



Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 01:14 PM EST

PDB ID : 8UGJ
EMDB ID : EMD-42227
Title : In-situ structure of typeB supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

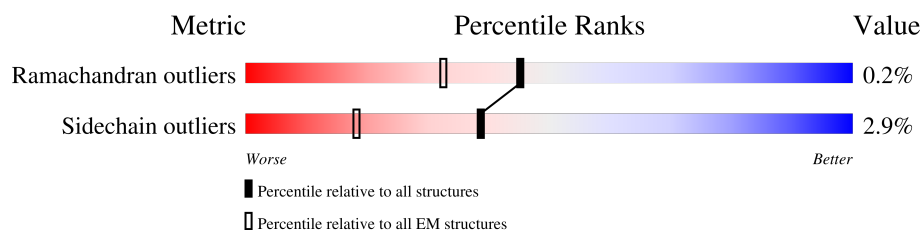
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	1A	115	<div> <div>12%</div> <div>92%</div> <div>8%</div> </div>
2	1B	258	<div> <div>57%</div> <div>40%</div> </div>
3	1C	264	<div> <div>78%</div> <div>21%</div> </div>
4	1D	476	<div> <div>88%</div> <div>10%</div> </div>
5	1E	249	<div> <div>12%</div> <div>84%</div> <div>14%</div> </div>
6	1F	464	<div> <div>11%</div> <div>91%</div> <div>7%</div> </div>
7	1G	727	<div> <div>92%</div> </div>
8	1H	318	<div> <div>96%</div> </div>
9	1I	239	<div> <div>74%</div> <div>26%</div> </div>

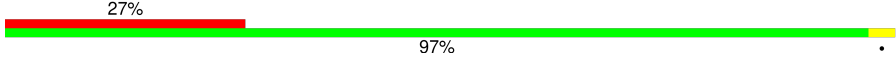



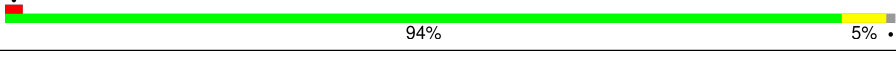
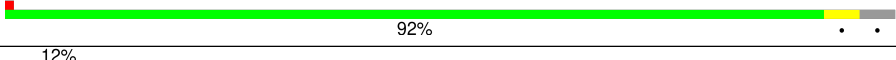

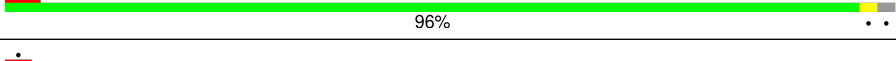
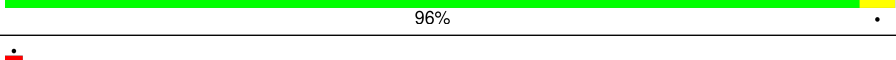
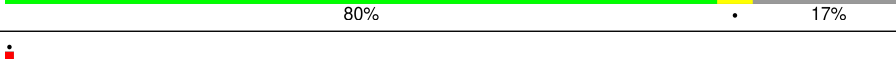
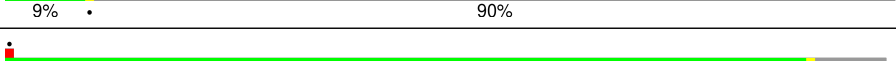
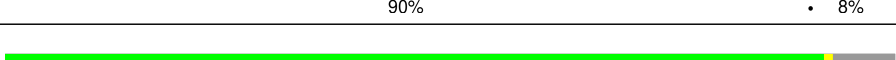
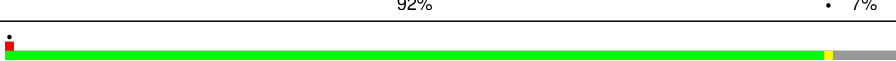
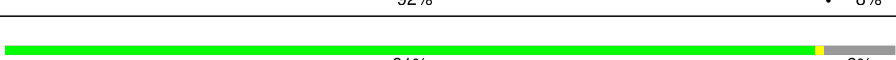
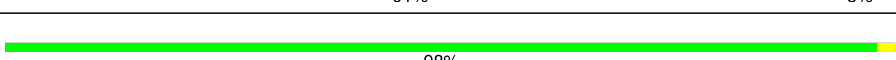
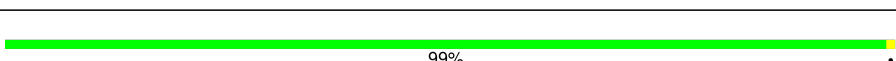
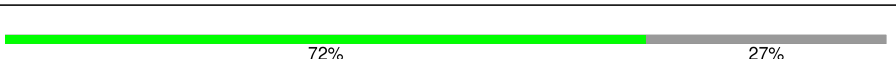
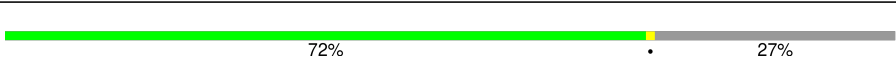




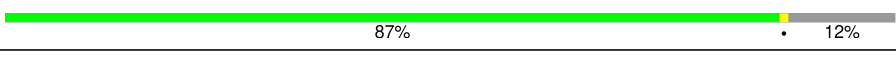


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Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	

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Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	

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Mol	Chain	Length	Quality of chain
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	60	
53	3W	60	
54	3X	56	
54	3Y	56	
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	128	
60	8F	128	
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	

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Mol	Chain	Length	Quality of chain
63	8I	75	
64	4J	80	
64	8J	80	
65	4K	80	
65	8K	80	
66	4L	63	
66	8L	63	
67	4M	70	
67	8M	70	
68	4N	82	
68	8N	82	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 134346 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		

- 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		

- 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		

There are 2 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

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	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		

- 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		

- 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		

There are 29 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
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

- 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		

- 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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	3I	47	Total	C	N	O	S	0	0
			340	211	65	63	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
			224	136	48	39	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3E	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3E	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3E	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3E	56	ARG	SER	conflict	UNP A0A4X1TWD8
3I	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3I	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3I	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3I	56	ARG	SER	conflict	UNP A0A4X1TWD8
3R	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3R	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3R	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3R	56	ARG	SER	conflict	UNP A0A4X1TWD8
3V	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3V	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3V	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3V	56	ARG	SER	conflict	UNP A0A4X1TWD8

- 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		

- 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		

- 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		

- Molecule 53 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3J	56	Total	C	N	O		0	0
			464	305	82	77			
53	3W	56	Total	C	N	O		0	0
			464	305	82	77			

- 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		

- 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
			4026	2693	625	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		

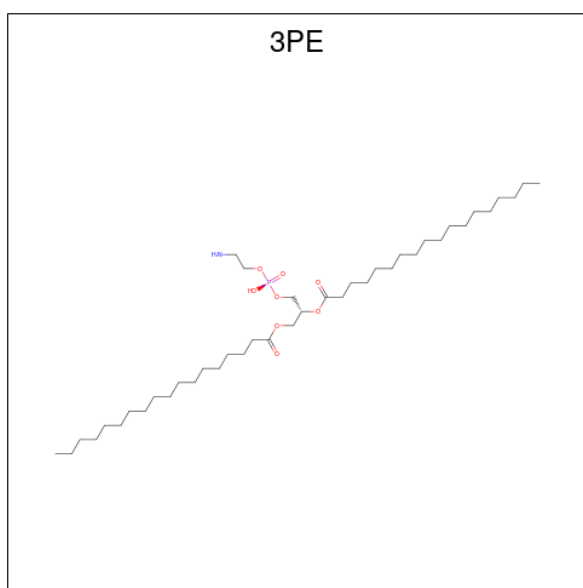
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

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 NDUF4.

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: $C_{41}H_{82}NO_8P$).



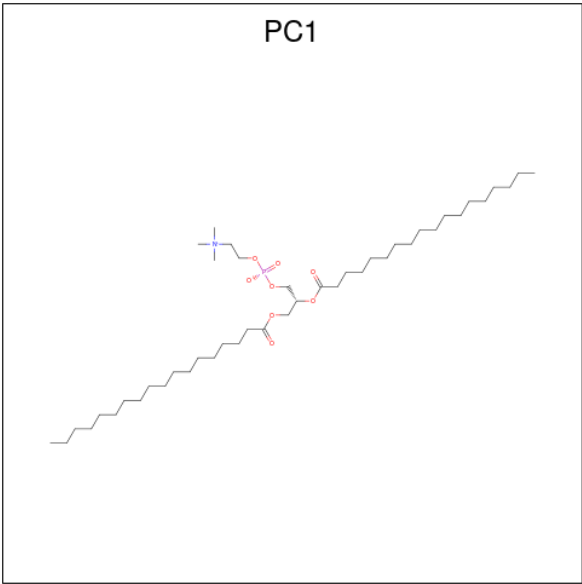
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1K	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1M	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1N	1	Total 49	C 39	N 1	O 8	P 1	0
69	1P	1	Total 35	C 25	N 1	O 8	P 1	0
69	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
69	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	1Y	1	Total 30	C 20	N 1	O 8	P 1	0
69	1Y	1	Total 33	C 23	N 1	O 8	P 1	0
69	1Y	1	Total 27	C 17	N 1	O 8	P 1	0
69	1d	1	Total 49	C 39	N 1	O 8	P 1	0
69	1j	1	Total 44	C 34	N 1	O 8	P 1	0
69	1m	1	Total 41	C 31	N 1	O 8	P 1	0
69	3A	1	Total 27	C 17	N 1	O 8	P 1	0
69	3A	1	Total 32	C 22	N 1	O 8	P 1	0
69	3C	1	Total 35	C 25	N 1	O 8	P 1	0
69	3C	1	Total 34	C 24	N 1	O 8	P 1	0
69	3D	1	Total 33	C 23	N 1	O 8	P 1	0
69	3G	1	Total 29	C 19	N 1	O 8	P 1	0
69	3N	1	Total 33	C 23	N 1	O 8	P 1	0
69	3N	1	Total 25	C 15	N 1	O 8	P 1	0
69	3P	1	Total 33	C 23	N 1	O 8	P 1	0
69	3R	1	Total 47	C 37	N 1	O 8	P 1	0
69	3Y	1	Total 30	C 20	N 1	O 8	P 1	0

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



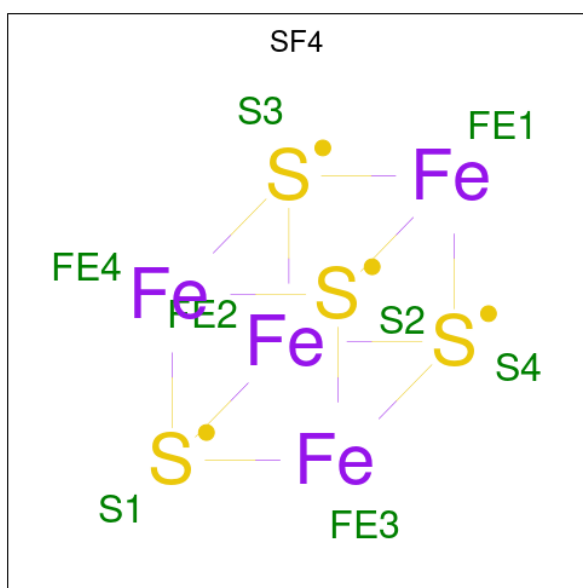
Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1I	1	Total	C	N	O	P	0
			44	34	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	1Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	

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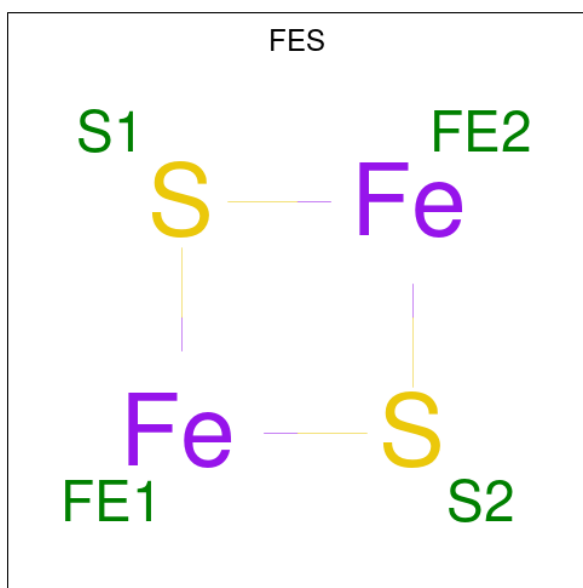
Mol	Chain	Residues	Atoms					AltConf
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	3J	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

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



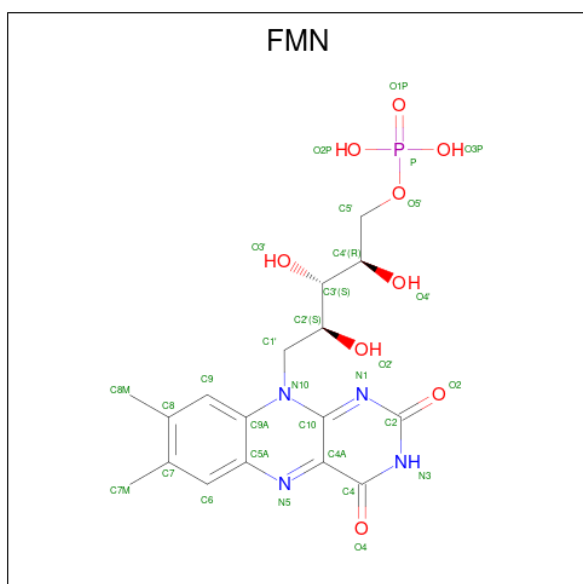
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

- 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	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

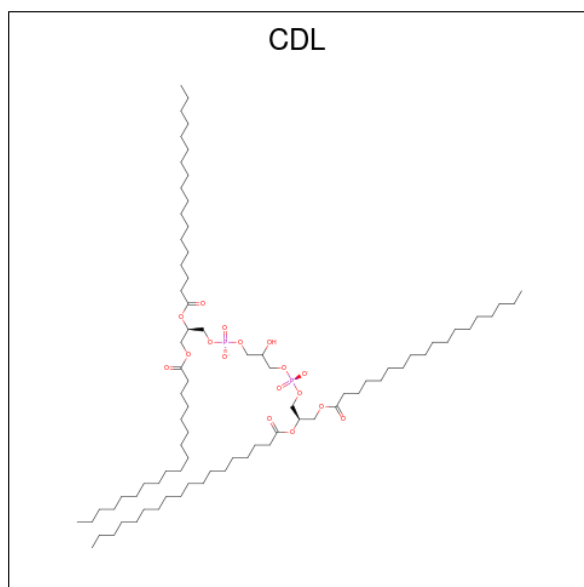


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

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



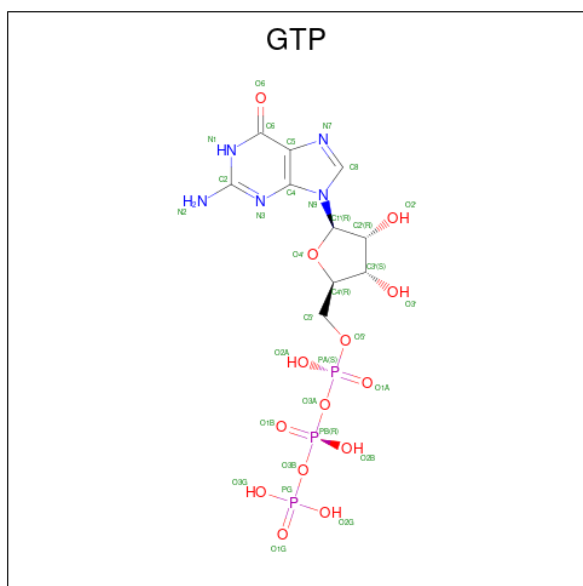
Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1h	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	3A	1	Total	C	O	P	0
			58	39	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	3G	1	Total	C	O	P	0
			52	33	17	2	
75	3G	1	Total	C	O	P	0
			56	37	17	2	
75	3N	1	Total	C	O	P	0
			43	24	17	2	
75	3P	1	Total	C	O	P	0
			56	37	17	2	
75	3T	1	Total	C	O	P	0
			57	38	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	8B	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: $C_{10}H_{16}N_5O_{14}P_3$).

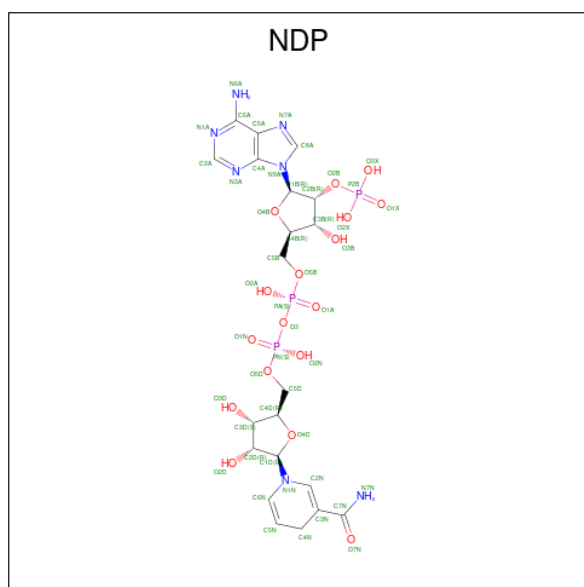


Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total 32	C 10	N 5	O 14	P 3	0

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

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

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



Mol	Chain	Residues	Atoms					AltConf
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 79 is ZINC ION (three-letter code: ZN) (formula: Zn).

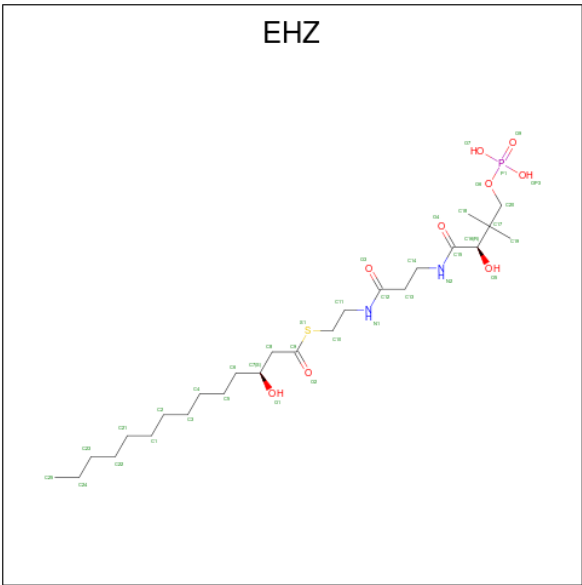
Mol	Chain	Residues	Atoms	AltConf
79	1R	1	Total Zn 1 1	0
79	4F	1	Total Zn 1 1	0

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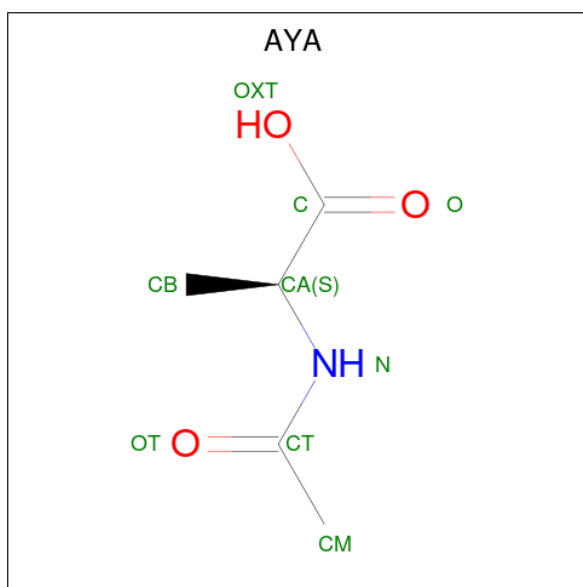
Mol	Chain	Residues	Atoms		AltConf
79	8F	1	Total	Zn	0
			1	1	

- Molecule 80 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



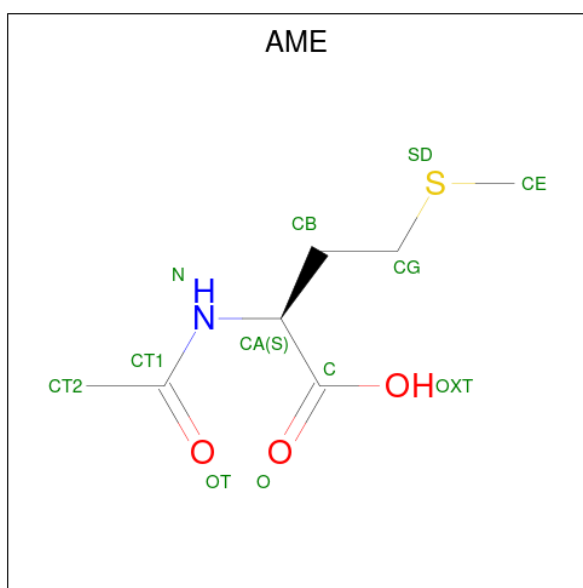
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 81 is N-ACETYLALANINE (three-letter code: AYA) (formula: C₅H₉NO₃).



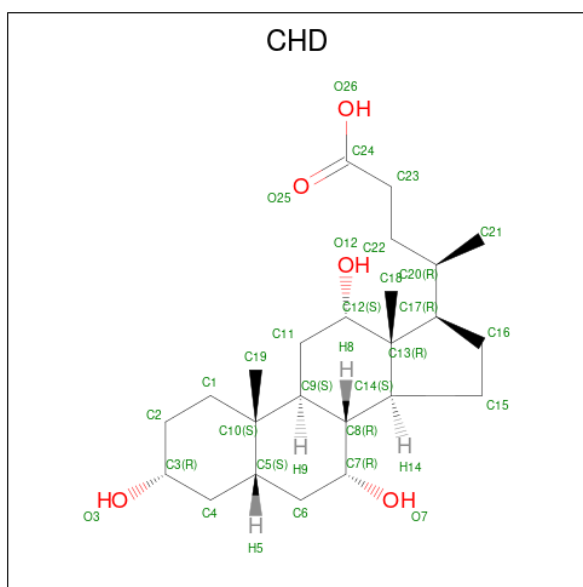
Mol	Chain	Residues	Atoms				AltConf
81	1Y	1	Total	C	N	O	0
			8	5	1	2	
81	1q	1	Total	C	N	O	0
			8	5	1	2	

- Molecule 82 is N-ACETYLMETHIONINE (three-letter code: AME) (formula: $C_7H_{13}NO_3S$).



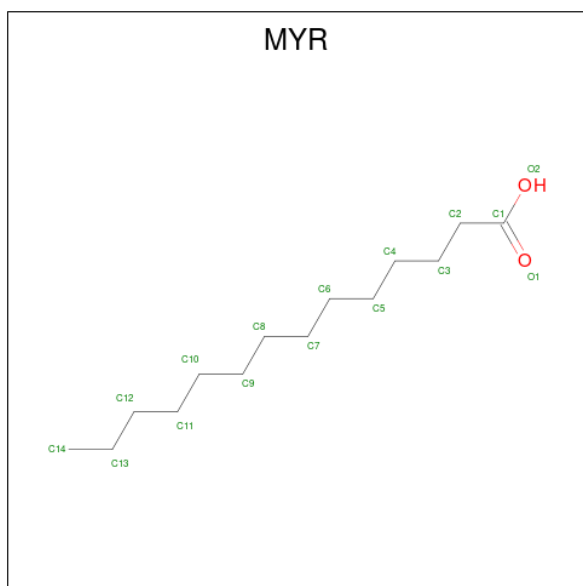
Mol	Chain	Residues	Atoms					AltConf
82	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 83 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



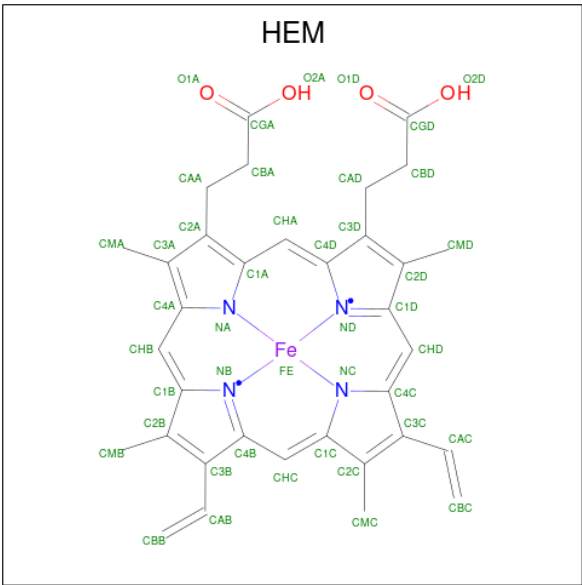
Mol	Chain	Residues	Atoms			AltConf
83	1i	1	Total	C	O	0
			29	24	5	

- Molecule 84 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



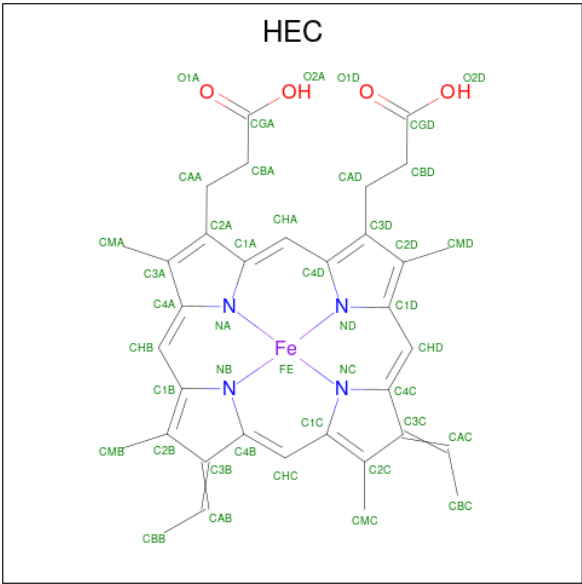
Mol	Chain	Residues	Atoms			AltConf
84	1l	1	Total	C	O	0
			15	14	1	

- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



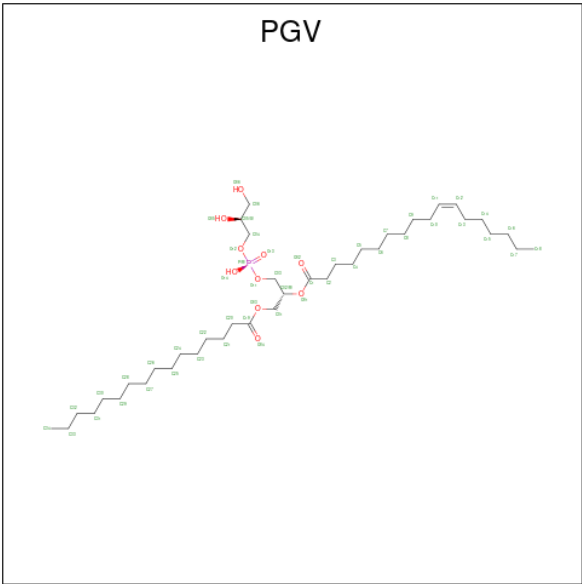
Mol	Chain	Residues	Atoms					AltConf
85	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 86 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
86	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 87 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).



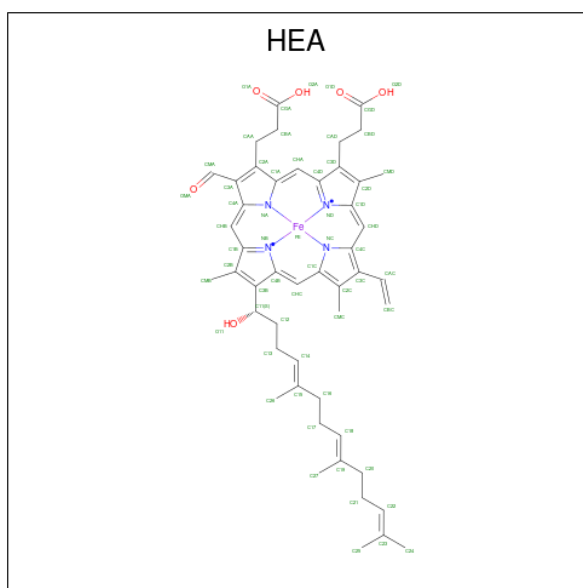
Mol	Chain	Residues	Atoms				AltConf
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4B	1	Total	C	O	P	0
			51	40	10	1	
87	4B	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
87	4C	1	Total 51	C 40	O 10	P 1	0
87	4G	1	Total 51	C 40	O 10	P 1	0
87	4J	1	Total 51	C 40	O 10	P 1	0
87	4K	1	Total 51	C 40	O 10	P 1	0
87	4L	1	Total 51	C 40	O 10	P 1	0
87	4M	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8B	1	Total 51	C 40	O 10	P 1	0
87	8B	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8G	1	Total 51	C 40	O 10	P 1	0
87	8J	1	Total 51	C 40	O 10	P 1	0
87	8K	1	Total 51	C 40	O 10	P 1	0
87	8L	1	Total 51	C 40	O 10	P 1	0

- Molecule 88 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
88	4A	1	Total	C	Fe	N	O
			60	49	1	4	6
88	4A	1	Total	C	Fe	N	O
			60	49	1	4	6
88	8A	1	Total	C	Fe	N	O
			60	49	1	4	6
88	8A	1	Total	C	Fe	N	O
			60	49	1	4	6

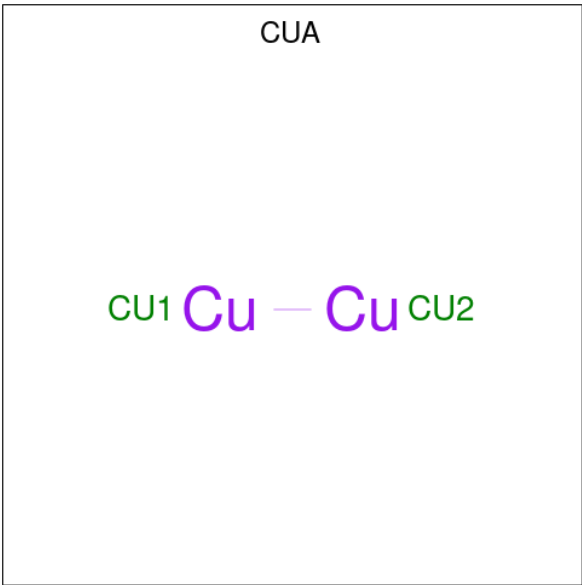
- Molecule 89 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 90 is SODIUM ION (three-letter code: NA) (formula: Na).

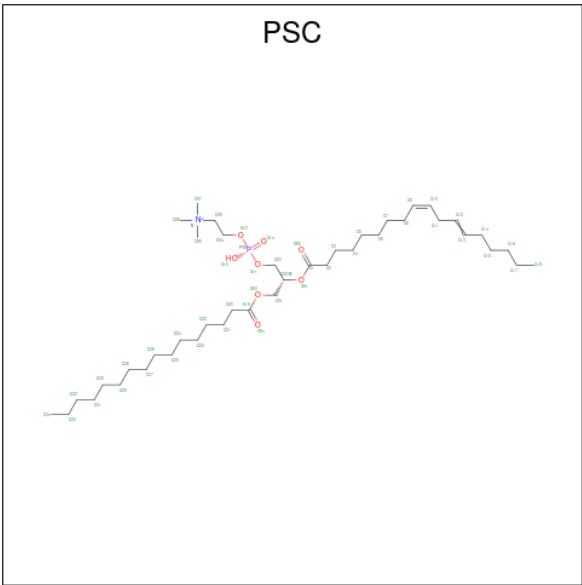
Mol	Chain	Residues	Atoms		AltConf
90	4A	1	Total	Na	0
			1	1	
90	8A	1	Total	Na	0
			1	1	

- Molecule 91 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
91	4B	1	Total	Cu	0
			2	2	
91	8B	1	Total	Cu	0
			2	2	

- Molecule 92 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).



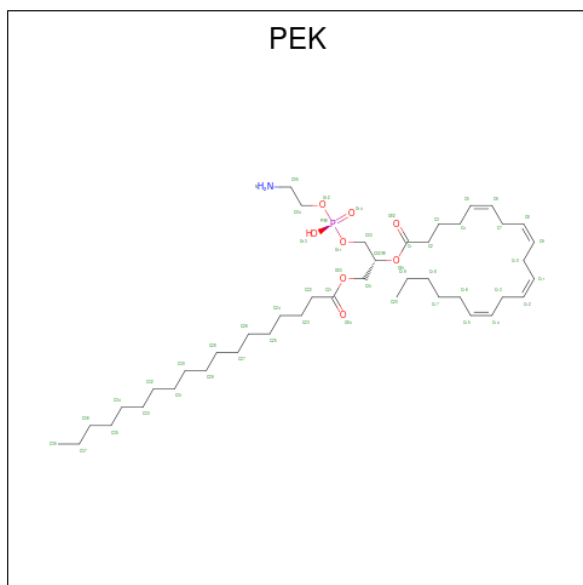
Mol	Chain	Residues	Atoms					AltConf
92	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
92	8B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 93 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
93	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
93	4G	1	Total	C	N	O	P	0
			53	43	1	8	1	
93	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	
93	8G	1	Total	C	N	O	P	0
			53	43	1	8	1	

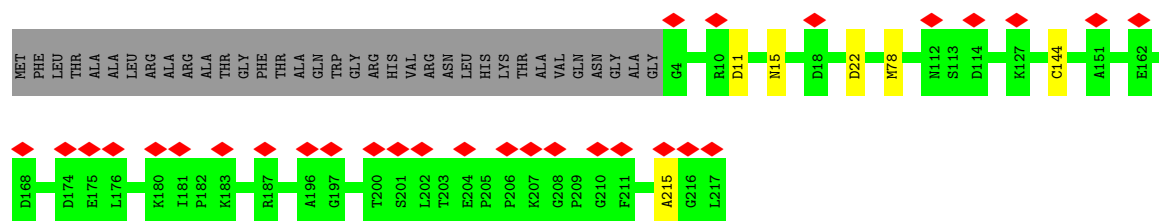
- Molecule 94 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
94	4H	1	Total	O	P	0
			5	4	1	
94	8H	1	Total	O	P	0
			5	4	1	

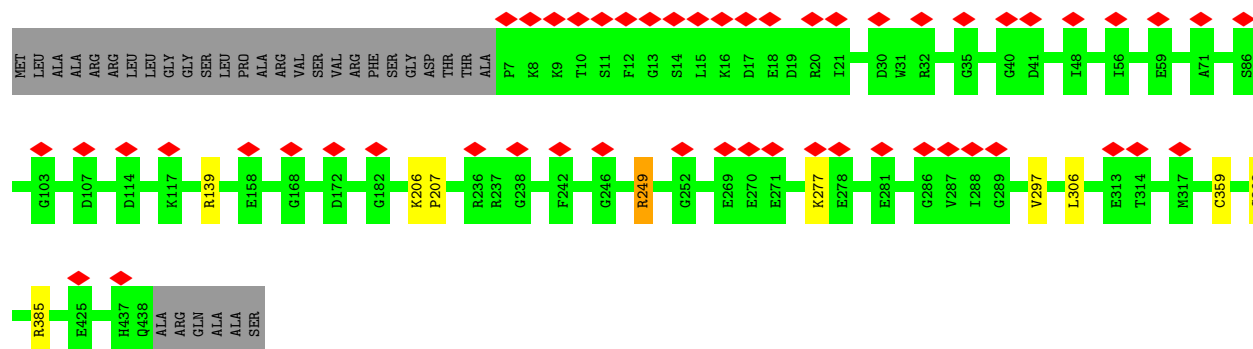
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 1E: 



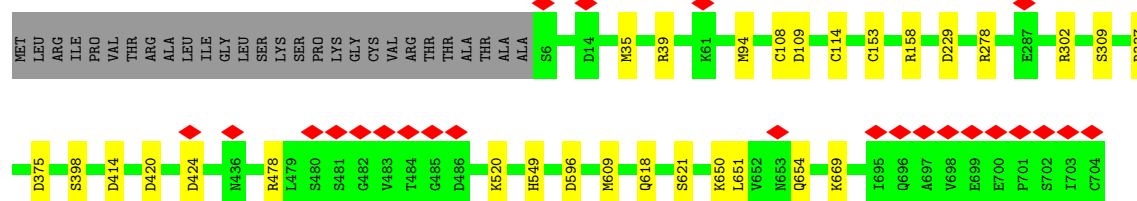
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F: 



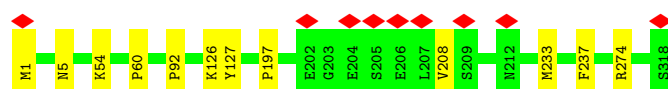
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G: 



- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

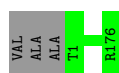
Chain 1H: 



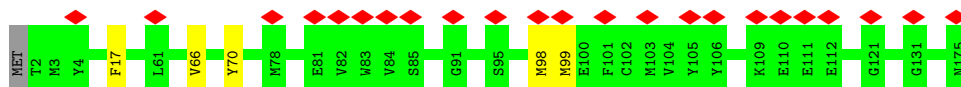
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 





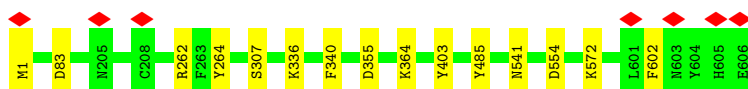
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



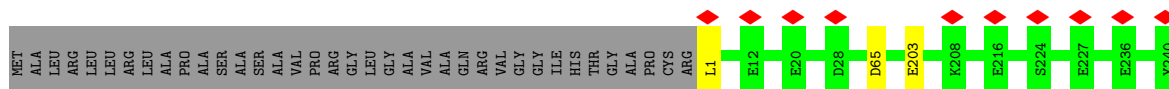
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

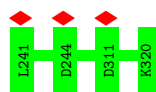


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



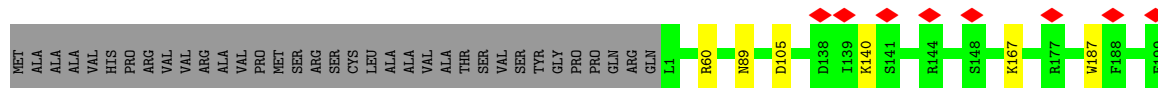
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





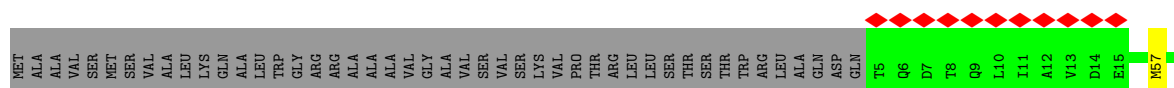
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P: 88% 9%



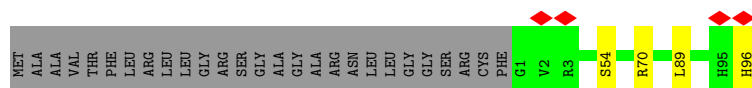
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q: 6% 71% 26%



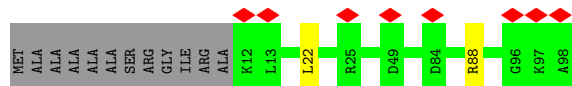
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R: 75% 22%



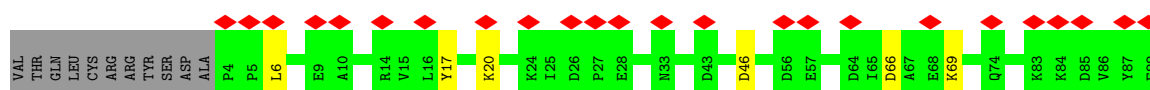
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S: 8% 86% 12%

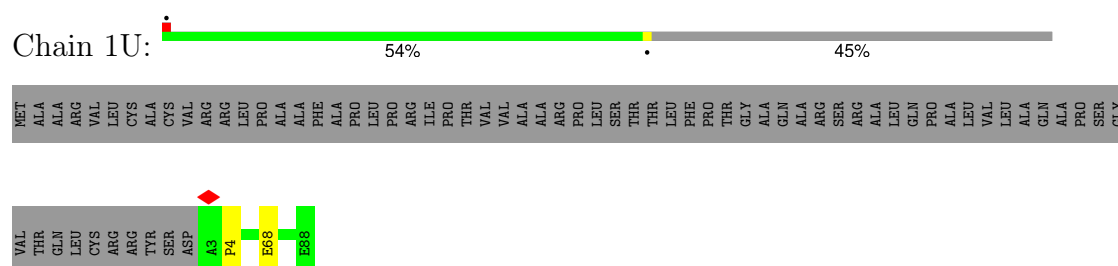


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

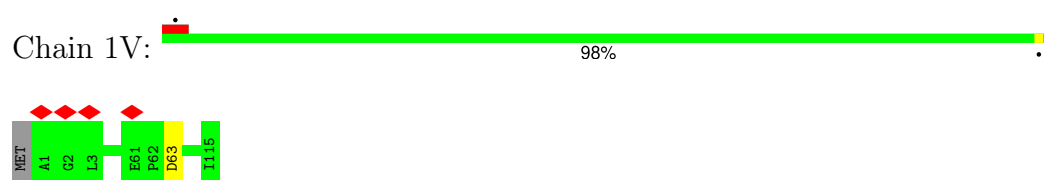
Chain 1T: 15% 51% 46%



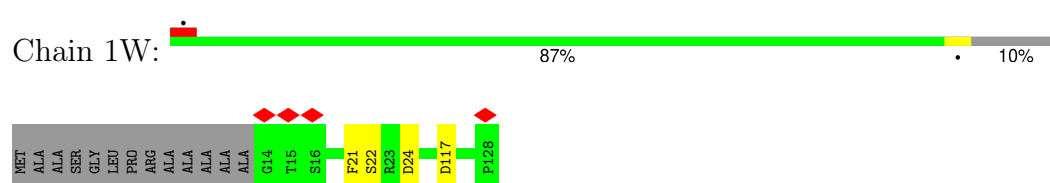
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



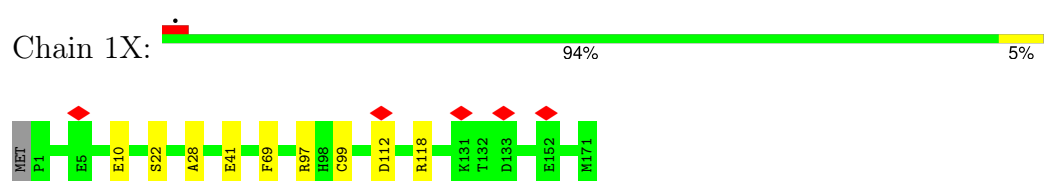
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



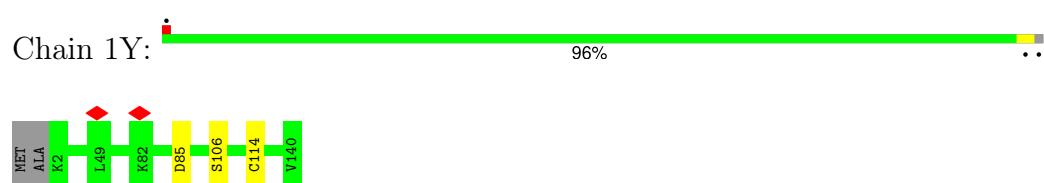
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



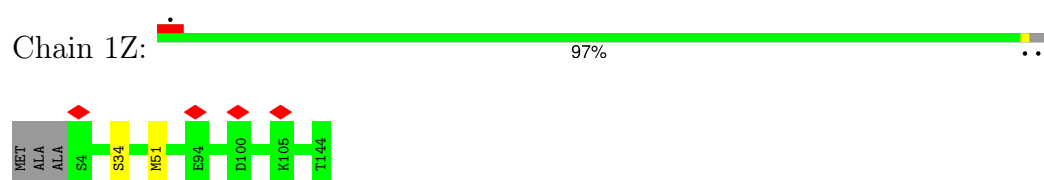
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



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

- Chain 1b:  7% 96% ..

The diagram shows a linear sequence of 100 residues, represented by colored blocks. The residues are grouped into segments: MET (grey), A1 (green), G2 (green), R3 (green), L34 (yellow), D59 (green), G60 (green), N61 (green), M62 (yellow), P63 (green), D64 (green), and L83 (green). Red diamonds indicate the positions of mutations: three diamonds are located above the A1 segment, one above the D59 segment, one above the N61 segment, and one above the P63 segment.

- Chain 1c: 63% 36%

NET
ALA
ALA
SER
ALA
LEU
PHE
ARG
PRO
PHE
SER
LYS
LEU
LEU
SER
SER
ARG
LEU
PRO
SER
GLY
SER
SER
ALA
ARG
SER
K1
E41
R44
E49

- Chain 1d:  96%

- Chain 1e:  5% 92% 7%

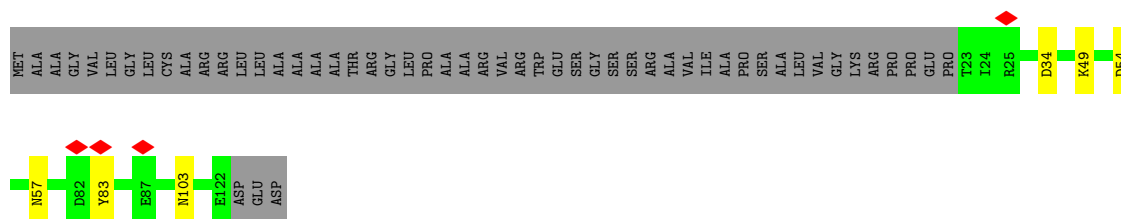
Diagram illustrating the structure of the 12S oxygen-binding domain of hemoglobin. The structure is shown as a ribbon diagram with various residues highlighted in yellow and red. Red diamonds indicate specific residues: R80, K87, E88, Y91, and H96. The residues are labeled as MET, P1, R8, R80, Q81, R82, K87, E88, Y91, H96, G99, LYS, GLU, ASP, PRO, ARG, and PRO.

- Chain 1f: 

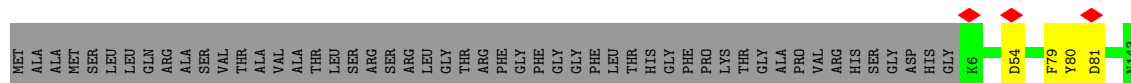
MET	ALA	ALA	ALA	ALA	ILE	LEU	LYS	LEU	GLU	GLY	THR	ARG	GLY	GLY	GLY	GLY	LYS	CYS	ASP	LYS	ASN	GLN	GLY	VAL	LYS	GLY	GLY	ARG	ARG	PHE	MET	ILE	SER	SER	ARG	SER	HIS	PRO	SER	SER	LEU	LEU	ALA	ALA	PRO	PRO	ASN	ASN	GLY	GLY	ARG	ARG	ARG	ARG	TRP	TRP	LEU	GLY	SER
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PRO	LEU	PRO	LEU	VAL	VAL	GLY	VAL	VAL	VAL	GLY	SER	GLU	ALA	ALA	ALA	PHE	MET	M1	N2	V3	L4	Q5	R8	D27	D31	N51	E52	E53	K57
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----

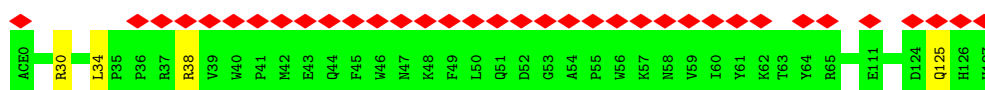
- Chain 1g:  61% 35%



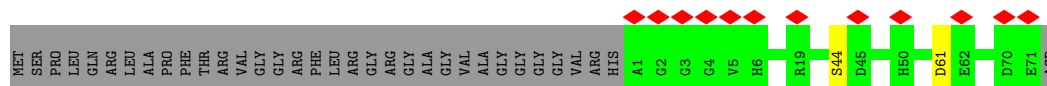
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



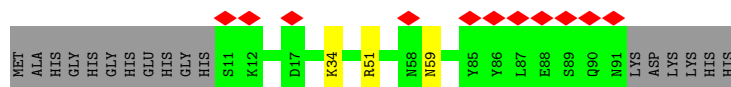
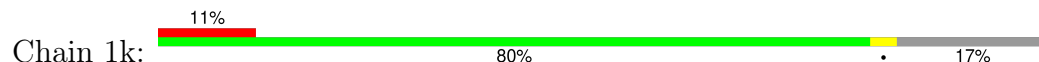
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



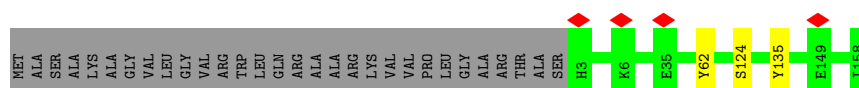
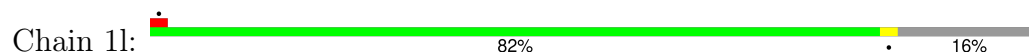
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



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



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



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

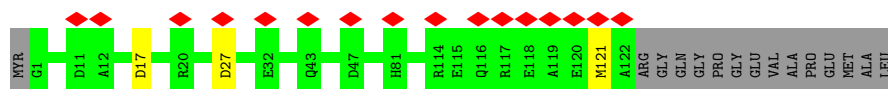
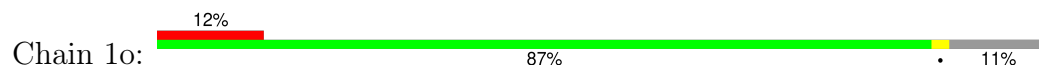




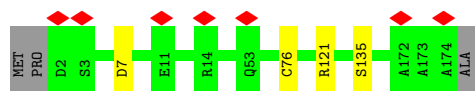
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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



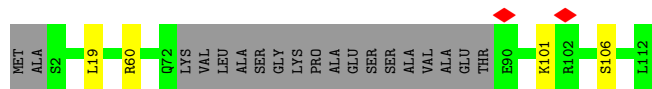
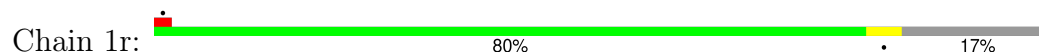
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



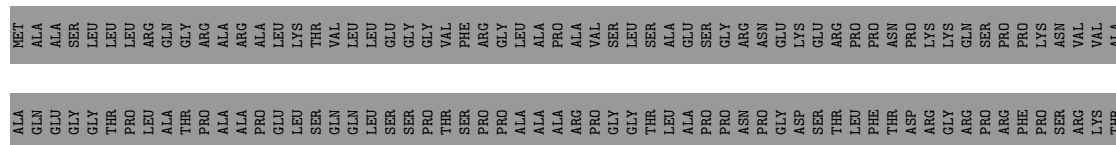
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

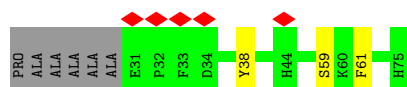


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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





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- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|------|------|------|------|------|
| MET | ALA | ALA | ALA | ALA | VAL | CYS | ARG | VAL | ALA | THR | GLY | SER | ARG | VAL | LEU | LEU | ARG | THR | CYS | ARG | SER | PRO | ALA | LEU | LEU | ARG | SER | PRO | ALA | ARG | GLY | THR | A2 | F58 | L112 | V117 | V224 | Y284 | F446 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|------|------|------|------|------|

- MET
 LYS
 LEU
 LEU
 ILE
 THR
 ARG
 ALA
 GLY
 SER
 PHE
 SER
 ARG
 ARG
 PHE
 TYR
 SER
 LYS
 LEU
 VAL
 ALA
 ALA
 PRO
 LYS
 LYS
 LEU
 LEU
 ALA
 ALA
 SER
 ALA
 ALA
 PRO
 GLY
 VAL
 PRO
 LEU
 LEU
 GLN
 P21
 D189
 R227
 G228
 K301
 S315
 N354
 E438
 LFT

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|------|------|-----|
| MET | LYS | LEU | ILE | THR | ARG | ALA | GLY | SER | PHE | SER | ARG | PHE | TYR | SER | LEU | LYS | VAL | ALA | PRO | LYS | ALA | LEU | ALA | SER | ALA | ALA | PRO | ALA | GLY | VAL | PRO | LEU | GLN | PRO | Q22 | S60 | A171 | F223 | M26 | E260 | F438 | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|------|------|-----|

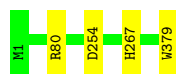
- 

Chain 3C:  98%



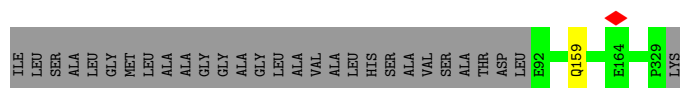
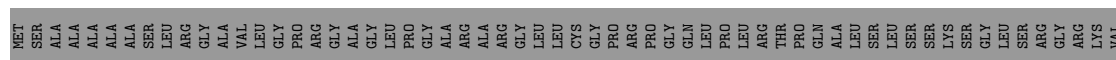
- Molecule 47: Cytochrome b

Chain 3P:  99%



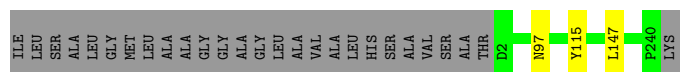
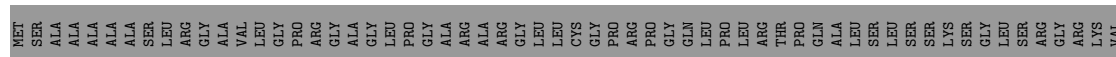
- Molecule 48: Cytochrome c1

Chain 3D:  72%  27%



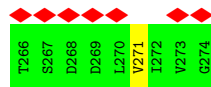
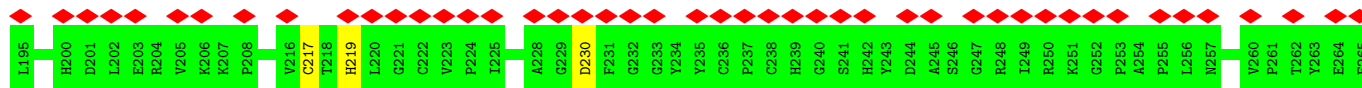
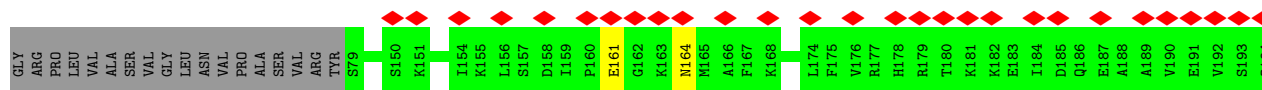
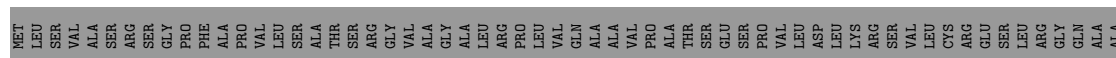
- Molecule 48: Cytochrome c1

Chain 3Q:  72%  27%

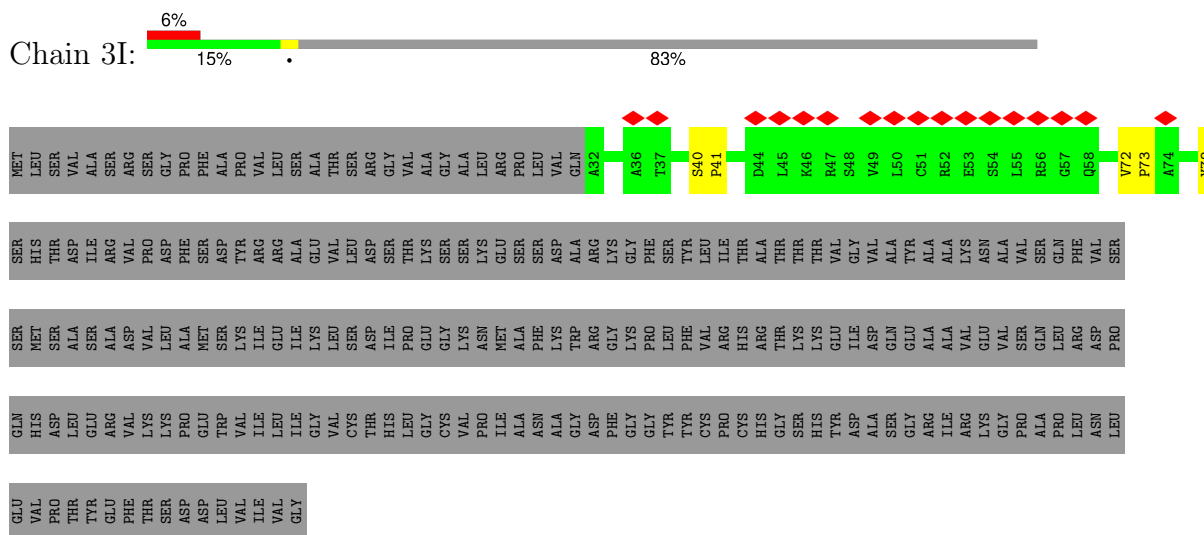


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3E:  30%  69%  28%



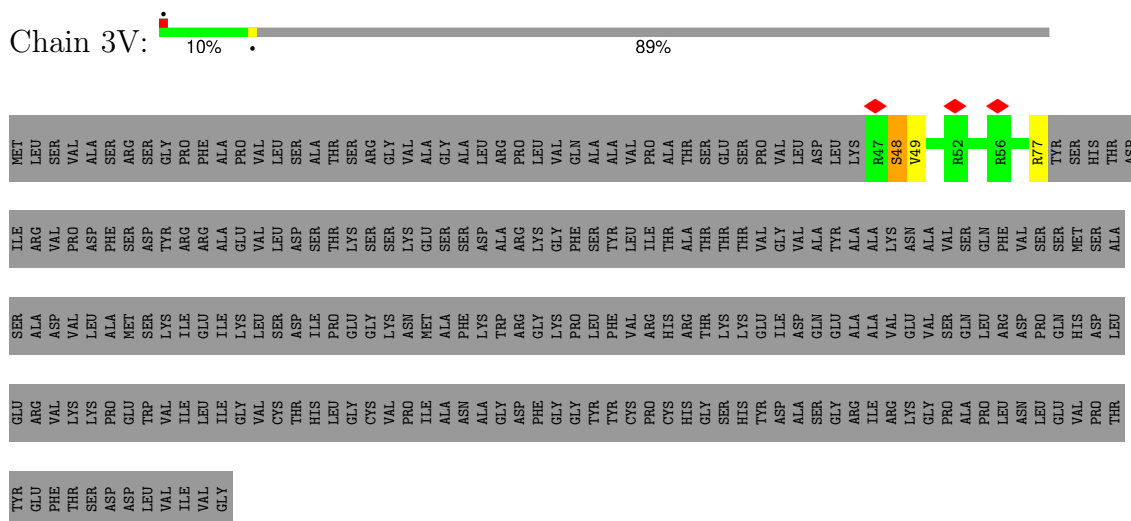
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial




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

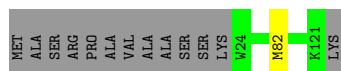


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial




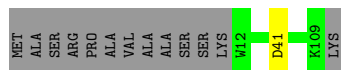
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3F:  87% 12%



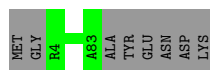
- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3S:  87% 12%



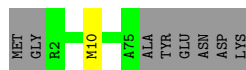
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3G:  90% 10%



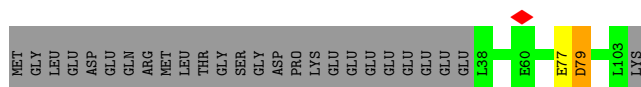
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T:  89% 10%



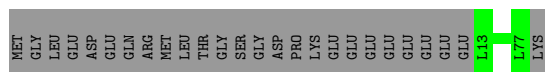
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H:  69% 29%




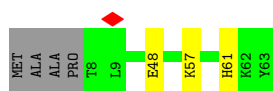
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U:  71% 29%



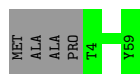
- Molecule 53: Complex III subunit 9

Chain 3J:  88% 5% 7%



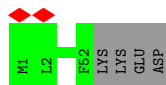
- Molecule 53: Complex III subunit 9

Chain 3W:  93% 7%




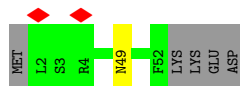
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X:  93% 7%



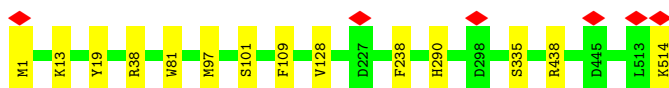
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y:  89% 9%



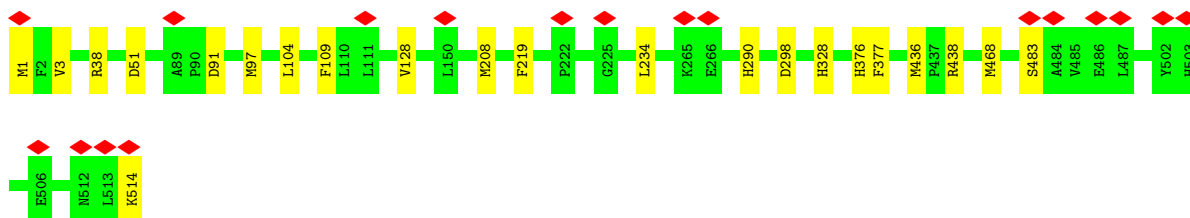
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A:  97%



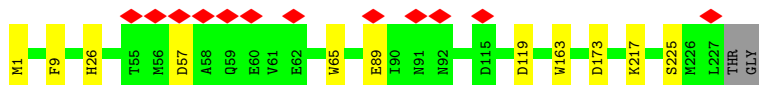
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 8A:  96%



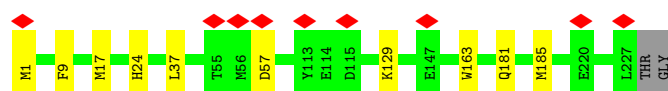
- Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B:  5% 94% 5%



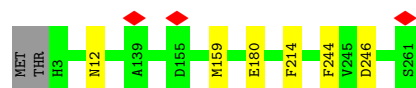
- Molecule 56: Cytochrome c oxidase subunit 2

Chain 8B:  95%



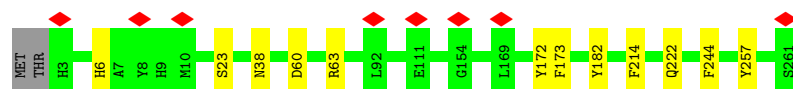
- Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C:  97%




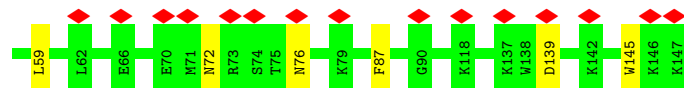
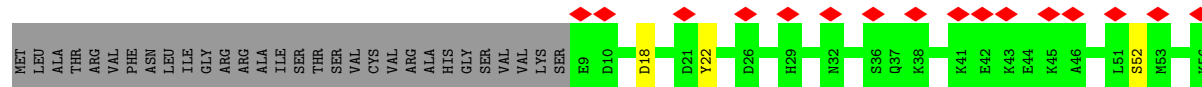
- Molecule 57: Cytochrome c oxidase subunit 3

Chain 8C:  95%




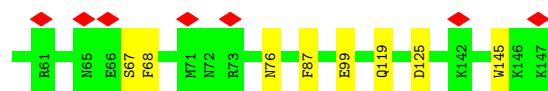
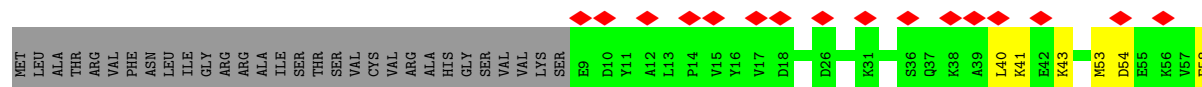
- Molecule 58: Cytochrome c oxidase subunit 4

Chain 4D:  77%



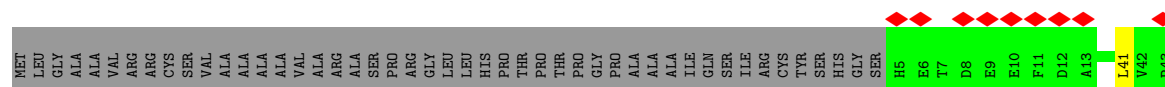
- Molecule 58: Cytochrome c oxidase subunit 4

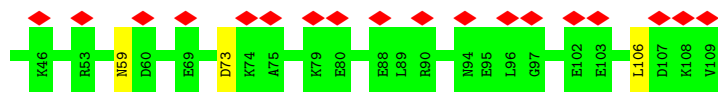
Chain 8D:  74%



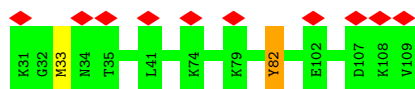
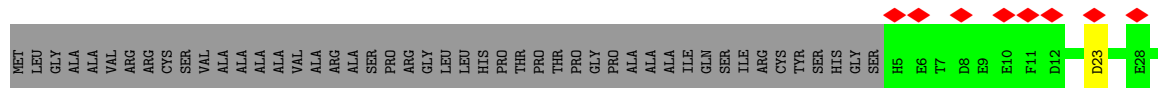
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 4E:  66%

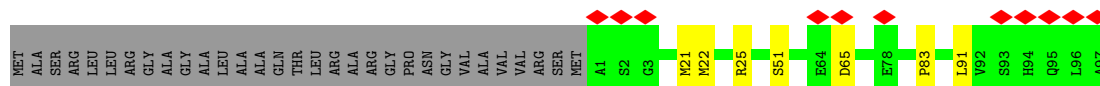




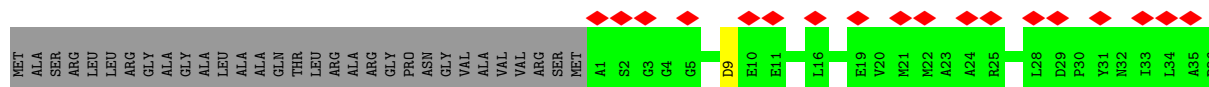
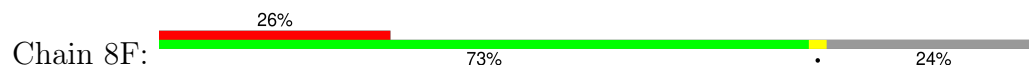
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



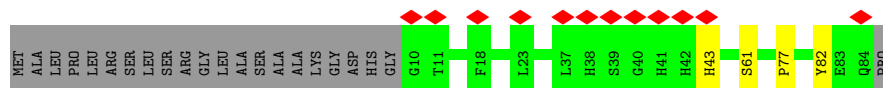
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



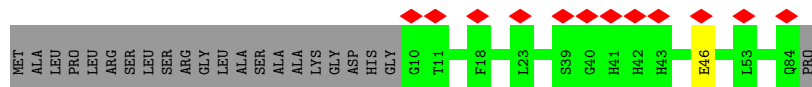
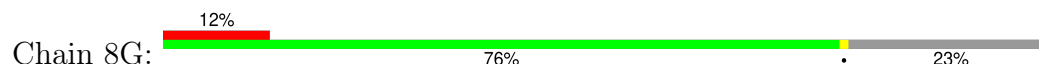
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



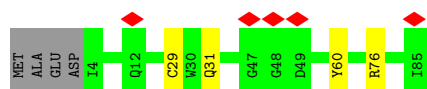
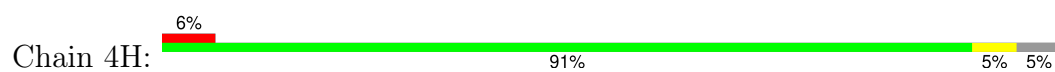
- Molecule 61: Cytochrome c oxidase subunit 6A2



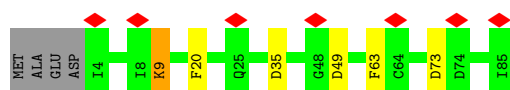
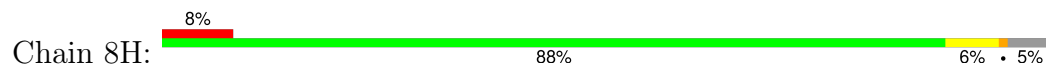
- Molecule 61: Cytochrome c oxidase subunit 6A2



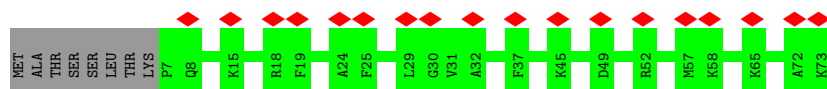
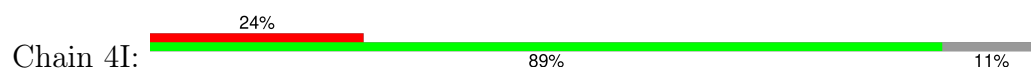
- Molecule 62: Cytochrome c oxidase subunit 6B1



