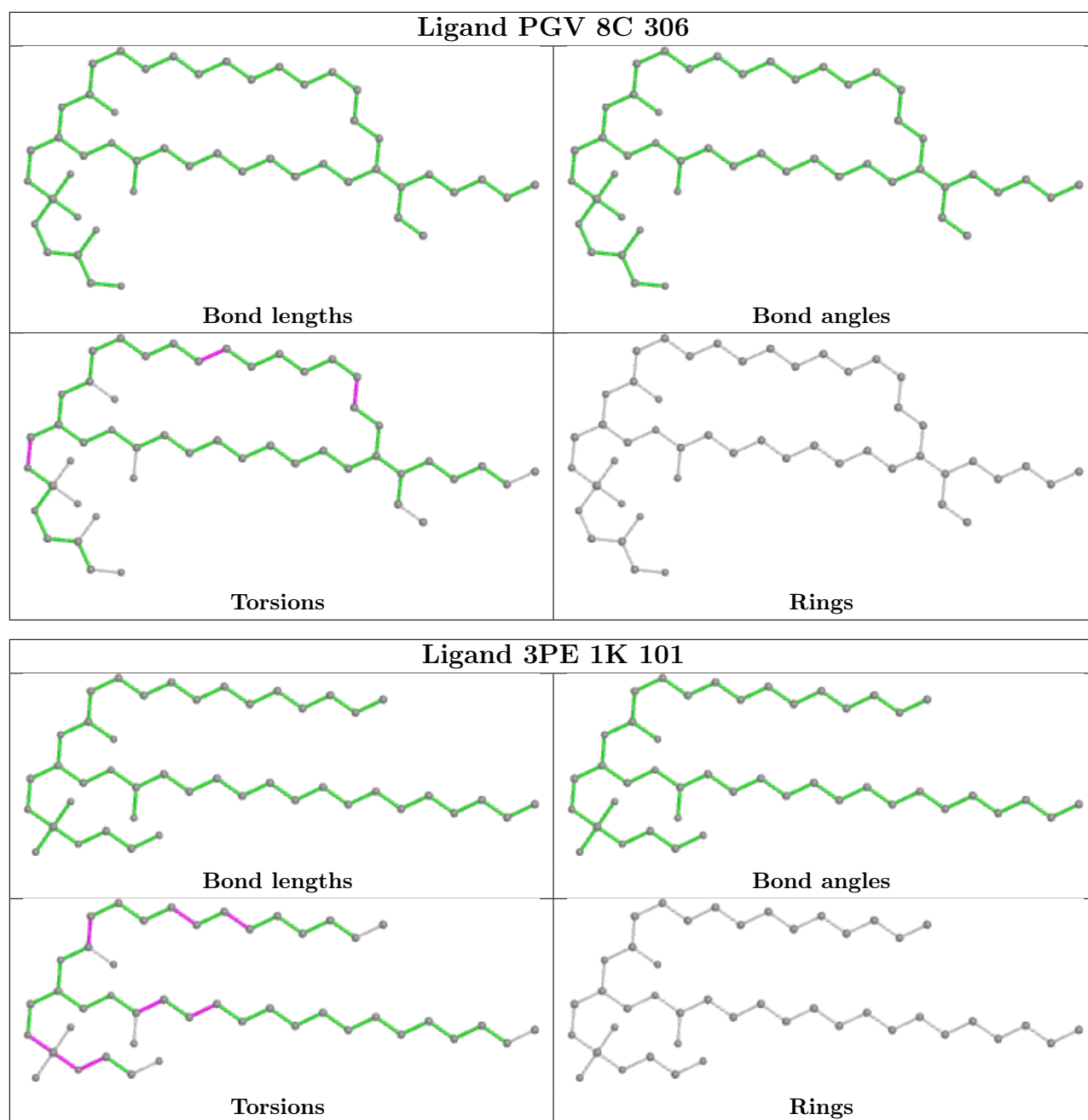


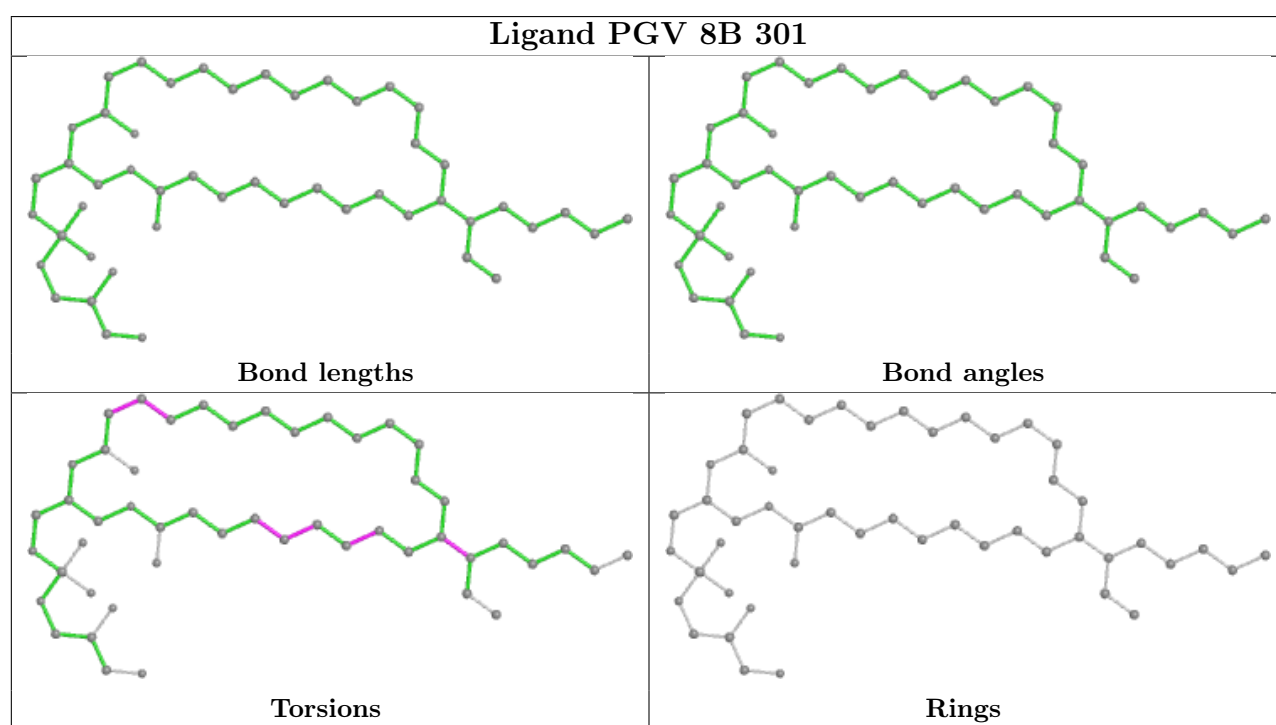
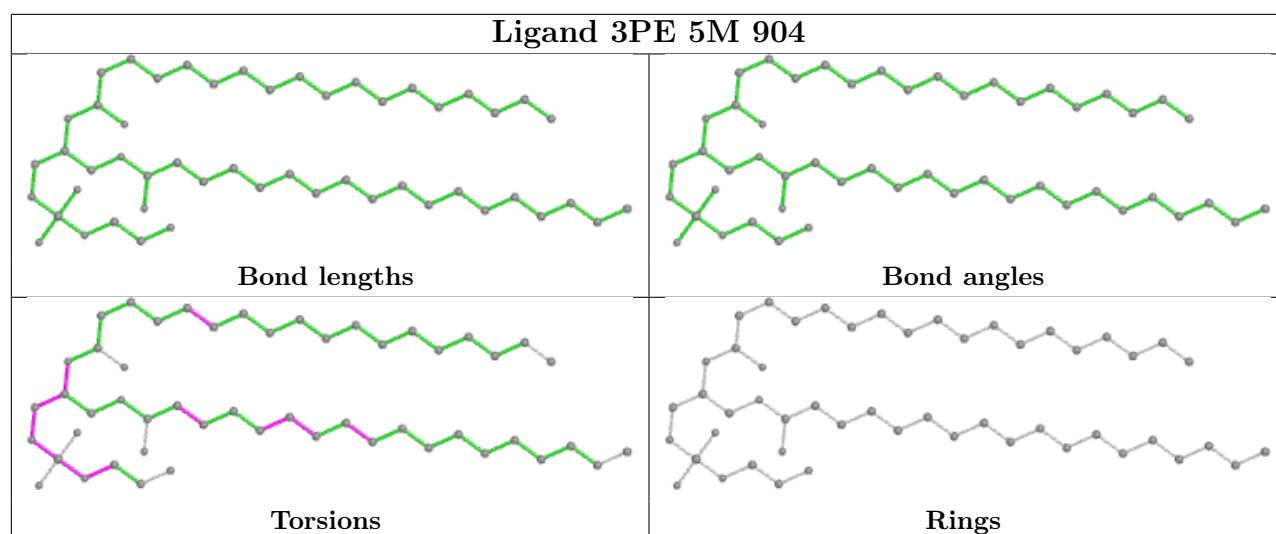
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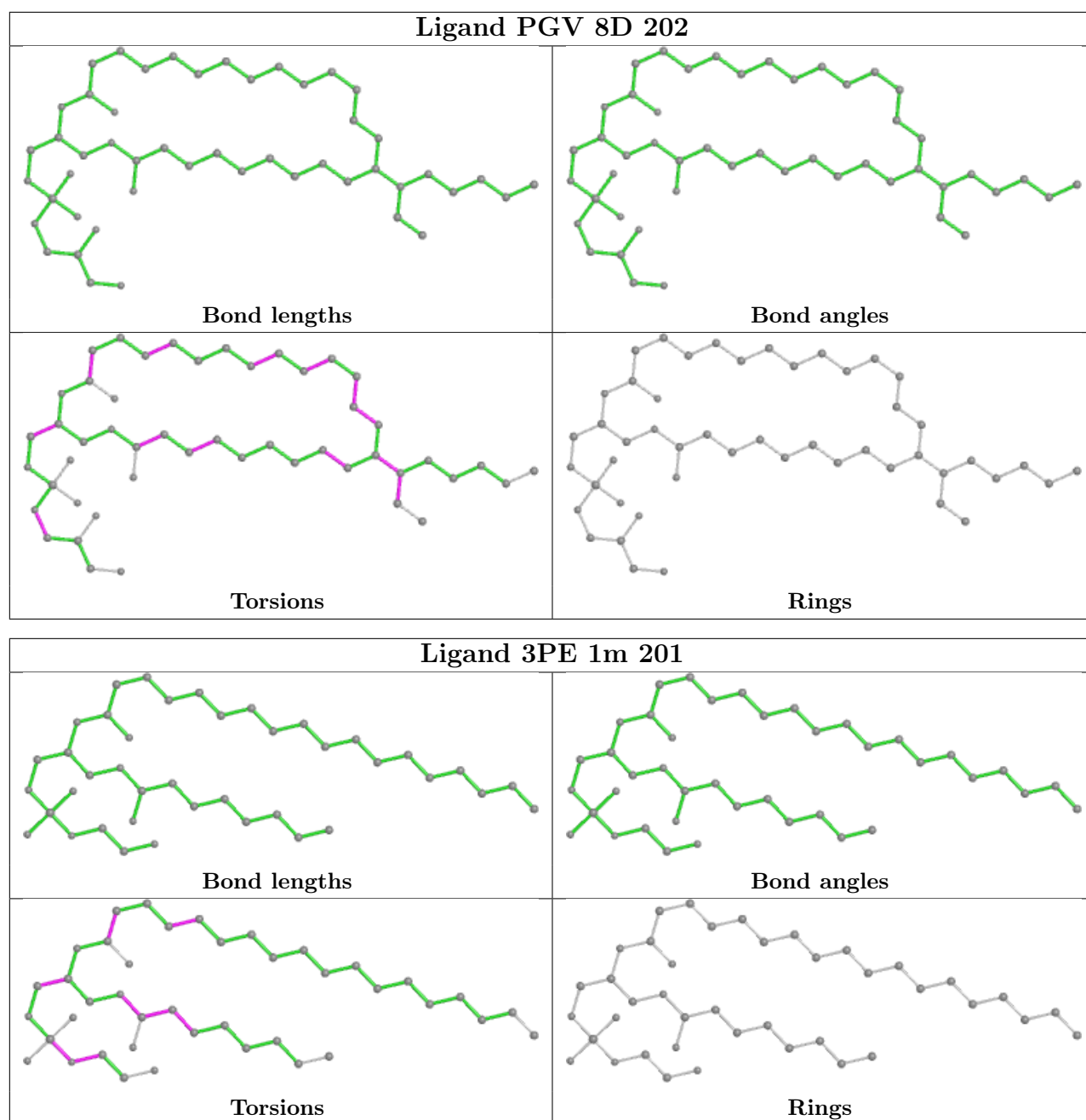


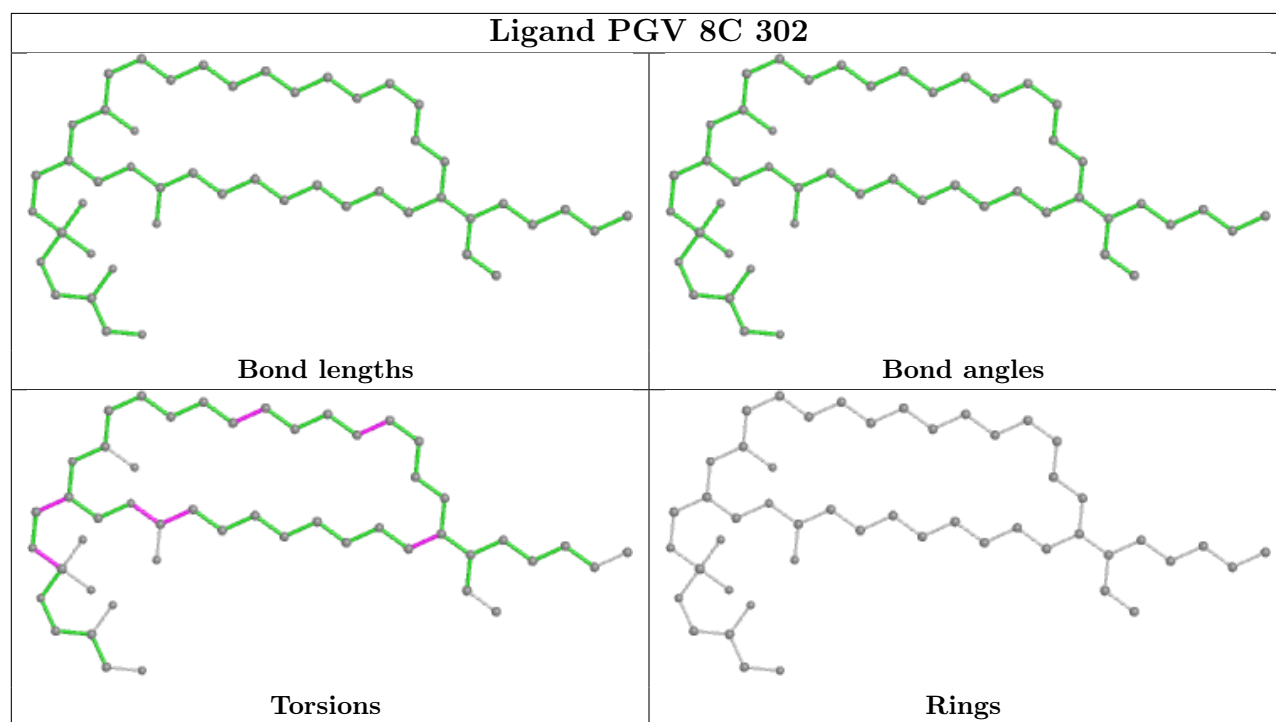
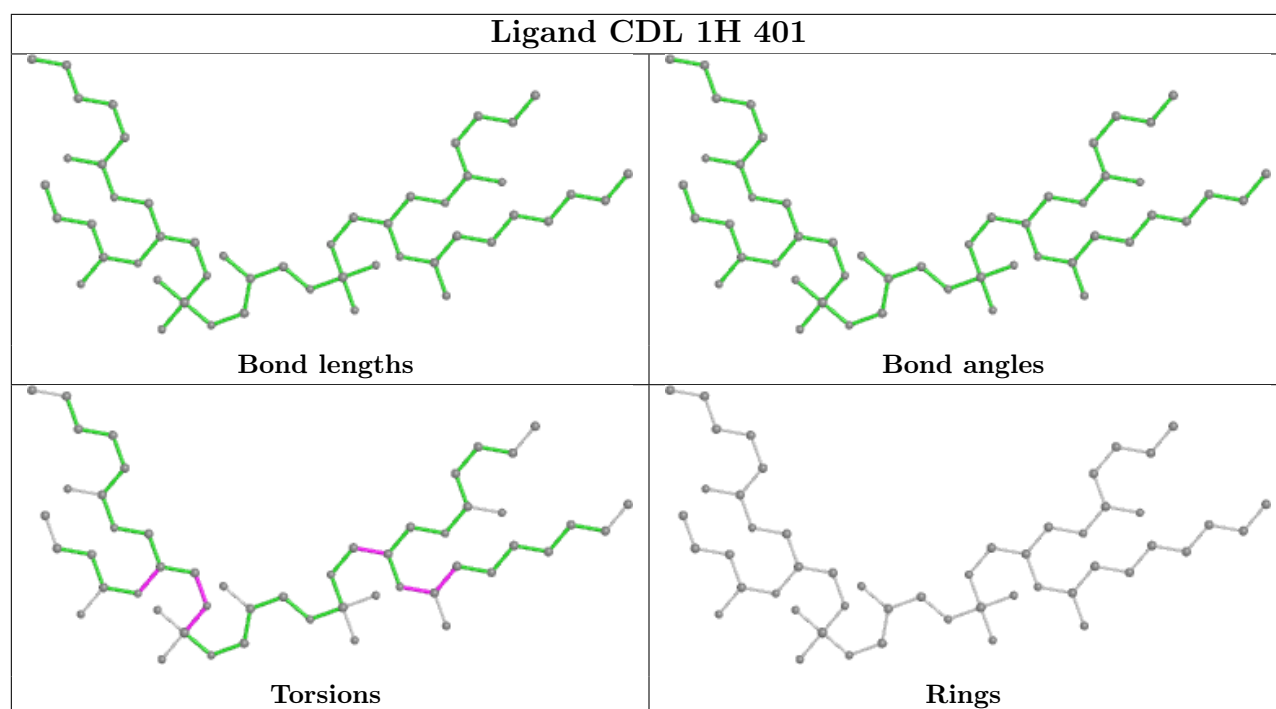


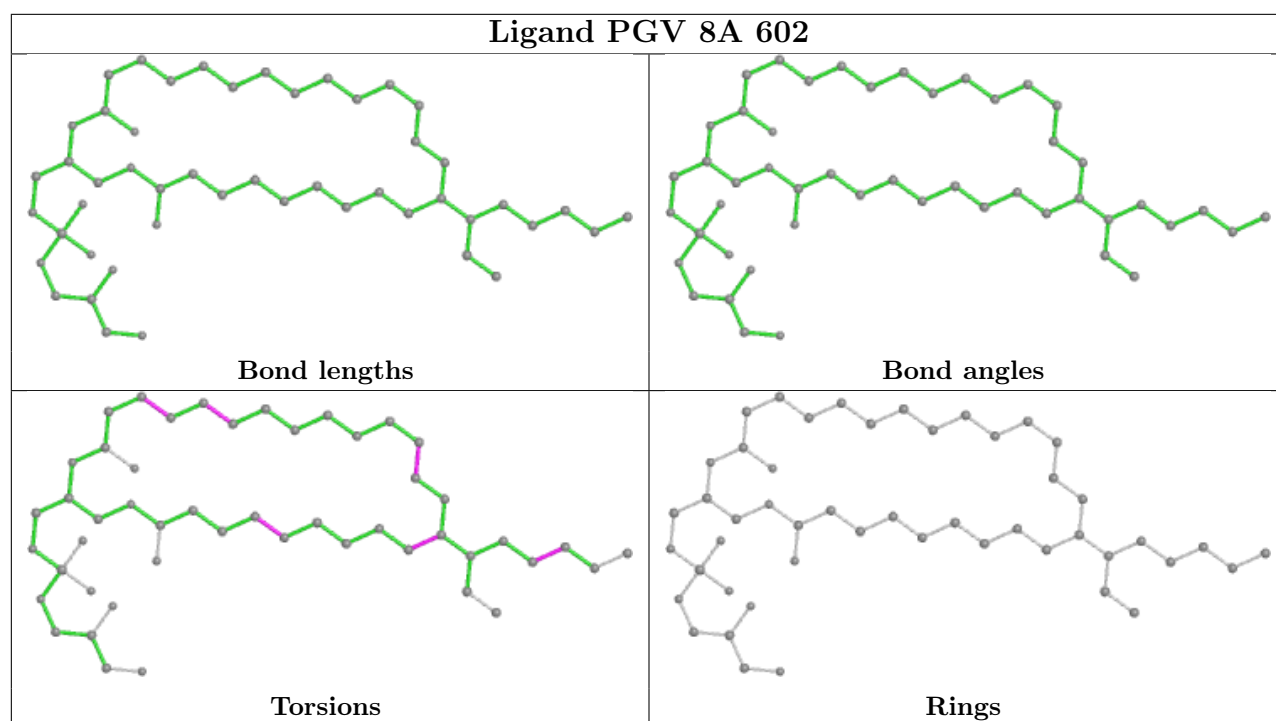
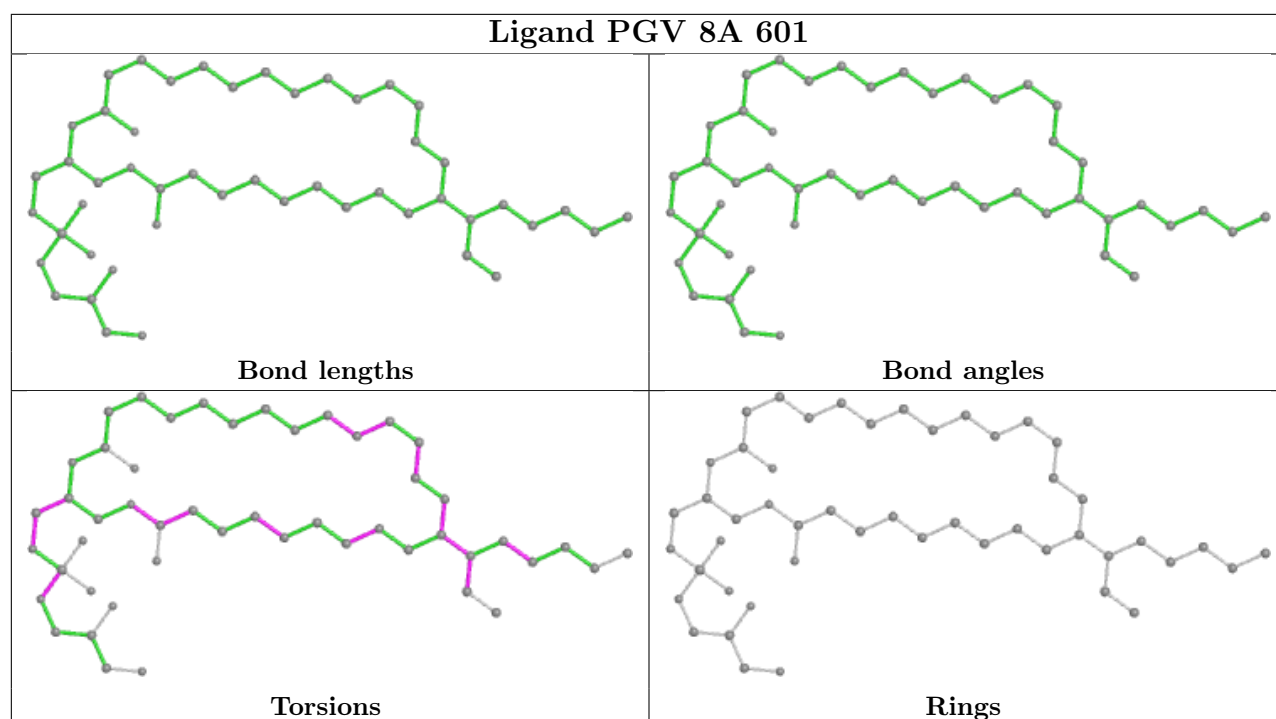


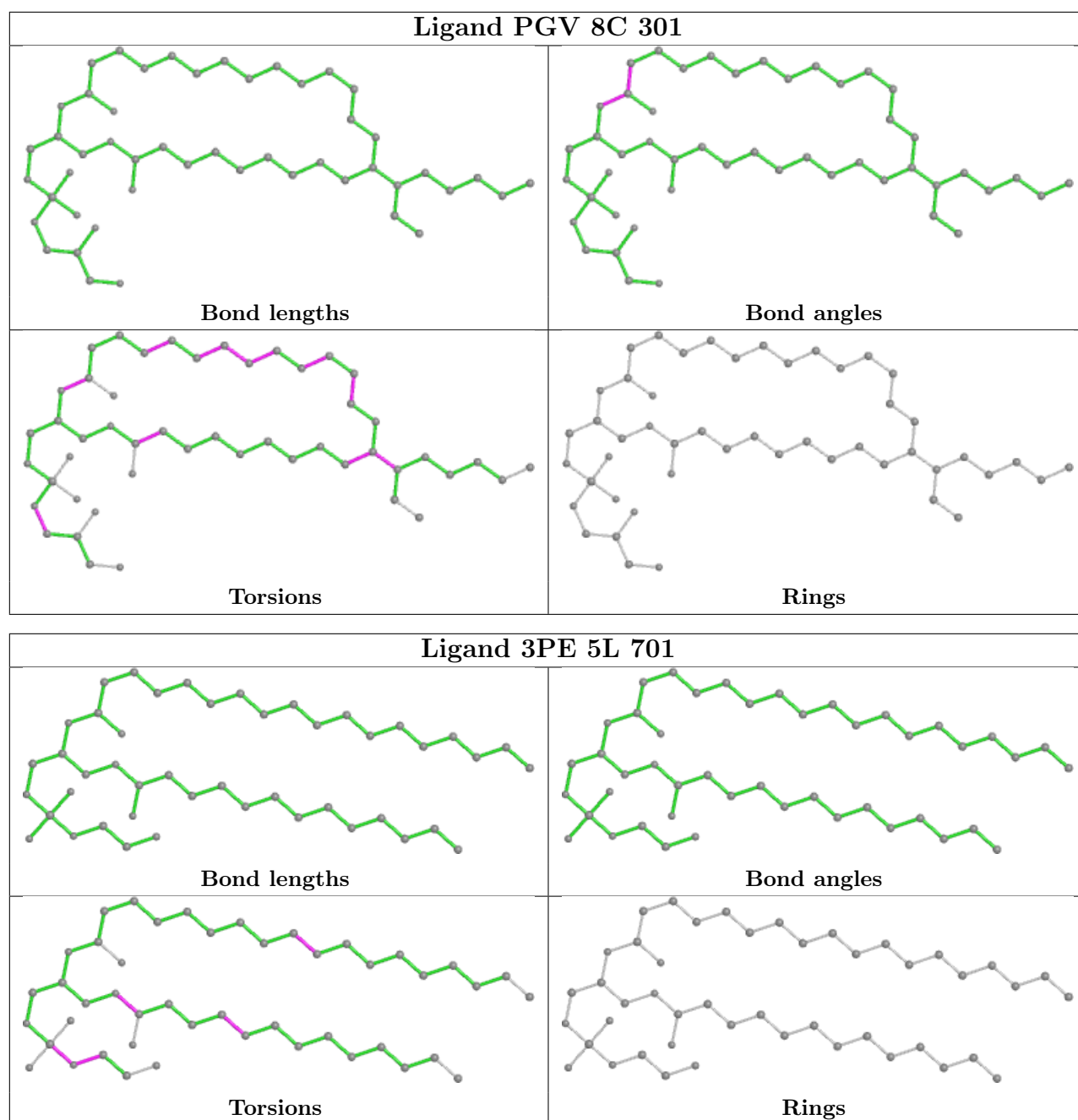




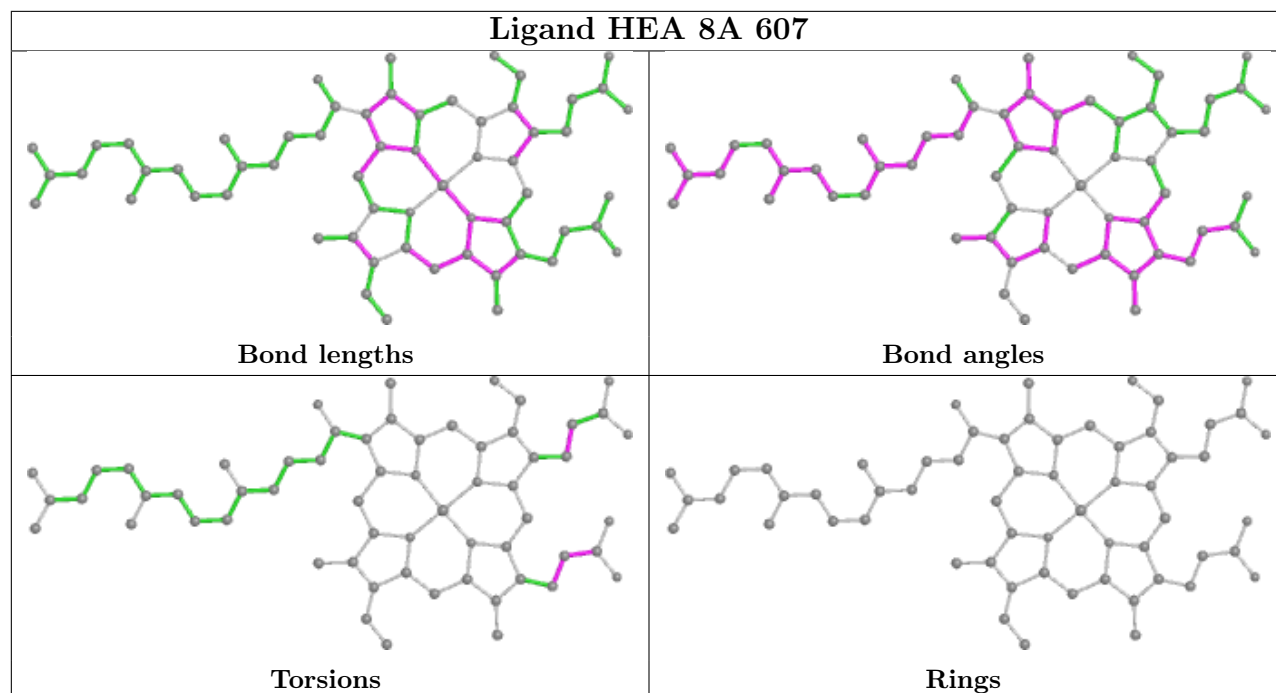




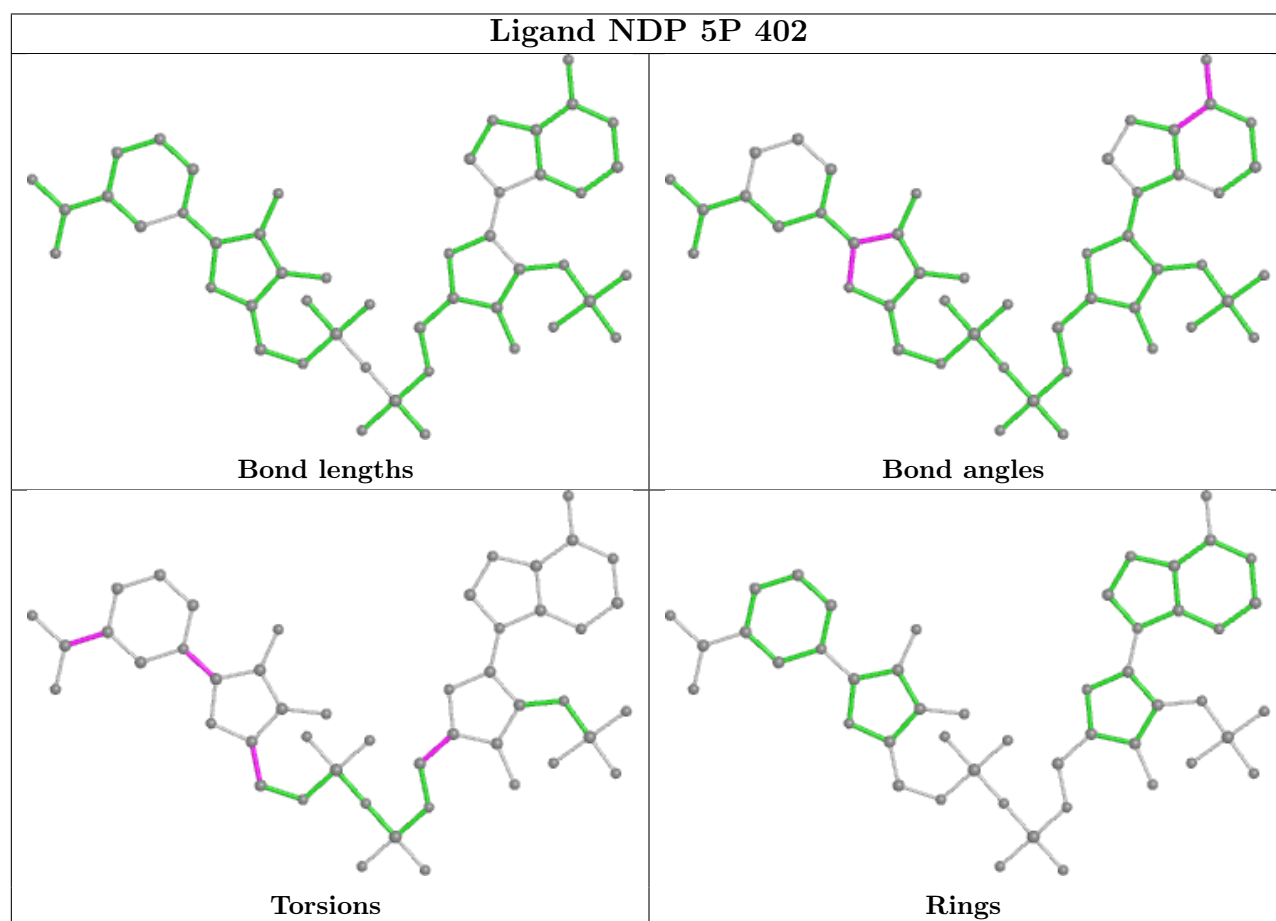


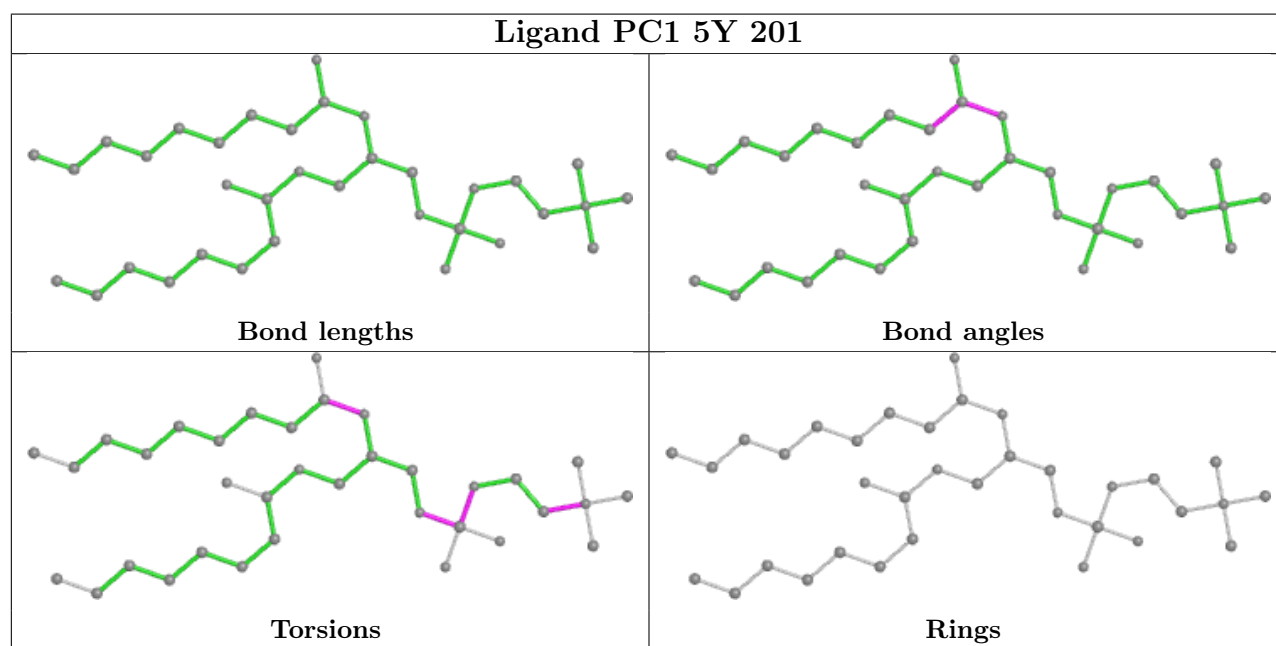
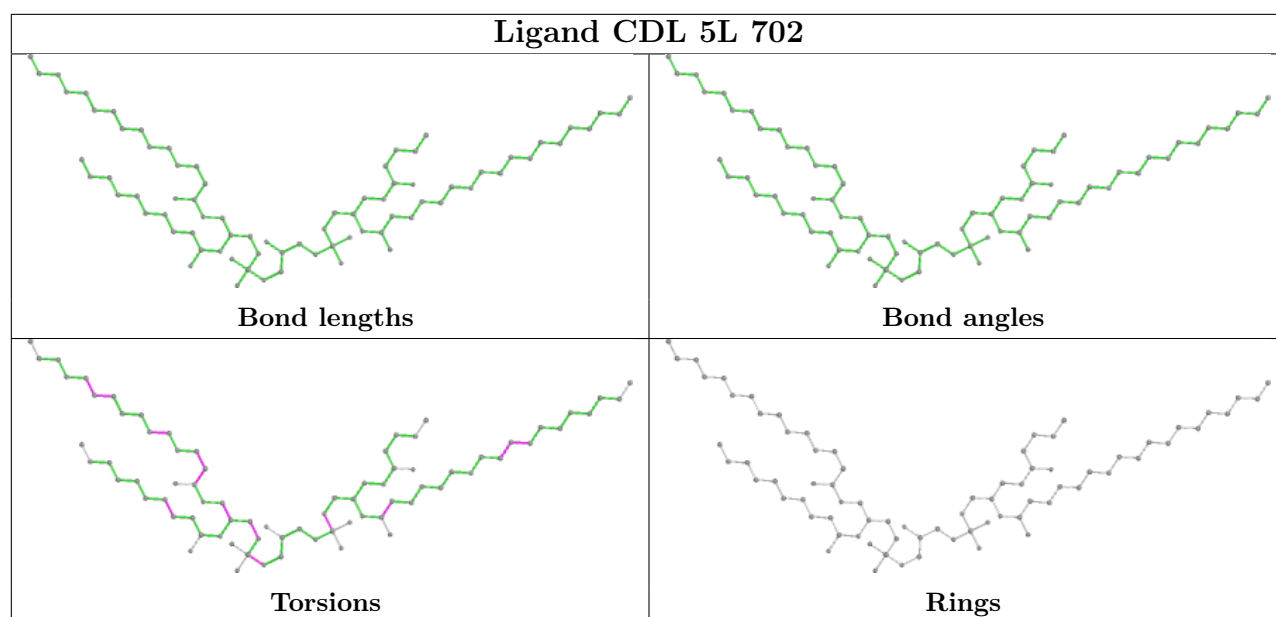