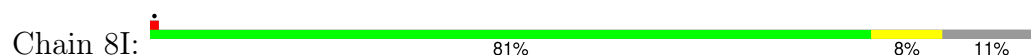
- Molecule 62: Cytochrome c oxidase subunit 6B1



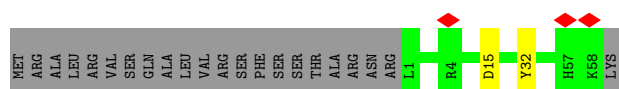
- Molecule 63: Cytochrome c oxidase subunit 6C



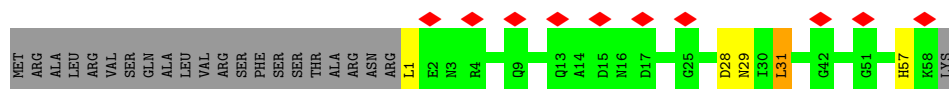
- Molecule 63: Cytochrome c oxidase subunit 6C



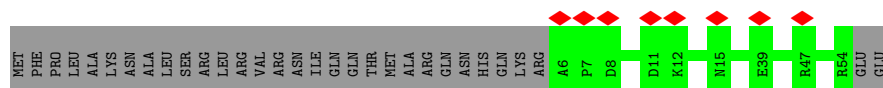
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



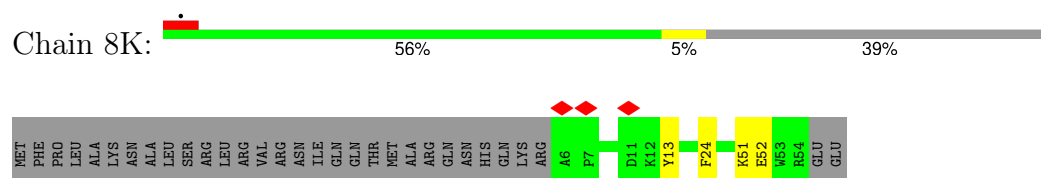
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



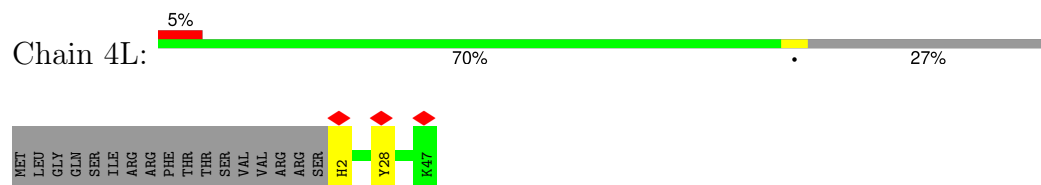
- Molecule 65: Cytochrome c oxidase subunit 7B



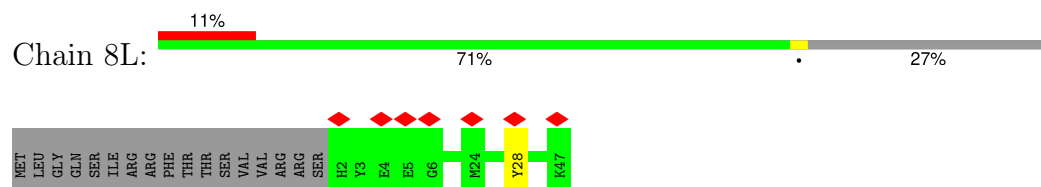
● Molecule 65: Cytochrome c oxidase subunit 7B



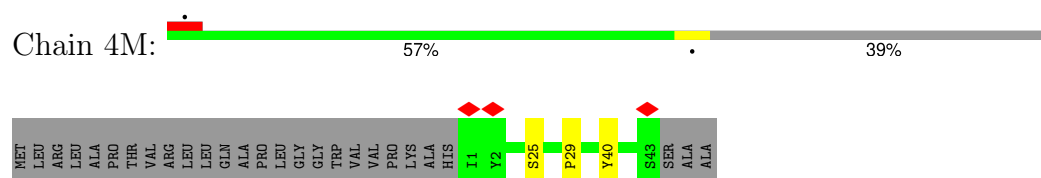
● Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



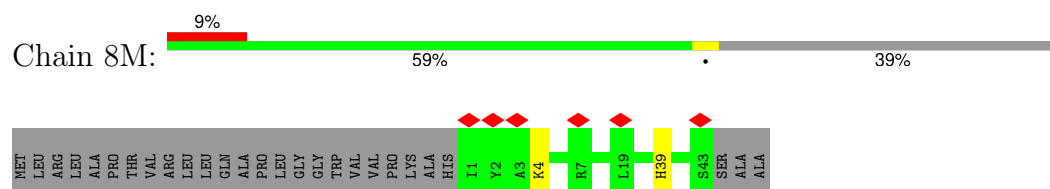
● Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



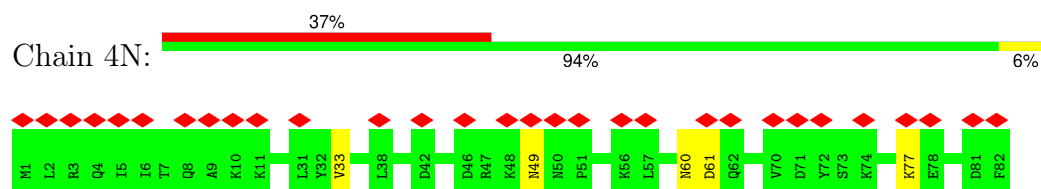
● Molecule 67: Cytochrome c oxidase subunit 8



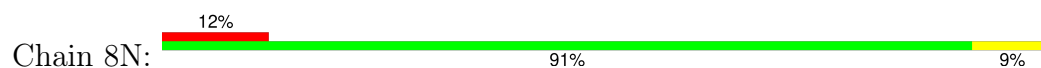
● Molecule 67: Cytochrome c oxidase subunit 8

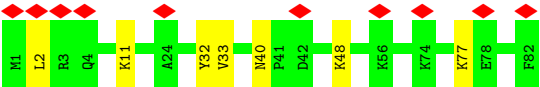


● Molecule 68: Cytochrome c oxidase subunit NDUF4A



● 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	320000	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	1.149	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	572.0, 572.0, 572.0	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.35	1/930 (0.1%)	0.50	0/1271
2	1B	0.27	0/1273	0.53	0/1722
3	1C	0.26	0/1791	0.50	0/2439
4	1D	0.26	0/3545	0.48	0/4806
5	1E	0.27	0/1698	0.49	0/2311
6	1F	0.27	0/3401	0.51	0/4595
7	1G	0.26	0/5451	0.51	0/7387
8	1H	0.30	0/2566	0.49	1/3509 (0.0%)
9	1I	0.26	0/1443	0.50	0/1952
10	1J	0.28	0/1364	0.48	0/1850
11	1K	0.26	0/751	0.51	0/1018
12	1L	0.27	0/4939	0.45	0/6718
13	1M	0.25	0/3713	0.45	0/5063
14	1N	0.27	0/2765	0.45	0/3758
15	1O	0.26	0/2650	0.49	0/3588
16	1P	0.27	0/2828	0.51	0/3834
17	1Q	0.26	0/1070	0.51	0/1446
18	1R	0.27	0/755	0.53	0/1018
19	1S	0.27	0/711	0.61	0/956
20	1T	0.28	0/701	0.49	0/946
20	1U	0.41	0/706	0.54	1/954 (0.1%)
21	1V	0.24	0/946	0.43	0/1281
22	1W	0.29	0/995	0.53	0/1340
23	1X	0.26	0/1436	0.51	0/1938
24	1Y	0.25	0/1037	0.45	0/1404
25	1Z	0.27	0/1199	0.51	0/1617
26	1a	0.26	0/577	0.51	0/777
27	1b	0.27	0/664	0.49	1/912 (0.1%)
28	1c	0.27	0/430	0.45	0/581
29	1d	0.26	0/1016	0.47	0/1374
30	1e	0.25	0/836	0.50	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	1f	0.26	0/499	0.57	0/673
32	1g	0.28	0/858	0.52	0/1165
33	1h	0.27	0/1184	0.50	0/1603
34	1i	0.26	0/1138	0.50	0/1551
35	1j	0.26	0/627	0.48	0/858
36	1k	0.32	0/668	0.49	0/903
37	1l	0.26	0/1365	0.50	0/1867
38	1m	0.35	1/1092 (0.1%)	0.52	0/1481
39	1n	0.44	2/1549 (0.1%)	0.73	2/2098 (0.1%)
40	1o	0.26	0/1069	0.57	0/1430
41	1p	0.25	0/1481	0.53	0/1997
42	1q	0.26	0/1253	0.52	0/1704
43	1r	0.29	0/777	0.57	0/1051
44	1s	0.25	0/394	0.52	0/533
45	3A	0.25	0/3481	0.48	0/4722
45	3N	0.25	0/3496	0.49	0/4723
46	3B	0.25	0/3190	0.47	0/4317
46	3O	0.26	0/3175	0.47	0/4292
47	3C	0.26	0/3123	0.44	0/4269
47	3P	0.26	0/3122	0.43	0/4269
48	3D	0.26	0/1946	0.48	0/2641
48	3Q	0.26	0/1962	0.48	0/2663
49	3E	0.27	0/1551	0.52	0/2098
49	3I	1.46	3/344 (0.9%)	1.87	8/468 (1.7%)
49	3R	0.58	2/1551 (0.1%)	0.80	2/2098 (0.1%)
49	3V	1.18	2/225 (0.9%)	2.23	4/303 (1.3%)
50	3F	0.24	0/888	0.48	0/1193
50	3S	0.24	0/888	0.48	0/1193
51	3G	0.25	0/649	0.52	0/878
51	3T	0.27	0/649	0.52	0/878
52	3H	0.30	0/539	0.67	1/724 (0.1%)
52	3U	0.27	0/539	0.54	0/724
53	3J	0.45	1/476 (0.2%)	0.56	0/641
53	3W	0.33	0/476	0.49	0/641
54	3X	0.23	0/445	0.48	0/608
54	3Y	0.24	0/437	0.50	0/598
55	4A	0.28	0/4156	0.44	0/5679
55	8A	0.38	2/4156 (0.0%)	0.54	4/5679 (0.1%)
56	4B	0.37	2/1865 (0.1%)	0.52	0/2544
56	8B	0.29	0/1865	0.59	1/2544 (0.0%)
57	4C	0.37	2/2179 (0.1%)	0.46	1/2981 (0.0%)
57	8C	0.31	0/2179	0.49	0/2981
58	4D	0.27	0/1197	0.50	0/1617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
58	8D	0.41	1/1197 (0.1%)	0.60	1/1617 (0.1%)
59	4E	0.31	0/871	0.62	0/1182
59	8E	0.43	1/871 (0.1%)	0.66	1/1182 (0.1%)
60	4F	0.33	0/749	0.67	1/1016 (0.1%)
60	8F	0.26	0/749	0.51	0/1016
61	4G	0.30	0/644	0.59	1/881 (0.1%)
61	8G	0.24	0/644	0.49	0/881
62	4H	0.27	0/708	0.48	0/956
62	8H	0.39	1/708 (0.1%)	0.56	0/956
63	4I	0.30	0/563	0.61	0/748
63	8I	0.33	0/563	0.60	1/748 (0.1%)
64	4J	0.27	0/466	0.51	0/631
64	8J	0.29	0/466	0.56	1/631 (0.2%)
65	4K	0.27	0/396	0.54	0/543
65	8K	0.30	0/396	0.58	0/543
66	4L	0.29	0/394	0.51	0/528
66	8L	0.37	0/394	0.51	0/528
67	4M	0.42	1/349 (0.3%)	0.61	1/477 (0.2%)
67	8M	0.46	0/349	0.61	0/477
68	4N	0.27	0/680	0.47	0/921
68	8N	0.35	0/680	0.61	0/921
All	All	0.30	22/131727 (0.0%)	0.53	33/178746 (0.0%)

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
6	1F	0	1
49	3V	0	1
68	8N	0	1
All	All	0	3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	3I	73	PRO	CG-CD	-20.55	0.82	1.50
49	3R	173	PRO	N-CD	16.09	1.70	1.47
49	3V	49	VAL	C-N	15.60	1.70	1.34
49	3I	73	PRO	N-CD	13.18	1.66	1.47
39	1n	144	PRO	N-CD	10.90	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	8A	483	SER	CB-OG	-10.24	1.28	1.42
49	3R	173	PRO	CG-CD	-9.45	1.19	1.50
57	4C	180	GLU	CD-OE1	-8.48	1.16	1.25
57	4C	159	MET	CG-SD	-8.11	1.60	1.81
56	4B	89	GLU	CD-OE1	-7.39	1.17	1.25
1	1A	18	VAL	CB-CG2	-7.16	1.37	1.52
49	3I	72	VAL	C-O	7.12	1.36	1.23
62	8H	9	LYS	CE-NZ	-6.52	1.32	1.49
38	1m	117	GLU	CD-OE1	-6.51	1.18	1.25
53	3J	48	GLU	CD-OE2	-6.36	1.18	1.25
39	1n	144	PRO	N-CA	-6.19	1.36	1.47
49	3V	48	SER	C-N	-6.16	1.19	1.34
59	8E	82	TYR	CE2-CZ	-6.08	1.30	1.38
58	8D	99	GLU	CD-OE2	-5.71	1.19	1.25
56	4B	65	TRP	CZ3-CH2	-5.64	1.31	1.40
55	8A	219	PHE	CG-CD1	-5.35	1.30	1.38
67	4M	40	TYR	CD2-CE2	-5.01	1.31	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3V	49	VAL	O-C-N	-27.17	79.22	122.70
49	3R	173	PRO	CA-N-CD	-22.76	79.64	111.50
49	3V	49	VAL	CA-C-N	19.61	160.33	117.20
39	1n	144	PRO	CA-N-CD	-19.35	84.41	111.50
49	3I	73	PRO	CB-CG-CD	18.83	179.94	106.50
49	3I	73	PRO	N-CD-CG	-18.09	76.06	103.20
49	3V	49	VAL	C-N-CA	13.30	154.96	121.70
49	3I	41	PRO	CA-N-CD	-12.82	93.55	111.50
49	3I	73	PRO	CA-CB-CG	-12.76	79.75	104.00
60	4F	83	PRO	CA-N-CD	-12.72	93.69	111.50
49	3R	172	LYS	C-N-CD	11.81	153.20	128.40
49	3I	73	PRO	CA-N-CD	-11.57	95.30	111.50
49	3I	40	SER	C-N-CD	-10.80	96.84	120.60
49	3I	72	VAL	C-N-CD	9.35	148.03	128.40
39	1n	143	THR	C-N-CD	9.01	147.32	128.40
49	3V	48	SER	C-N-CA	-8.48	100.50	121.70
52	3H	77	GLU	C-N-CA	8.01	141.71	121.70
59	8E	82	TYR	CZ-CE2-CD2	7.96	126.96	119.80
55	8A	208	MET	CG-SD-CE	-7.69	87.90	100.20
8	1H	60	PRO	CA-N-CD	-7.50	101.00	111.50
55	8A	208	MET	CB-CG-SD	6.52	131.97	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	8A	234	LEU	CA-CB-CG	6.52	130.29	115.30
56	8B	37	LEU	CA-CB-CG	6.11	129.35	115.30
20	1U	4	PRO	CA-N-CD	-6.03	103.06	111.50
61	4G	77	PRO	CA-N-CD	-5.80	103.39	111.50
55	8A	104	LEU	CA-CB-CG	5.79	128.63	115.30
63	8I	17	LEU	CA-CB-CG	5.35	127.61	115.30
58	8D	40	LEU	CB-CG-CD2	-5.34	101.92	111.00
49	3I	41	PRO	N-CD-CG	-5.26	95.31	103.20
67	4M	40	TYR	CZ-CE2-CD2	5.25	124.53	119.80
64	8J	31	LEU	CA-CB-CG	5.20	127.25	115.30
57	4C	159	MET	CG-SD-CE	5.06	108.30	100.20
27	1b	34	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
49	3V	48	SER	Mainchain
68	8N	48	LYS	Peptide

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%)	103 (91%)	8 (7%)	2 (2%)	7	6
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	199 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1D	427/476 (90%)	412 (96%)	15 (4%)	0	100	100
5	1E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	25	32
6	1F	430/464 (93%)	402 (94%)	25 (6%)	3 (1%)	19	23
7	1G	697/727 (96%)	668 (96%)	28 (4%)	1 (0%)	48	60
8	1H	316/318 (99%)	294 (93%)	20 (6%)	2 (1%)	22	27
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	22	27
11	1K	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	13	15
12	1L	604/606 (100%)	563 (93%)	41 (7%)	0	100	100
13	1M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	1N	345/347 (99%)	335 (97%)	9 (3%)	1 (0%)	37	47
15	1O	318/357 (89%)	305 (96%)	13 (4%)	0	100	100
16	1P	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	1T	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
23	1X	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	22	27
24	1Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
25	1Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	5 (9%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	8 (8%)	0	100	100
33	1h	136/189 (72%)	136 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	1i	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	1m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100
40	1o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
45	3A	436/480 (91%)	428 (98%)	6 (1%)	2 (0%)	25	32
45	3N	444/480 (92%)	427 (96%)	16 (4%)	1 (0%)	44	55
46	3B	414/453 (91%)	403 (97%)	11 (3%)	0	100	100
46	3O	413/453 (91%)	404 (98%)	8 (2%)	1 (0%)	44	55
47	3C	377/379 (100%)	366 (97%)	11 (3%)	0	100	100
47	3P	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
48	3D	235/326 (72%)	229 (97%)	6 (3%)	0	100	100
48	3Q	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
49	3E	194/274 (71%)	177 (91%)	16 (8%)	1 (0%)	25	32
49	3I	45/274 (16%)	43 (96%)	2 (4%)	0	100	100
49	3R	194/274 (71%)	172 (89%)	18 (9%)	4 (2%)	5	5
49	3V	29/274 (11%)	29 (100%)	0	0	100	100
50	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	3S	96/111 (86%)	96 (100%)	0	0	100	100
51	3G	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	63/91 (69%)	62 (98%)	0	1 (2%)	8	7
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/60 (90%)	52 (96%)	1 (2%)	1 (2%)	6	6
53	3W	54/60 (90%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	3X	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
55	4A	512/514 (100%)	497 (97%)	14 (3%)	1 (0%)	44	55
55	8A	512/514 (100%)	497 (97%)	13 (2%)	2 (0%)	30	39
56	4B	225/229 (98%)	215 (96%)	10 (4%)	0	100	100
56	8B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
58	8D	137/169 (81%)	132 (96%)	5 (4%)	0	100	100
59	4E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
59	8E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
60	4F	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
60	8F	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	75 (94%)	5 (6%)	0	100	100
62	8H	80/86 (93%)	74 (92%)	6 (8%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
63	8I	65/75 (87%)	64 (98%)	1 (2%)	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%)	44 (94%)	3 (6%)	0	100	100
65	8K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
66	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
66	8L	44/63 (70%)	44 (100%)	0	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	10	11
68	8N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	10	11
All	All	15889/19086 (83%)	15257 (96%)	603 (4%)	29 (0%)	45	55

All (29) Ramachandran outliers are listed below:

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
1	1A	52	SER
8	1H	208	VAL
49	3R	181	LYS
49	3R	228	ALA
68	8N	33	VAL
1	1A	109	LYS
6	1F	249	ARG
6	1F	297	VAL
49	3R	273	VAL
68	4N	33	VAL
46	3O	171	ALA
49	3R	150	SER
7	1G	654	GLN
11	1K	2	PRO
45	3A	231	PHE
5	1E	215	ALA
6	1F	207	PRO
45	3A	350	THR
52	3H	79	ASP
55	8A	128	VAL
55	4A	128	VAL
55	8A	3	VAL
14	1N	110	PRO

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%)	20 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1B	131/212 (62%)	123 (94%)	8 (6%)	15	22
3	1C	190/227 (84%)	187 (98%)	3 (2%)	58	74
4	1D	371/405 (92%)	363 (98%)	8 (2%)	47	65
5	1E	183/207 (88%)	178 (97%)	5 (3%)	40	57
6	1F	346/368 (94%)	339 (98%)	7 (2%)	50	68
7	1G	588/610 (96%)	560 (95%)	28 (5%)	21	32
8	1H	274/274 (100%)	266 (97%)	8 (3%)	37	54
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/141 (99%)	136 (97%)	4 (3%)	37	54
11	1K	84/84 (100%)	79 (94%)	5 (6%)	16	23
12	1L	539/539 (100%)	525 (97%)	14 (3%)	41	58
13	1M	408/408 (100%)	402 (98%)	6 (2%)	60	76
14	1N	310/310 (100%)	306 (99%)	4 (1%)	65	79
15	1O	283/307 (92%)	280 (99%)	3 (1%)	70	83
16	1P	296/323 (92%)	284 (96%)	12 (4%)	26	39
17	1Q	117/152 (77%)	112 (96%)	5 (4%)	25	36
18	1R	79/97 (81%)	75 (95%)	4 (5%)	20	29
19	1S	77/82 (94%)	75 (97%)	2 (3%)	41	58
20	1T	79/133 (59%)	73 (92%)	6 (8%)	11	14
20	1U	79/133 (59%)	78 (99%)	1 (1%)	65	79
21	1V	100/101 (99%)	99 (99%)	1 (1%)	73	85
22	1W	107/112 (96%)	103 (96%)	4 (4%)	29	43
23	1X	153/154 (99%)	145 (95%)	8 (5%)	19	28
24	1Y	101/102 (99%)	98 (97%)	3 (3%)	36	52
25	1Z	123/124 (99%)	121 (98%)	2 (2%)	58	74
26	1a	58/58 (100%)	57 (98%)	1 (2%)	56	72
27	1b	69/70 (99%)	68 (99%)	1 (1%)	62	77
28	1c	45/66 (68%)	44 (98%)	1 (2%)	47	65
29	1d	106/109 (97%)	104 (98%)	2 (2%)	52	69
30	1e	87/94 (93%)	85 (98%)	2 (2%)	45	63
31	1f	54/113 (48%)	53 (98%)	1 (2%)	52	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	1g	92/129 (71%)	86 (94%)	6 (6%)	14	20
33	1h	121/158 (77%)	117 (97%)	4 (3%)	33	48
34	1i	120/120 (100%)	116 (97%)	4 (3%)	33	48
35	1j	62/84 (74%)	60 (97%)	2 (3%)	34	50
36	1k	63/76 (83%)	60 (95%)	3 (5%)	21	32
37	1l	141/161 (88%)	138 (98%)	3 (2%)	48	66
38	1m	113/114 (99%)	107 (95%)	6 (5%)	19	28
39	1n	156/160 (98%)	151 (97%)	5 (3%)	34	50
40	1o	110/119 (92%)	107 (97%)	3 (3%)	40	57
41	1p	154/156 (99%)	150 (97%)	4 (3%)	41	58
42	1q	131/131 (100%)	125 (95%)	6 (5%)	23	33
43	1r	85/98 (87%)	81 (95%)	4 (5%)	22	32
44	1s	44/351 (12%)	41 (93%)	3 (7%)	13	18
45	3A	367/397 (92%)	362 (99%)	5 (1%)	62	77
45	3N	372/397 (94%)	368 (99%)	4 (1%)	70	83
46	3B	328/355 (92%)	325 (99%)	3 (1%)	75	87
46	3O	327/355 (92%)	324 (99%)	3 (1%)	75	87
47	3C	332/332 (100%)	326 (98%)	6 (2%)	54	71
47	3P	332/332 (100%)	328 (99%)	4 (1%)	67	81
48	3D	202/259 (78%)	201 (100%)	1 (0%)	86	93
48	3Q	204/259 (79%)	201 (98%)	3 (2%)	60	76
49	3E	166/226 (74%)	161 (97%)	5 (3%)	36	52
49	3I	37/226 (16%)	36 (97%)	1 (3%)	40	57
49	3R	166/226 (74%)	160 (96%)	6 (4%)	30	44
49	3V	24/226 (11%)	23 (96%)	1 (4%)	25	37
50	3F	90/99 (91%)	89 (99%)	1 (1%)	70	83
50	3S	90/99 (91%)	89 (99%)	1 (1%)	70	83
51	3G	67/73 (92%)	67 (100%)	0	100	100
51	3T	67/73 (92%)	66 (98%)	1 (2%)	60	76
52	3H	62/85 (73%)	61 (98%)	1 (2%)	58	74
52	3U	62/85 (73%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	3J	46/48 (96%)	45 (98%)	1 (2%)	47	65
53	3W	46/48 (96%)	46 (100%)	0	100	100
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	40 (98%)	1 (2%)	44	61
55	4A	424/424 (100%)	412 (97%)	12 (3%)	38	55
55	8A	424/424 (100%)	410 (97%)	14 (3%)	33	48
56	4B	210/211 (100%)	202 (96%)	8 (4%)	28	42
56	8B	210/211 (100%)	202 (96%)	8 (4%)	28	42
57	4C	223/225 (99%)	219 (98%)	4 (2%)	54	71
57	8C	223/225 (99%)	211 (95%)	12 (5%)	18	27
58	4D	124/149 (83%)	115 (93%)	9 (7%)	11	16
58	8D	124/149 (83%)	112 (90%)	12 (10%)	6	8
59	4E	92/124 (74%)	88 (96%)	4 (4%)	25	36
59	8E	92/124 (74%)	89 (97%)	3 (3%)	33	48
60	4F	80/100 (80%)	74 (92%)	6 (8%)	11	15
60	8F	80/100 (80%)	77 (96%)	3 (4%)	28	42
61	4G	65/80 (81%)	62 (95%)	3 (5%)	23	33
61	8G	65/80 (81%)	64 (98%)	1 (2%)	60	76
62	4H	73/76 (96%)	69 (94%)	4 (6%)	18	26
62	8H	73/76 (96%)	67 (92%)	6 (8%)	9	12
63	4I	54/61 (88%)	54 (100%)	0	100	100
63	8I	54/61 (88%)	49 (91%)	5 (9%)	7	9
64	4J	49/68 (72%)	47 (96%)	2 (4%)	26	39
64	8J	49/68 (72%)	44 (90%)	5 (10%)	6	7
65	4K	38/66 (58%)	38 (100%)	0	100	100
65	8K	38/66 (58%)	34 (90%)	4 (10%)	5	6
66	4L	39/55 (71%)	37 (95%)	2 (5%)	20	29
66	8L	39/55 (71%)	38 (97%)	1 (3%)	41	58
67	4M	37/57 (65%)	35 (95%)	2 (5%)	18	27
67	8M	37/57 (65%)	35 (95%)	2 (5%)	18	27
68	4N	70/70 (100%)	66 (94%)	4 (6%)	17	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
68	8N	70/70 (100%)	65 (93%)	5 (7%)	12 17
All	All	13845/16096 (86%)	13439 (97%)	406 (3%)	39 54

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	16	LEU
1	1A	22	PHE
1	1A	51	PHE
1	1A	66	ASP
1	1A	87	MET
2	1B	25	ARG
2	1B	41	ARG
2	1B	50	PHE
2	1B	84	ASP
2	1B	100	LEU
2	1B	101	ARG
2	1B	125	TYR
2	1B	134	ARG
3	1C	23	SER
3	1C	33	LEU
3	1C	120	SER
4	1D	40	LYS
4	1D	71	GLU
4	1D	108	TYR
4	1D	119	SER
4	1D	164	MET
4	1D	209	ASP
4	1D	297	TYR
4	1D	413	ASP
5	1E	11	ASP
5	1E	15	ASN
5	1E	22	ASP
5	1E	78	MET
5	1E	144	CYS
6	1F	139	ARG
6	1F	249	ARG
6	1F	277	LYS
6	1F	306	LEU
6	1F	359	CYS
6	1F	362	CYS
6	1F	385	ARG

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Mol	Chain	Res	Type
7	1G	35	MET
7	1G	39	ARG
7	1G	94	MET
7	1G	108	CYS
7	1G	109	ASP
7	1G	114	CYS
7	1G	153	CYS
7	1G	158	ARG
7	1G	229	ASP
7	1G	278	ARG
7	1G	302	ARG
7	1G	309	SER
7	1G	337	ARG
7	1G	375	ASP
7	1G	398	SER
7	1G	414	ASP
7	1G	420	ASP
7	1G	424	ASP
7	1G	478	ARG
7	1G	520	LYS
7	1G	549	HIS
7	1G	596	ASP
7	1G	609	MET
7	1G	618	GLN
7	1G	621	SER
7	1G	650	LYS
7	1G	651	LEU
7	1G	669	LYS
8	1H	5	ASN
8	1H	54	LYS
8	1H	126	LYS
8	1H	127	TYR
8	1H	197	PRO
8	1H	233	MET
8	1H	237	PHE
8	1H	274	ARG
10	1J	17	PHE
10	1J	70	TYR
10	1J	98	MET
10	1J	99	MET
11	1K	3	LEU
11	1K	21	MET

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Mol	Chain	Res	Type
11	1K	50	ASN
11	1K	53	PHE
11	1K	69	CYS
12	1L	83	ASP
12	1L	262	ARG
12	1L	264	TYR
12	1L	307	SER
12	1L	336	LYS
12	1L	340	PHE
12	1L	355	ASP
12	1L	364	LYS
12	1L	403	TYR
12	1L	485	TYR
12	1L	541	ASN
12	1L	554	ASP
12	1L	572	LYS
12	1L	602	PHE
13	1M	57	PHE
13	1M	122	PHE
13	1M	256	TYR
13	1M	263	MET
13	1M	410	MET
13	1M	416	ARG
14	1N	97	MET
14	1N	104	MET
14	1N	159	MET
14	1N	282	MET
15	1O	1	LEU
15	1O	65	ASP
15	1O	203	GLU
16	1P	60	ARG
16	1P	89	ASN
16	1P	105	ASP
16	1P	140	LYS
16	1P	167	LYS
16	1P	187	TRP
16	1P	253	PHE
16	1P	263	TYR
16	1P	275	PHE
16	1P	281	ARG
16	1P	292	MET
16	1P	335	LYS

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Mol	Chain	Res	Type
17	1Q	57	MET
17	1Q	73	SER
17	1Q	77	ASP
17	1Q	79	LEU
17	1Q	123	SER
18	1R	54	SER
18	1R	70	ARG
18	1R	89	LEU
18	1R	96	HIS
19	1S	22	LEU
19	1S	88	ARG
20	1T	6	LEU
20	1T	17	TYR
20	1T	20	LYS
20	1T	46	ASP
20	1T	66	ASP
20	1T	69	LYS
20	1U	68	GLU
21	1V	63	ASP
22	1W	21	PHE
22	1W	22	SER
22	1W	24	ASP
22	1W	117	ASP
23	1X	10	GLU
23	1X	22	SER
23	1X	41	GLU
23	1X	69	PHE
23	1X	97	ARG
23	1X	99	CYS
23	1X	112	ASP
23	1X	118	ARG
24	1Y	85	ASP
24	1Y	106	SER
24	1Y	114	CYS
25	1Z	34	SER
25	1Z	51	MET
26	1a	68	ASN
27	1b	62	MET
28	1c	44	ARG
29	1d	64	TYR
29	1d	96	SER
30	1e	8	ARG

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Mol	Chain	Res	Type
30	1e	82	ARG
31	1f	27	ASP
32	1g	34	ASP
32	1g	49	LYS
32	1g	54	ASP
32	1g	57	ASN
32	1g	83	TYR
32	1g	103	ASN
33	1h	54	ASP
33	1h	79	PHE
33	1h	80	TYR
33	1h	81	ASP
34	1i	30	ARG
34	1i	34	LEU
34	1i	38	ARG
34	1i	125	GLN
35	1j	44	SER
35	1j	61	ASP
36	1k	34	LYS
36	1k	51	ARG
36	1k	59	ASN
37	1l	62	TYR
37	1l	124	SER
37	1l	135	TYR
38	1m	4	LYS
38	1m	25	SER
38	1m	40	SER
38	1m	56	LEU
38	1m	84	LYS
38	1m	121	ASP
39	1n	12	GLN
39	1n	20	LYS
39	1n	44	ARG
39	1n	89	SER
39	1n	116	ASP
40	1o	17	ASP
40	1o	27	ASP
40	1o	121	MET
41	1p	7	ASP
41	1p	76	CYS
41	1p	121	ARG
41	1p	135	SER

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Mol	Chain	Res	Type
42	1q	15	SER
42	1q	55	PHE
42	1q	95	ASP
42	1q	108	TYR
42	1q	115	PHE
42	1q	145	LYS
43	1r	19	LEU
43	1r	60	ARG
43	1r	101	LYS
43	1r	106	SER
44	1s	38	TYR
44	1s	59	SER
44	1s	61	PHE
45	3A	45	SER
45	3A	58	PHE
45	3A	142	ASP
45	3A	146	ARG
45	3A	308	GLN
46	3B	189	ASP
46	3B	301	LYS
46	3B	315	SER
47	3C	80	ARG
47	3C	90	PHE
47	3C	183	PHE
47	3C	215	MET
47	3C	234	PHE
47	3C	379	TRP
48	3D	159	GLN
49	3E	161	GLU
49	3E	164	ASN
49	3E	217	CYS
49	3E	219	HIS
49	3E	230	ASP
50	3F	82	MET
52	3H	79	ASP
49	3I	78	TYR
53	3J	61	HIS
45	3N	58	PHE
45	3N	112	LEU
45	3N	117	VAL
45	3N	284	TYR
46	3O	60	SER

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Mol	Chain	Res	Type
46	3O	223	PHE
46	3O	260	GLU
47	3P	80	ARG
47	3P	254	ASP
47	3P	267	HIS
47	3P	379	TRP
48	3Q	97	ASN
48	3Q	115	TYR
48	3Q	147	LEU
49	3R	79	SER
49	3R	82	ASP
49	3R	149	MET
49	3R	178	HIS
49	3R	196	ARG
49	3R	234	TYR
50	3S	41	ASP
51	3T	10	MET
49	3V	77	ARG
54	3Y	49	ASN
55	4A	13	LYS
55	4A	19	TYR
55	4A	38	ARG
55	4A	81	TRP
55	4A	97	MET
55	4A	101	SER
55	4A	109	PHE
55	4A	238	PHE
55	4A	290	HIS
55	4A	335	SER
55	4A	438	ARG
55	4A	514	LYS
56	4B	9	PHE
56	4B	26	HIS
56	4B	57	ASP
56	4B	119	ASP
56	4B	163	TRP
56	4B	173	ASP
56	4B	217	LYS
56	4B	225	SER
57	4C	12	ASN
57	4C	214	PHE
57	4C	244	PHE

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Mol	Chain	Res	Type
57	4C	246	ASP
58	4D	18	ASP
58	4D	22	TYR
58	4D	52	SER
58	4D	59	LEU
58	4D	72	ASN
58	4D	76	ASN
58	4D	87	PHE
58	4D	139	ASP
58	4D	145	TRP
59	4E	41	LEU
59	4E	59	ASN
59	4E	73	ASP
59	4E	106	LEU
60	4F	21	MET
60	4F	22	MET
60	4F	25	ARG
60	4F	51	SER
60	4F	65	ASP
60	4F	91	LEU
61	4G	43	HIS
61	4G	61	SER
61	4G	82	TYR
62	4H	29	CYS
62	4H	31	GLN
62	4H	60	TYR
62	4H	76	ARG
64	4J	15	ASP
64	4J	32	TYR
66	4L	2	HIS
66	4L	28	TYR
67	4M	25	SER
67	4M	29	PRO
68	4N	49	ASN
68	4N	60	ASN
68	4N	61	ASP
68	4N	77	LYS
55	8A	38	ARG
55	8A	51	ASP
55	8A	91	ASP
55	8A	97	MET
55	8A	109	PHE

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Mol	Chain	Res	Type
55	8A	290	HIS
55	8A	298	ASP
55	8A	328	HIS
55	8A	376	HIS
55	8A	377	PHE
55	8A	436	MET
55	8A	438	ARG
55	8A	468	MET
55	8A	514	LYS
56	8B	9	PHE
56	8B	17	MET
56	8B	24	HIS
56	8B	57	ASP
56	8B	129	LYS
56	8B	163	TRP
56	8B	181	GLN
56	8B	185	MET
57	8C	6	HIS
57	8C	23	SER
57	8C	38	ASN
57	8C	60	ASP
57	8C	63	ARG
57	8C	172	TYR
57	8C	173	PHE
57	8C	182	TYR
57	8C	214	PHE
57	8C	222	GLN
57	8C	244	PHE
57	8C	257	TYR
58	8D	41	LYS
58	8D	43	LYS
58	8D	53	MET
58	8D	54	ASP
58	8D	58	GLU
58	8D	67	SER
58	8D	68	PHE
58	8D	76	ASN
58	8D	87	PHE
58	8D	119	GLN
58	8D	125	ASP
58	8D	145	TRP
59	8E	23	ASP

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Mol	Chain	Res	Type
59	8E	33	MET
59	8E	82	TYR
60	8F	9	ASP
60	8F	42	THR
60	8F	54	ASN
61	8G	46	GLU
62	8H	9	LYS
62	8H	20	PHE
62	8H	35	ASP
62	8H	49	ASP
62	8H	63	PHE
62	8H	73	ASP
63	8I	16	ARG
63	8I	34	PHE
63	8I	35	TYR
63	8I	49	ASP
63	8I	54	TYR
64	8J	1	LEU
64	8J	28	ASP
64	8J	29	ASN
64	8J	31	LEU
64	8J	57	HIS
65	8K	13	TYR
65	8K	24	PHE
65	8K	51	LYS
65	8K	52	GLU
66	8L	28	TYR
67	8M	4	LYS
67	8M	39	HIS
68	8N	2	LEU
68	8N	11	LYS
68	8N	32	TYR
68	8N	40	ASN
68	8N	77	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	162	GLN
5	1E	37	ASN
6	1F	250	ASN
7	1G	101	HIS

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Mol	Chain	Res	Type
7	1G	259	ASN
9	1I	150	ASN
12	1L	23	ASN
12	1L	194	ASN
13	1M	220	HIS
14	1N	204	ASN
16	1P	136	ASN
19	1S	24	GLN
19	1S	47	ASN
22	1W	70	ASN
24	1Y	78	GLN
24	1Y	88	ASN
29	1d	46	ASN
29	1d	97	HIS
34	1i	47	ASN
39	1n	12	GLN
40	1o	116	GLN
41	1p	106	GLN
41	1p	123	ASN
42	1q	87	HIS
42	1q	123	GLN
43	1r	12	ASN
43	1r	35	GLN
44	1s	44	HIS
44	1s	65	GLN
45	3A	430	GLN
45	3N	9	GLN
49	3R	257	ASN
57	4C	50	ASN
57	4C	231	HIS
58	4D	29	HIS
58	4D	72	ASN
58	4D	76	ASN
59	4E	78	HIS
60	4F	32	ASN
62	4H	31	GLN
55	8A	328	HIS
56	8B	6	GLN
56	8B	24	HIS
56	8B	52	HIS
57	8C	6	HIS
57	8C	50	ASN

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Mol	Chain	Res	Type
57	8C	76	GLN
57	8C	122	HIS
59	8E	78	HIS
62	8H	25	GLN
62	8H	28	ASN
68	8N	12	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
56	FME	4B	1	56	8,9,10	0.56	0	8,9,11	0.99	1 (12%)
13	FME	1M	1	13	8,9,10	0.56	0	8,9,11	1.04	1 (12%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	1.07	1 (12%)
11	FME	1K	1	11	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
12	FME	1L	1	12	8,9,10	0.57	0	8,9,11	0.90	1 (12%)
8	FME	1H	1	8	8,9,10	0.56	0	8,9,11	1.01	1 (12%)
55	FME	4A	1	55	8,9,10	0.55	0	8,9,11	1.01	1 (12%)
55	FME	8A	1	55	8,9,10	0.55	0	8,9,11	1.16	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	1.02	1 (12%)
56	FME	8B	1	56	8,9,10	0.56	0	8,9,11	0.83	1 (12%)

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
56	FME	4B	1	56	-	3/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
11	FME	1K	1	11	-	3/7/9/11	-
12	FME	1L	1	12	-	1/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
55	FME	4A	1	55	-	1/7/9/11	-
55	FME	8A	1	55	-	1/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
56	FME	8B	1	56	-	1/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1M	1	FME	O-C-CA	-2.63	118.01	124.77
11	1K	1	FME	O-C-CA	-2.61	118.07	124.77
1	1A	1	FME	O-C-CA	-2.60	118.08	124.77
8	1H	1	FME	O-C-CA	-2.57	118.17	124.77
55	8A	1	FME	O-C-CA	-2.48	118.38	124.77
14	1N	1	FME	O-C-CA	-2.46	118.44	124.77
55	4A	1	FME	O-C-CA	-2.44	118.50	124.77
56	4B	1	FME	O-C-CA	-2.38	118.65	124.77
12	1L	1	FME	O-C-CA	-2.38	118.66	124.77
56	8B	1	FME	O-C-CA	-2.29	118.87	124.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	CB-CA-N-CN
56	8B	1	FME	O1-CN-N-CA
55	4A	1	FME	CA-CB-CG-SD
11	1K	1	FME	N-CA-CB-CG
55	8A	1	FME	CA-CB-CG-SD
11	1K	1	FME	C-CA-CB-CG
11	1K	1	FME	CB-CG-SD-CE
12	1L	1	FME	CB-CA-N-CN
56	4B	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 11 are monoatomic - leaving 135 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	$\# Z > 2$
70	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.37	0
87	PGV	8A	602	-	50,50,50	0.28	0	53,56,56	0.30	0
70	PC1	1H	402	-	53,53,53	0.28	0	59,61,61	0.35	0
69	3PE	3P	503	-	32,32,50	0.33	0	35,37,55	0.37	0
71	SF4	1F	502	6	0,12,12	-	-	-		
69	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.33	0
69	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.49	0
87	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.32	0
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.37	0
75	CDL	4B	303	-	99,99,99	0.27	0	105,111,111	0.30	0
78	NDP	1P	402	-	47,52,52	0.65	0	61,80,80	0.96	3 (4%)
75	CDL	8B	303	-	99,99,99	0.27	0	105,111,111	0.30	0
87	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.30	0
70	PC1	1H	403	-	47,47,53	0.29	0	53,55,61	0.36	0
87	PGV	8B	301	-	50,50,50	0.28	0	53,56,56	0.32	0
69	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.37	0
69	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.44	0
86	HEC	3D	501	48	30,49,50	2.39	12 (40%)	28,80,82	2.18	5 (17%)
92	PSC	4B	305	-	51,51,51	0.29	0	57,59,59	0.47	1 (1%)
83	CHD	1i	201	-	32,32,32	0.51	0	51,51,51	0.57	0
87	PGV	8B	302	-	50,50,50	0.28	0	53,56,56	0.37	0
70	PC1	1Y	207	-	45,45,53	0.29	0	51,53,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	PGV	4K	101	-	50,50,50	0.28	0	53,56,56	0.31	0
71	SF4	1G	802	7	0,12,12	-	-	-		
70	PC1	3R	303	-	44,44,53	0.29	0	50,52,61	0.36	0
75	CDL	3N	502	-	42,42,99	0.37	0	48,54,111	0.52	0
71	SF4	1I	201	9	0,12,12	-	-	-		
87	PGV	4B	302	-	50,50,50	0.29	0	53,56,56	0.36	0
85	HEM	3P	501	47	42,50,50	1.29	5 (11%)	46,82,82	1.78	10 (21%)
70	PC1	1A	203	-	34,34,53	0.33	0	40,42,61	0.39	0
69	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.64	1 (3%)
93	PEK	8G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
75	CDL	1d	203	-	64,64,99	0.32	0	70,76,111	0.41	0
69	3PE	1N	901	-	48,48,50	0.28	0	51,53,55	0.36	0
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
93	PEK	4C	307	-	51,51,52	0.26	0	54,56,57	0.42	0
87	PGV	4G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
87	PGV	4J	101	-	50,50,50	0.30	0	53,56,56	0.38	0
75	CDL	3T	101	-	56,56,99	0.35	0	62,68,111	0.48	0
69	3PE	1Y	205	-	32,32,50	0.32	0	35,37,55	0.52	0
76	GTP	1O	401	77	29,34,34	1.01	3 (10%)	35,54,54	0.76	0
70	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.48	0
75	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.69	1 (1%)
69	3PE	1Y	202	-	30,30,50	0.32	0	33,35,55	0.53	0
71	SF4	1G	801	7	0,12,12	-	-	-		
75	CDL	3G	103	-	55,55,99	0.34	0	61,67,111	0.48	0
75	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.39	0
69	3PE	1d	201	-	48,48,50	0.27	0	51,53,55	0.36	0
88	HEA	8A	604	55	58,67,67	2.20	20 (34%)	63,103,103	2.45	24 (38%)
70	PC1	1M	503	-	34,34,53	0.32	0	40,42,61	0.52	0
71	SF4	1B	201	2	0,12,12	-	-	-		
69	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.49	0
87	PGV	8C	301	-	50,50,50	0.27	0	53,56,56	0.35	0
84	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.29	0
75	CDL	3P	504	-	55,55,99	0.35	0	61,67,111	0.52	0
94	PO4	4H	101	-	4,4,4	0.97	0	6,6,6	0.47	0
81	AYA	1q	202	-	6,7,8	0.62	0	6,8,10	0.89	0
87	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.72	1 (1%)
69	3PE	3C	503	-	34,34,50	0.32	0	37,39,55	0.45	0
87	PGV	8L	101	-	50,50,50	0.28	0	53,56,56	0.41	0
75	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.43	0
93	PEK	8C	308	-	51,51,52	0.26	0	54,56,57	0.41	0
72	FES	1E	301	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	PGV	4C	306	-	50,50,50	0.29	0	53,56,56	0.36	0
69	3PE	1K	101	-	43,43,50	0.30	0	46,48,55	0.34	0
70	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.33	0
70	PC1	1B	203	-	47,47,53	0.29	0	53,55,61	0.42	0
85	HEM	3C	502	-	42,50,50	1.30	6 (14%)	46,82,82	1.72	8 (17%)
88	HEA	8A	605	55	58,67,67	2.21	20 (34%)	63,103,103	2.41	27 (42%)
80	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.05	1 (2%)
69	3PE	3R	302	-	46,46,50	0.28	0	49,51,55	0.36	0
87	PGV	4A	603	-	50,50,50	0.28	0	53,56,56	0.35	0
86	HEC	3Q	501	48	32,50,50	2.32	12 (37%)	30,82,82	2.18	6 (20%)
69	3PE	3A	503	-	31,31,50	0.41	0	34,36,55	0.48	0
70	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.35	0
75	CDL	1q	203	-	60,60,99	0.34	0	66,72,111	0.42	0
70	PC1	1d	202	-	38,38,53	0.31	0	44,46,61	0.47	0
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
92	PSC	8B	305	-	51,51,51	0.29	0	57,59,59	0.42	0
75	CDL	8C	306	-	99,99,99	0.27	0	105,111,111	0.40	0
87	PGV	8C	305	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
70	PC1	3J	101	-	46,46,53	0.28	0	52,54,61	0.32	0
87	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.40	0
69	3PE	1M	506	-	49,49,50	0.28	0	52,54,55	0.33	0
72	FES	1G	803	7	0,4,4	-	-	-	-	-
88	HEA	4A	605	55	58,67,67	2.19	20 (34%)	63,103,103	2.42	27 (42%)
85	HEM	3C	501	47	42,50,50	1.29	5 (11%)	46,82,82	1.79	8 (17%)
70	PC1	1A	202	-	34,34,53	0.37	0	40,42,61	0.44	0
71	SF4	1I	202	9	0,12,12	-	-	-	-	-
69	3PE	1Y	203	-	39,39,50	0.31	0	42,44,55	0.50	0
69	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.42	0
69	3PE	1P	403	-	34,34,50	0.31	0	37,39,55	0.43	0
70	PC1	1M	505	-	43,43,53	0.31	0	49,51,61	0.40	0
69	3PE	1m	201	-	40,40,50	0.29	0	43,45,55	0.40	0
69	3PE	1M	502	-	47,47,50	0.27	0	50,52,55	0.33	0
72	FES	3E	301	49	0,4,4	-	-	-	-	-
93	PEK	4G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
91	CUA	4B	304	56	0,1,1	-	-	-	-	-
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
87	PGV	4C	303	-	50,50,50	0.28	0	53,56,56	0.39	0
87	PGV	8A	601	-	50,50,50	0.29	0	53,56,56	0.41	0
81	AYA	1Y	201	-	6,7,8	0.64	0	6,8,10	0.86	0
91	CUA	8B	304	56	0,1,1	-	-	-	-	-
87	PGV	4L	101	-	50,50,50	0.28	0	53,56,56	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	1M	504	-	50,50,50	0.28	0	53,55,55	0.46	0
87	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.32	0
72	FES	3R	301	49	0,4,4	-	-	-		
75	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.60	1 (1%)
88	HEA	4A	604	55	58,67,67	2.19	20 (34%)	63,103,103	2.46	26 (41%)
75	CDL	3A	501	-	57,57,99	0.33	0	63,69,111	0.42	0
69	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.56	0
75	CDL	1h	202	-	79,79,99	0.31	0	85,91,111	0.42	0
69	3PE	3C	504	-	33,33,50	0.33	0	36,38,55	0.41	0
87	PGV	4C	304	-	50,50,50	0.29	0	53,56,56	0.47	1 (1%)
87	PGV	8A	603	-	50,50,50	0.28	0	53,56,56	0.33	0
75	CDL	3G	102	-	51,51,99	0.35	0	57,63,111	0.56	0
87	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.31	0
80	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.12	1 (2%)
75	CDL	4C	305	-	99,99,99	0.27	0	105,111,111	0.39	0
87	PGV	8J	101	-	50,50,50	0.28	0	53,56,56	0.40	0
82	AME	1h	201	-	9,10,11	0.51	0	9,11,13	0.99	1 (11%)
69	3PE	1Y	204	-	29,29,50	0.34	0	32,34,55	0.80	1 (3%)
69	3PE	1Y	206	-	26,26,50	0.35	0	29,31,55	0.55	0
87	PGV	4B	301	-	50,50,50	0.27	0	53,56,56	0.31	0
87	PGV	8G	101	-	50,50,50	0.29	0	53,56,56	0.45	1 (1%)
87	PGV	8C	307	-	50,50,50	0.29	0	53,56,56	0.35	0
87	PGV	8C	304	-	50,50,50	0.28	0	53,56,56	0.38	0
87	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
85	HEM	3P	502	47	42,50,50	1.30	5 (11%)	46,82,82	1.74	8 (17%)
87	PGV	4C	301	-	50,50,50	0.29	0	53,56,56	0.74	1 (1%)
94	PO4	8H	101	-	4,4,4	0.97	0	6,6,6	0.44	0
70	PC1	1I	203	-	43,43,53	0.29	0	49,51,61	0.32	0
69	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.34	0
73	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
75	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	1P	401	-	-	5/36/36/57	-
87	PGV	8A	602	-	-	8/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	1H	402	-	-	6/57/57/57	-
69	3PE	3P	503	-	-	6/36/36/54	-
71	SF4	1F	502	6	-	-	0/6/5/5
69	3PE	1L	701	-	-	4/49/49/54	-
69	3PE	3D	502	-	-	1/36/36/54	-
87	PGV	8C	303	-	-	10/55/55/55	-
75	CDL	1L	702	-	-	13/86/86/110	-
75	CDL	4B	303	-	-	14/110/110/110	-
78	NDP	1P	402	-	-	3/30/77/77	0/5/5/5
75	CDL	8B	303	-	-	15/110/110/110	-
87	PGV	4M	101	-	-	7/55/55/55	-
70	PC1	1H	403	-	-	4/51/51/57	-
87	PGV	8B	301	-	-	7/55/55/55	-
69	3PE	3G	101	-	-	3/32/32/54	-
69	3PE	1j	101	-	-	3/47/47/54	-
86	HEC	3D	501	48	-	3/9/53/54	-
92	PSC	4B	305	-	-	14/55/55/55	-
83	CHD	1i	201	-	-	2/9/74/74	0/4/4/4
87	PGV	8B	302	-	-	5/55/55/55	-
70	PC1	1Y	207	-	-	8/49/49/57	-
87	PGV	4K	101	-	-	14/55/55/55	-
71	SF4	1G	802	7	-	-	0/6/5/5
70	PC1	3R	303	-	-	3/48/48/57	-
75	CDL	3N	502	-	-	8/53/53/110	-
71	SF4	1I	201	9	-	-	0/6/5/5
87	PGV	4B	302	-	-	5/55/55/55	-
85	HEM	3P	501	47	-	7/12/54/54	-
70	PC1	1A	203	-	-	2/38/38/57	-
69	3PE	3A	502	-	-	7/30/30/54	-
93	PEK	8G	102	-	-	6/56/56/56	-
75	CDL	1d	203	-	-	11/75/75/110	-
69	3PE	1N	901	-	-	11/52/52/54	-
69	3PE	1L	703	-	-	6/48/48/54	-
93	PEK	4C	307	-	-	3/55/55/56	-
87	PGV	4G	101	-	-	10/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	PGV	4J	101	-	-	7/55/55/55	-
75	CDL	3T	101	-	-	9/67/67/110	-
69	3PE	1Y	205	-	-	2/36/36/54	-
76	GTP	1O	401	77	-	4/18/38/38	0/3/3/3
70	PC1	3X	101	-	-	2/32/32/57	-
75	CDL	1N	902	-	-	15/71/71/110	-
69	3PE	1Y	202	-	-	9/34/34/54	-
71	SF4	1G	801	7	-	-	0/6/5/5
75	CDL	3G	103	-	-	8/66/66/110	-
75	CDL	1X	201	-	-	17/96/96/110	-
69	3PE	1d	201	-	-	7/52/52/54	-
88	HEA	8A	604	55	-	6/32/76/76	-
70	PC1	1M	503	-	-	6/38/38/57	-
71	SF4	1B	201	2	-	-	0/6/5/5
69	3PE	3N	501	-	-	10/35/35/54	-
87	PGV	8C	301	-	-	3/55/55/55	-
84	MYR	1l	201	-	-	1/12/12/13	-
75	CDL	3P	504	-	-	17/66/66/110	-
81	AYA	1q	202	-	-	0/5/6/8	-
87	PGV	8C	302	-	-	15/55/55/55	-
69	3PE	3C	503	-	-	11/38/38/54	-
87	PGV	8L	101	-	-	5/55/55/55	-
75	CDL	4D	201	-	-	15/110/110/110	-
93	PEK	8C	308	-	-	2/55/55/56	-
72	FES	1E	301	5	-	-	0/1/1/1
87	PGV	4C	306	-	-	2/55/55/55	-
69	3PE	1K	101	-	-	9/47/47/54	-
70	PC1	1q	201	-	-	3/52/52/57	-
70	PC1	1B	203	-	-	10/51/51/57	-
85	HEM	3C	502	-	-	4/12/54/54	-
88	HEA	8A	605	55	-	6/32/76/76	-
80	EHZ	1n	201	-	-	4/42/44/45	-
69	3PE	3R	302	-	-	4/50/50/54	-
87	PGV	4A	603	-	-	3/55/55/55	-
86	HEC	3Q	501	48	-	3/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3A	503	-	-	6/35/35/54	-
70	PC1	1B	202	-	-	3/49/49/57	-
75	CDL	1q	203	-	-	6/71/71/110	-
70	PC1	1d	202	-	-	7/42/42/57	-
69	3PE	1A	201	-	-	7/50/50/54	-
92	PSC	8B	305	-	-	16/55/55/55	-
75	CDL	8C	306	-	-	18/110/110/110	-
87	PGV	8C	305	-	-	6/55/55/55	-
70	PC1	3J	101	-	-	1/50/50/57	-
87	PGV	4A	601	-	-	14/55/55/55	-
69	3PE	1M	506	-	-	7/53/53/54	-
72	FES	1G	803	7	-	-	0/1/1/1
88	HEA	4A	605	55	-	5/32/76/76	-
85	HEM	3C	501	47	-	5/12/54/54	-
70	PC1	1A	202	-	-	4/38/38/57	-
71	SF4	1I	202	9	-	-	0/6/5/5
69	3PE	1Y	203	-	-	14/43/43/54	-
69	3PE	3Y	101	-	-	5/33/33/54	-
69	3PE	1P	403	-	-	5/38/38/54	-
70	PC1	1M	505	-	-	13/47/47/57	-
69	3PE	1m	201	-	-	9/44/44/54	-
69	3PE	1M	502	-	-	13/51/51/54	-
93	PEK	4G	102	-	-	6/56/56/56	-
72	FES	3E	301	49	-	-	0/1/1/1
70	PC1	1h	203	-	-	12/50/50/57	-
87	PGV	4C	303	-	-	9/55/55/55	-
87	PGV	8A	601	-	-	11/55/55/55	-
81	AYA	1Y	201	-	-	0/5/6/8	-
87	PGV	4L	101	-	-	5/55/55/55	-
69	3PE	1M	504	-	-	10/54/54/54	-
87	PGV	4A	602	-	-	1/55/55/55	-
72	FES	3R	301	49	-	-	0/1/1/1
75	CDL	1H	401	-	-	4/61/61/110	-
88	HEA	4A	604	55	-	8/32/76/76	-
75	CDL	3A	501	-	-	1/68/68/110	-
69	3PE	3N	503	-	-	5/28/28/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	1h	202	-	-	19/90/90/110	-
69	3PE	3C	504	-	-	8/37/37/54	-
87	PGV	4C	304	-	-	4/55/55/55	-
87	PGV	8A	603	-	-	4/55/55/55	-
75	CDL	3G	102	-	-	8/62/62/110	-
87	PGV	4C	302	-	-	9/55/55/55	-
80	EHZ	1T	101	20	-	10/42/44/45	-
75	CDL	4C	305	-	-	18/110/110/110	-
87	PGV	8J	101	-	-	9/55/55/55	-
82	AME	1h	201	-	-	2/9/10/12	-
69	3PE	1Y	204	-	-	9/33/33/54	-
69	3PE	1Y	206	-	-	5/30/30/54	-
87	PGV	4B	301	-	-	2/55/55/55	-
87	PGV	8G	101	-	-	8/55/55/55	-
87	PGV	8C	307	-	-	3/55/55/55	-
87	PGV	8C	304	-	-	13/55/55/55	-
87	PGV	8K	101	-	-	13/55/55/55	-
85	HEM	3P	502	47	-	6/12/54/54	-
87	PGV	4C	301	-	-	11/55/55/55	-
70	PC1	1I	203	-	-	5/47/47/57	-
69	3PE	1M	501	-	-	6/48/48/54	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
75	CDL	8D	201	-	-	14/110/110/110	-

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3D	501	HEC	C2B-C3B	6.50	1.48	1.40
86	3D	501	HEC	C3C-C2C	6.49	1.48	1.40
86	3Q	501	HEC	C2B-C3B	6.48	1.48	1.40
86	3Q	501	HEC	C3C-C2C	6.44	1.48	1.40
88	8A	604	HEA	C3A-C2A	5.56	1.47	1.40
88	8A	604	HEA	C3B-C2B	5.50	1.47	1.34
88	8A	605	HEA	C3B-C2B	5.47	1.47	1.34
88	4A	604	HEA	C3A-C2A	5.47	1.47	1.40
88	4A	604	HEA	C3B-C2B	5.45	1.47	1.34
88	4A	605	HEA	C3B-C2B	5.43	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	8A	605	HEA	C3A-C2A	5.40	1.47	1.40
88	4A	605	HEA	C3A-C2A	5.31	1.47	1.40
88	8A	605	HEA	CHC-C4B	5.22	1.47	1.34
88	4A	605	HEA	CHD-C1D	5.21	1.47	1.34
88	4A	604	HEA	CHC-C4B	5.18	1.47	1.34
88	8A	605	HEA	CHD-C1D	5.18	1.47	1.34
88	4A	605	HEA	CHC-C4B	5.18	1.47	1.34
88	4A	604	HEA	CHD-C1D	5.14	1.47	1.34
88	8A	604	HEA	CHD-C1D	5.10	1.47	1.34
88	8A	604	HEA	CHC-C4B	5.09	1.47	1.34
88	8A	605	HEA	C3A-C4A	5.05	1.48	1.41
88	4A	605	HEA	C3A-C4A	5.01	1.48	1.41
88	8A	604	HEA	C3A-C4A	5.00	1.48	1.41
88	4A	604	HEA	C3A-C4A	4.99	1.48	1.41
88	8A	605	HEA	C3D-C2D	4.97	1.47	1.36
88	4A	605	HEA	C3D-C2D	4.89	1.47	1.36
88	8A	605	HEA	C3C-C2C	4.83	1.46	1.40
88	8A	604	HEA	C3D-C2D	4.83	1.47	1.36
88	4A	604	HEA	C3D-C2D	4.78	1.47	1.36
88	8A	604	HEA	C3C-C2C	4.70	1.46	1.40
88	4A	605	HEA	C3C-C2C	4.69	1.46	1.40
88	4A	604	HEA	C3C-C2C	4.56	1.46	1.40
86	3D	501	HEC	C2A-C3A	3.38	1.47	1.37
86	3D	501	HEC	C3D-C2D	3.37	1.47	1.37
85	3C	502	HEM	C1B-NB	-3.35	1.34	1.40
85	3P	502	HEM	C1B-NB	-3.35	1.34	1.40
86	3Q	501	HEC	C2A-C3A	3.31	1.47	1.37
85	3C	502	HEM	C4D-ND	-3.25	1.34	1.40
85	3P	502	HEM	C4D-ND	-3.22	1.34	1.40
85	3P	501	HEM	C1B-NB	-3.21	1.34	1.40
86	3Q	501	HEC	C3D-C2D	3.21	1.47	1.37
85	3C	501	HEM	C1B-NB	-3.17	1.34	1.40
85	3C	501	HEM	C4D-ND	-3.16	1.34	1.40
85	3P	501	HEM	C4D-ND	-3.15	1.34	1.40
86	3D	501	HEC	C3C-C4C	3.07	1.48	1.43
86	3Q	501	HEC	C3C-C4C	3.07	1.48	1.43
88	8A	604	HEA	C2A-C1A	2.95	1.49	1.42
86	3D	501	HEC	C4B-C3B	2.94	1.48	1.43
88	4A	605	HEA	C2A-C1A	2.91	1.49	1.42
88	4A	604	HEA	C2A-C1A	2.89	1.49	1.42
86	3Q	501	HEC	C4B-C3B	2.88	1.48	1.43
88	8A	605	HEA	C2A-C1A	2.87	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3D	501	HEC	C2A-C1A	2.84	1.48	1.42
86	3Q	501	HEC	C2A-C1A	2.81	1.48	1.42
88	4A	604	HEA	C4B-C3B	2.80	1.49	1.44
86	3Q	501	HEC	C3A-C4A	2.80	1.48	1.42
86	3D	501	HEC	C3A-C4A	2.77	1.48	1.42
88	8A	604	HEA	C4B-C3B	2.73	1.49	1.44
88	8A	605	HEA	C1D-ND	-2.69	1.35	1.40
76	1O	401	GTP	C5-C6	-2.68	1.42	1.47
88	4A	604	HEA	C1D-ND	-2.68	1.35	1.40
88	8A	605	HEA	C4B-C3B	2.66	1.49	1.44
88	4A	605	HEA	C1D-ND	-2.62	1.35	1.40
88	4A	605	HEA	C4B-C3B	2.62	1.49	1.44
88	8A	605	HEA	C4B-NB	-2.60	1.35	1.40
88	8A	604	HEA	C1D-ND	-2.59	1.35	1.40
88	4A	604	HEA	C4D-C3D	2.57	1.49	1.45
88	8A	604	HEA	FE-NB	2.56	2.12	1.98
88	4A	605	HEA	C4B-NB	-2.56	1.35	1.40
88	4A	604	HEA	FE-ND	2.56	2.12	1.98
88	4A	604	HEA	FE-NB	2.55	2.12	1.98
88	8A	604	HEA	FE-ND	2.54	2.12	1.98
88	4A	605	HEA	FE-ND	2.53	2.12	1.98
88	4A	604	HEA	C4B-NB	-2.53	1.35	1.40
86	3D	501	HEC	C1D-CHD	2.52	1.48	1.41
88	8A	604	HEA	C4B-NB	-2.52	1.35	1.40
86	3D	501	HEC	C4D-CHA	2.52	1.48	1.41
88	8A	605	HEA	FE-ND	2.52	2.12	1.98
86	3Q	501	HEC	C1D-CHD	2.51	1.48	1.41
88	4A	605	HEA	FE-NB	2.50	2.12	1.98
88	8A	605	HEA	FE-NB	2.48	2.11	1.98
86	3Q	501	HEC	C4D-CHA	2.47	1.47	1.41
86	3Q	501	HEC	C1B-CHB	2.45	1.47	1.41
86	3D	501	HEC	C1B-CHB	2.45	1.47	1.41
86	3Q	501	HEC	C1C-CHC	2.44	1.47	1.41
88	8A	604	HEA	C4D-C3D	2.43	1.49	1.45
86	3D	501	HEC	C1C-CHC	2.39	1.47	1.41
85	3C	501	HEM	FE-NB	2.38	2.11	1.98
85	3P	501	HEM	FE-NB	2.37	2.11	1.98
85	3C	501	HEM	CHB-C1B	2.33	1.40	1.34
88	4A	605	HEA	C4C-CHD	2.31	1.47	1.41
85	3C	502	HEM	FE-NB	2.31	2.10	1.98
88	4A	605	HEA	C1D-C2D	2.31	1.49	1.44
85	3P	501	HEM	CHB-C1B	2.30	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	3P	502	HEM	FE-NB	2.29	2.10	1.98
88	8A	605	HEA	C1C-CHC	2.28	1.47	1.41
88	8A	605	HEA	C4C-CHD	2.28	1.47	1.41
85	3P	502	HEM	CHB-C1B	2.28	1.40	1.34
88	8A	605	HEA	C11-C3B	-2.27	1.48	1.51
88	8A	605	HEA	C4D-C3D	2.27	1.48	1.45
85	3C	502	HEM	CHB-C1B	2.26	1.40	1.34
88	4A	604	HEA	C1C-CHC	2.25	1.47	1.41
88	4A	605	HEA	C1C-CHC	2.24	1.47	1.41
88	4A	605	HEA	C11-C3B	-2.23	1.48	1.51
88	8A	605	HEA	C1D-C2D	2.22	1.49	1.44
88	4A	604	HEA	C4C-CHD	2.21	1.47	1.41
88	4A	605	HEA	C4D-C3D	2.20	1.48	1.45
88	8A	604	HEA	C1D-C2D	2.17	1.48	1.44
85	3P	502	HEM	C1D-ND	-2.17	1.34	1.38
88	8A	604	HEA	C1C-CHC	2.16	1.47	1.41
88	8A	604	HEA	C4C-CHD	2.15	1.47	1.41
85	3P	501	HEM	C1D-ND	-2.14	1.34	1.38
76	1O	401	GTP	C8-N7	-2.11	1.31	1.34
85	3C	502	HEM	C1D-ND	-2.11	1.34	1.38
88	8A	604	HEA	C1B-C2B	2.08	1.48	1.44
88	8A	604	HEA	CHA-C4D	2.07	1.46	1.40
88	4A	604	HEA	CHA-C4D	2.07	1.46	1.40
88	4A	604	HEA	C1D-C2D	2.06	1.48	1.44
85	3C	501	HEM	C1D-ND	-2.05	1.34	1.38
88	8A	605	HEA	CHB-C1B	2.05	1.46	1.40
88	4A	604	HEA	C1B-C2B	2.04	1.48	1.44
88	8A	605	HEA	C1B-C2B	2.03	1.48	1.44
88	4A	605	HEA	CHB-C1B	2.03	1.46	1.40
88	4A	604	HEA	CHB-C1B	2.02	1.46	1.40
85	3C	502	HEM	C4B-NB	-2.01	1.34	1.38
76	1O	401	GTP	C5-C4	-2.01	1.38	1.43
88	4A	605	HEA	CHA-C4D	2.01	1.46	1.40
88	8A	604	HEA	C11-C3B	-2.01	1.48	1.51

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	605	HEA	C3D-C4D-ND	6.64	116.77	110.35
88	8A	605	HEA	C3D-C4D-ND	6.63	116.76	110.35
88	4A	604	HEA	C3D-C4D-ND	6.54	116.67	110.35
88	8A	604	HEA	C3D-C4D-ND	6.47	116.60	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1T	101	EHZ	C10-S1-C9	6.20	120.16	101.84
88	8A	604	HEA	C2B-C1B-NB	6.02	116.86	109.90
86	3D	501	HEC	C1D-C2D-C3D	-5.99	102.83	107.00
80	1n	201	EHZ	C10-S1-C9	5.93	119.36	101.84
86	3Q	501	HEC	C1D-C2D-C3D	-5.89	102.89	107.00
88	4A	605	HEA	C2B-C1B-NB	5.89	116.71	109.90
88	4A	604	HEA	C2B-C1B-NB	5.83	116.64	109.90
88	8A	604	HEA	C3B-C4B-NB	5.79	116.50	109.84
88	8A	605	HEA	C2B-C1B-NB	5.70	116.49	109.90
88	4A	604	HEA	C2D-C1D-ND	5.66	116.34	109.84
88	8A	604	HEA	C2D-C1D-ND	5.64	116.32	109.84
88	8A	605	HEA	C2D-C1D-ND	5.63	116.31	109.84
88	4A	604	HEA	C3B-C4B-NB	5.59	116.26	109.84
88	4A	605	HEA	C3B-C4B-NB	5.52	116.19	109.84
88	4A	605	HEA	C2D-C1D-ND	5.52	116.19	109.84
88	8A	605	HEA	C3B-C4B-NB	5.38	116.03	109.84
86	3D	501	HEC	CMC-C2C-C3C	5.32	132.08	125.82
86	3Q	501	HEC	CMC-C2C-C3C	5.26	132.00	125.82
86	3Q	501	HEC	CMB-C2B-C3B	5.17	131.90	125.82
86	3D	501	HEC	CMB-C2B-C3B	5.14	131.87	125.82
85	3C	501	HEM	CHC-C4B-NB	5.08	129.90	124.44
78	1P	402	NDP	P2B-O2B-C2B	-4.98	110.14	123.43
85	3P	501	HEM	CHC-C4B-NB	4.92	129.72	124.44
85	3P	502	HEM	CHC-C4B-NB	4.91	129.71	124.44
85	3C	502	HEM	CHC-C4B-NB	4.90	129.71	124.44
85	3C	501	HEM	CHD-C1D-ND	4.38	129.15	124.44
88	4A	604	HEA	CHA-C4D-ND	-4.37	119.74	124.44
85	3P	501	HEM	CHD-C1D-ND	4.34	129.10	124.44
85	3P	502	HEM	CHD-C1D-ND	4.28	129.04	124.44
88	4A	605	HEA	C1D-C2D-C3D	-4.23	102.53	106.98
88	8A	604	HEA	C3C-C4C-NC	4.23	114.67	109.21
88	8A	605	HEA	C1D-C2D-C3D	-4.22	102.54	106.98
88	8A	604	HEA	C1D-C2D-C3D	-4.07	102.70	106.98
88	8A	604	HEA	CBA-CAA-C2A	-4.04	105.89	112.55
75	1N	902	CDL	OB6-CB5-C51	4.02	118.25	111.09
88	4A	604	HEA	C3C-C4C-NC	3.99	114.37	109.21
85	3C	502	HEM	CHD-C1D-ND	3.99	128.72	124.44
88	4A	604	HEA	C1D-C2D-C3D	-3.89	102.89	106.98
87	4C	301	PGV	O01-C1-C2	3.82	119.74	111.48
88	8A	605	HEA	CHA-C4D-ND	-3.81	120.33	124.44
88	8A	605	HEA	C3C-C4C-NC	3.81	114.13	109.21
88	4A	605	HEA	C3C-C4C-NC	3.80	114.12	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	605	HEA	C1B-C2B-C3B	-3.73	102.47	106.80
88	8A	604	HEA	C1B-C2B-C3B	-3.72	102.49	106.80
88	8A	605	HEA	C1B-C2B-C3B	-3.70	102.51	106.80
88	4A	604	HEA	CBA-CAA-C2A	-3.64	106.55	112.55
87	8C	302	PGV	O01-C1-C2	3.58	119.23	111.48
88	4A	604	HEA	C1B-C2B-C3B	-3.58	102.65	106.80
85	3C	501	HEM	CHA-C4D-ND	3.51	128.73	124.37
88	4A	604	HEA	CAD-C3D-C4D	3.47	130.75	124.70
85	3P	502	HEM	C1B-NB-C4B	3.45	109.30	105.21
88	8A	604	HEA	CHA-C4D-ND	-3.45	120.73	124.44
88	4A	604	HEA	C4D-C3D-C2D	-3.44	101.89	106.89
85	3C	502	HEM	C1B-NB-C4B	3.44	109.28	105.21
85	3P	501	HEM	CHB-C1B-NB	3.43	128.62	124.37
85	3P	501	HEM	CHA-C4D-ND	3.42	128.62	124.37
88	8A	605	HEA	C13-C12-C11	-3.36	109.03	114.39
85	3C	502	HEM	CHA-C4D-ND	3.35	128.53	124.37
88	4A	605	HEA	CHA-C4D-ND	-3.35	120.83	124.44
88	4A	605	HEA	C13-C12-C11	-3.33	109.07	114.39
88	8A	604	HEA	C13-C14-C15	-3.30	120.06	127.62
88	8A	605	HEA	C4D-C3D-C2D	-3.30	102.08	106.89
88	4A	604	HEA	C13-C14-C15	-3.28	120.11	127.62
88	8A	604	HEA	C4D-C3D-C2D	-3.27	102.13	106.89
85	3C	501	HEM	CHB-C1B-NB	3.26	128.41	124.37
88	4A	605	HEA	C4D-C3D-C2D	-3.23	102.19	106.89
85	3P	502	HEM	CHA-C4D-ND	3.21	128.35	124.37
85	3C	501	HEM	C1B-NB-C4B	3.19	108.99	105.21
85	3P	501	HEM	C1B-NB-C4B	3.19	108.98	105.21
88	8A	604	HEA	C4B-C3B-C2B	-3.18	102.09	107.44
88	8A	605	HEA	C13-C14-C15	-3.17	120.36	127.62
88	4A	604	HEA	C4B-C3B-C2B	-3.16	102.12	107.44
88	4A	605	HEA	C13-C14-C15	-3.15	120.41	127.62
88	8A	604	HEA	CHB-C1B-NB	-3.13	121.07	124.44
85	3P	502	HEM	CHB-C1B-NB	3.09	128.20	124.37
69	1Y	204	3PE	O21-C21-C22	3.07	118.13	111.48
85	3C	502	HEM	CHB-C1B-NB	3.04	128.14	124.37
88	4A	605	HEA	C4B-C3B-C2B	-3.03	102.34	107.44
88	4A	604	HEA	C26-C15-C16	3.00	120.44	115.23
88	8A	604	HEA	C26-C15-C16	3.00	120.44	115.23
88	8A	604	HEA	CAD-C3D-C4D	3.00	129.92	124.70
88	8A	605	HEA	C4B-C3B-C2B	-2.99	102.41	107.44
88	4A	604	HEA	CHB-C1B-NB	-2.87	121.34	124.44
88	4A	605	HEA	CMC-C2C-C3C	2.85	130.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	8A	605	HEA	CMC-C2C-C3C	2.84	130.36	124.68
85	3P	502	HEM	C3B-C4B-NB	-2.83	107.44	109.47
88	8A	605	HEA	CBA-CAA-C2A	-2.82	107.91	112.55
82	1h	201	AME	O-C-CA	-2.80	117.58	124.77
85	3C	502	HEM	C3B-C4B-NB	-2.78	107.47	109.47
88	4A	605	HEA	C26-C15-C16	2.78	120.05	115.23
86	3Q	501	HEC	CBD-CAD-C3D	-2.76	107.89	112.54
88	8A	604	HEA	CMC-C2C-C3C	2.76	130.19	124.68
88	4A	605	HEA	CBA-CAA-C2A	-2.75	108.03	112.55
88	4A	605	HEA	C17-C18-C19	-2.69	121.46	127.62
88	8A	605	HEA	C26-C15-C16	2.68	119.88	115.23
88	4A	605	HEA	CHB-C1B-NB	-2.67	121.56	124.44
78	1P	402	NDP	O4D-C1D-C2D	-2.66	100.92	106.62
88	8A	604	HEA	C4B-NB-C1B	-2.66	102.06	105.21
88	8A	605	HEA	C27-C19-C20	2.65	119.82	115.23
88	4A	604	HEA	CMC-C2C-C3C	2.64	129.96	124.68
85	3P	501	HEM	CHD-C1D-C2D	-2.61	120.90	125.03
88	8A	605	HEA	CHB-C1B-NB	-2.60	121.64	124.44
85	3C	501	HEM	CHD-C1D-C2D	-2.59	120.93	125.03
88	4A	605	HEA	C27-C19-C20	2.59	119.72	115.23
85	3P	501	HEM	C3B-C4B-NB	-2.55	107.64	109.47
88	8A	605	HEA	C17-C18-C19	-2.54	121.81	127.62
85	3C	501	HEM	C3B-C4B-NB	-2.53	107.65	109.47
88	4A	604	HEA	C1D-ND-C4D	-2.53	102.21	105.21
88	8A	604	HEA	C17-C18-C19	-2.52	121.86	127.62
88	8A	604	HEA	C1D-ND-C4D	-2.50	102.24	105.21
85	3P	502	HEM	CHD-C1D-C2D	-2.49	121.10	125.03
88	4A	605	HEA	C4B-NB-C1B	-2.47	102.28	105.21
88	8A	605	HEA	C1D-ND-C4D	-2.45	102.31	105.21
88	4A	604	HEA	C4B-NB-C1B	-2.44	102.32	105.21
88	4A	605	HEA	C1D-ND-C4D	-2.43	102.33	105.21
88	4A	605	HEA	C25-C23-C24	2.43	120.18	114.59
86	3Q	501	HEC	CAA-CBA-CGA	-2.40	107.37	113.83
88	4A	604	HEA	C17-C18-C19	-2.39	122.15	127.62
88	4A	605	HEA	CMB-C2B-C1B	2.37	128.74	125.03
88	4A	604	HEA	CMB-C2B-C1B	2.37	128.74	125.03
88	8A	604	HEA	CMB-C2B-C1B	2.37	128.73	125.03
88	8A	604	HEA	CHD-C1D-C2D	-2.35	120.28	126.94
88	4A	604	HEA	CHD-C1D-C2D	-2.35	120.28	126.94
88	4A	604	HEA	C27-C19-C20	2.33	119.26	115.23
92	4B	305	PSC	O01-C1-C2	2.30	116.46	111.48
88	8A	605	HEA	CAD-C3D-C4D	2.29	128.69	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	3D	501	HEC	CMA-C3A-C2A	2.29	129.26	124.94
88	4A	604	HEA	C13-C12-C11	-2.29	110.73	114.39
88	8A	605	HEA	CMB-C2B-C1B	2.28	128.59	125.03
69	3A	502	3PE	O21-C21-C22	2.27	116.40	111.48
88	8A	604	HEA	C25-C23-C24	2.27	119.81	114.59
85	3C	502	HEM	CHD-C1D-C2D	-2.26	121.45	125.03
85	3P	501	HEM	CBA-CAA-C2A	-2.26	108.74	112.54
88	8A	605	HEA	C25-C23-C24	2.26	119.78	114.59
88	4A	605	HEA	CAD-C3D-C4D	2.26	128.63	124.70
78	1P	402	NDP	C5A-C6A-N6A	2.25	123.74	120.31
88	8A	604	HEA	CMD-C2D-C1D	2.25	128.54	125.03
88	8A	605	HEA	C4B-NB-C1B	-2.24	102.55	105.21
88	4A	605	HEA	CMD-C2D-C1D	2.24	128.53	125.03
88	8A	605	HEA	CHD-C1D-C2D	-2.22	120.67	126.94
86	3Q	501	HEC	CMA-C3A-C2A	2.21	129.12	124.94
88	4A	604	HEA	C25-C23-C24	2.20	119.65	114.59
88	4A	604	HEA	CMD-C2D-C1D	2.19	128.46	125.03
88	4A	605	HEA	CHD-C1D-C2D	-2.19	120.75	126.94
85	3P	502	HEM	C4D-ND-C1D	2.17	107.77	105.21
85	3C	501	HEM	CHA-C4D-C3D	-2.14	121.28	125.23
87	8G	101	PGV	O01-C1-C2	2.12	116.06	111.48
86	3D	501	HEC	CAA-CBA-CGA	-2.11	108.14	113.83
88	8A	604	HEA	C21-C22-C23	-2.11	120.59	127.64
87	4G	101	PGV	O01-C1-C2	2.11	116.04	111.48
85	3C	502	HEM	C4D-ND-C1D	2.10	107.70	105.21
73	1F	501	FMN	C4-N3-C2	-2.10	121.92	125.64
88	4A	605	HEA	CHB-C1B-C2B	-2.09	121.72	125.03
75	1H	401	CDL	OB6-CB5-C51	2.09	116.00	111.48
87	4C	304	PGV	O01-C1-C2	2.09	116.00	111.48
85	3P	501	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
88	8A	605	HEA	CMD-C2D-C1D	2.06	128.26	125.03
87	8C	305	PGV	O01-C1-C2	2.05	115.92	111.48
88	8A	605	HEA	C21-C22-C23	-2.05	120.82	127.64
88	4A	605	HEA	C21-C22-C23	-2.03	120.86	127.64
85	3P	501	HEM	CHB-C1B-C2B	-2.03	121.18	126.94
88	4A	604	HEA	C21-C22-C23	-2.03	120.88	127.64
88	8A	605	HEA	CHB-C1B-C2B	-2.00	121.86	125.03

There are no chirality outliers.

All (877) 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-O13
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	703	3PE	C2-C1-O11-P
69	1M	501	3PE	C11-O13-P-O14
69	1M	502	3PE	C1-O11-P-O12
69	1M	502	3PE	C2-C1-O11-P
69	1M	502	3PE	O32-C31-O31-C3
69	1M	502	3PE	C32-C31-O31-C3
69	1M	504	3PE	C2-C1-O11-P
69	1M	506	3PE	C1-O11-P-O14
69	1N	901	3PE	C1-O11-P-O12
69	1N	901	3PE	C1-O11-P-O13
69	1N	901	3PE	C1-O11-P-O14
69	1P	403	3PE	C1-O11-P-O12
69	1Y	202	3PE	C1-O11-P-O13
69	1Y	202	3PE	C2-C1-O11-P
69	1Y	203	3PE	C1-O11-P-O13
69	1Y	203	3PE	C1-O11-P-O14
69	1Y	203	3PE	C2-C1-O11-P
69	1Y	203	3PE	O22-C21-O21-C2
69	1Y	203	3PE	C22-C21-O21-C2
69	1Y	204	3PE	O22-C21-O21-C2
69	1Y	204	3PE	C22-C21-O21-C2
69	1Y	206	3PE	C11-O13-P-O14
69	1Y	206	3PE	C12-C11-O13-P
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	3A	502	3PE	O32-C31-O31-C3
69	3A	502	3PE	C32-C31-O31-C3
69	3A	502	3PE	O22-C21-O21-C2
69	3A	502	3PE	C22-C21-O21-C2
69	3A	503	3PE	C1-O11-P-O14
69	3A	503	3PE	C2-C1-O11-P
69	3C	503	3PE	C11-O13-P-O11
69	3C	503	3PE	C11-O13-P-O12
69	3C	503	3PE	C11-O13-P-O14
69	3C	504	3PE	O21-C2-C3-O31
69	3G	101	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	3G	101	3PE	C32-C31-O31-C3
69	3N	501	3PE	C1-O11-P-O13
69	3N	501	3PE	C1-O11-P-O14
69	3N	501	3PE	C2-C1-O11-P
69	3N	503	3PE	O22-C21-O21-C2
69	3N	503	3PE	C22-C21-O21-C2
69	3P	503	3PE	C11-O13-P-O11
69	3P	503	3PE	C11-O13-P-O12
69	3P	503	3PE	C11-O13-P-O14
69	3Y	101	3PE	C2-C1-O11-P
70	1B	203	PC1	O22-C21-O21-C2
70	1B	203	PC1	C22-C21-O21-C2
70	1I	203	PC1	C1-O11-P-O14
70	1M	503	PC1	C11-O13-P-O11
70	1M	503	PC1	O22-C21-O21-C2
70	1M	503	PC1	C22-C21-O21-C2
70	1M	505	PC1	C1-O11-P-O12
70	1d	202	PC1	O22-C21-O21-C2
70	1d	202	PC1	C22-C21-O21-C2
70	1h	203	PC1	C11-O13-P-O14
70	1h	203	PC1	O32-C31-O31-C3
70	1h	203	PC1	C32-C31-O31-C3
70	3R	303	PC1	O32-C31-O31-C3
70	3R	303	PC1	C32-C31-O31-C3
70	3X	101	PC1	C1-O11-P-O14
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	OA6-CA4-CA6-OA8
75	1L	702	CDL	CB3-OB5-PB2-OB4
75	1N	902	CDL	OA6-CA4-CA6-OA8
75	1N	902	CDL	CB3-OB5-PB2-OB3
75	1X	201	CDL	C1-CA2-OA2-PA1
75	1X	201	CDL	CA2-OA2-PA1-OA4
75	1X	201	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CA2-OA2-PA1-OA4
75	1h	202	CDL	CA2-OA2-PA1-OA5
75	1h	202	CDL	C1-CB2-OB2-PB2
75	1h	202	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	OB7-CB5-OB6-CB4
75	1h	202	CDL	C51-CB5-OB6-CB4
75	1h	202	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
75	1h	202	CDL	C71-CB7-OB8-CB6
75	3G	102	CDL	CB2-OB2-PB2-OB3
75	3G	102	CDL	CB2-OB2-PB2-OB4
75	3G	102	CDL	CB2-OB2-PB2-OB5
75	3G	103	CDL	CB2-OB2-PB2-OB4
75	3G	103	CDL	CB2-OB2-PB2-OB5
75	3P	504	CDL	OB9-CB7-OB8-CB6
75	3P	504	CDL	C71-CB7-OB8-CB6
75	3T	101	CDL	CA3-OA5-PA1-OA3
75	3T	101	CDL	CA3-OA5-PA1-OA4
75	3T	101	CDL	OB9-CB7-OB8-CB6
75	3T	101	CDL	C71-CB7-OB8-CB6
75	4B	303	CDL	OA9-CA7-OA8-CA6
75	4B	303	CDL	C31-CA7-OA8-CA6
75	4B	303	CDL	CB3-OB5-PB2-OB2
75	4B	303	CDL	CB3-OB5-PB2-OB3
75	4C	305	CDL	C1-CA2-OA2-PA1
75	4C	305	CDL	OB7-CB5-OB6-CB4
75	4C	305	CDL	C51-CB5-OB6-CB4
75	4C	305	CDL	OB9-CB7-OB8-CB6
75	4C	305	CDL	C71-CB7-OB8-CB6
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	8B	303	CDL	OA9-CA7-OA8-CA6
75	8B	303	CDL	C31-CA7-OA8-CA6
75	8B	303	CDL	CB3-OB5-PB2-OB3
75	8C	306	CDL	C1-CA2-OA2-PA1
75	8C	306	CDL	OB7-CB5-OB6-CB4
75	8C	306	CDL	C51-CB5-OB6-CB4
75	8C	306	CDL	OB9-CB7-OB8-CB6
75	8C	306	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-OB3
75	8D	201	CDL	OB7-CB5-OB6-CB4
75	8D	201	CDL	C51-CB5-OB6-CB4
75	8D	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
75	8D	201	CDL	C71-CB7-OB8-CB6
76	1O	401	GTP	C5'-O5'-PA-O1A
80	1T	101	EHZ	N2-C15-C16-O5
84	1l	201	MYR	O1-C1-C2-C3
85	3C	501	HEM	C2B-C3B-CAB-CBB
85	3C	501	HEM	C4B-C3B-CAB-CBB
85	3C	502	HEM	C2B-C3B-CAB-CBB
85	3P	501	HEM	C2B-C3B-CAB-CBB
85	3P	501	HEM	C4B-C3B-CAB-CBB
85	3P	502	HEM	C2B-C3B-CAB-CBB
87	4A	601	PGV	O04-C19-O03-C01
87	4A	601	PGV	C20-C19-O03-C01
87	4A	603	PGV	C02-C03-O11-P
87	4C	301	PGV	C05-C04-O12-P
87	4C	301	PGV	O02-C1-O01-C02
87	4C	301	PGV	C2-C1-O01-C02
87	4C	302	PGV	C03-O11-P-O14
87	4C	302	PGV	O04-C19-O03-C01
87	4C	302	PGV	C20-C19-O03-C01
87	4C	303	PGV	C03-O11-P-O13
87	4C	304	PGV	O02-C1-O01-C02
87	4C	304	PGV	C2-C1-O01-C02
87	4G	101	PGV	O02-C1-O01-C02
87	4G	101	PGV	C2-C1-O01-C02
87	4G	101	PGV	O04-C19-O03-C01
87	4G	101	PGV	C20-C19-O03-C01
87	4K	101	PGV	C03-O11-P-O12
87	4K	101	PGV	C03-O11-P-O14
87	4K	101	PGV	O04-C19-O03-C01
87	4K	101	PGV	C20-C19-O03-C01
87	8A	601	PGV	O04-C19-O03-C01
87	8A	601	PGV	C20-C19-O03-C01
87	8A	603	PGV	C02-C03-O11-P
87	8B	301	PGV	C03-O11-P-O12
87	8B	301	PGV	C03-O11-P-O13
87	8B	301	PGV	C04-O12-P-O11
87	8C	302	PGV	C04-O12-P-O11
87	8C	302	PGV	C04-O12-P-O13
87	8C	302	PGV	C05-C04-O12-P
87	8C	302	PGV	O02-C1-O01-C02
87	8C	302	PGV	C2-C1-O01-C02
87	8C	303	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
87	8C	303	PGV	O04-C19-O03-C01
87	8C	303	PGV	C20-C19-O03-C01
87	8C	304	PGV	C03-O11-P-O12
87	8C	304	PGV	C03-O11-P-O13
87	8C	305	PGV	O02-C1-O01-C02
87	8C	305	PGV	C2-C1-O01-C02
87	8G	101	PGV	O02-C1-O01-C02
87	8G	101	PGV	C2-C1-O01-C02
87	8G	101	PGV	O04-C19-O03-C01
87	8G	101	PGV	C20-C19-O03-C01
87	8K	101	PGV	C03-O11-P-O12
87	8K	101	PGV	C03-O11-P-O14
87	8K	101	PGV	O04-C19-O03-C01
87	8K	101	PGV	C20-C19-O03-C01
92	4B	305	PSC	C03-O11-P-O12
92	4B	305	PSC	C03-O11-P-O13
92	4B	305	PSC	C02-C03-O11-P
92	4B	305	PSC	O02-C1-O01-C02
92	4B	305	PSC	C2-C1-O01-C02
92	8B	305	PSC	C03-O11-P-O12
92	8B	305	PSC	C03-O11-P-O13
92	8B	305	PSC	O02-C1-O01-C02
92	8B	305	PSC	C2-C1-O01-C02
80	1T	101	EHZ	C13-C12-N1-C11
75	4C	305	CDL	O1-C1-CA2-OA2
75	4D	201	CDL	O1-C1-CB2-OB2
75	8C	306	CDL	O1-C1-CA2-OA2
75	8D	201	CDL	O1-C1-CB2-OB2
75	1N	902	CDL	C51-CB5-OB6-CB4
75	1N	902	CDL	OB7-CB5-OB6-CB4
88	4A	604	HEA	C19-C20-C21-C22
88	8A	604	HEA	C19-C20-C21-C22
75	1N	902	CDL	C1-CA2-OA2-PA1
92	8B	305	PSC	C02-C03-O11-P
80	1T	101	EHZ	O3-C12-N1-C11
75	4C	305	CDL	CB2-C1-CA2-OA2
75	8C	306	CDL	CB2-C1-CA2-OA2
78	1P	402	NDP	O4D-C1D-N1N-C6N
69	3C	503	3PE	C21-C22-C23-C24
70	1q	201	PC1	C31-C32-C33-C34
87	4B	302	PGV	C1-C2-C3-C4
70	1Y	207	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
70	1H	403	PC1	C31-C32-C33-C34
87	8B	302	PGV	C1-C2-C3-C4
69	1m	201	3PE	C31-C32-C33-C34
87	4J	101	PGV	C21-C22-C23-C24
87	8J	101	PGV	C21-C22-C23-C24
75	3G	102	CDL	O1-C1-CB2-OB2
70	1h	203	PC1	C2-C1-O11-P
73	1F	501	FMN	C4'-C5'-O5'-P
69	1N	901	3PE	C32-C33-C34-C35
87	4C	302	PGV	C5-C6-C7-C8
87	8C	303	PGV	C5-C6-C7-C8
75	1d	203	CDL	CA5-C11-C12-C13
88	4A	605	HEA	C2A-CAA-CBA-CGA
87	8C	302	PGV	C26-C27-C28-C29
69	1L	703	3PE	C39-C3A-C3B-C3C
69	1M	501	3PE	C26-C27-C28-C29
75	1q	203	CDL	C16-C17-C18-C19
69	3P	503	3PE	C1-C2-C3-O31
75	1N	902	CDL	CB3-CB4-CB6-OB8
93	8C	308	PEK	C21-C22-C23-C24
69	1d	201	3PE	C3C-C3D-C3E-C3F
70	1Y	207	PC1	C23-C24-C25-C26
69	3A	503	3PE	C36-C37-C38-C39
75	8B	303	CDL	C59-C60-C61-C62
69	1Y	204	3PE	C23-C24-C25-C26
70	1M	505	PC1	C23-C24-C25-C26
75	4B	303	CDL	C59-C60-C61-C62
87	4B	301	PGV	C22-C23-C24-C25
69	3C	504	3PE	C2-C1-O11-P
87	4C	306	PGV	C02-C03-O11-P
69	1M	504	3PE	C38-C39-C3A-C3B
85	3C	501	HEM	C3D-CAD-CBD-CGD
69	3A	503	3PE	C32-C33-C34-C35
69	3R	302	3PE	C35-C36-C37-C38
69	1M	501	3PE	C21-C22-C23-C24
87	8B	301	PGV	C22-C23-C24-C25
80	1T	101	EHZ	C21-C22-C23-C24
92	8B	305	PSC	C25-C26-C27-C28
92	4B	305	PSC	C25-C26-C27-C28
75	1d	203	CDL	C32-C33-C34-C35
75	1L	702	CDL	CA7-C31-C32-C33
87	8C	302	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
69	1d	201	3PE	C31-C32-C33-C34
75	3T	101	CDL	OA5-CA3-CA4-OA6
69	3R	302	3PE	C27-C28-C29-C2A
87	8L	101	PGV	C21-C22-C23-C24
85	3C	502	HEM	C4B-C3B-CAB-CBB
85	3P	502	HEM	C4B-C3B-CAB-CBB
69	1M	502	3PE	C22-C23-C24-C25
69	1A	201	3PE	C36-C37-C38-C39
75	1h	202	CDL	C60-C61-C62-C63
87	4K	101	PGV	C02-C03-O11-P
87	8C	304	PGV	C02-C03-O11-P
87	8C	307	PGV	C02-C03-O11-P
75	8D	201	CDL	C71-C72-C73-C74
70	1B	203	PC1	C28-C29-C2A-C2B
87	4L	101	PGV	C6-C7-C8-C9
87	4L	101	PGV	C21-C22-C23-C24
87	8A	602	PGV	C22-C23-C24-C25
69	1L	703	3PE	C33-C34-C35-C36
80	1T	101	EHZ	O4-C15-C16-O5
69	1M	502	3PE	C3B-C3C-C3D-C3E
75	3T	101	CDL	OA5-CA3-CA4-CA6
75	4C	305	CDL	C36-C37-C38-C39
93	4C	307	PEK	C21-C22-C23-C24
69	1N	901	3PE	C2E-C2F-C2G-C2H
75	3T	101	CDL	C52-C53-C54-C55
87	8L	101	PGV	C6-C7-C8-C9
75	1X	201	CDL	C23-C24-C25-C26
69	1Y	203	3PE	C31-C32-C33-C34
75	3G	103	CDL	CA5-C11-C12-C13
69	1L	703	3PE	C1-C2-C3-O31
69	1M	502	3PE	C1-C2-C3-O31
69	3C	504	3PE	C1-C2-C3-O31
70	1B	203	PC1	C1-C2-C3-O31
70	1h	203	PC1	C1-C2-C3-O31
75	1N	902	CDL	CA3-CA4-CA6-OA8
75	8C	306	CDL	C36-C37-C38-C39
75	1L	702	CDL	C57-C58-C59-C60
70	1I	203	PC1	C24-C25-C26-C27
70	1h	203	PC1	C32-C33-C34-C35
75	8D	201	CDL	C62-C63-C64-C65
87	4C	304	PGV	C02-C03-O11-P
87	8K	101	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
93	8G	102	PEK	C21-C22-C23-C24
70	1h	203	PC1	C2A-C2B-C2C-C2D
70	1H	402	PC1	O11-C1-C2-O21
87	8B	302	PGV	C24-C25-C26-C27
87	8K	101	PGV	C22-C23-C24-C25
87	4B	302	PGV	C24-C25-C26-C27
69	1N	901	3PE	O21-C2-C3-O31
87	8C	304	PGV	O03-C01-C02-O01
75	1N	902	CDL	C32-C31-CA7-OA8
87	8C	302	PGV	C3-C4-C5-C6
88	8A	605	HEA	C3B-C11-C12-C13
75	1L	702	CDL	C11-C12-C13-C14
75	4B	303	CDL	C38-C39-C40-C41
75	1X	201	CDL	C61-C62-C63-C64
87	4C	301	PGV	C7-C8-C9-C10
75	1N	902	CDL	C12-C13-C14-C15
75	8C	306	CDL	C59-C60-C61-C62
87	8C	302	PGV	C27-C28-C29-C30
69	1N	901	3PE	C2-C1-O11-P
75	3N	502	CDL	CB4-CB3-OB5-PB2
87	4K	101	PGV	C05-C04-O12-P
87	8B	301	PGV	C05-C04-O12-P
87	8C	305	PGV	C02-C03-O11-P
87	8K	101	PGV	C05-C04-O12-P
70	1M	505	PC1	C32-C33-C34-C35
75	4D	201	CDL	C71-C72-C73-C74
69	1M	506	3PE	C21-C22-C23-C24
69	1M	506	3PE	C27-C28-C29-C2A
87	4A	601	PGV	C21-C22-C23-C24
69	1N	901	3PE	O11-C1-C2-C3
69	3A	503	3PE	O11-C1-C2-C3
69	3C	504	3PE	O11-C1-C2-C3
75	1d	203	CDL	OA5-CA3-CA4-CA6
75	3P	504	CDL	OB5-CB3-CB4-CB6
87	8A	602	PGV	C01-C02-C03-O11
75	3G	102	CDL	C72-C71-CB7-OB8
93	4G	102	PEK	O03-C21-C22-C23
93	8G	102	PEK	O03-C21-C22-C23
69	3Y	101	3PE	C31-C32-C33-C34
70	1q	201	PC1	C2A-C2B-C2C-C2D
75	4D	201	CDL	CA2-C1-CB2-OB2
75	1h	202	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
69	1Y	202	3PE	C1-C2-C3-O31
69	1Y	204	3PE	C1-C2-C3-O31
69	3N	501	3PE	C1-C2-C3-O31
75	1L	702	CDL	CA3-CA4-CA6-OA8
75	4B	303	CDL	CB3-CB4-CB6-OB8
75	8B	303	CDL	CB3-CB4-CB6-OB8
87	4J	101	PGV	O03-C01-C02-C03
75	1h	202	CDL	C34-C35-C36-C37
69	1d	201	3PE	C28-C29-C2A-C2B
70	1B	203	PC1	C35-C36-C37-C38
69	3G	101	3PE	C31-C32-C33-C34
75	4C	305	CDL	C59-C60-C61-C62
93	4G	102	PEK	C21-C22-C23-C24
69	1M	504	3PE	O11-C1-C2-O21
69	1m	201	3PE	O11-C1-C2-O21
69	3A	502	3PE	O11-C1-C2-O21
87	4C	302	PGV	O01-C02-C03-O11
87	8C	303	PGV	O01-C02-C03-O11
69	1M	502	3PE	C34-C35-C36-C37
69	1Y	204	3PE	C2-C1-O11-P
75	3T	101	CDL	CA4-CA3-OA5-PA1
75	4B	303	CDL	C1-CA2-OA2-PA1
87	4G	101	PGV	C02-C03-O11-P
87	8G	101	PGV	C02-C03-O11-P
70	1M	505	PC1	C2A-C2B-C2C-C2D
82	1h	201	AME	C-CA-N-CT1
70	1I	203	PC1	C37-C38-C39-C3A
69	1Y	203	3PE	C22-C23-C24-C25
75	1L	702	CDL	C33-C34-C35-C36
75	1q	203	CDL	C52-C51-CB5-OB6
69	1Y	204	3PE	O21-C2-C3-O31
69	3N	501	3PE	O21-C2-C3-O31
69	3N	503	3PE	O21-C2-C3-O31
75	3N	502	CDL	OA6-CA4-CA6-OA8
75	4B	303	CDL	OB6-CB4-CB6-OB8
87	4C	303	PGV	O03-C01-C02-O01
87	8J	101	PGV	O03-C01-C02-O01
75	8B	303	CDL	C38-C39-C40-C41
92	4B	305	PSC	C9-C10-C11-C12
92	4B	305	PSC	C10-C11-C12-C13
92	8B	305	PSC	C9-C10-C11-C12
92	8B	305	PSC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
93	4G	102	PEK	C5-C6-C7-C8
93	4G	102	PEK	C9-C10-C11-C12
93	8G	102	PEK	C5-C6-C7-C8
93	8G	102	PEK	C9-C10-C11-C12
69	1M	504	3PE	C31-C32-C33-C34
87	4J	101	PGV	C19-C20-C21-C22
70	1A	202	PC1	C22-C23-C24-C25
75	3P	504	CDL	CA5-C11-C12-C13
75	1L	702	CDL	C37-C38-C39-C40
87	4L	101	PGV	C3-C4-C5-C6
75	1X	201	CDL	C36-C37-C38-C39
76	1O	401	GTP	PB-O3A-PA-O5'
75	1h	202	CDL	CB7-C71-C72-C73
75	4D	201	CDL	C59-C60-C61-C62
87	8J	101	PGV	C19-C20-C21-C22
75	4C	305	CDL	C52-C53-C54-C55
70	1H	402	PC1	O11-C1-C2-C3
75	4B	303	CDL	OA5-CA3-CA4-CA6
75	1X	201	CDL	C58-C59-C60-C61
87	4C	303	PGV	C02-C03-O11-P
87	8C	304	PGV	C24-C25-C26-C27
87	4C	303	PGV	C24-C25-C26-C27
69	1A	201	3PE	O21-C21-C22-C23
70	1Y	207	PC1	O31-C31-C32-C33
75	4D	201	CDL	C62-C63-C64-C65
69	1Y	204	3PE	O31-C31-C32-C33
69	1N	901	3PE	O11-C1-C2-O21
75	1d	203	CDL	OA5-CA3-CA4-OA6
75	4B	303	CDL	OA5-CA3-CA4-OA6
87	8A	601	PGV	O01-C02-C03-O11
69	1M	501	3PE	C1-C2-C3-O31
69	1N	901	3PE	C1-C2-C3-O31
69	3N	503	3PE	C1-C2-C3-O31
75	3P	504	CDL	CB3-CB4-CB6-OB8
87	8J	101	PGV	O03-C01-C02-C03
88	4A	604	HEA	O11-C11-C12-C13
88	8A	604	HEA	O11-C11-C12-C13
75	3G	103	CDL	C52-C53-C54-C55
87	4C	301	PGV	C26-C27-C28-C29
75	1h	202	CDL	C38-C39-C40-C41
69	1K	101	3PE	C12-C11-O13-P
69	1L	701	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
69	1M	504	3PE	C12-C11-O13-P
69	1Y	203	3PE	C12-C11-O13-P
69	1m	201	3PE	C12-C11-O13-P
69	3C	503	3PE	C12-C11-O13-P
69	3C	504	3PE	C12-C11-O13-P
69	3P	503	3PE	C12-C11-O13-P
70	1A	203	PC1	C12-C11-O13-P
70	1B	203	PC1	C12-C11-O13-P
70	1P	401	PC1	C12-C11-O13-P
93	4C	307	PEK	C05-C04-O12-P
93	4G	102	PEK	C05-C04-O12-P
93	8C	308	PEK	C05-C04-O12-P
93	8G	102	PEK	C05-C04-O12-P
75	8C	306	CDL	C52-C53-C54-C55
69	1L	703	3PE	O21-C2-C3-O31
69	3P	503	3PE	O21-C2-C3-O31
70	1H	403	PC1	O21-C2-C3-O31
70	1h	203	PC1	O21-C2-C3-O31
75	3P	504	CDL	OB6-CB4-CB6-OB8
75	8B	303	CDL	OB6-CB4-CB6-OB8
87	4J	101	PGV	O03-C01-C02-O01
75	1d	203	CDL	C71-C72-C73-C74
75	3P	504	CDL	C31-C32-C33-C34
87	4K	101	PGV	C22-C23-C24-C25
75	1X	201	CDL	C35-C36-C37-C38
87	8L	101	PGV	C3-C4-C5-C6
70	1A	202	PC1	O13-C11-C12-N
70	1B	203	PC1	O13-C11-C12-N
70	1P	401	PC1	O13-C11-C12-N
70	1Y	207	PC1	O13-C11-C12-N
70	1h	203	PC1	O13-C11-C12-N
76	1O	401	GTP	PA-O3A-PB-O1B
85	3P	501	HEM	C3D-CAD-CBD-CGD
75	8D	201	CDL	CA2-C1-CB2-OB2
88	8A	605	HEA	C2A-CAA-CBA-CGA
75	8D	201	CDL	C59-C60-C61-C62
87	8B	302	PGV	C20-C21-C22-C23
70	1I	203	PC1	C23-C24-C25-C26
87	4B	302	PGV	C27-C28-C29-C30
86	3D	501	HEC	C3D-CAD-CBD-CGD
87	4A	601	PGV	C11-C10-C9-C8
69	1M	504	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
69	1m	201	3PE	O11-C1-C2-C3
75	8B	303	CDL	OA5-CA3-CA4-CA6
87	4A	601	PGV	C01-C02-C03-O11
87	4M	101	PGV	C01-C02-C03-O11
75	1d	203	CDL	C1-CA2-OA2-PA1
75	1h	202	CDL	CB4-CB3-OB5-PB2
87	4A	601	PGV	C02-C03-O11-P
87	8A	601	PGV	C29-C30-C31-C32
80	1n	201	EHZ	C11-C10-S1-C9
87	4C	301	PGV	C3-C4-C5-C6
87	8B	302	PGV	C27-C28-C29-C30
69	3A	503	3PE	O11-C1-C2-O21
70	1M	505	PC1	O11-C1-C2-O21
75	8B	303	CDL	OA5-CA3-CA4-OA6
87	4A	601	PGV	O01-C02-C03-O11
87	4M	101	PGV	O01-C02-C03-O11
87	8A	602	PGV	O01-C02-C03-O11
75	4C	305	CDL	C11-C12-C13-C14
75	4C	305	CDL	C16-C17-C18-C19
69	1Y	202	3PE	O21-C2-C3-O31
70	1B	203	PC1	O21-C2-C3-O31
75	1N	902	CDL	OB6-CB4-CB6-OB8
70	1Y	207	PC1	C36-C37-C38-C39
87	4G	101	PGV	C22-C23-C24-C25
69	1M	502	3PE	C24-C25-C26-C27
70	1H	402	PC1	C1-C2-C3-O31
80	1T	101	EHZ	C10-C11-N1-C12
80	1n	201	EHZ	C10-C11-N1-C12
70	1H	403	PC1	C39-C3A-C3B-C3C
69	1A	201	3PE	C11-O13-P-O11
69	1A	201	3PE	C11-O13-P-O14
69	1K	101	3PE	C1-O11-P-O12
69	1K	101	3PE	C11-O13-P-O14
69	1M	502	3PE	C1-O11-P-O13
69	1M	504	3PE	C11-O13-P-O14
69	1M	506	3PE	C11-O13-P-O14
69	1P	403	3PE	C1-O11-P-O13
69	1P	403	3PE	C1-O11-P-O14
69	1Y	202	3PE	C11-O13-P-O14
69	1Y	203	3PE	C11-O13-P-O14
69	1d	201	3PE	C11-O13-P-O14
69	1j	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
69	1m	201	3PE	C11-O13-P-O14
69	3C	503	3PE	C1-O11-P-O14
69	3N	501	3PE	C1-O11-P-O12
69	3N	501	3PE	C11-O13-P-O14
69	3N	503	3PE	C11-O13-P-O14
70	1A	203	PC1	C1-O11-P-O14
70	1M	503	PC1	C1-O11-P-O14
70	1M	505	PC1	C1-O11-P-O14
70	1M	505	PC1	C1-O11-P-O13
70	1d	202	PC1	C1-O11-P-O14
75	1N	902	CDL	CA3-OA5-PA1-OA3
75	1X	201	CDL	CA2-OA2-PA1-OA5
75	1X	201	CDL	CB2-OB2-PB2-OB3
75	1d	203	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	CB2-OB2-PB2-OB4
75	1h	202	CDL	CB2-OB2-PB2-OB5
75	3G	103	CDL	CA2-OA2-PA1-OA3
75	3G	103	CDL	CB3-OB5-PB2-OB3
75	3N	502	CDL	CB3-OB5-PB2-OB3
75	3P	504	CDL	CA3-OA5-PA1-OA3
75	3P	504	CDL	CB3-OB5-PB2-OB3
75	3T	101	CDL	CA3-OA5-PA1-OA2
75	4B	303	CDL	CB3-OB5-PB2-OB4
75	4D	201	CDL	CB2-OB2-PB2-OB3
75	8B	303	CDL	CB3-OB5-PB2-OB2
75	8B	303	CDL	CB3-OB5-PB2-OB4
75	8D	201	CDL	CB2-OB2-PB2-OB3
87	4A	601	PGV	C04-O12-P-O13
87	4C	302	PGV	C03-O11-P-O12
87	4K	101	PGV	C04-O12-P-O13
87	8A	601	PGV	C04-O12-P-O13
87	8B	301	PGV	C04-O12-P-O13
87	8C	302	PGV	C04-O12-P-O14
87	8C	304	PGV	C03-O11-P-O14
87	8C	305	PGV	C03-O11-P-O14
87	8K	101	PGV	C04-O12-P-O13
92	4B	305	PSC	C04-O12-P-O14
92	8B	305	PSC	C04-O12-P-O14
69	1M	506	3PE	C28-C29-C2A-C2B
70	1H	402	PC1	C2-C1-O11-P
70	1M	505	PC1	C2-C1-O11-P
75	1d	203	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
75	3P	504	CDL	CB4-CB3-OB5-PB2
75	8B	303	CDL	C1-CA2-OA2-PA1
87	8A	601	PGV	C02-C03-O11-P
69	1Y	203	3PE	C33-C34-C35-C36
70	1d	202	PC1	C37-C38-C39-C3A
87	8C	301	PGV	C11-C12-C13-C14
92	8B	305	PSC	C12-C13-C14-C15
92	8B	305	PSC	C19-C20-C21-C22
75	1H	401	CDL	CA3-CA4-OA6-CA5
88	4A	604	HEA	C15-C16-C17-C18
69	3Y	101	3PE	O11-C1-C2-C3
70	1M	505	PC1	O11-C1-C2-C3
75	8C	306	CDL	OB5-CB3-CB4-CB6
87	8K	101	PGV	C2-C3-C4-C5
87	8C	304	PGV	C9-C10-C11-C12
87	8C	305	PGV	C9-C10-C11-C12
87	8K	101	PGV	C9-C10-C11-C12
69	1Y	203	3PE	O11-C1-C2-O21
69	3C	504	3PE	O11-C1-C2-O21
75	1L	702	CDL	OA5-CA3-CA4-OA6
75	3P	504	CDL	OB5-CB3-CB4-OB6
69	1m	201	3PE	C23-C24-C25-C26
69	1M	504	3PE	C24-C25-C26-C27
69	1Y	205	3PE	C33-C34-C35-C36
87	4K	101	PGV	C2-C3-C4-C5
69	1M	502	3PE	O21-C2-C3-O31
87	4B	301	PGV	C30-C31-C32-C33
69	1m	201	3PE	O21-C21-C22-C23
69	3C	504	3PE	O31-C31-C32-C33
70	3X	101	PC1	O21-C21-C22-C23
69	3C	503	3PE	C29-C2A-C2B-C2C
87	8C	301	PGV	C11-C10-C9-C8
88	4A	605	HEA	C3B-C11-C12-C13
87	8C	302	PGV	C1-C2-C3-C4
87	4C	303	PGV	C5-C6-C7-C8
87	4C	301	PGV	C1-C2-C3-C4
80	1n	201	EHZ	C7-C8-C9-O2
87	4K	101	PGV	C9-C10-C11-C12
87	4L	101	PGV	C9-C10-C11-C12
69	3C	504	3PE	C23-C24-C25-C26
75	8C	306	CDL	C11-C12-C13-C14
75	8C	306	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
75	8C	306	CDL	C51-C52-C53-C54
70	1B	202	PC1	C36-C37-C38-C39
80	1T	101	EHZ	C1-C21-C22-C23
75	1L	702	CDL	C38-C39-C40-C41
70	1Y	207	PC1	C25-C26-C27-C28
87	4M	101	PGV	C3-C4-C5-C6
69	1d	201	3PE	C2-C1-O11-P
69	3R	302	3PE	C21-C22-C23-C24
87	4J	101	PGV	C2-C3-C4-C5
75	1X	201	CDL	OB5-CB3-CB4-OB6
92	8B	305	PSC	O01-C02-C03-O11
87	4A	602	PGV	C11-C12-C13-C14
87	4C	301	PGV	C9-C10-C11-C12
87	4C	304	PGV	C9-C10-C11-C12
87	4M	101	PGV	C9-C10-C11-C12
87	8L	101	PGV	C9-C10-C11-C12
92	4B	305	PSC	C12-C13-C14-C15
69	1Y	202	3PE	C31-C32-C33-C34
75	4C	305	CDL	C51-C52-C53-C54
69	1P	403	3PE	C37-C38-C39-C3A
87	8A	602	PGV	C9-C10-C11-C12
87	8C	303	PGV	C9-C10-C11-C12
87	8J	101	PGV	C9-C10-C11-C12
75	1X	201	CDL	C55-C56-C57-C58
69	3Y	101	3PE	O21-C2-C3-O31
70	1M	505	PC1	O21-C2-C3-O31
87	8B	302	PGV	C11-C10-C9-C8
75	1L	702	CDL	C58-C59-C60-C61
75	8B	303	CDL	C11-C12-C13-C14
87	8C	304	PGV	C13-C14-C15-C16
87	4A	601	PGV	C29-C30-C31-C32
87	4B	302	PGV	C20-C21-C22-C23
75	1L	702	CDL	CA4-CA3-OA5-PA1
87	8C	304	PGV	C5-C6-C7-C8
69	1M	502	3PE	C2A-C2B-C2C-C2D
75	1N	902	CDL	O1-C1-CB2-OB2
69	3N	501	3PE	C33-C34-C35-C36
87	4C	303	PGV	C9-C10-C11-C12
87	8A	603	PGV	C11-C12-C13-C14
87	8C	302	PGV	C11-C12-C13-C14
87	8C	307	PGV	C11-C12-C13-C14
87	8A	601	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
85	3C	501	HEM	CAA-CBA-CGA-O1A
85	3C	501	HEM	CAA-CBA-CGA-O2A
85	3P	501	HEM	CAA-CBA-CGA-O2A
85	3P	502	HEM	CAA-CBA-CGA-O1A
88	8A	604	HEA	CAD-CBD-CGD-O1D
69	1Y	202	3PE	O31-C31-C32-C33
69	1M	504	3PE	C1-C2-O21-C21
69	1Y	202	3PE	C1-C2-O21-C21
69	1Y	205	3PE	C1-C2-O21-C21
87	8C	304	PGV	C01-C02-O01-C1
88	8A	604	HEA	CAD-CBD-CGD-O2D
70	1B	202	PC1	C3D-C3E-C3F-C3G
75	1X	201	CDL	C31-C32-C33-C34
87	4A	603	PGV	C11-C12-C13-C14
88	4A	604	HEA	CAD-CBD-CGD-O1D
88	8A	605	HEA	CAD-CBD-CGD-O1D
75	1N	902	CDL	C32-C31-CA7-OA9
69	1N	901	3PE	C23-C24-C25-C26
70	1h	203	PC1	C2B-C2C-C2D-C2E
69	3C	503	3PE	O11-C1-C2-O21
92	4B	305	PSC	O01-C02-C03-O11
87	8G	101	PGV	C7-C8-C9-C10
87	8A	603	PGV	C15-C16-C17-C18
69	1M	506	3PE	C25-C26-C27-C28
87	8G	101	PGV	C9-C10-C11-C12
75	1N	902	CDL	C1-CB2-OB2-PB2
75	3N	502	CDL	C1-CB2-OB2-PB2
85	3C	502	HEM	CAA-CBA-CGA-O1A
88	8A	605	HEA	C26-C15-C16-C17
75	4C	305	CDL	OB5-CB3-CB4-CB6
92	4B	305	PSC	C2-C3-C4-C5
69	3A	502	3PE	O21-C2-C3-O31
75	1q	203	CDL	OB6-CB4-CB6-OB8
75	3G	103	CDL	OB6-CB4-CB6-OB8
75	4D	201	CDL	OA6-CA4-CA6-OA8
85	3P	501	HEM	CAD-CBD-CGD-O1D
85	3P	502	HEM	CAD-CBD-CGD-O1D
87	4K	101	PGV	C3-C4-C5-C6
87	8K	101	PGV	C3-C4-C5-C6
93	4G	102	PEK	O04-C21-C22-C23
78	1P	402	NDP	O4D-C4D-C5D-O5D
78	1P	402	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
87	4M	101	PGV	C22-C23-C24-C25
88	4A	605	HEA	CAD-CBD-CGD-O2D
75	1d	203	CDL	C72-C73-C74-C75
93	8G	102	PEK	O04-C21-C22-C23
87	4C	301	PGV	C11-C12-C13-C14
87	4M	101	PGV	C11-C12-C13-C14
87	8L	101	PGV	C11-C12-C13-C14
70	1P	401	PC1	C33-C34-C35-C36
69	3C	503	3PE	C25-C26-C27-C28
75	3A	501	CDL	O1-C1-CA2-OA2
87	4C	301	PGV	C6-C7-C8-C9
85	3P	501	HEM	CAA-CBA-CGA-O1A
88	4A	604	HEA	CAD-CBD-CGD-O2D
88	8A	605	HEA	CAD-CBD-CGD-O2D
87	8J	101	PGV	C5-C6-C7-C8
75	3N	502	CDL	CA4-CA6-OA8-CA7
69	3N	501	3PE	C22-C23-C24-C25
69	3Y	101	3PE	C2-C3-O31-C31
85	3P	502	HEM	CAD-CBD-CGD-O2D
87	8C	304	PGV	O03-C01-C02-C03
85	3C	502	HEM	CAA-CBA-CGA-O2A
86	3Q	501	HEC	CAA-CBA-CGA-O2A
87	8C	307	PGV	C5-C6-C7-C8
87	4G	101	PGV	C9-C10-C11-C12
87	4J	101	PGV	C9-C10-C11-C12
87	4B	302	PGV	C11-C10-C9-C8
87	8A	603	PGV	C2-C3-C4-C5
75	1h	202	CDL	OB5-CB3-CB4-OB6
85	3P	502	HEM	CAA-CBA-CGA-O2A
92	8B	305	PSC	C15-C16-C17-C18
87	8C	302	PGV	C6-C7-C8-C9
85	3P	501	HEM	CAD-CBD-CGD-O2D
87	4A	601	PGV	C11-C12-C13-C14
87	4C	302	PGV	C9-C10-C11-C12
87	4C	306	PGV	C11-C12-C13-C14
87	8A	602	PGV	C11-C12-C13-C14
87	8C	302	PGV	C9-C10-C11-C12
69	1K	101	3PE	O21-C21-C22-C23
70	1B	202	PC1	C3C-C3D-C3E-C3F
88	4A	605	HEA	CAD-CBD-CGD-O1D
70	1P	401	PC1	C24-C25-C26-C27
69	1Y	203	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
75	1L	702	CDL	OA5-CA3-CA4-CA6
75	1h	202	CDL	OB5-CB3-CB4-CB6
88	4A	604	HEA	C27-C19-C20-C21
88	4A	605	HEA	C26-C15-C16-C17
69	3R	302	3PE	C22-C23-C24-C25
69	1d	201	3PE	O21-C2-C3-O31
92	4B	305	PSC	C19-C20-C21-C22
86	3D	501	HEC	CAA-CBA-CGA-O2A
75	4B	303	CDL	C12-C11-CA5-OA6
87	4C	303	PGV	C13-C14-C15-C16
87	8J	101	PGV	C2-C3-C4-C5
75	4C	305	CDL	C81-C82-C83-C84
69	1M	506	3PE	C2B-C2C-C2D-C2E
70	1M	505	PC1	C28-C29-C2A-C2B
69	1K	101	3PE	C24-C25-C26-C27
87	4K	101	PGV	C11-C12-C13-C14
87	8A	601	PGV	C9-C10-C11-C12
87	8K	101	PGV	C11-C12-C13-C14
87	8B	301	PGV	C30-C31-C32-C33
83	1i	201	CHD	C22-C23-C24-O26
69	3C	503	3PE	C2C-C2D-C2E-C2F
75	3G	102	CDL	C72-C71-CB7-OB9
86	3Q	501	HEC	CAA-CBA-CGA-O1A
69	1L	703	3PE	C29-C2A-C2B-C2C
69	1Y	206	3PE	C3-C2-O21-C21
69	3C	503	3PE	C1-C2-O21-C21
87	4C	303	PGV	C01-C02-O01-C1
75	1X	201	CDL	C34-C35-C36-C37
69	3N	501	3PE	C26-C27-C28-C29
69	1K	101	3PE	C26-C27-C28-C29
75	3G	102	CDL	C12-C13-C14-C15
82	1h	201	AME	CB-CA-N-CT1
87	8C	304	PGV	C05-C04-O12-P
75	3G	102	CDL	CA2-C1-CB2-OB2
70	1M	503	PC1	C11-C12-N-C15
75	4C	305	CDL	C75-C76-C77-C78
70	1M	505	PC1	C1-C2-C3-O31
75	3N	502	CDL	CA3-CA4-CA6-OA8
70	3R	303	PC1	C27-C28-C29-C2A
88	8A	605	HEA	O11-C11-C12-C13
69	3D	502	3PE	C24-C25-C26-C27
87	4A	601	PGV	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
83	1i	201	CHD	C22-C23-C24-O25
80	1T	101	EHZ	C15-C16-C17-C19
70	1h	203	PC1	C22-C23-C24-C25
69	1A	201	3PE	C2A-C2B-C2C-C2D
87	8A	602	PGV	C3-C4-C5-C6
86	3D	501	HEC	CAA-CBA-CGA-O1A
87	4C	303	PGV	C3-C4-C5-C6
93	4C	307	PEK	O03-C01-C02-O01
69	3A	502	3PE	O11-C1-C2-C3
70	1B	203	PC1	O11-C1-C2-C3
87	4C	302	PGV	C01-C02-C03-O11
87	8C	303	PGV	C01-C02-C03-O11
92	4B	305	PSC	C01-C02-C03-O11
92	8B	305	PSC	C01-C02-C03-O11
87	4K	101	PGV	C1-C2-C3-C4
75	8C	306	CDL	C62-C63-C64-C65
87	4G	101	PGV	C7-C8-C9-C10
69	1Y	203	3PE	C2D-C2E-C2F-C2G
70	1M	505	PC1	C2D-C2E-C2F-C2G
87	8C	303	PGV	C14-C15-C16-C17
76	1O	401	GTP	PA-O3A-PB-O2B
70	1A	202	PC1	C23-C24-C25-C26
80	1n	201	EHZ	C21-C1-C2-C3
87	8C	303	PGV	C26-C27-C28-C29
75	3G	103	CDL	C11-C12-C13-C14
75	8C	306	CDL	C71-C72-C73-C74
87	8K	101	PGV	C5-C6-C7-C8
92	8B	305	PSC	C4-C5-C6-C7
75	8C	306	CDL	C18-C19-C20-C21
87	4A	601	PGV	C24-C25-C26-C27
75	1d	203	CDL	C32-C31-CA7-OA8
87	8C	303	PGV	C6-C7-C8-C9
69	1Y	206	3PE	O21-C21-C22-C23
87	8A	601	PGV	O03-C19-C20-C21
70	1I	203	PC1	C22-C23-C24-C25
70	1H	402	PC1	C31-C32-C33-C34
75	3P	504	CDL	C32-C31-CA7-OA8
87	8A	602	PGV	C21-C22-C23-C24
80	1T	101	EHZ	C4-C5-C6-C7
88	8A	604	HEA	CAA-CBA-CGA-O1A
69	1d	201	3PE	C35-C36-C37-C38
87	4C	301	PGV	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
70	1d	202	PC1	O21-C21-C22-C23
88	4A	604	HEA	CAA-CBA-CGA-O1A
88	8A	604	HEA	CAA-CBA-CGA-O2A
69	1P	403	3PE	O21-C21-C22-C23
87	4A	601	PGV	O03-C19-C20-C21
75	4C	305	CDL	C18-C19-C20-C21
75	1q	203	CDL	C52-C51-CB5-OB7
88	4A	604	HEA	CAA-CBA-CGA-O2A
69	1M	504	3PE	C32-C33-C34-C35
75	1X	201	CDL	OB5-CB3-CB4-CB6
73	1F	501	FMN	N10-C1'-C2'-O2'
75	1X	201	CDL	CB2-C1-CA2-OA2
70	1H	402	PC1	C36-C37-C38-C39
75	8C	306	CDL	C75-C76-C77-C78
69	1M	502	3PE	C29-C2A-C2B-C2C
69	1Y	202	3PE	C3-C2-O21-C21
75	3N	502	CDL	CB3-CB4-OB6-CB5
75	3N	502	CDL	CB6-CB4-OB6-CB5
75	1X	201	CDL	C63-C64-C65-C66
87	8J	101	PGV	C30-C31-C32-C33
87	8C	304	PGV	C3-C4-C5-C6
69	1K	101	3PE	C34-C35-C36-C37
70	1P	401	PC1	C32-C33-C34-C35
75	3P	504	CDL	C72-C71-CB7-OB8
75	3P	504	CDL	C13-C14-C15-C16
87	8A	602	PGV	C05-C04-O12-P
70	1Y	207	PC1	O32-C31-C32-C33
70	1q	201	PC1	C32-C33-C34-C35
75	4C	305	CDL	C71-C72-C73-C74
69	1Y	203	3PE	C27-C28-C29-C2A
87	8G	101	PGV	C22-C23-C24-C25
75	1q	203	CDL	CA5-C11-C12-C13
75	8B	303	CDL	CB5-C51-C52-C53
75	1h	202	CDL	C74-C75-C76-C77
75	1N	902	CDL	CA7-C31-C32-C33
70	3J	101	PC1	C22-C23-C24-C25
70	1M	503	PC1	C11-C12-N-C14
75	4B	303	CDL	C13-C14-C15-C16
87	4G	101	PGV	C23-C24-C25-C26
87	4L	101	PGV	C11-C12-C13-C14
70	1d	202	PC1	O22-C21-C22-C23
69	1L	701	3PE	C28-C29-C2A-C2B

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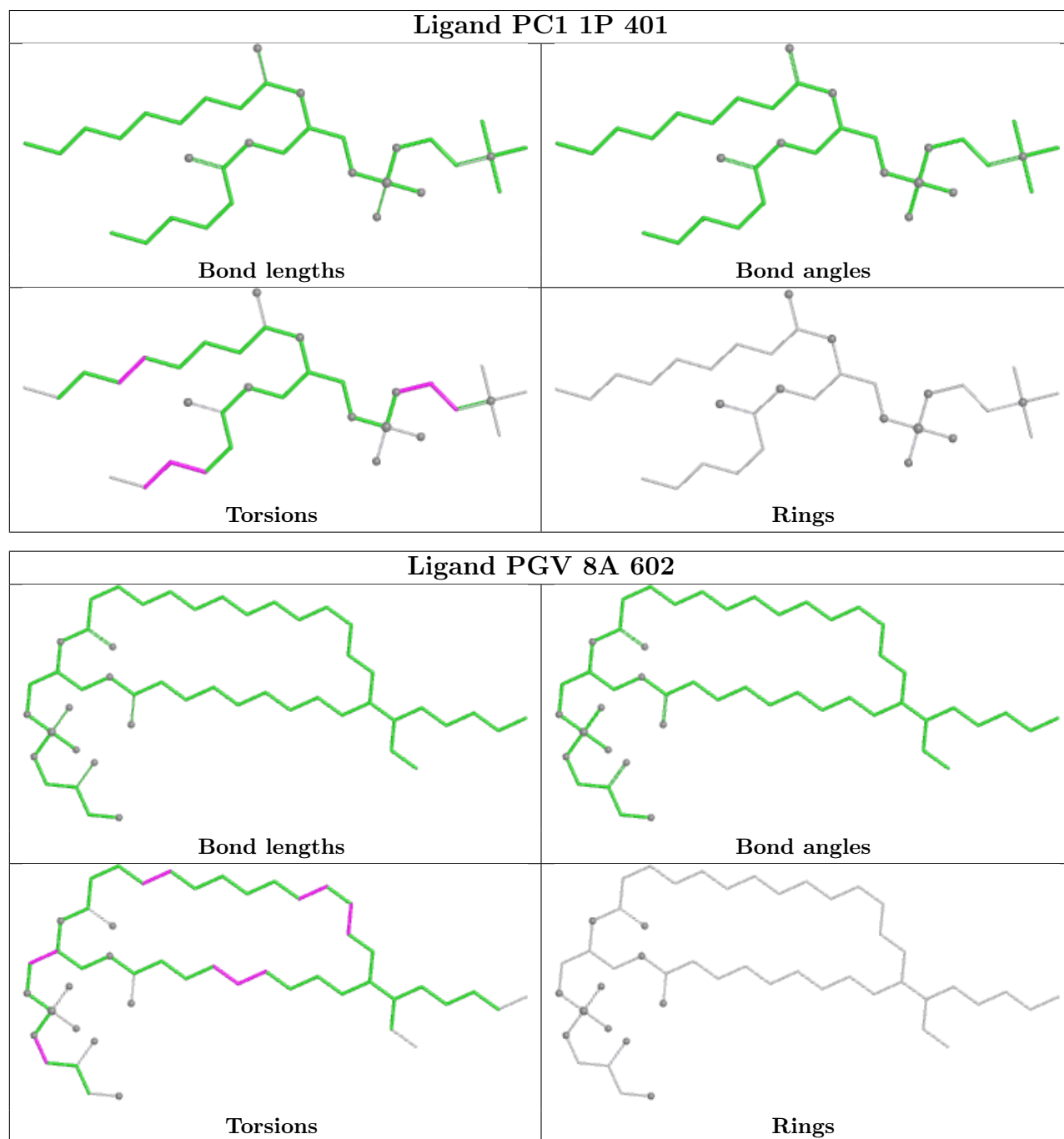
Mol	Chain	Res	Type	Atoms
87	4A	603	PGV	C6-C7-C8-C9
69	1M	501	3PE	C23-C24-C25-C26
87	8A	601	PGV	O04-C19-C20-C21
69	1M	501	3PE	O21-C2-C3-O31
75	8D	201	CDL	OA6-CA4-CA6-OA8
87	8J	101	PGV	C27-C28-C29-C30
86	3Q	501	HEC	CAD-CBD-CGD-O2D
75	1d	203	CDL	C32-C31-CA7-OA9
87	4J	101	PGV	C27-C28-C29-C30
87	8C	301	PGV	C26-C27-C28-C29
69	1A	201	3PE	C27-C28-C29-C2A
70	1A	202	PC1	O31-C31-C32-C33
87	8C	305	PGV	C7-C8-C9-C10
69	1Y	206	3PE	O22-C21-C22-C23
75	3P	504	CDL	C32-C31-CA7-OA9
87	4A	601	PGV	O04-C19-C20-C21
75	8B	303	CDL	C12-C11-CA5-OA6
70	1Y	207	PC1	C3A-C3B-C3C-C3D
70	1H	403	PC1	O11-C1-C2-C3
87	8A	601	PGV	C01-C02-C03-O11
75	1q	203	CDL	C12-C11-CA5-OA6
80	1T	101	EHZ	C2-C3-C4-C5
87	4M	101	PGV	C20-C21-C22-C23
92	8B	305	PSC	C2-C3-C4-C5
75	3P	504	CDL	C72-C71-CB7-OB9
75	3P	504	CDL	CB5-C51-C52-C53
70	1B	203	PC1	O31-C31-C32-C33
70	1h	203	PC1	O31-C31-C32-C33
75	4D	201	CDL	C32-C31-CA7-OA8
87	4G	101	PGV	O03-C19-C20-C21
87	8C	302	PGV	O03-C19-C20-C21
87	4K	101	PGV	C5-C6-C7-C8
69	1Y	204	3PE	O22-C21-C22-C23
69	1Y	204	3PE	O21-C21-C22-C23
70	1d	202	PC1	O31-C31-C32-C33
87	4C	302	PGV	C26-C27-C28-C29

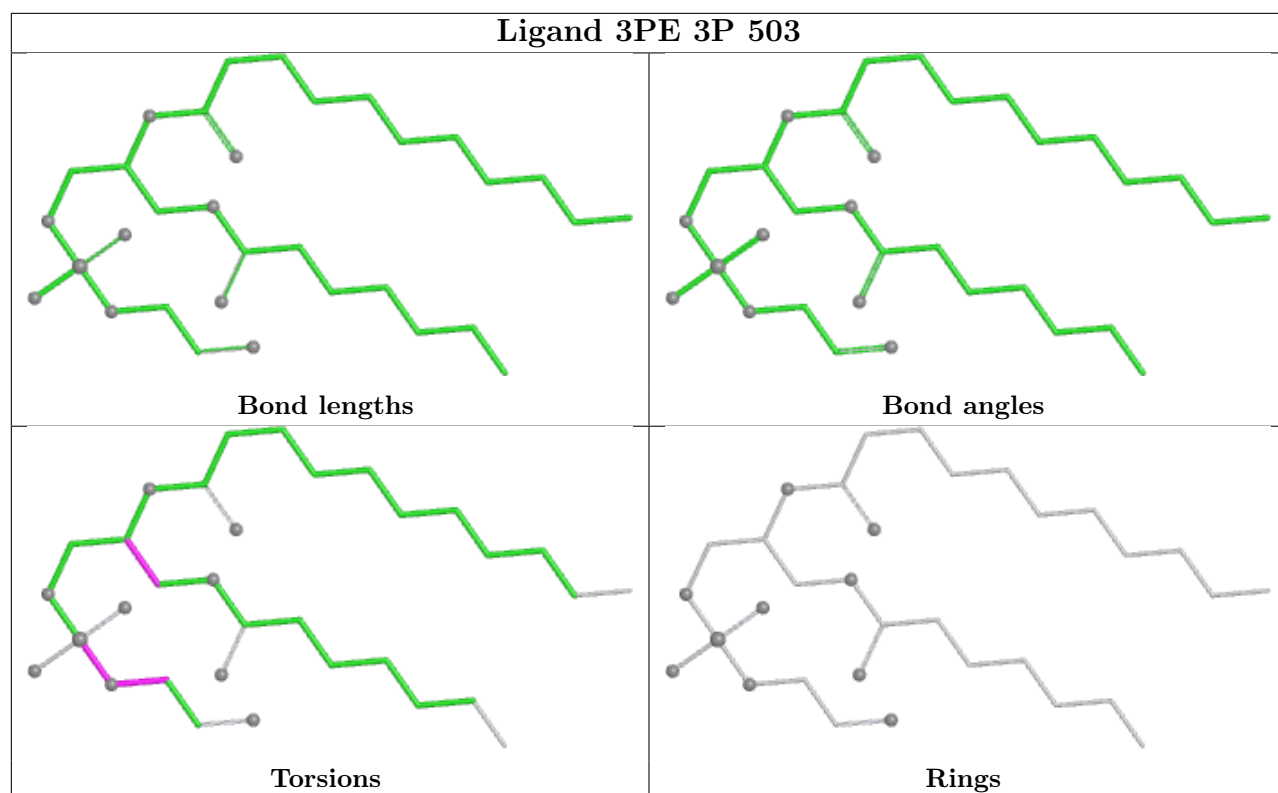
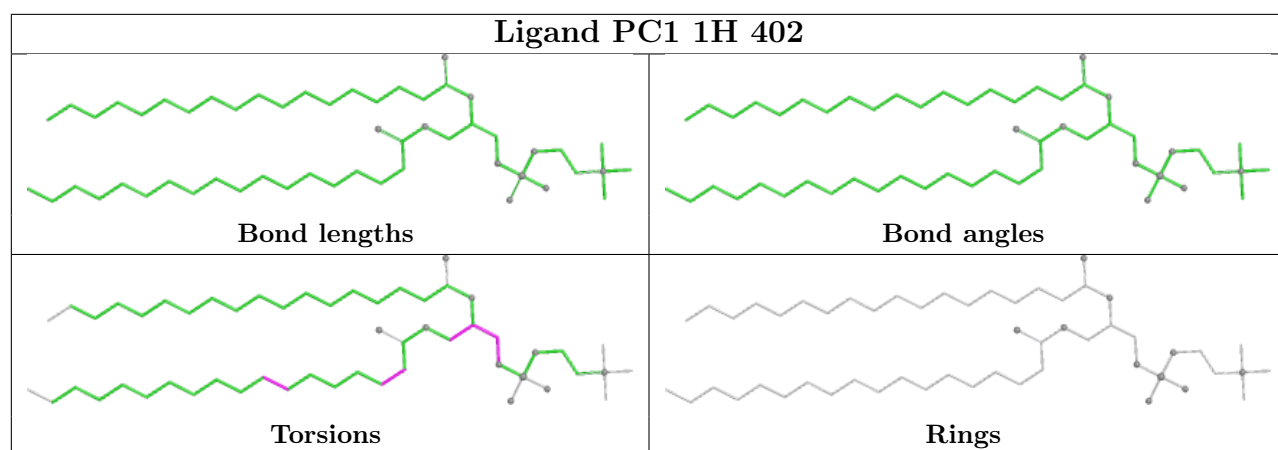
There are no ring outliers.