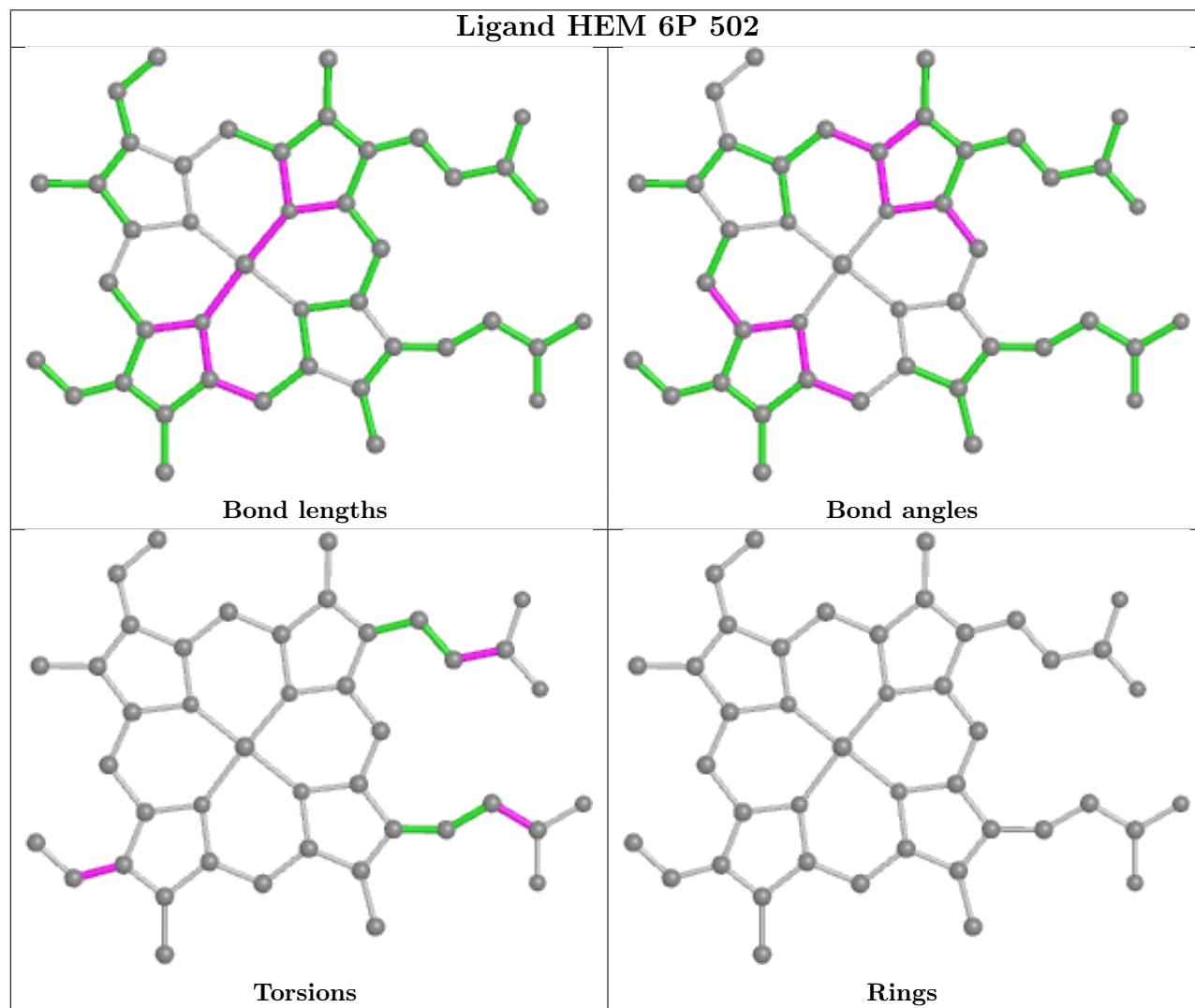
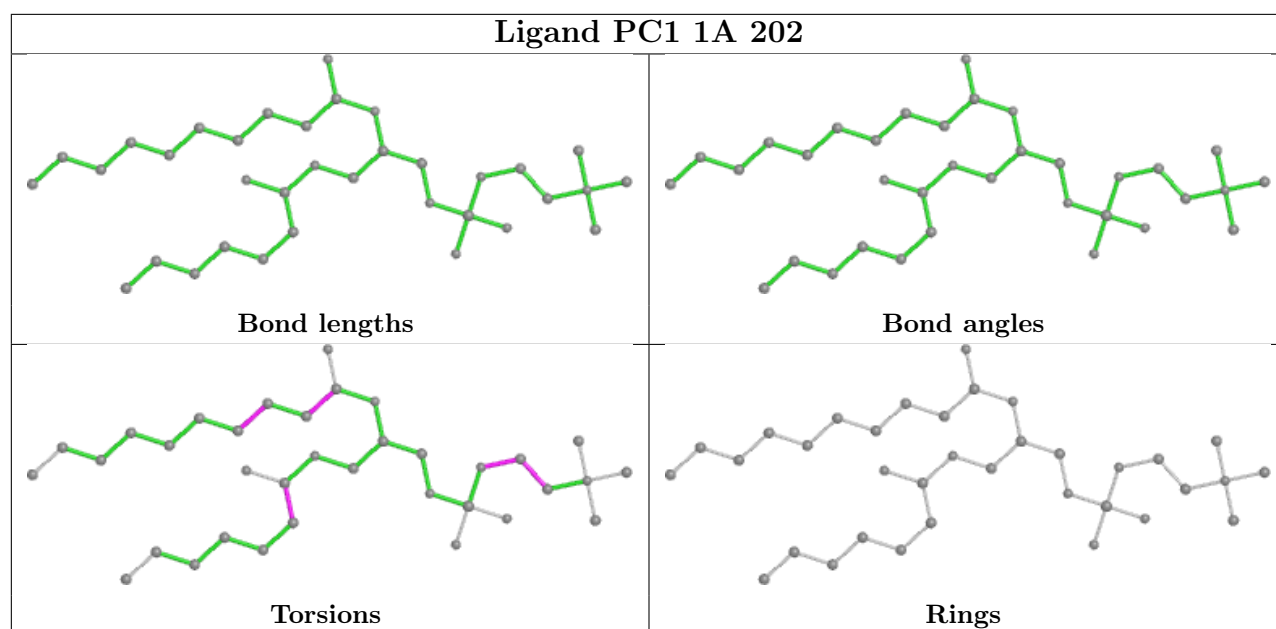
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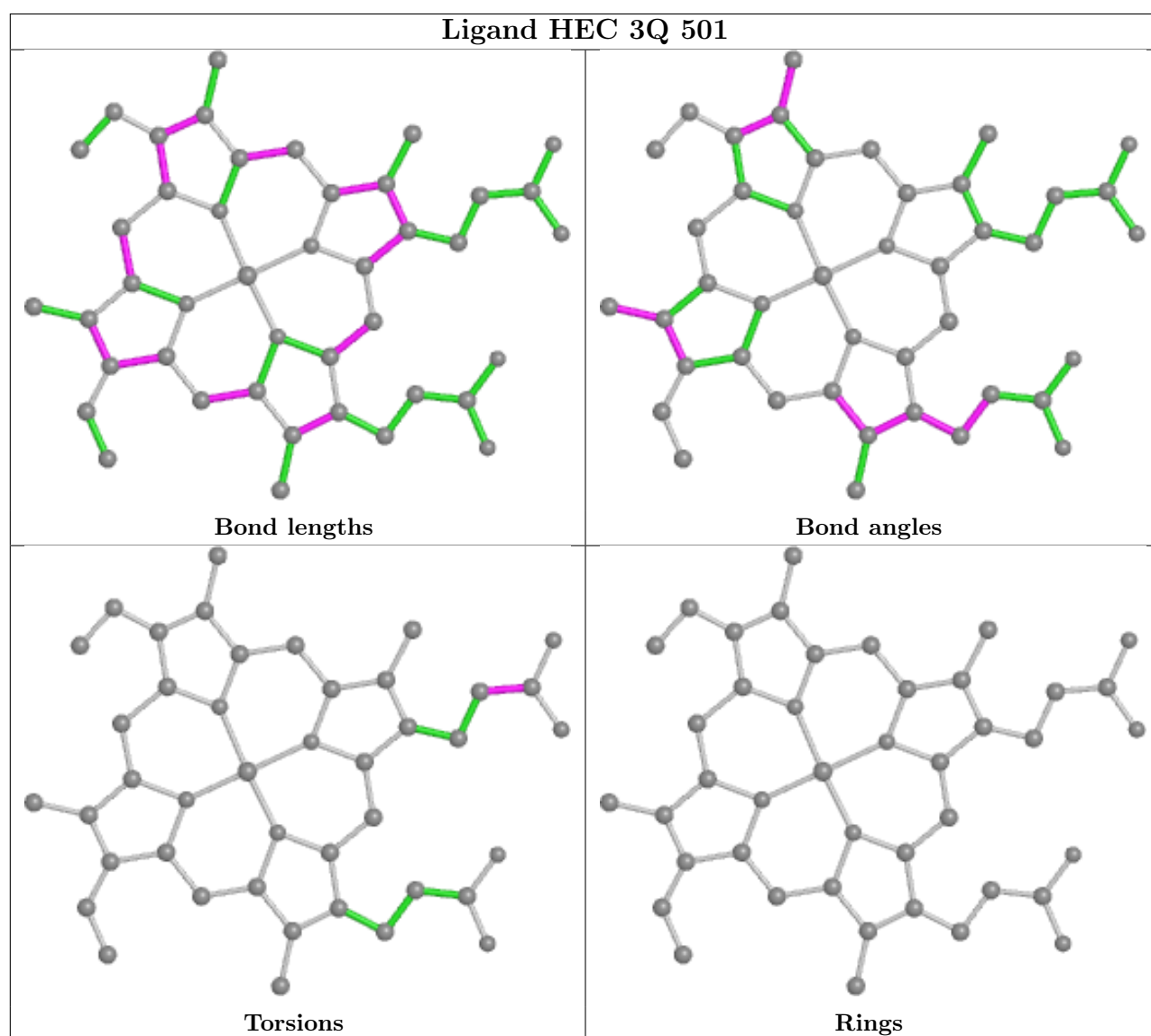
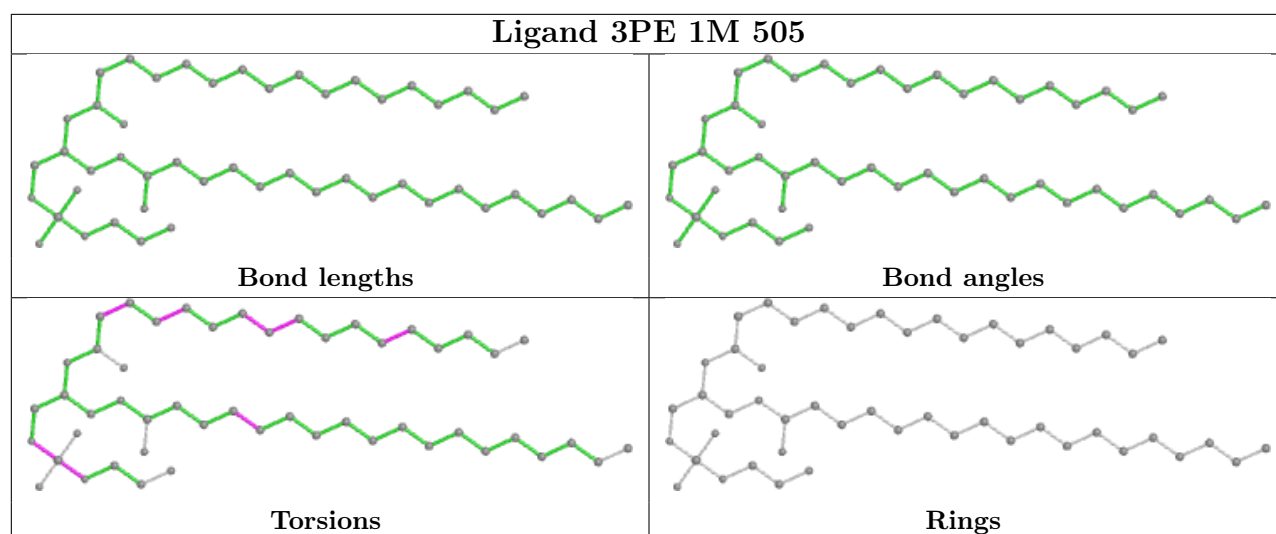


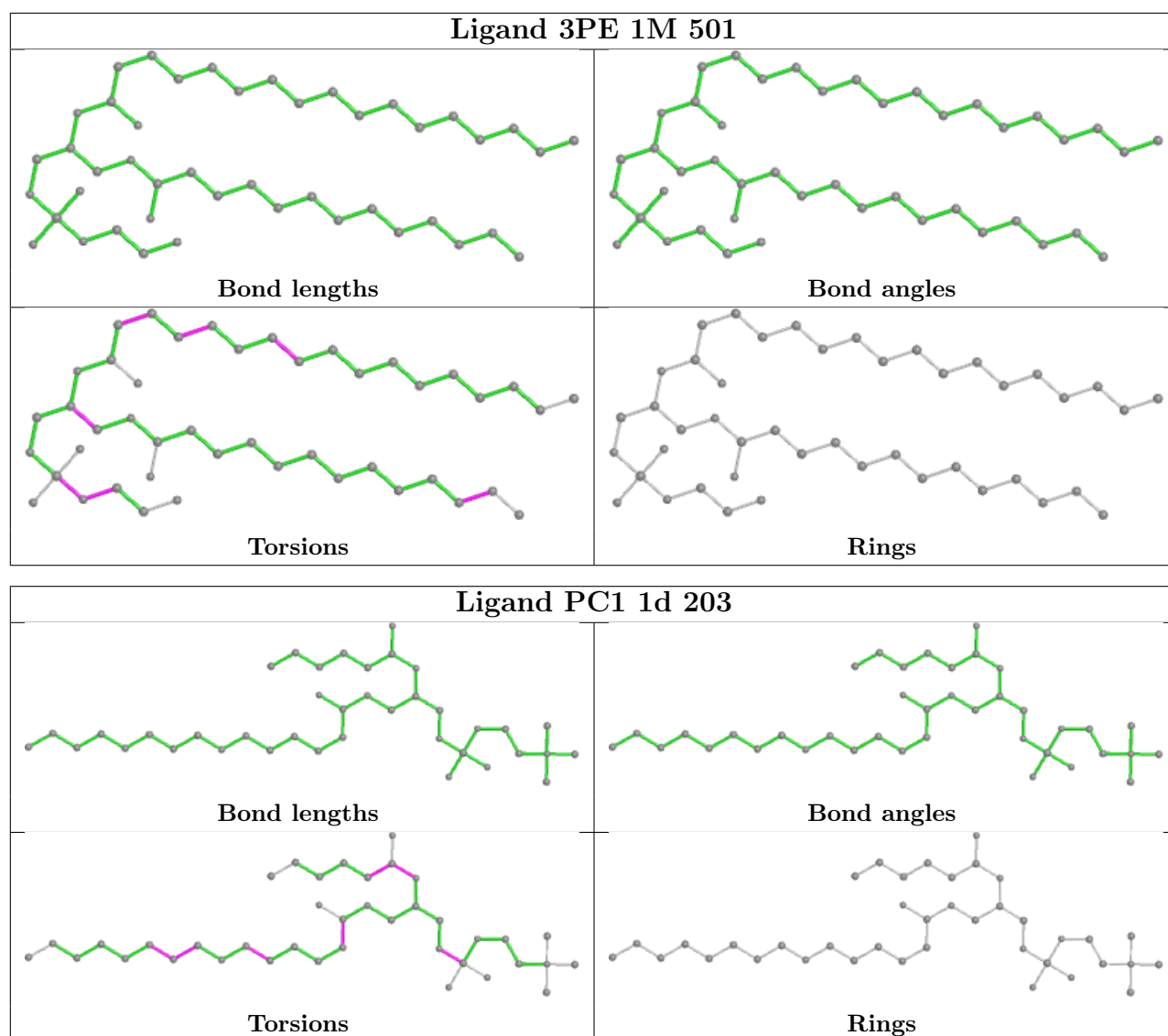
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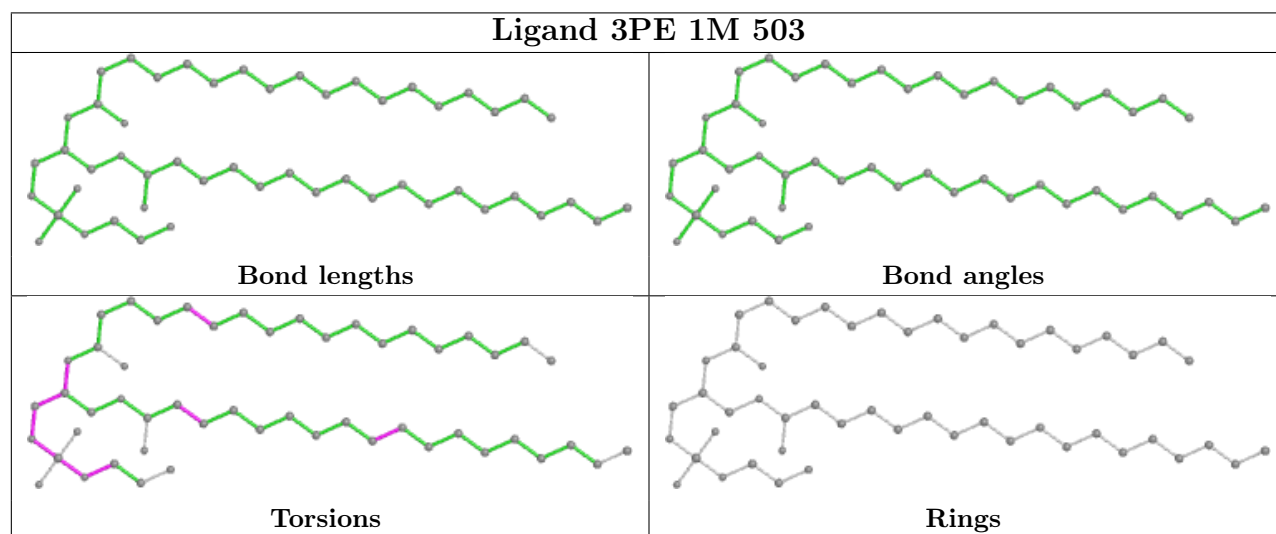
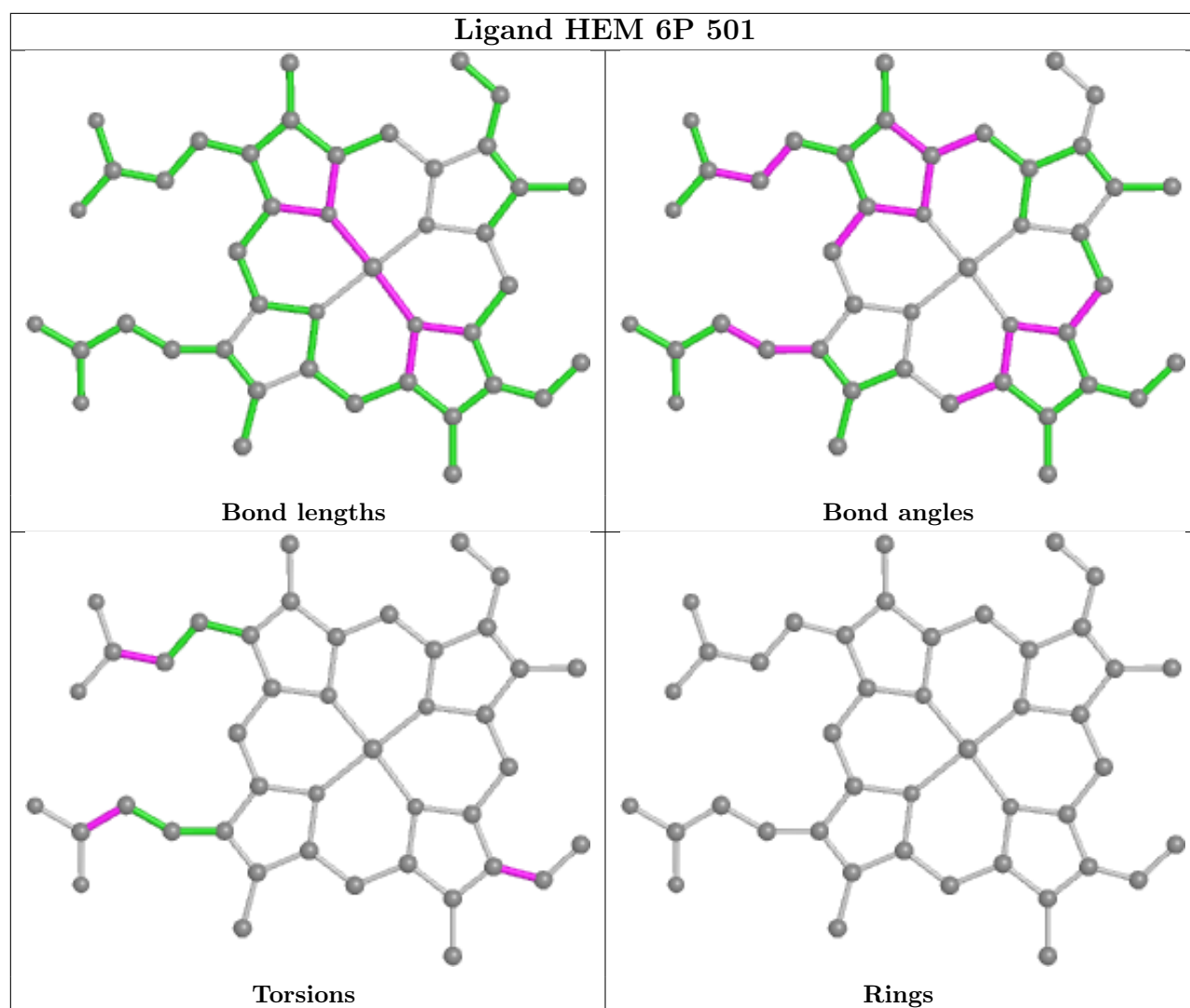


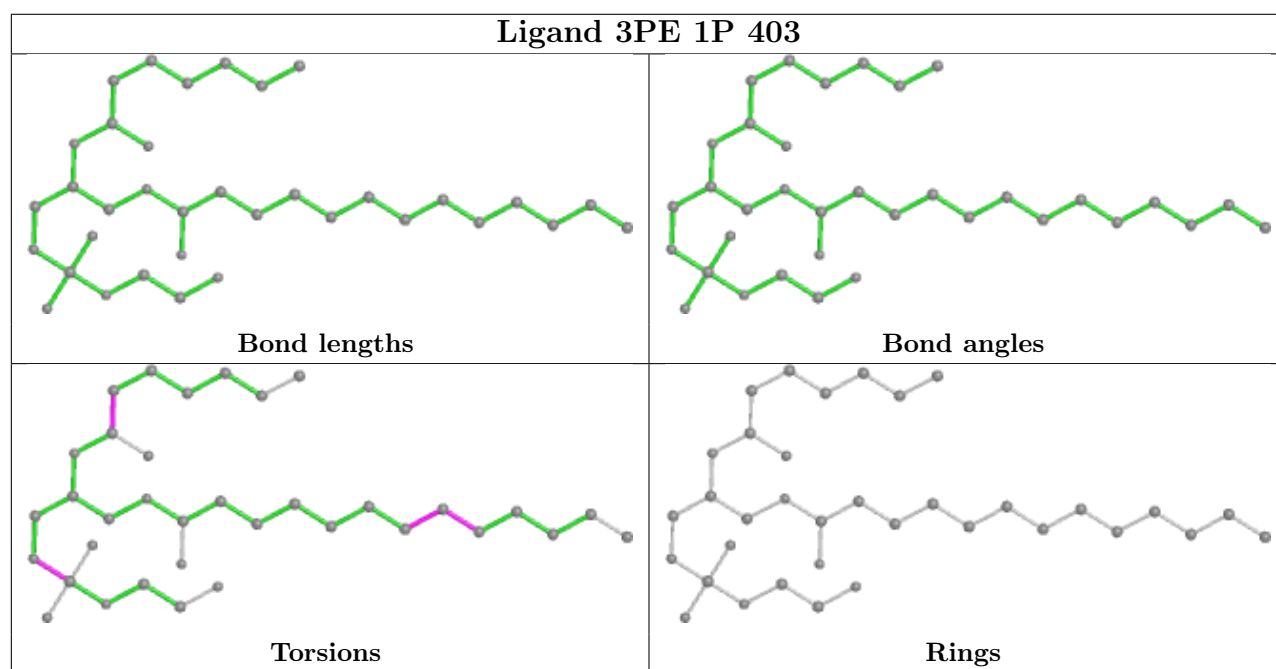
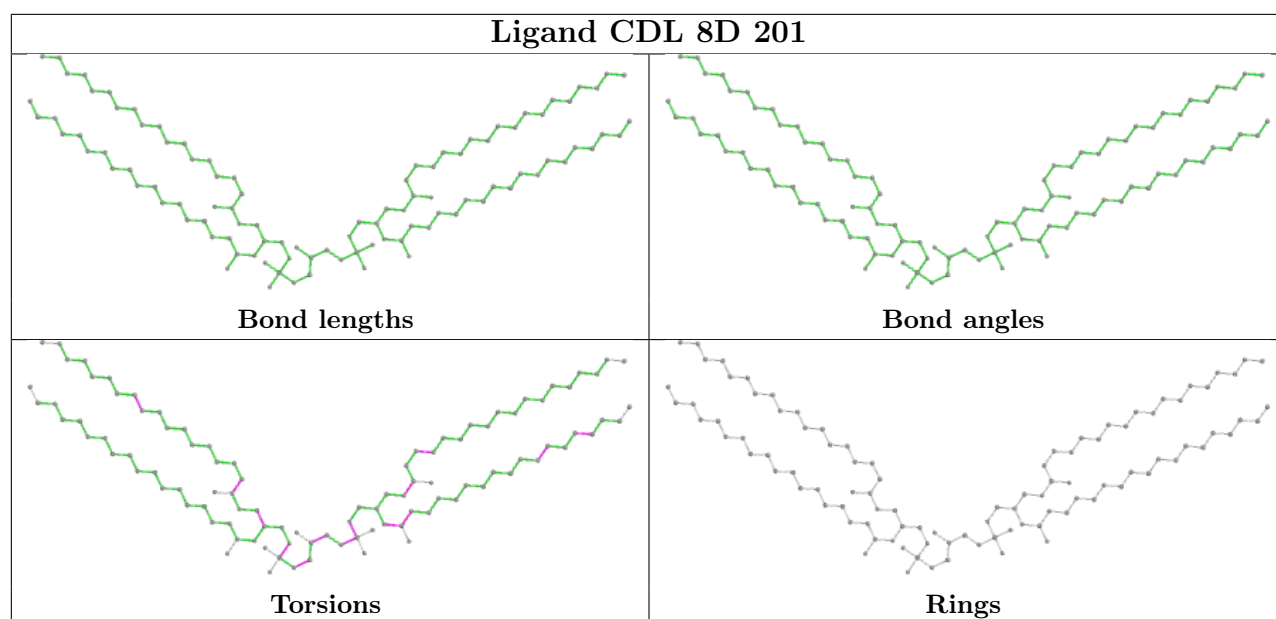