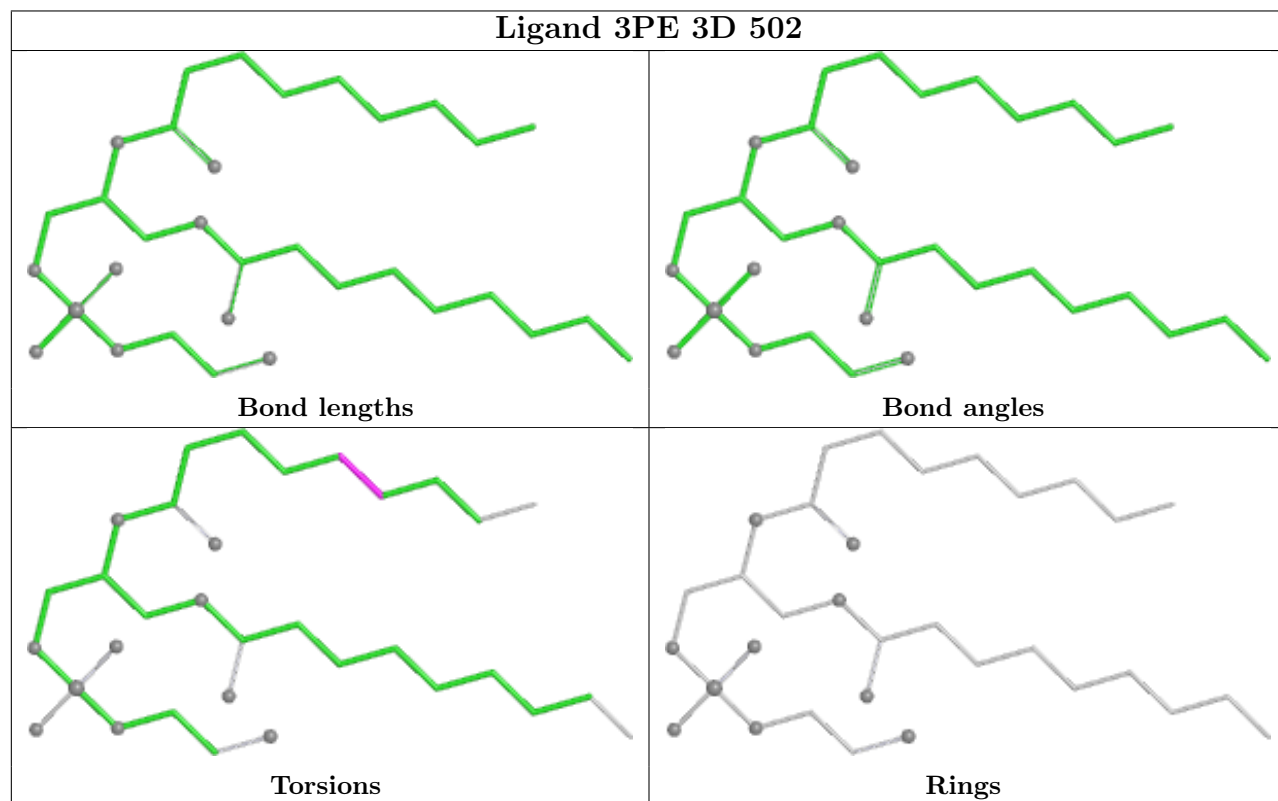
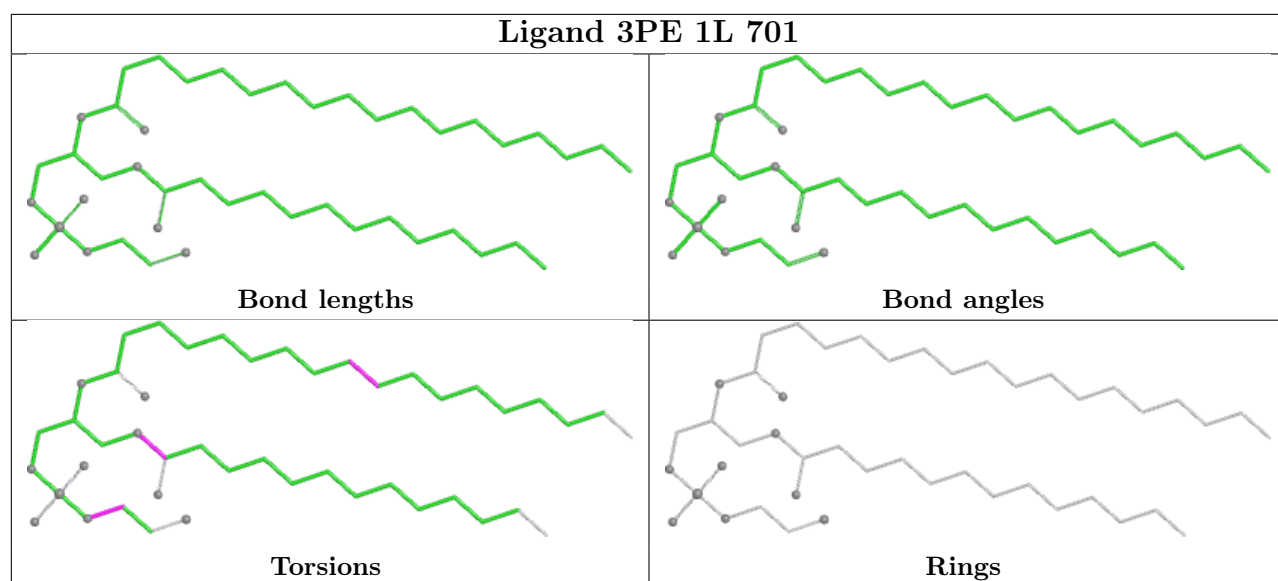
No monomer is involved in short contacts.

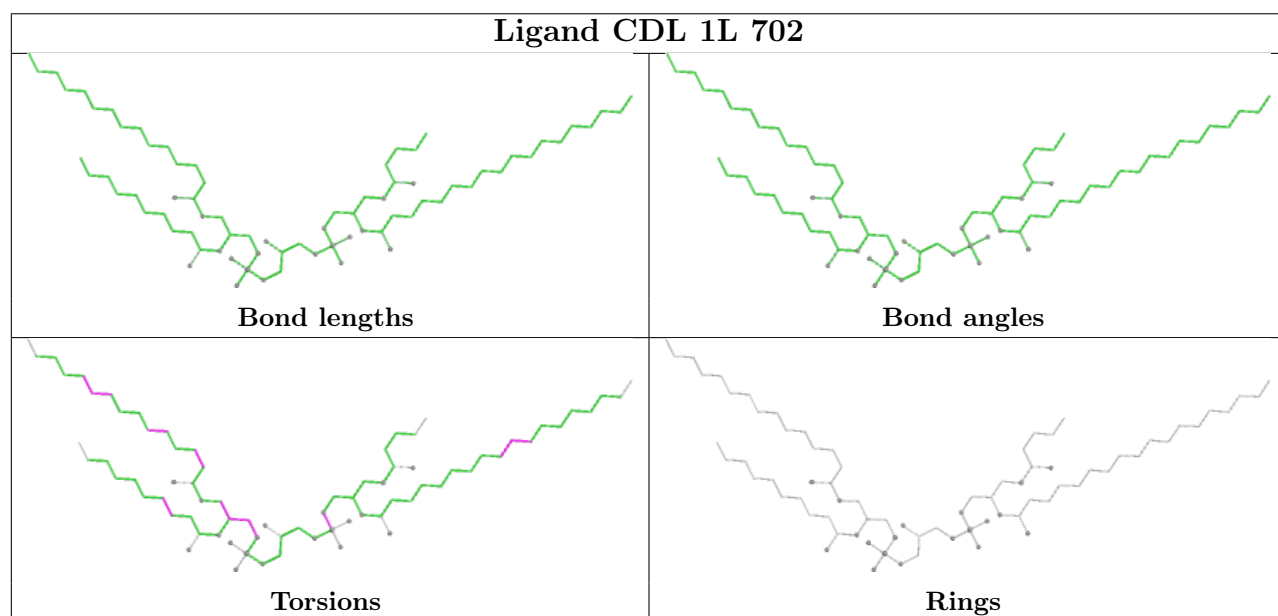
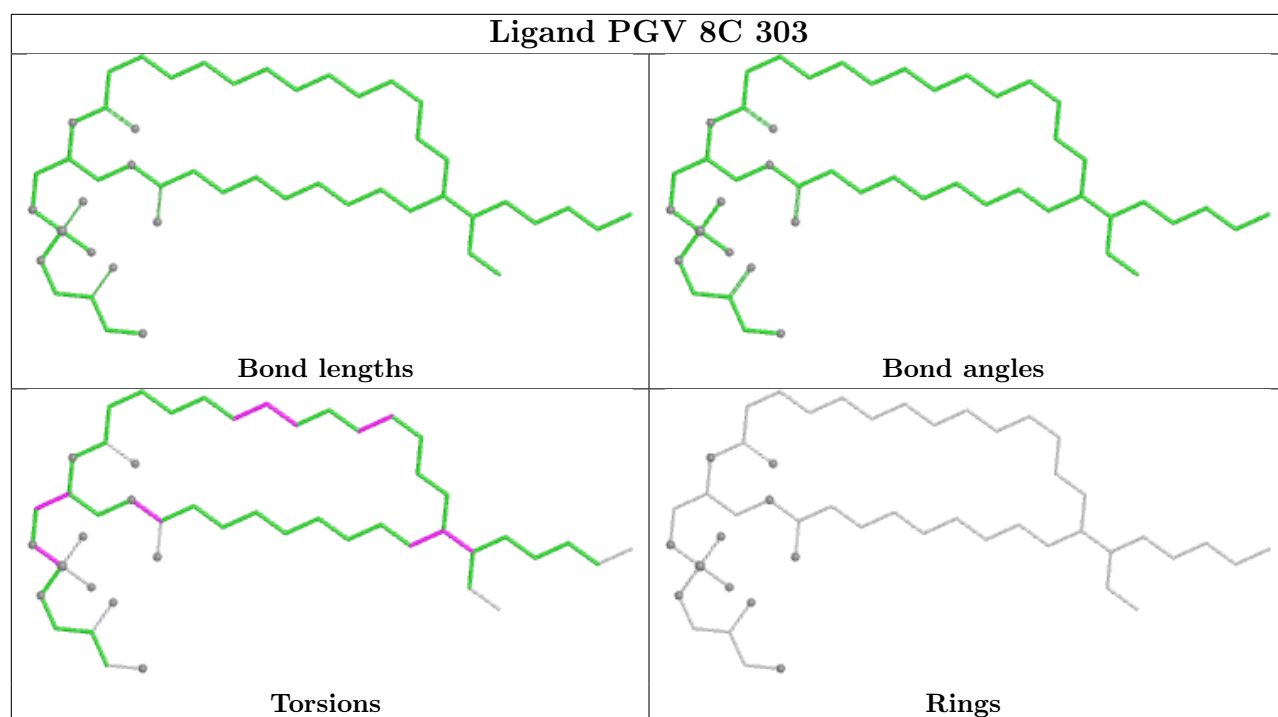
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

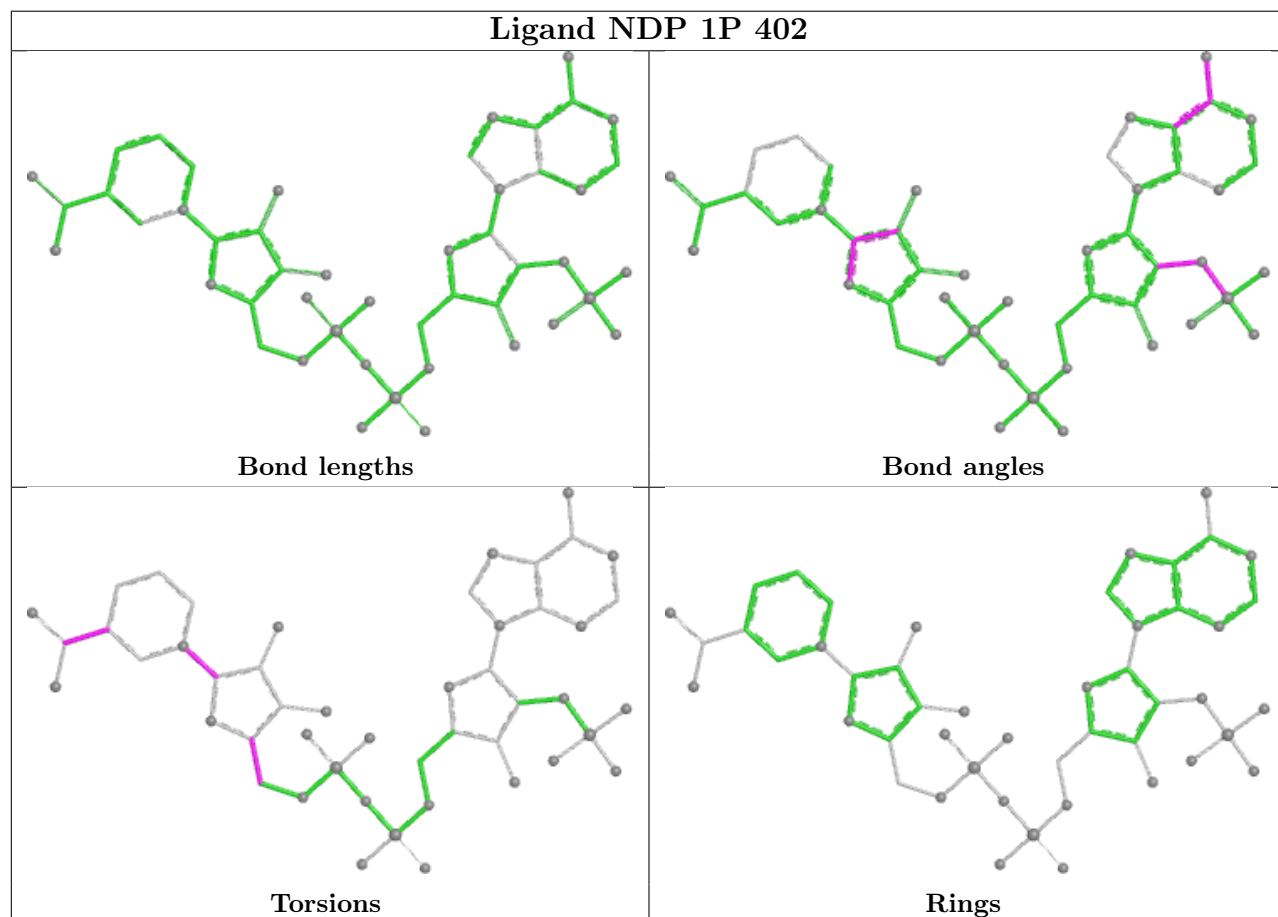
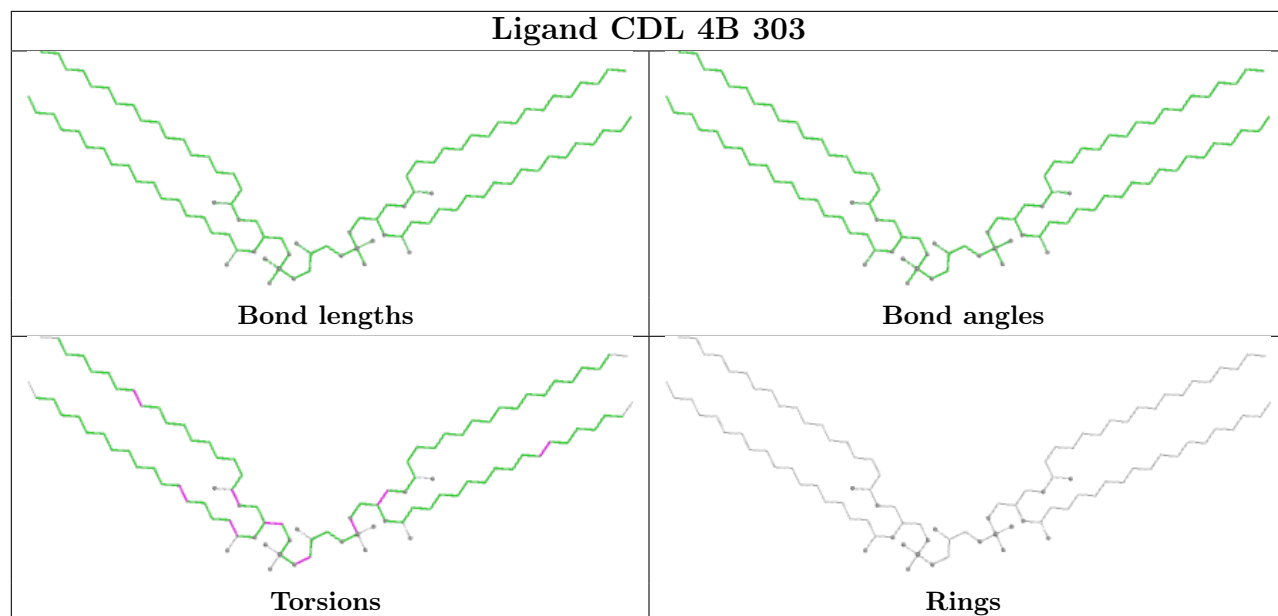
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

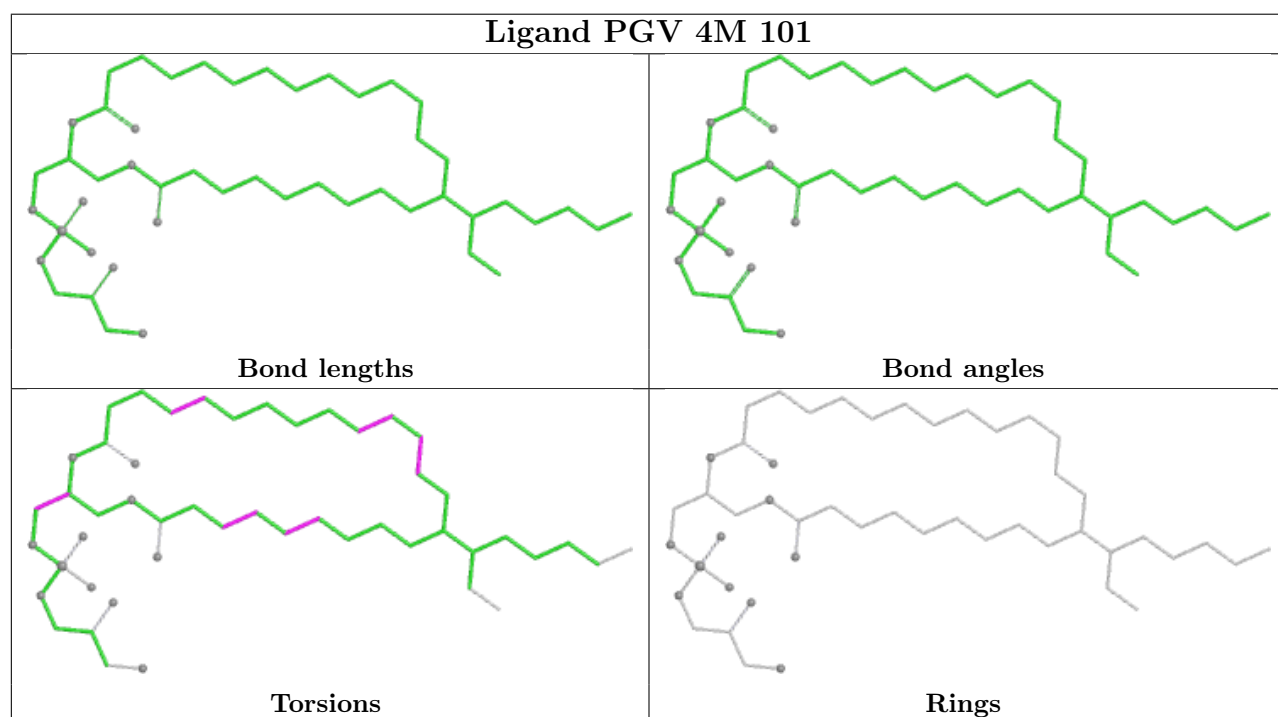
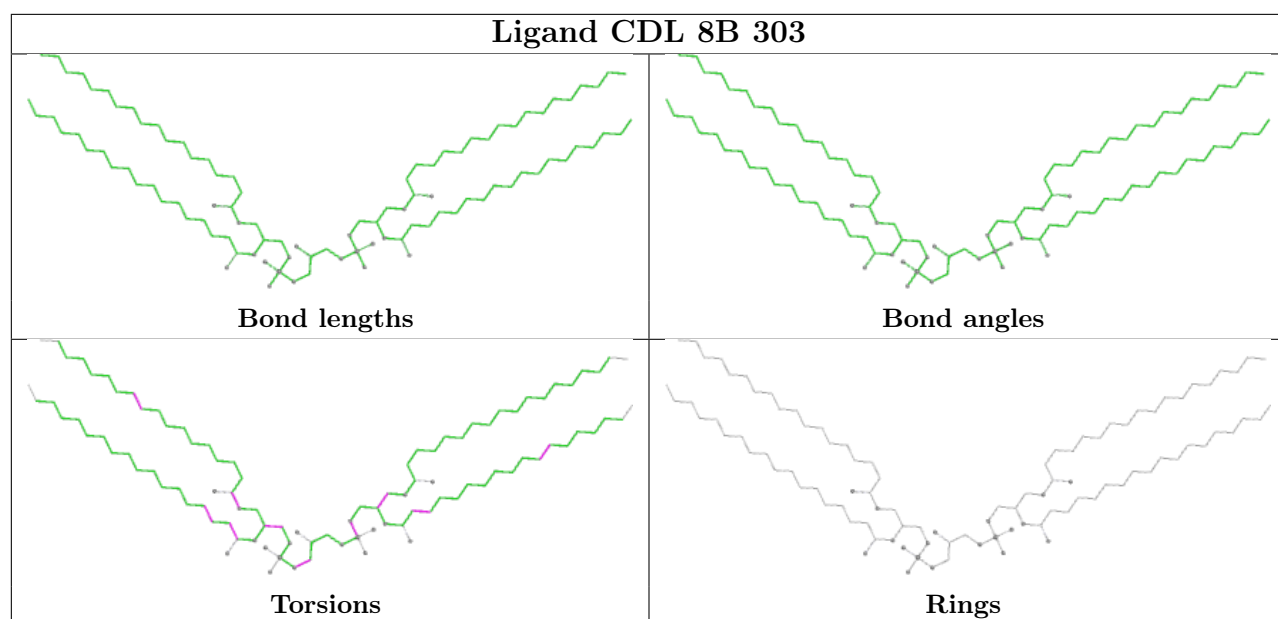


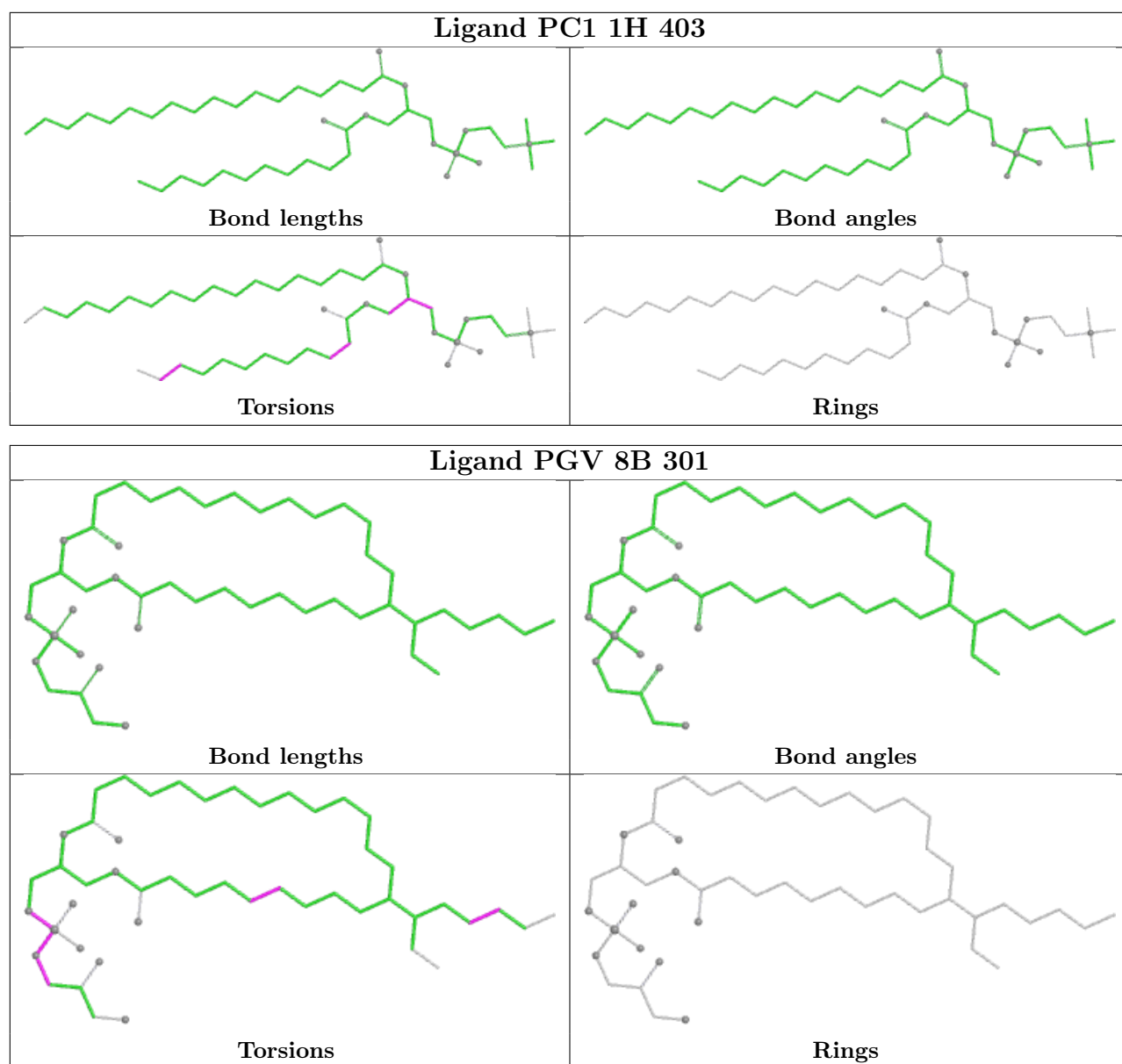


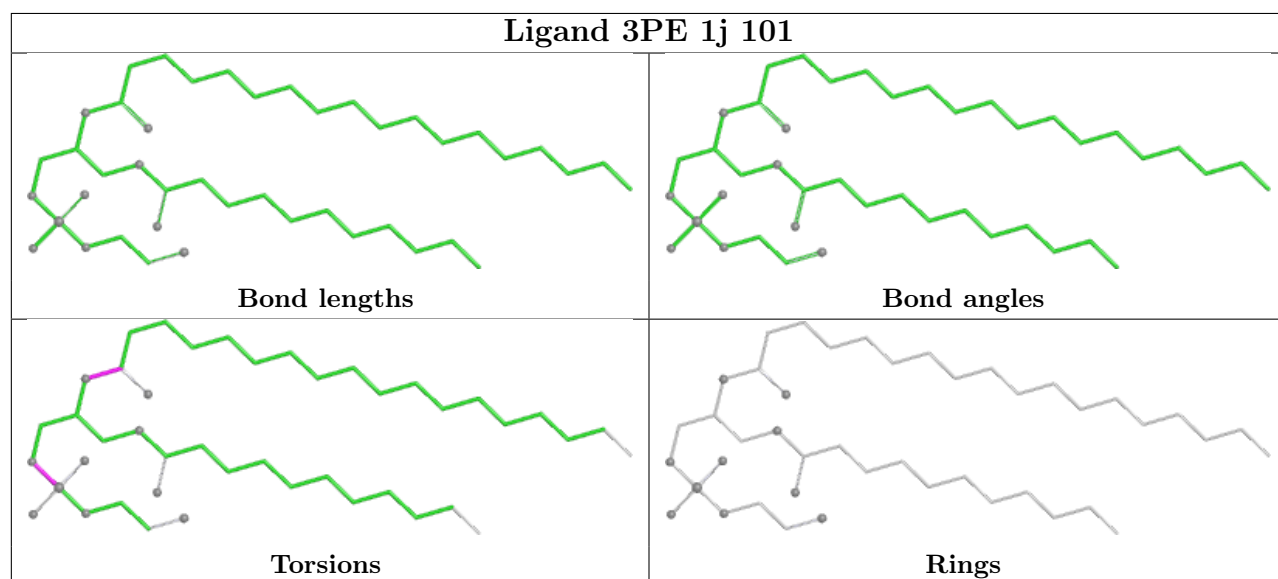
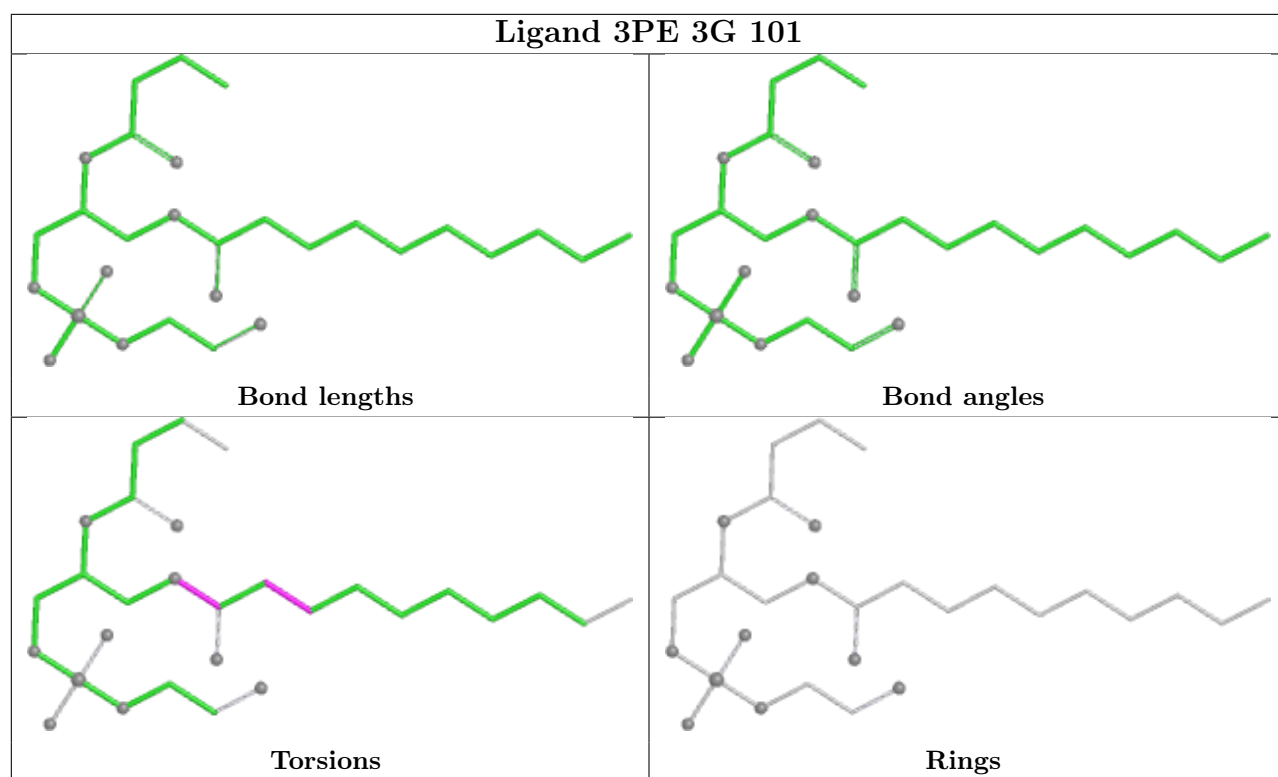


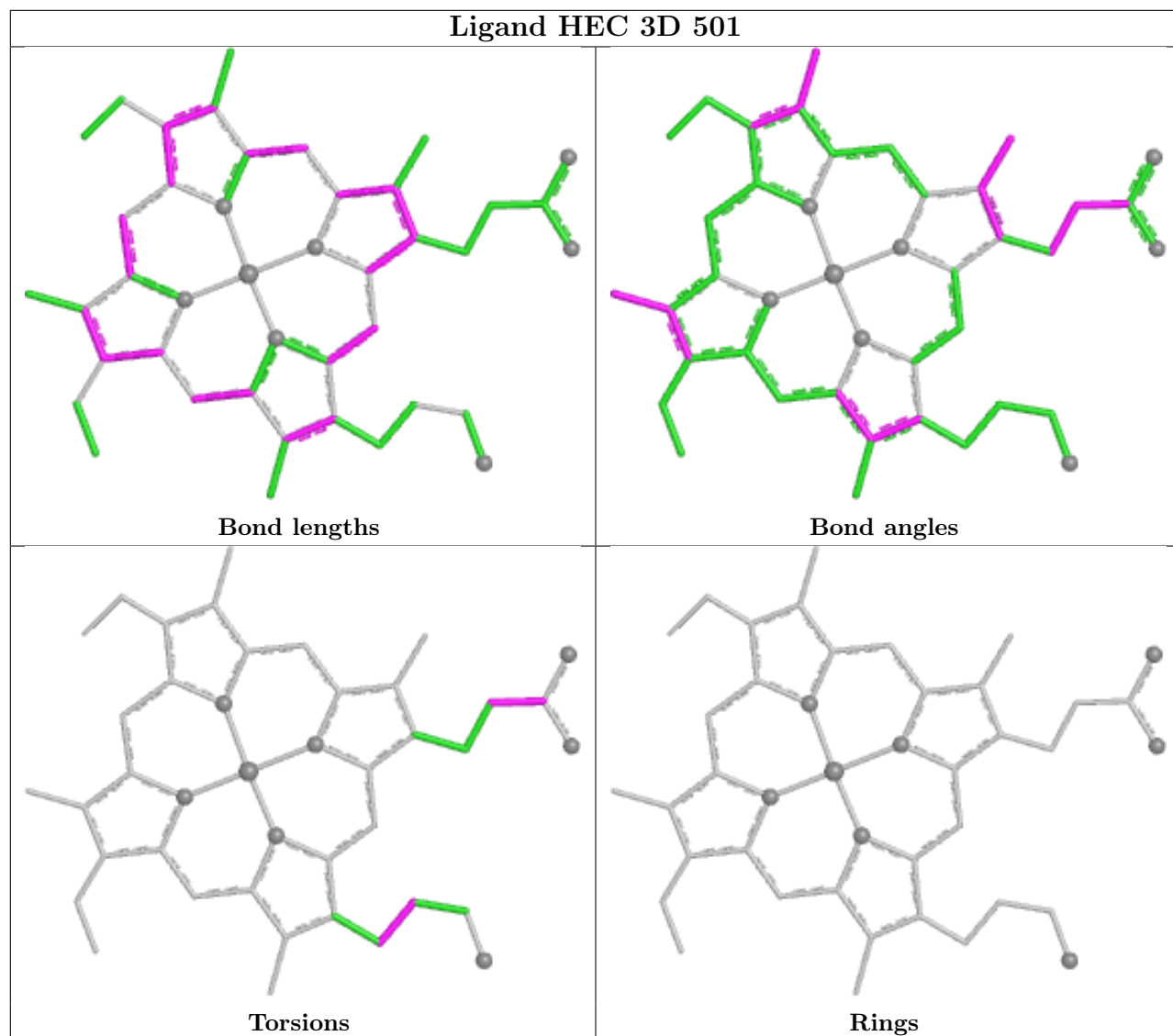


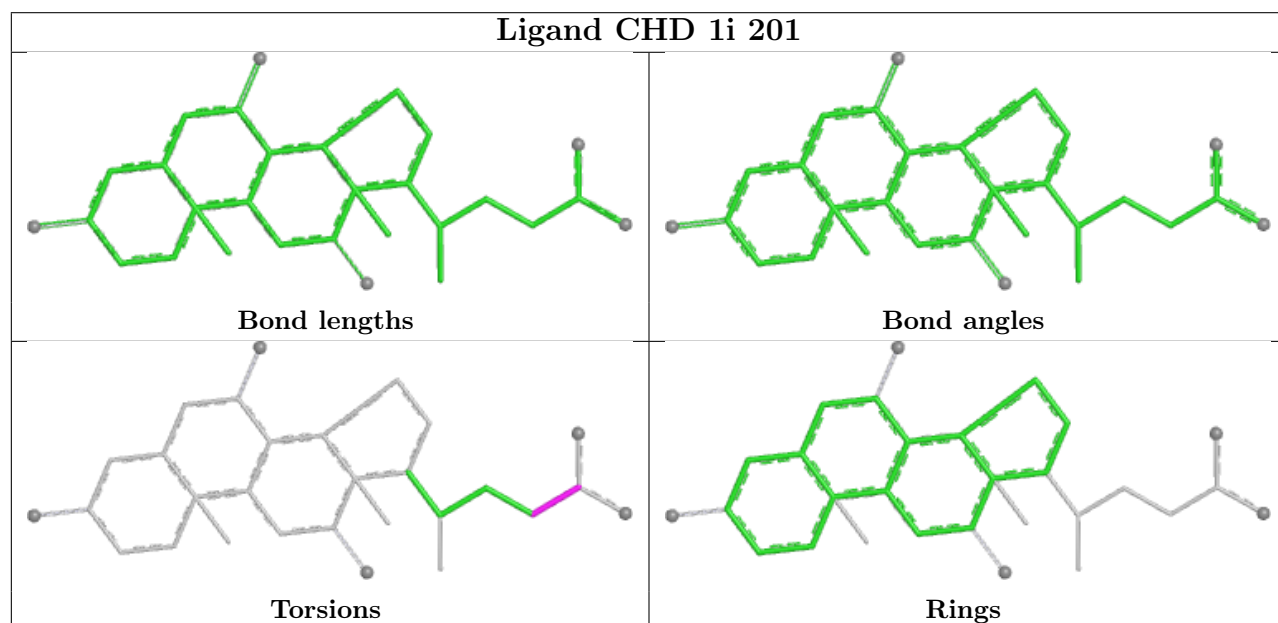
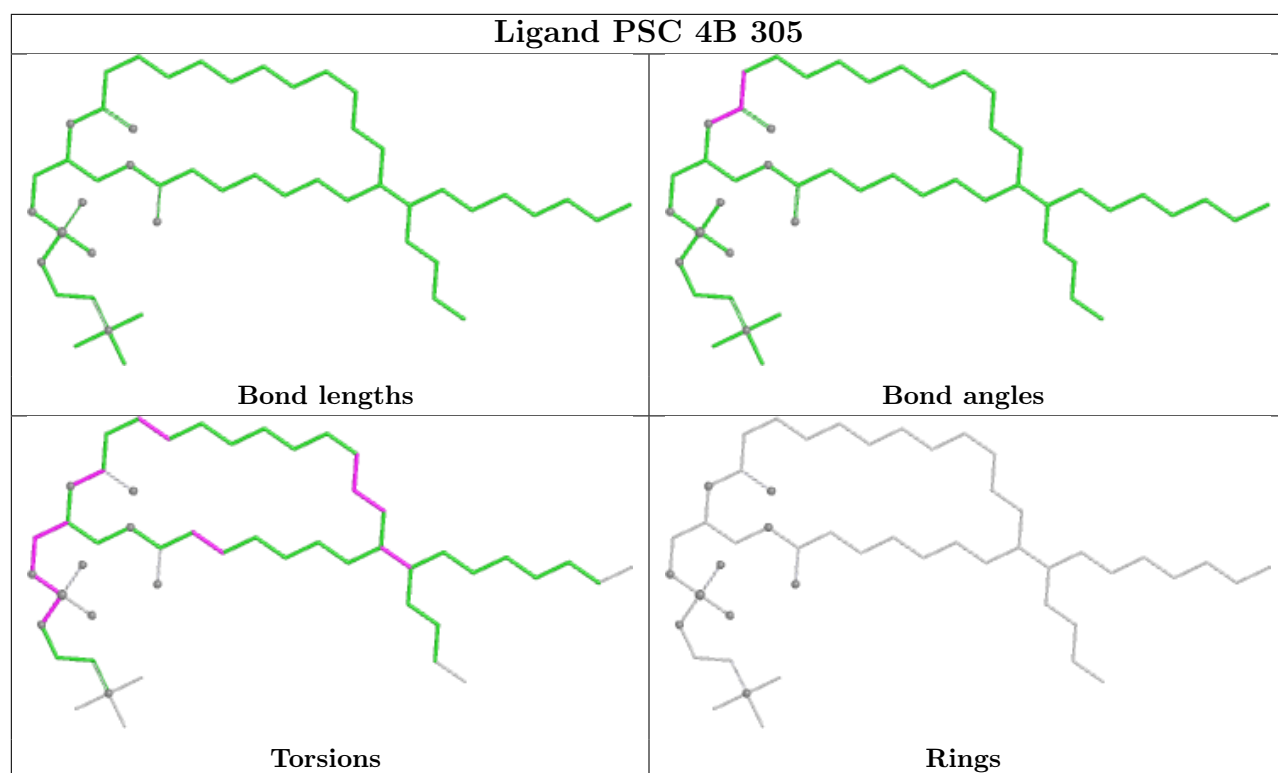


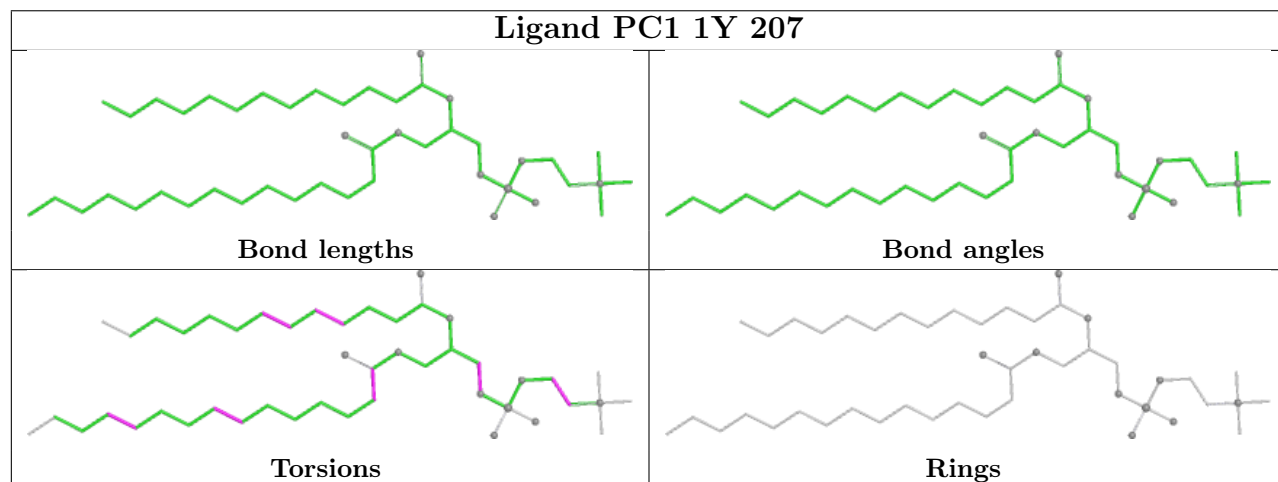
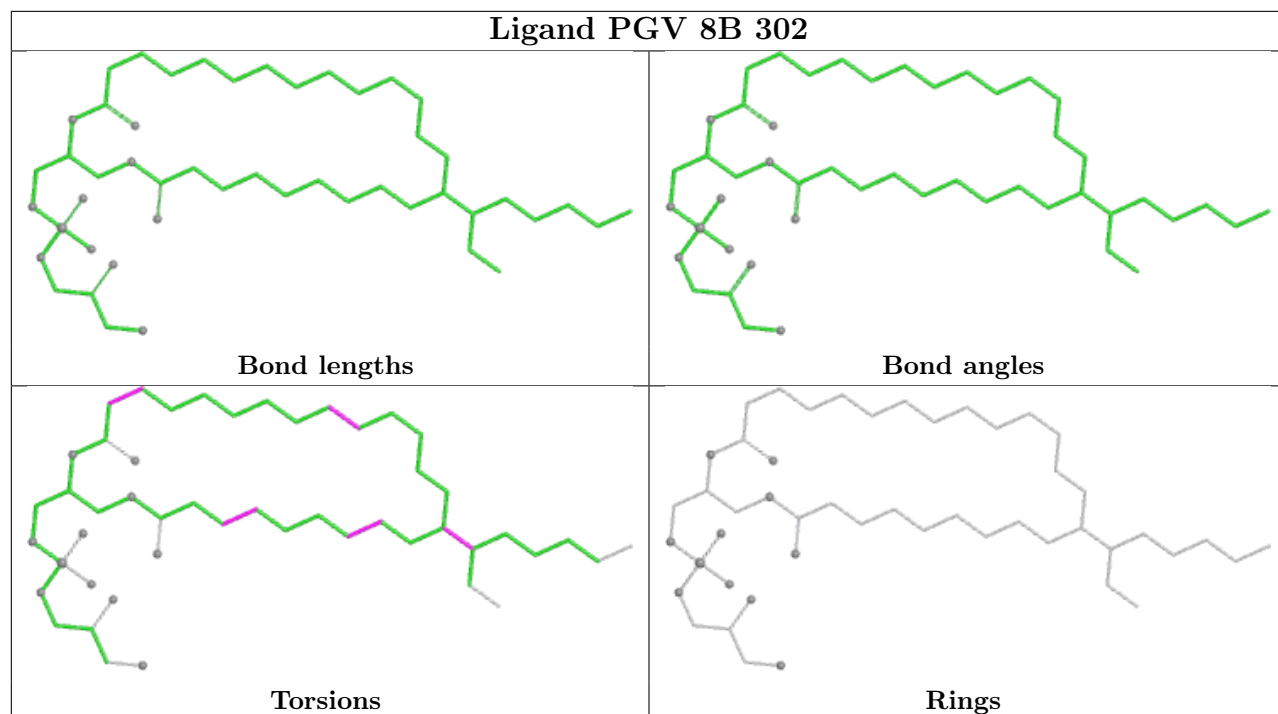


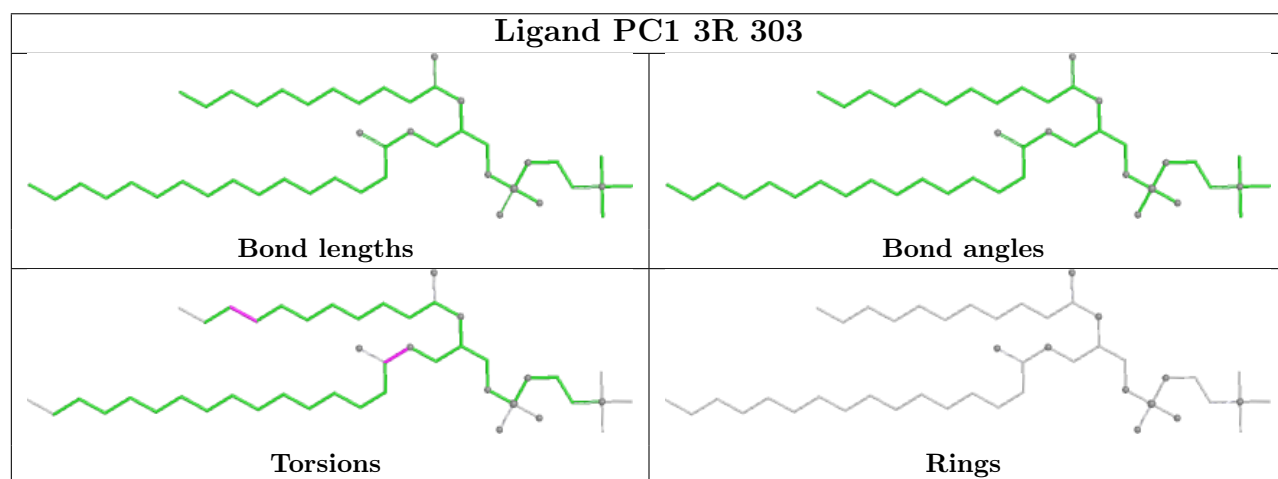
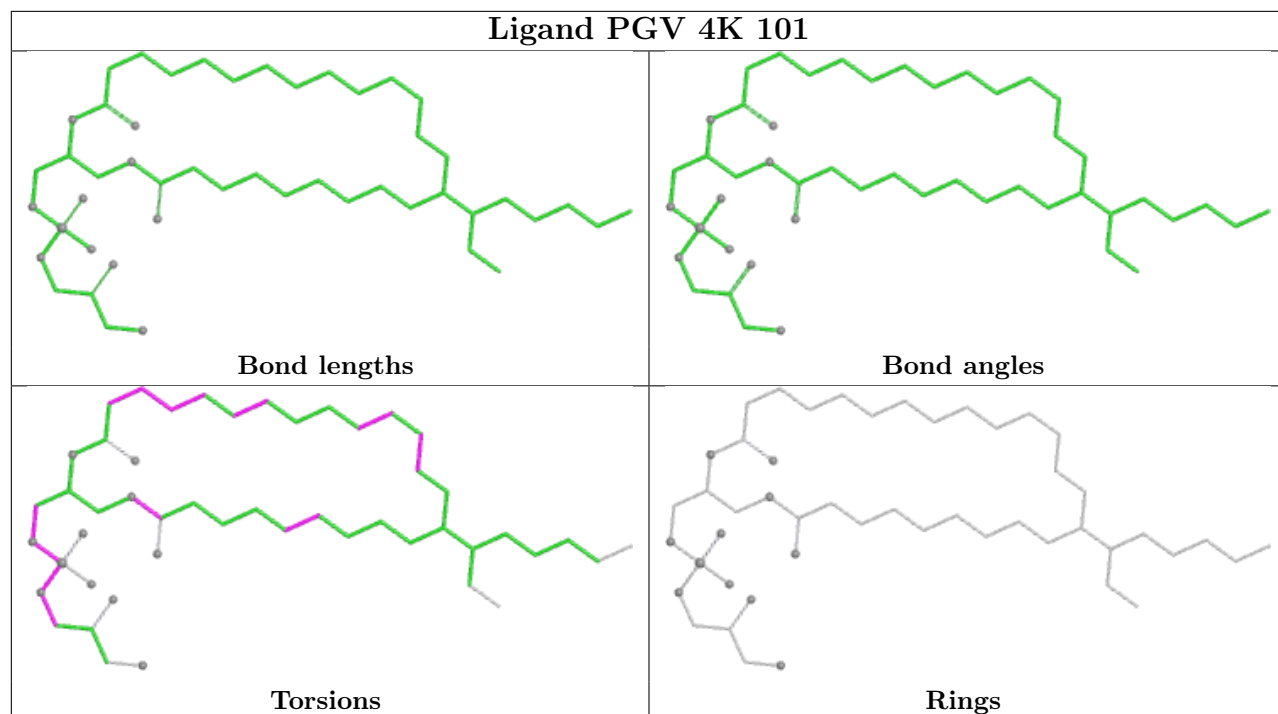


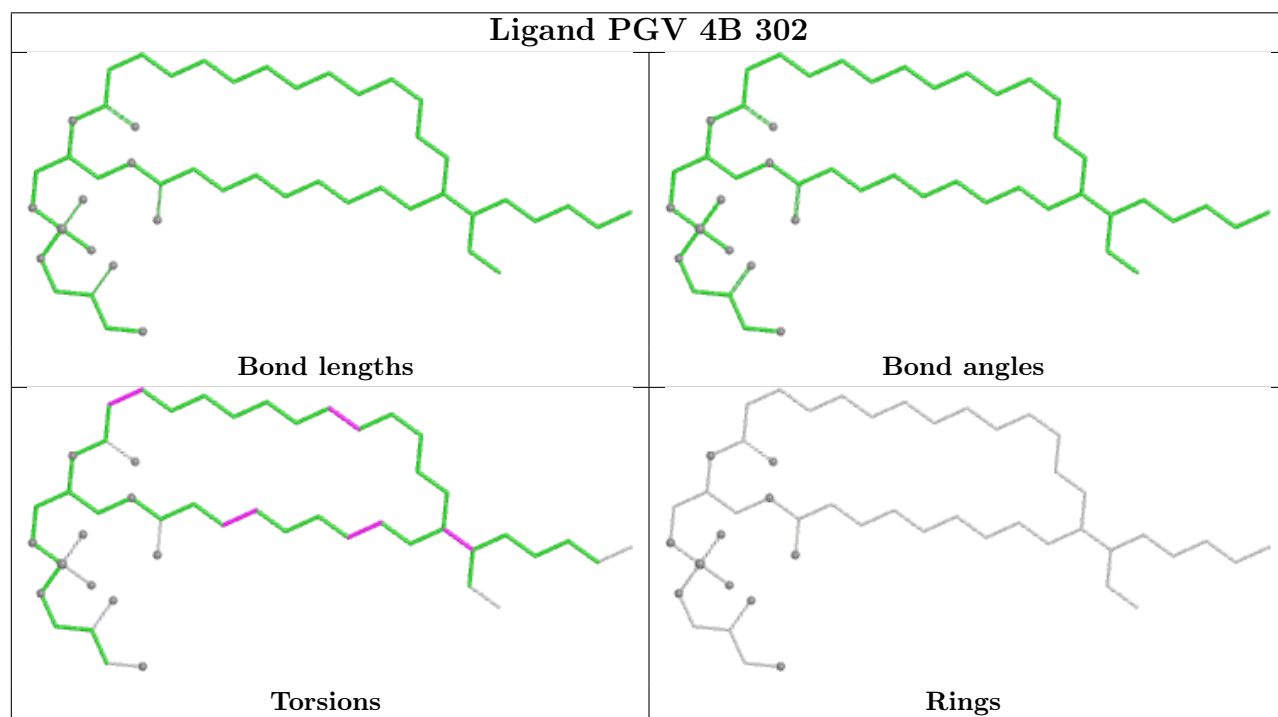
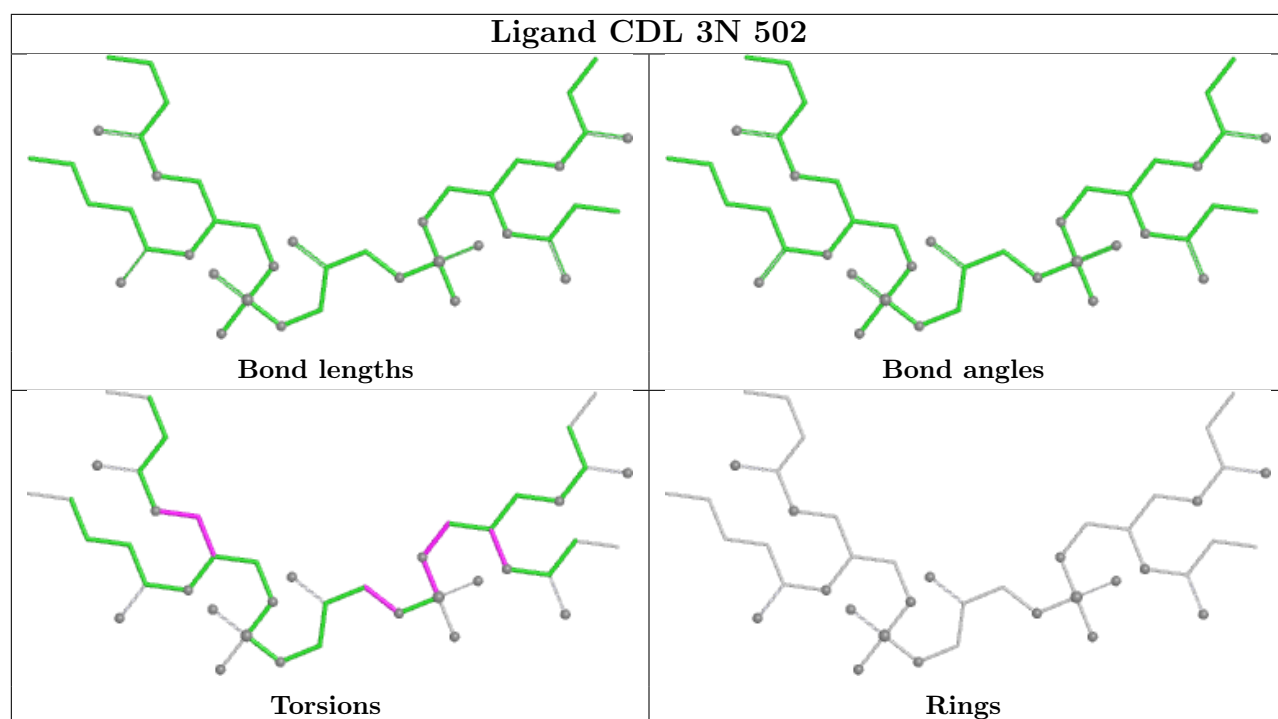




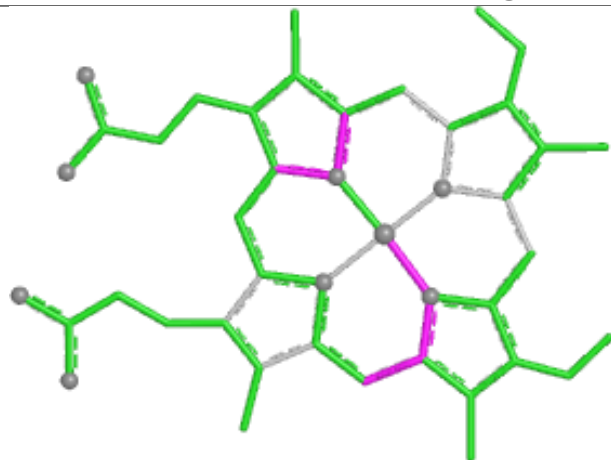




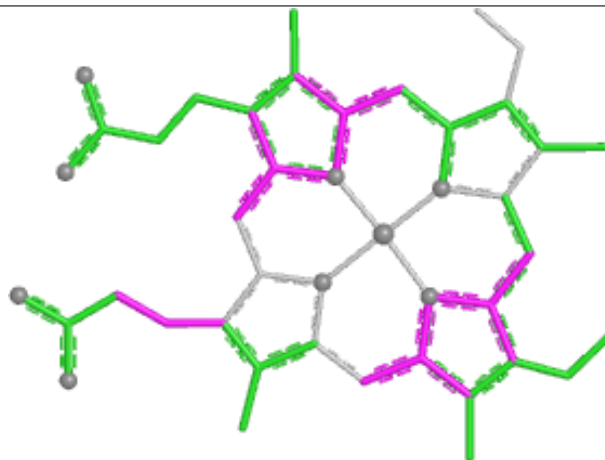




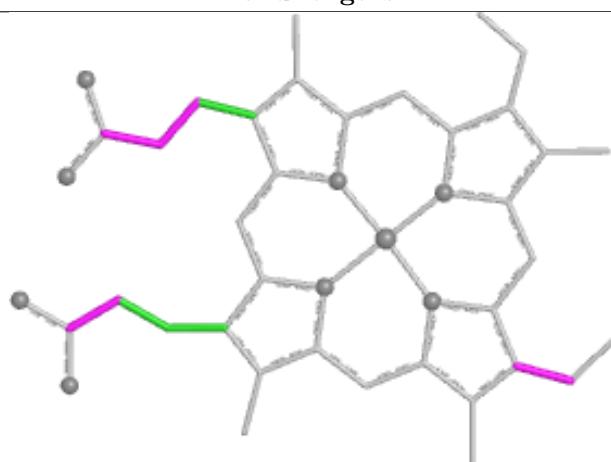
Ligand HEM 3P 501



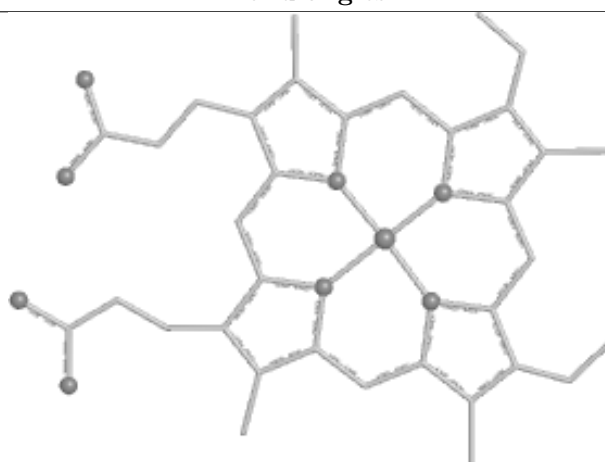
Bond lengths



Bond angles

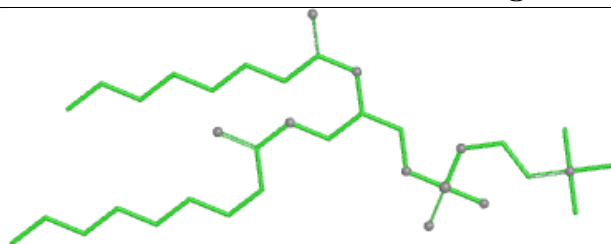


Torsions

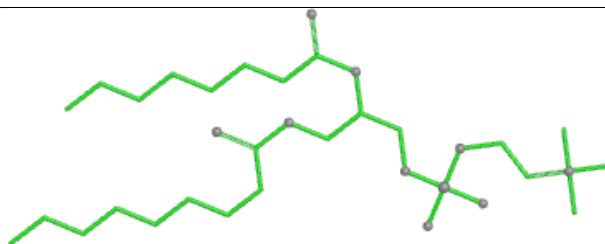


Rings

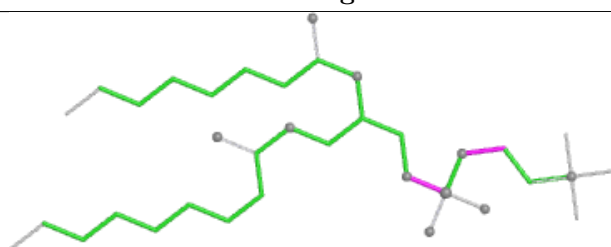
Ligand PC1 1A 203



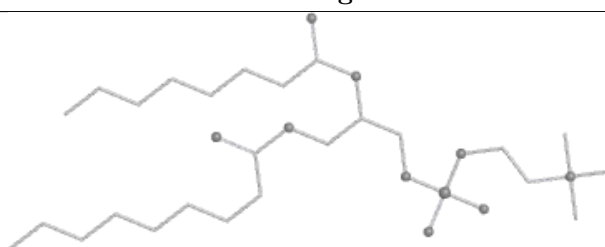
Bond lengths



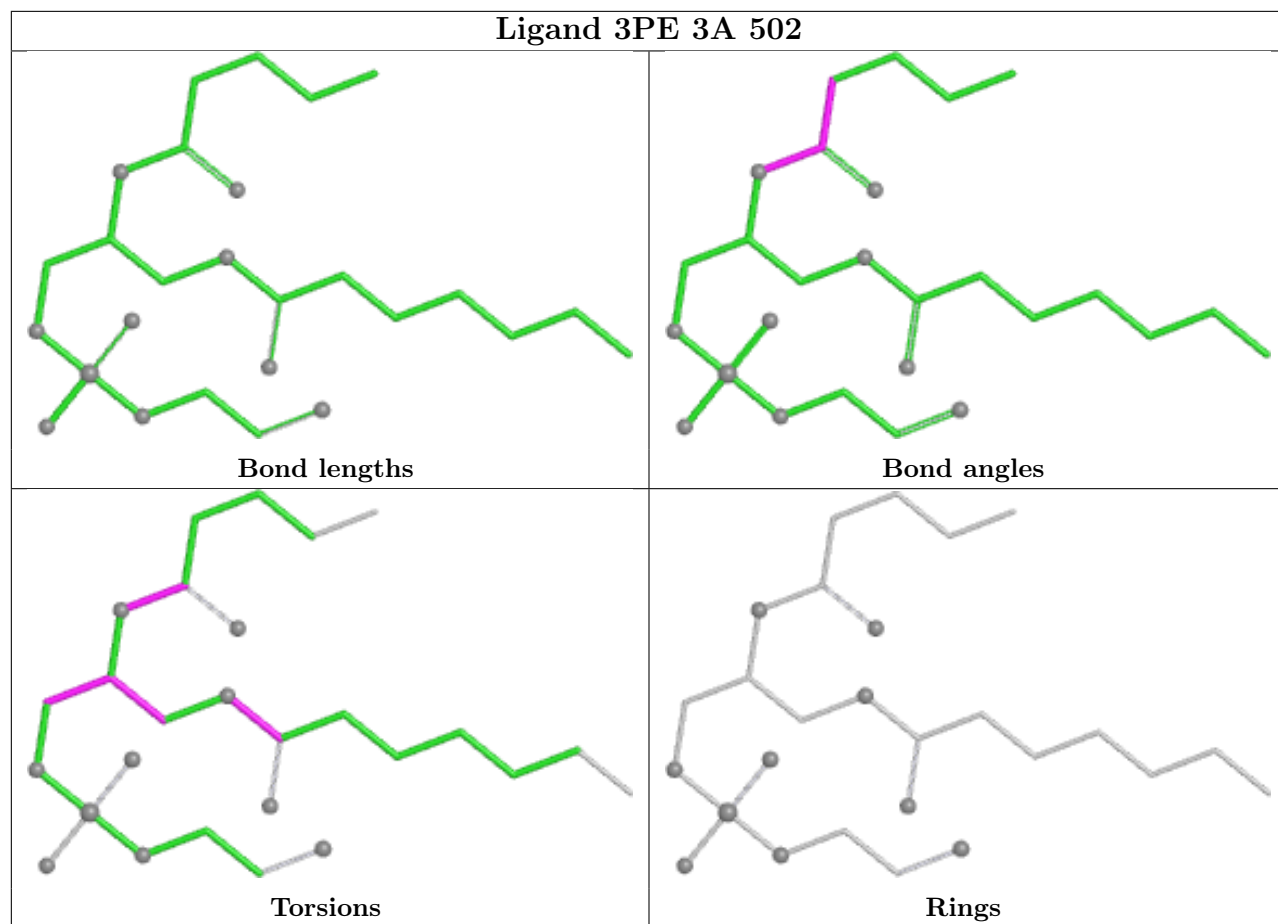
Bond angles

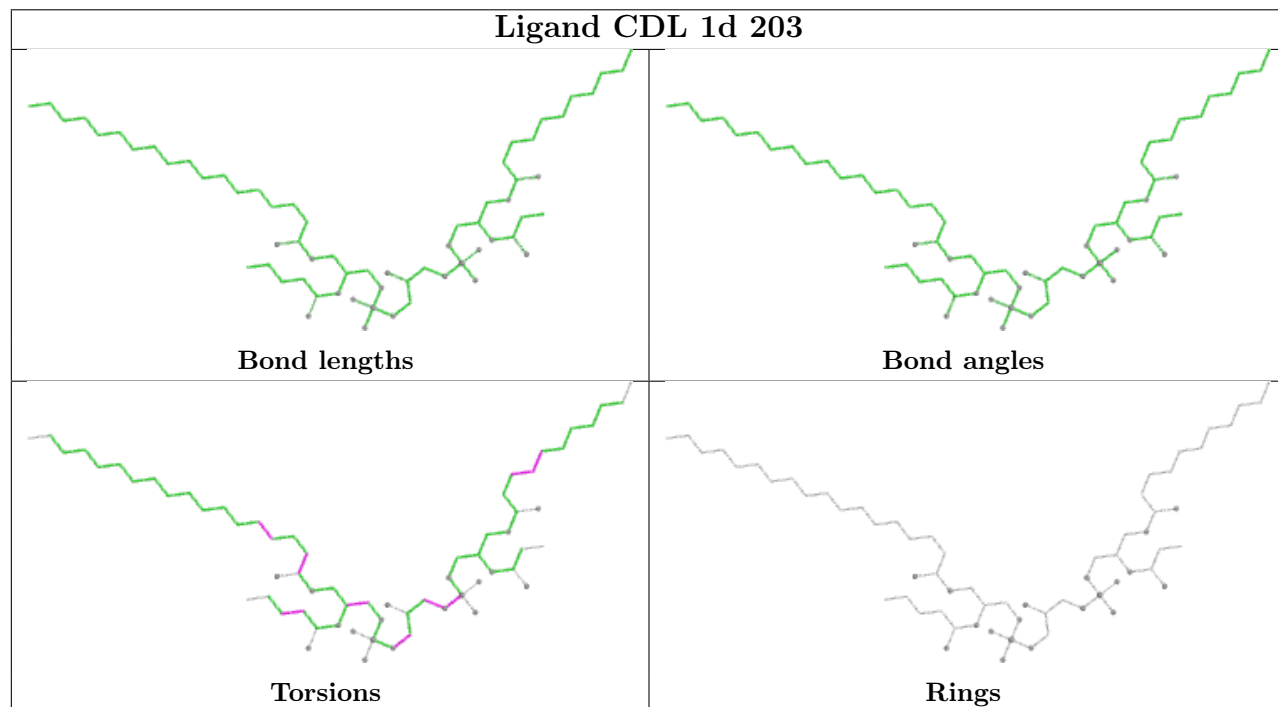
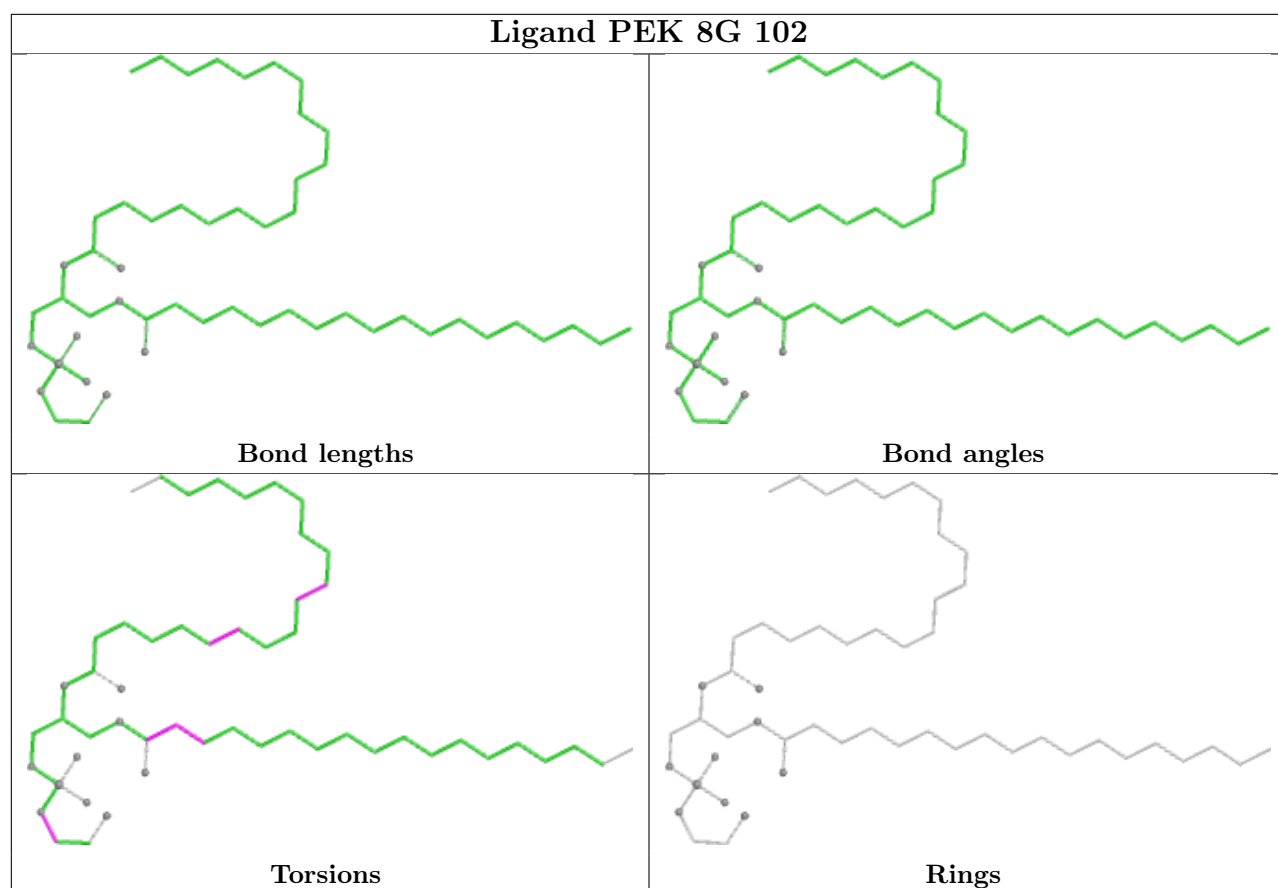


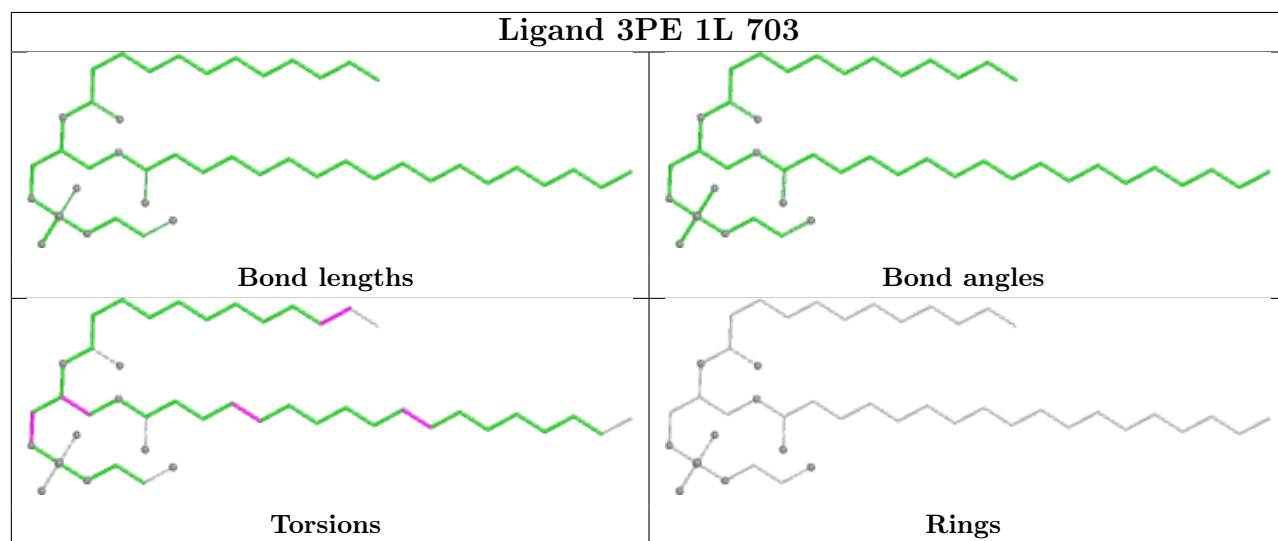
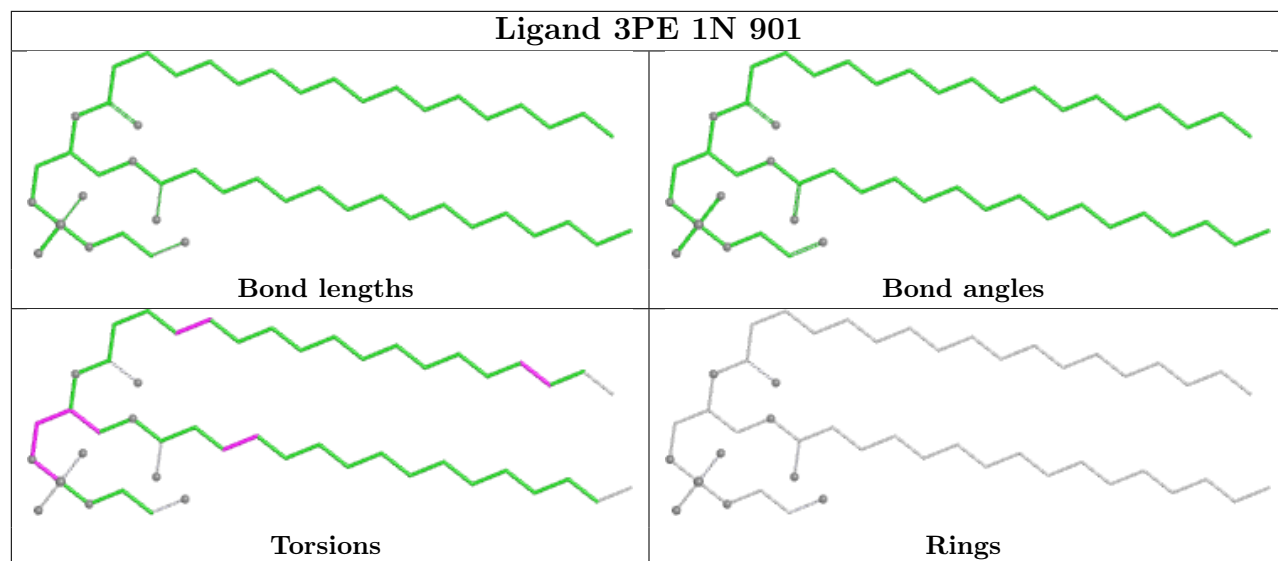
Torsions

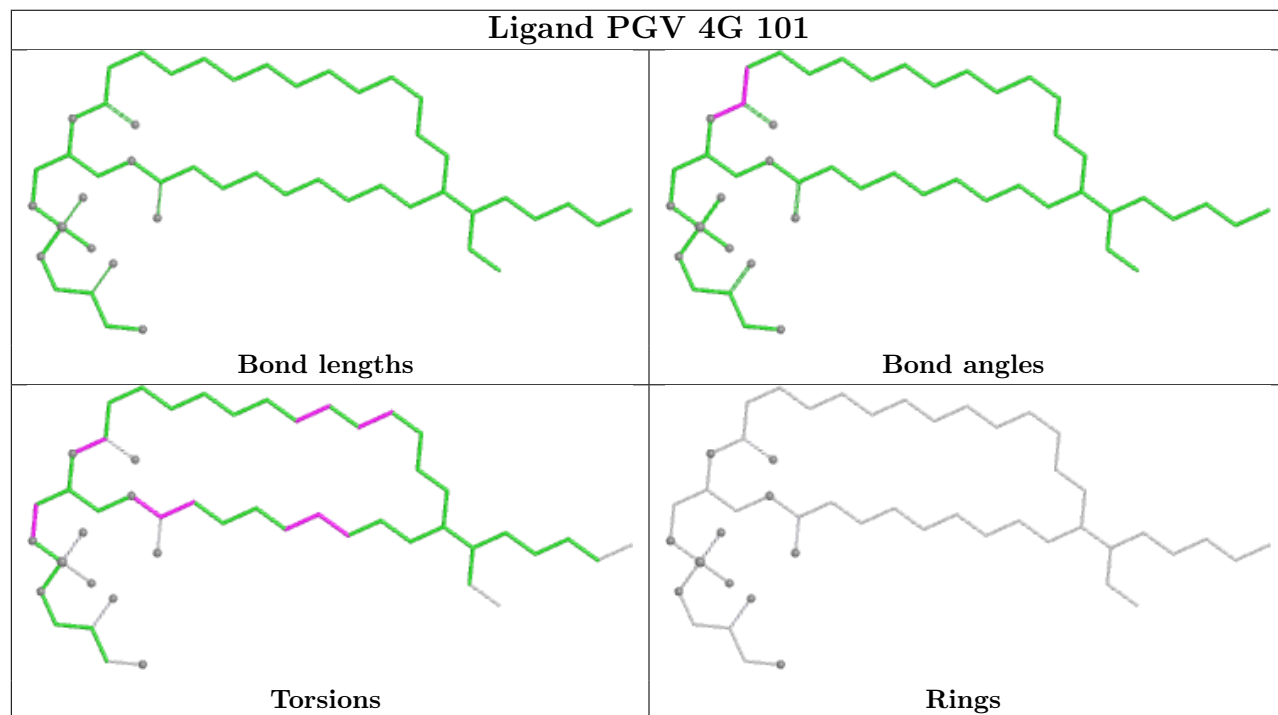
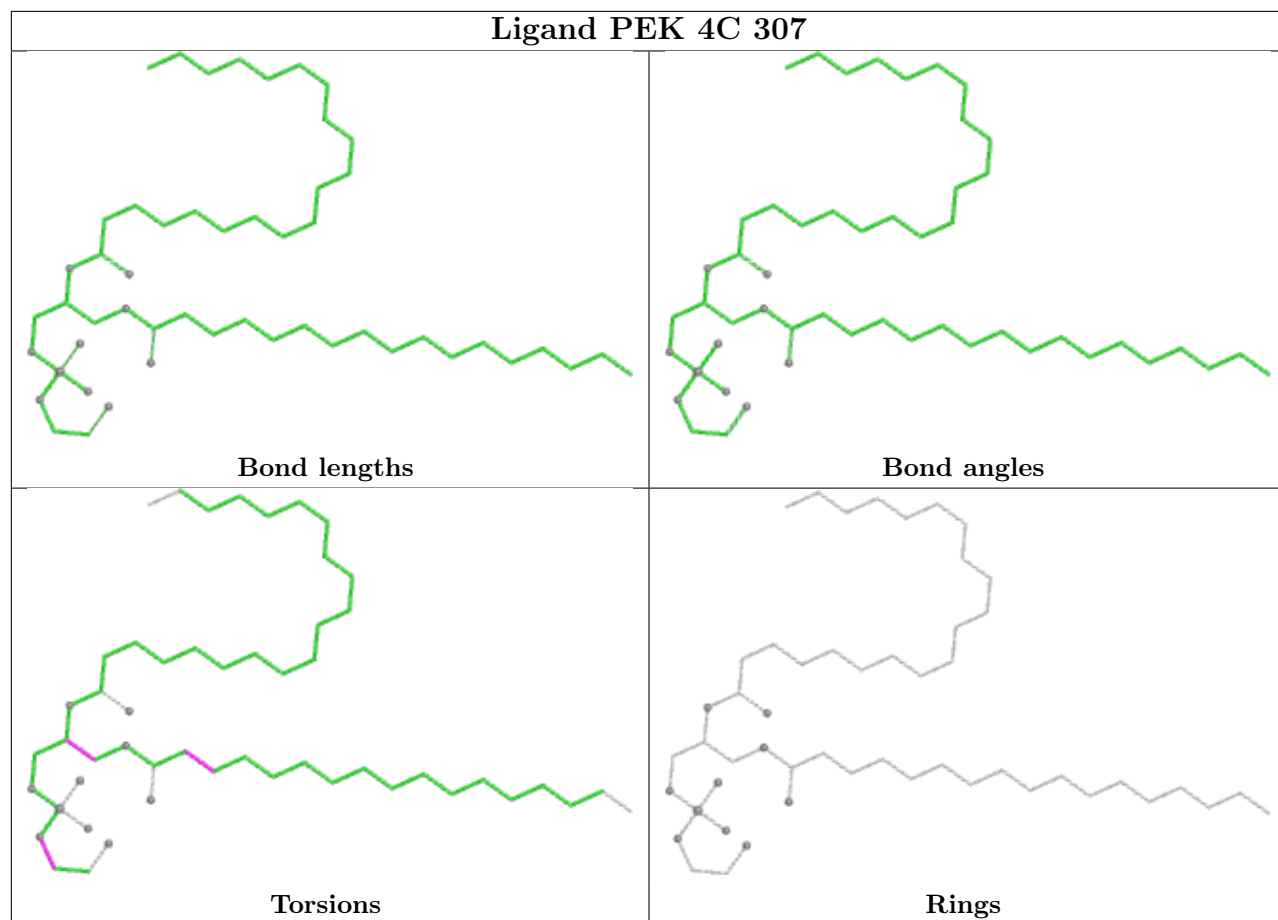


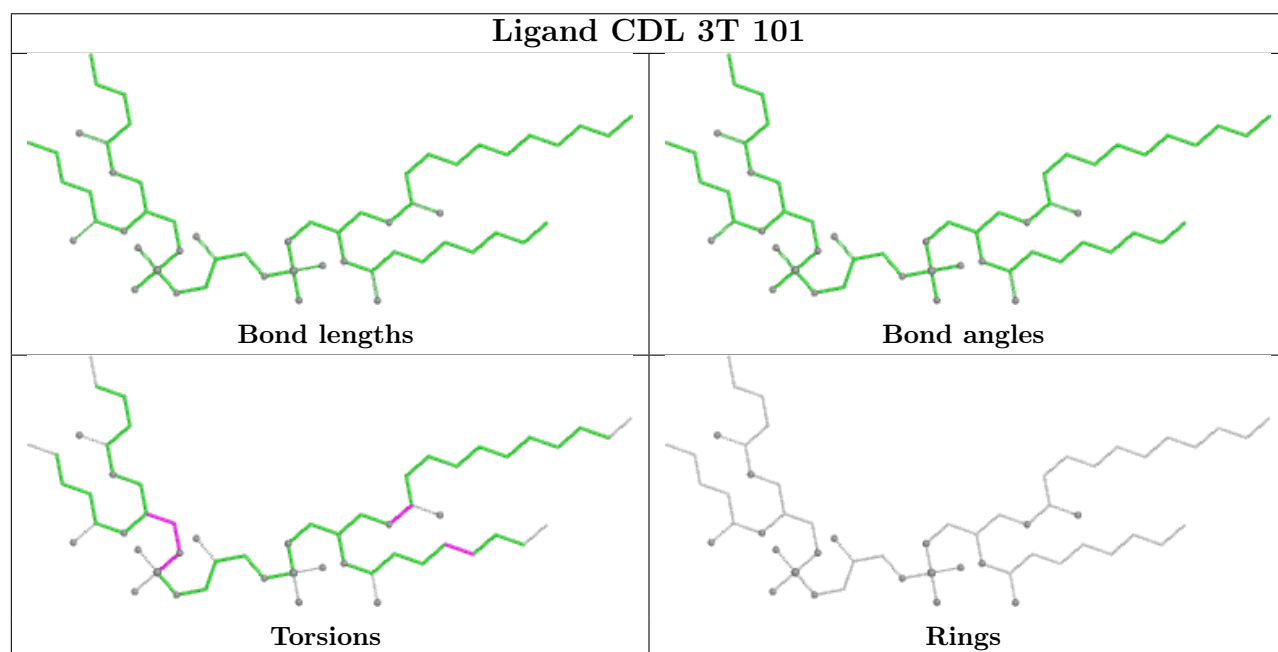
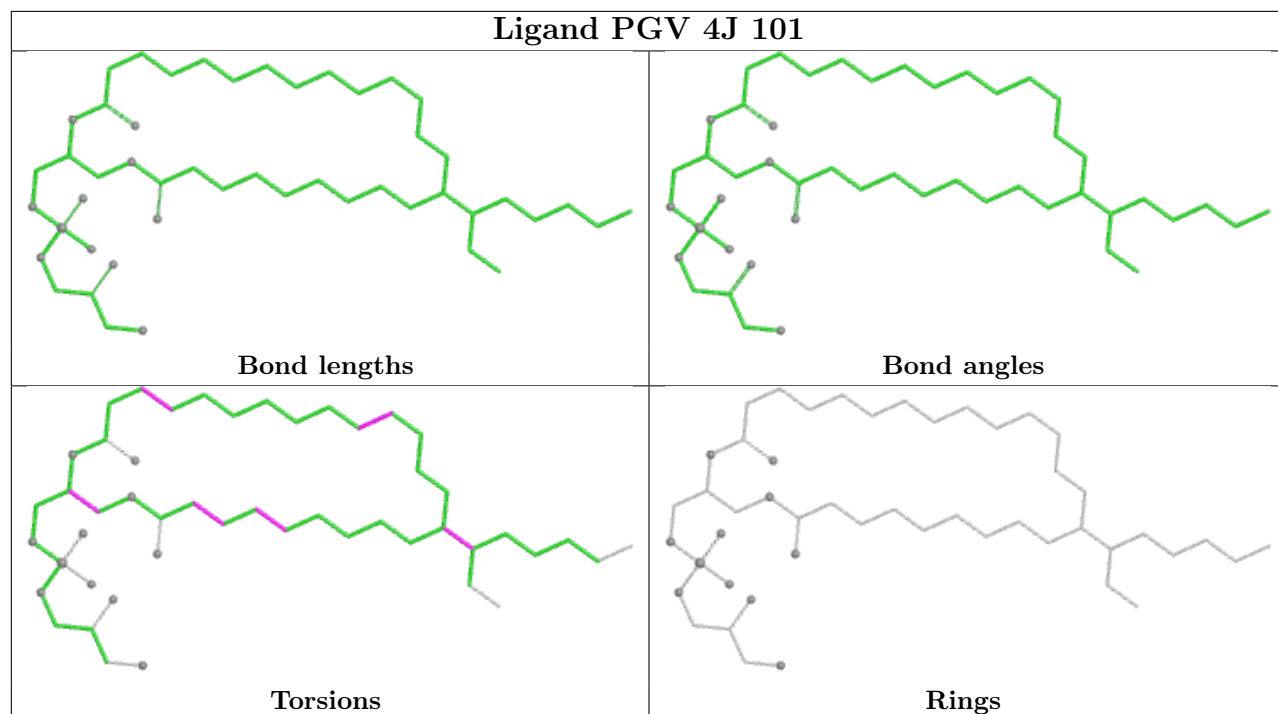
Rings

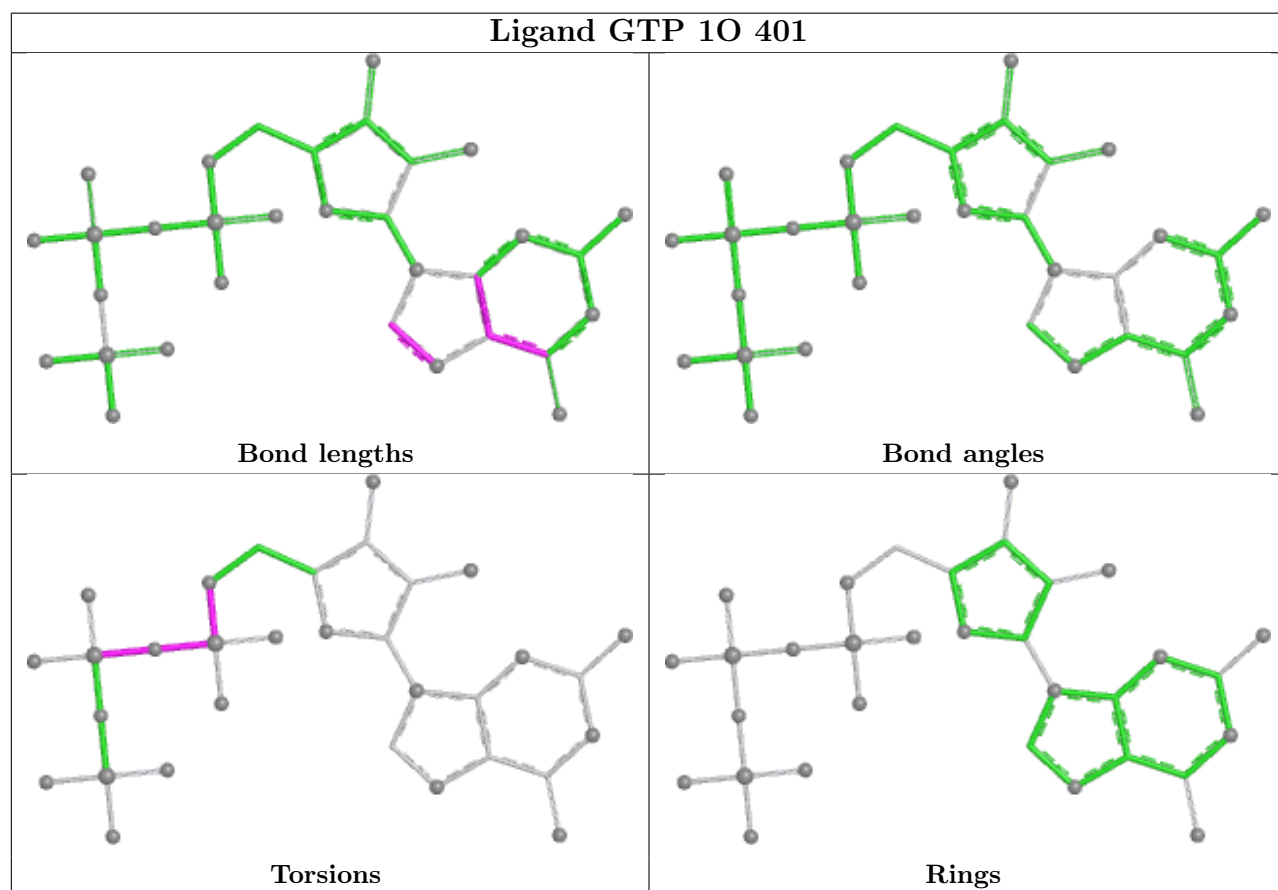
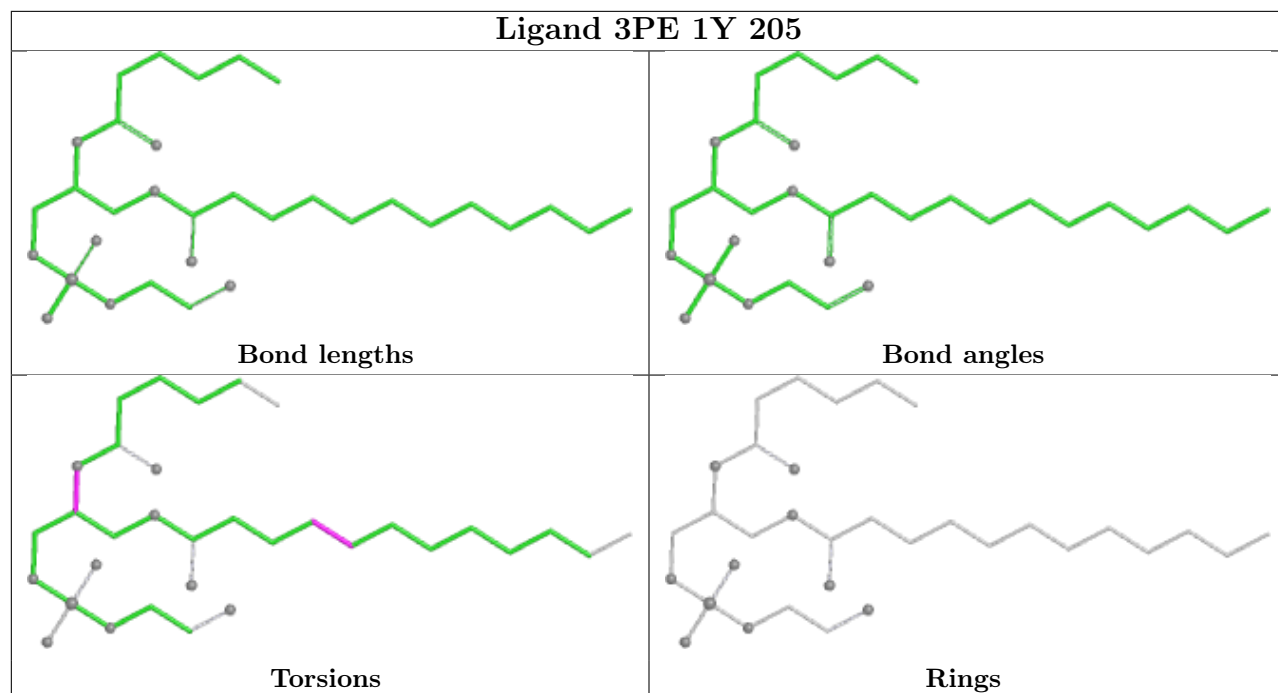


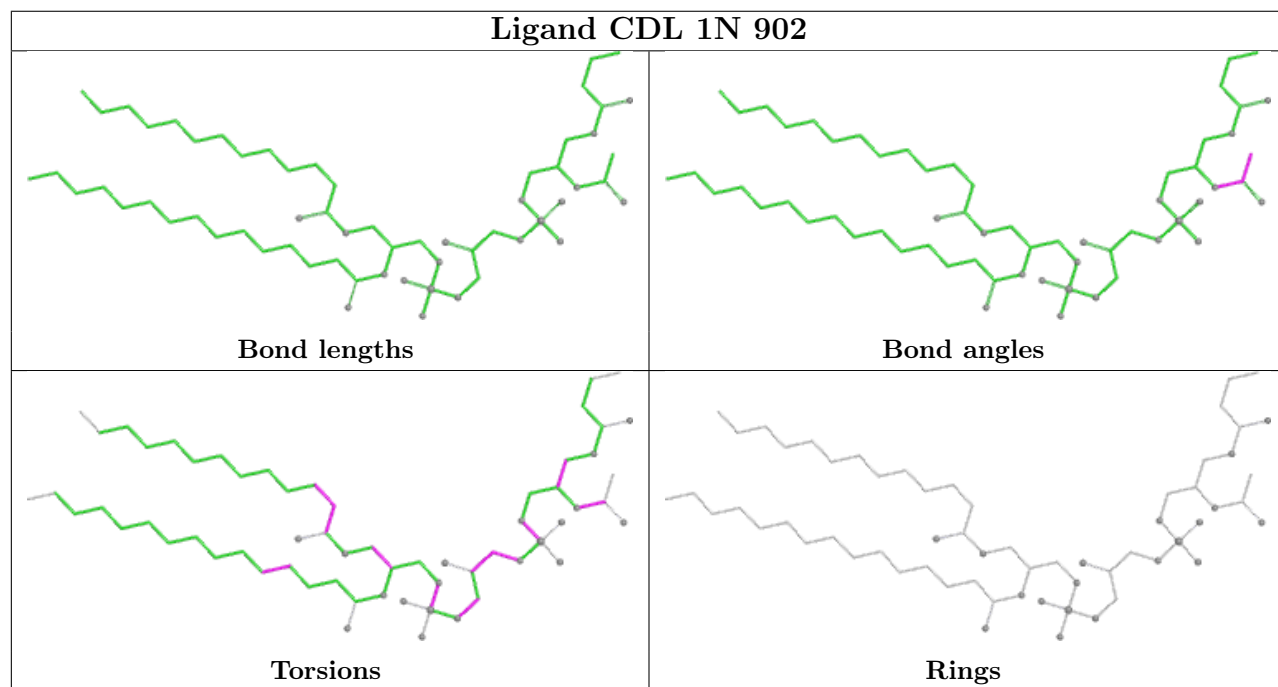
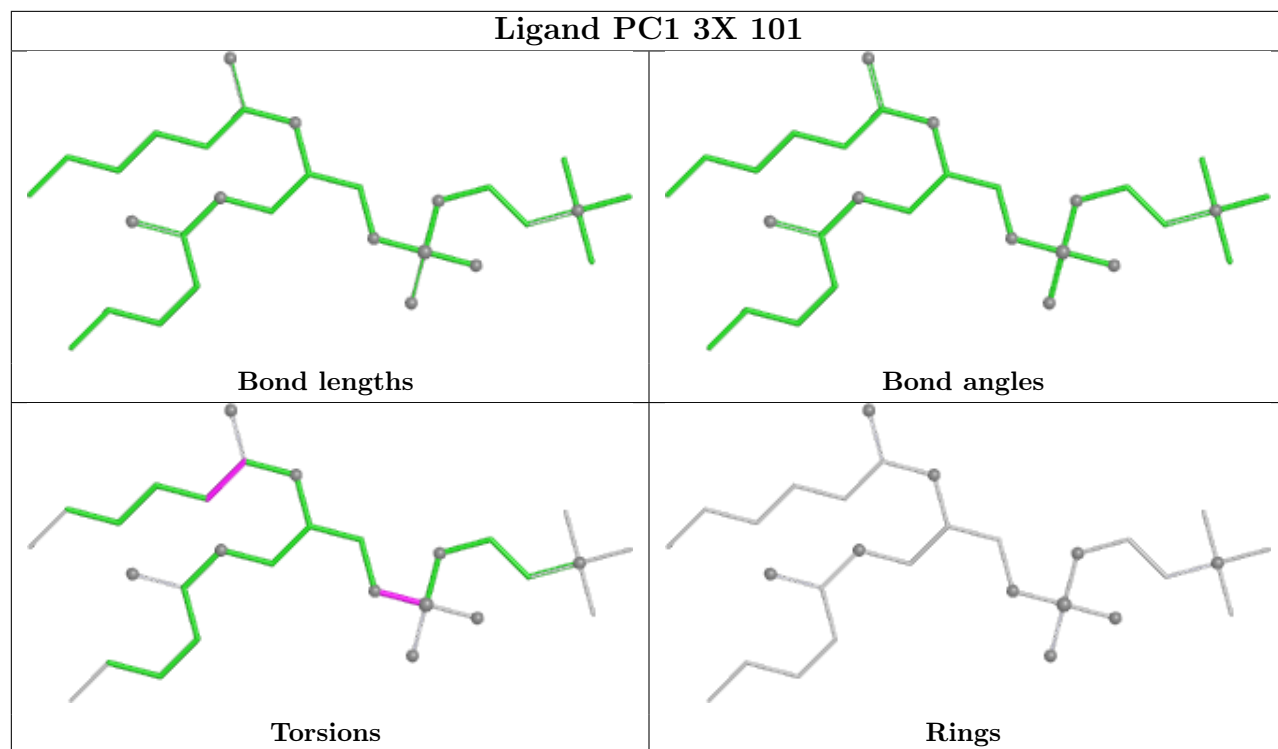


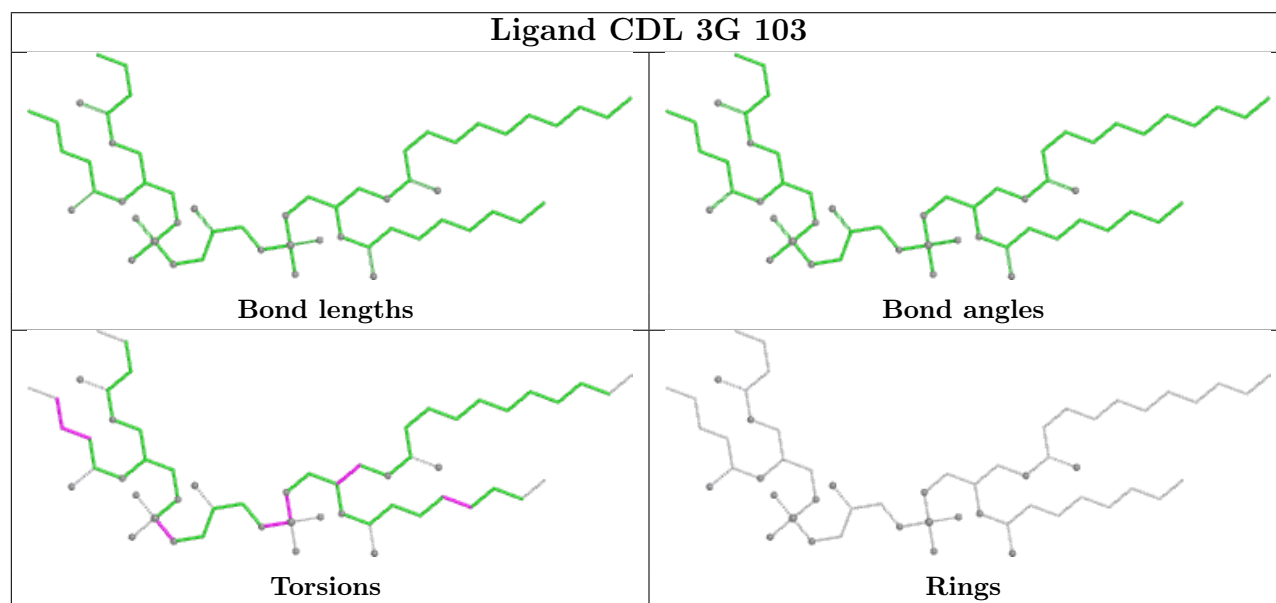
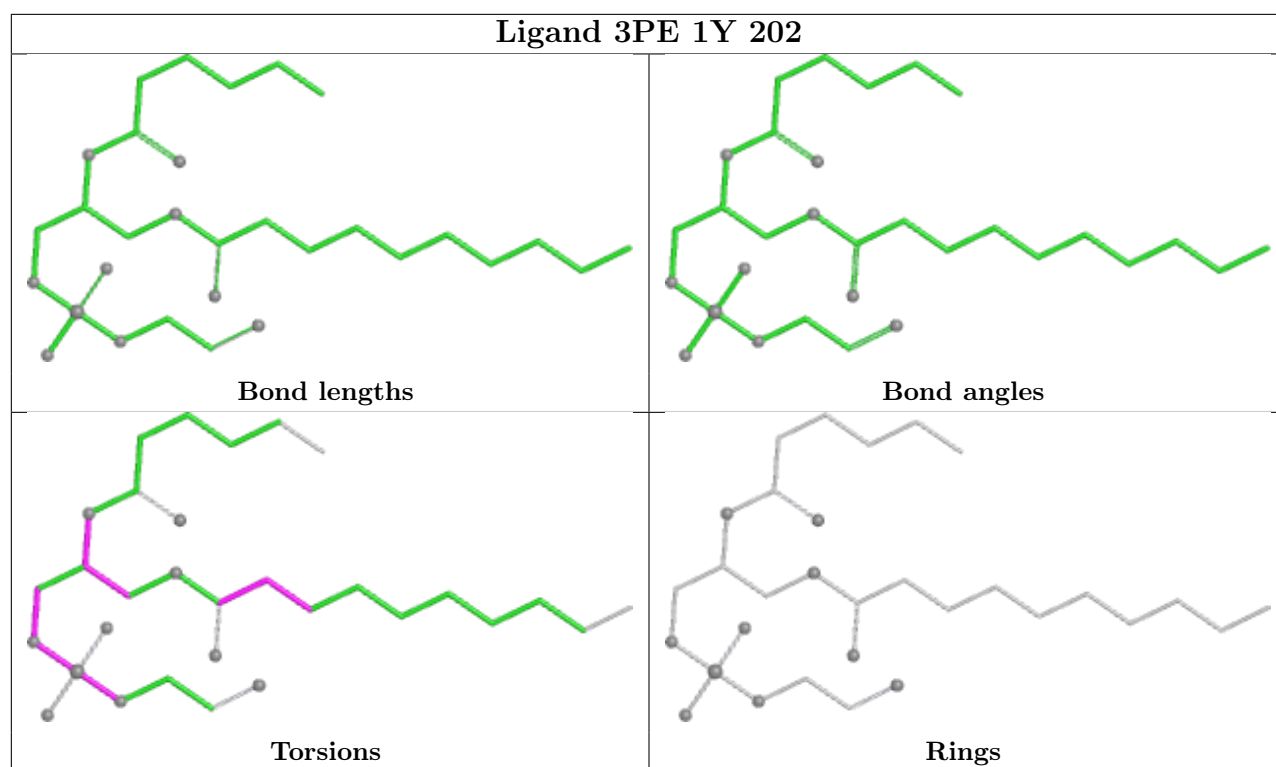


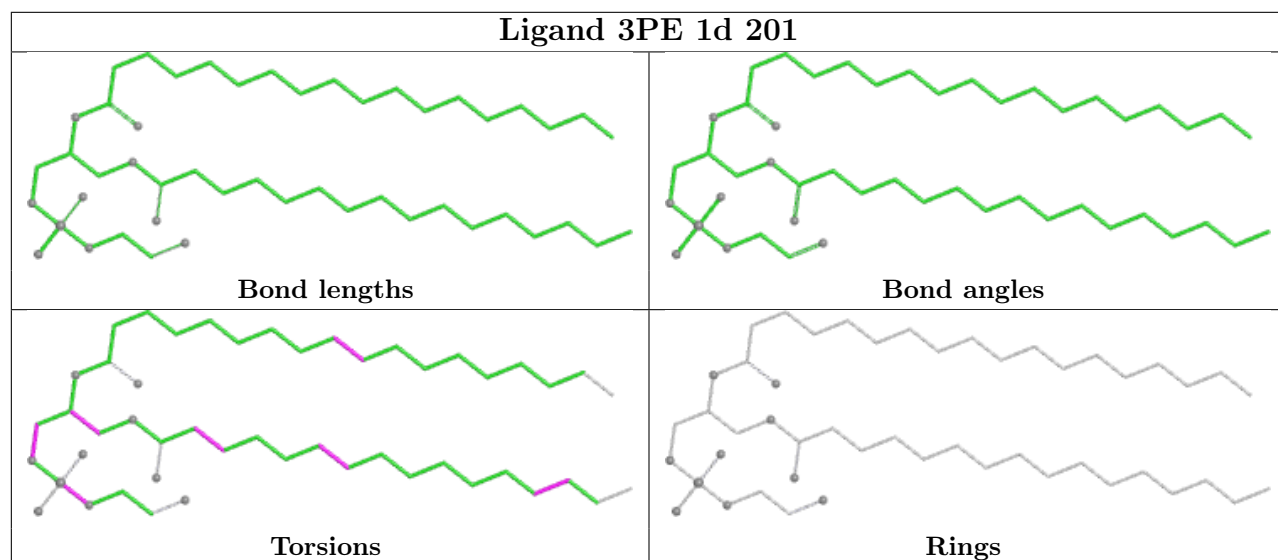
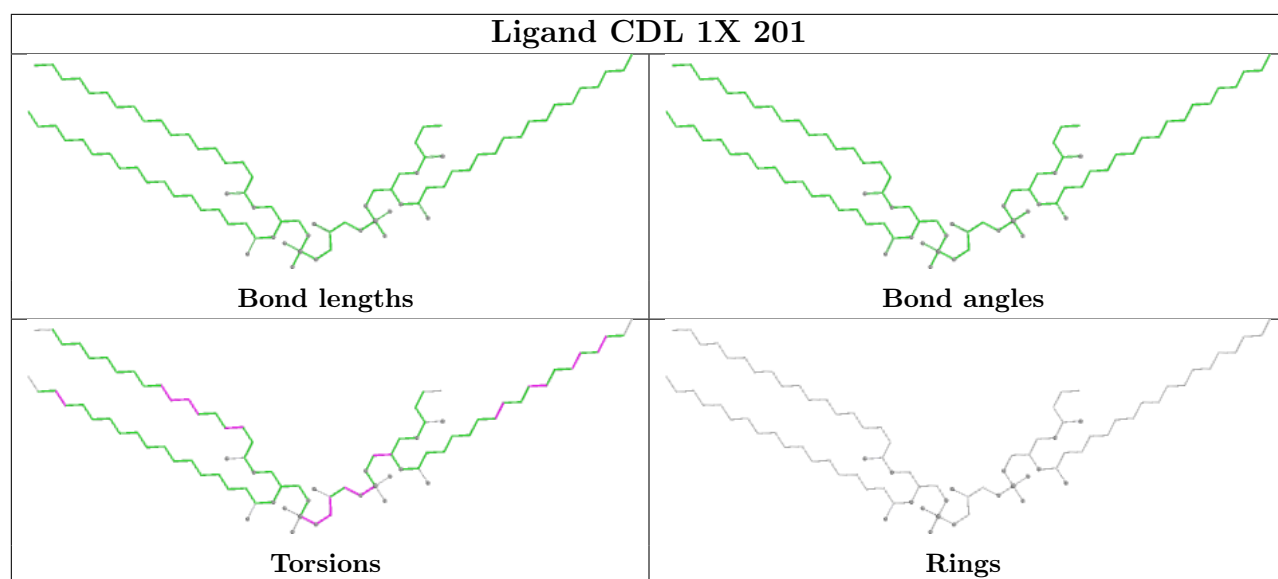


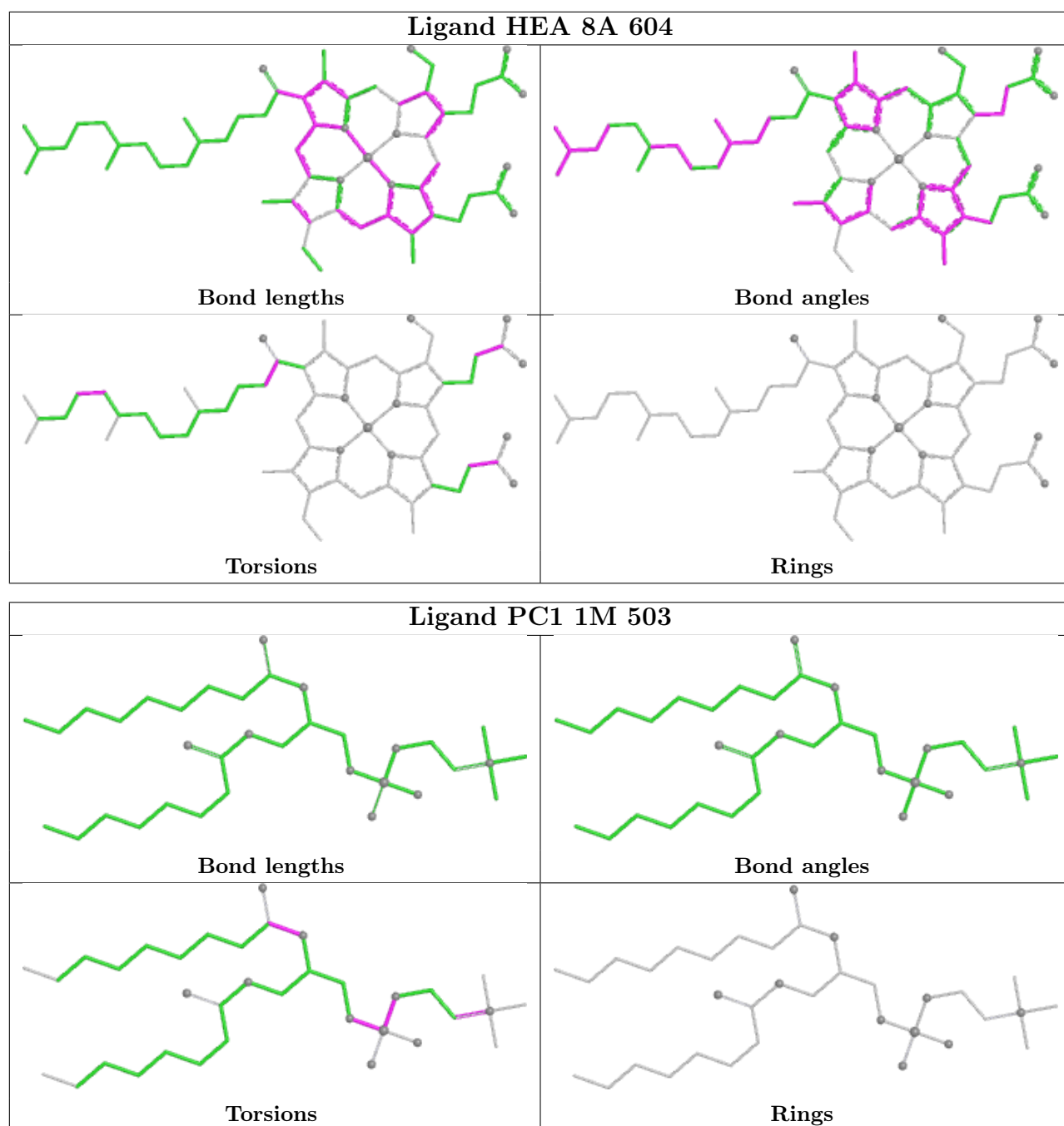


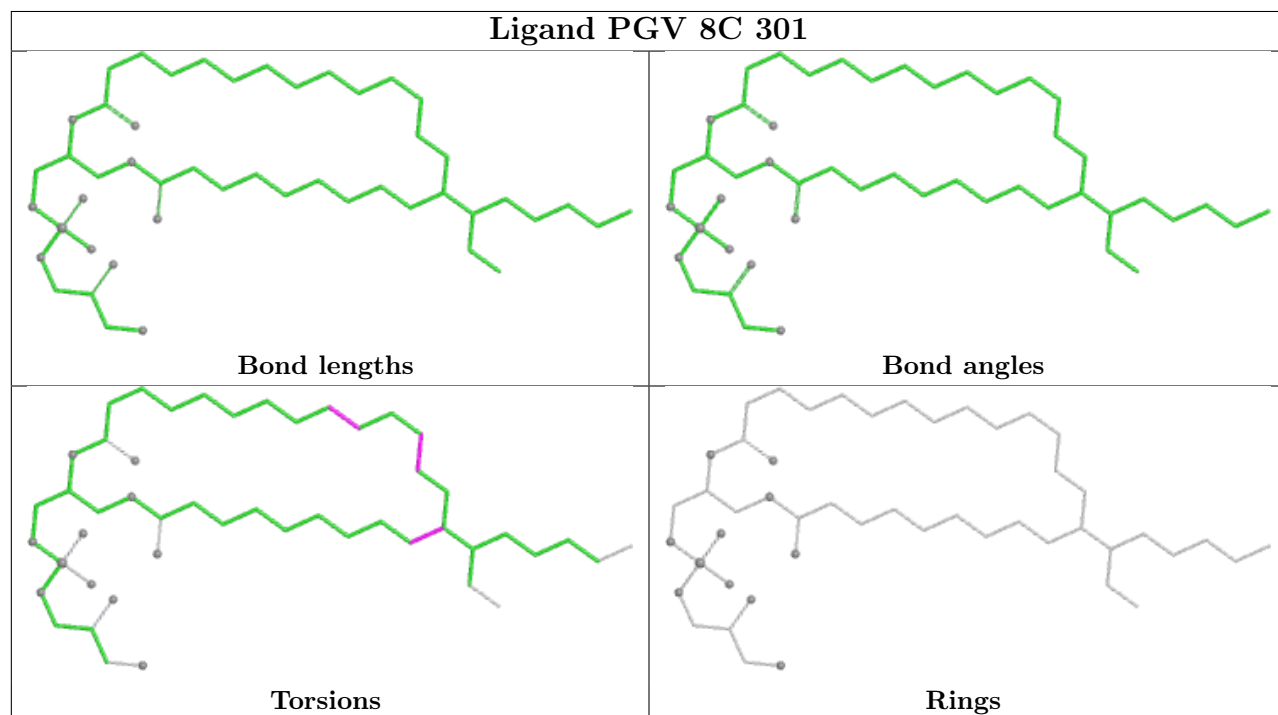
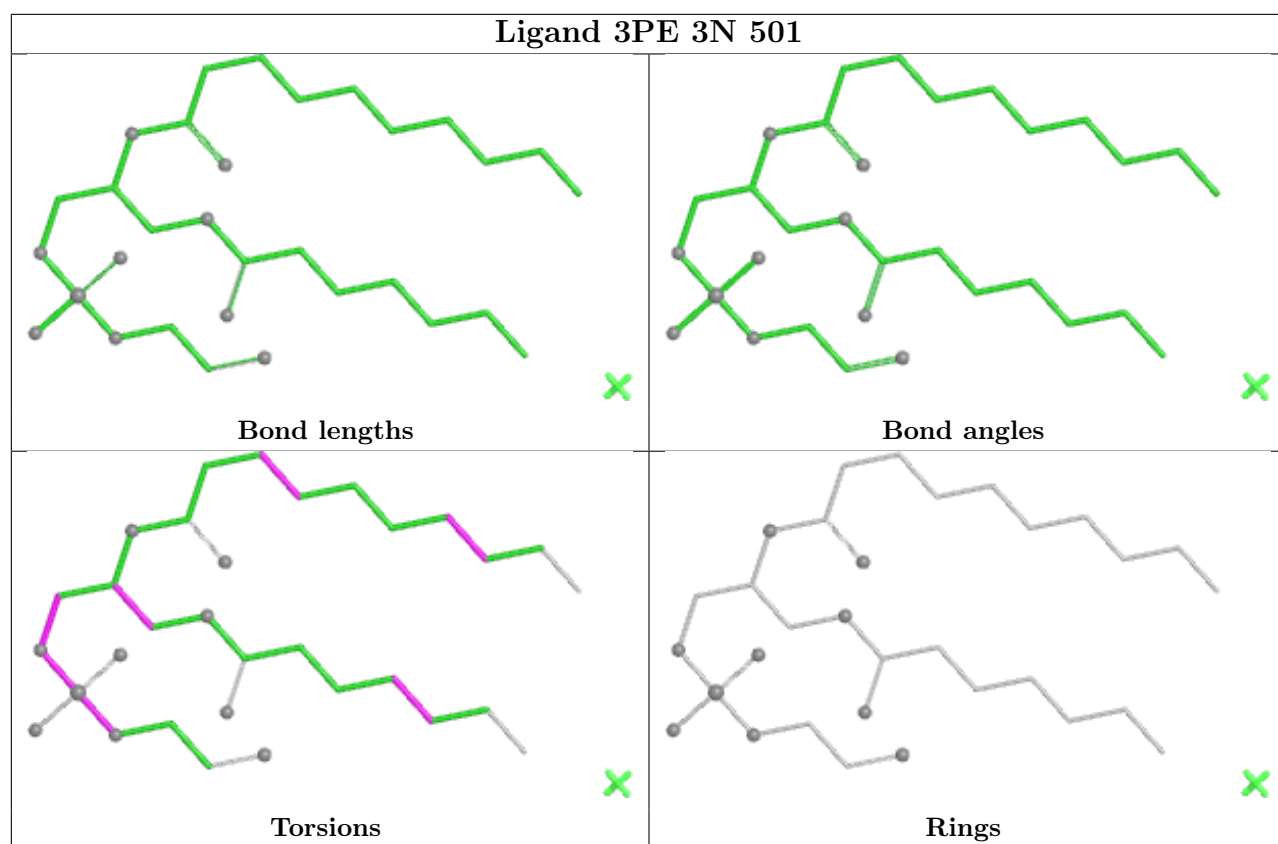


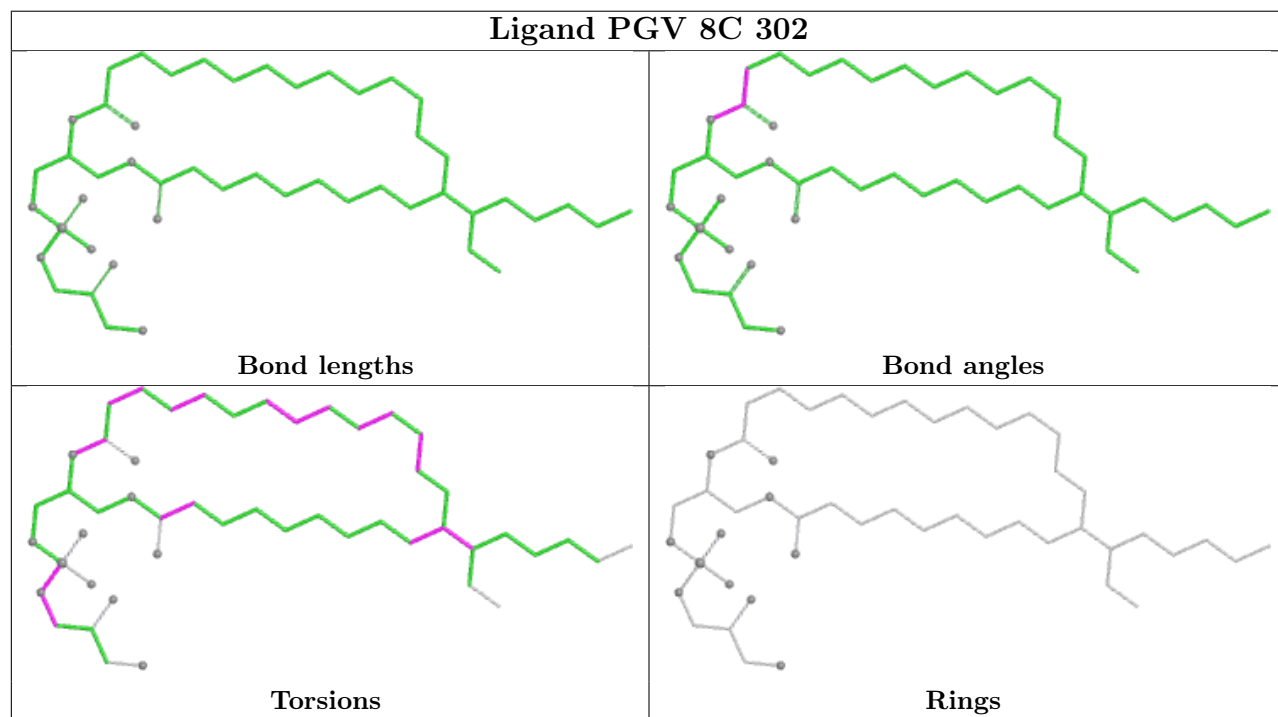
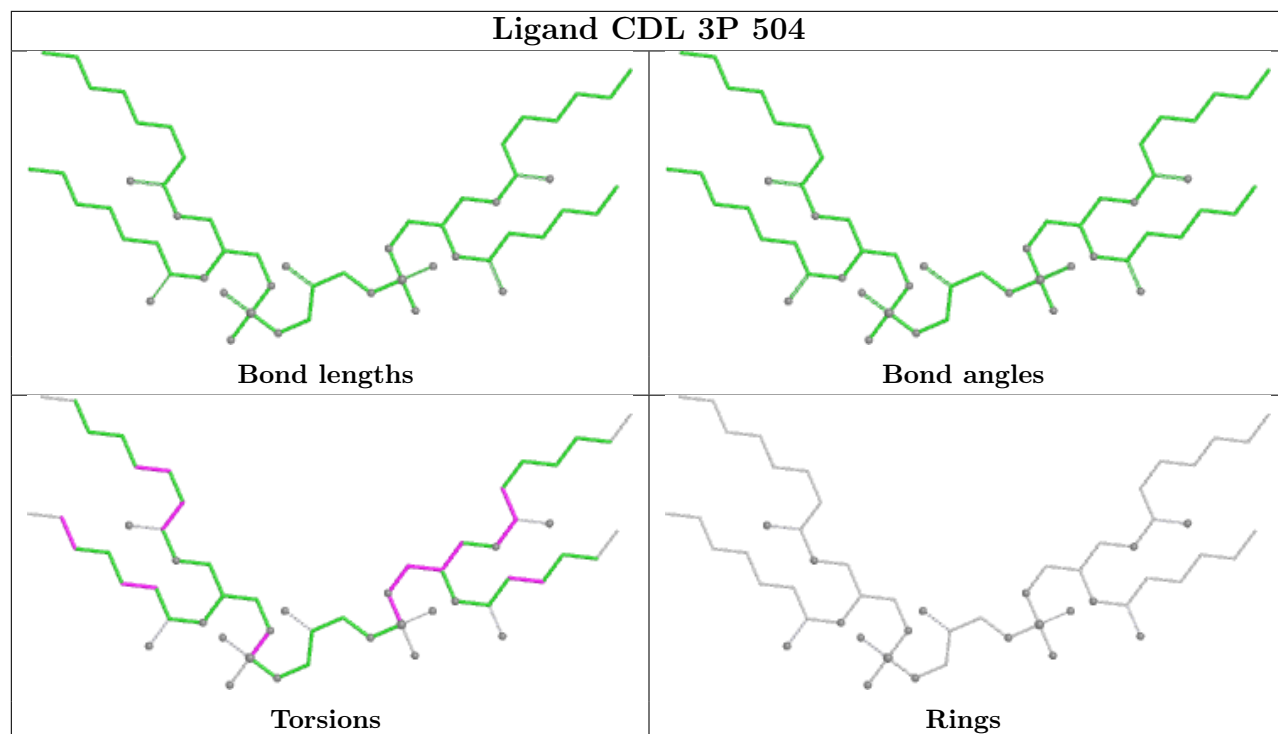


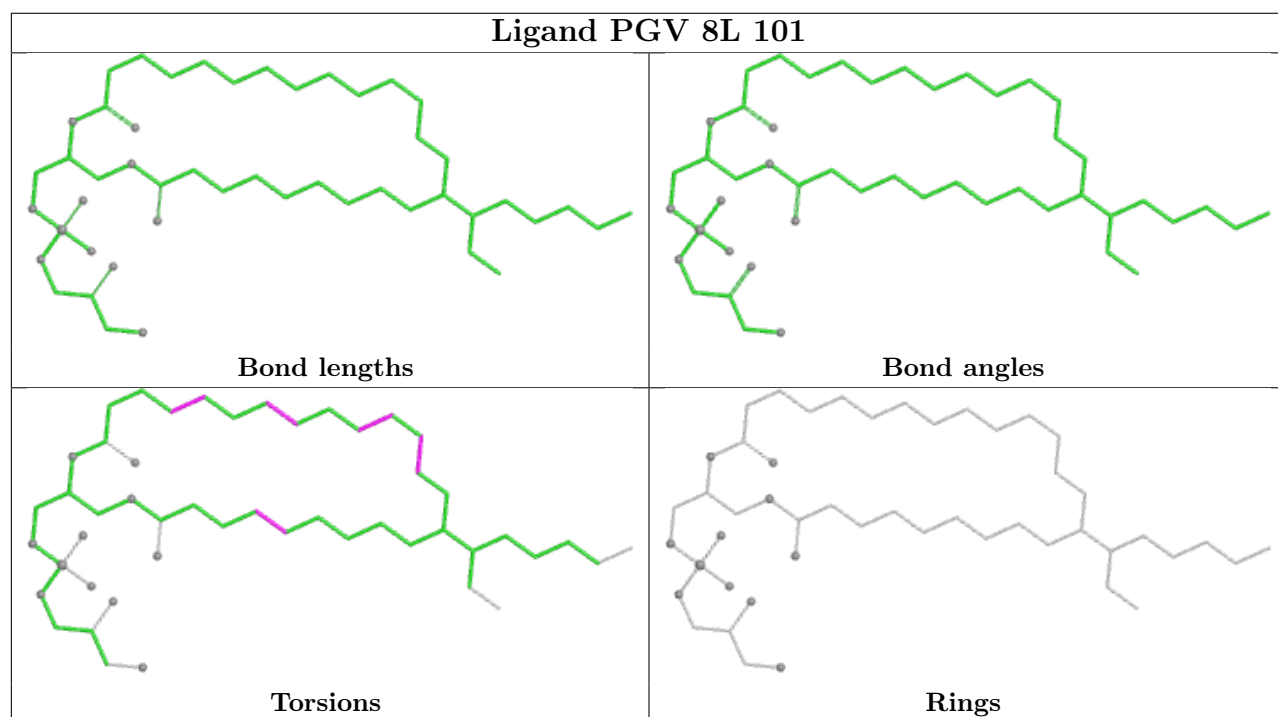
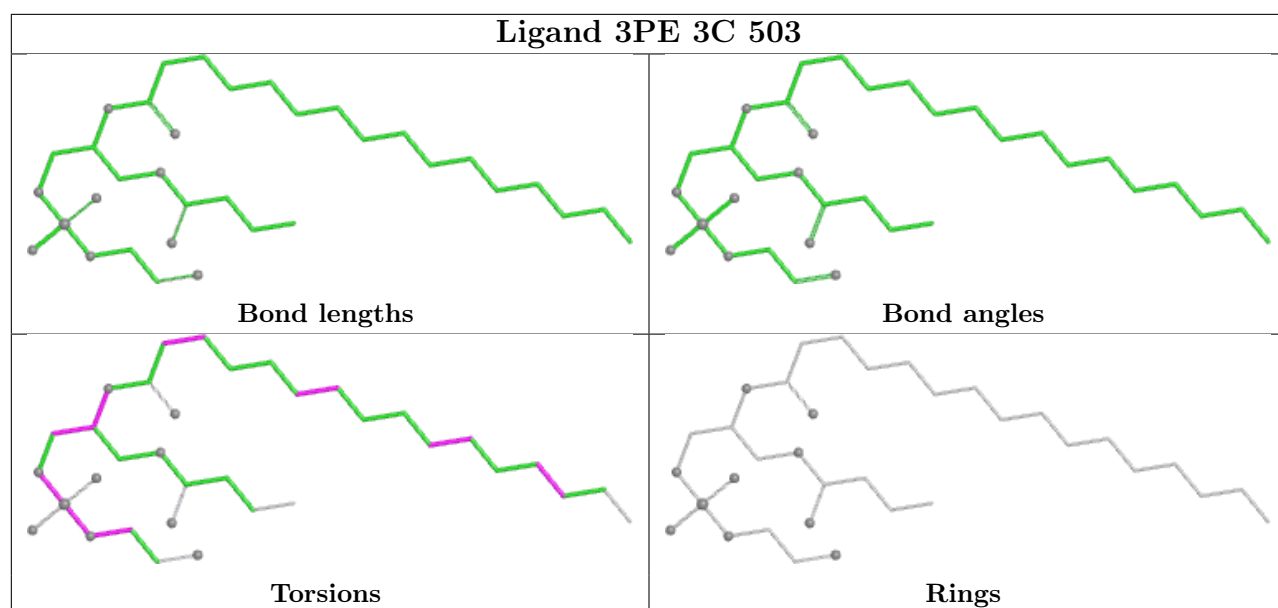


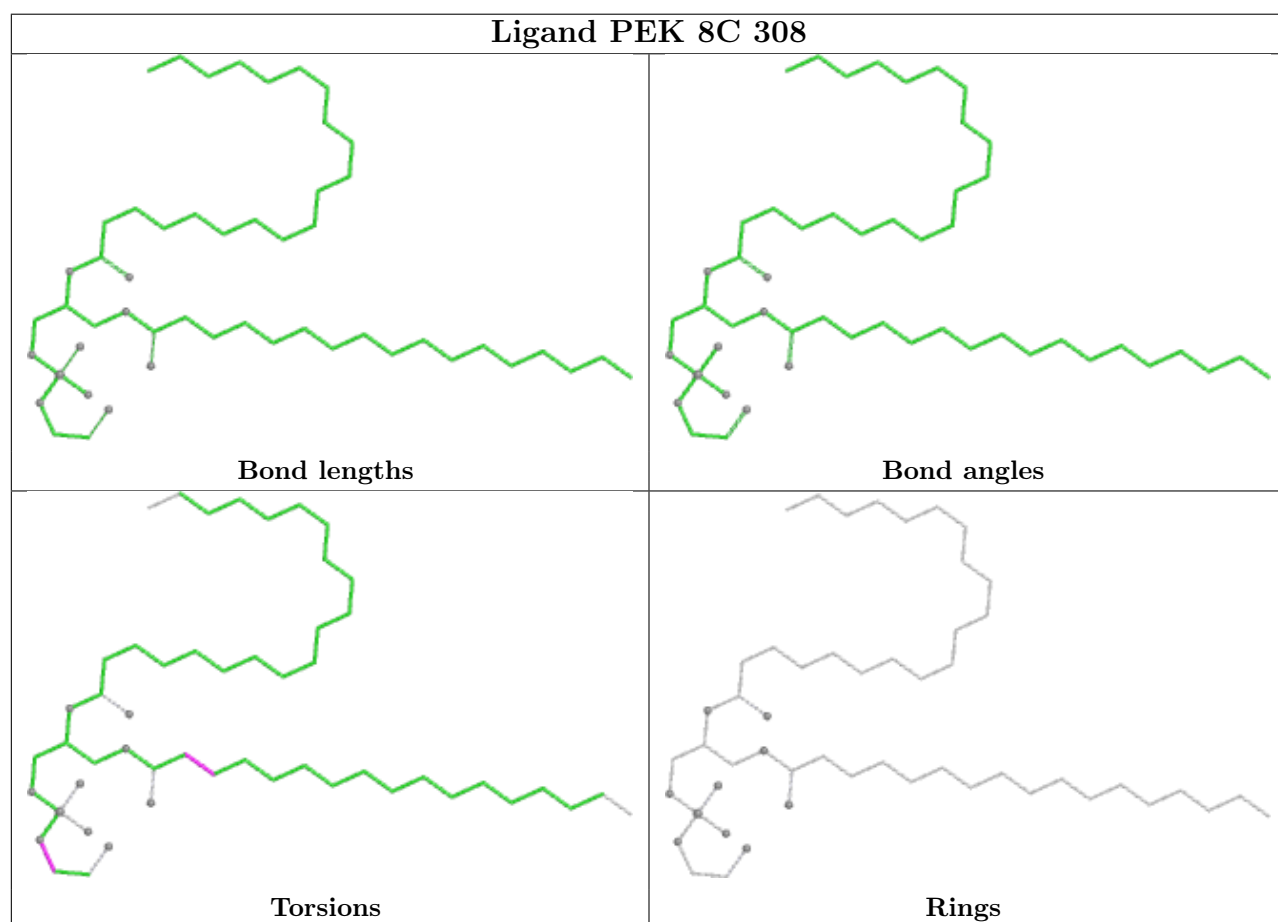
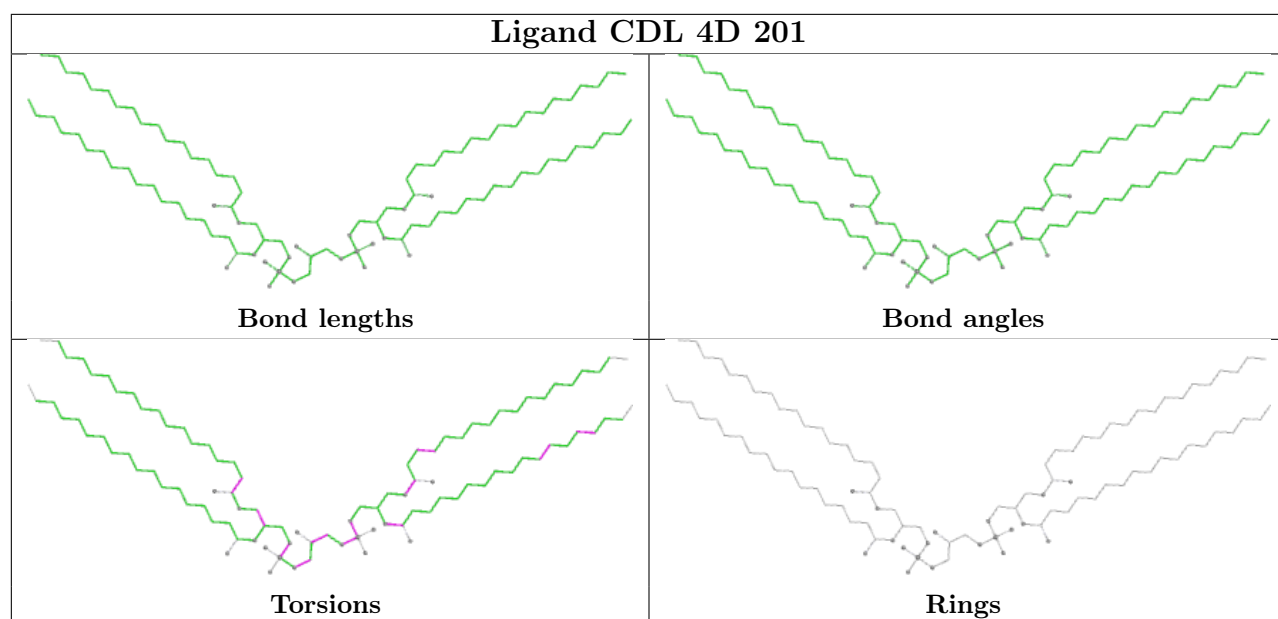