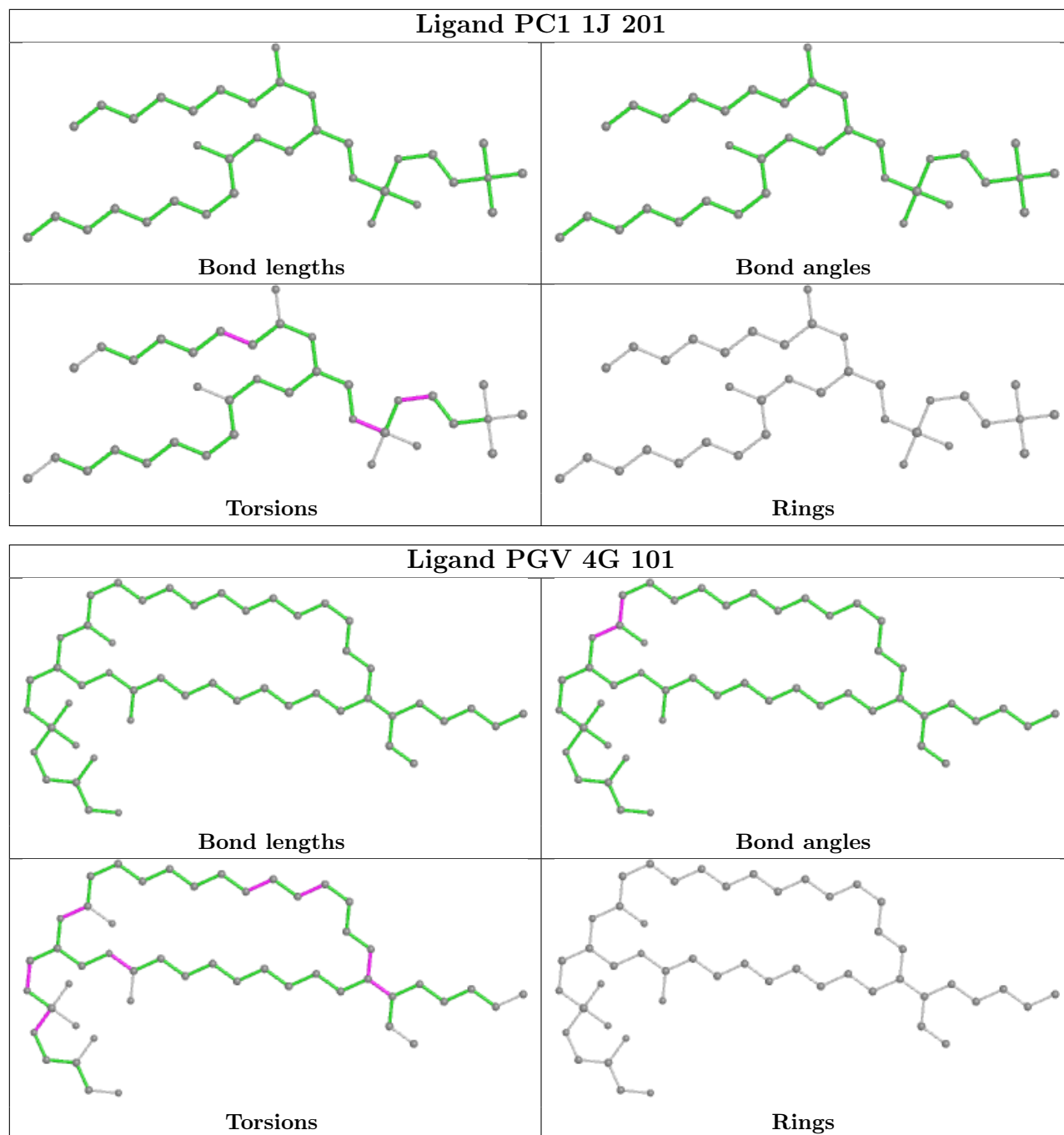




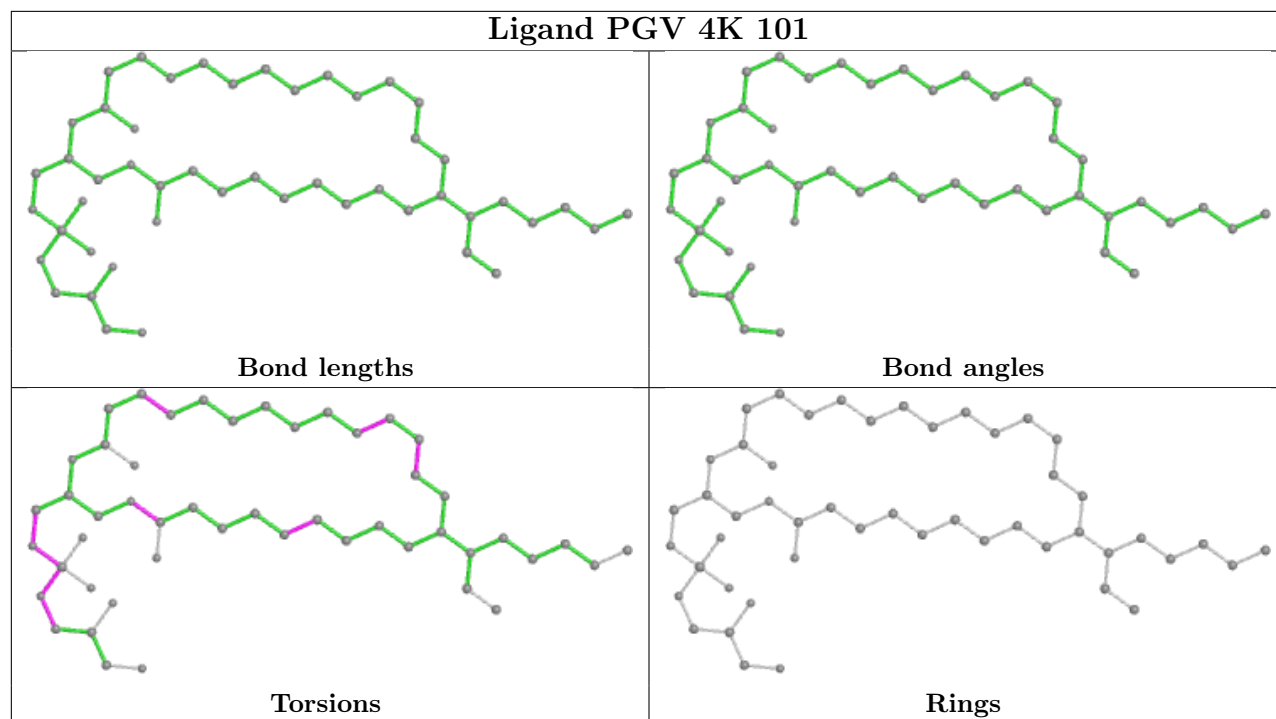




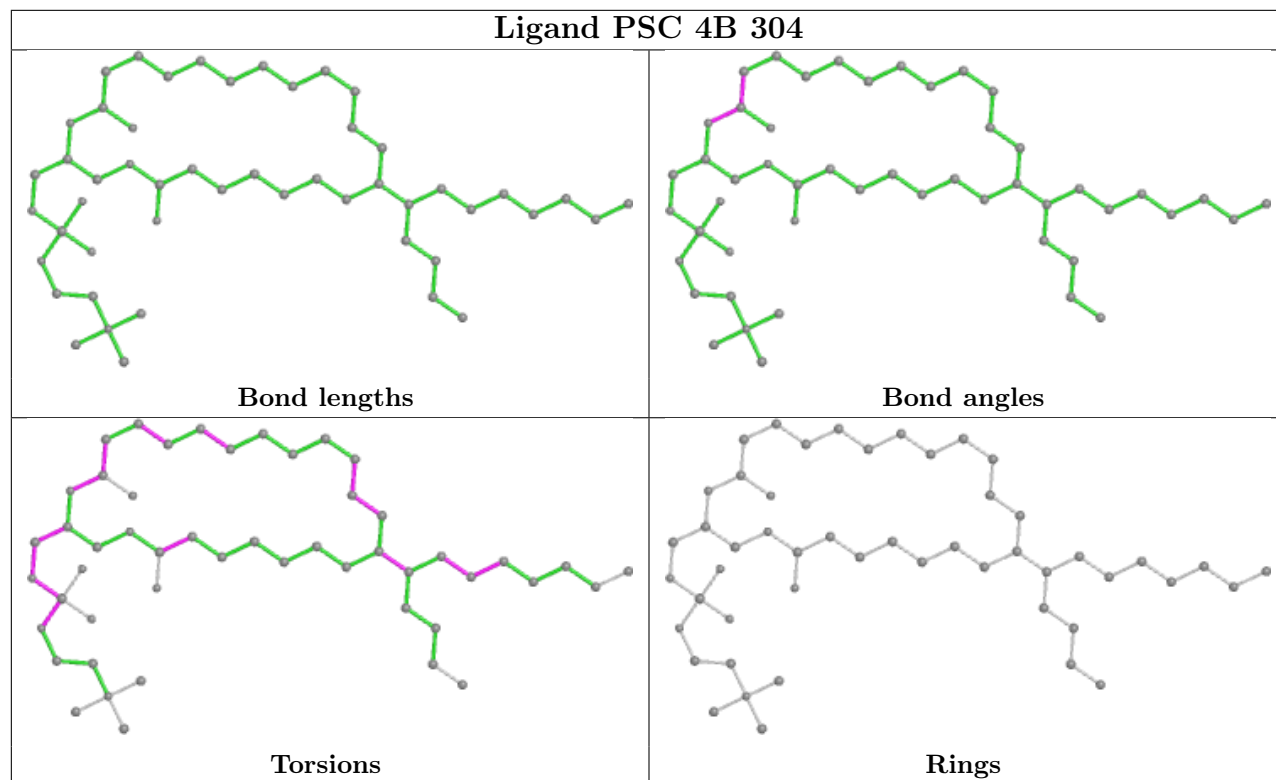


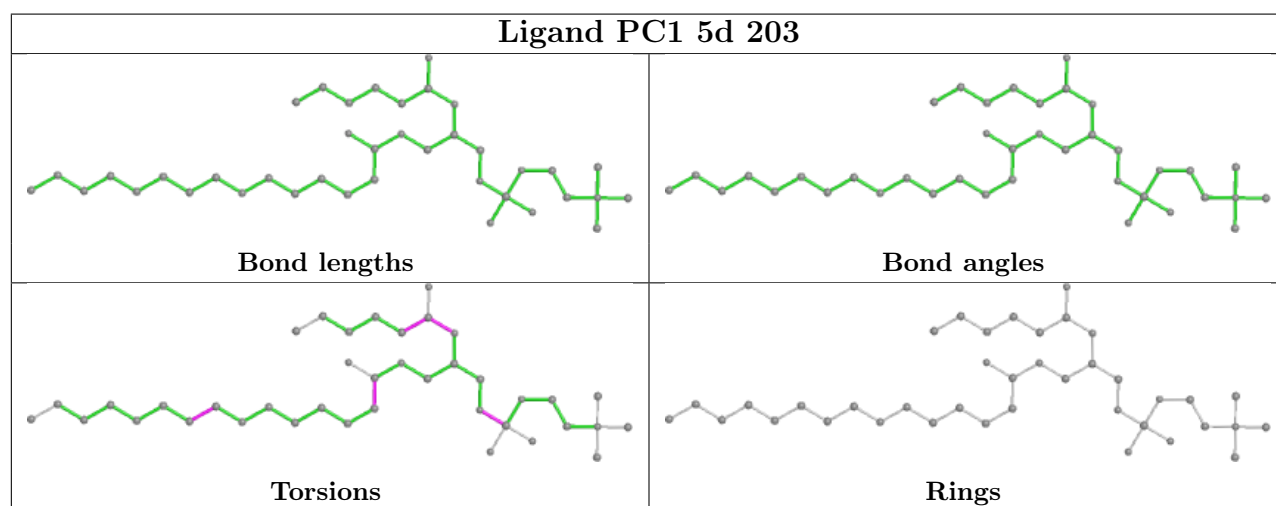
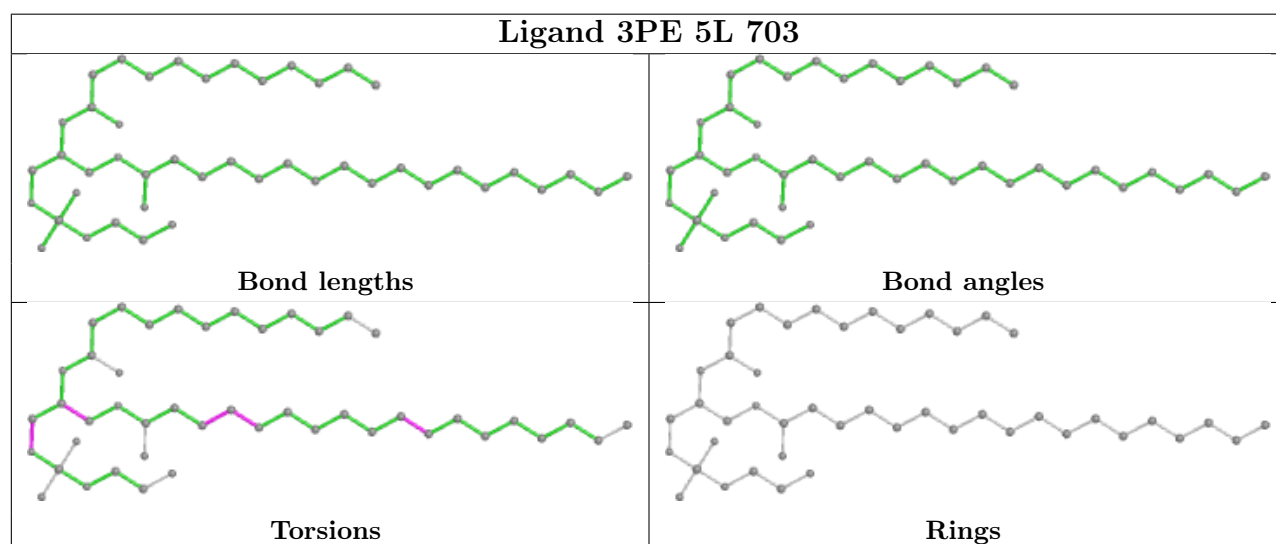
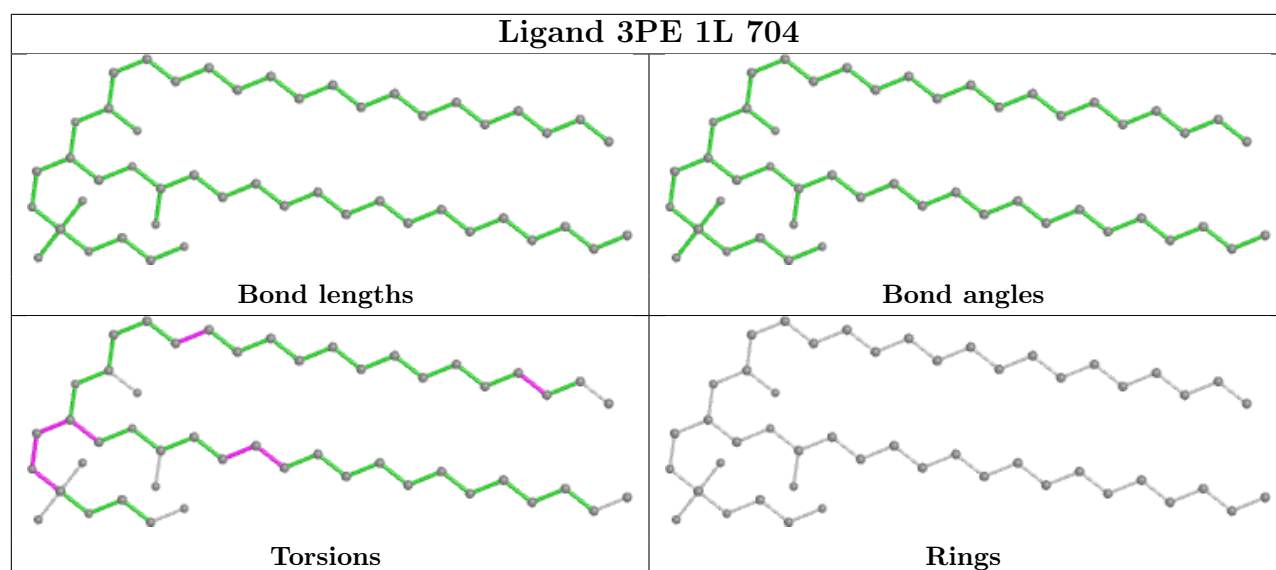


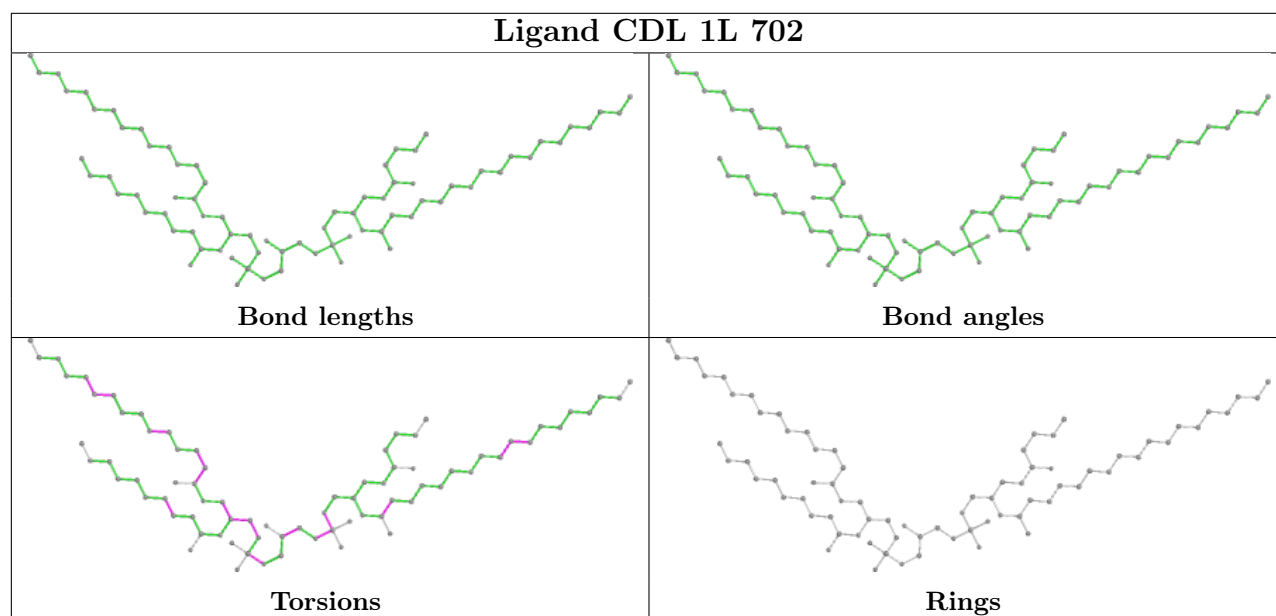
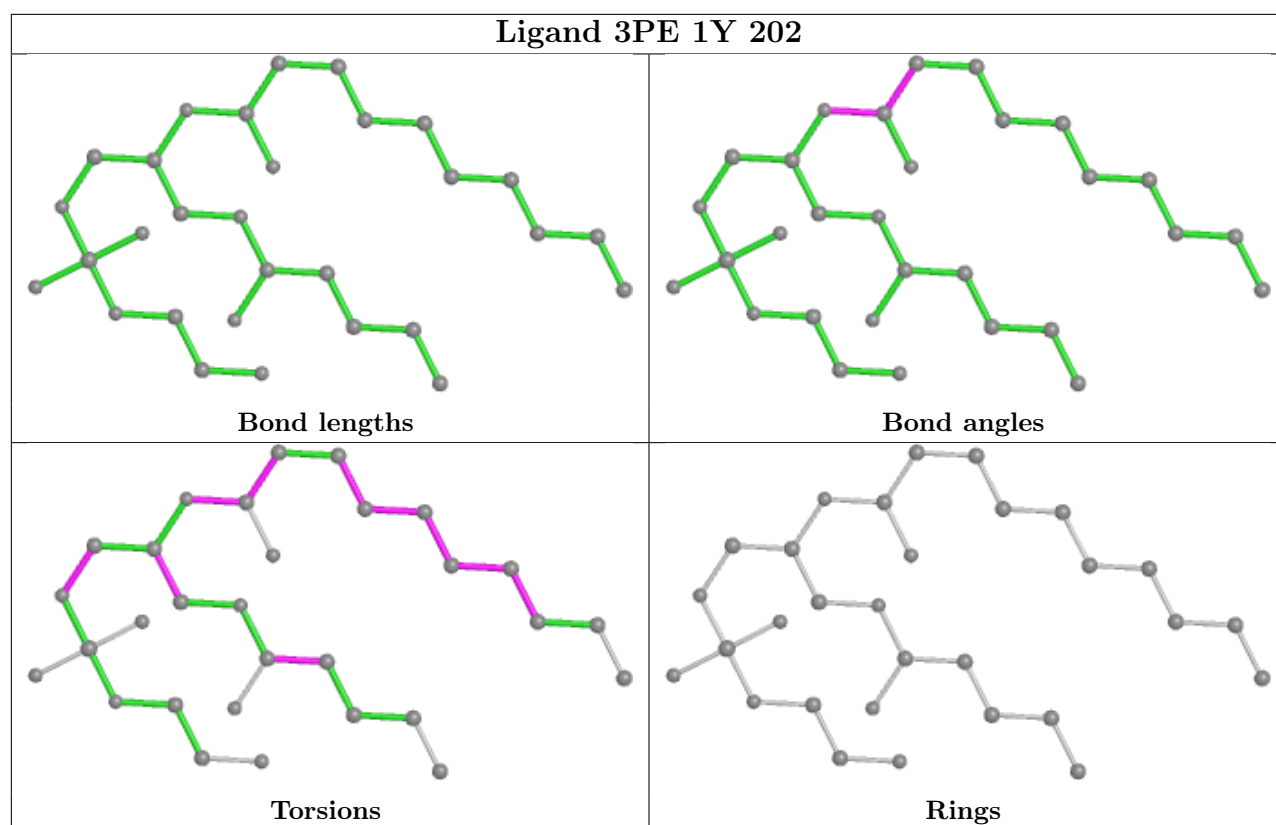
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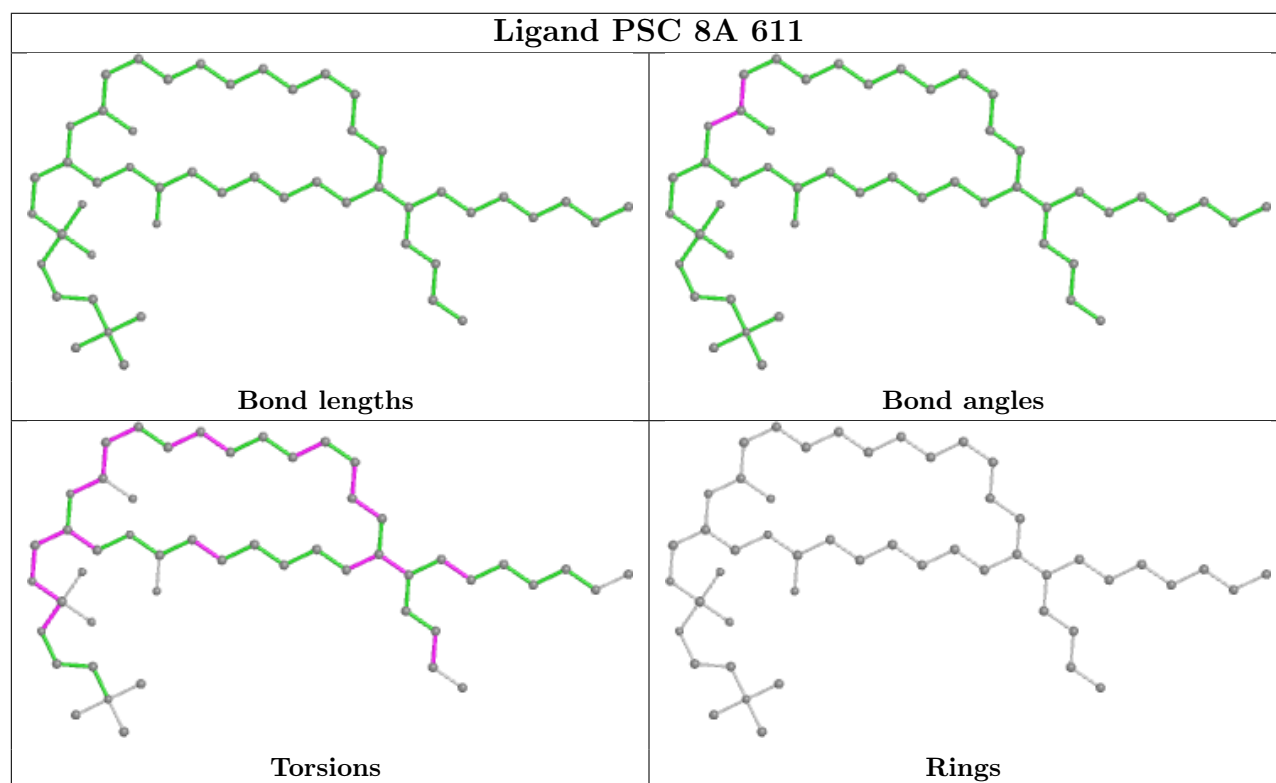
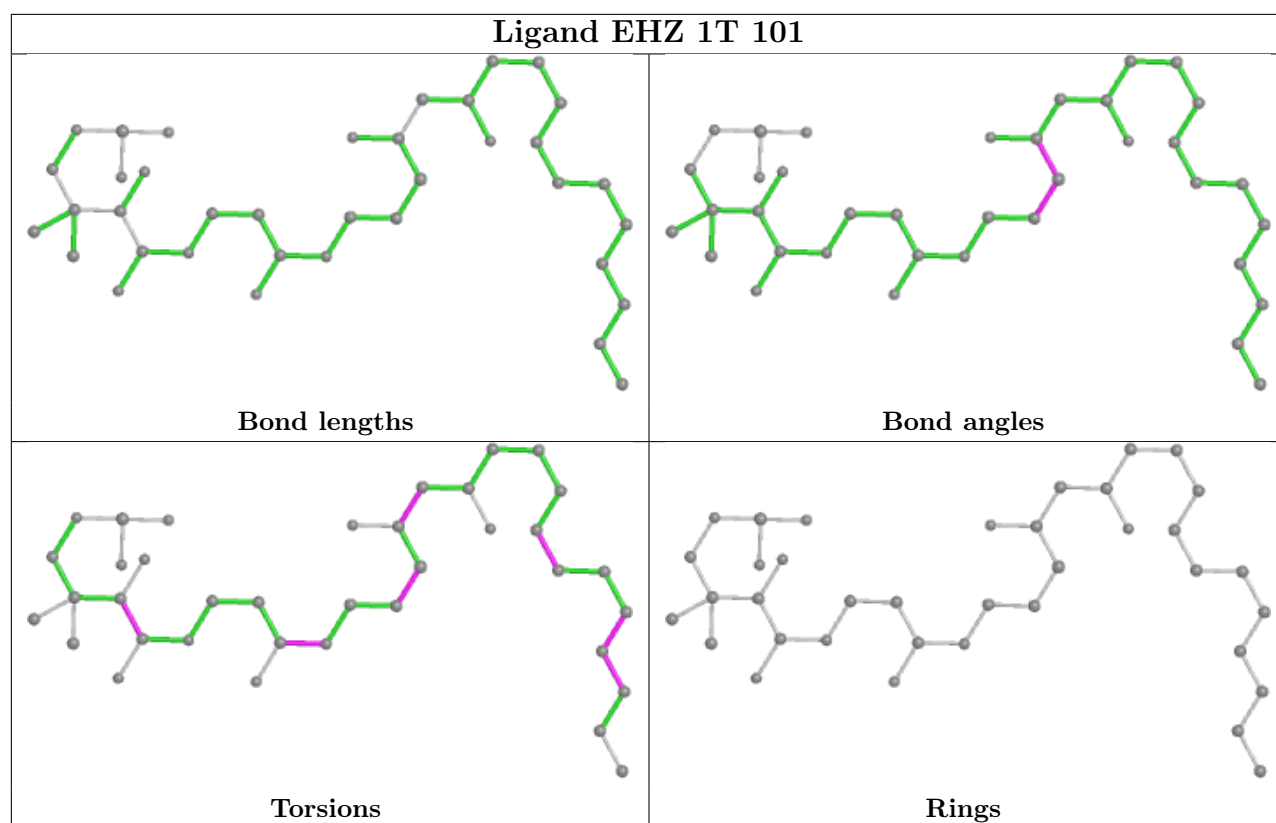


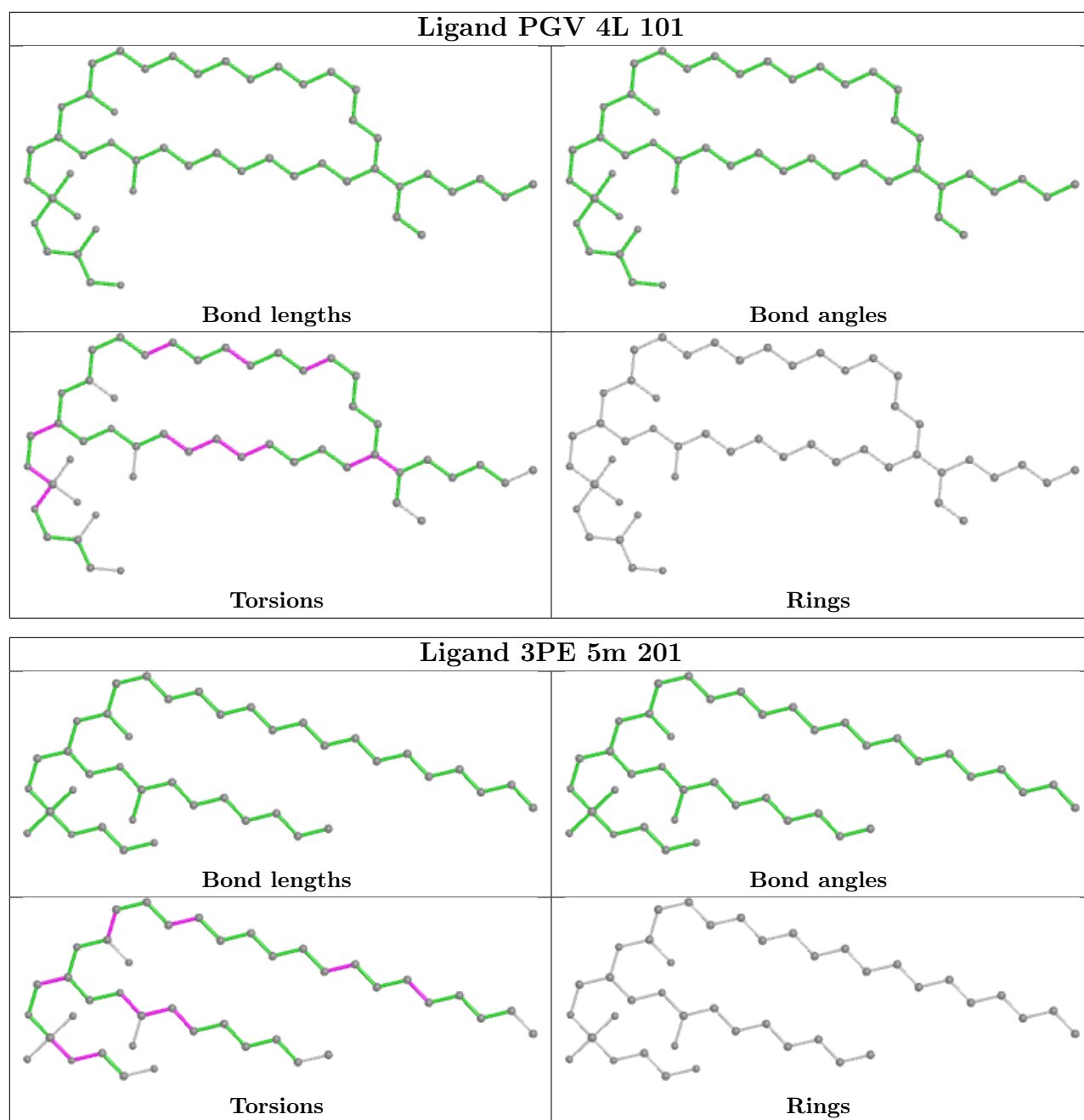
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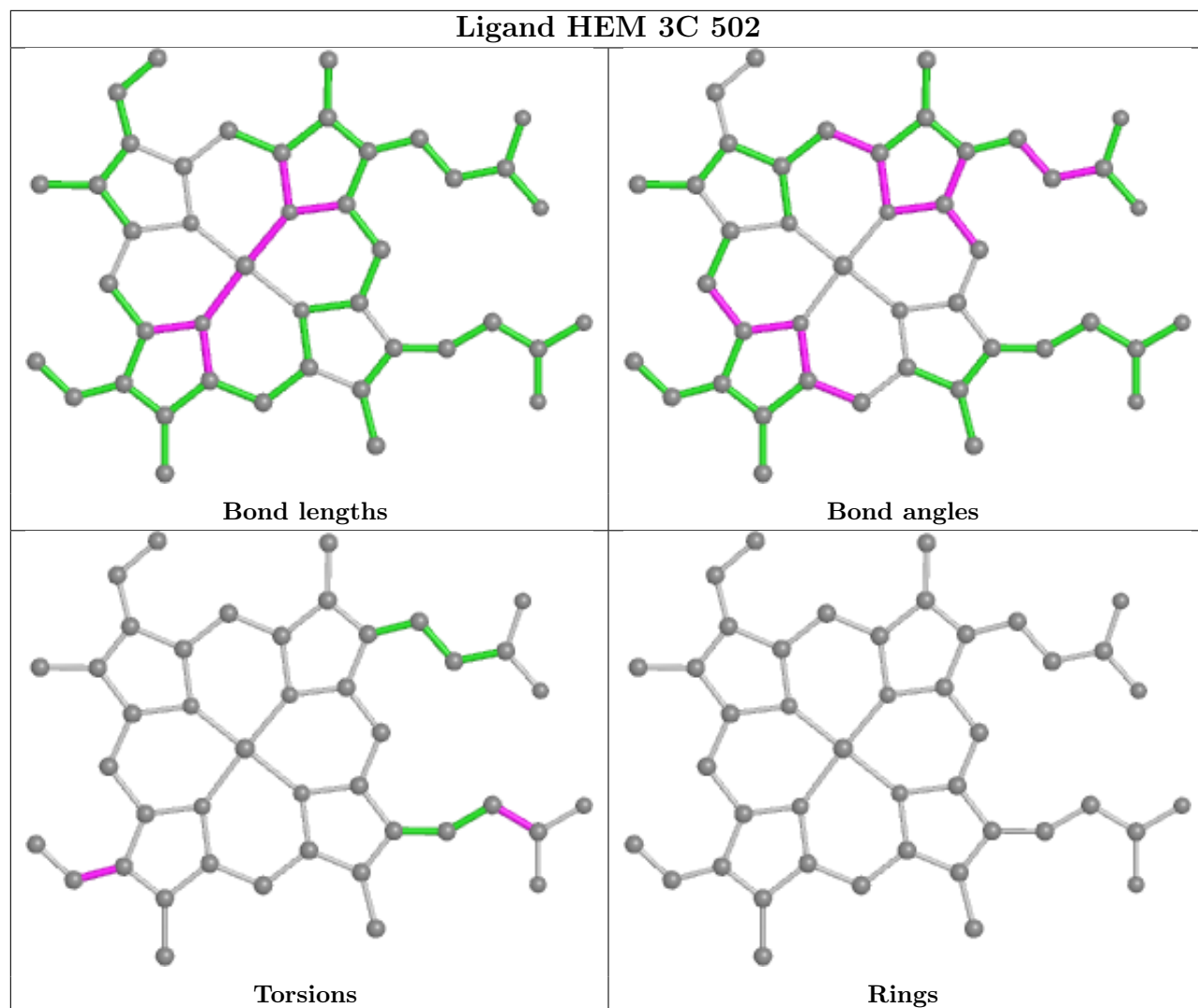