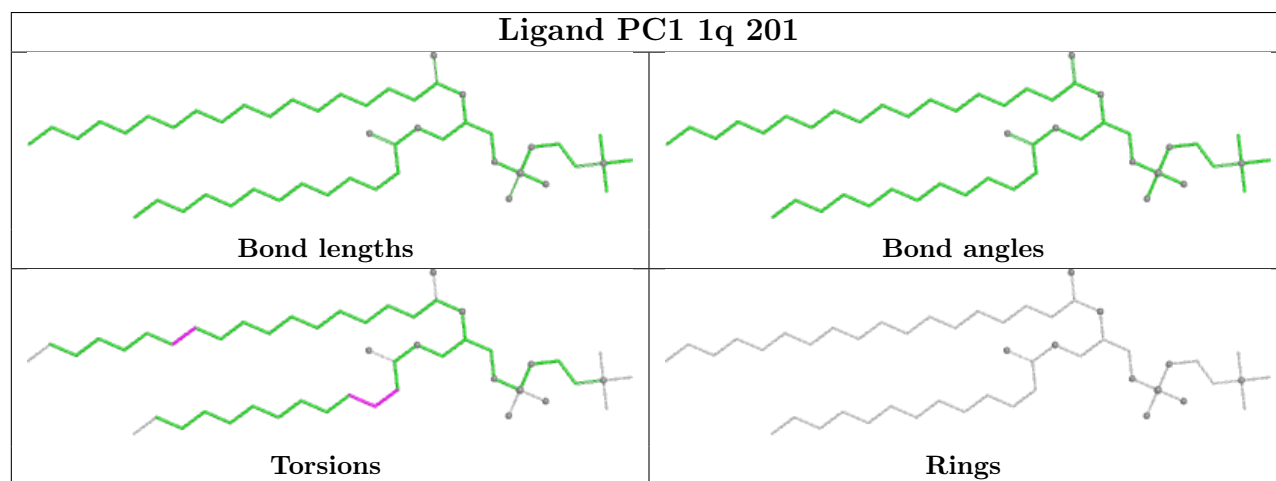
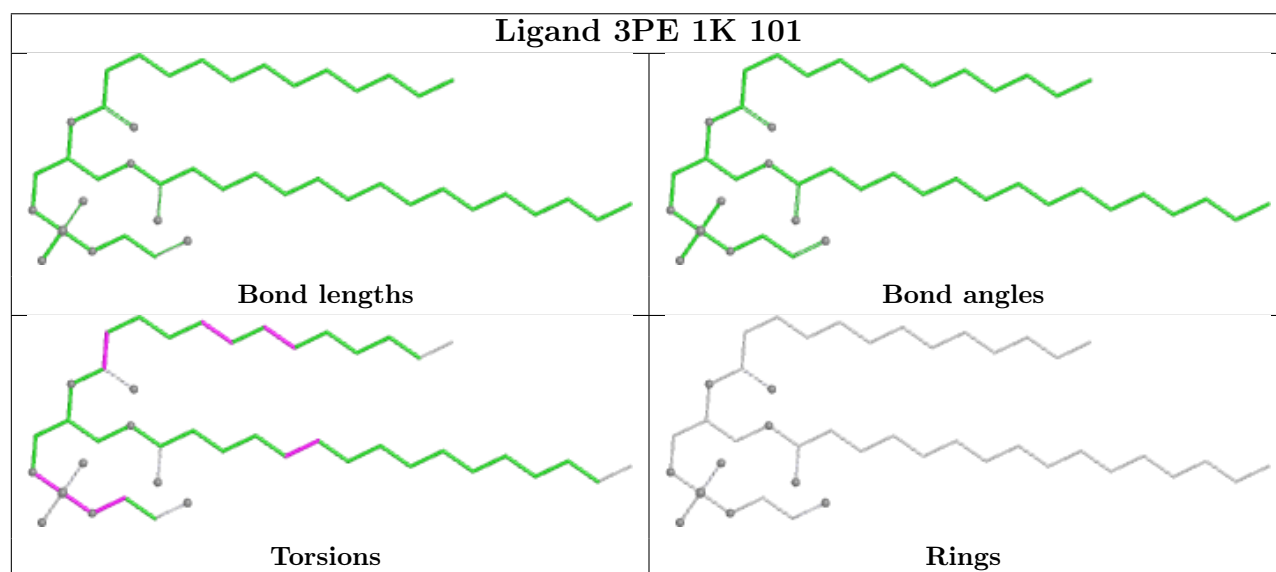
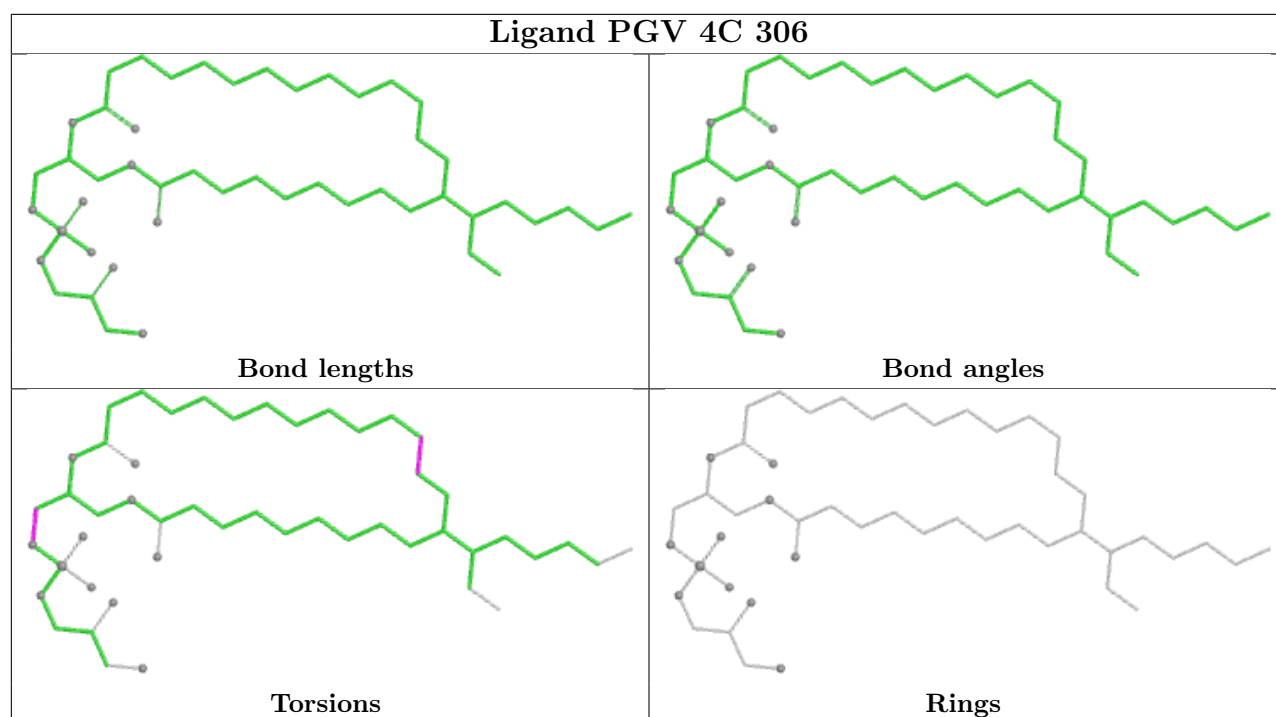


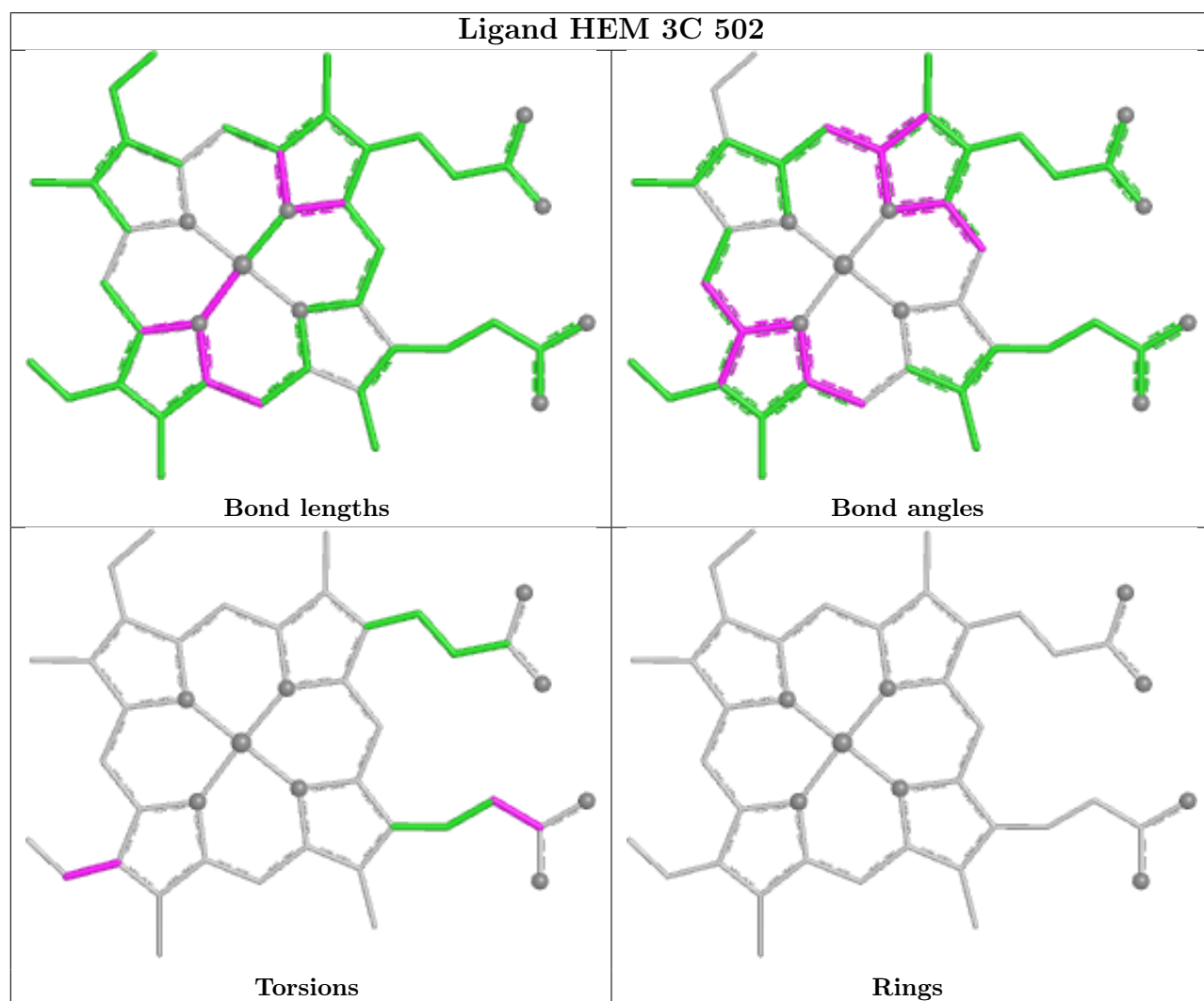
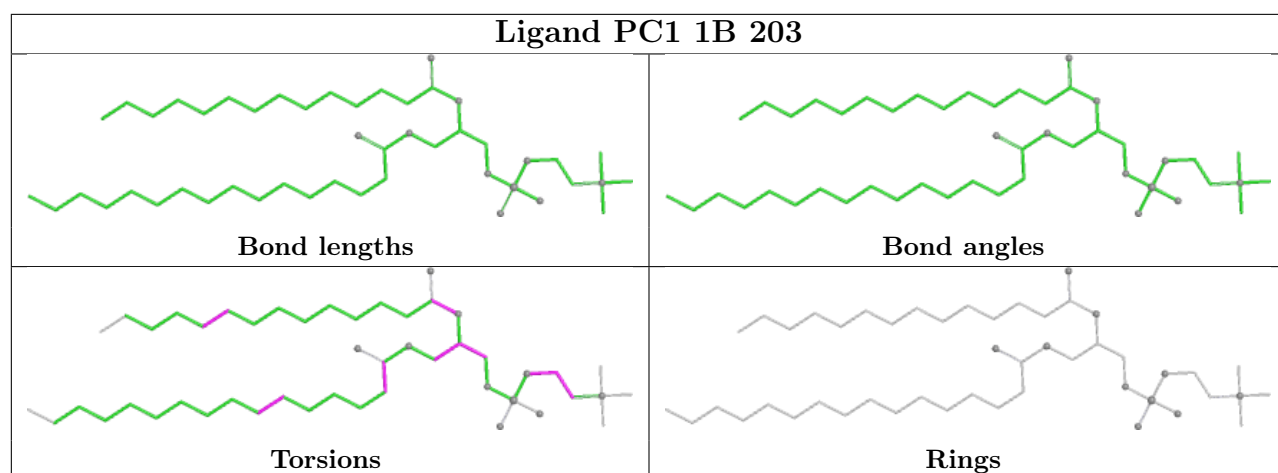


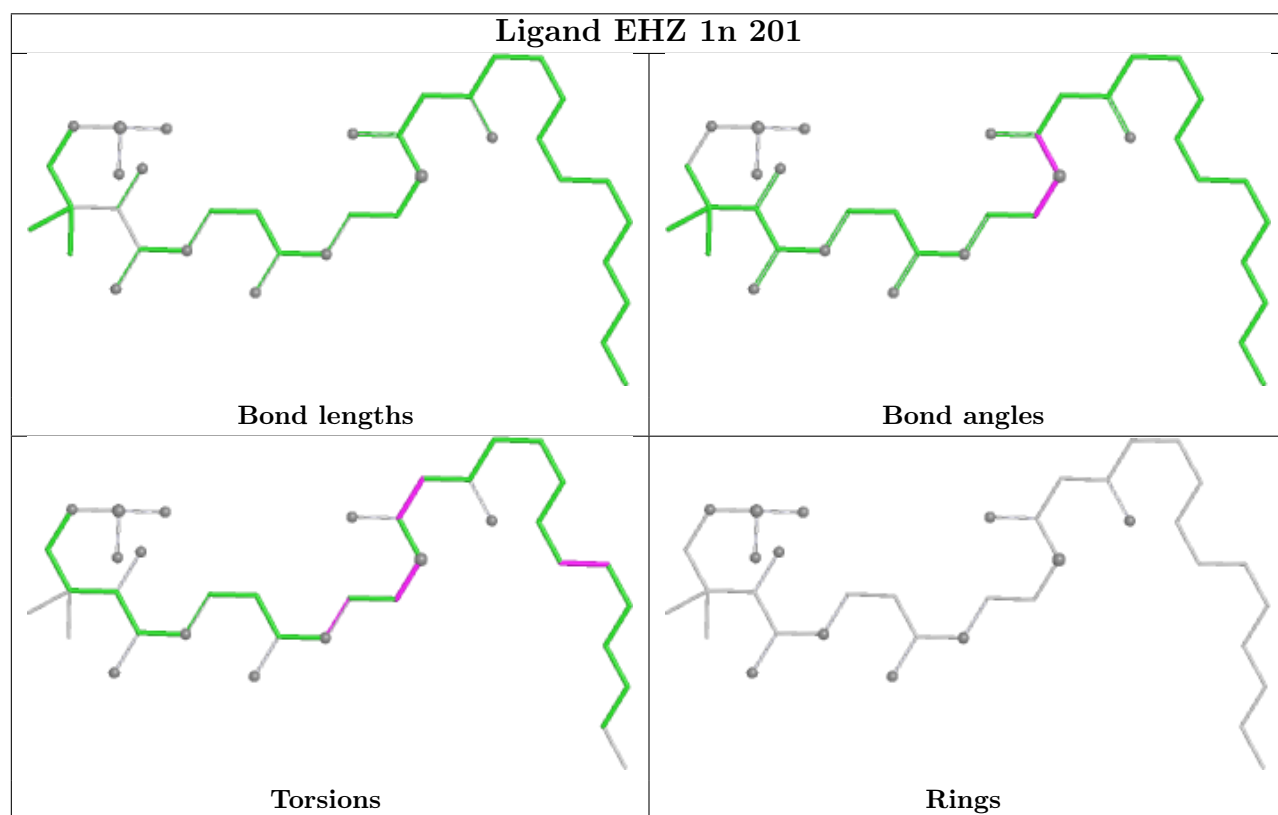
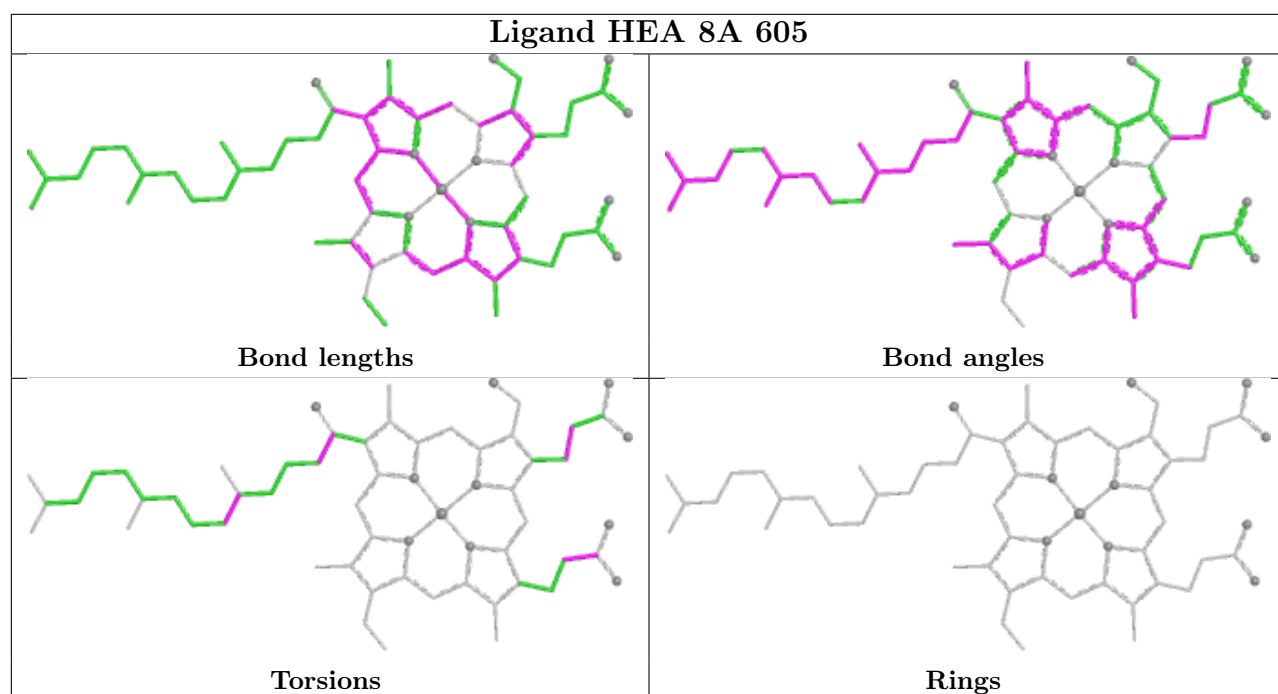


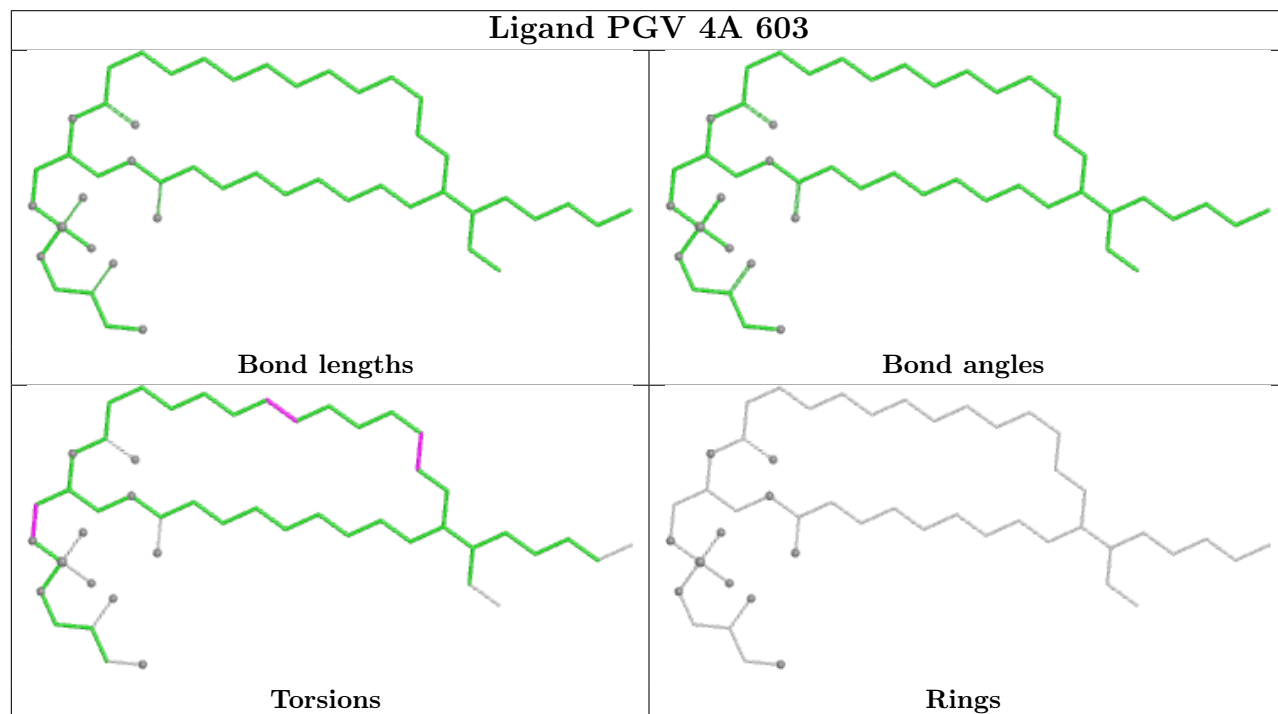
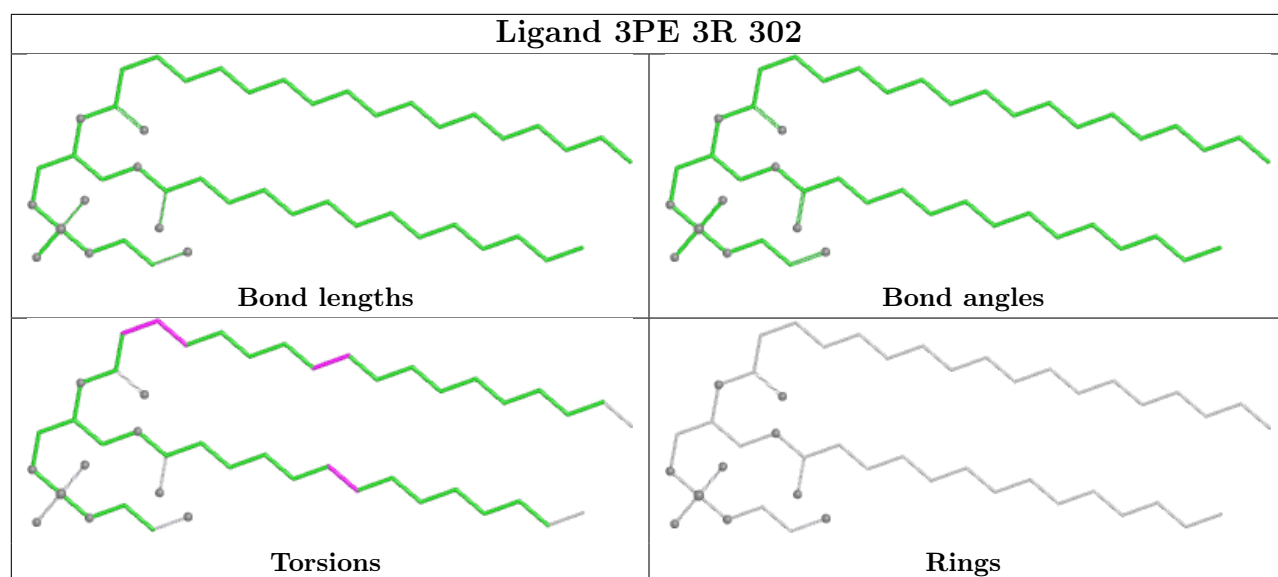




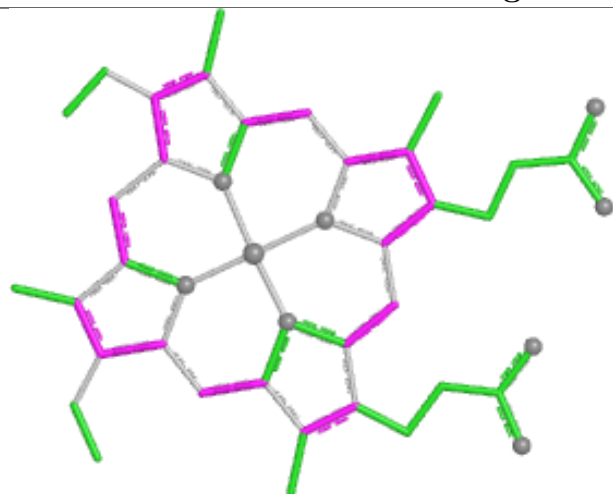




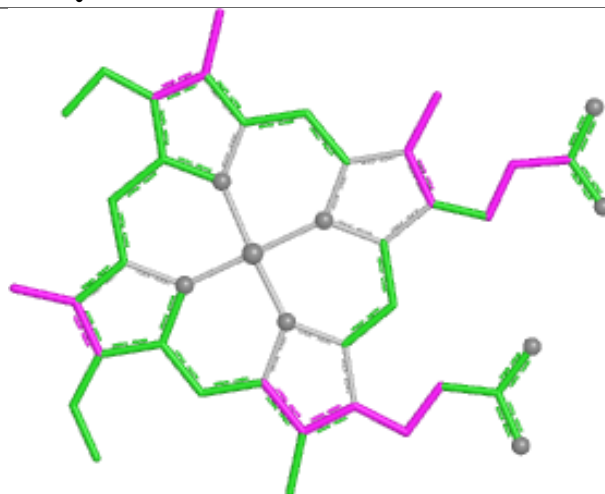




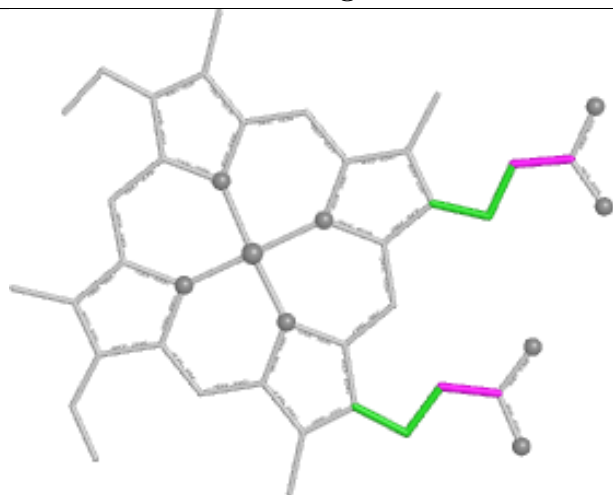
Ligand HEC 3Q 501



Bond lengths



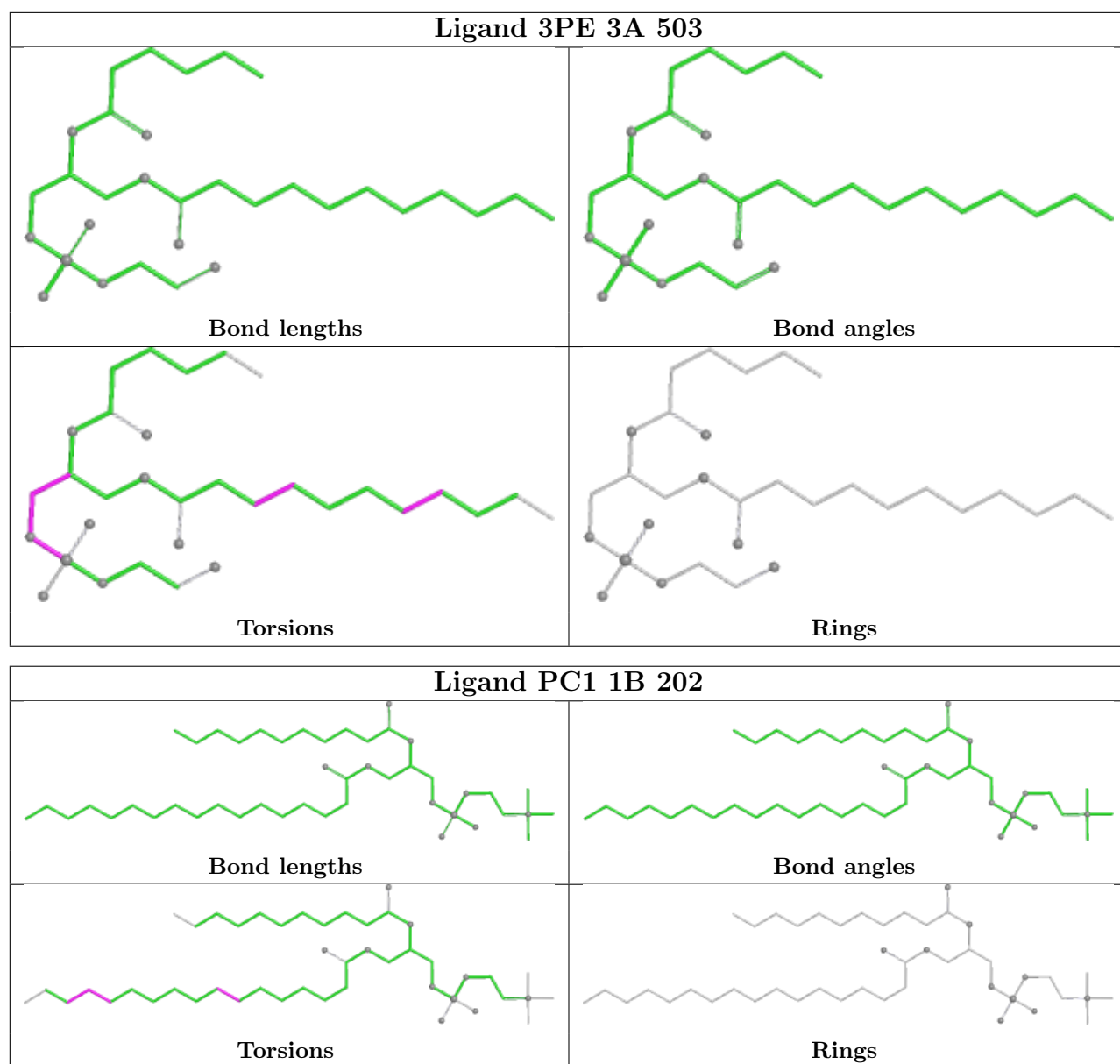
Bond angles

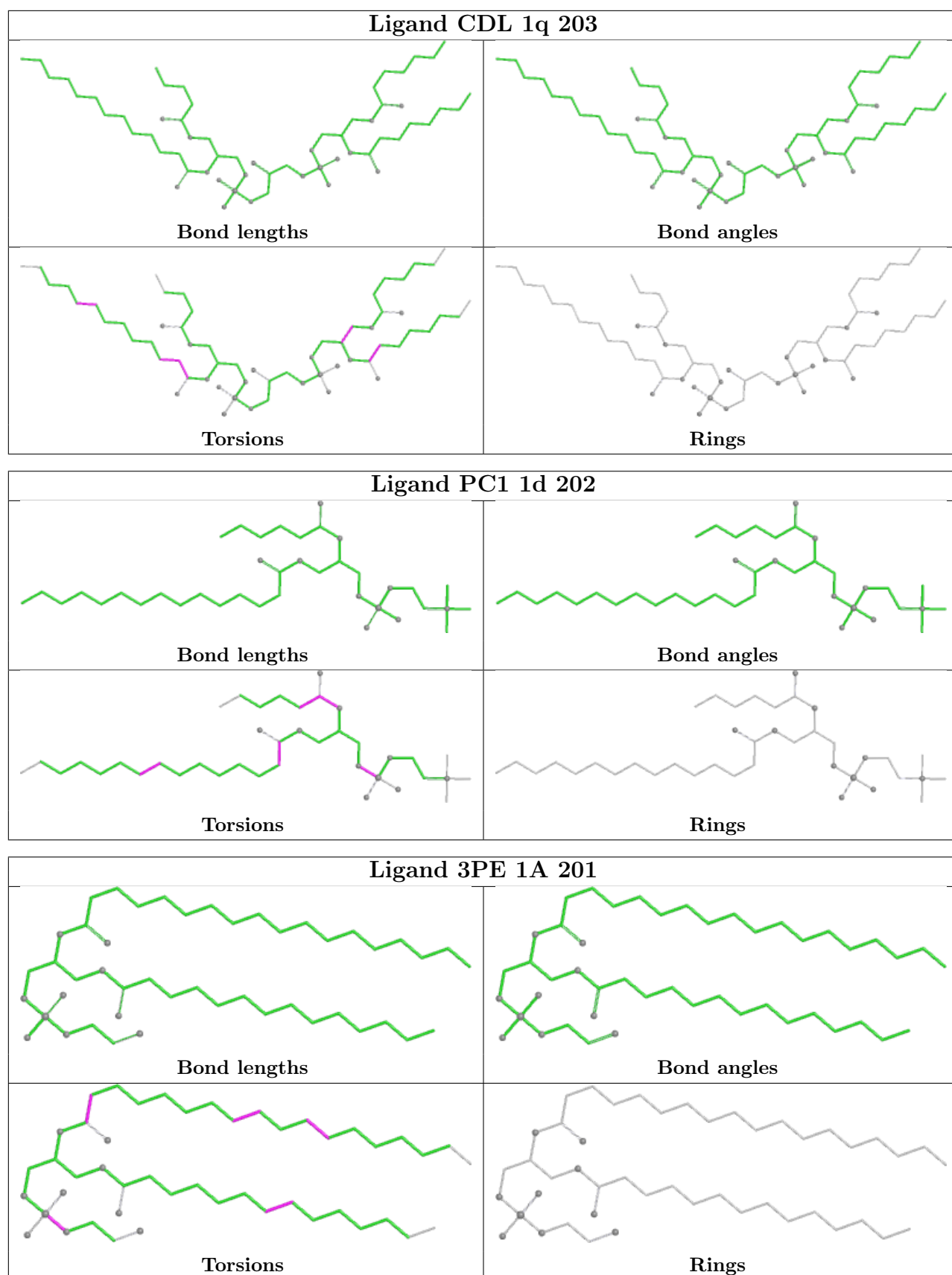


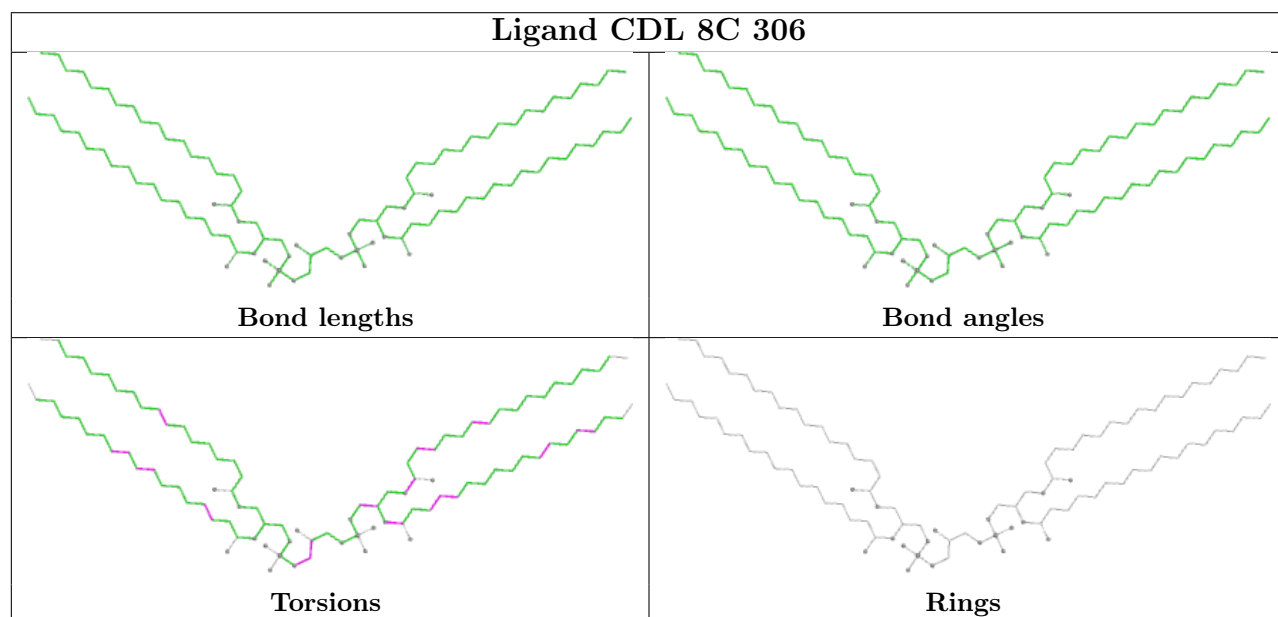
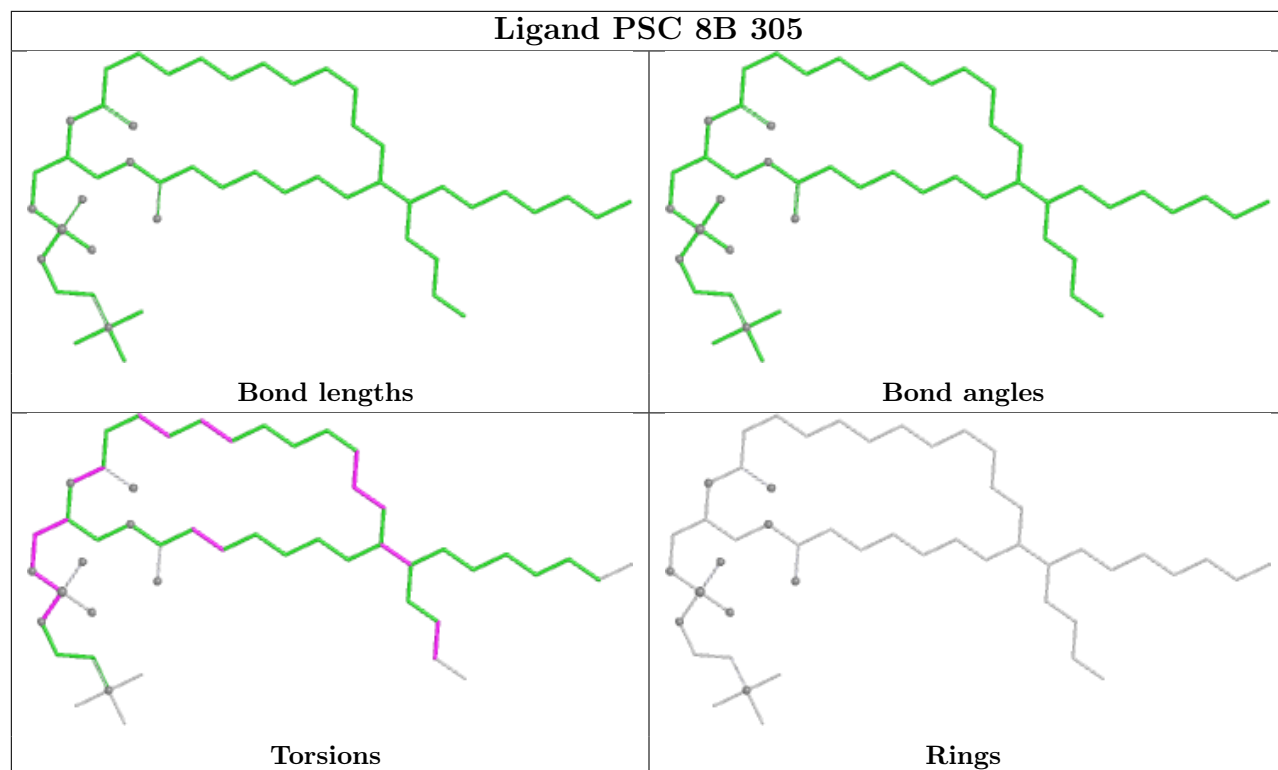
Torsions

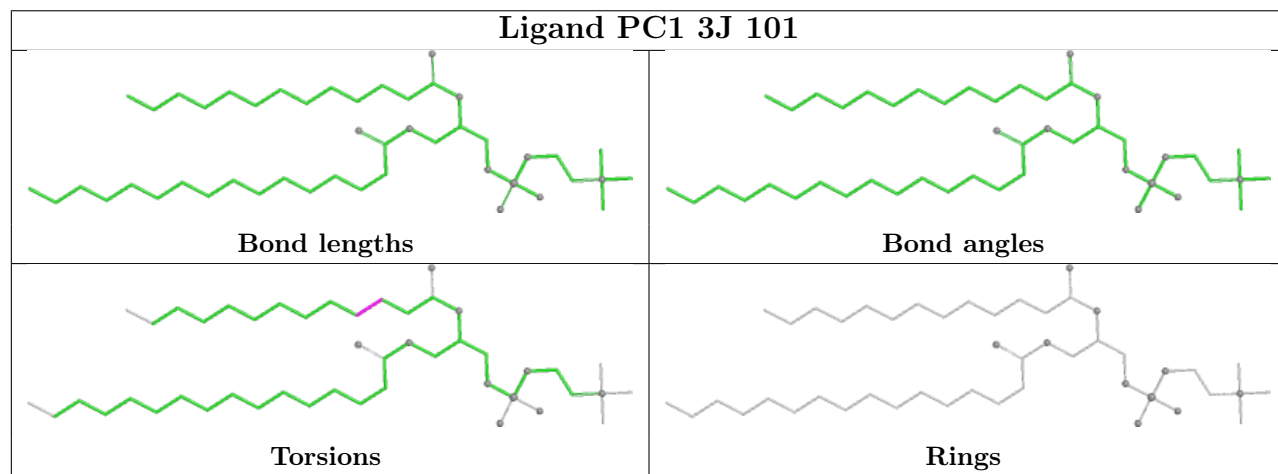
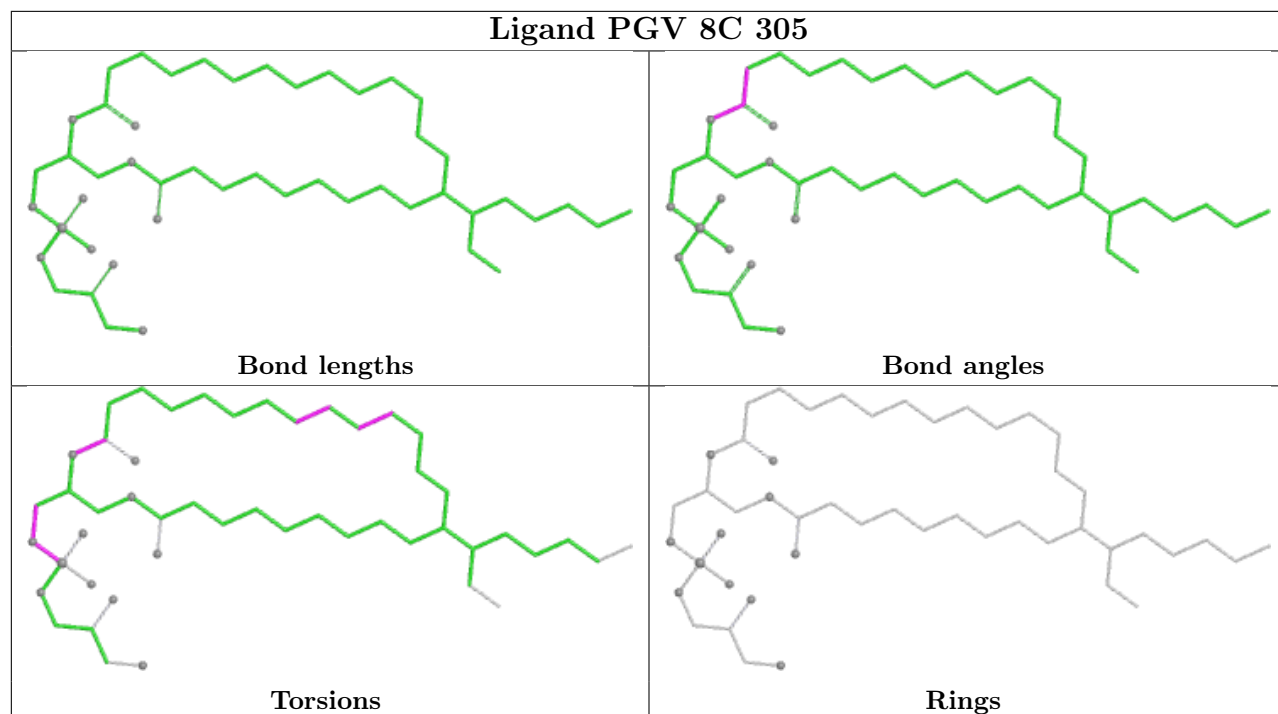


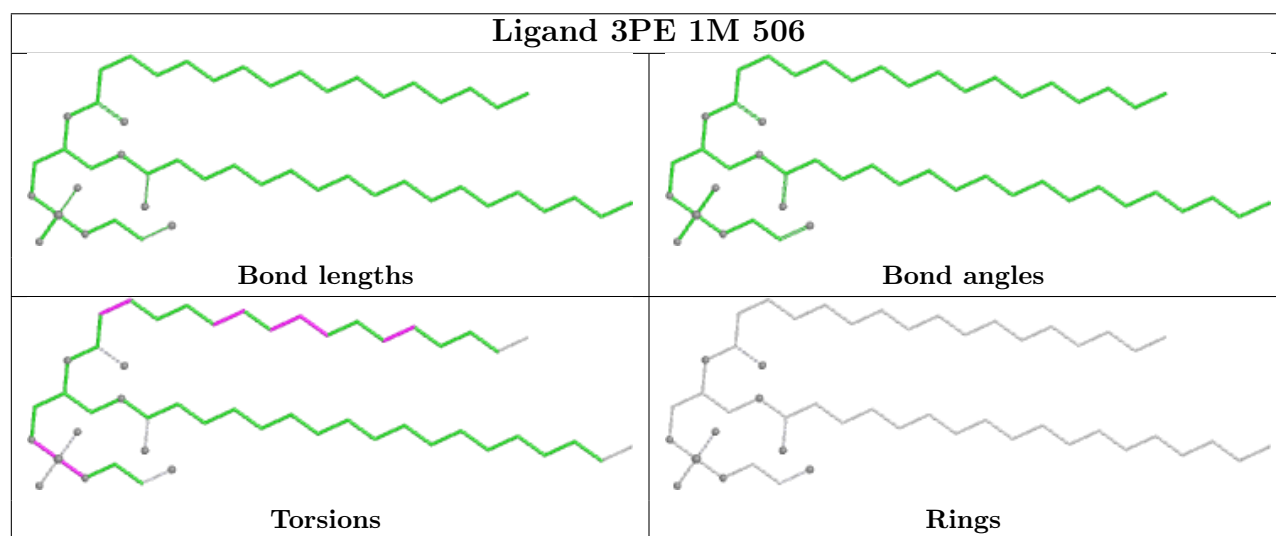
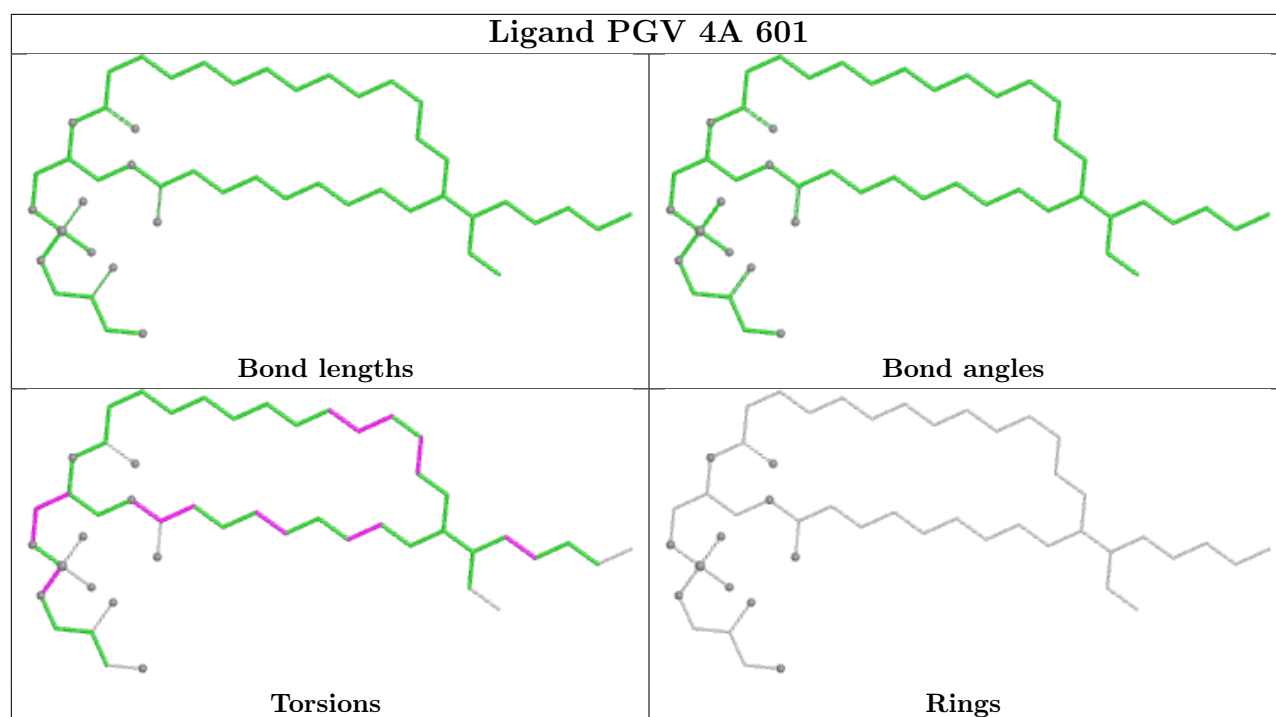
Rings



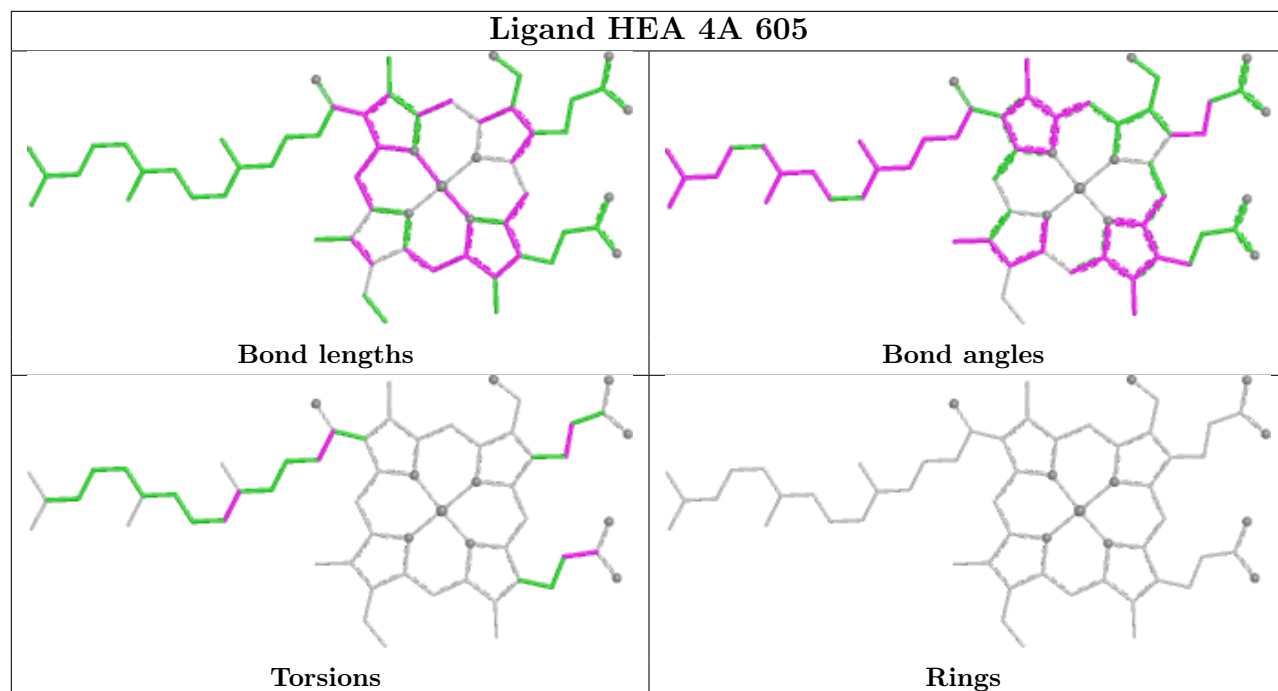




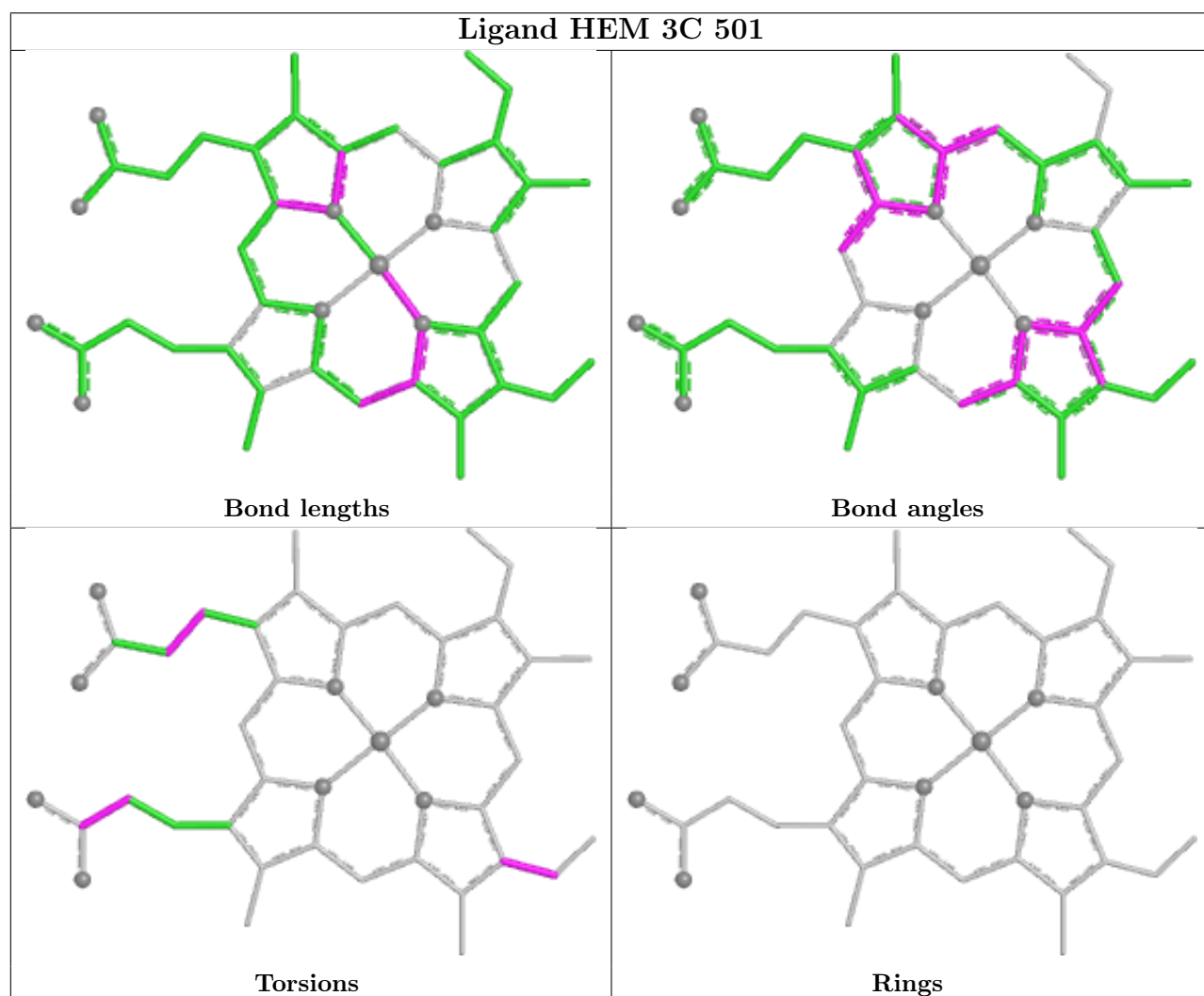


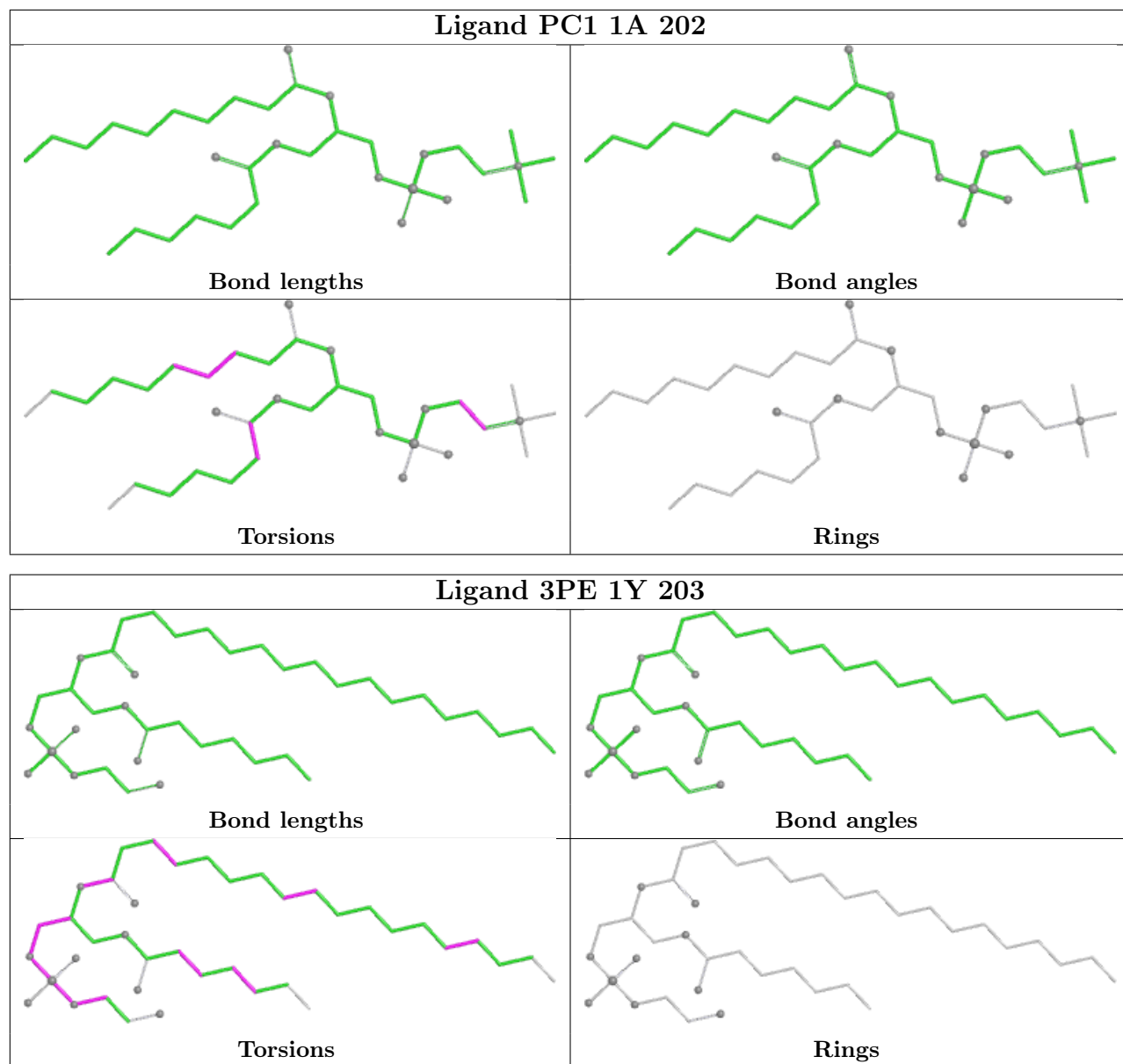


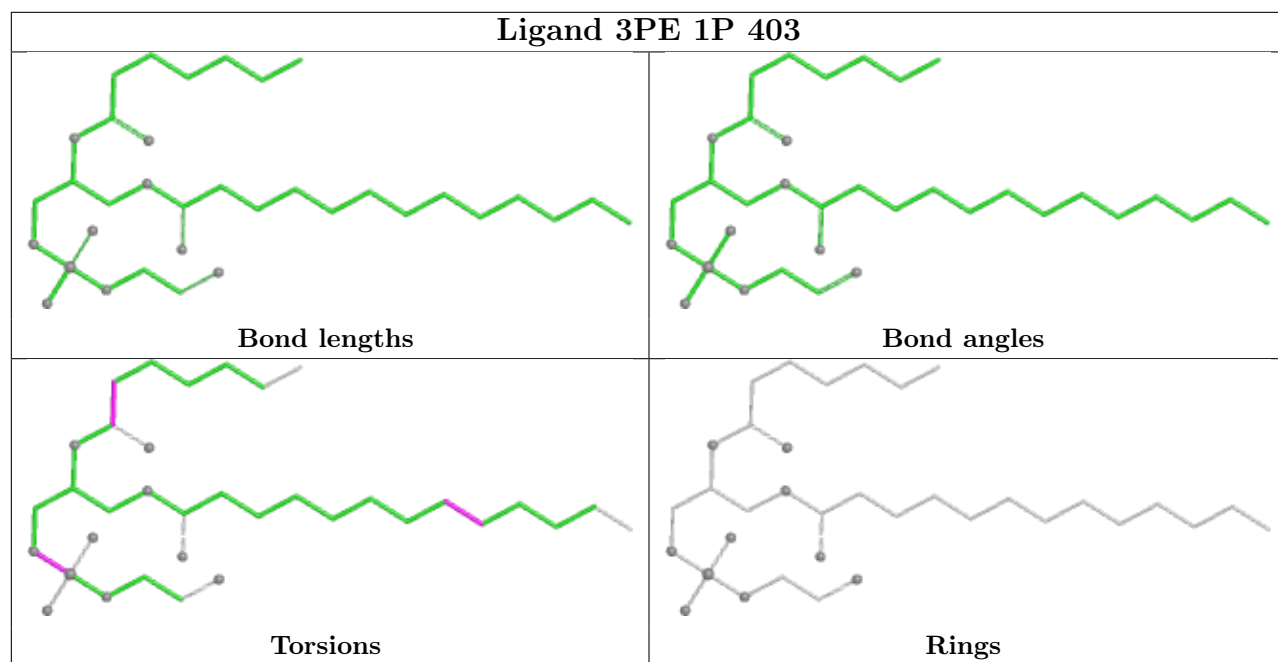
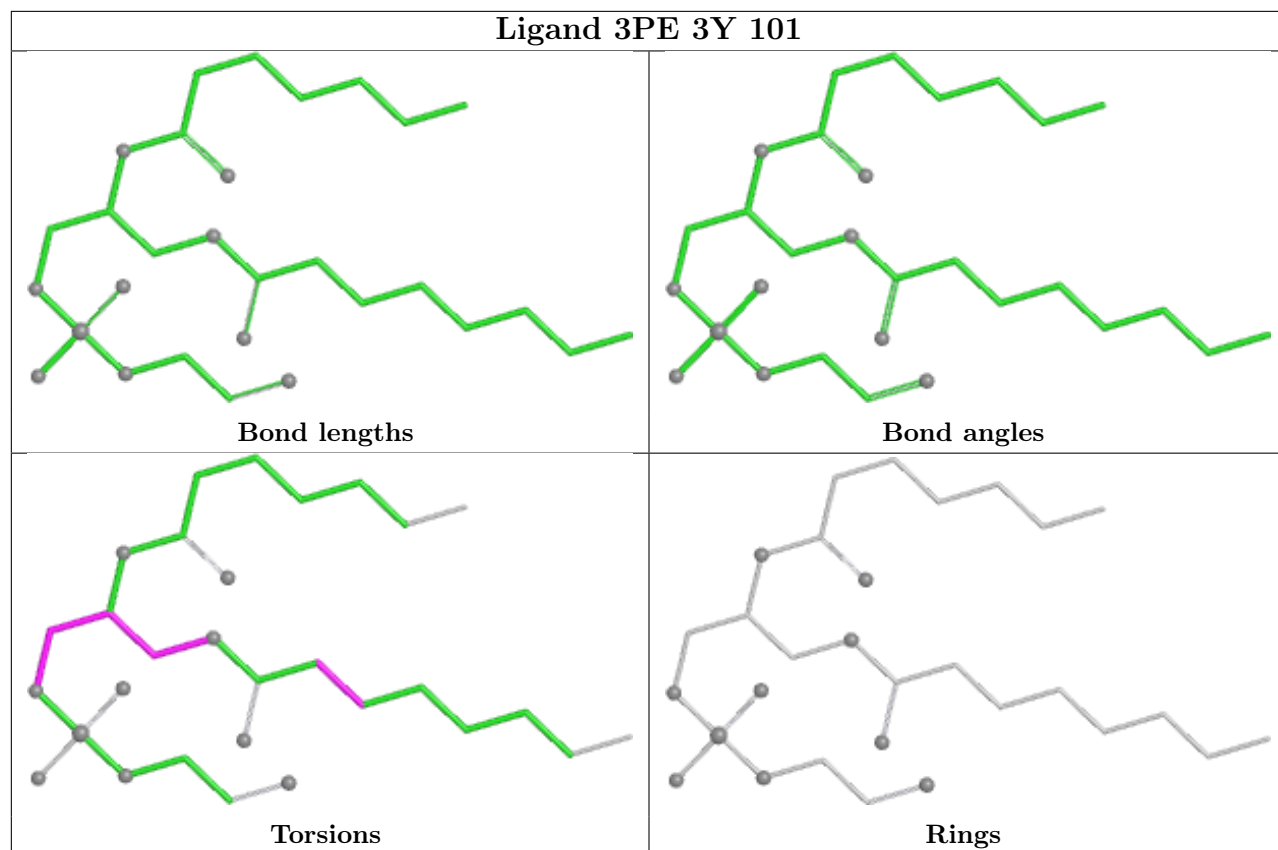
Ligand HEA 4A 605