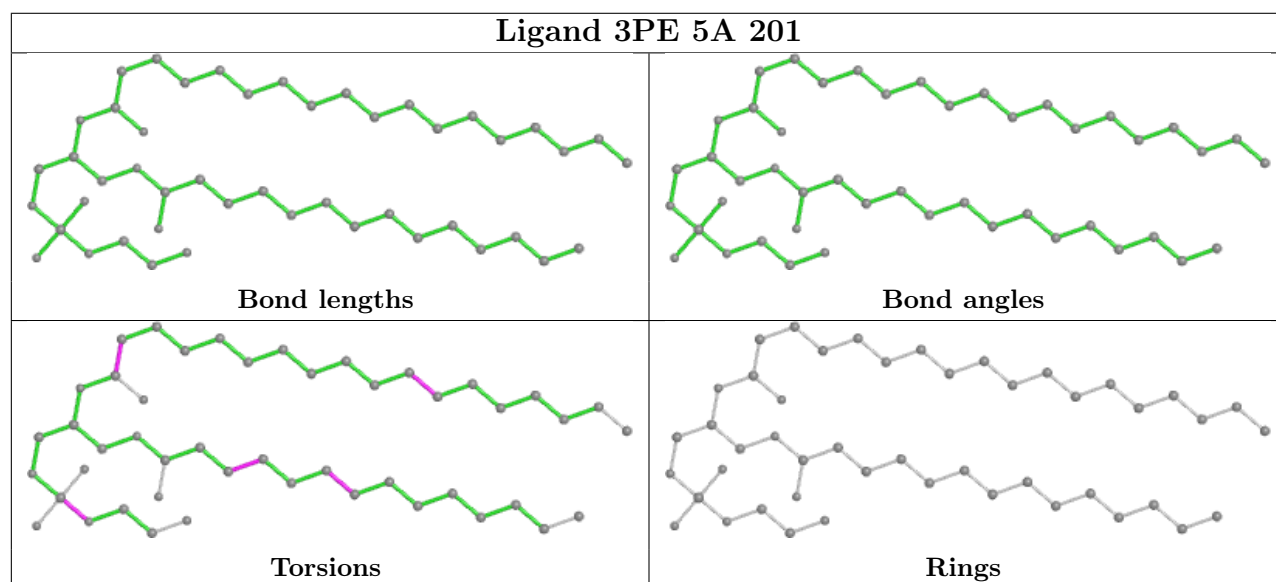
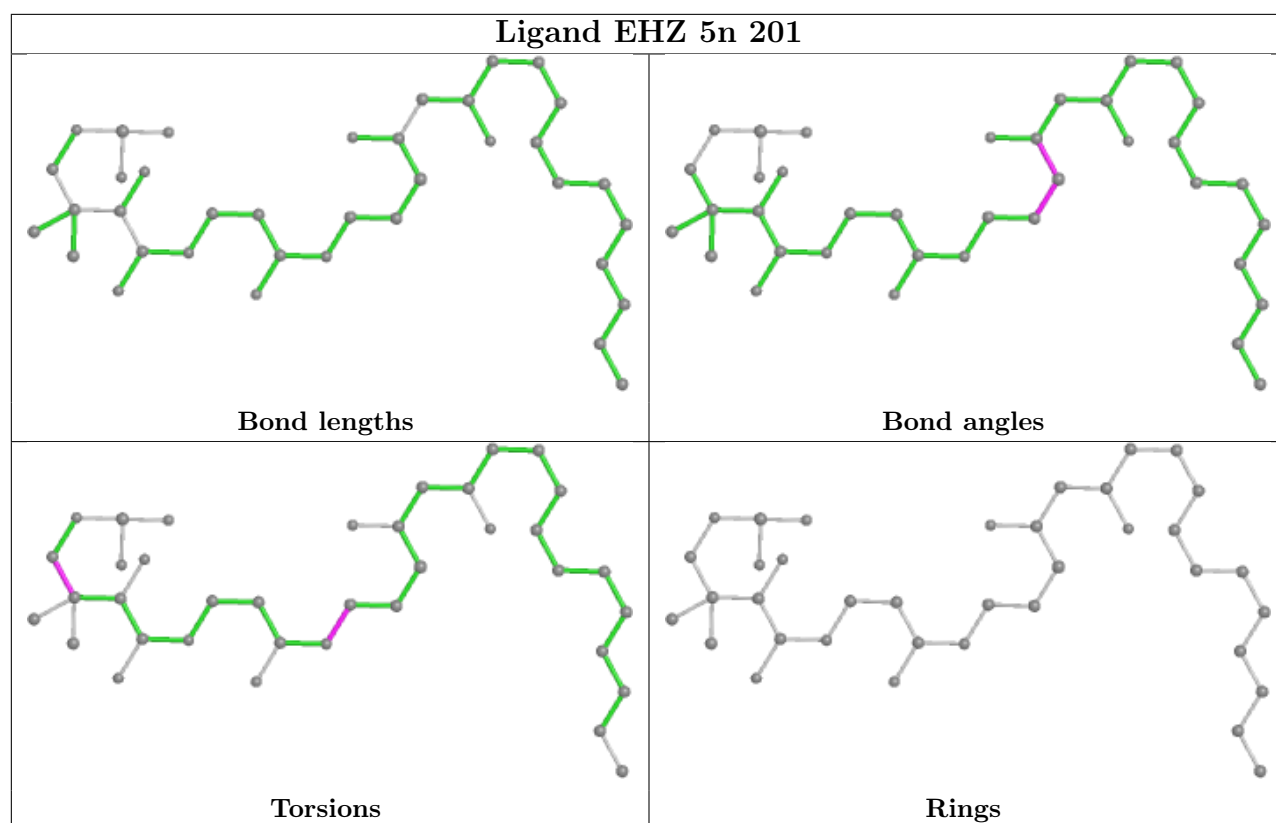


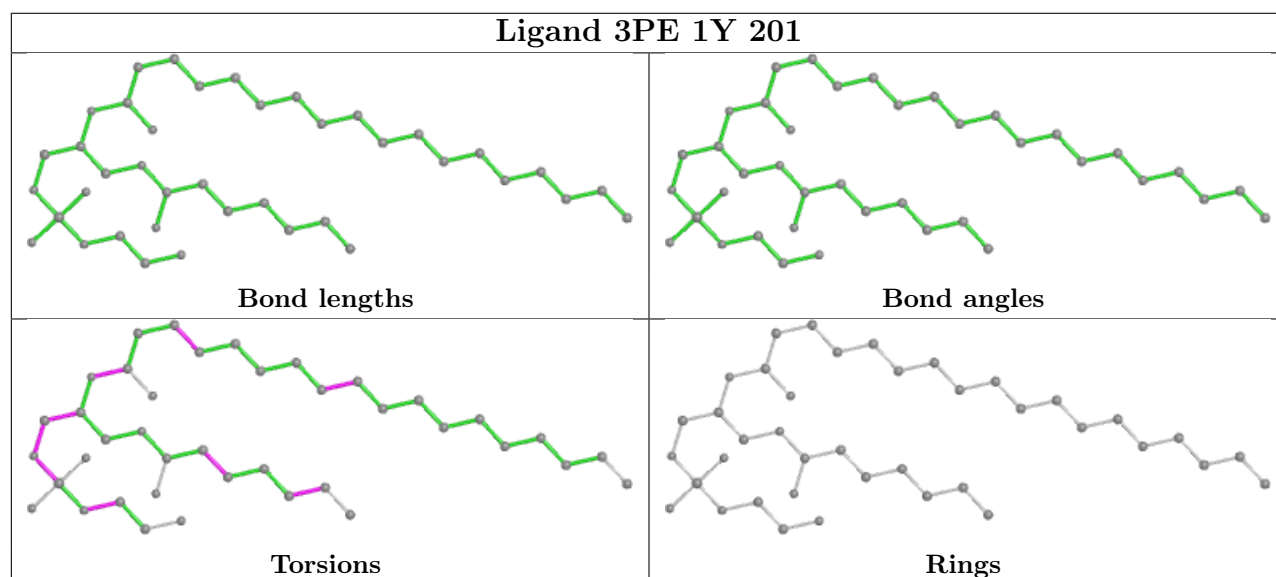
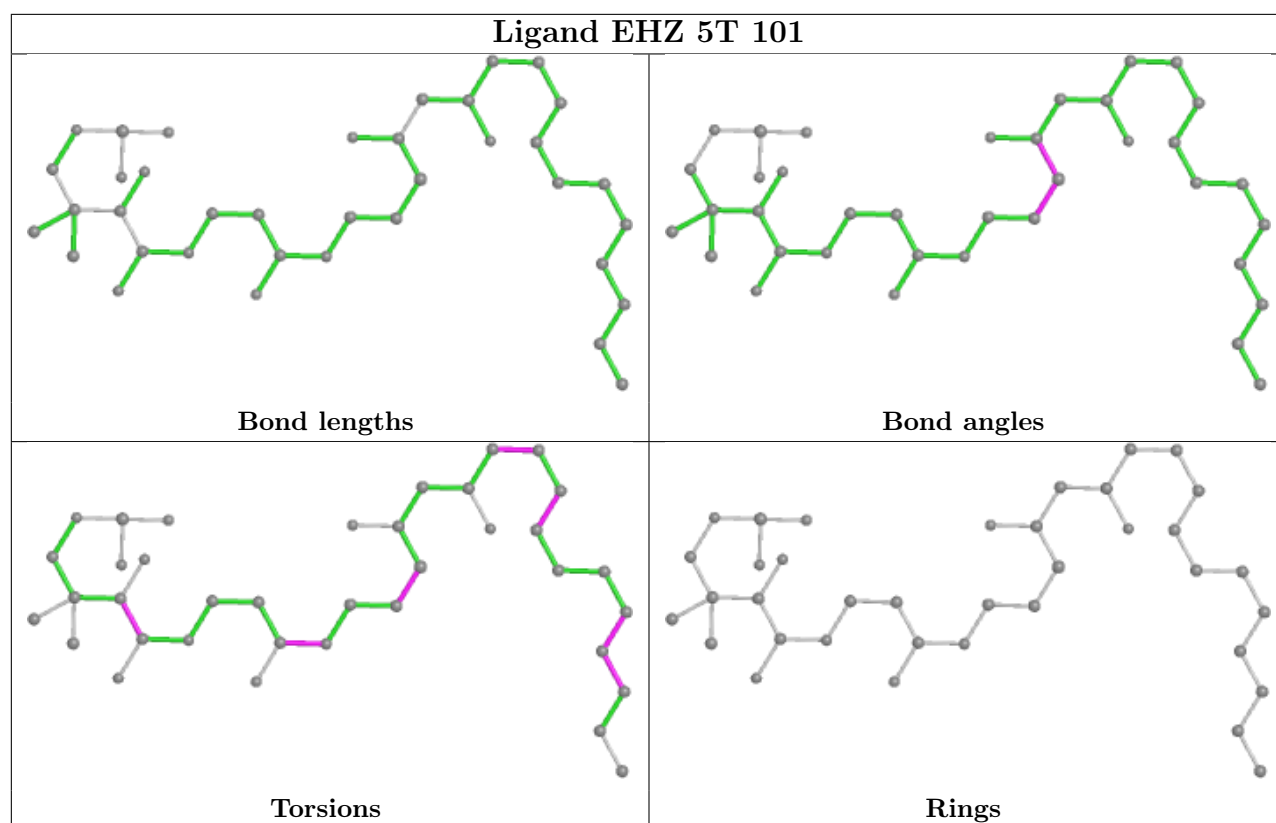


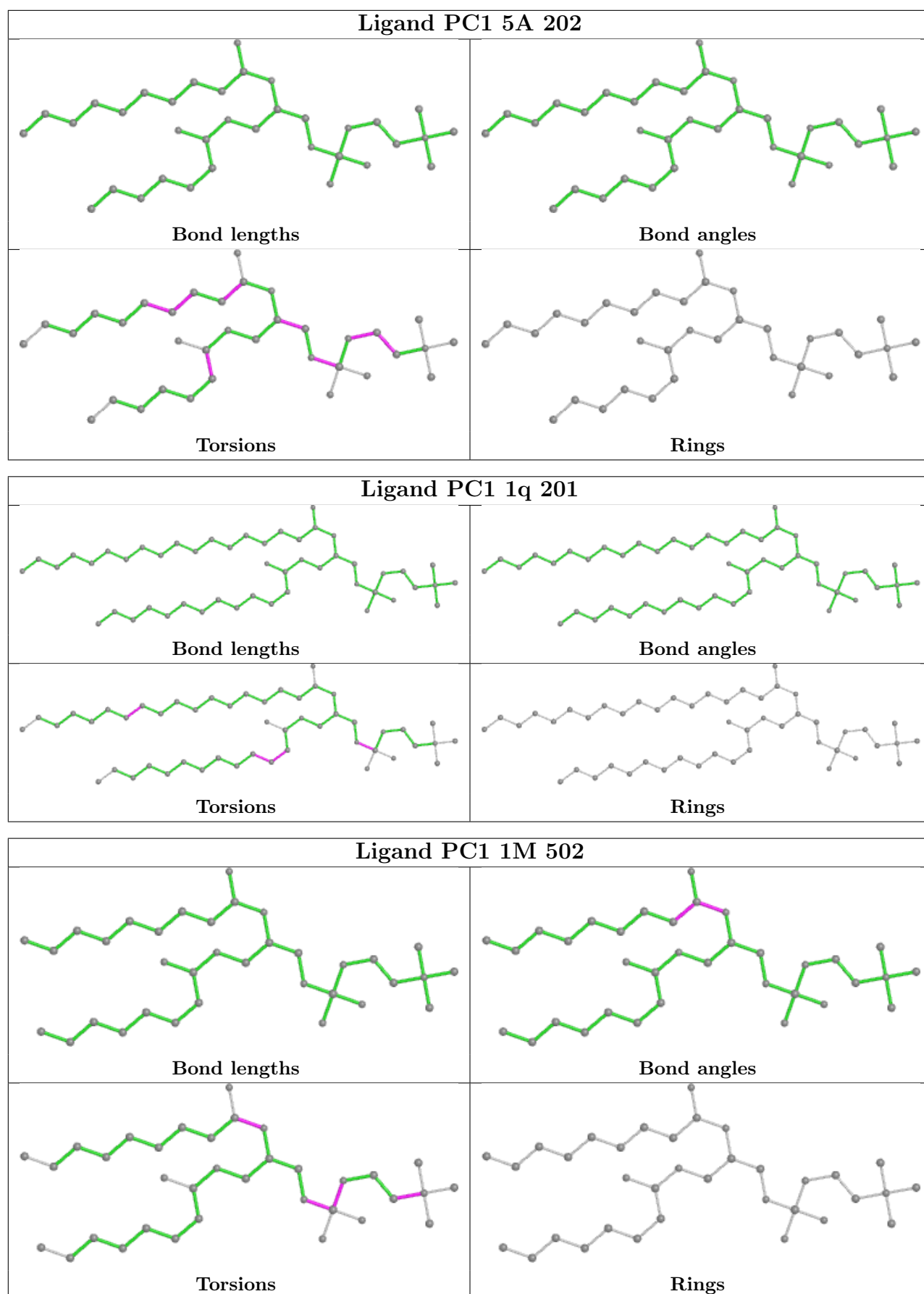


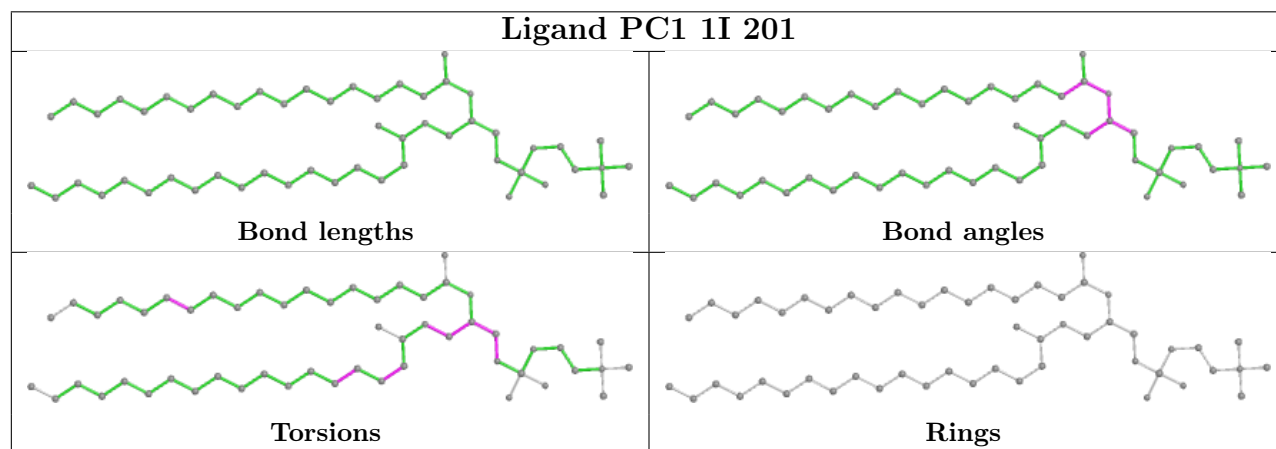
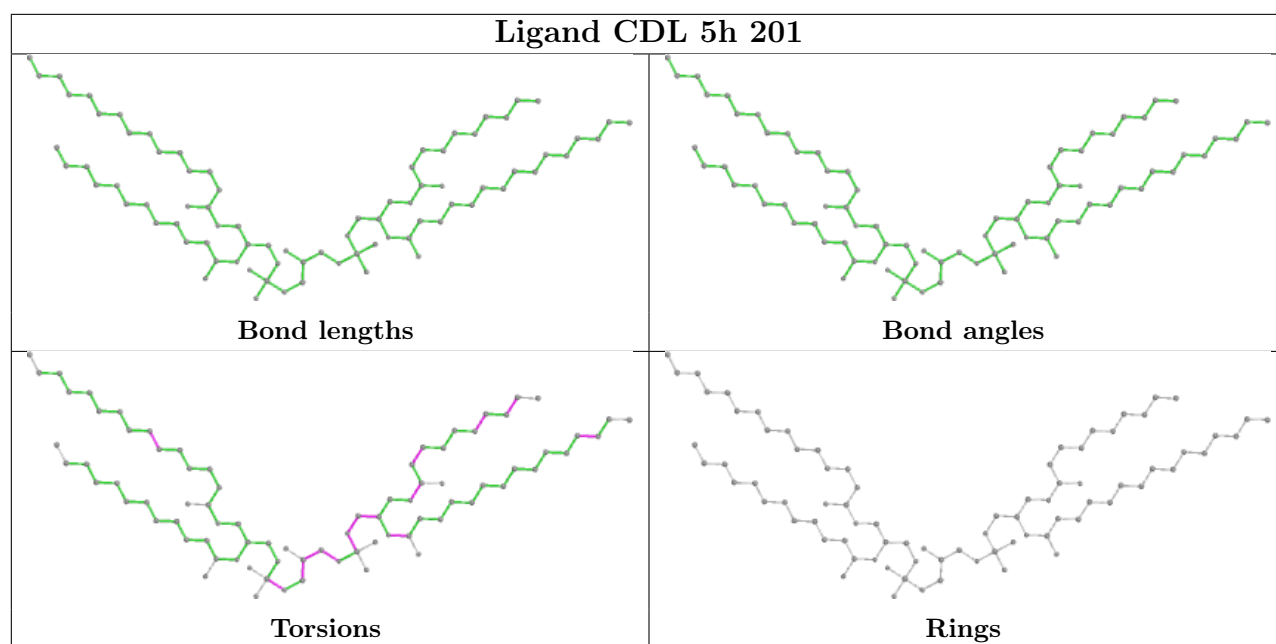


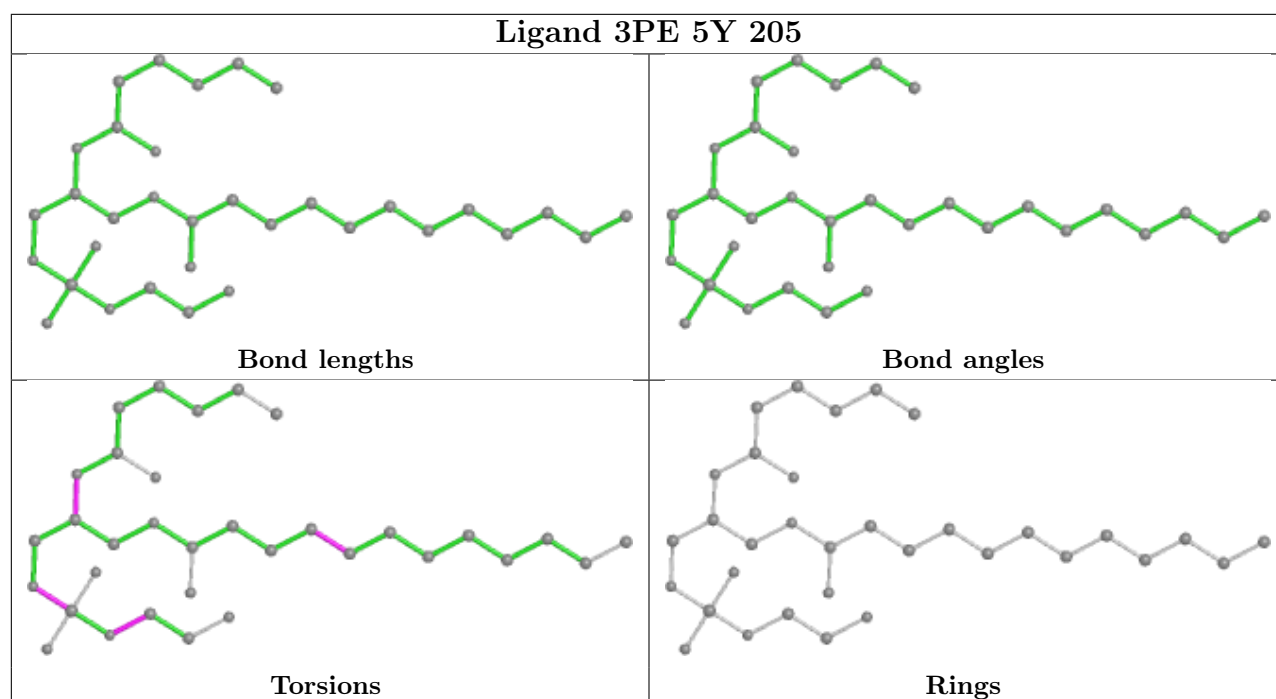
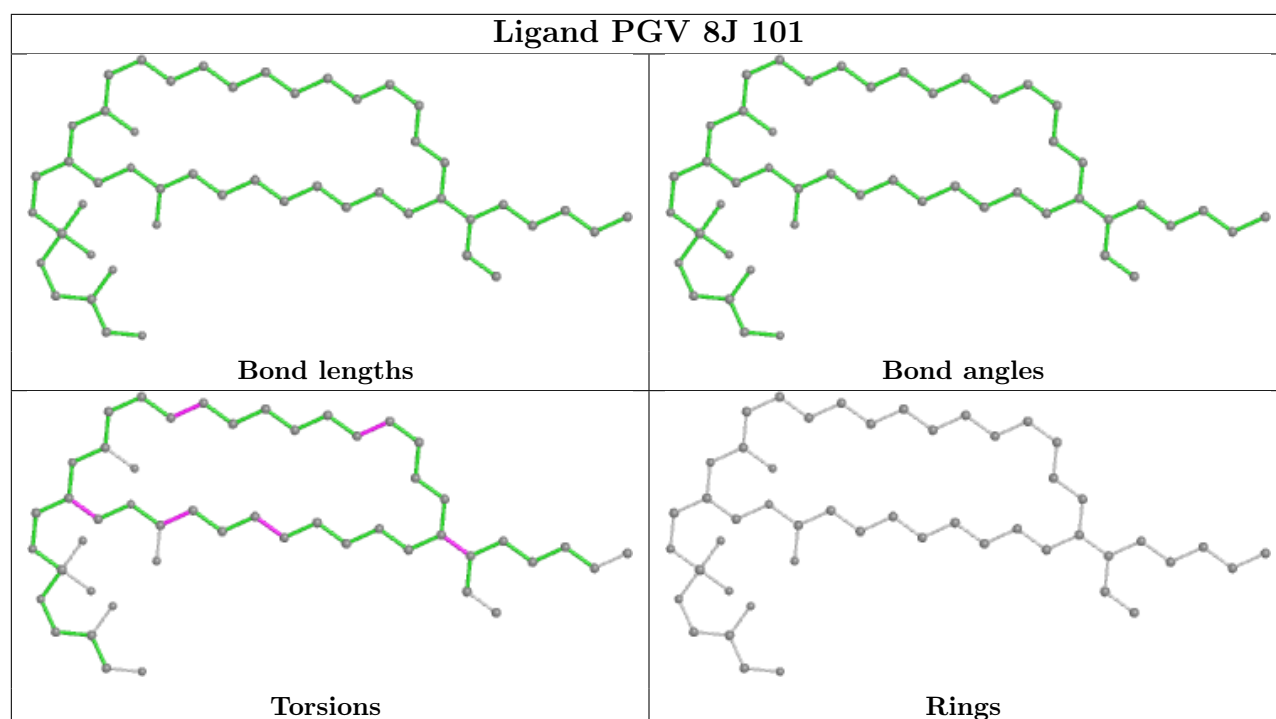


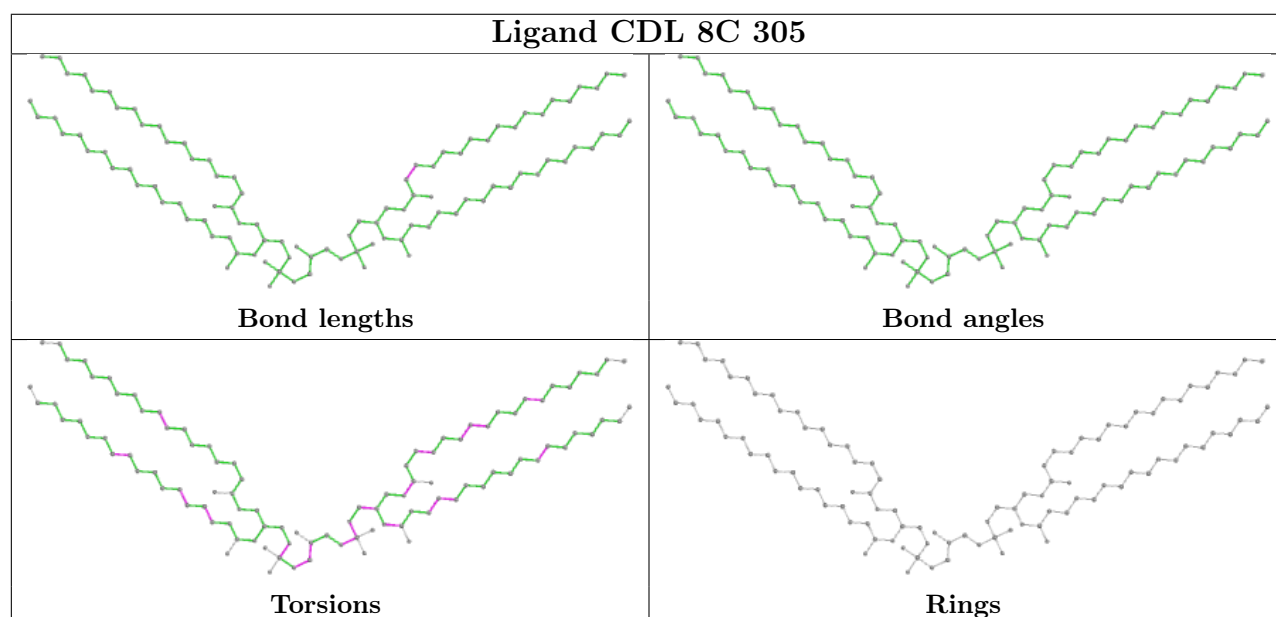
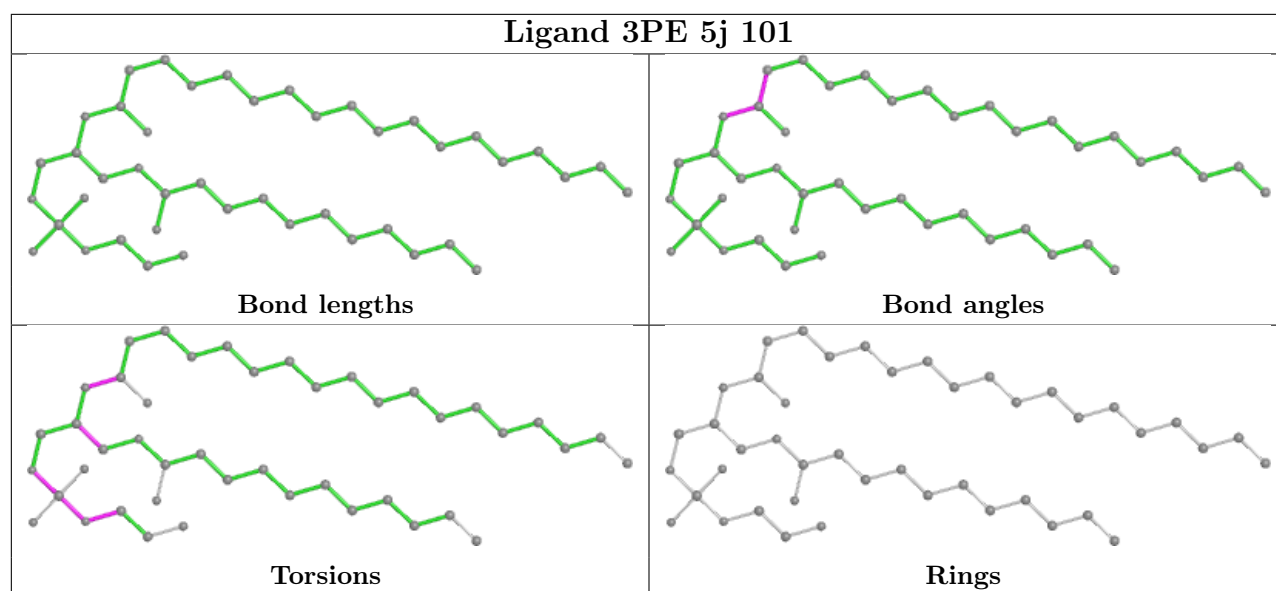


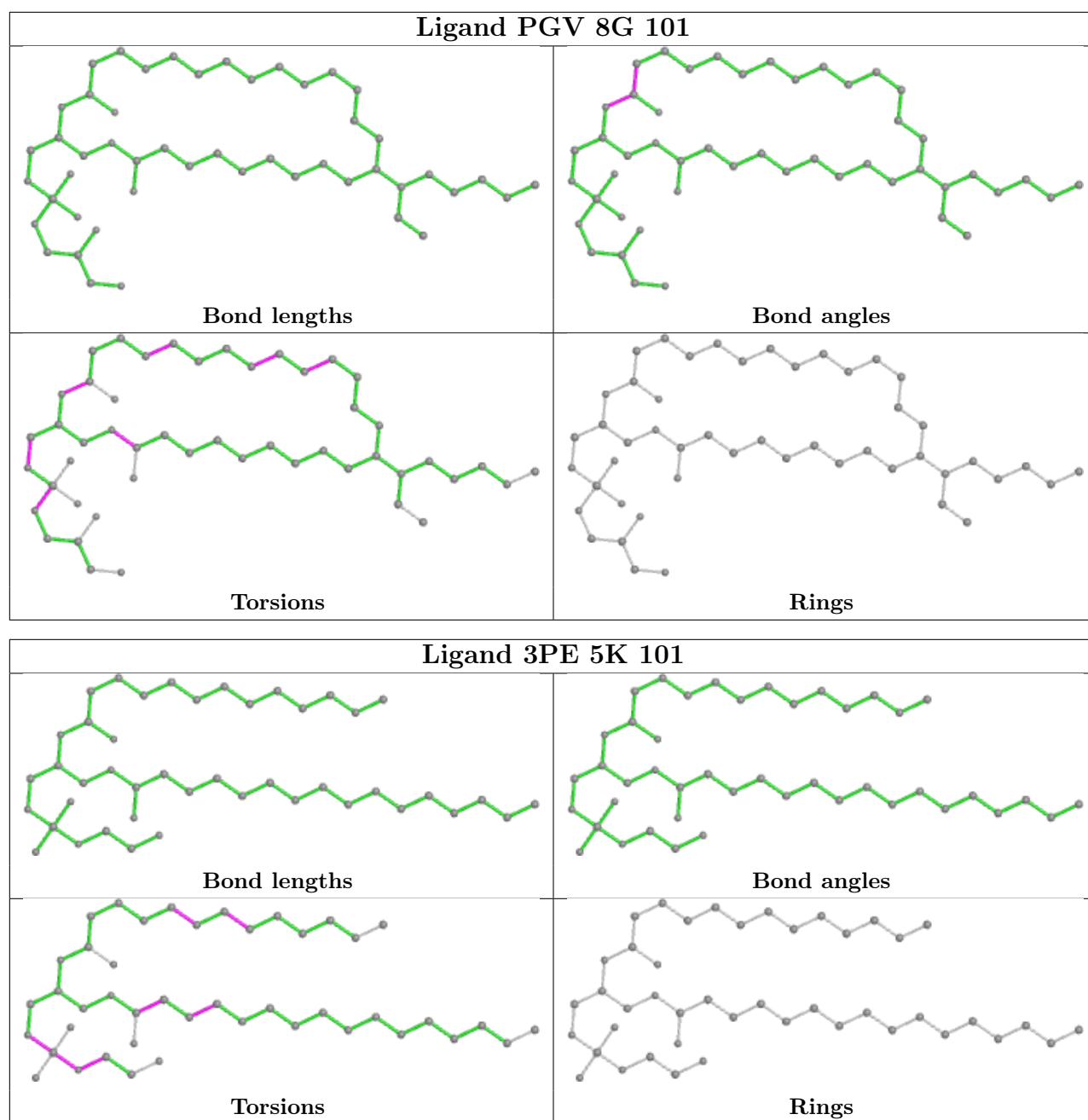


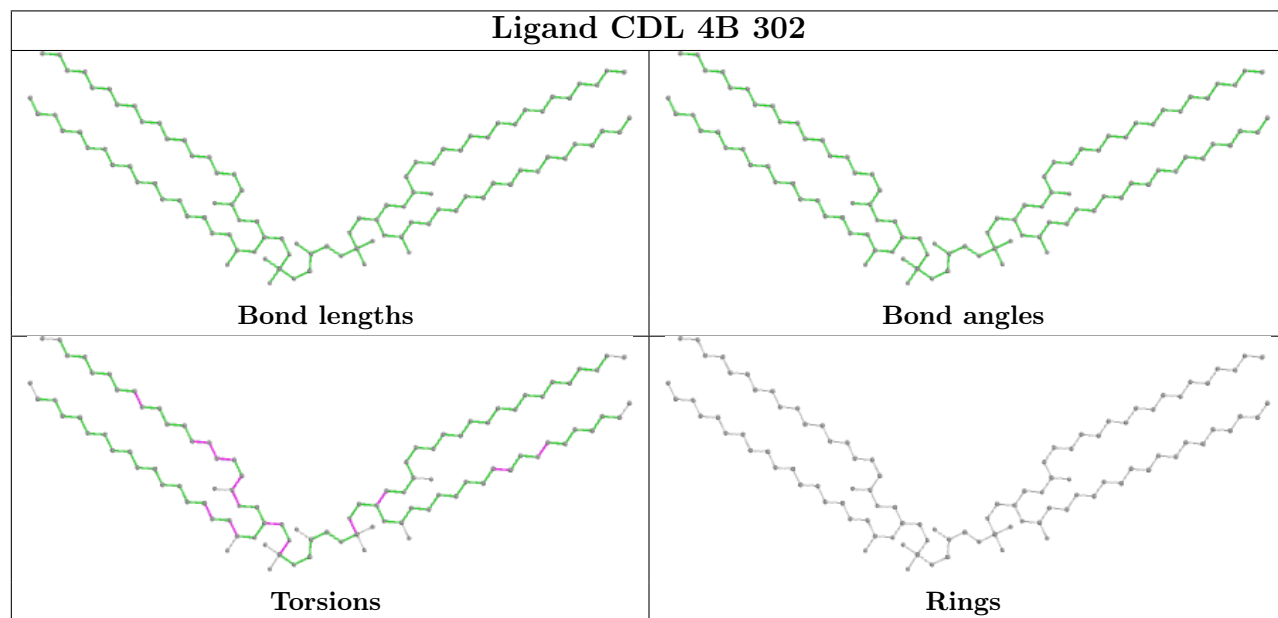
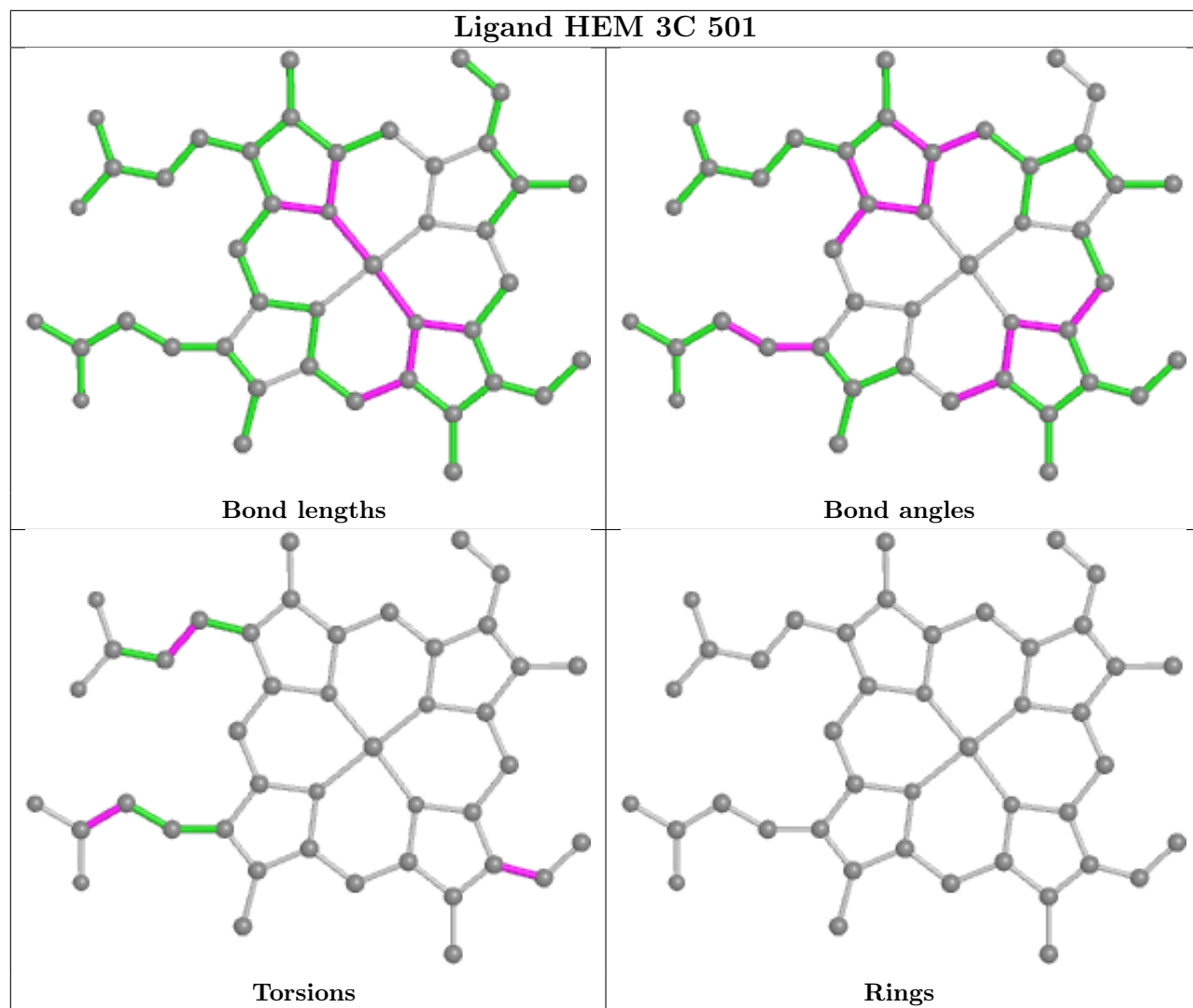


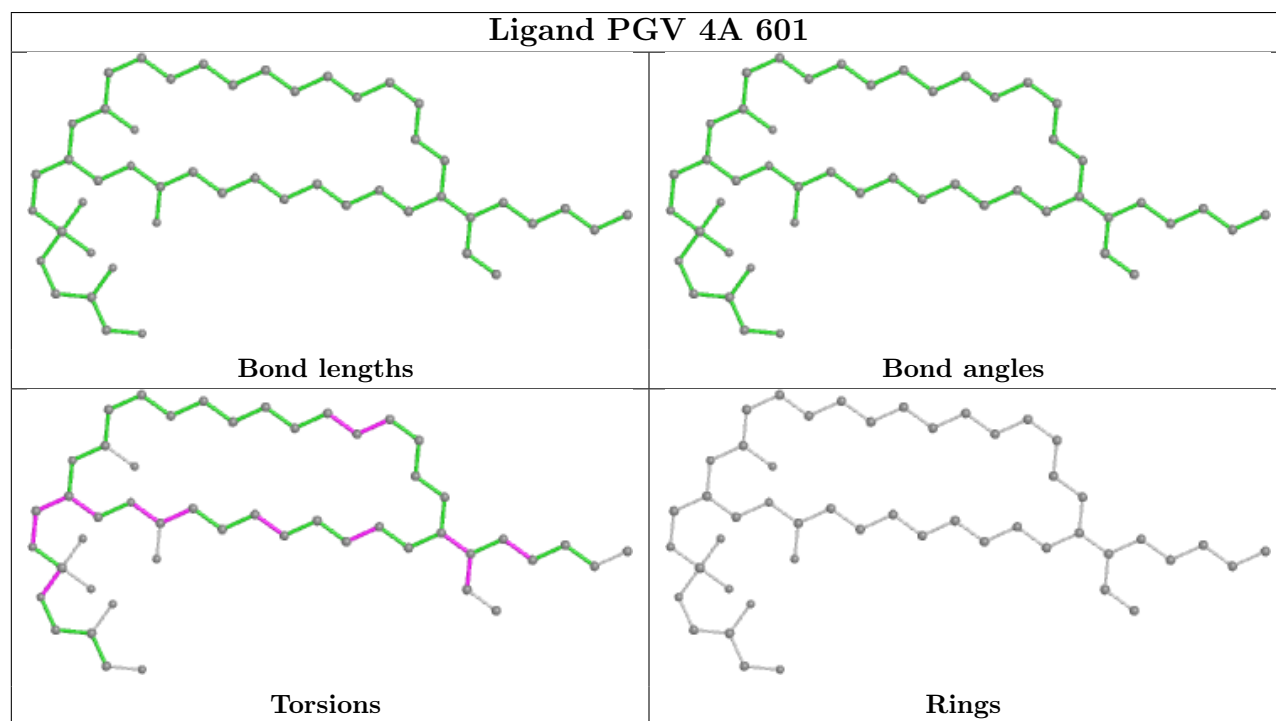
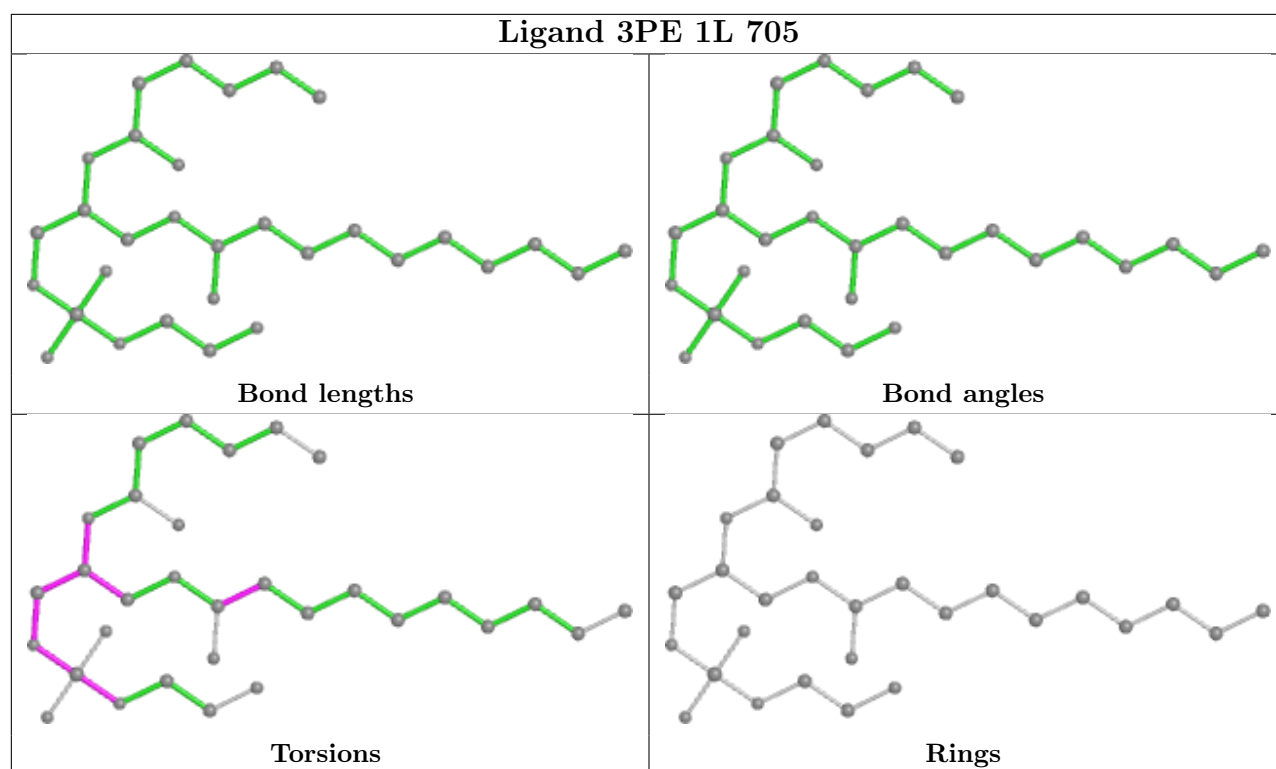


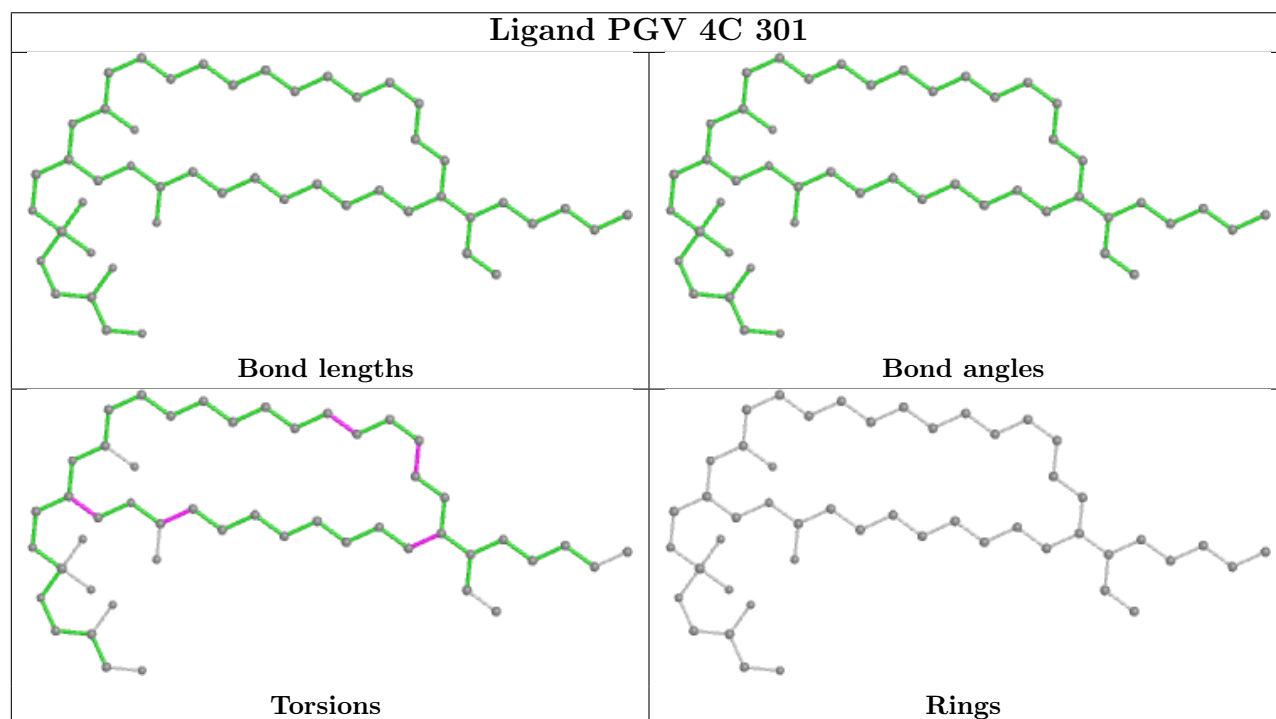
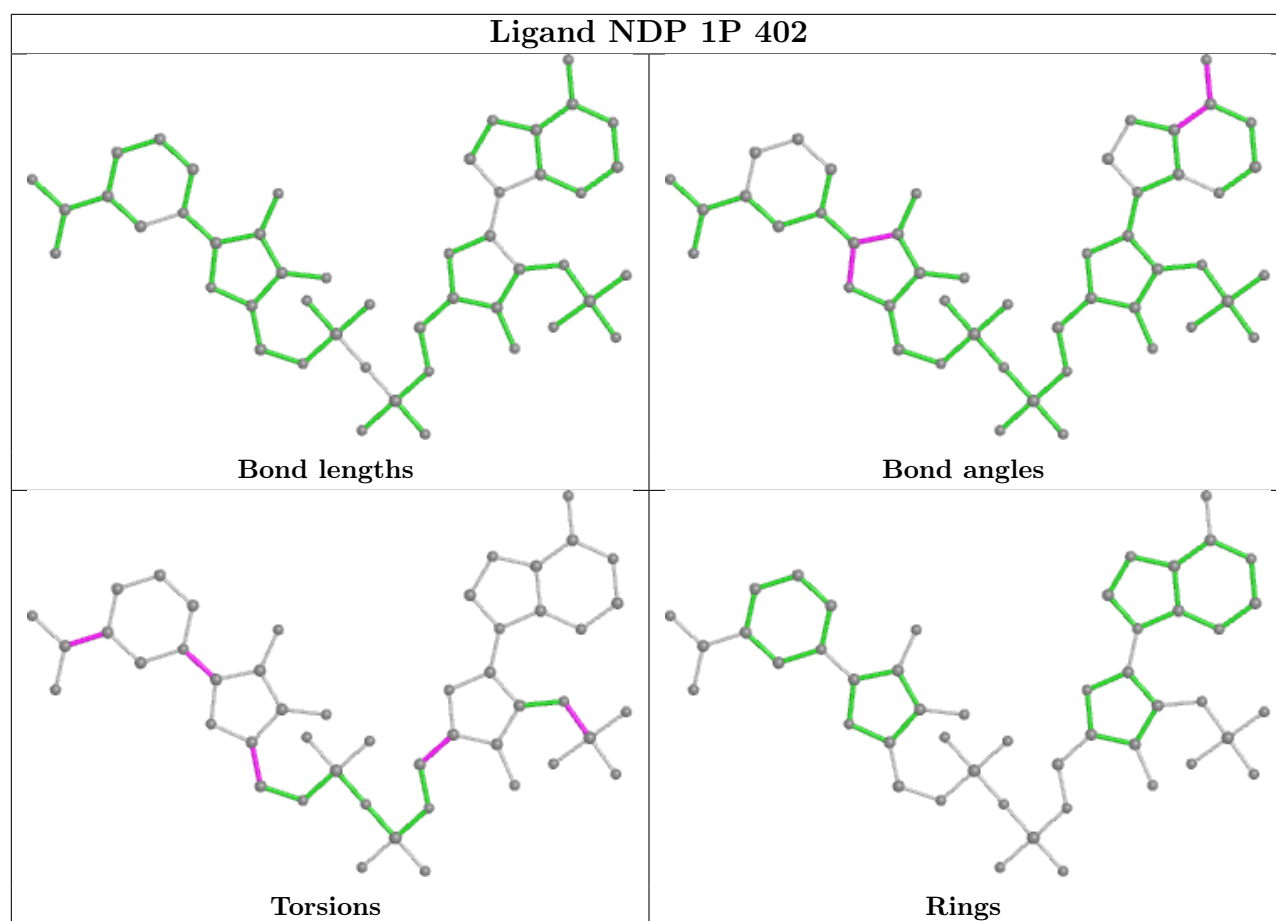


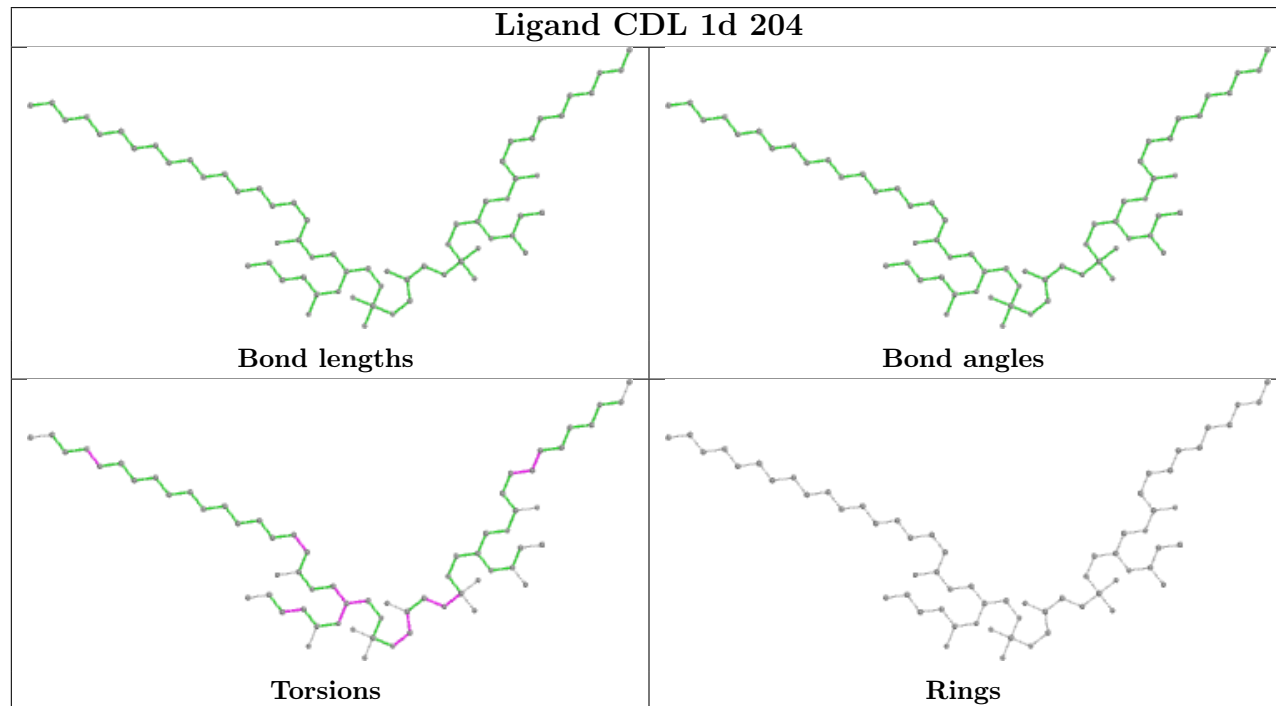
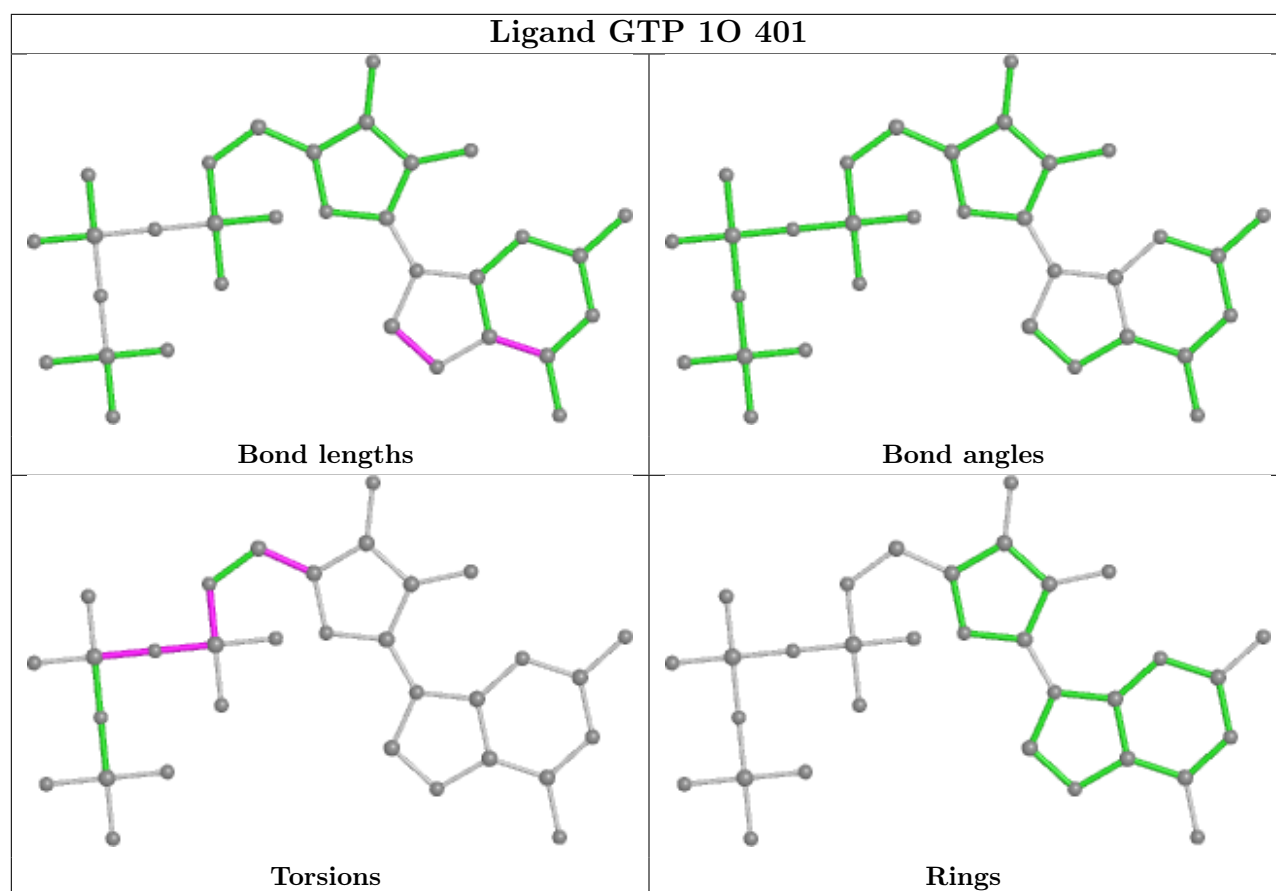


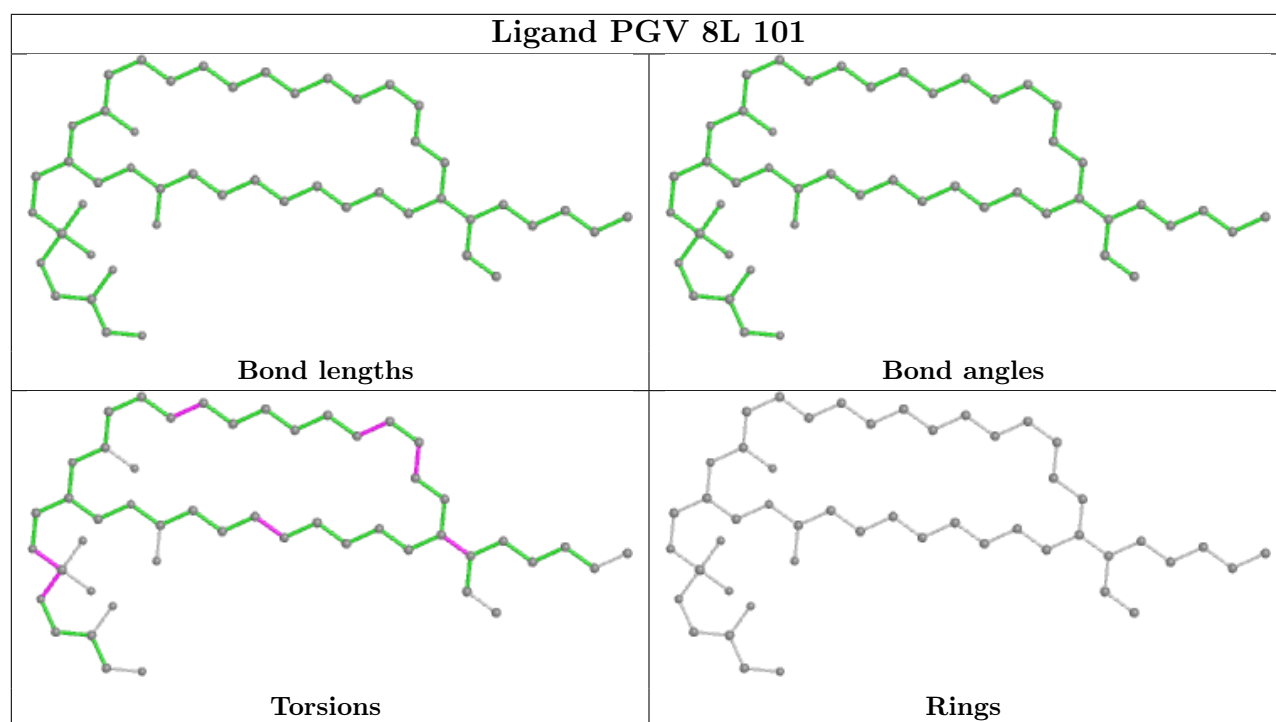


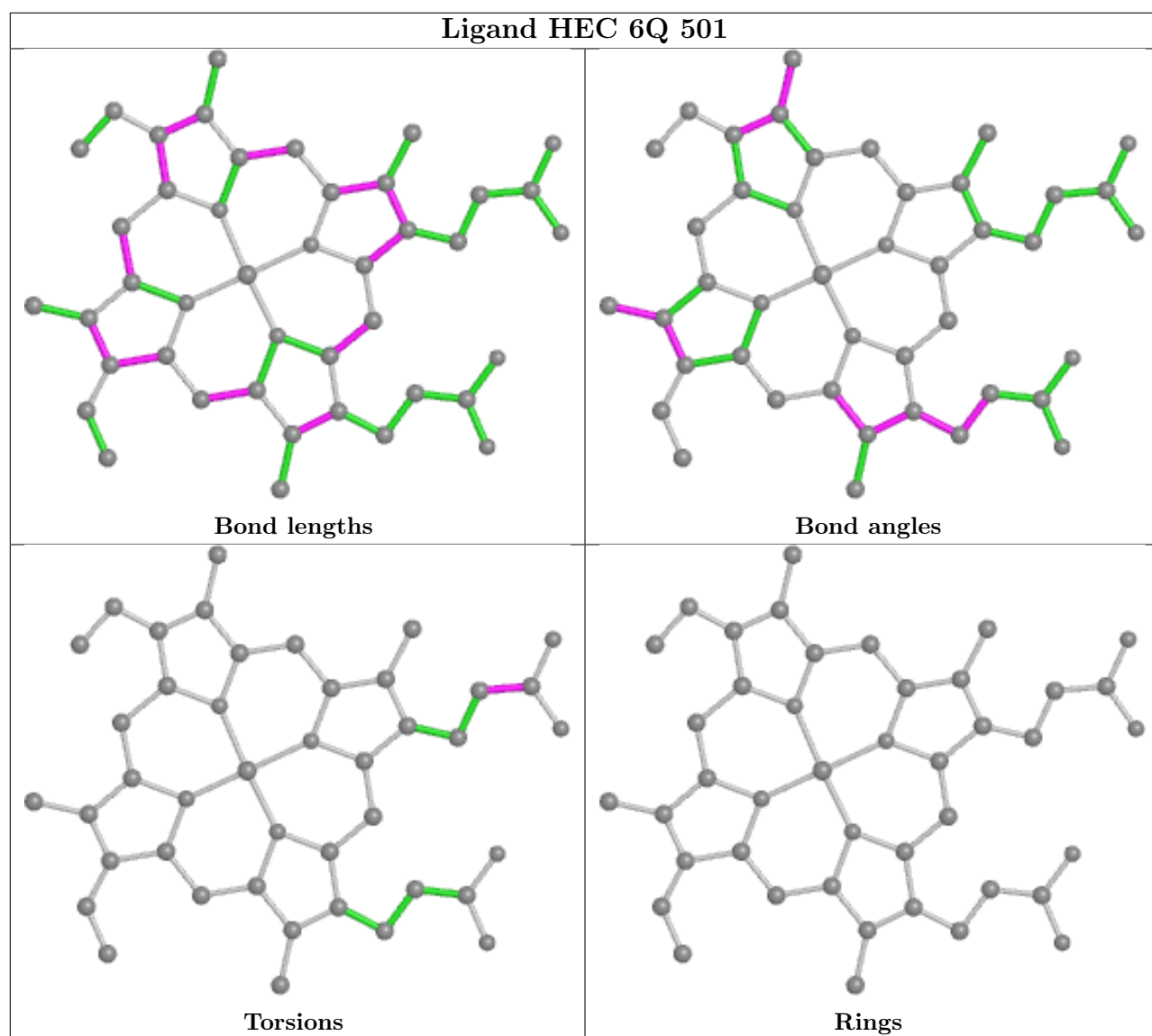




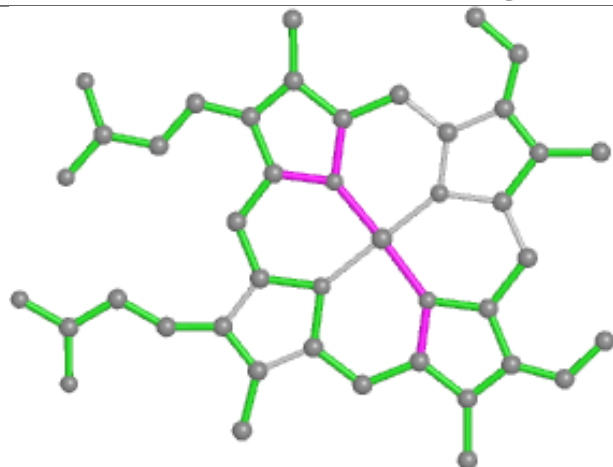




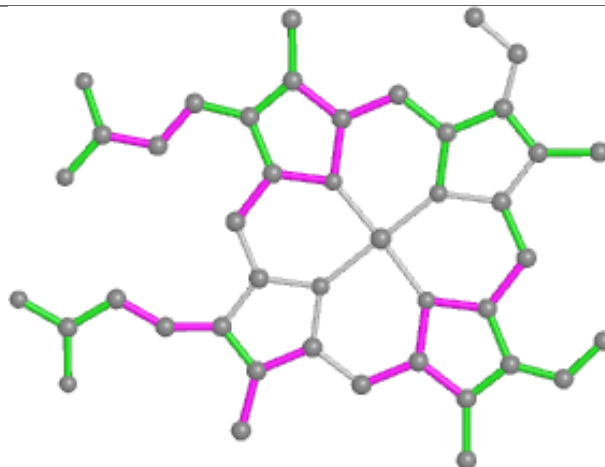




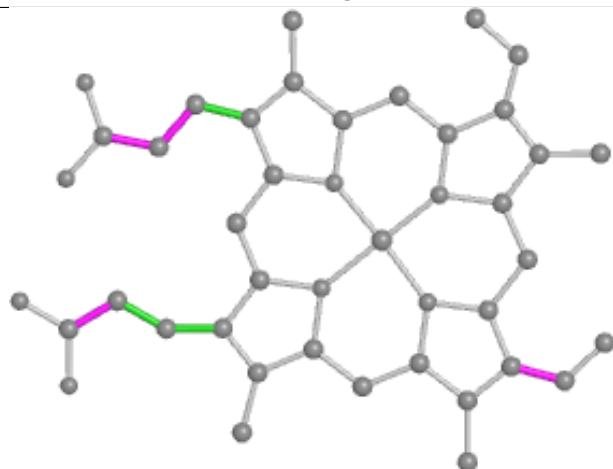
Ligand HEM 3P 501



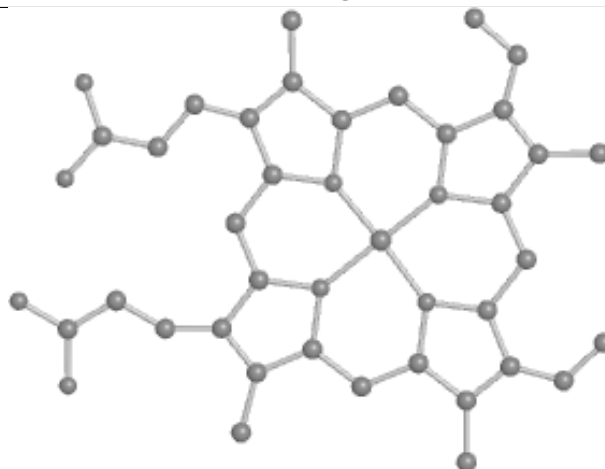
Bond lengths



Bond angles

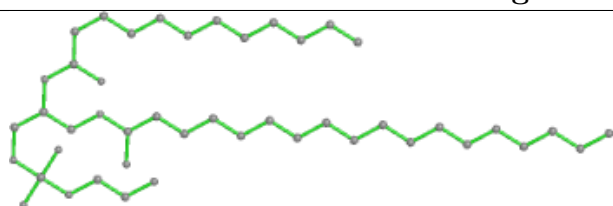


Torsions

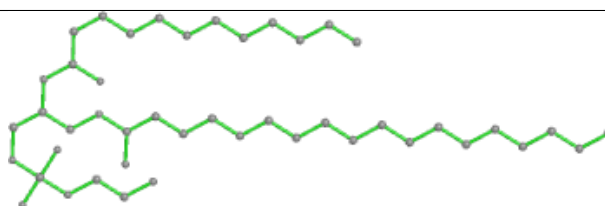


Rings

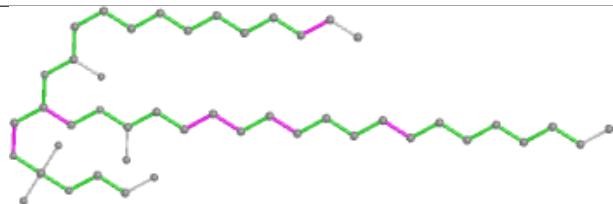
Ligand 3PE 1L 703



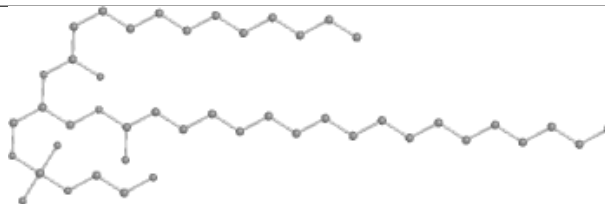
Bond lengths



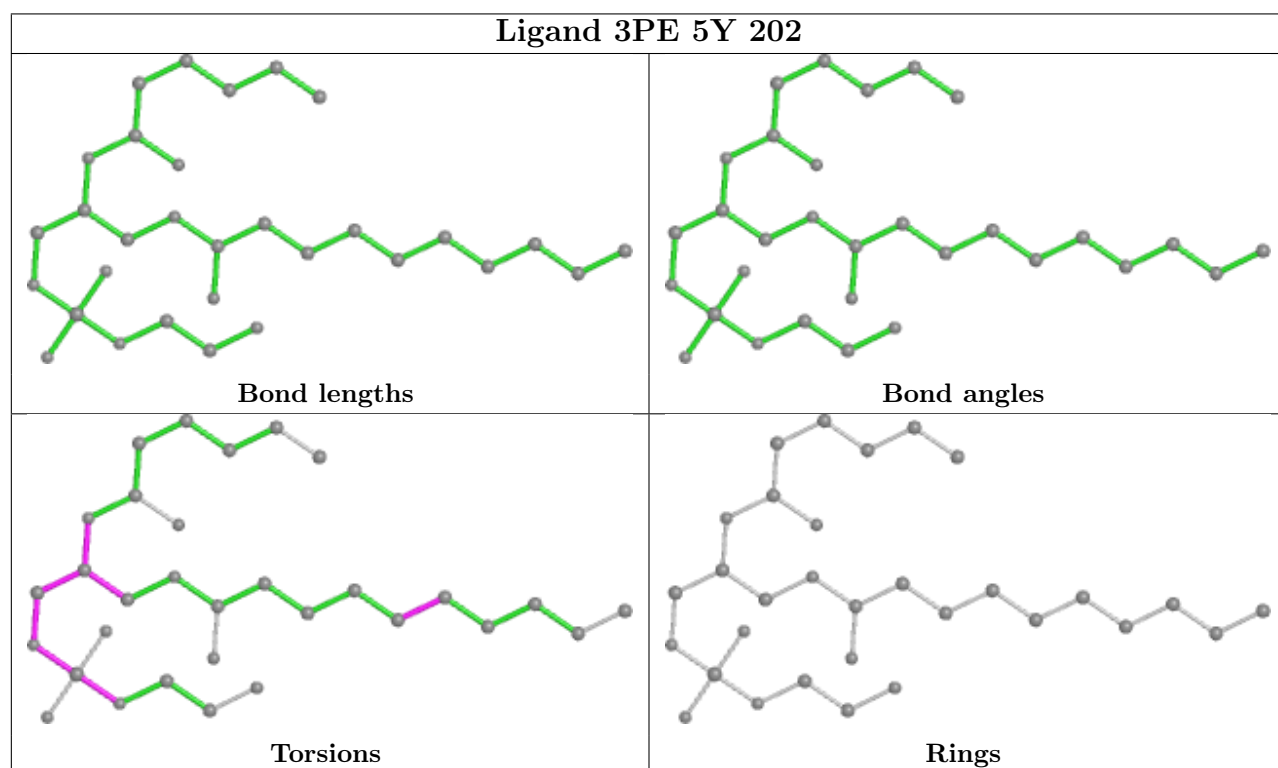
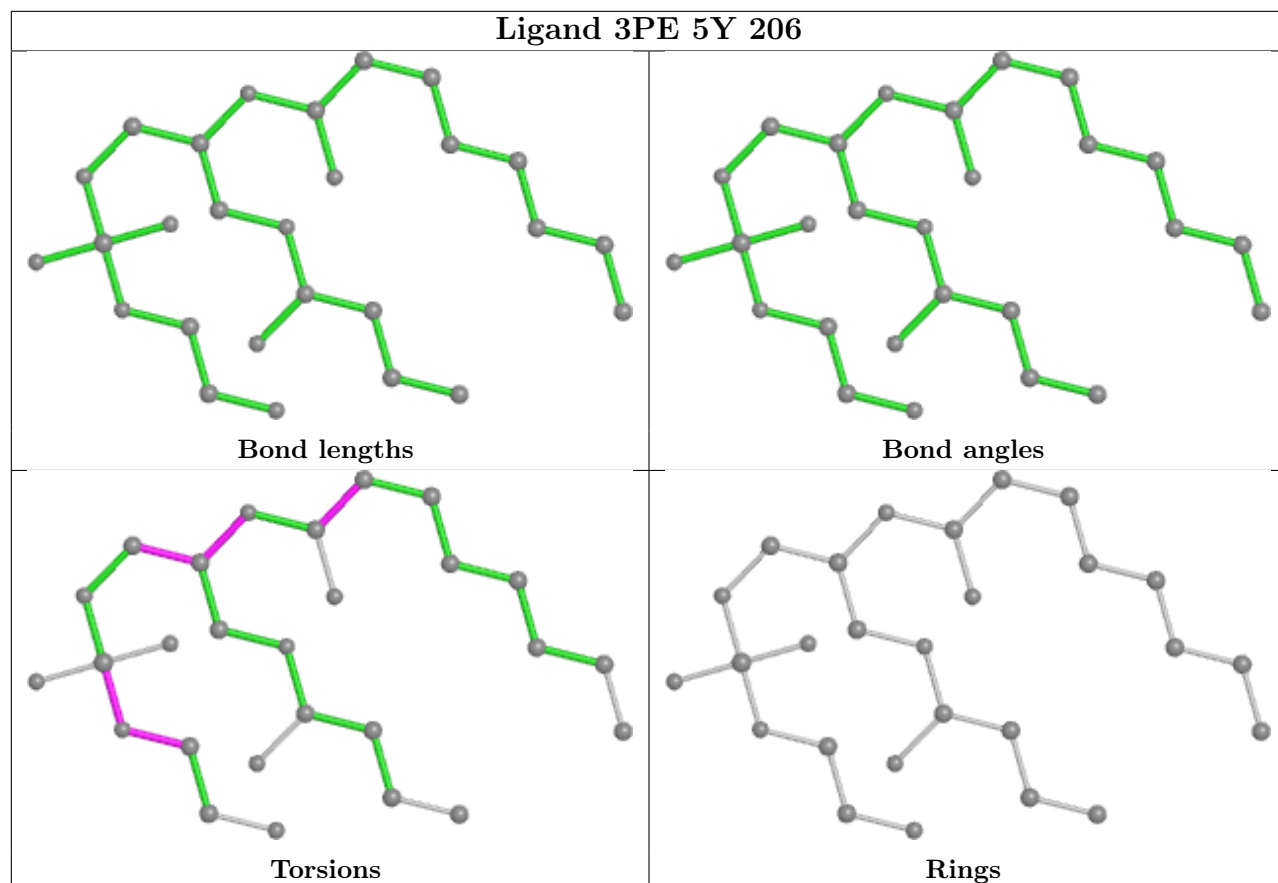
Bond angles