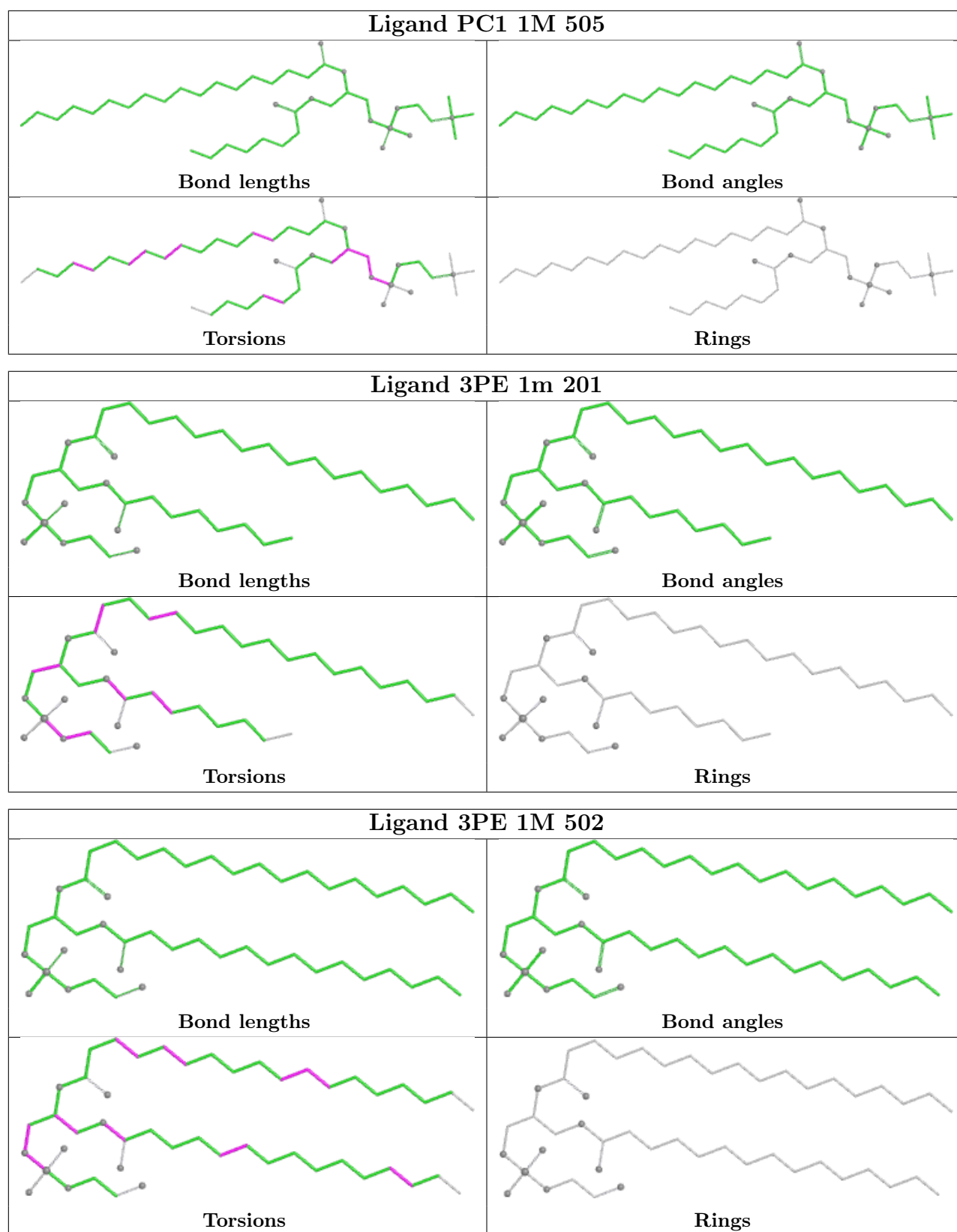


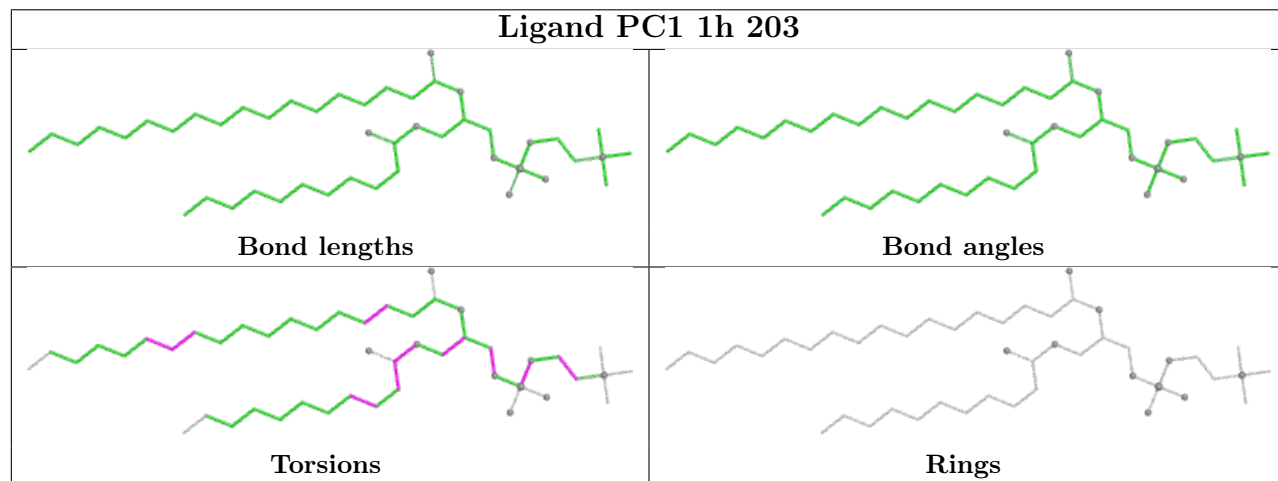
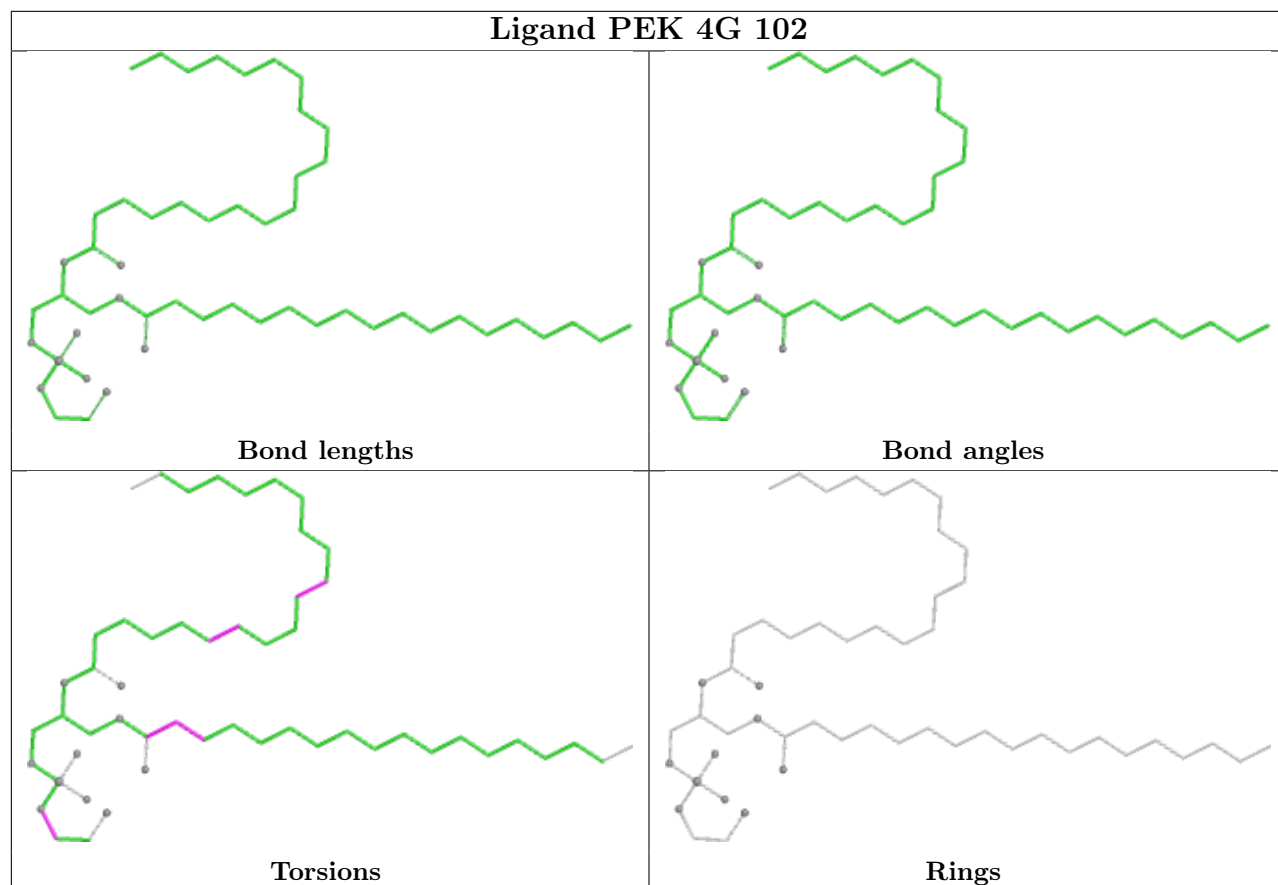
Ligand HEM 3C 501

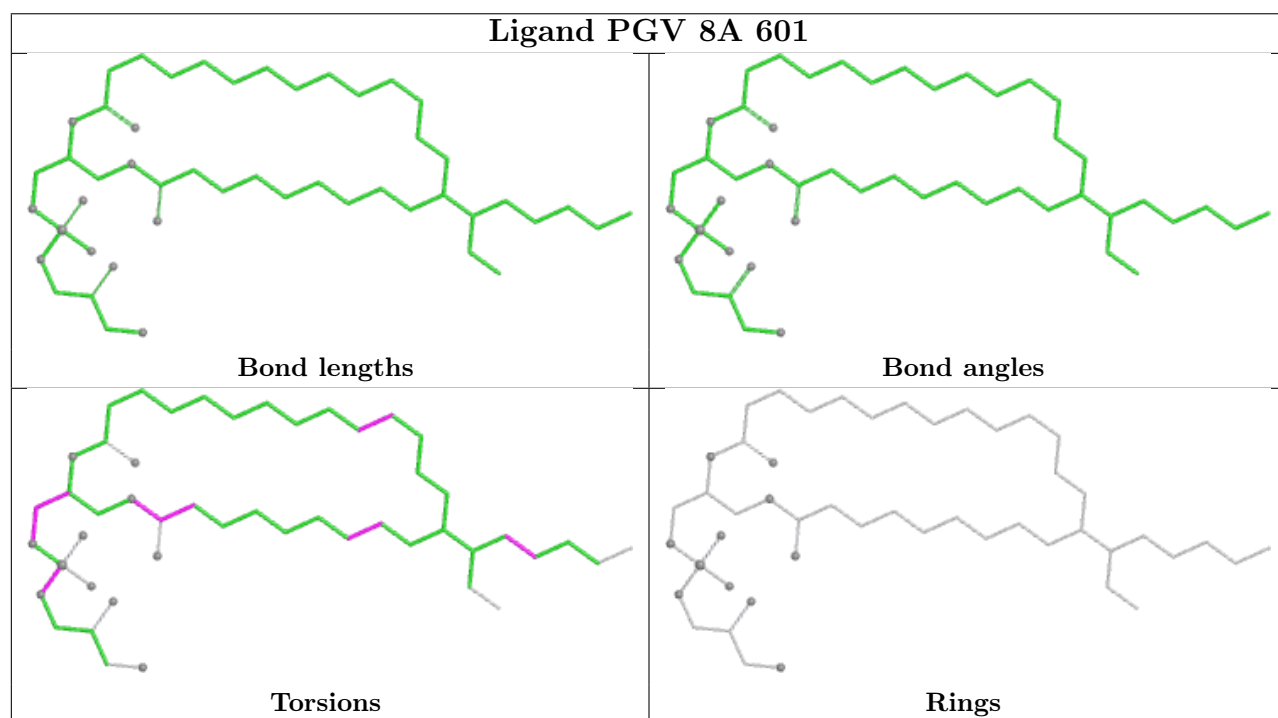
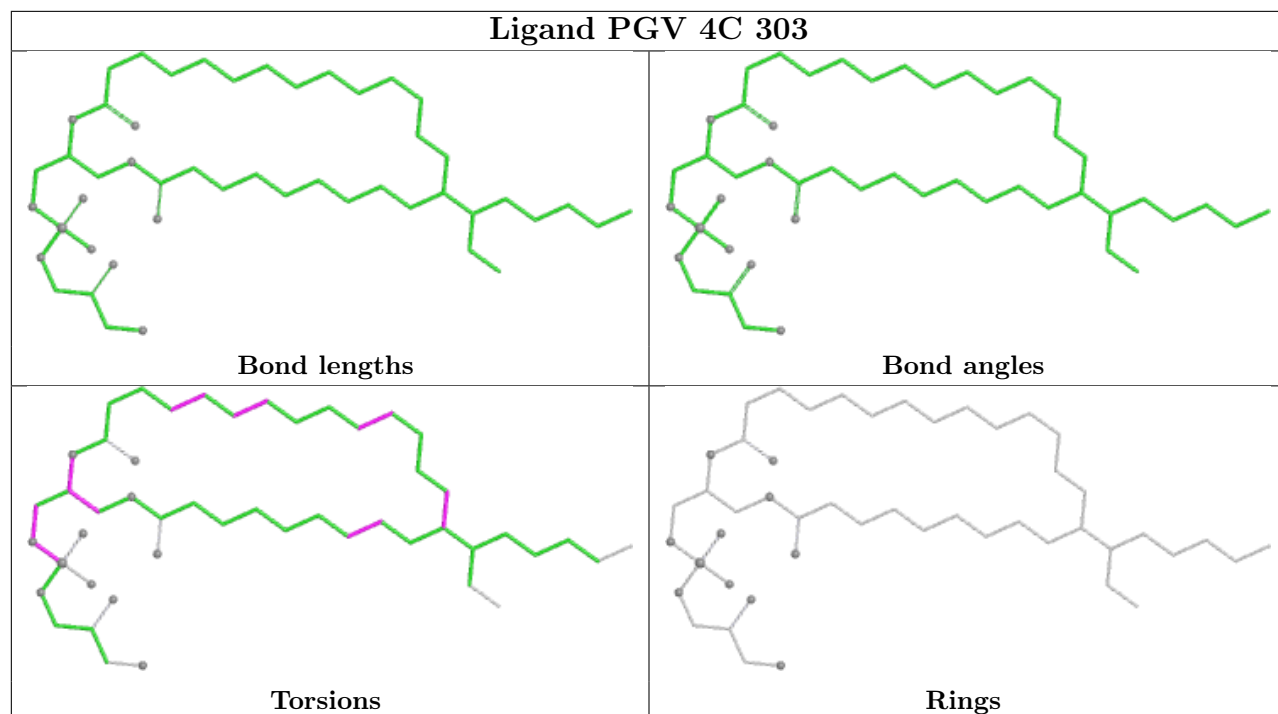


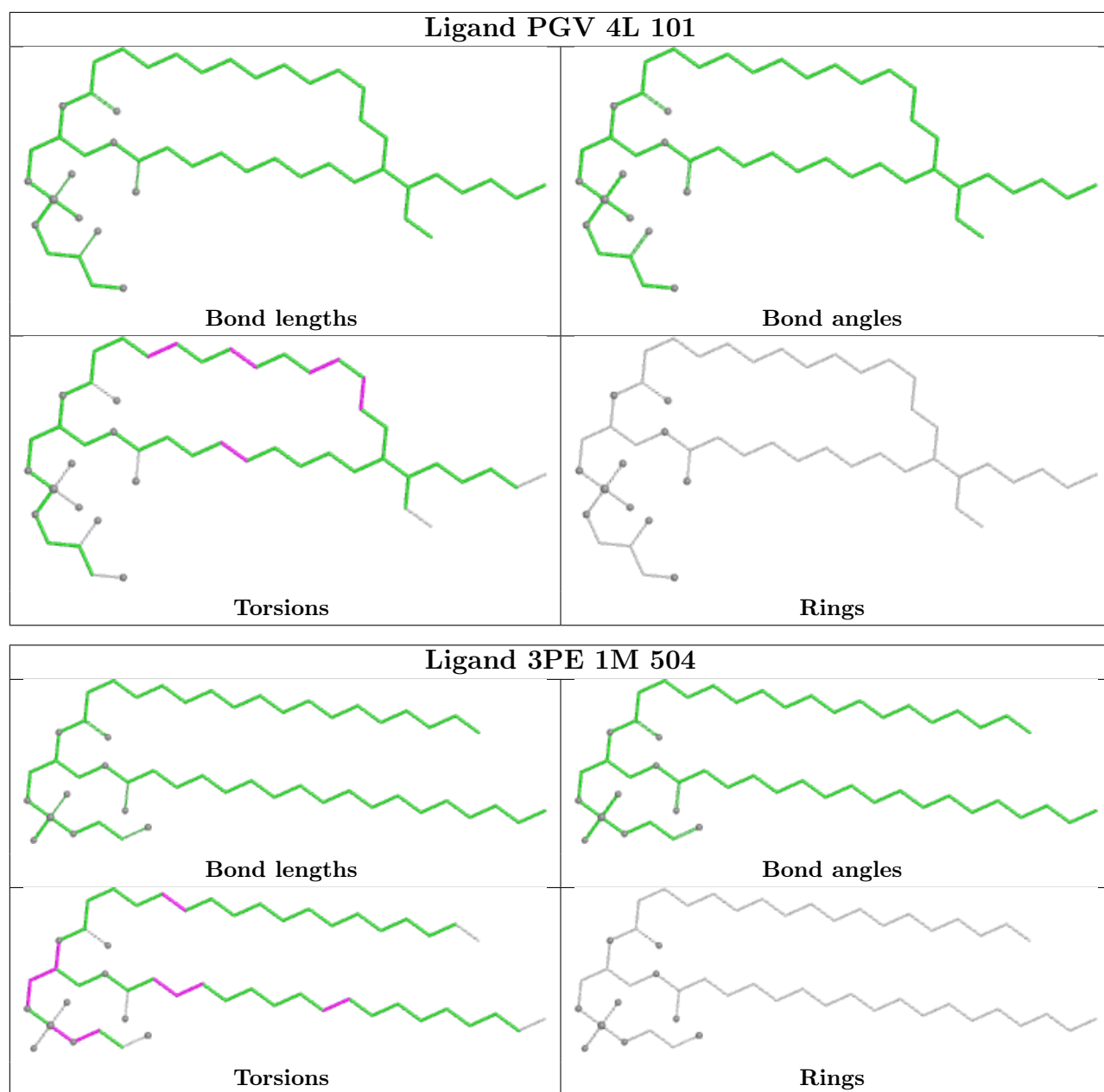


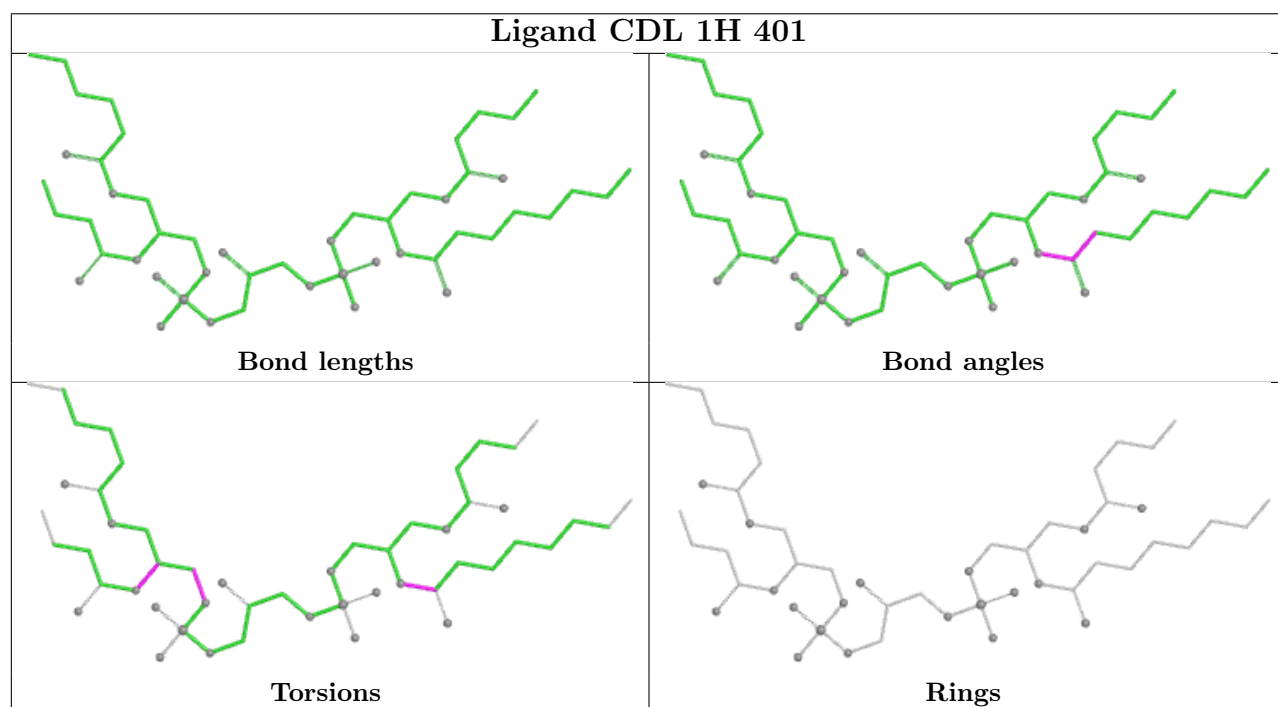
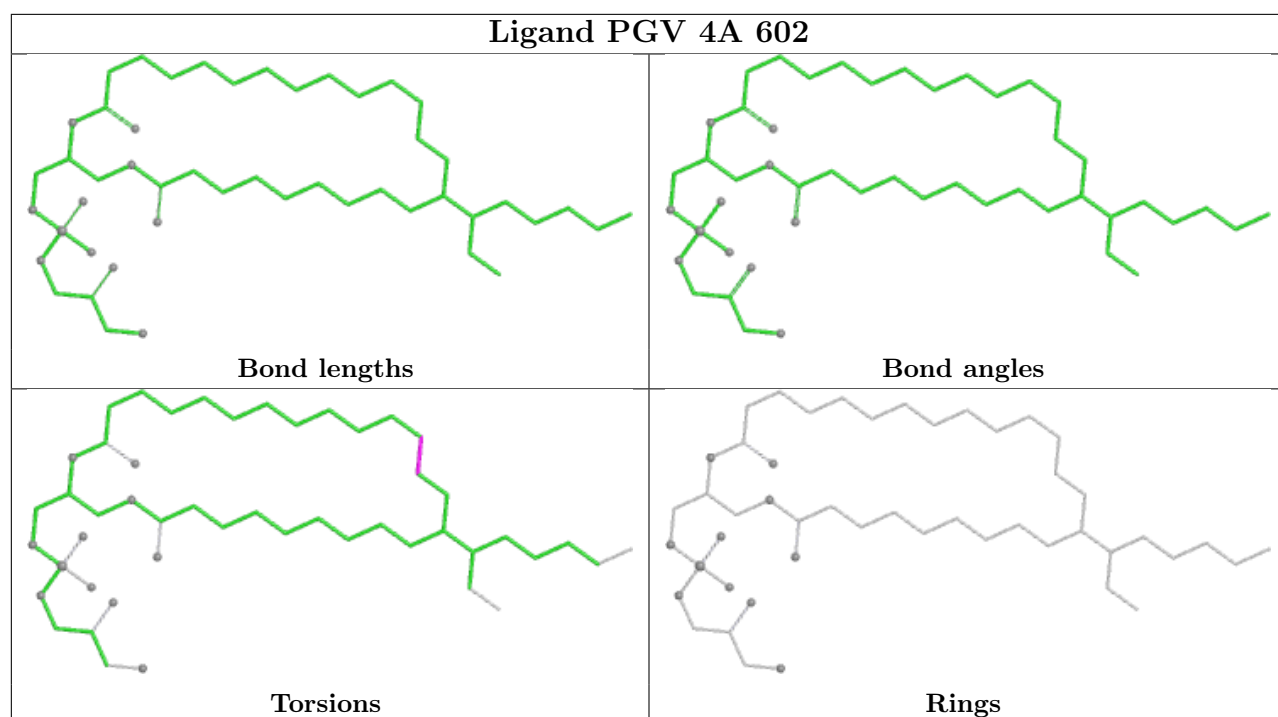


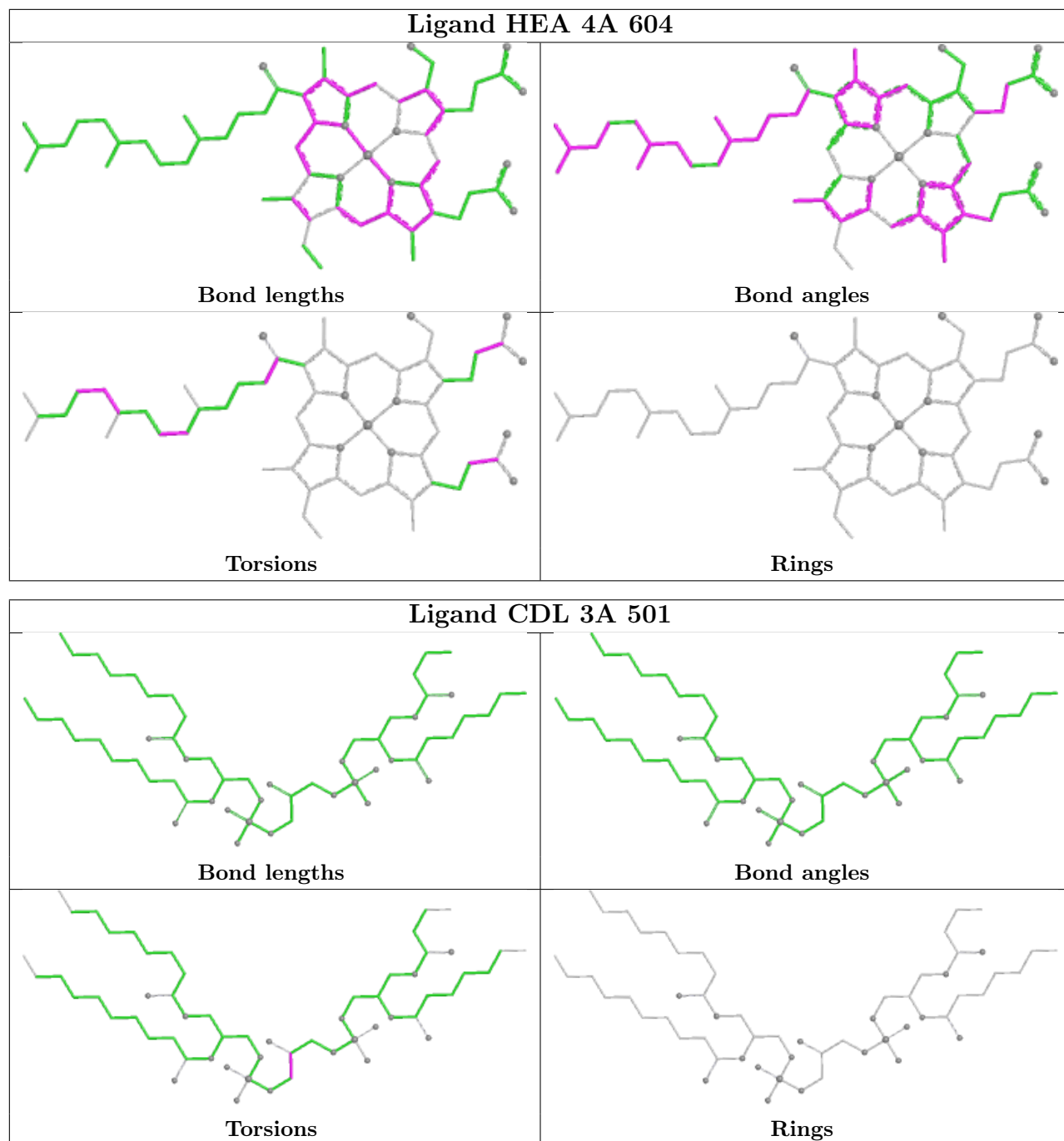


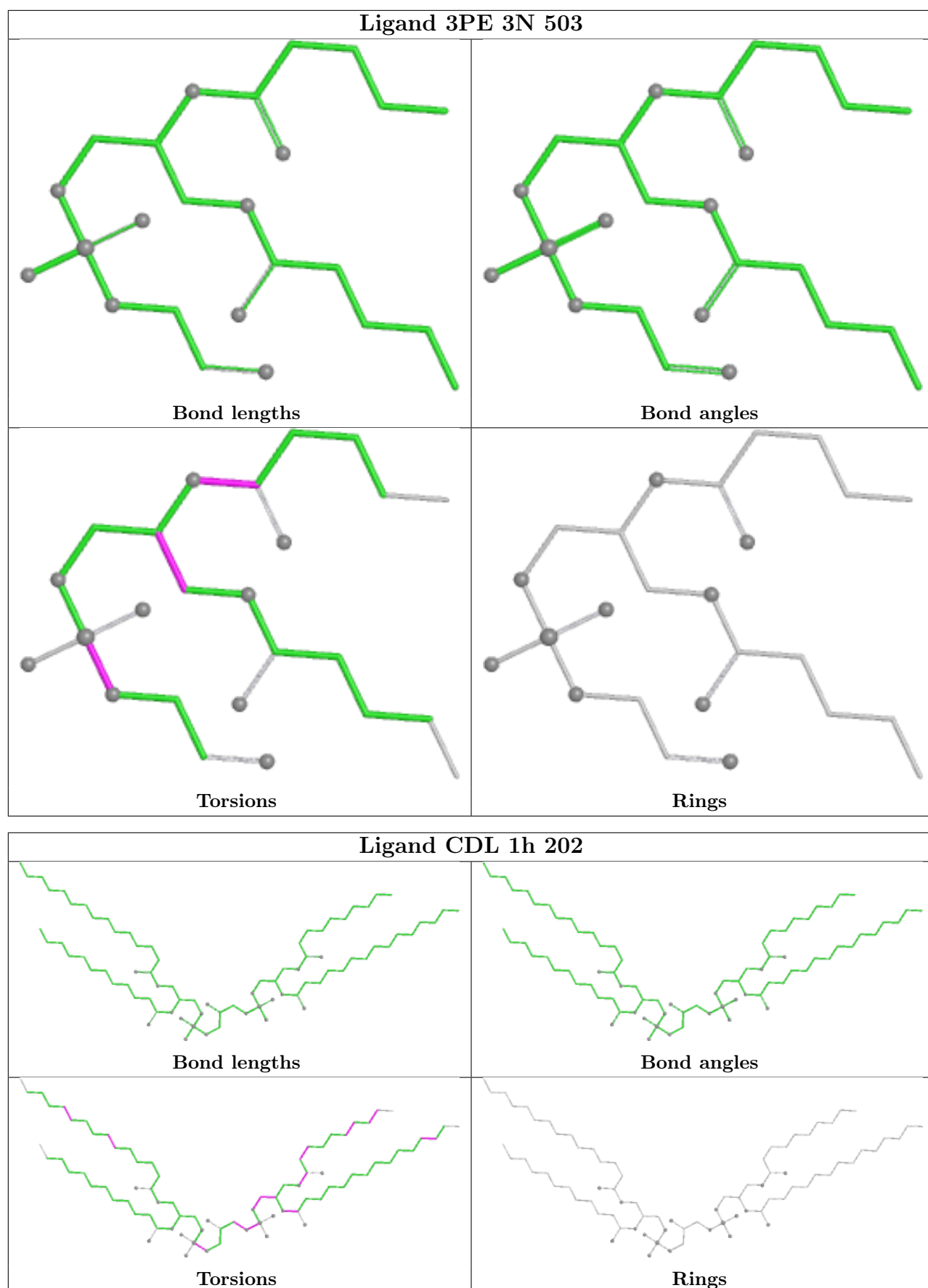


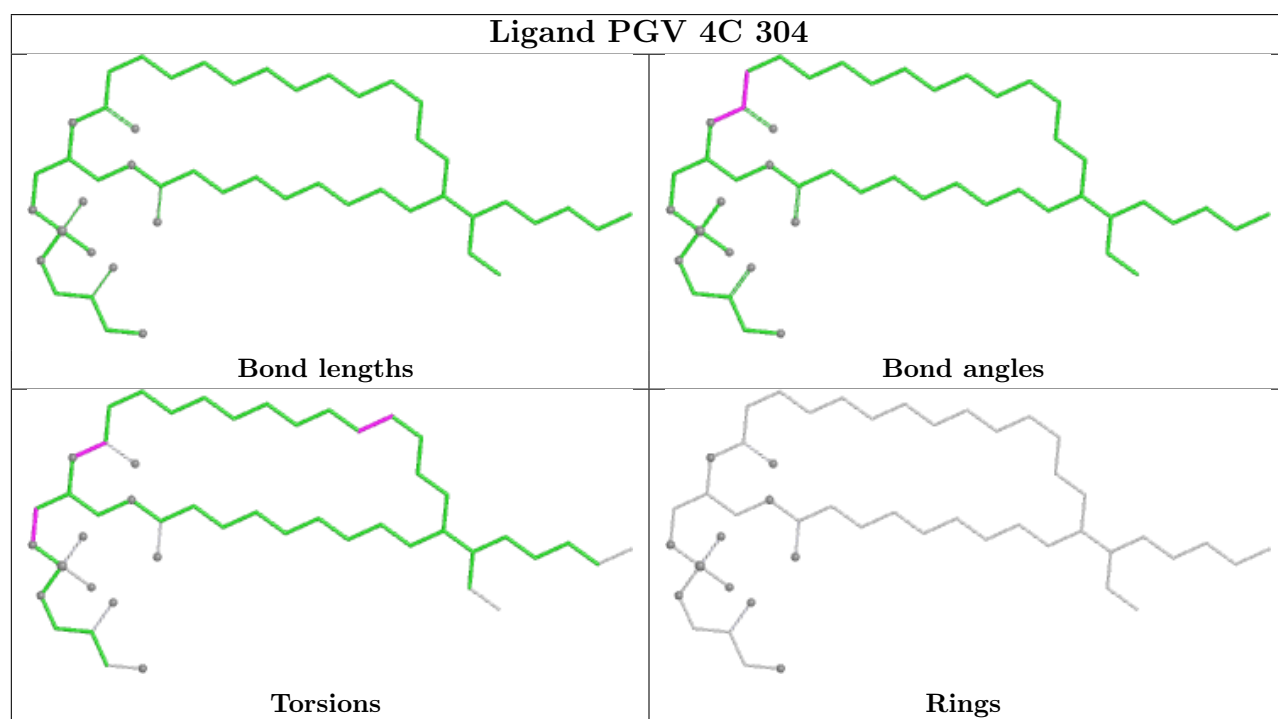
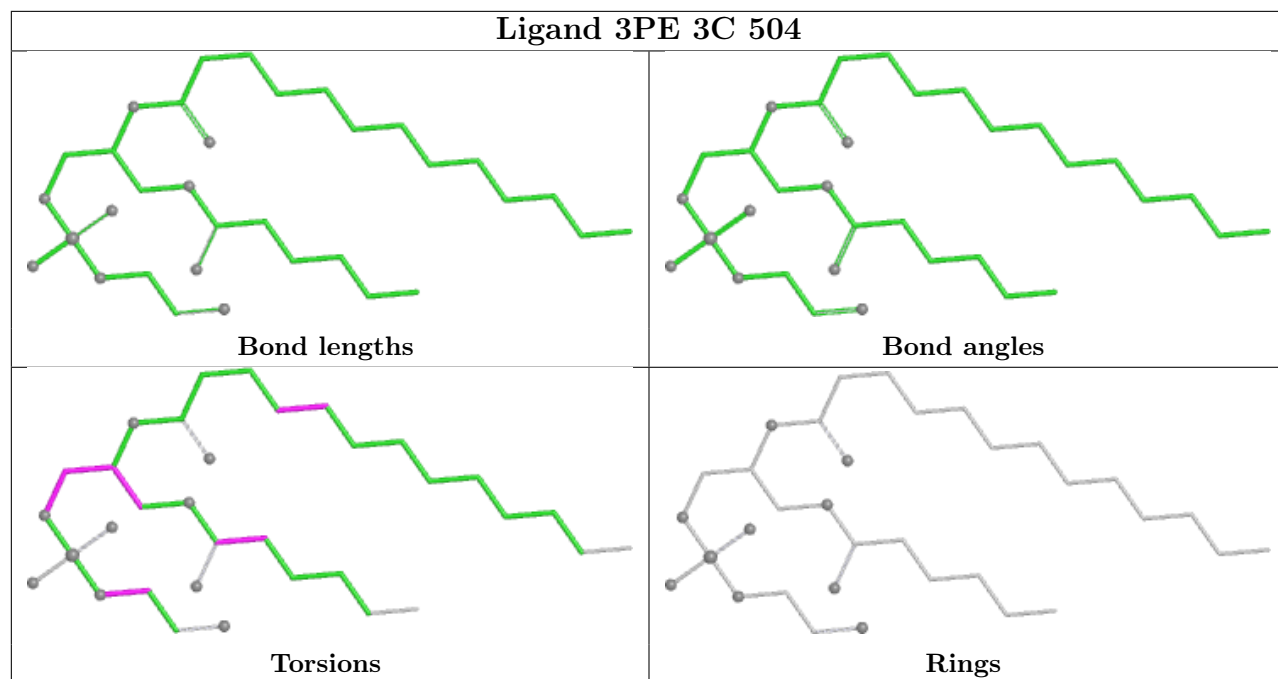


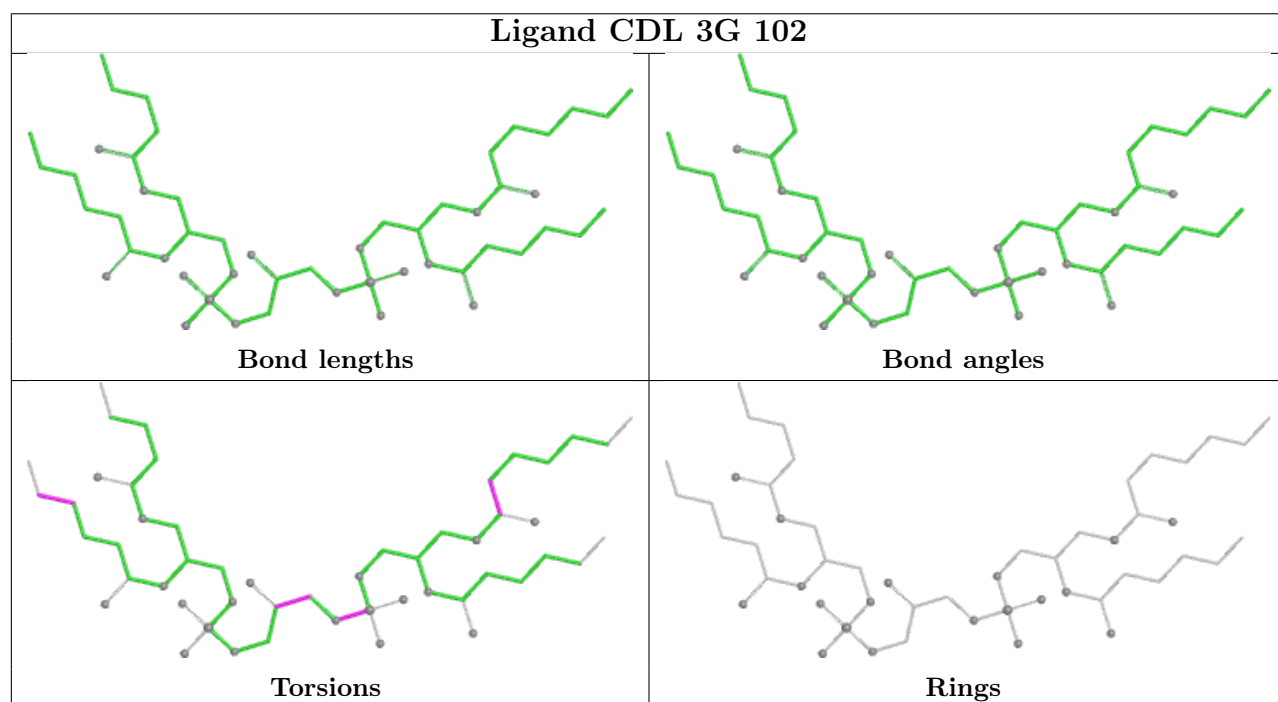
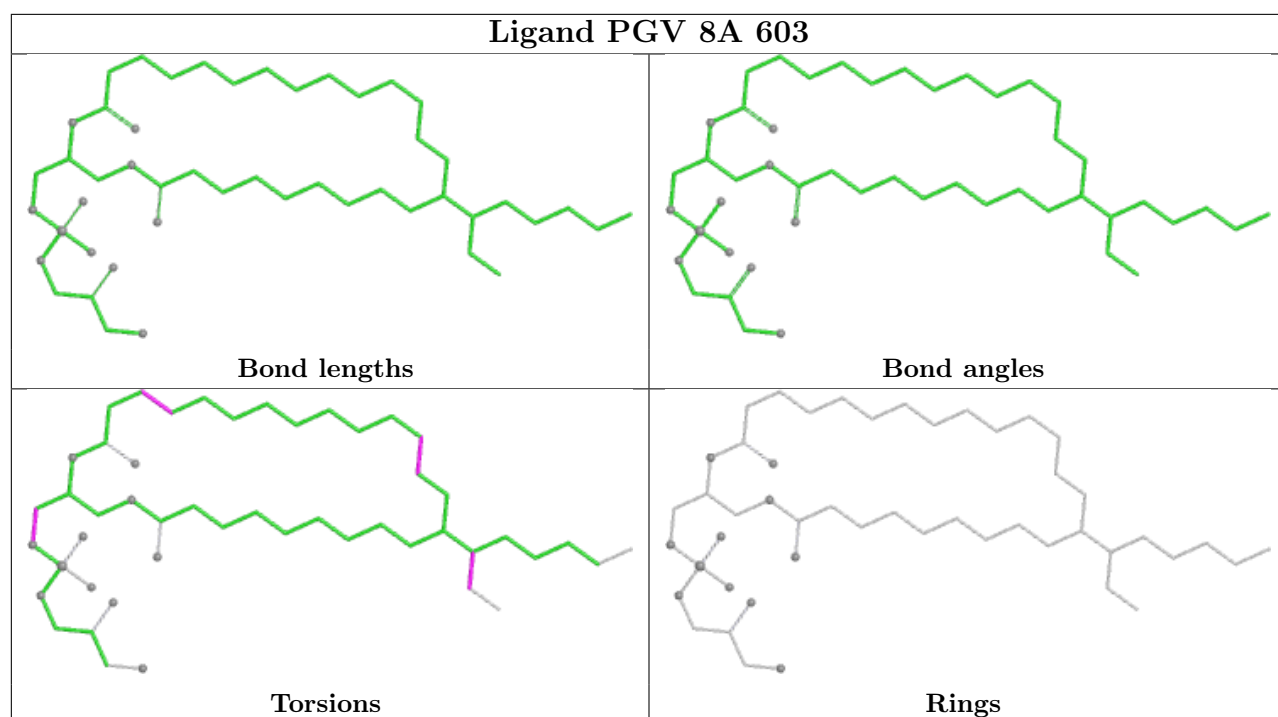


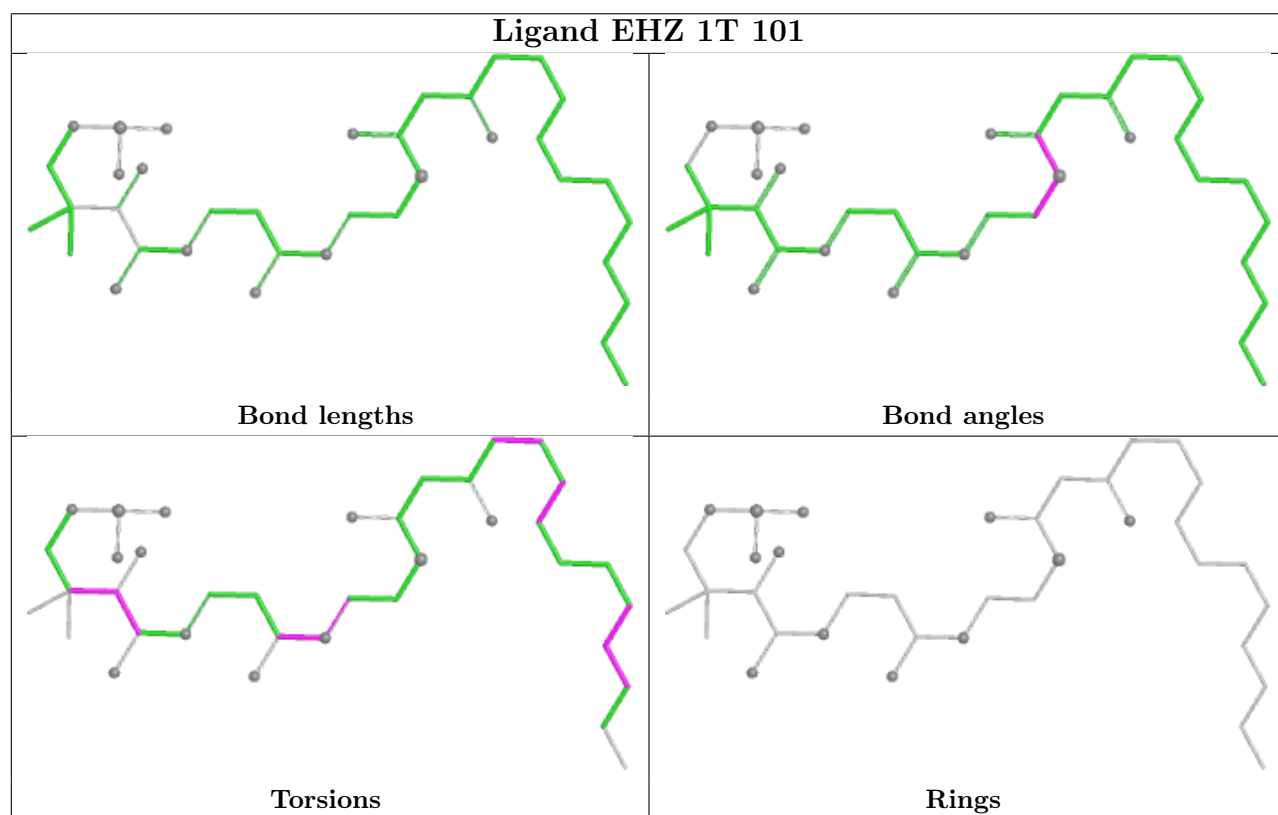
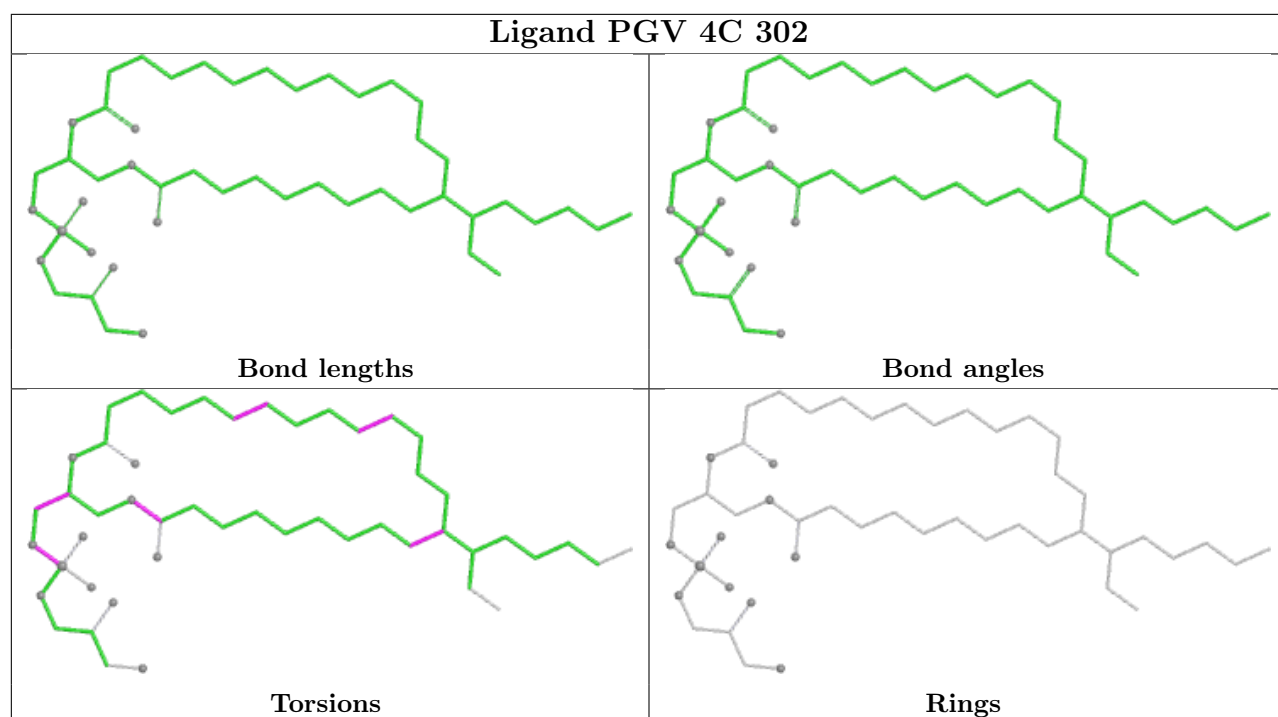


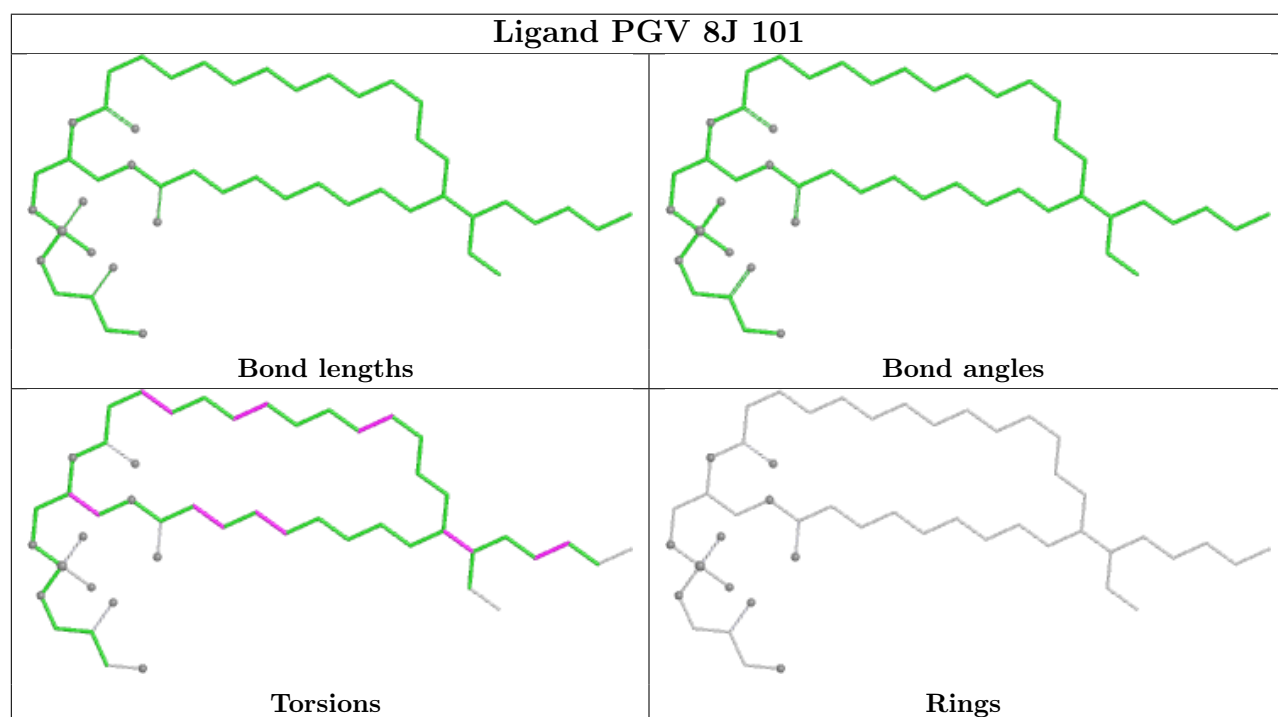
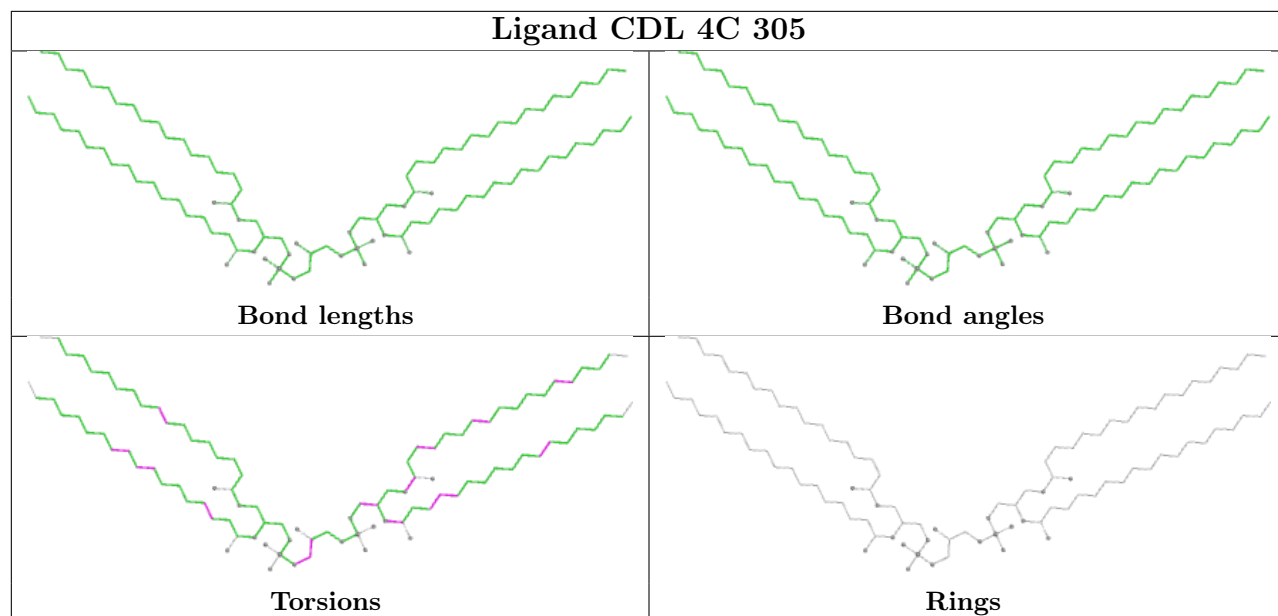


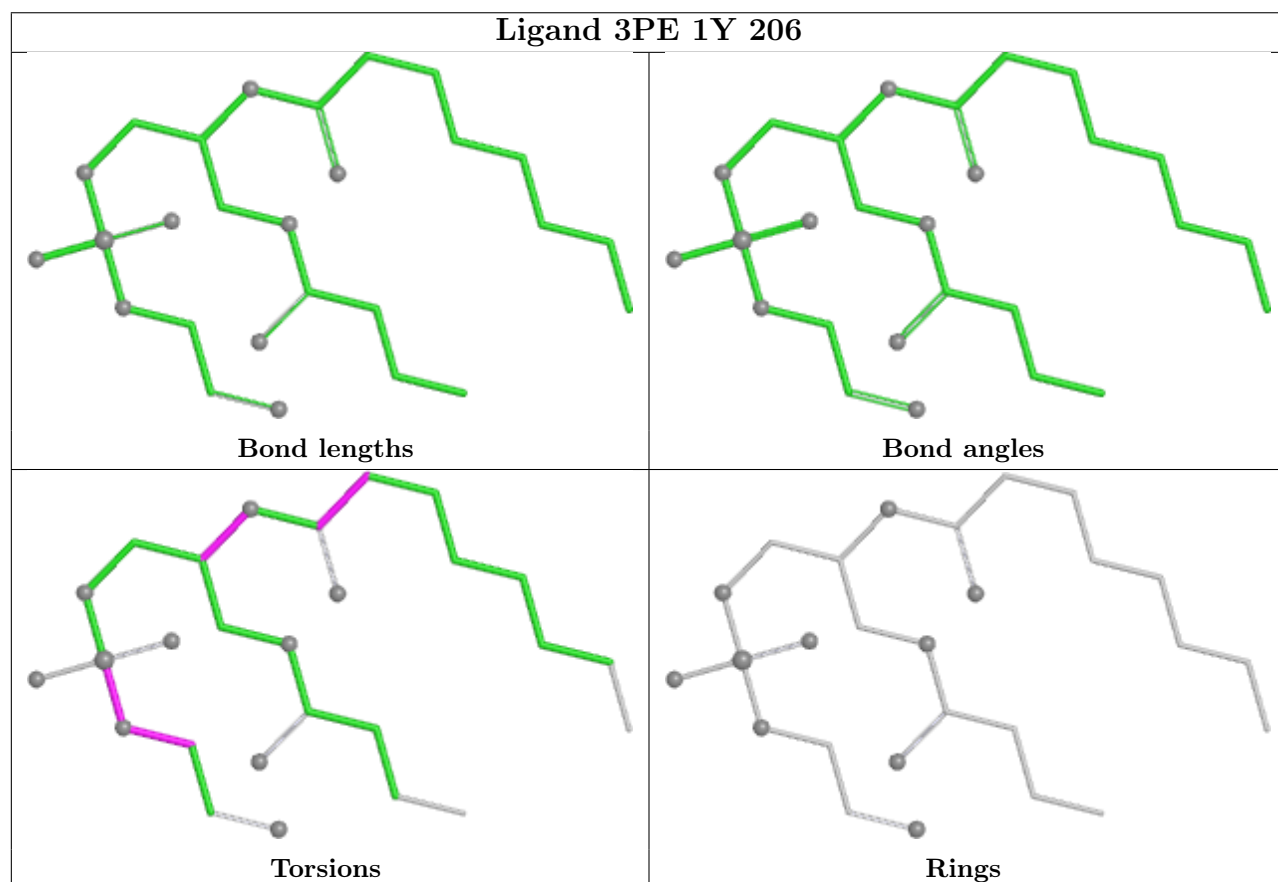
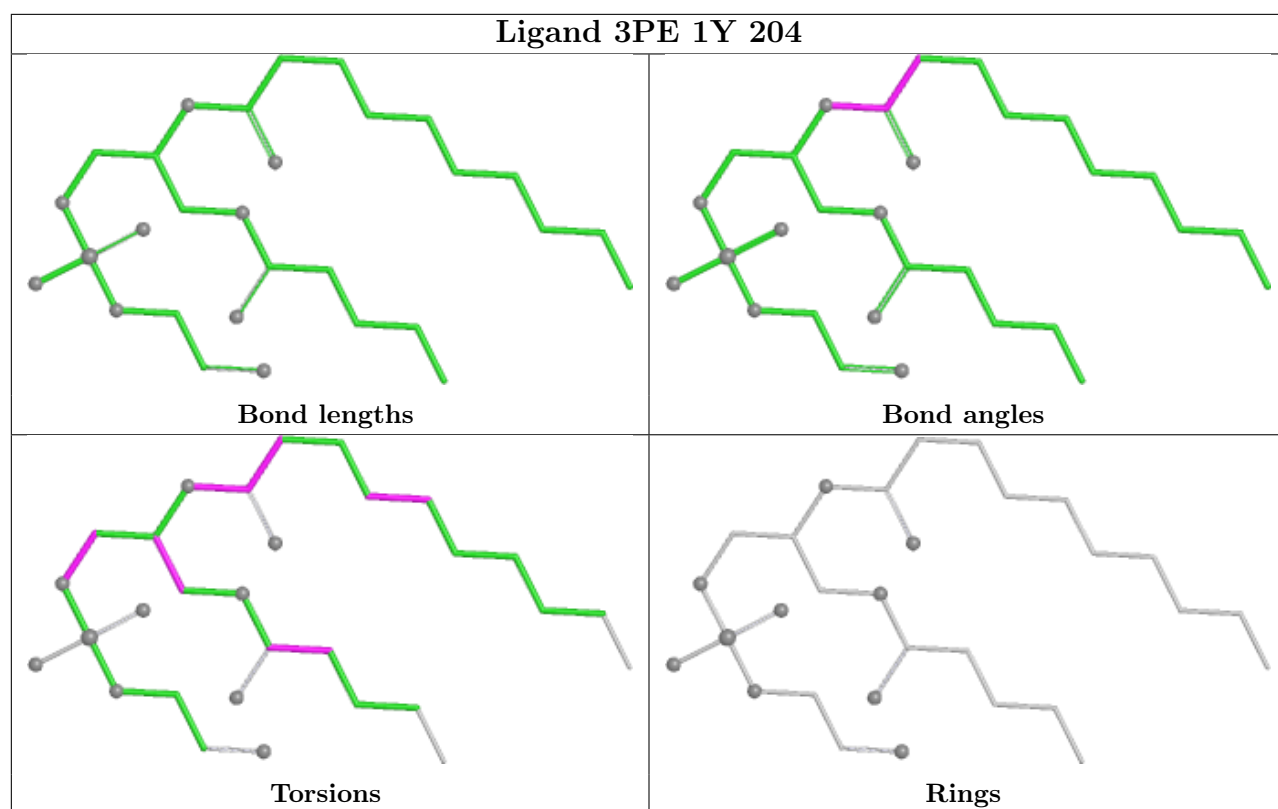


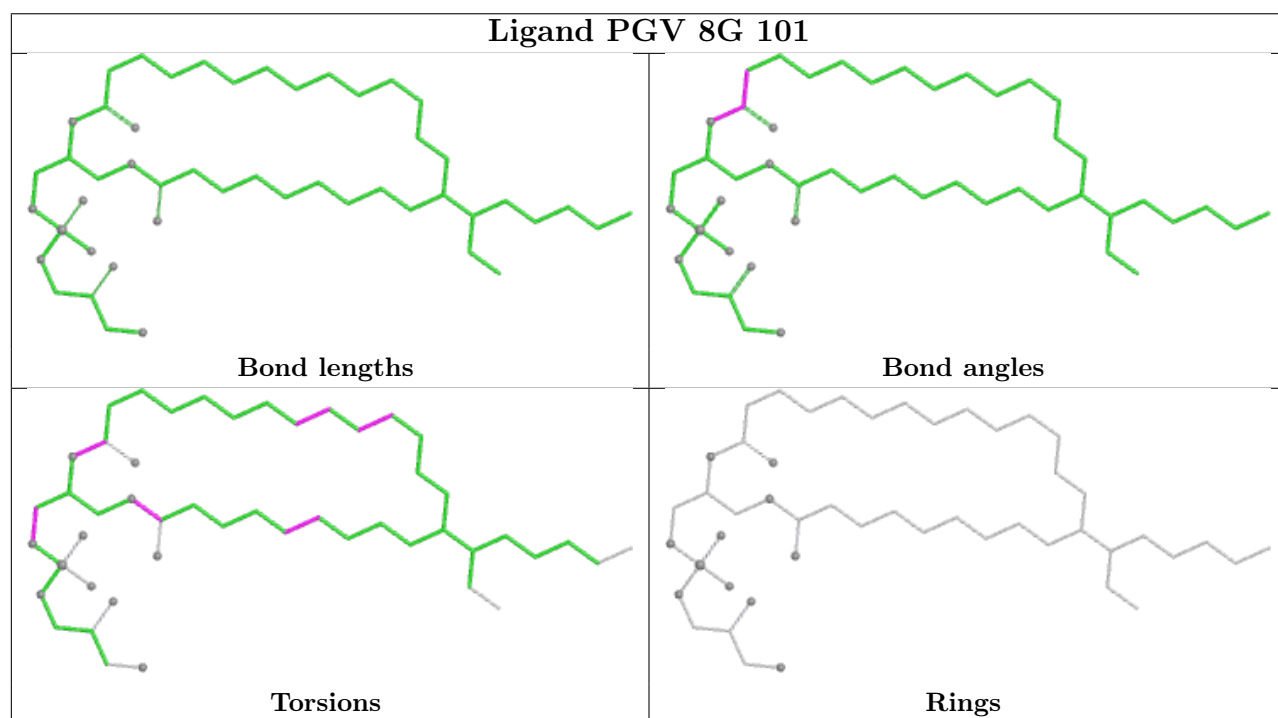
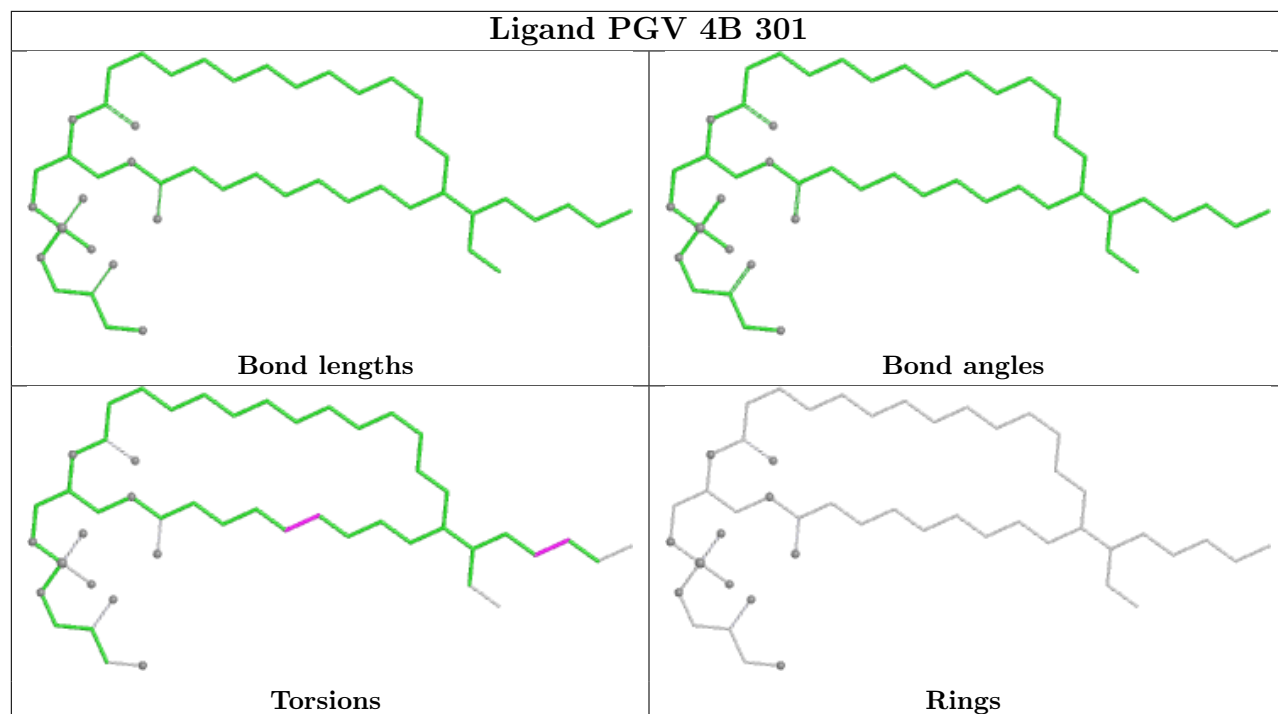