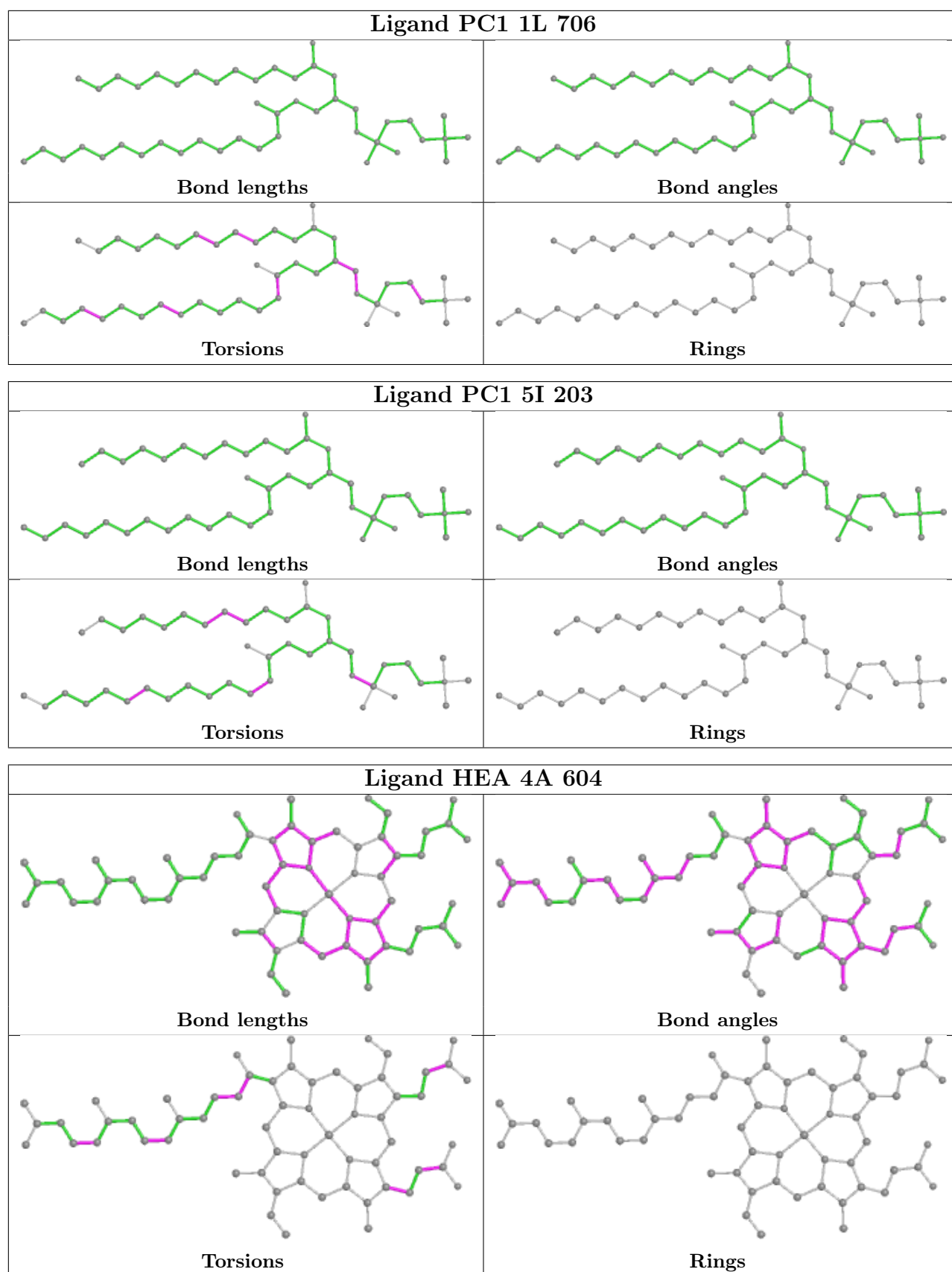


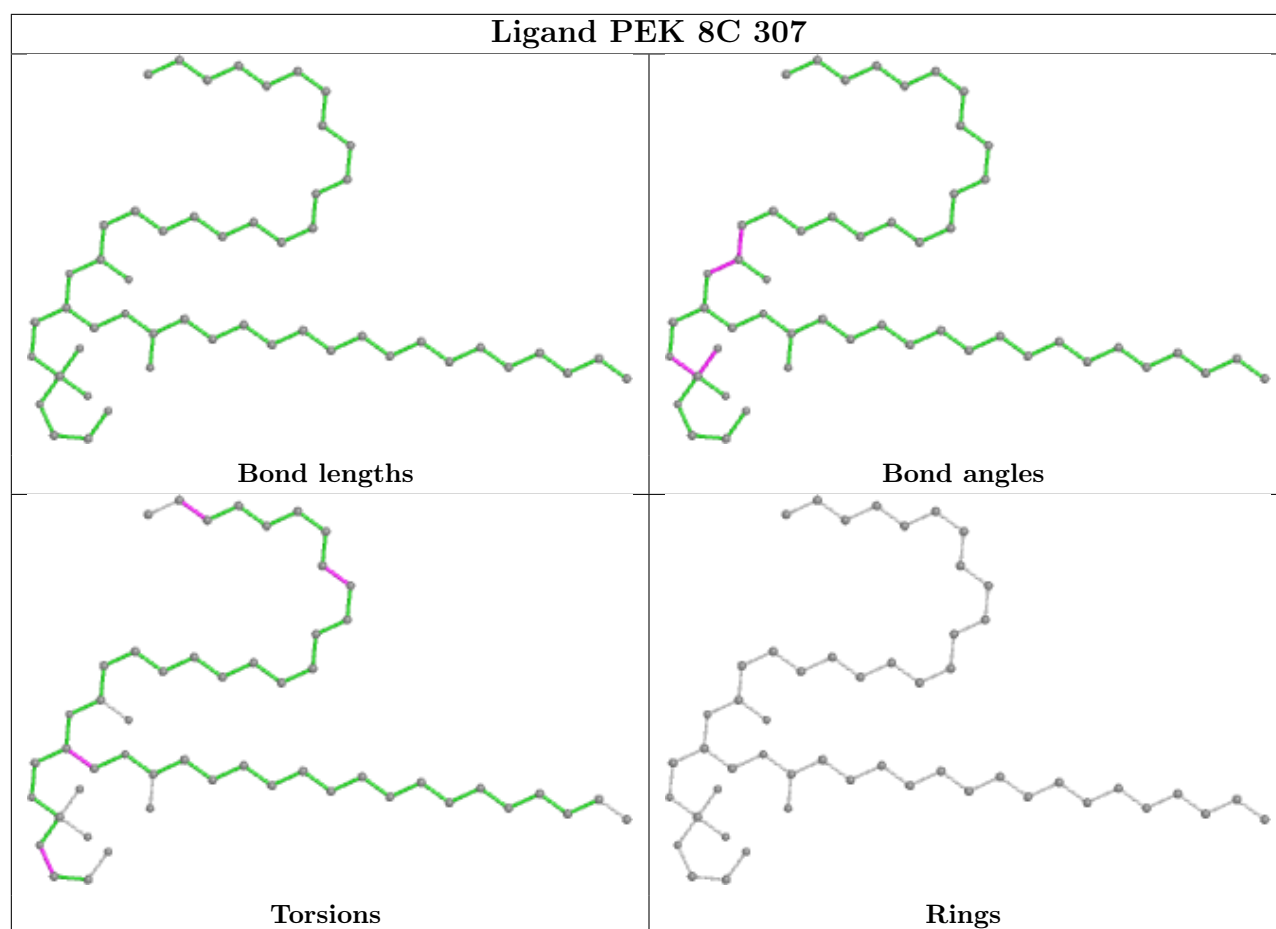
Torsions

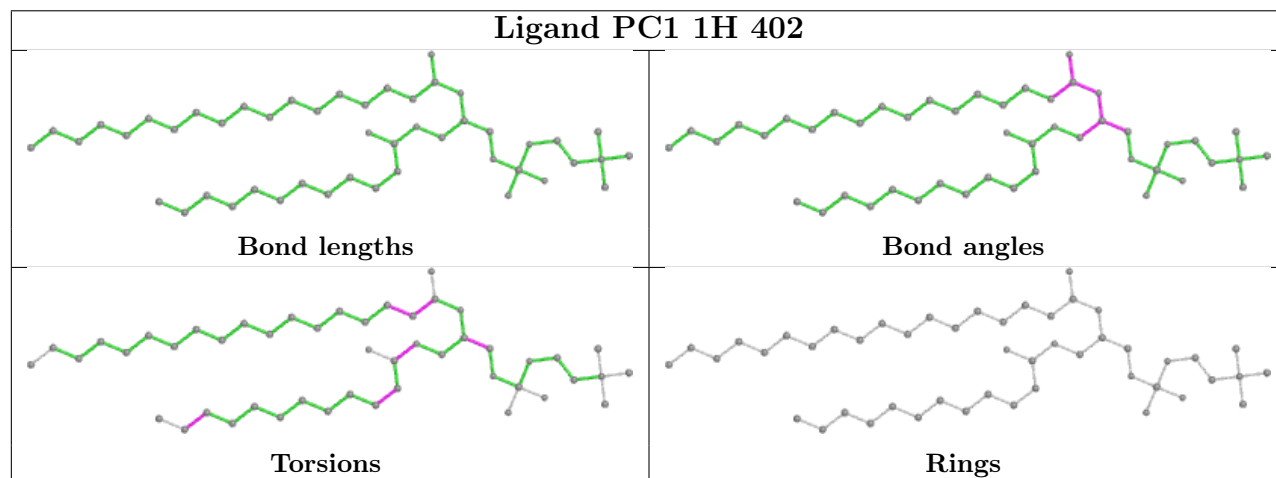
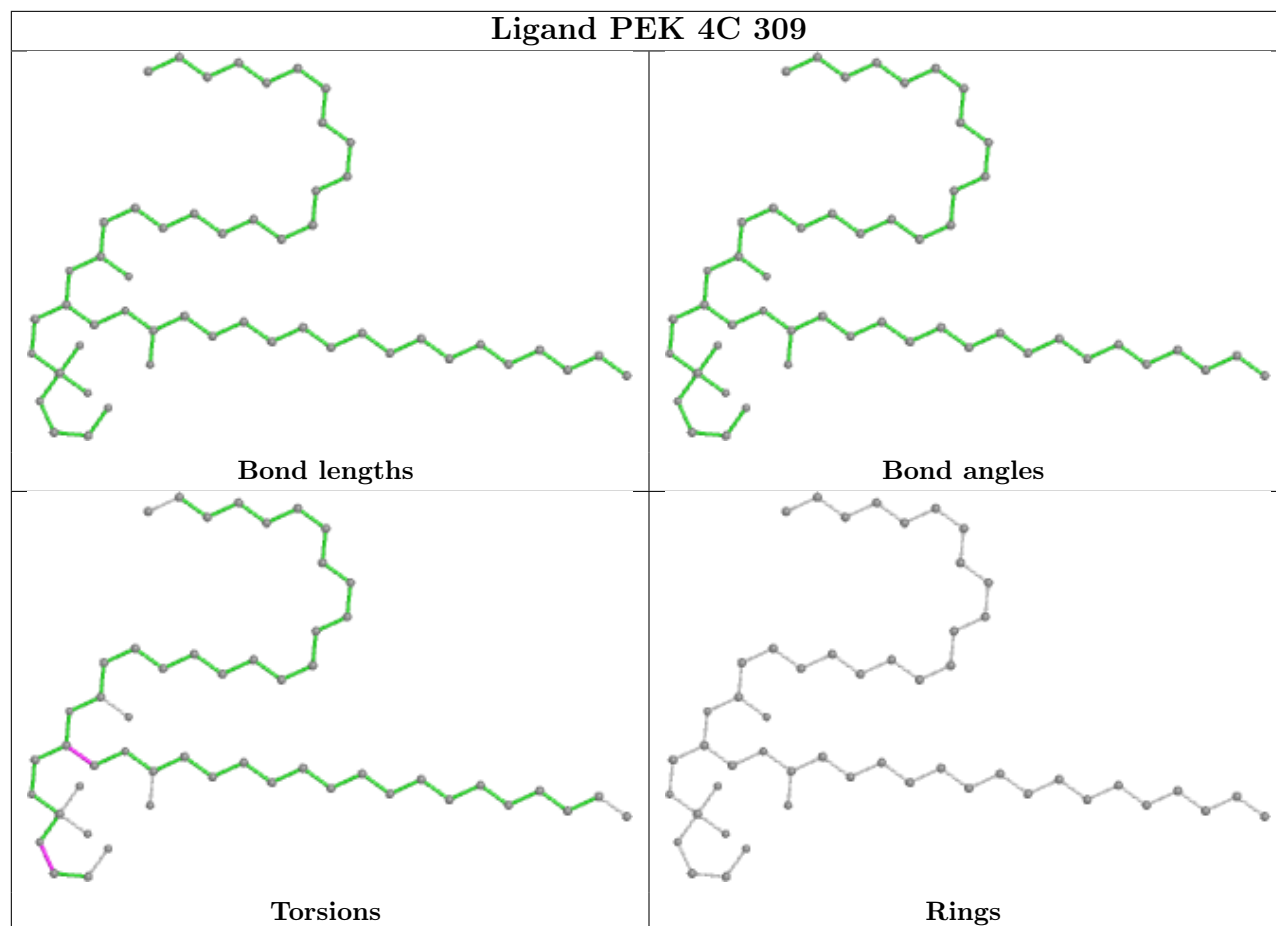


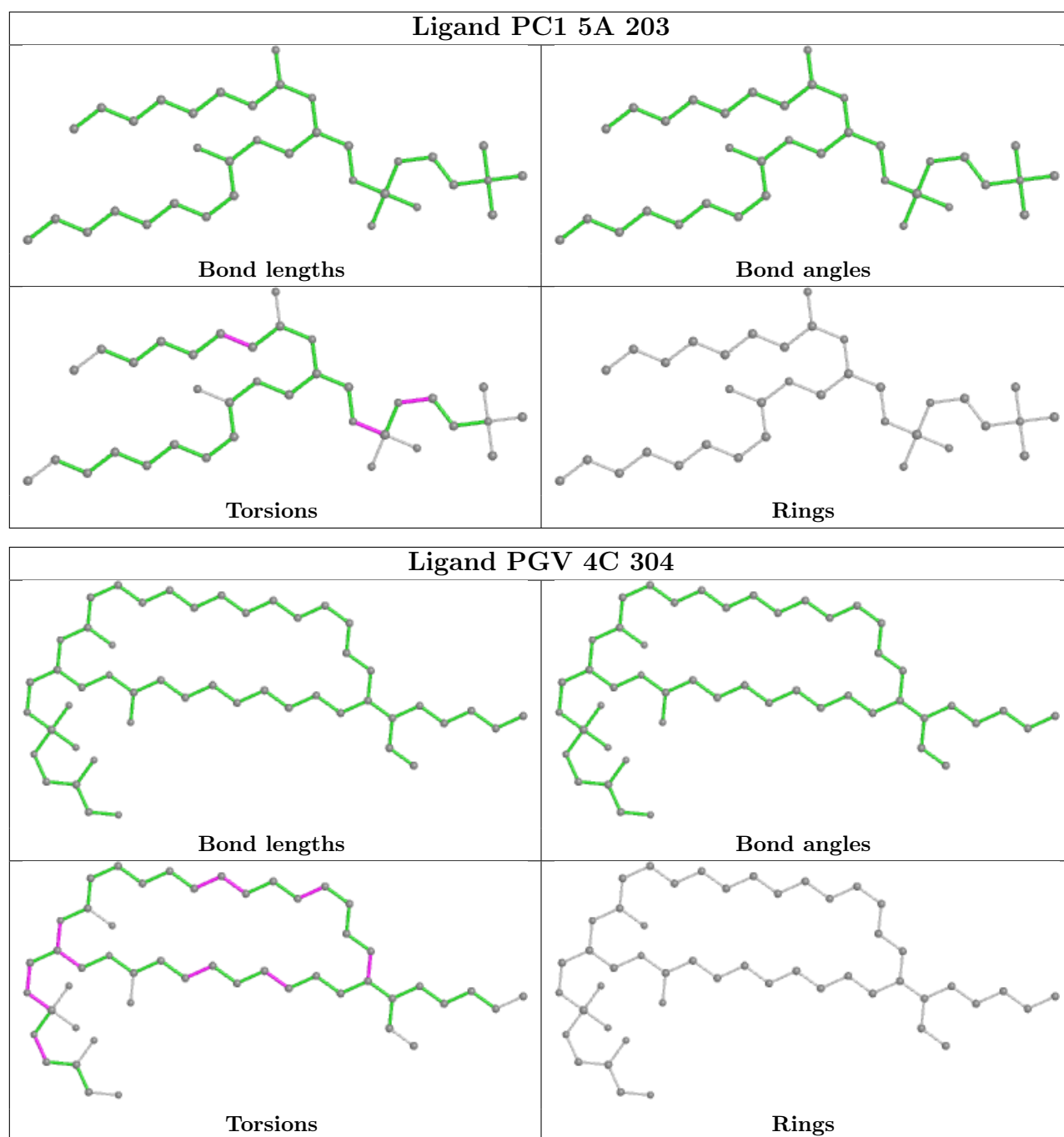
Rings

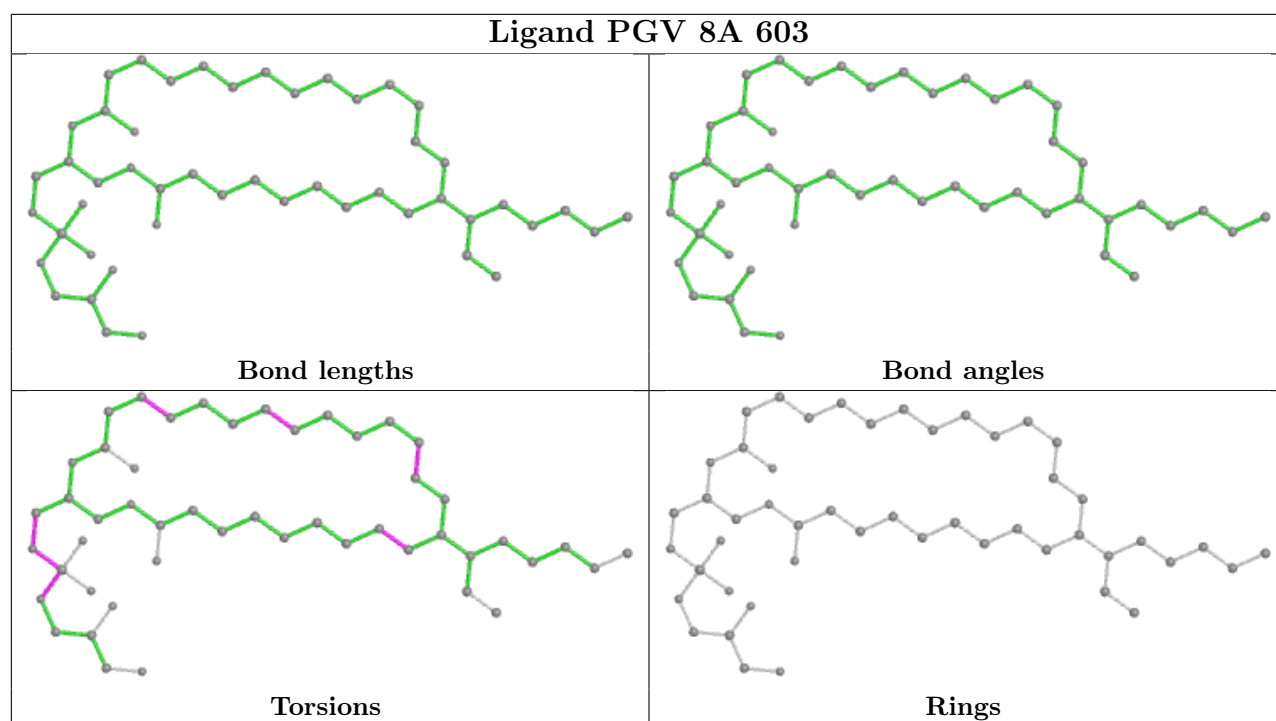
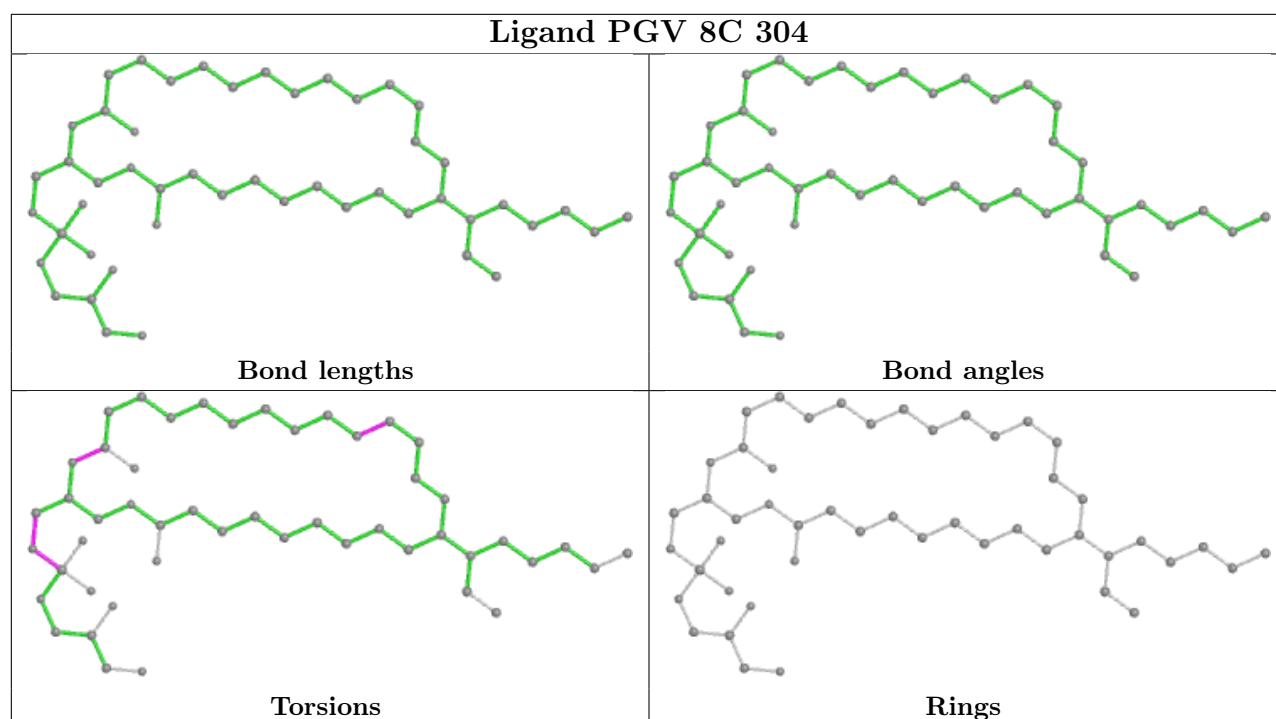


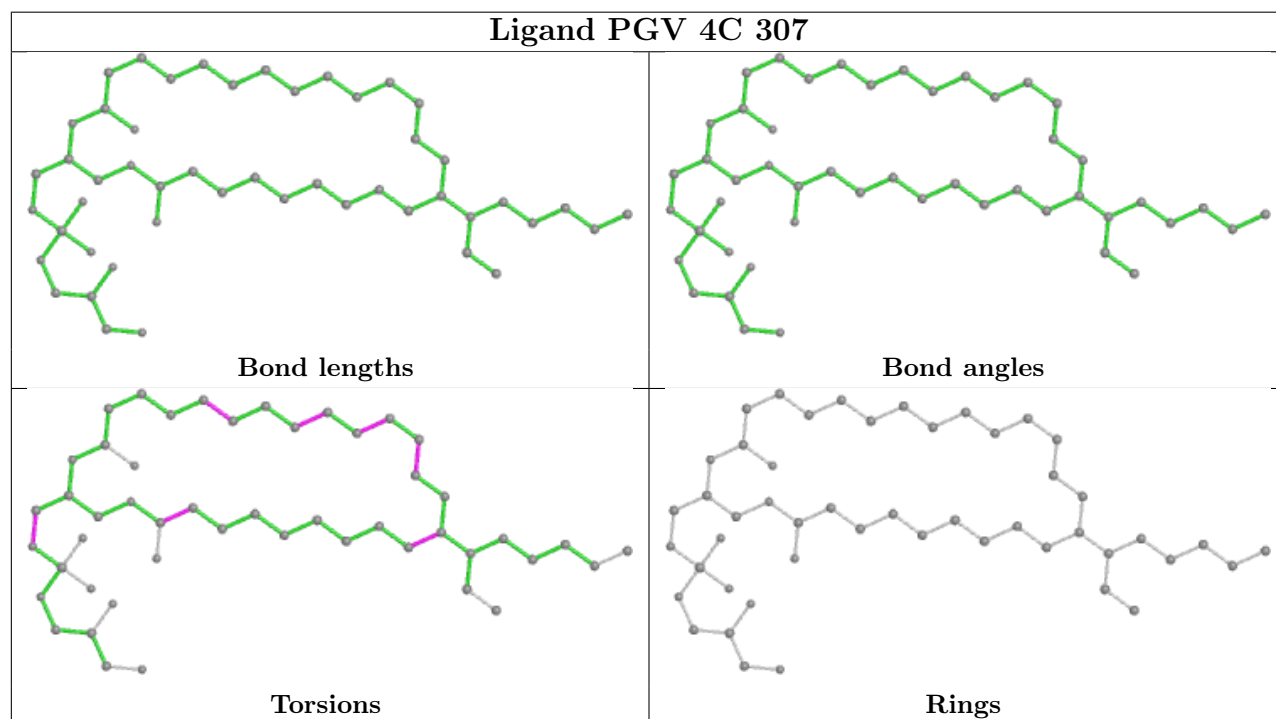
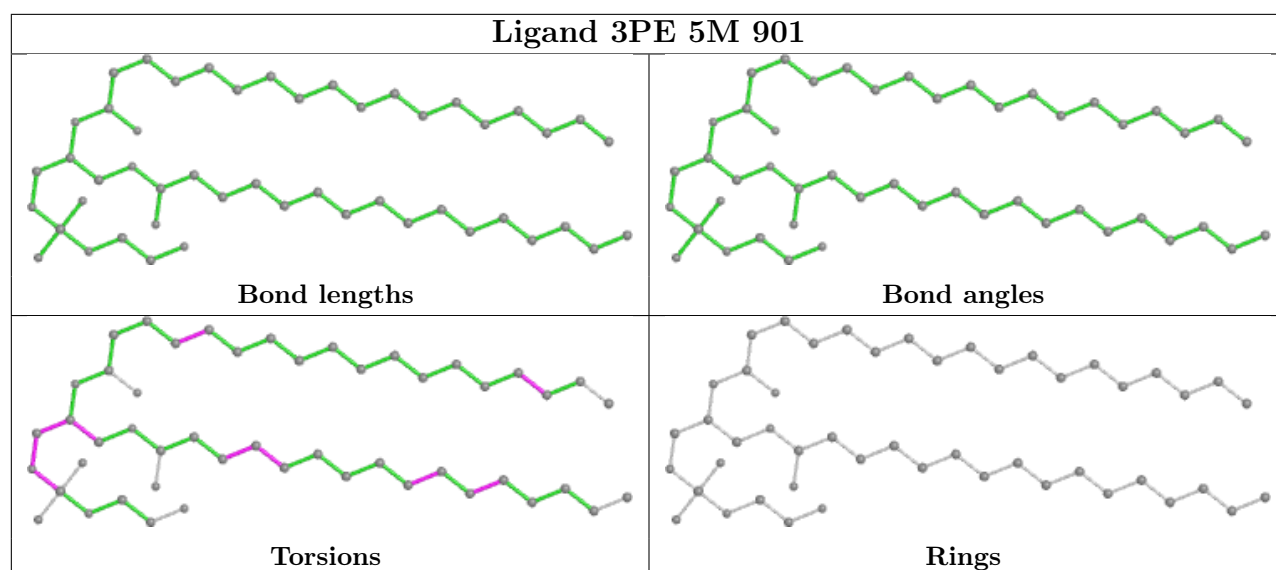


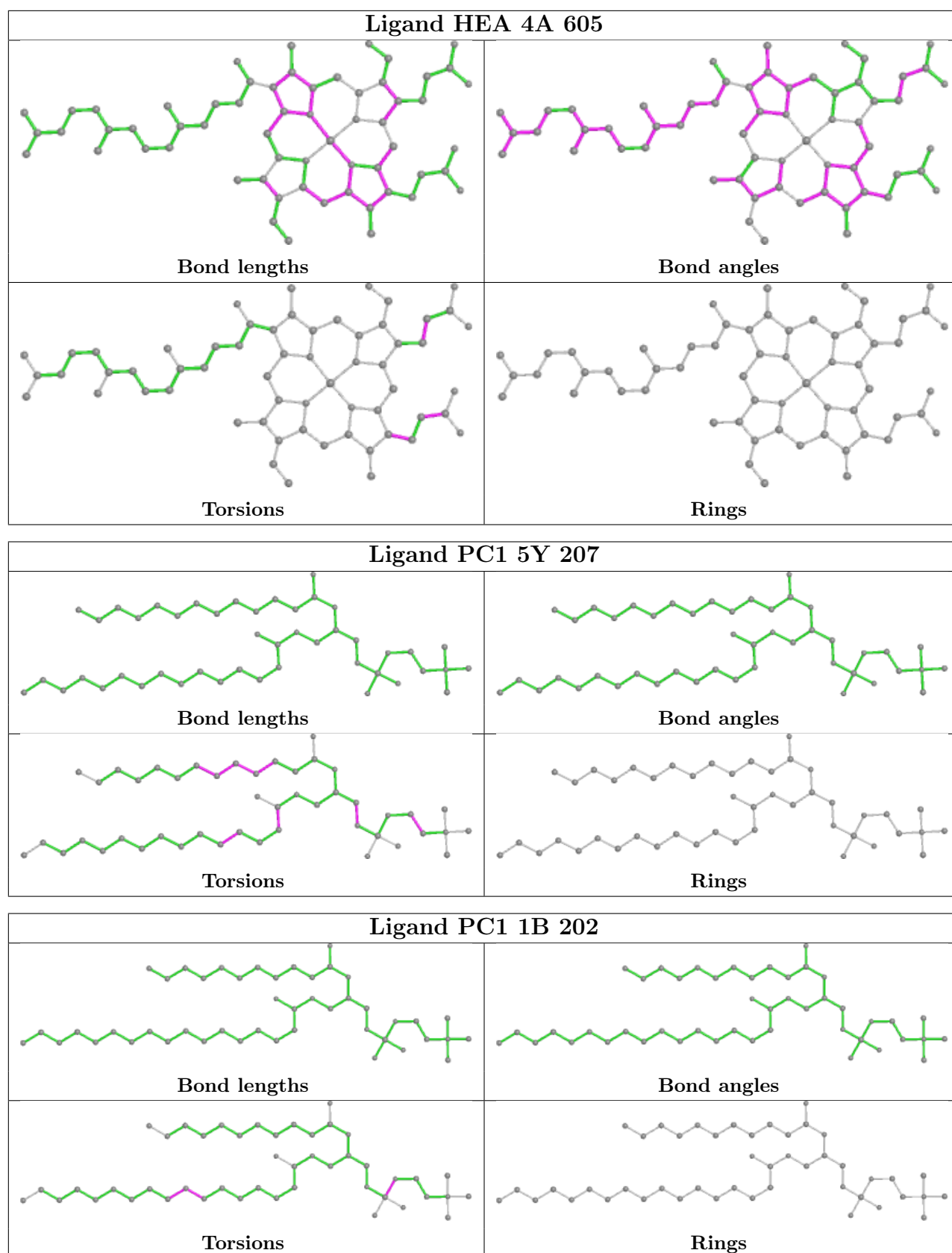


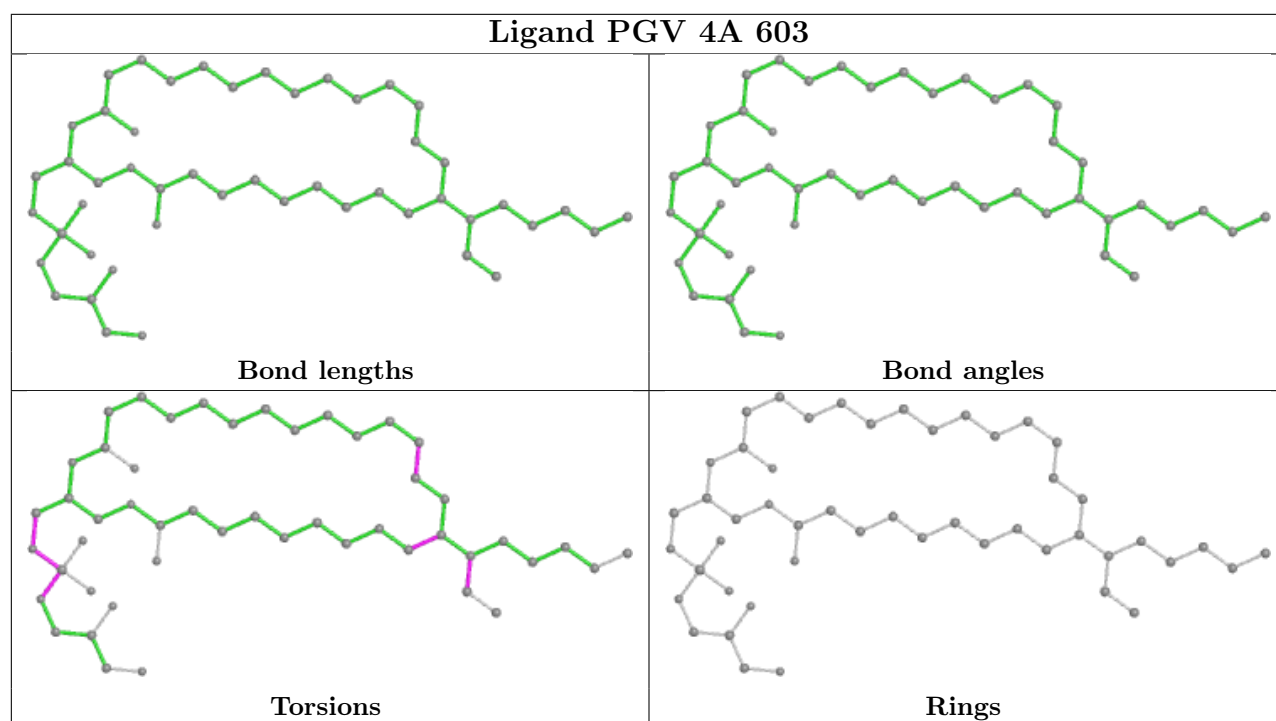
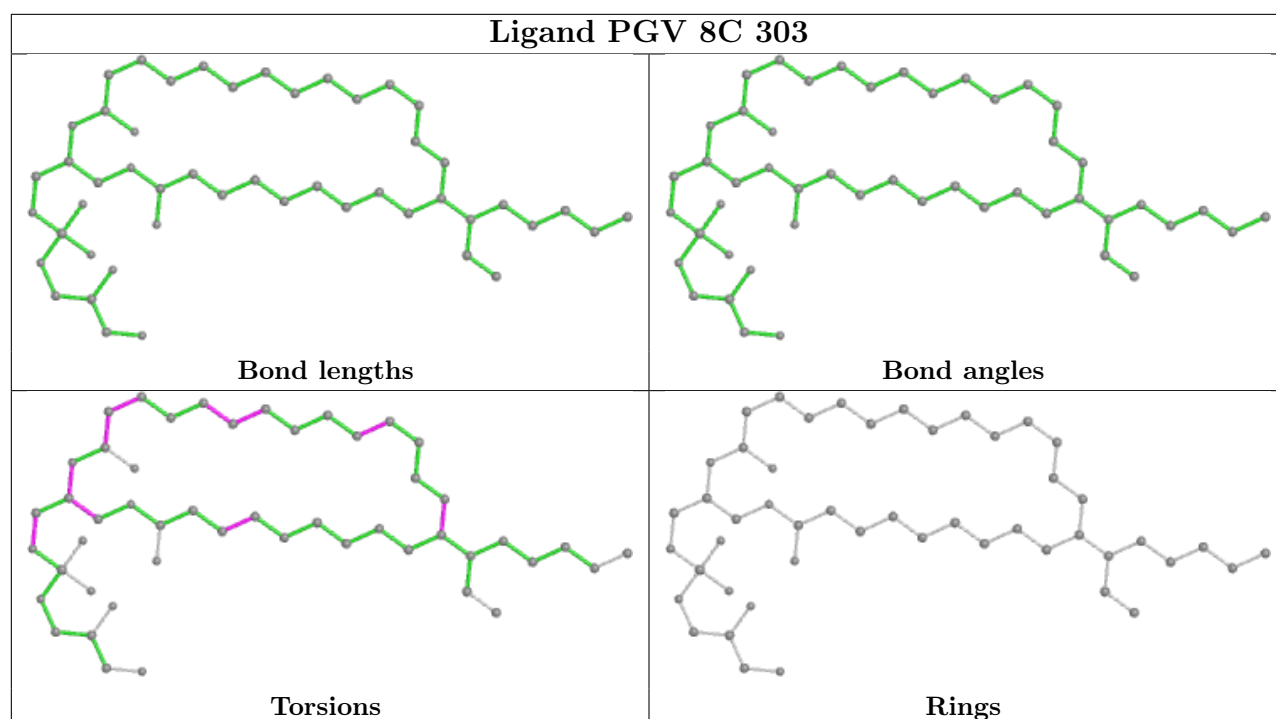


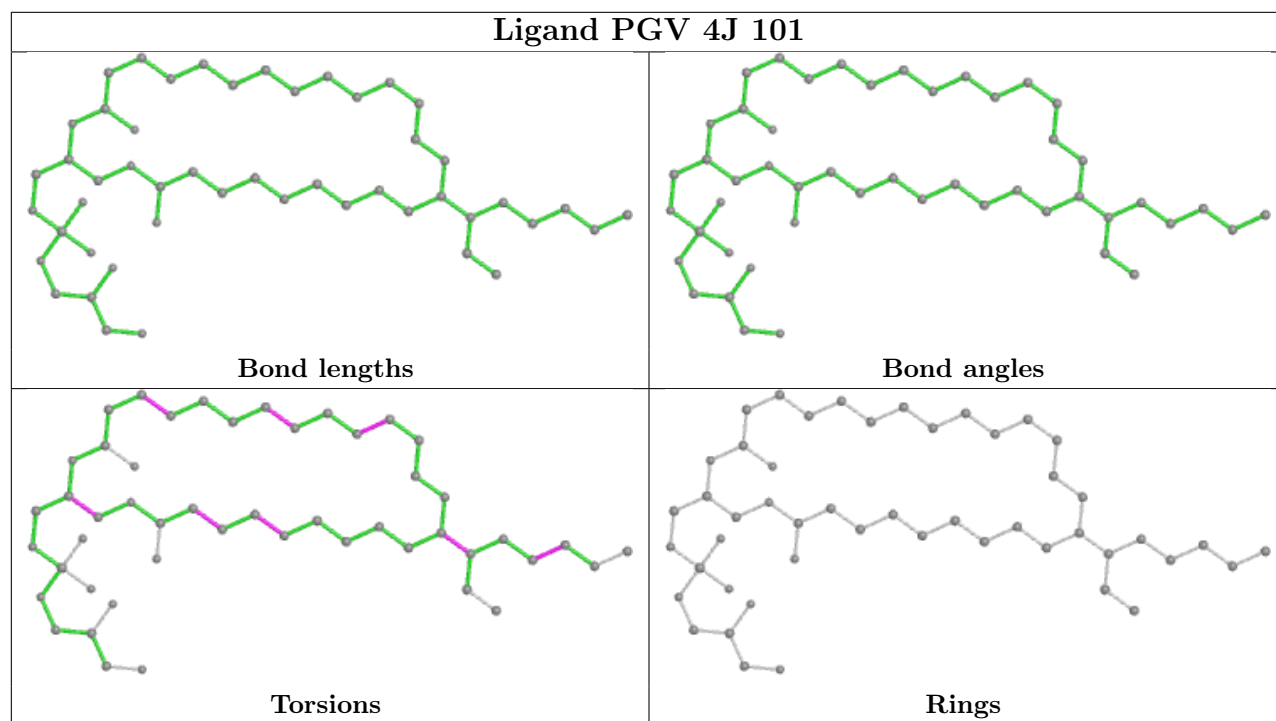
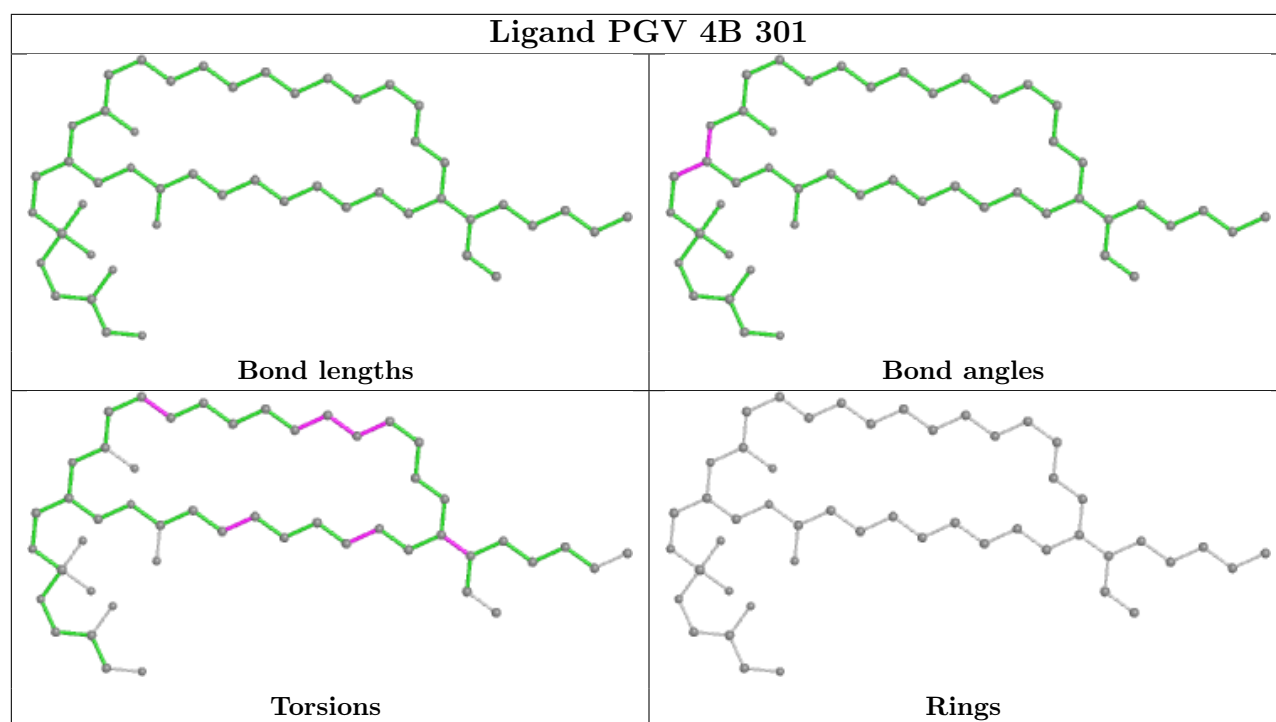


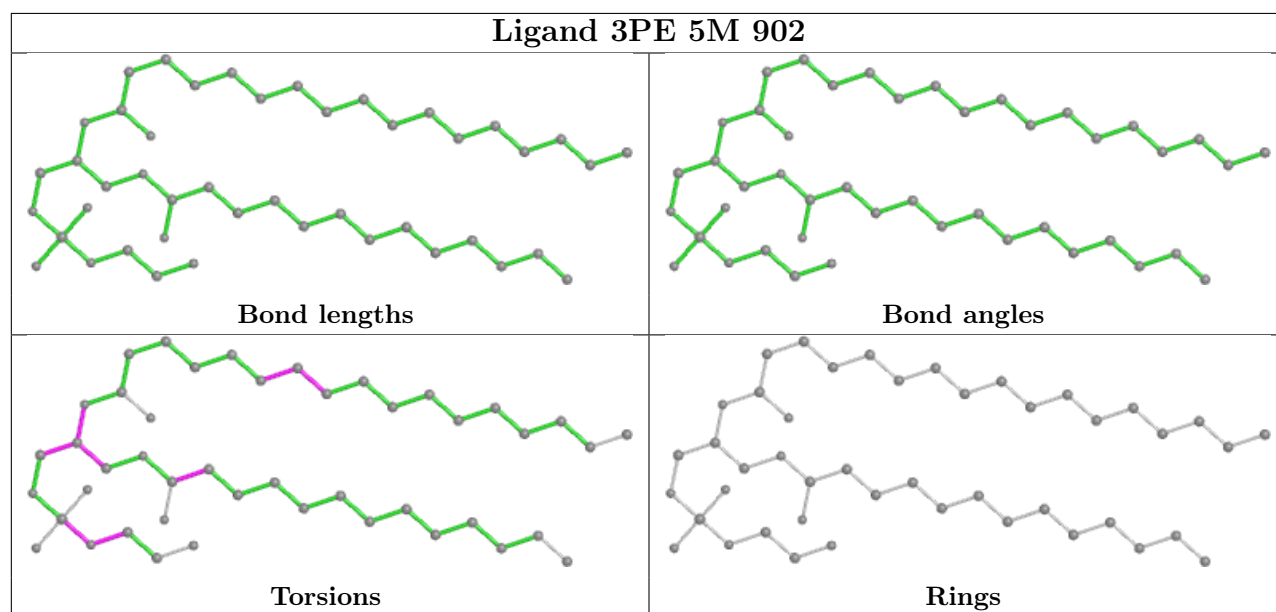
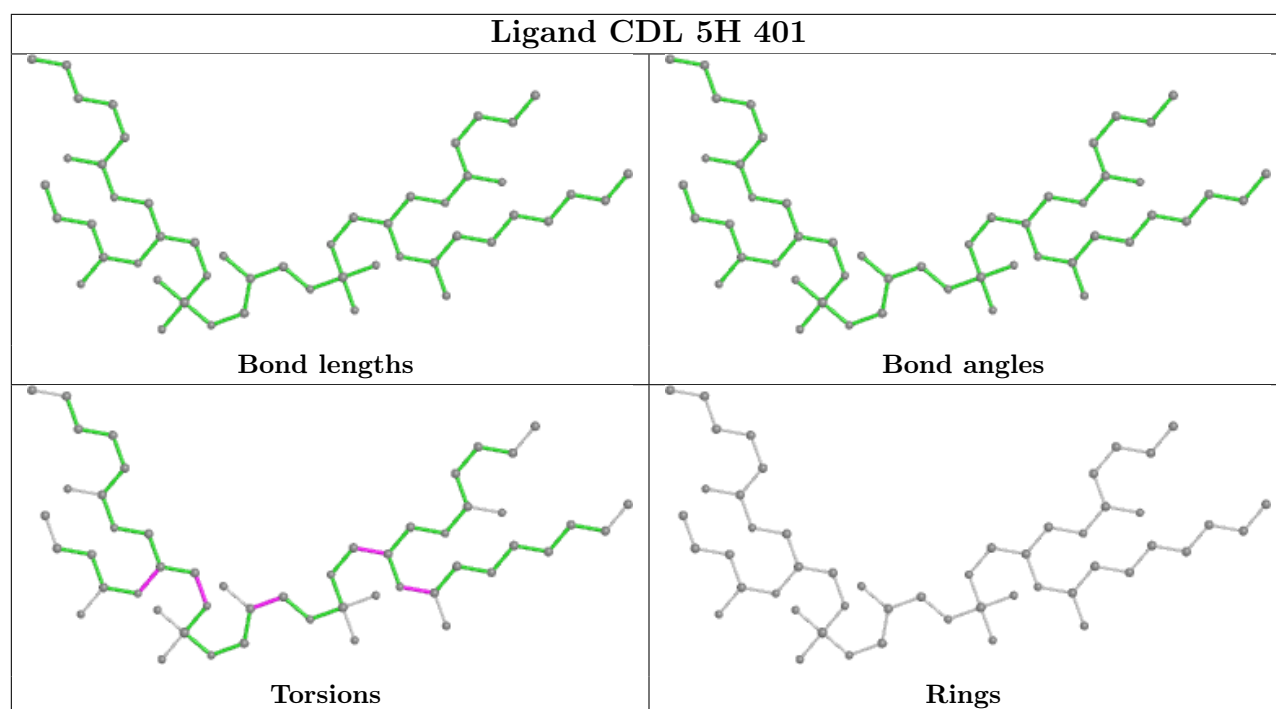


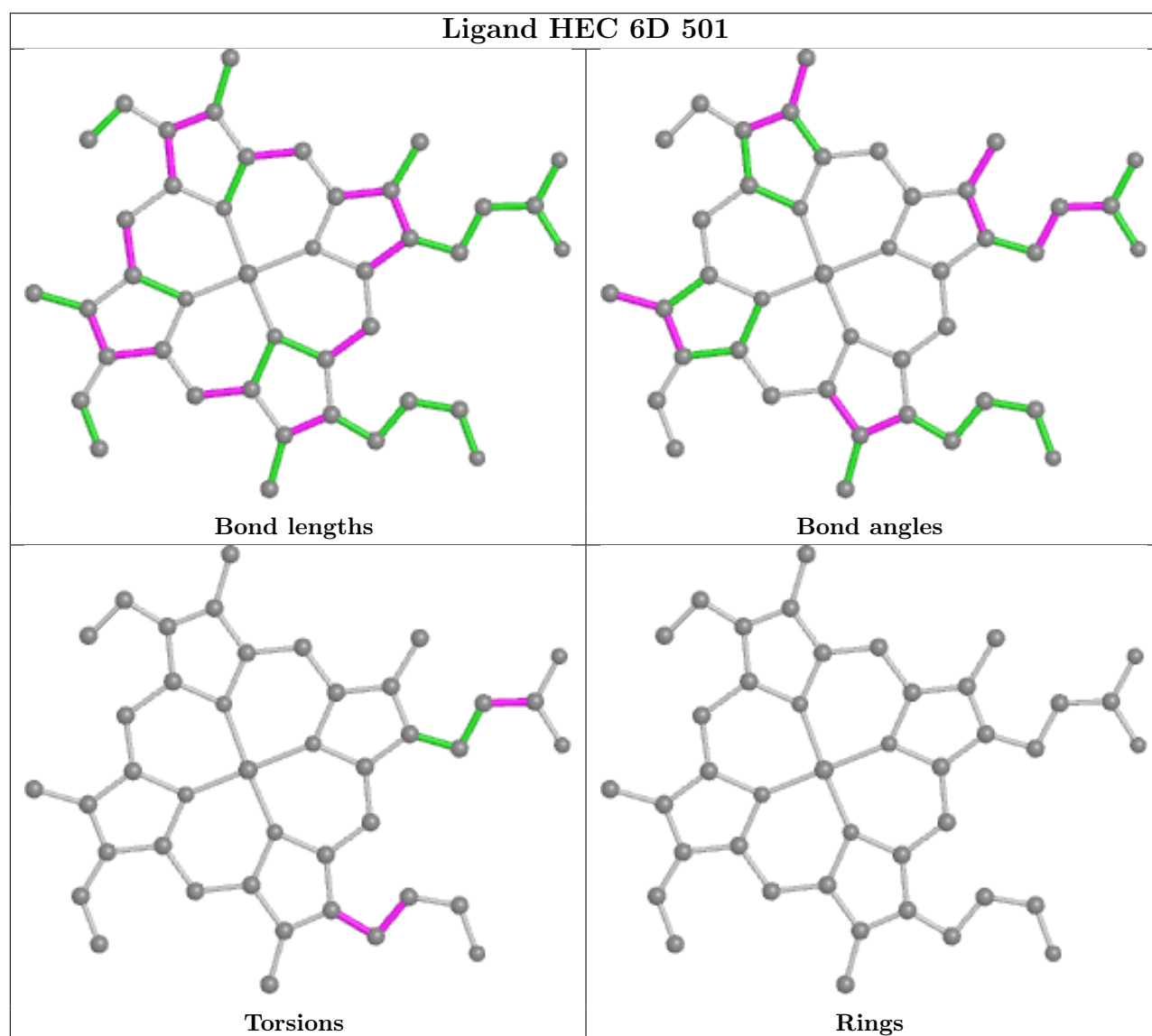
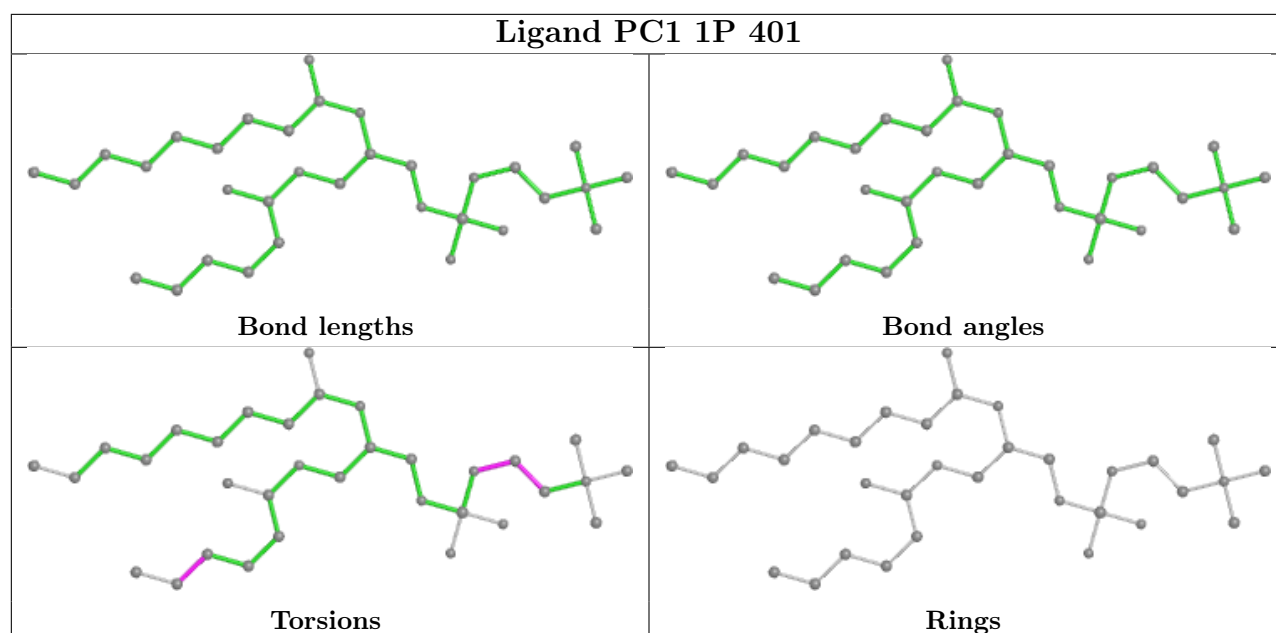












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	1h	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1h	124:GLN	C	125:TYR	N	1.12

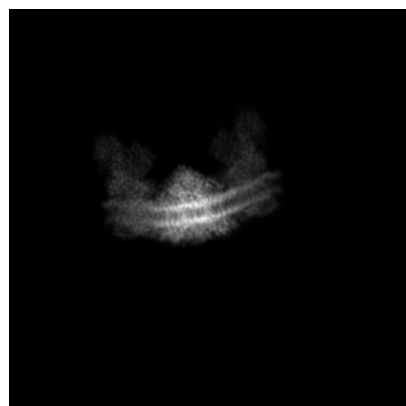
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42233. These allow visual inspection of the internal detail of the map and identification of artifacts.

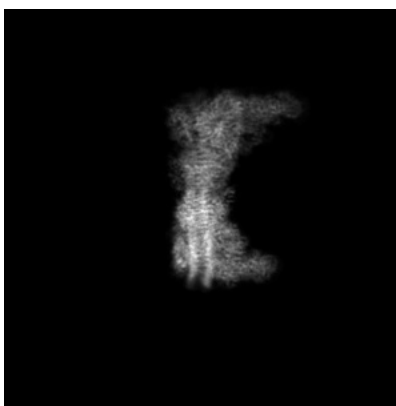
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

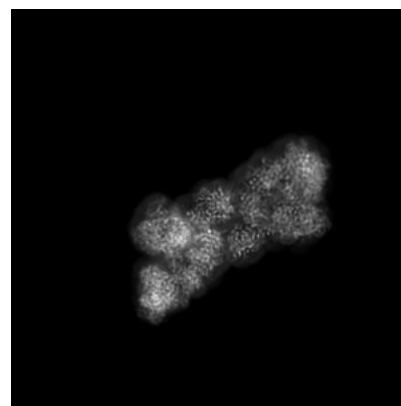
6.1.1 Primary map



X

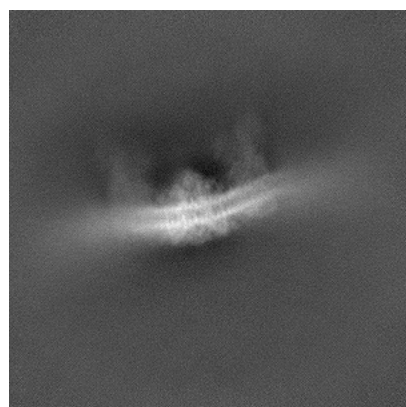


Y

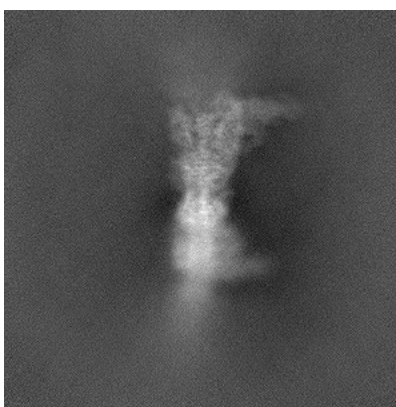


Z

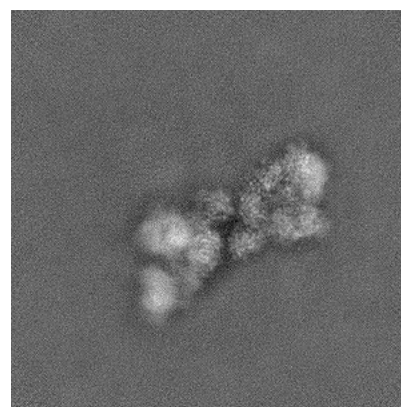
6.1.2 Raw map



X



Y

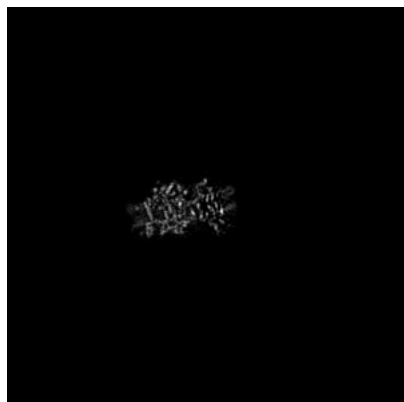


Z

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

6.2 Central slices [i](#)

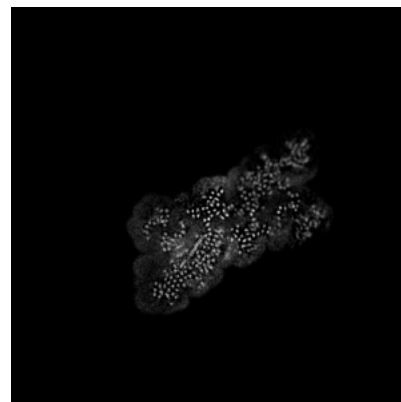
6.2.1 Primary map



X Index: 256

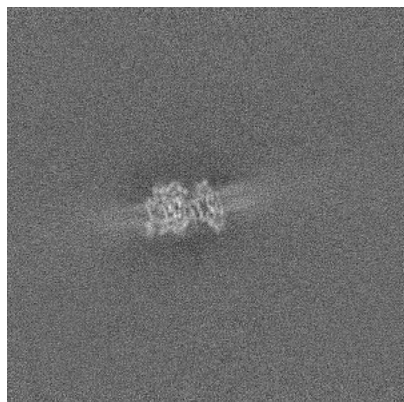


Y Index: 256



Z Index: 256

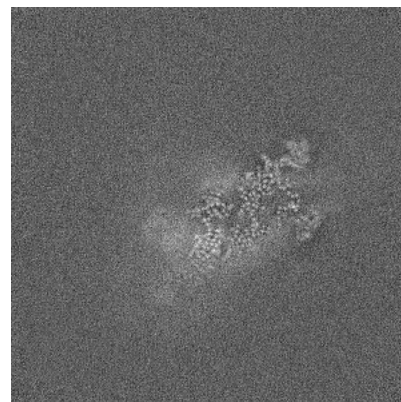
6.2.2 Raw map



X Index: 256



Y Index: 256

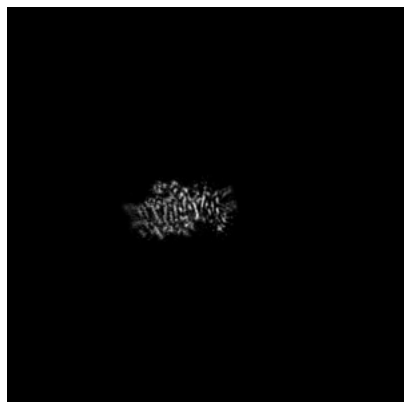


Z Index: 256

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

6.3 Largest variance slices [i](#)

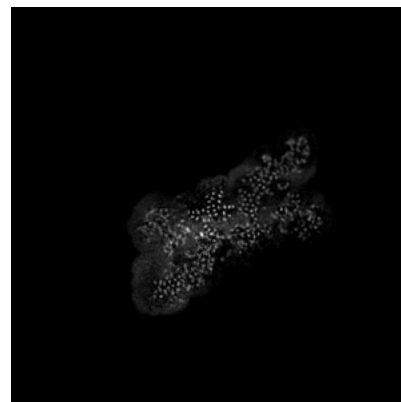
6.3.1 Primary map



X Index: 252

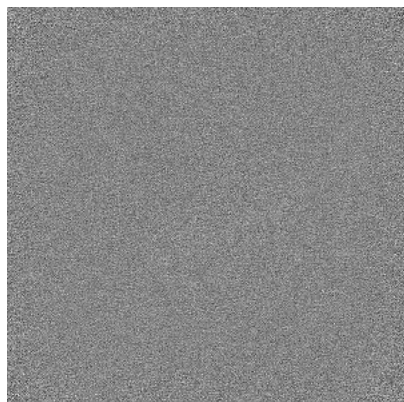


Y Index: 222

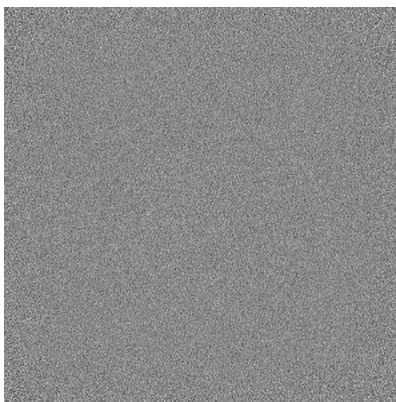


Z Index: 260

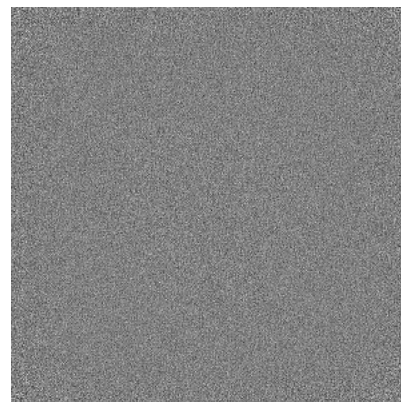
6.3.2 Raw map



X Index: 0



Y Index: 0

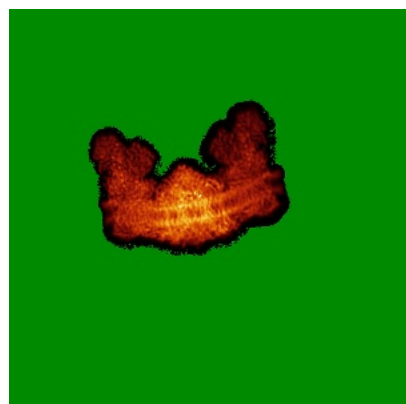


Z Index: 0

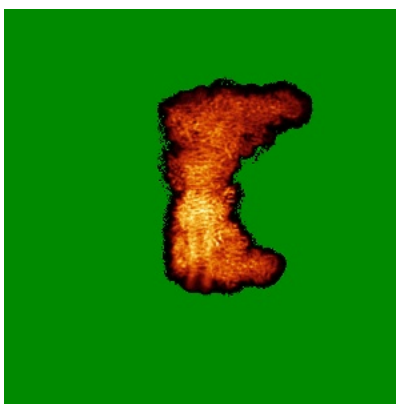
The images above show the largest variance slices of the map in three orthogonal directions.