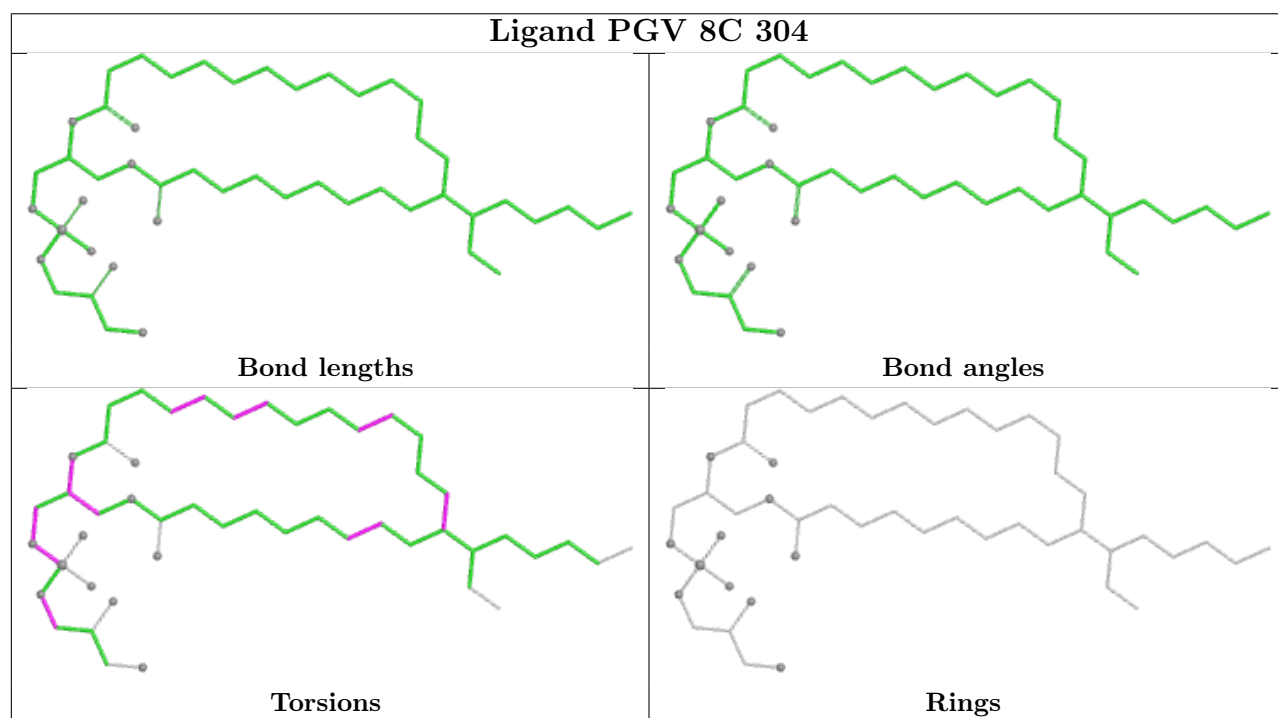
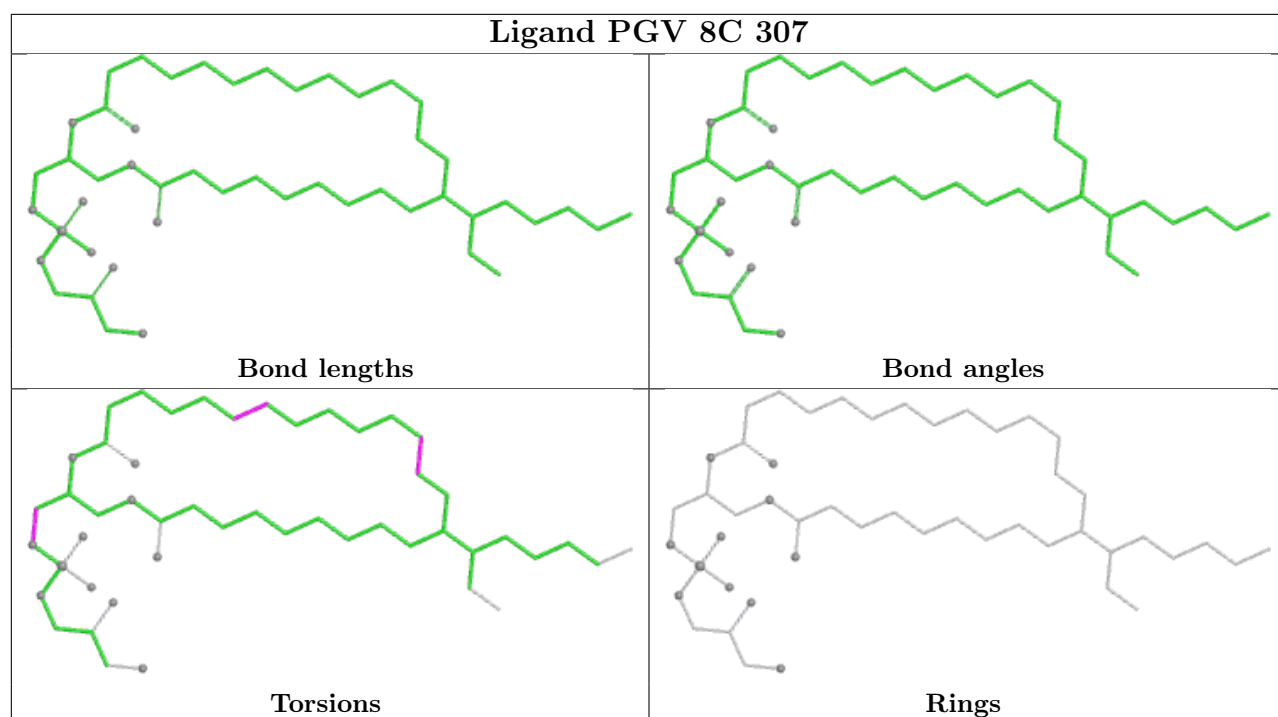




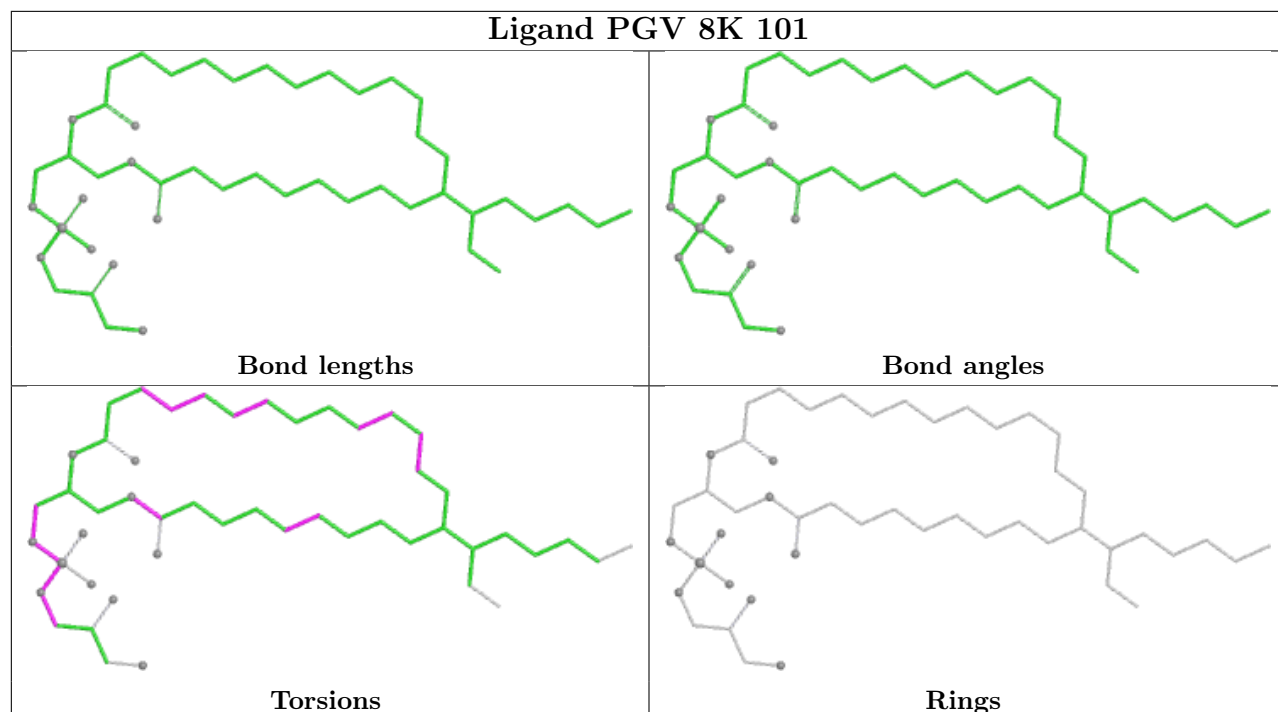




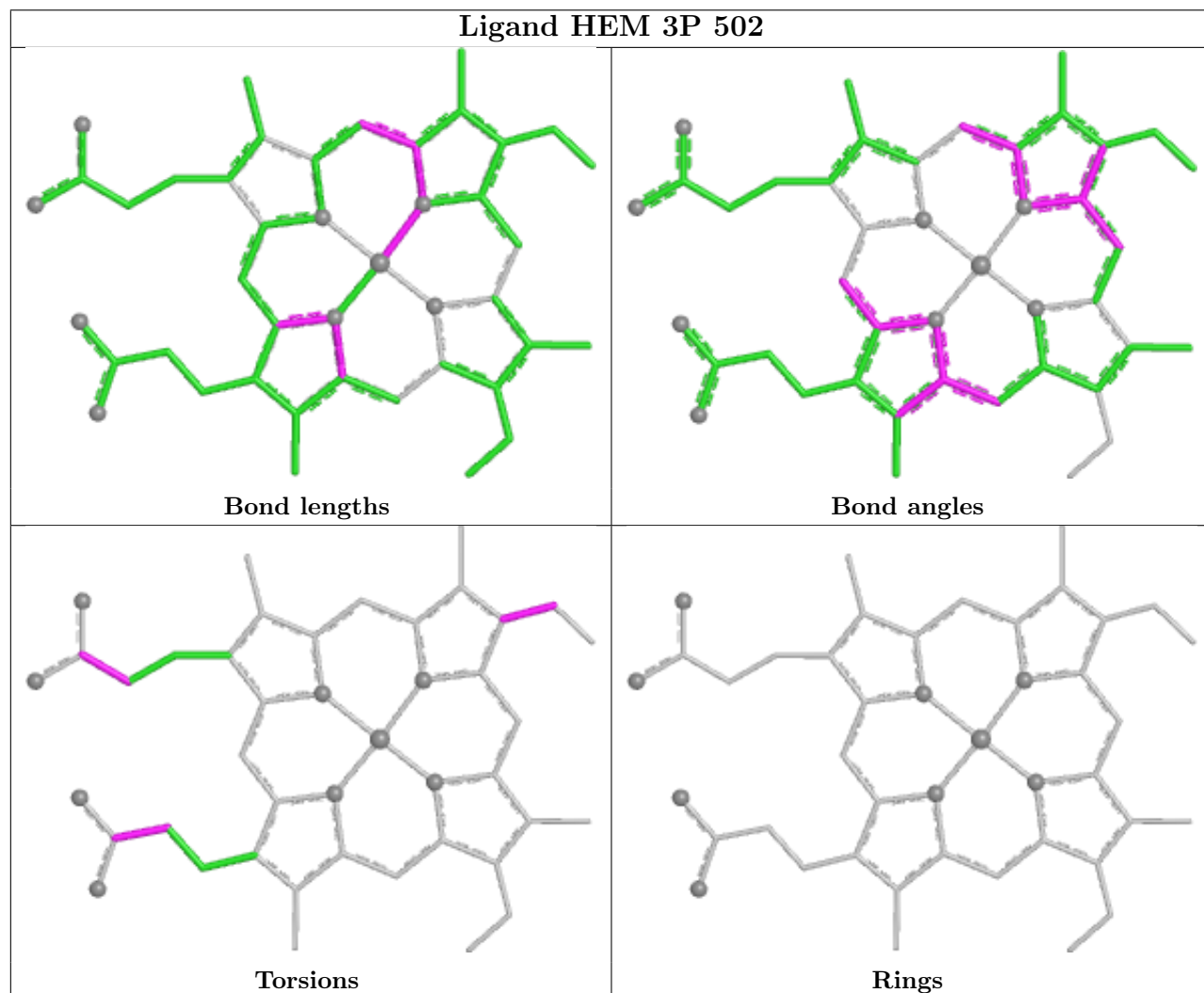


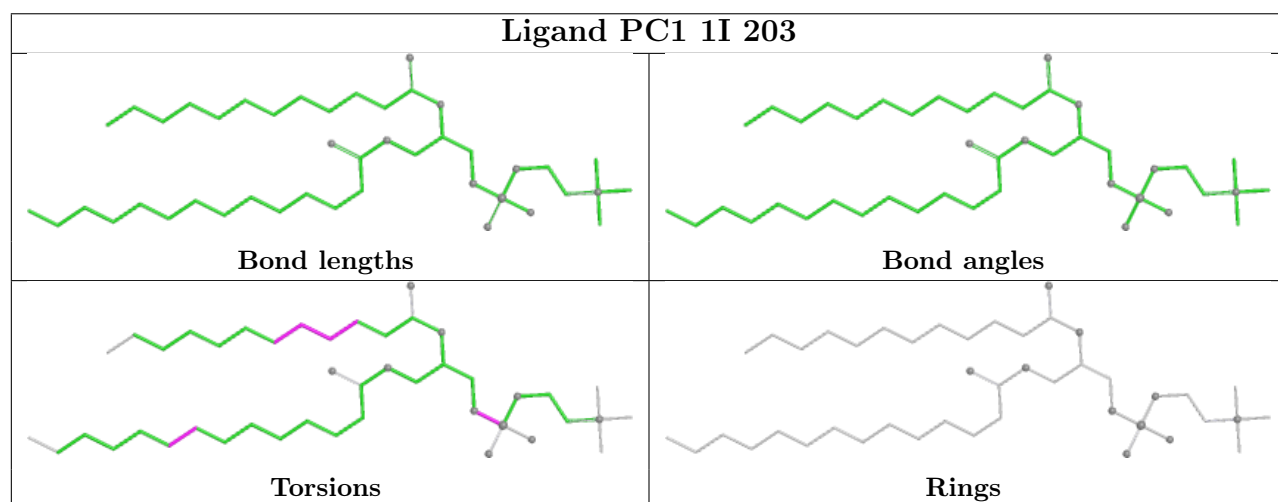
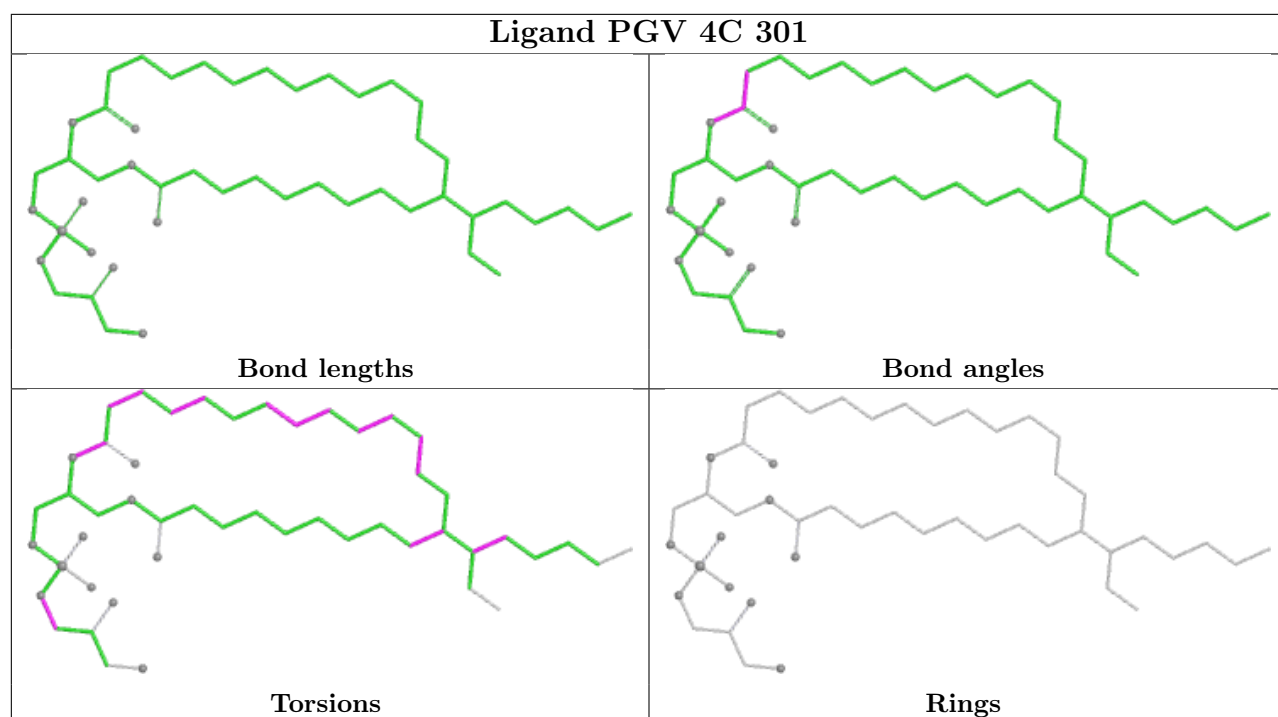


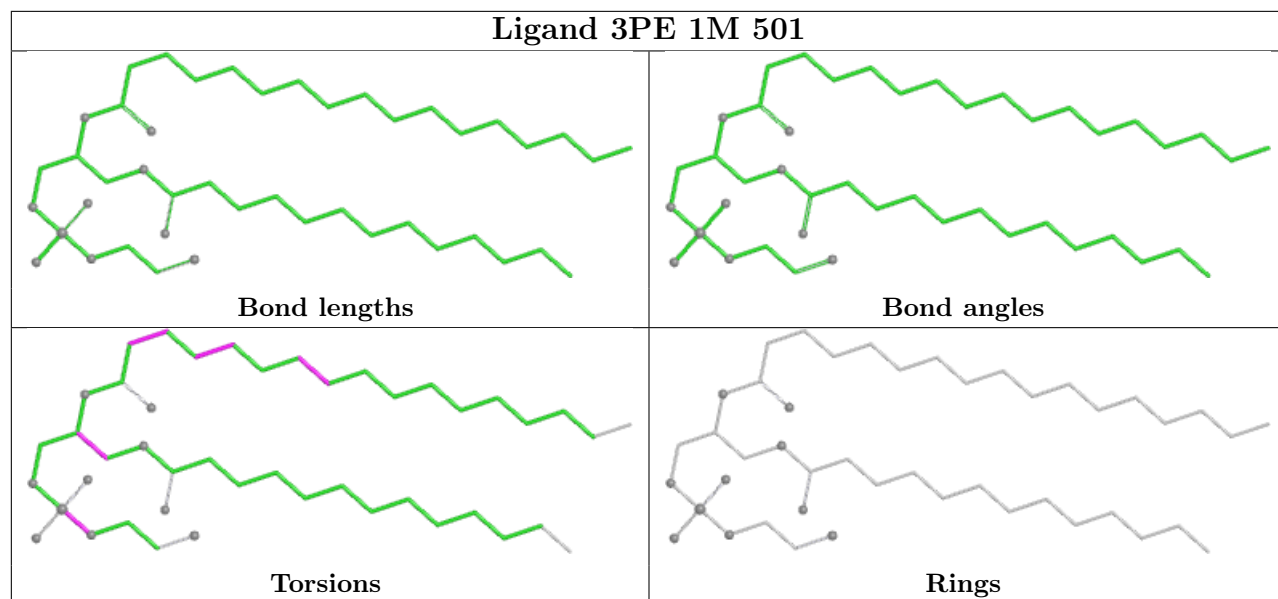
Ligand PGV 8K 101



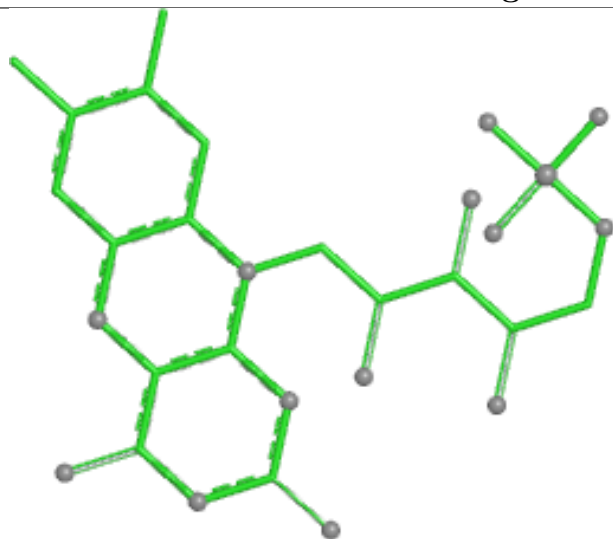
Ligand HEM 3P 502



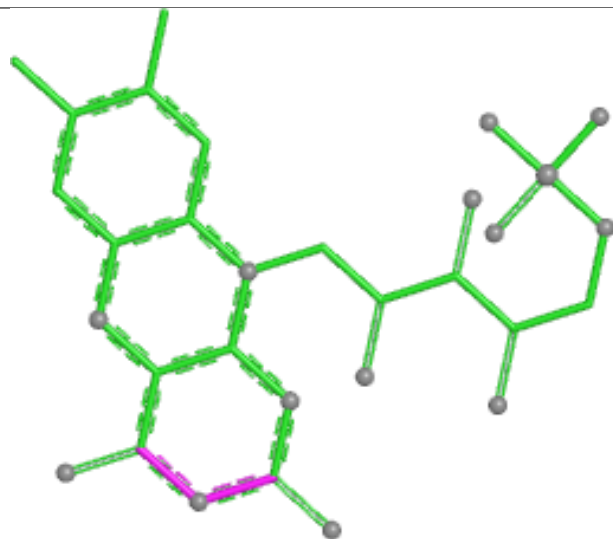




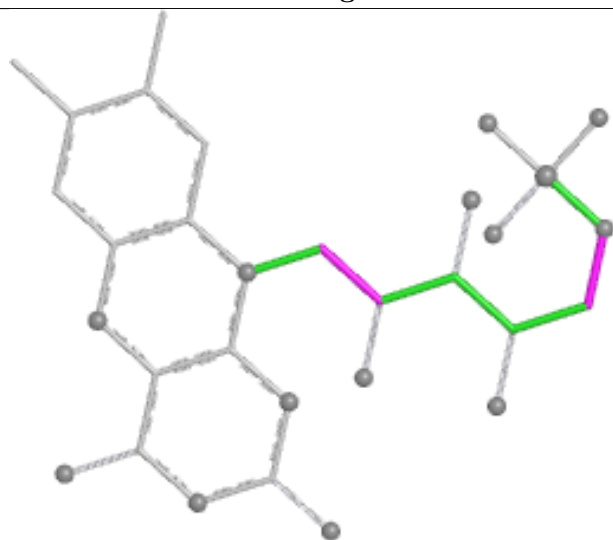
Ligand FMN 1F 501



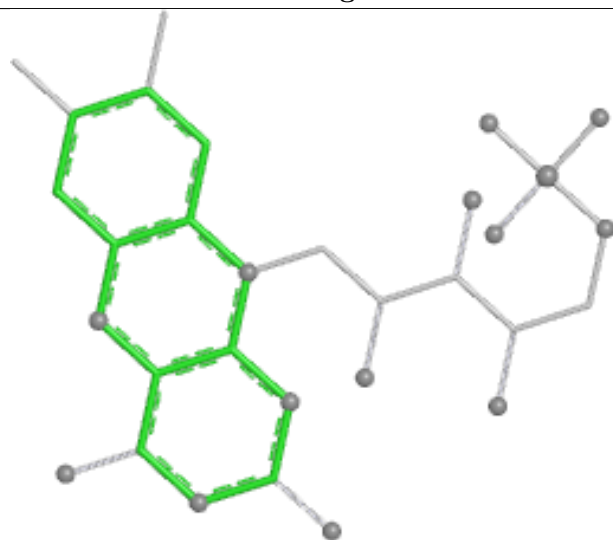
Bond lengths



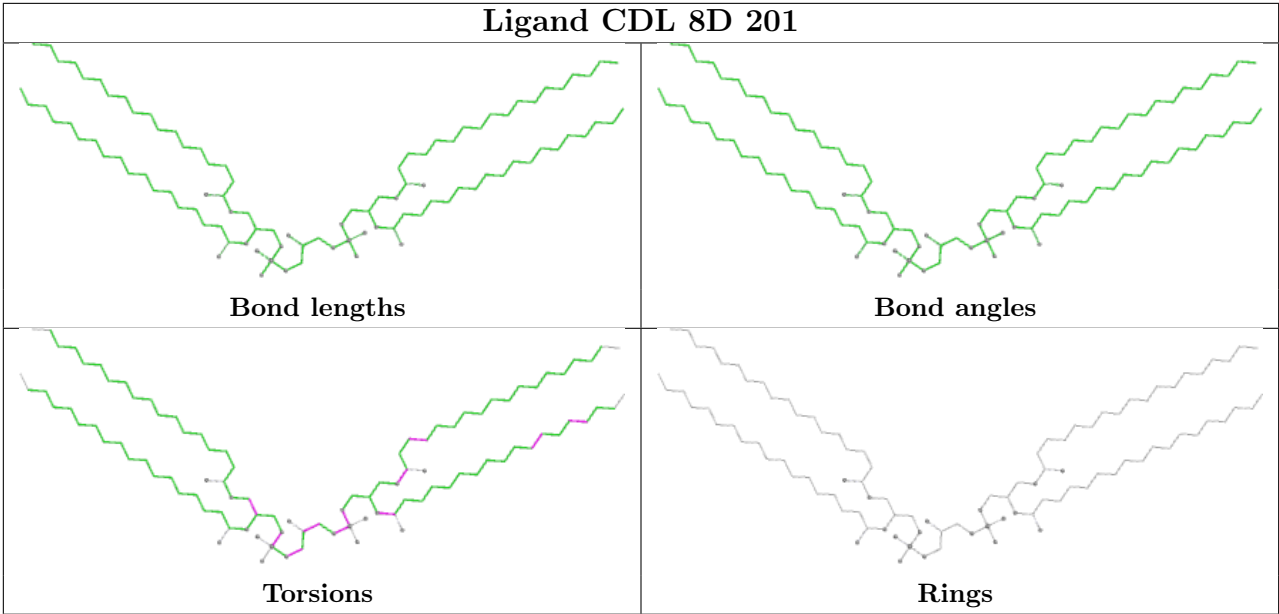
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	3V	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3V	49:VAL	C	50:LEU	N	1.69
1	3V	48:SER	C	49:VAL	N	1.19

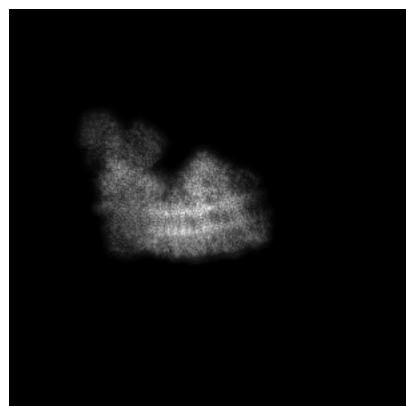
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42227. These allow visual inspection of the internal detail of the map and identification of artifacts.

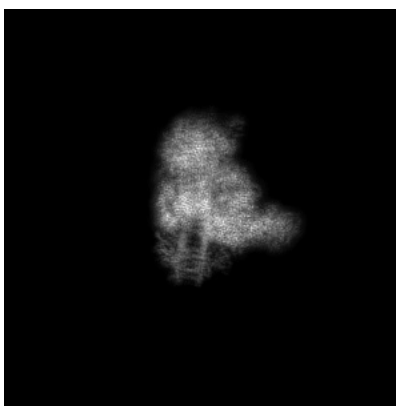
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

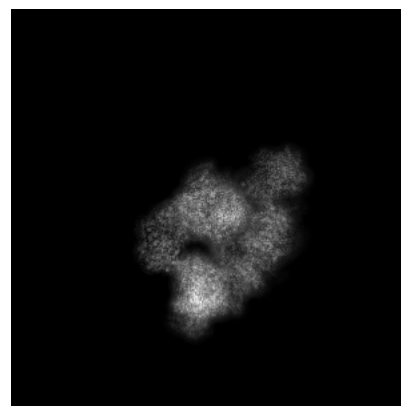
6.1.1 Primary map



X

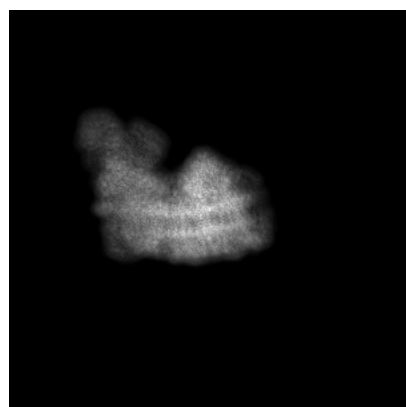


Y

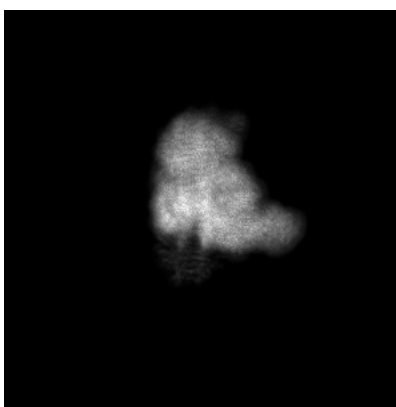


Z

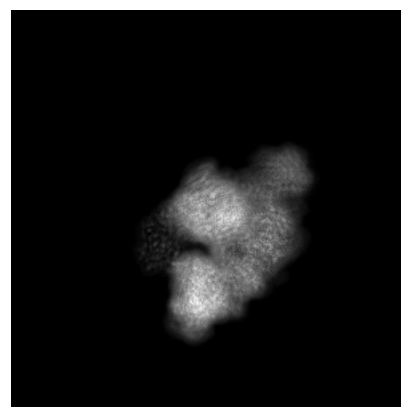
6.1.2 Raw map



X



Y

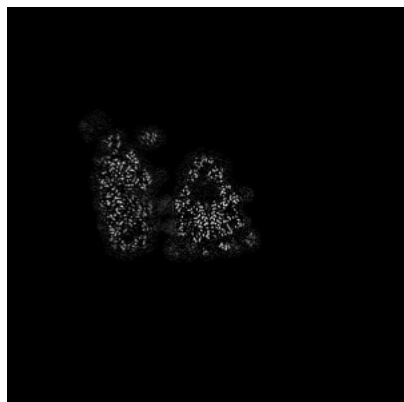


Z

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

6.2 Central slices [i](#)

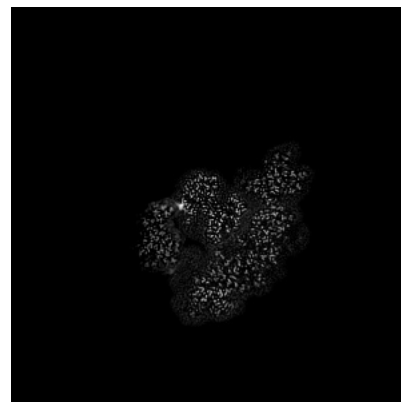
6.2.1 Primary map



X Index: 275

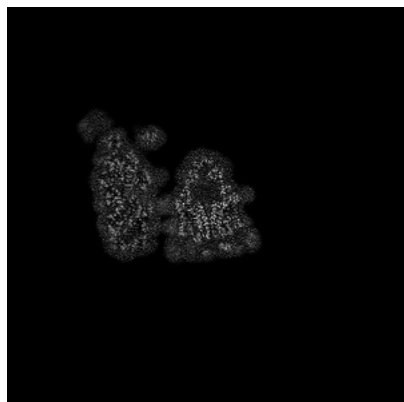


Y Index: 275

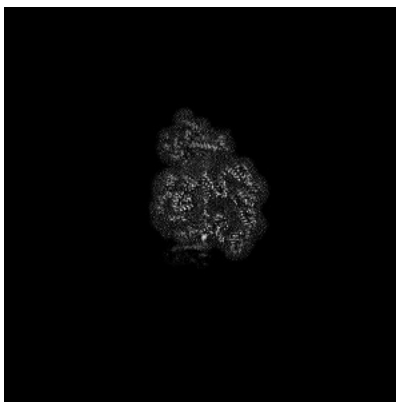


Z Index: 275

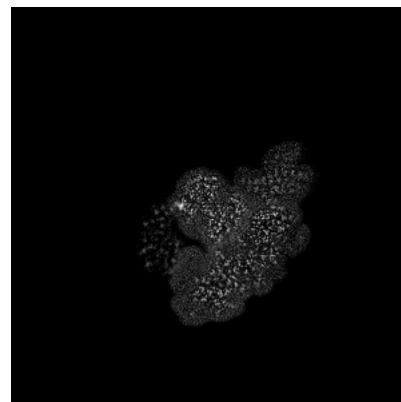
6.2.2 Raw map



X Index: 275



Y Index: 275

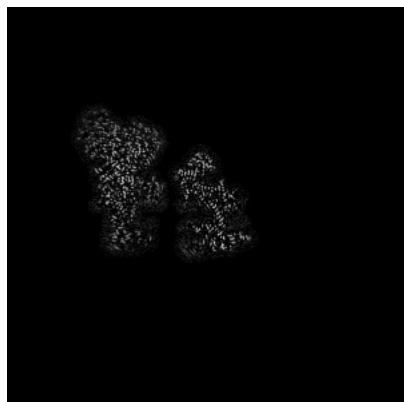


Z Index: 275

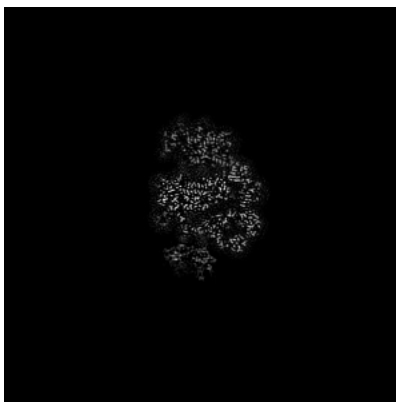
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

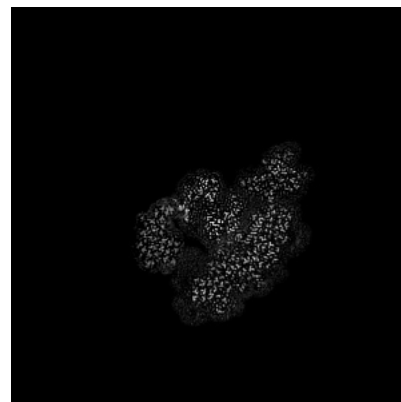
6.3.1 Primary map



X Index: 256

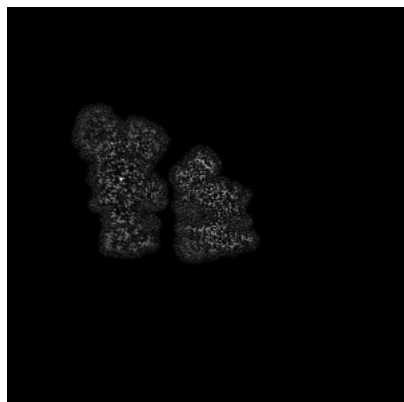


Y Index: 264

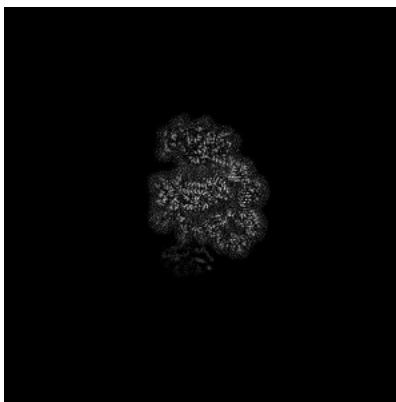


Z Index: 272

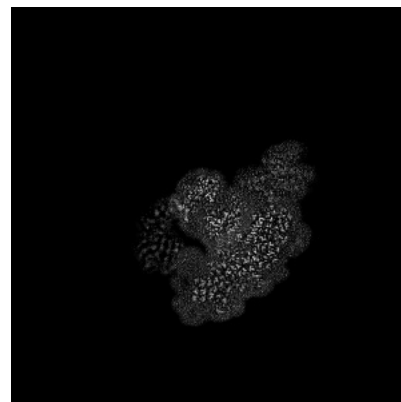
6.3.2 Raw map



X Index: 260



Y Index: 264

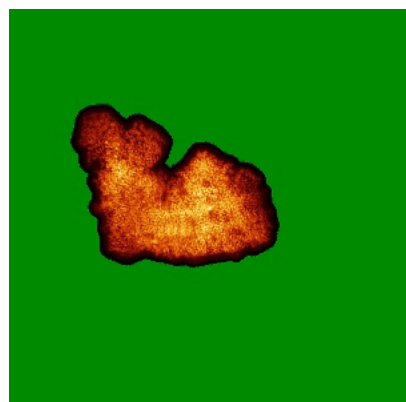


Z Index: 272

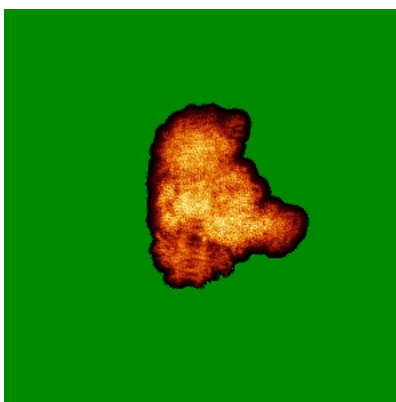
The images above show the largest variance slices of the map in three orthogonal directions.

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

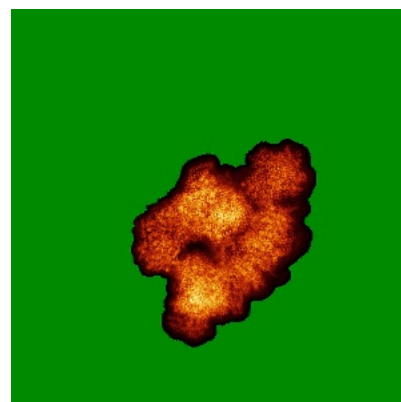
6.4.1 Primary map



X

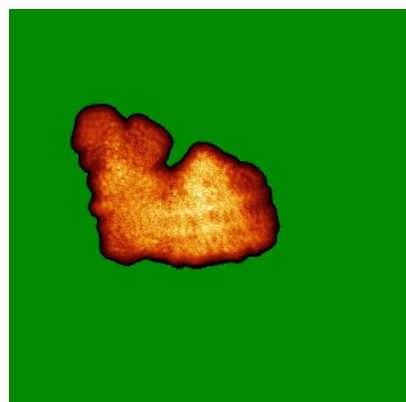


Y

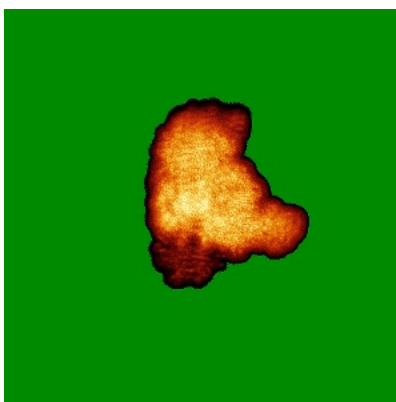


Z

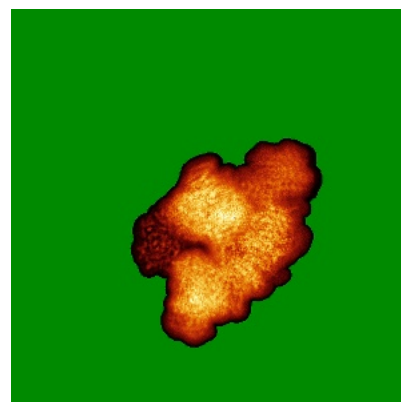
6.4.2 Raw map



X



Y

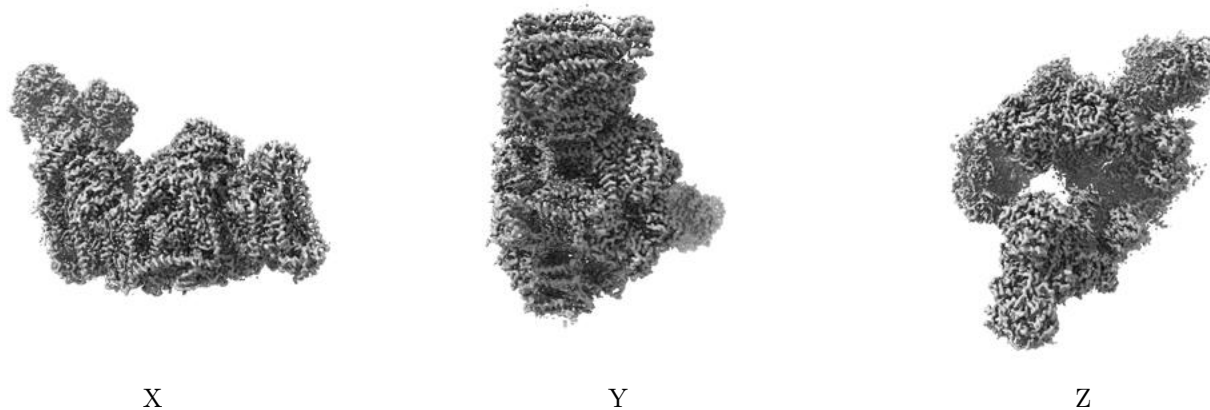


Z

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.

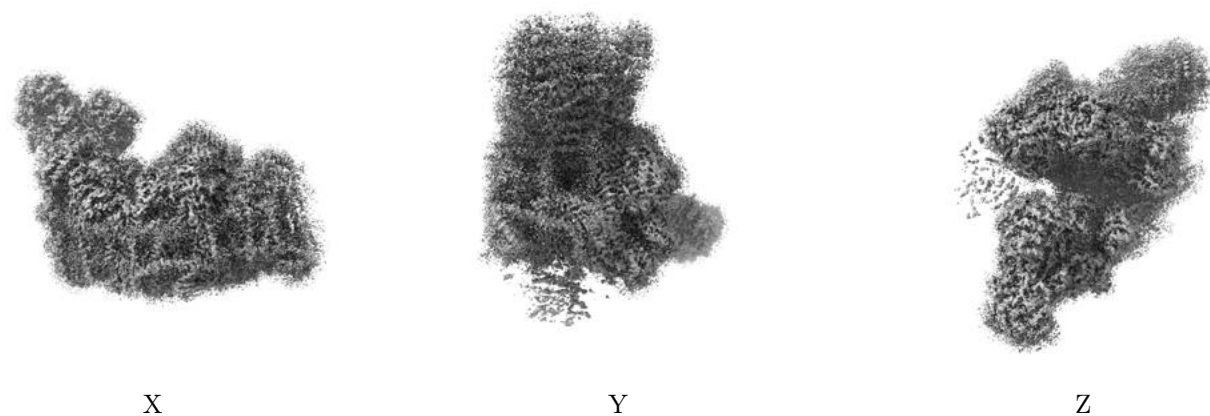
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

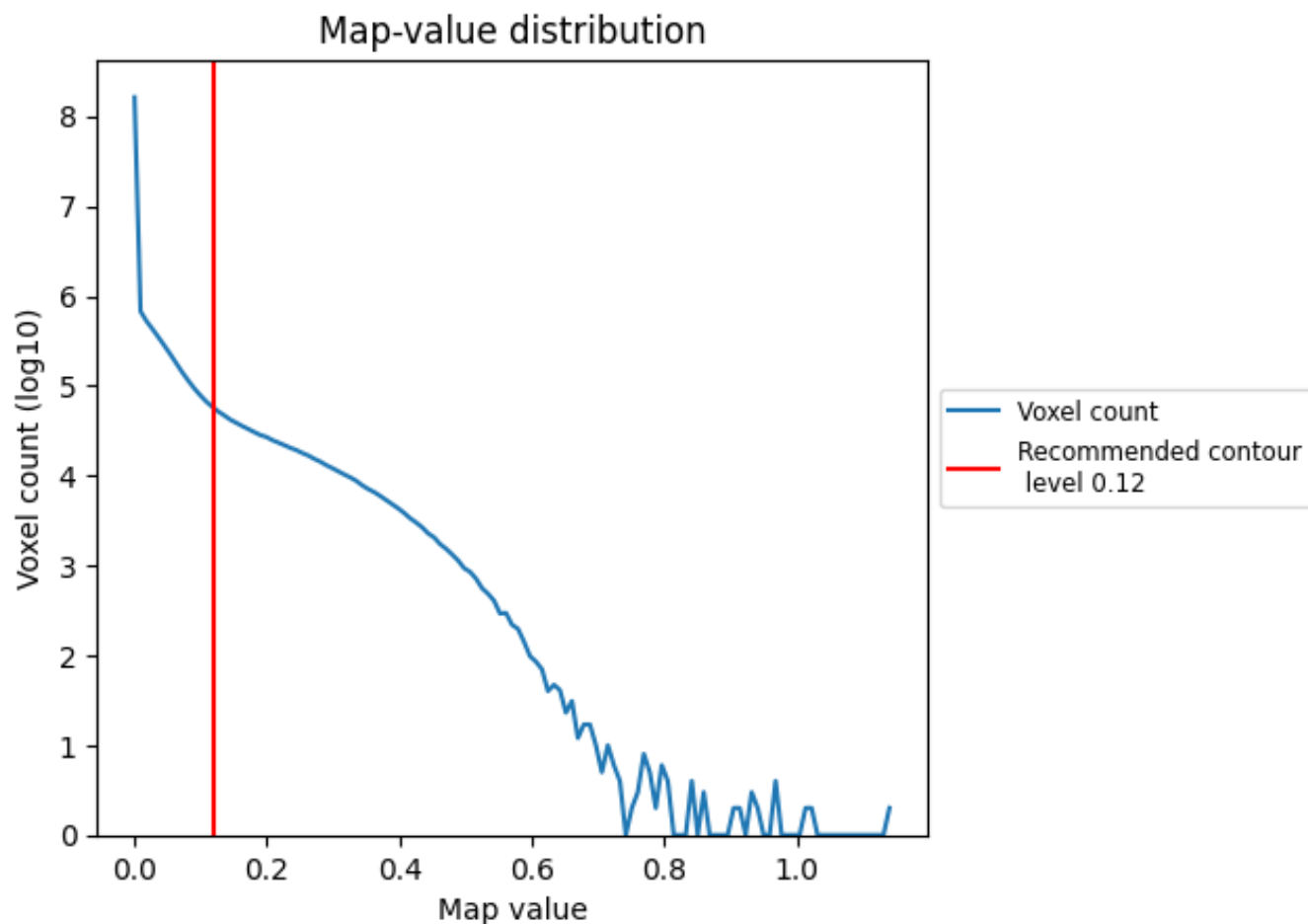
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

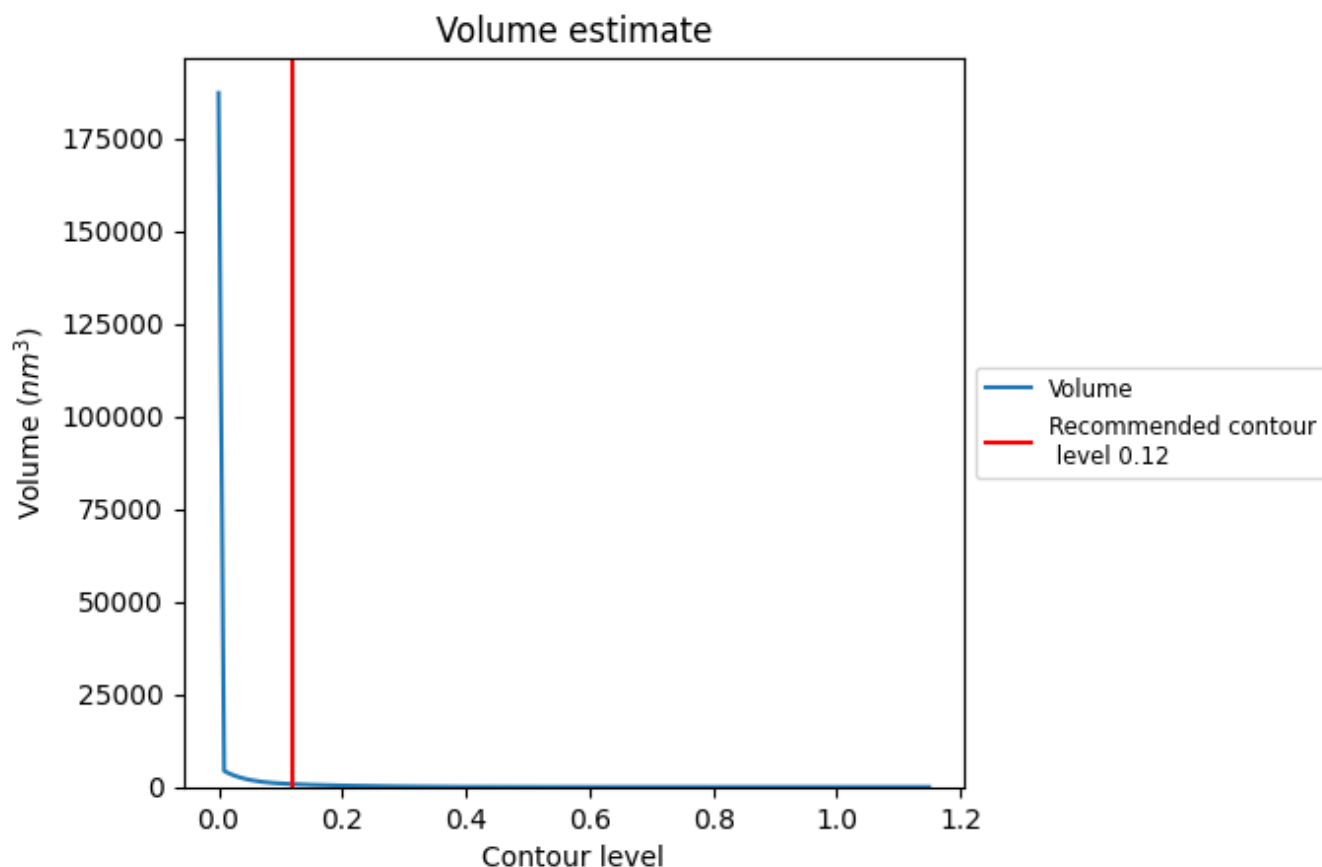
This section contains the results of statistical analysis of the map.

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.

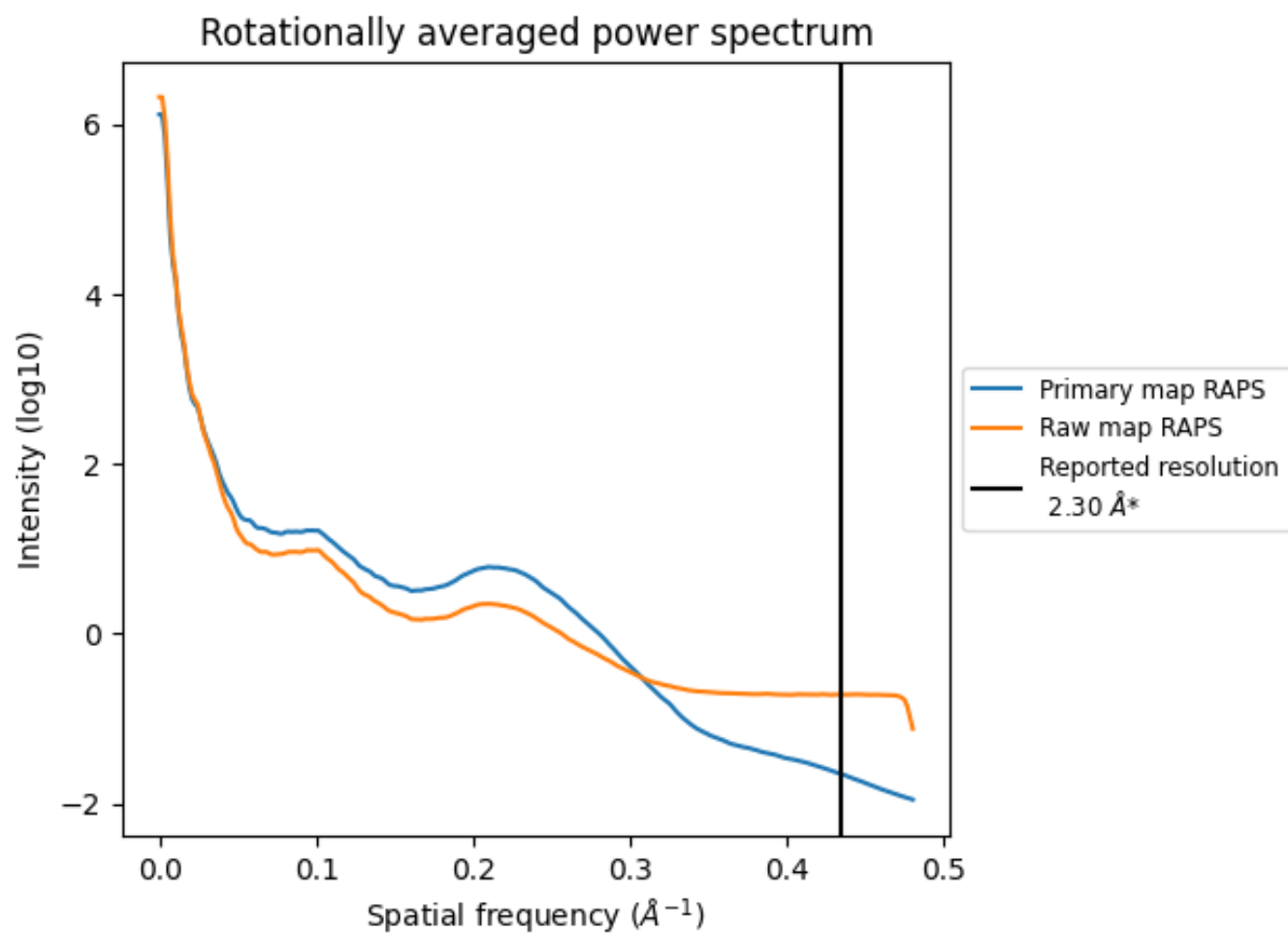
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm^3 ; this corresponds to an approximate mass of 696 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 ⓘ

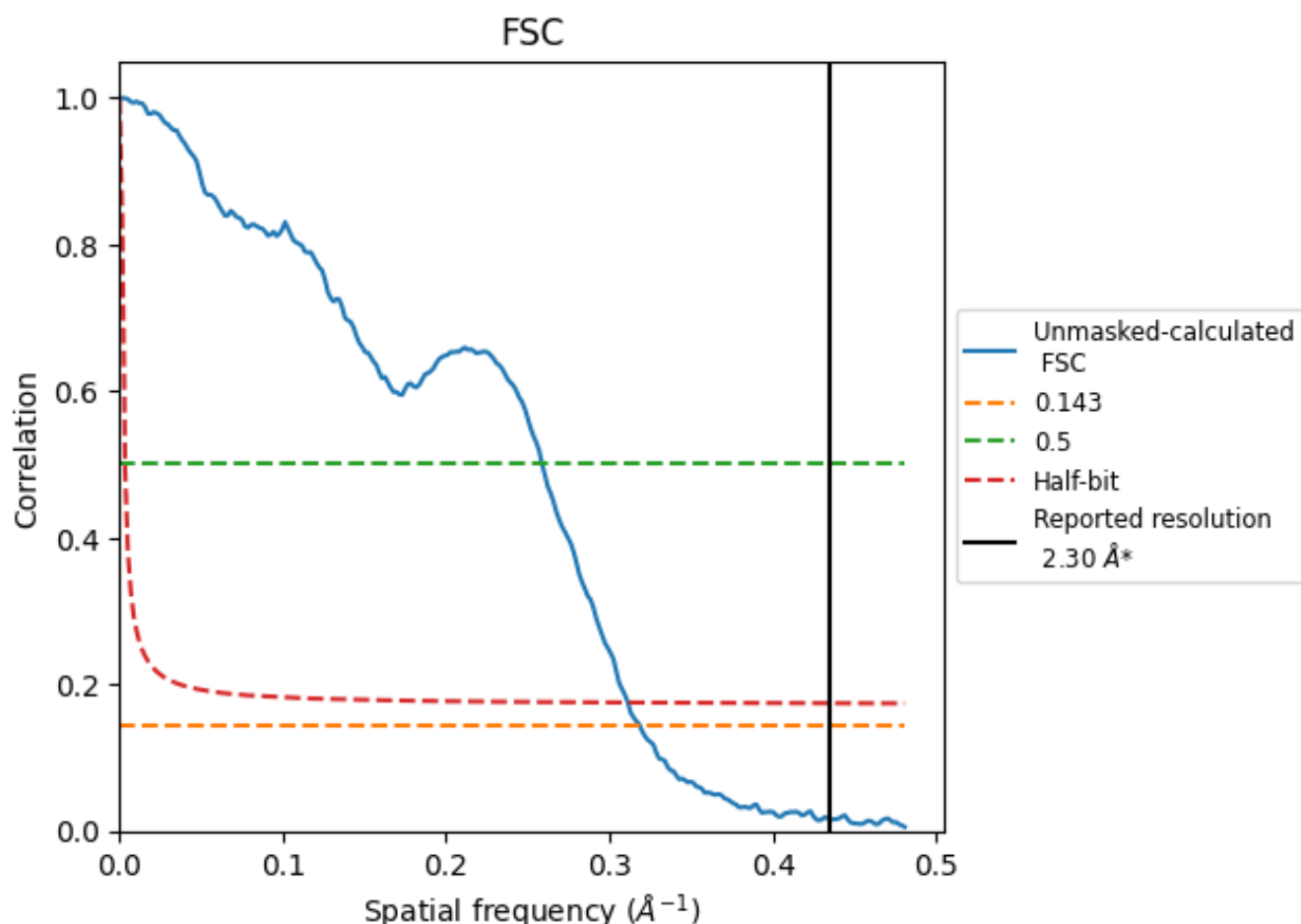


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

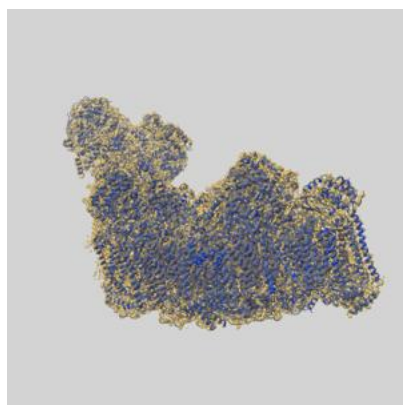
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.86	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.3 by more than 10 %

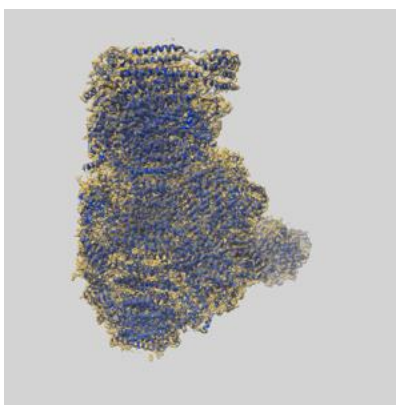
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42227 and PDB model 8UGJ. Per-residue inclusion information can be found in section 3 on page 38.

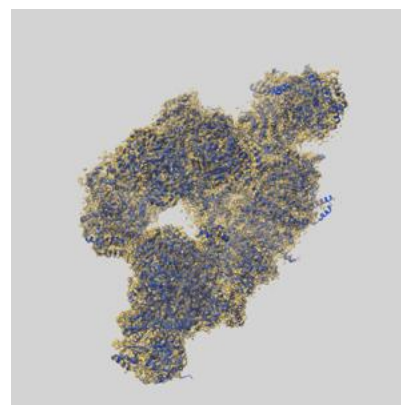
9.1 Map-model overlay [i](#)



X



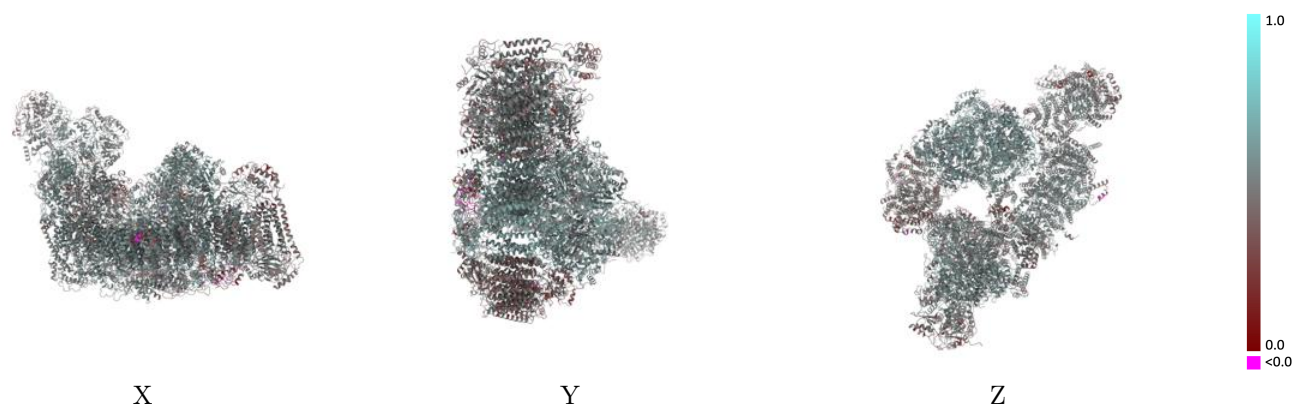
Y



Z

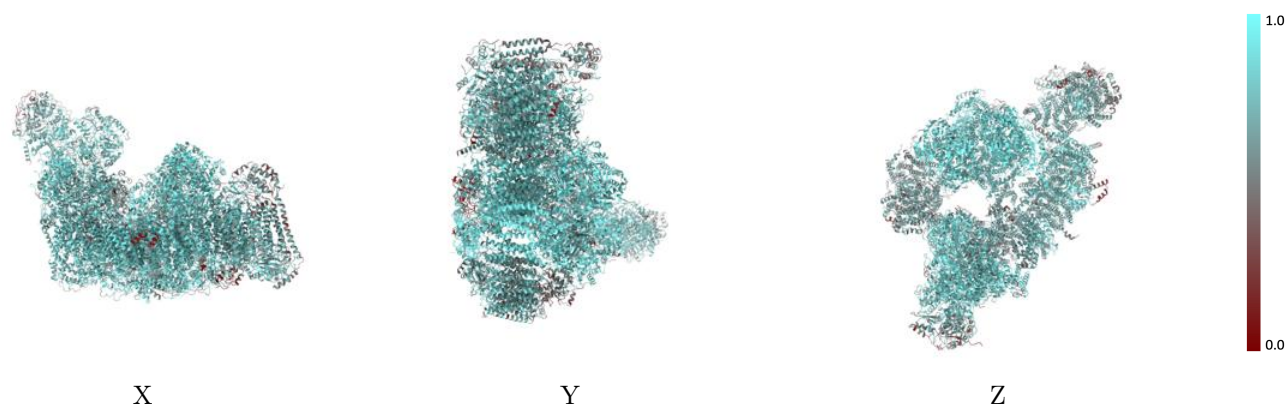
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



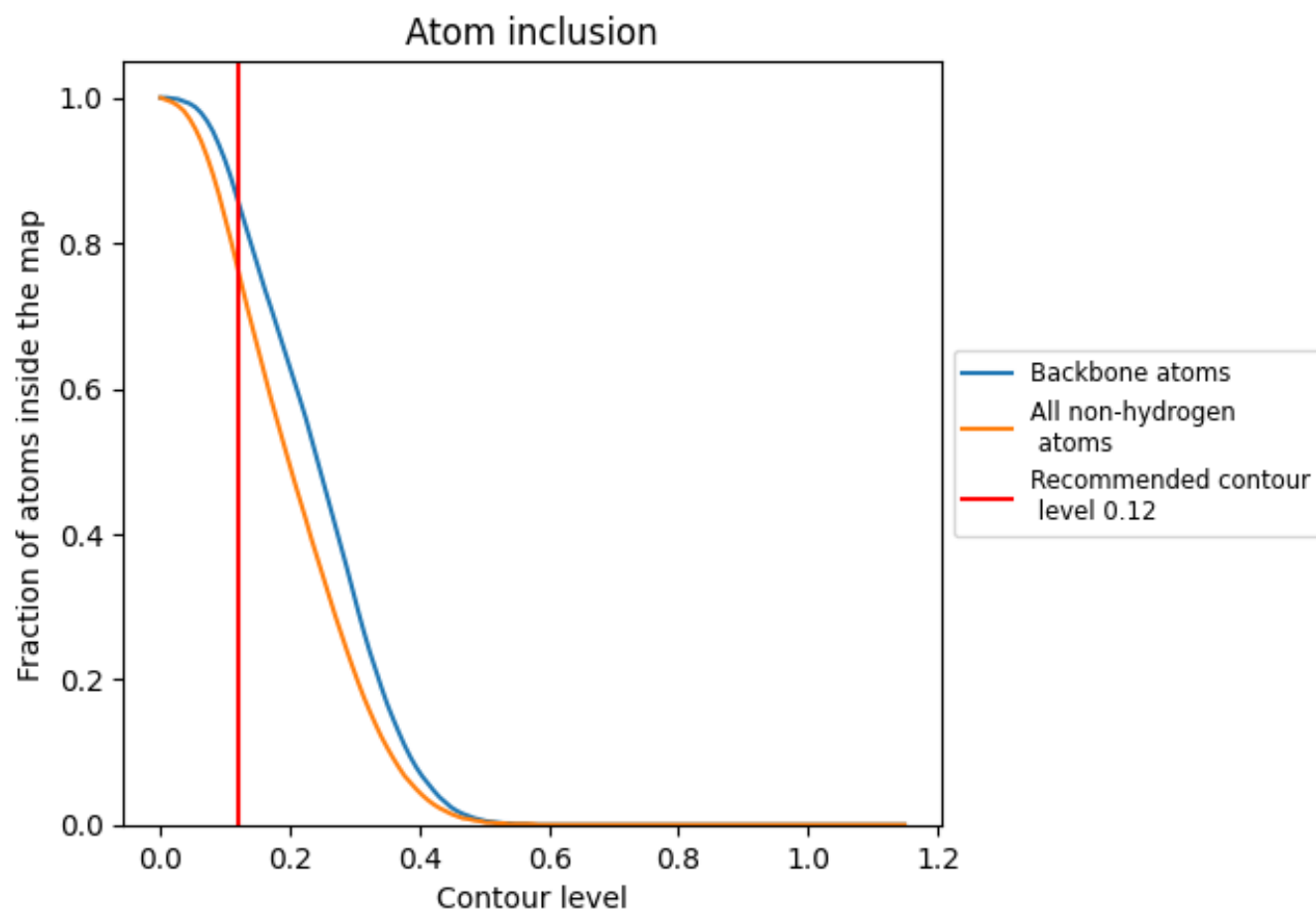
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.4950
1A	 0.6590	 0.4580
1B	 0.8660	 0.5350
1C	 0.8720	 0.5560
1D	 0.8450	 0.5410
1E	 0.6430	 0.4590
1F	 0.6550	 0.4660
1G	 0.8050	 0.5150
1H	 0.8060	 0.5140
1I	 0.8950	 0.5560
1J	 0.6710	 0.4620
1K	 0.7730	 0.5060
1L	 0.8300	 0.5200
1M	 0.8490	 0.5390
1N	 0.8340	 0.5390
1O	 0.7540	 0.4680
1P	 0.7610	 0.4890
1Q	 0.7830	 0.5130
1R	 0.8030	 0.5350
1S	 0.7300	 0.4740
1T	 0.5330	 0.3490
1U	 0.7690	 0.4940
1V	 0.7410	 0.4990
1W	 0.8070	 0.5110
1X	 0.7450	 0.5010
1Y	 0.7760	 0.4830
1Z	 0.7800	 0.5210
1a	 0.8400	 0.5270
1b	 0.7490	 0.4940
1c	 0.7170	 0.4900
1d	 0.7770	 0.5180
1e	 0.7480	 0.5190
1f	 0.6950	 0.4990
1g	 0.7700	 0.5060
1h	 0.7590	 0.5160









































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Chain	Atom inclusion	Q-score
1i	 0.5600	 0.4240
1j	 0.6760	 0.4540
1k	 0.6750	 0.4500
1l	 0.8060	 0.5080
1m	 0.8060	 0.5160
1n	 0.8200	 0.5110
1o	 0.7010	 0.4450
1p	 0.7580	 0.5020
1q	 0.7880	 0.5240
1r	 0.8190	 0.5450
1s	 0.6280	 0.4670
3A	 0.8560	 0.5540
3B	 0.8650	 0.5550
3C	 0.9140	 0.5770
3D	 0.9080	 0.5710
3E	 0.5160	 0.3660
3F	 0.8710	 0.5680
3G	 0.8490	 0.5510
3H	 0.7930	 0.5240
3I	 0.4830	 0.4250
3J	 0.8800	 0.5130
3N	 0.9010	 0.5680
3O	 0.8710	 0.5560
3P	 0.9170	 0.5790
3Q	 0.9170	 0.5760
3R	 0.5040	 0.3410
3S	 0.8830	 0.5740
3T	 0.9110	 0.5600
3U	 0.8120	 0.5130
3V	 0.7290	 0.5270
3W	 0.9180	 0.5770
3X	 0.8590	 0.5500
3Y	 0.8180	 0.5350
4A	 0.7670	 0.4960
4B	 0.6290	 0.4440
4C	 0.6810	 0.4580
4D	 0.5470	 0.4050
4E	 0.5240	 0.3980
4F	 0.6500	 0.4690
4G	 0.5720	 0.4200
4H	 0.7020	 0.4510
4I	 0.5490	 0.4430

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Chain	Atom inclusion	Q-score
4J	 0.6570	 0.4500
4K	 0.4960	 0.4260
4L	 0.6710	 0.4540
4M	 0.5840	 0.4440
4N	 0.4840	 0.4220
8A	 0.7010	 0.4270
8B	 0.6480	 0.3960
8C	 0.6210	 0.3890
8D	 0.5890	 0.3680
8E	 0.5910	 0.3680
8F	 0.4800	 0.3690
8G	 0.5780	 0.3700
8H	 0.7180	 0.4000
8I	 0.7430	 0.4120
8J	 0.5710	 0.3790
8K	 0.6140	 0.3890
8L	 0.5740	 0.3870
8M	 0.6250	 0.3910
8N	 0.6560	 0.3990