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

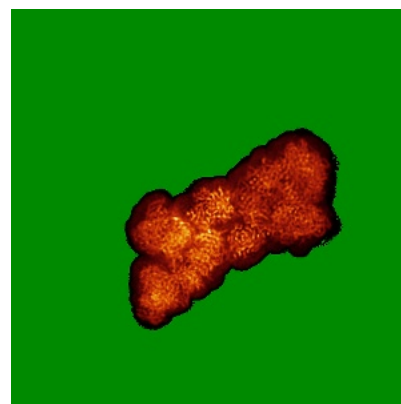
6.4.1 Primary map



X

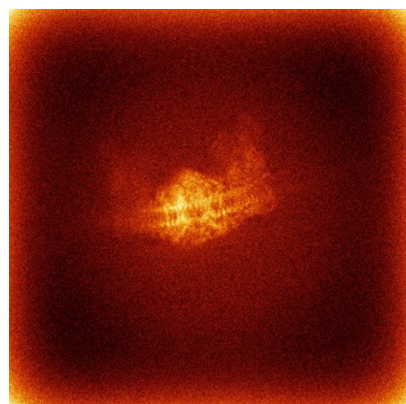


Y

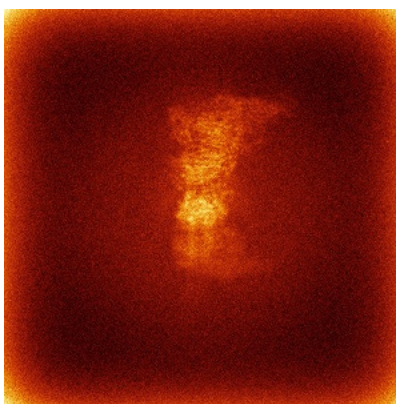


Z

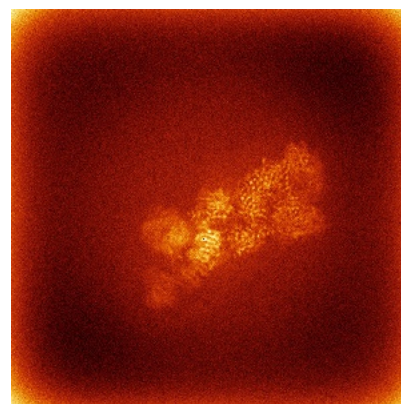
6.4.2 Raw map



X



Y

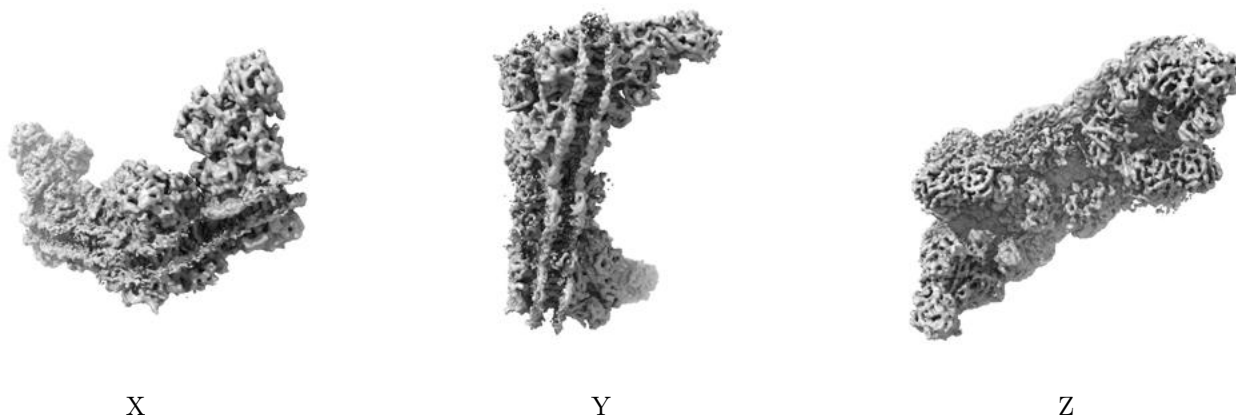


Z

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

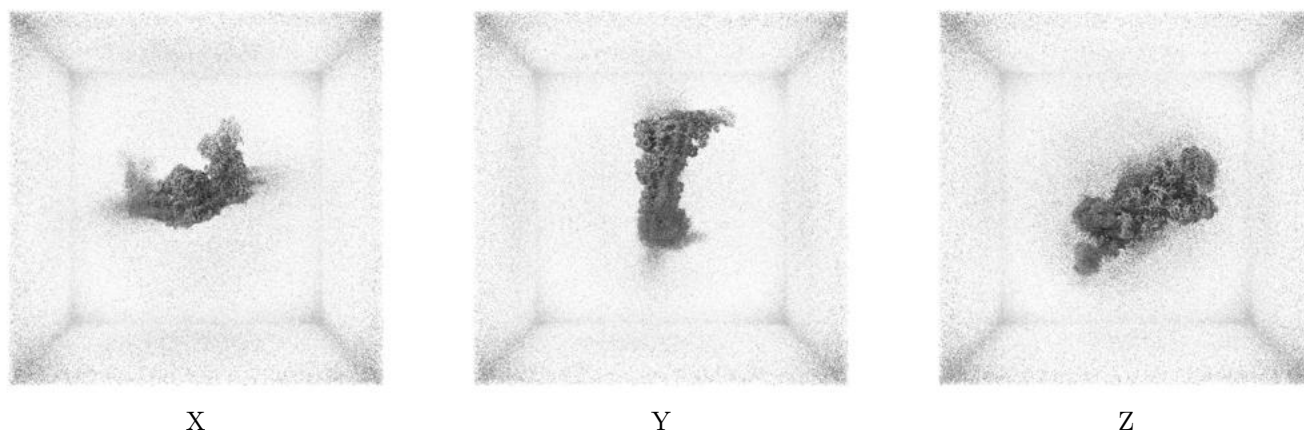
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

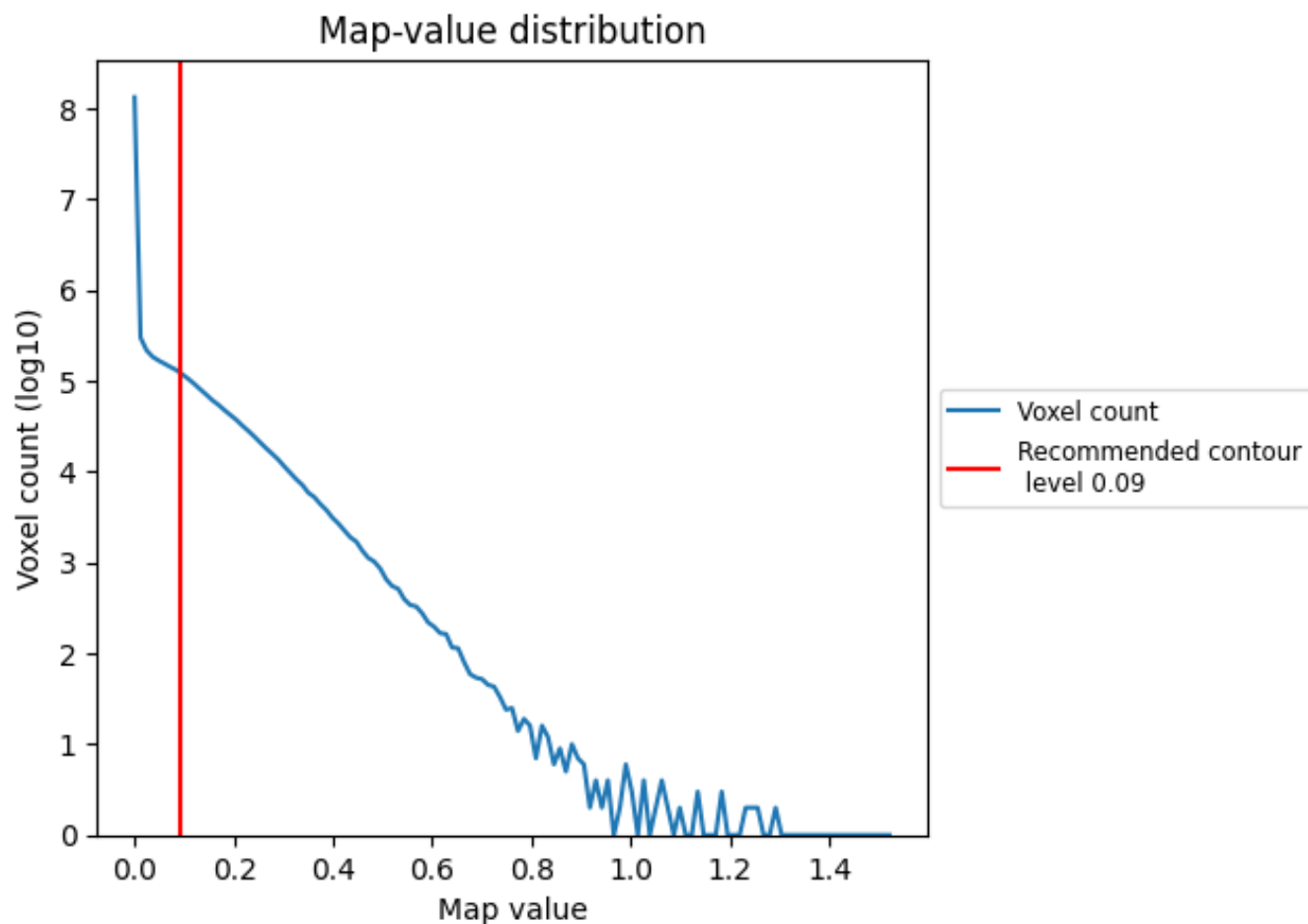
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

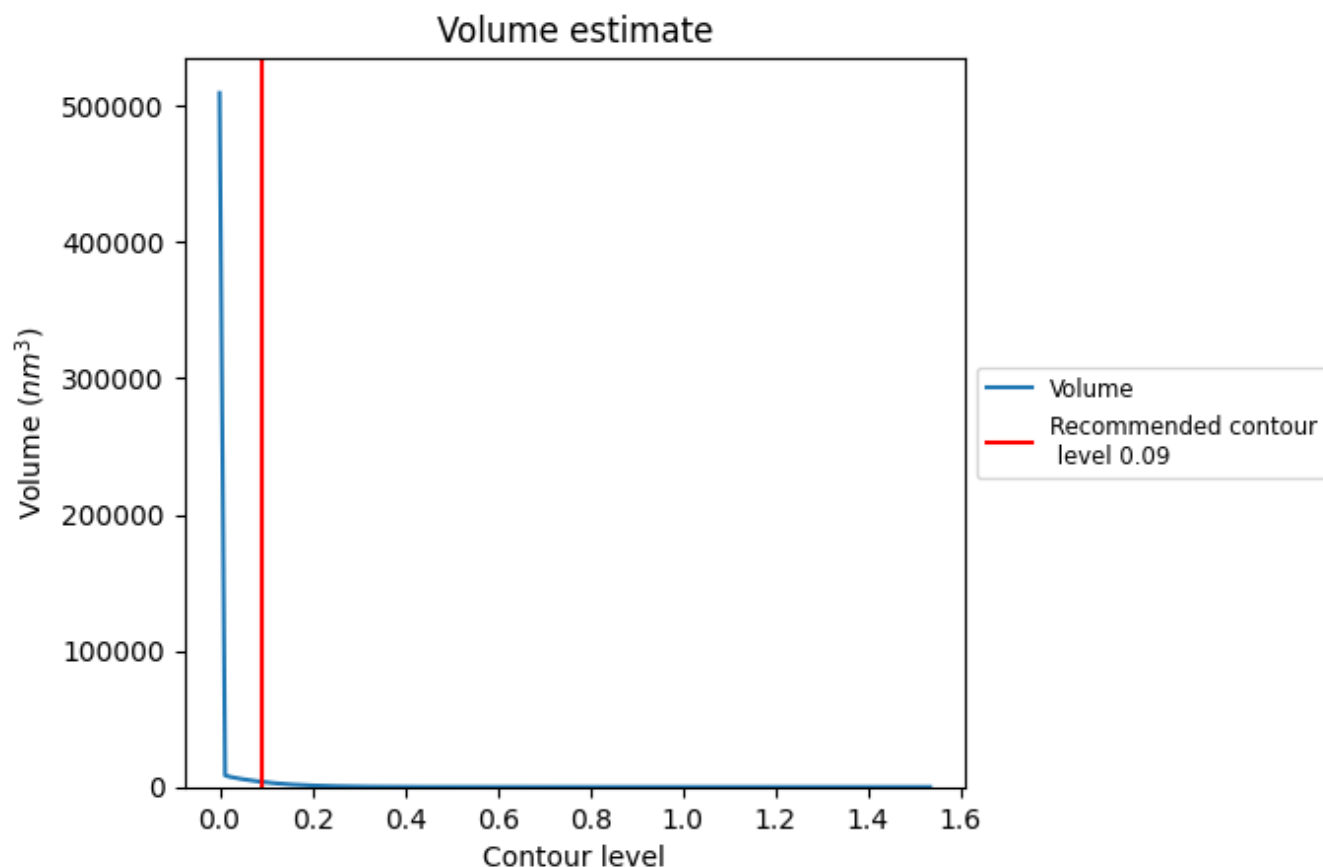
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

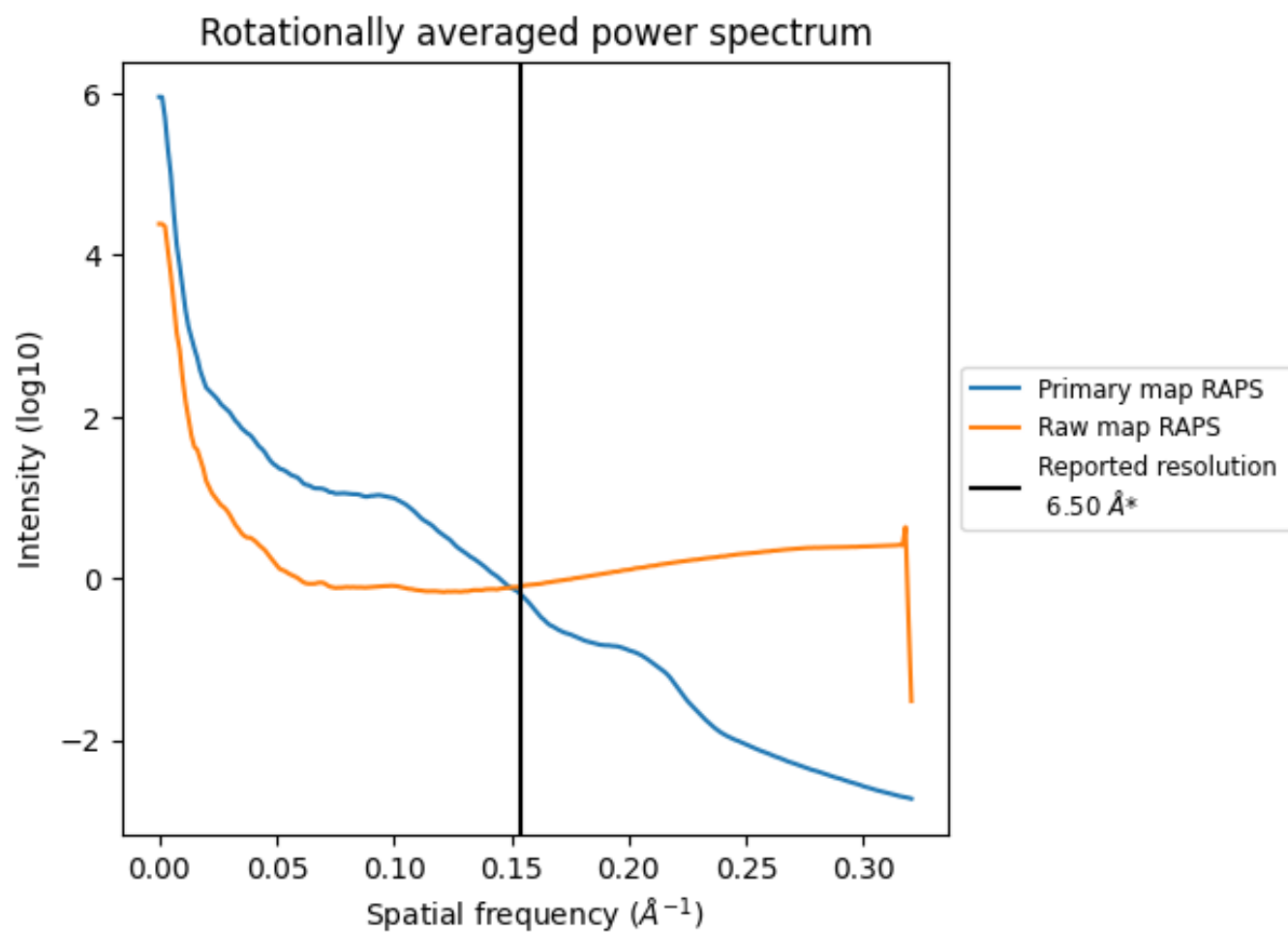
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3822 nm^3 ; this corresponds to an approximate mass of 3453 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 ⓘ

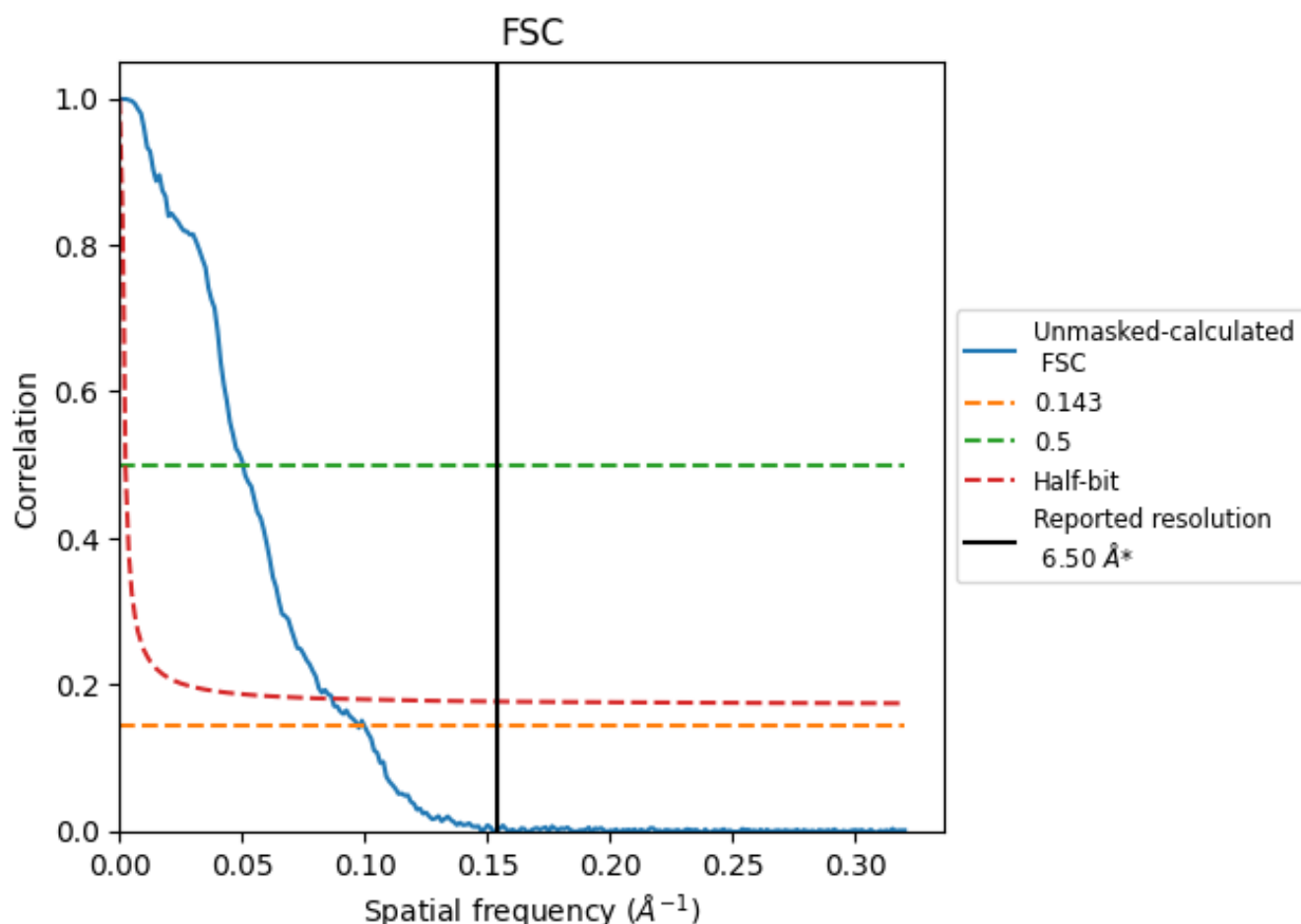


*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

8.2 Resolution estimates [i](#)

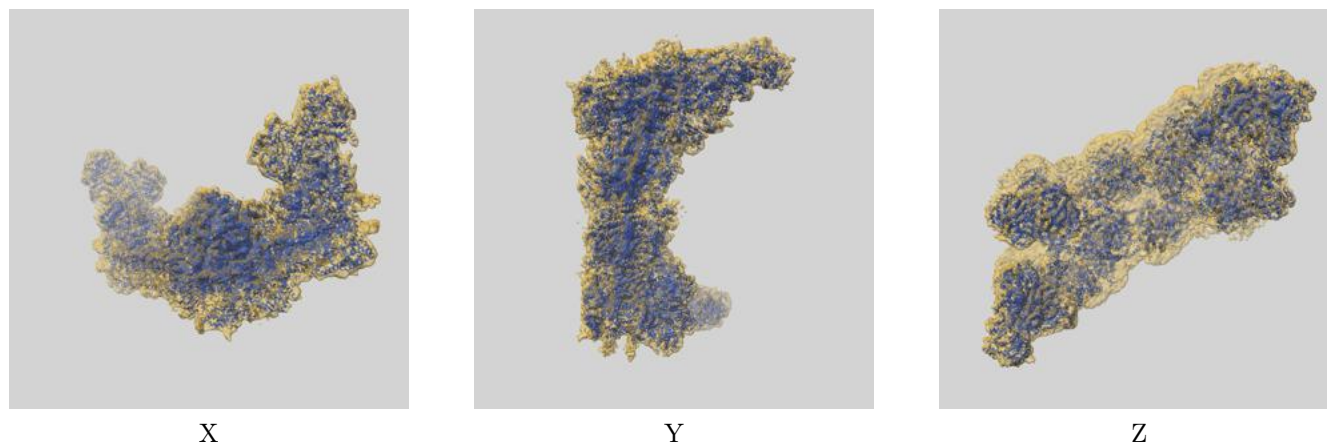
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.28	19.84	11.52

*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 10.28 differs from the reported value 6.5 by more than 10 %

9 Map-model fit [i](#)

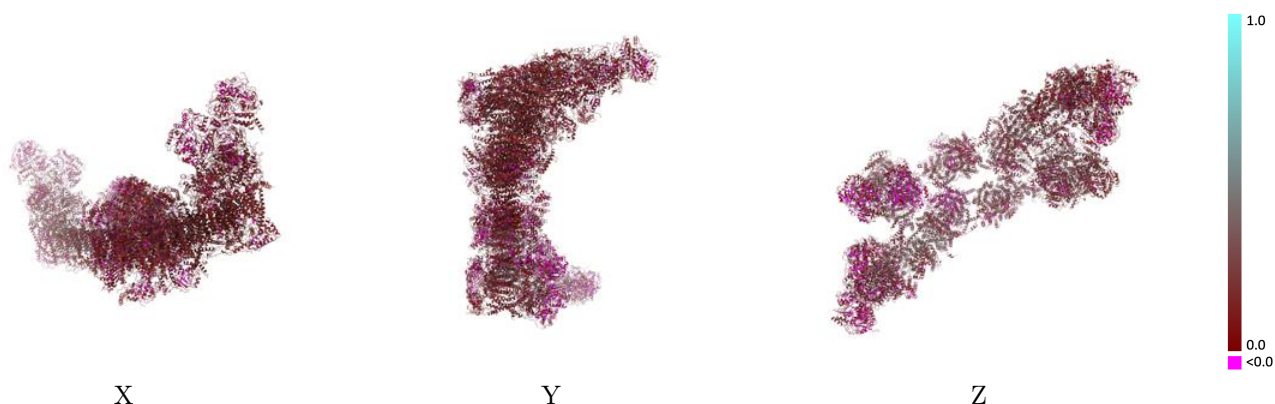
This section contains information regarding the fit between EMDB map EMD-42233 and PDB model 8UGR. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



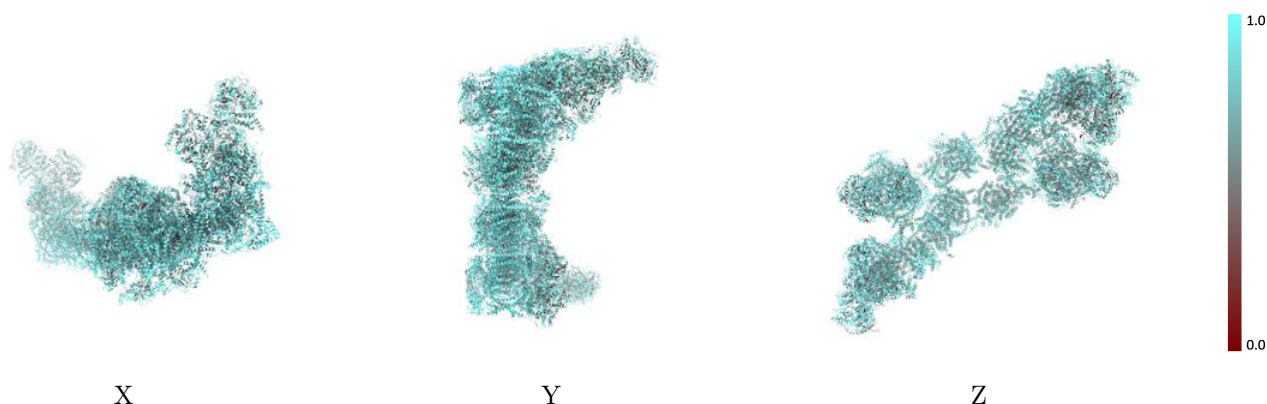
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



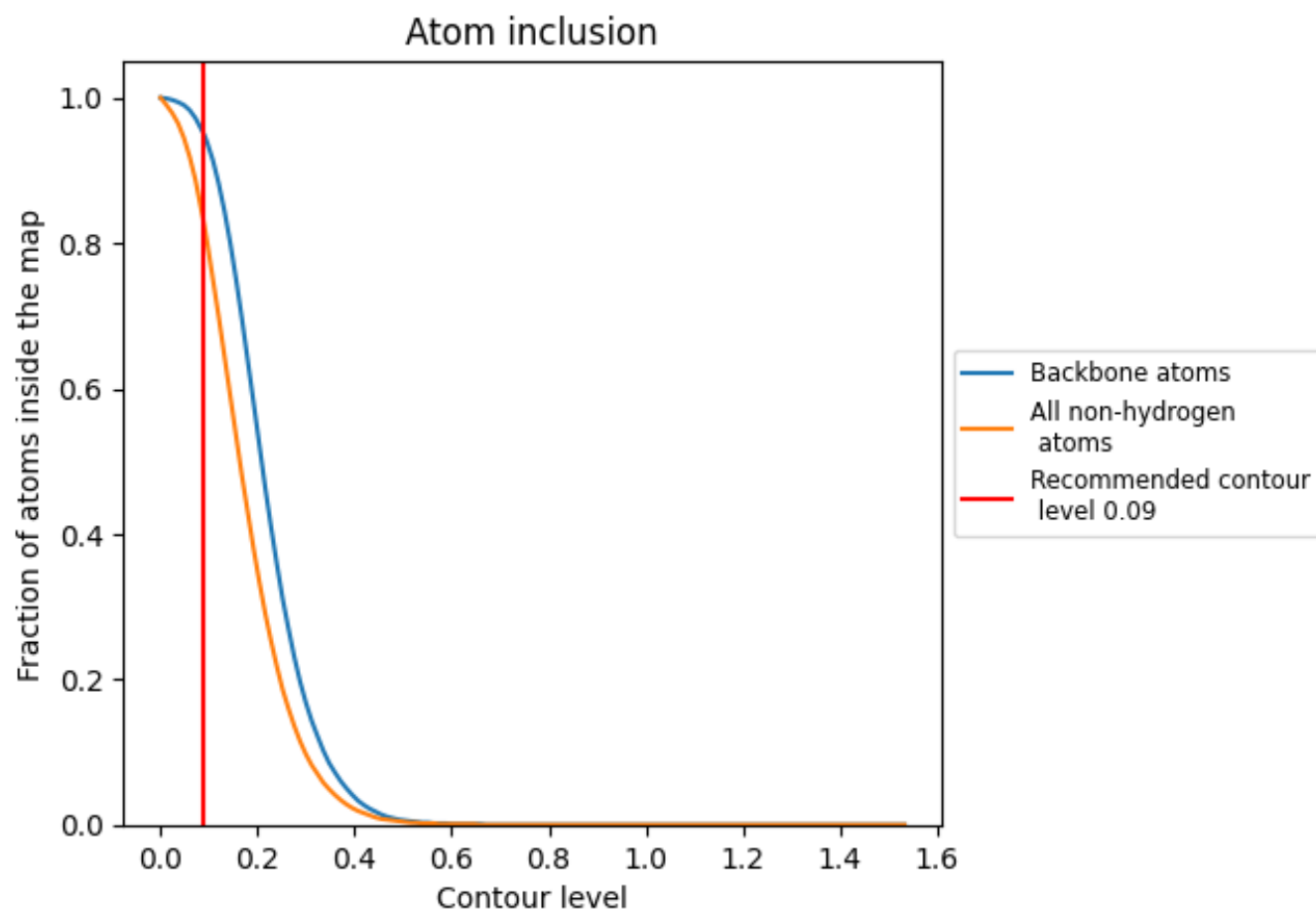
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.1640
1A	 0.7810	 0.1770
1B	 0.8050	 0.2190
1C	 0.8000	 0.1750
1D	 0.8160	 0.1950
1E	 0.7730	 0.1490
1F	 0.7460	 0.0960
1G	 0.7630	 0.1300
1H	 0.8300	 0.1690
1I	 0.8500	 0.2150
1J	 0.8640	 0.1710
1K	 0.8430	 0.1960
1L	 0.8990	 0.1430
1M	 0.9080	 0.2170
1N	 0.8990	 0.2450
1O	 0.9130	 0.1940
1P	 0.8220	 0.1840
1Q	 0.7280	 0.1670
1R	 0.9180	 0.2740
1S	 0.7860	 0.1280
1T	 0.8500	 0.1710
1U	 0.8110	 0.0840
1V	 0.7570	 0.1290
1W	 0.7880	 0.2200
1X	 0.8550	 0.1170
1Y	 0.9300	 0.1460
1Z	 0.8650	 0.1450
1a	 0.8490	 0.1500
1b	 0.8790	 0.1350
1c	 0.9410	 0.1880
1d	 0.8990	 0.2020
1e	 0.8730	 0.1950
1f	 0.9600	 0.2150
1g	 0.9420	 0.2150
1h	 0.9000	 0.2050























































































Continued on next page...

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Chain	Atom inclusion	Q-score
1i	 0.9340	 0.1700
1j	 0.9080	 0.1040
1k	 0.8890	 0.1040
1l	 0.9310	 0.1500
1m	 0.9690	 0.1570
1n	 0.9040	 0.1210
1o	 0.9550	 0.0990
1p	 0.9640	 0.2230
1q	 0.8860	 0.2210
1r	 0.8340	 0.1970
1s	 0.8190	 0.1440
3A	 0.7990	 0.1440
3B	 0.7850	 0.1130
3C	 0.8970	 0.2060
3D	 0.8690	 0.1830
3E	 0.8660	 0.1660
3F	 0.9090	 0.1920
3G	 0.9320	 0.2200
3H	 0.8890	 0.1880
3I	 0.5060	 0.1000
3J	 0.9340	 0.1950
3N	 0.9090	 0.0730
3O	 0.7770	 0.0680
3P	 0.9560	 0.2070
3Q	 0.9400	 0.1550
3R	 0.8070	 0.0940
3S	 0.9690	 0.1920
3T	 0.9980	 0.2110
3U	 0.9790	 0.1550
3V	 0.7260	 0.0540
3W	 0.9640	 0.0990
3X	 0.9900	 0.1100
3Y	 0.9160	 0.1960
4A	 0.8040	 0.1340
4B	 0.7970	 0.1320
4C	 0.8150	 0.1280
4D	 0.8760	 0.1460
4E	 0.8650	 0.1650
4F	 0.8550	 0.1950
4G	 0.9620	 0.1570
4H	 0.8330	 0.1530
4I	 0.9030	 0.1600





















































































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Chain	Atom inclusion	Q-score
4J	 0.9360	 0.1790
4K	 0.9690	 0.1790
4L	 0.8780	 0.1360
4M	 0.9270	 0.1730
4N	 0.8490	 0.1880
5A	 0.6690	 0.1480
5B	 0.7630	 0.1710
5C	 0.7090	 0.1680
5D	 0.7110	 0.1670
5E	 0.7260	 0.1680
5F	 0.7090	 0.1420
5G	 0.7110	 0.1380
5H	 0.7540	 0.1630
5I	 0.8000	 0.1580
5J	 0.8290	 0.1710
5K	 0.8010	 0.1620
5L	 0.8130	 0.1490
5M	 0.7790	 0.1580
5N	 0.8230	 0.1820
5O	 0.8270	 0.1800
5P	 0.7980	 0.1540
5Q	 0.6260	 0.1510
5R	 0.8460	 0.1950
5S	 0.7230	 0.1580
5T	 0.6920	 0.1580
5U	 0.6990	 0.1460
5V	 0.7170	 0.1800
5W	 0.7340	 0.1850
5X	 0.9300	 0.1860
5Y	 0.8280	 0.1740
5Z	 0.8680	 0.1990
5a	 0.8660	 0.1750
5b	 0.8980	 0.1810
5c	 0.8990	 0.1810
5d	 0.8240	 0.1740
5e	 0.9400	 0.2020
5f	 0.8860	 0.1940
5g	 0.8590	 0.1980
5h	 0.8410	 0.1670
5i	 0.8680	 0.1670
5j	 0.8350	 0.1640
5k	 0.8690	 0.1640





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Chain	Atom inclusion	Q-score
5l	 0.8910	 0.1890
5m	 0.8490	 0.1700
5n	 0.8120	 0.1630
5o	 0.9260	 0.1740
5p	 0.9190	 0.1880
5q	 0.8750	 0.2050
5r	 0.7860	 0.2200
5s	 0.8280	 0.1690
6A	 0.7840	 0.1820
6B	 0.7560	 0.2090
6C	 0.7690	 0.1910
6D	 0.8500	 0.1770
6E	 0.7830	 0.1330
6F	 0.7520	 0.2040
6G	 0.8310	 0.1980
6H	 0.8390	 0.1970
6I	 0.4390	 0.1080
6J	 0.8890	 0.1770
6N	 0.8100	 0.1730
6O	 0.7600	 0.2010
6P	 0.8020	 0.1850
6Q	 0.8520	 0.1810
6R	 0.7420	 0.1360
6S	 0.8250	 0.1910
6T	 0.9190	 0.1890
6U	 0.9100	 0.1870
6V	 0.5950	 0.1620
6W	 0.8850	 0.1770
6X	 0.9420	 0.2070
6Y	 0.8860	 0.2100
8A	 0.7410	 0.1270
8B	 0.7730	 0.1400
8C	 0.7210	 0.1170
8D	 0.8260	 0.1590
8E	 0.7620	 0.1590
8F	 0.7720	 0.1790
8G	 0.8490	 0.1450
8H	 0.8370	 0.1620
8I	 0.8800	 0.1760
8J	 0.9120	 0.1780
8K	 0.9360	 0.1510
8L	 0.8280	 0.1400

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Chain	Atom inclusion	Q-score
8M	 0.9370	 0.1760
8N	 0.8230	 0.1840