



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 03:05 PM UTC

PDB ID : 9FZL / pdb_00009fzl
EMDB ID : EMD-50491
Title : Perkinsus marinus respiratory supercomplex CII2CIII2CIV2 in an intermediate state
Authors : Wu, F.; Amunts, A.
Deposited on : 2024-07-05
Resolution : 2.20 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

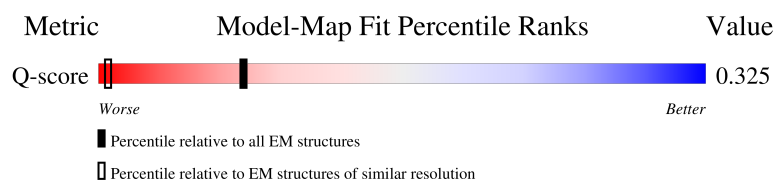
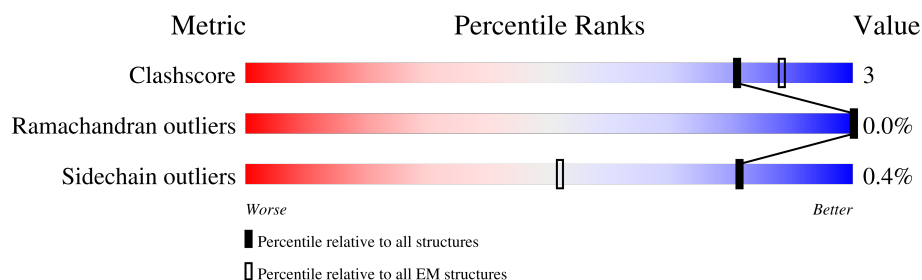
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 Å.

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



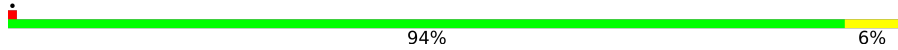
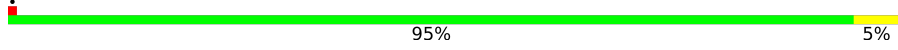
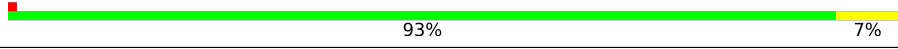
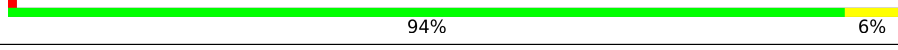
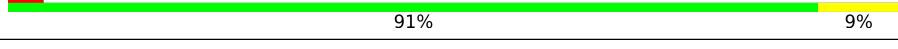
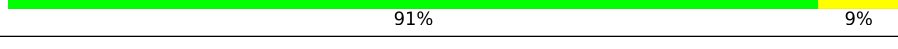
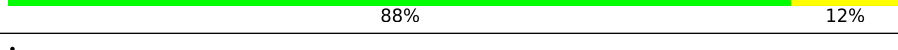
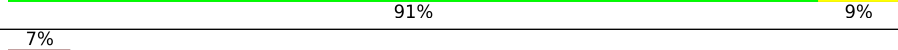
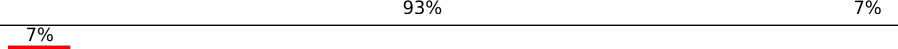
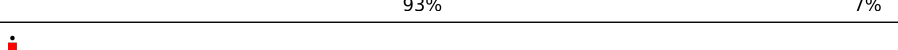
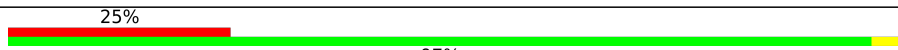
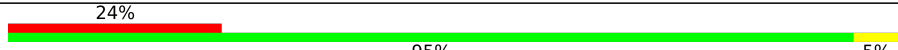
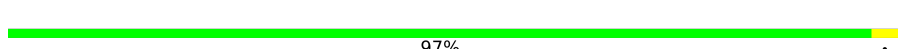
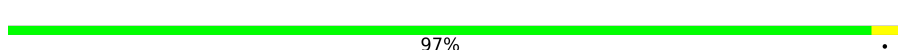
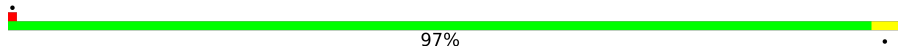
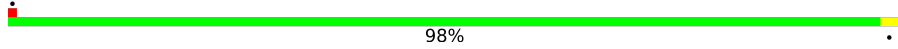
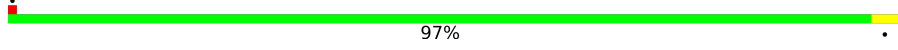
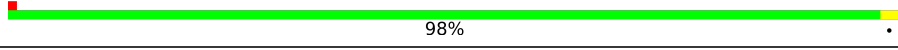
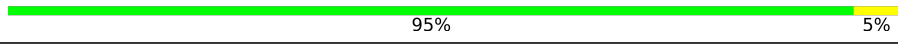
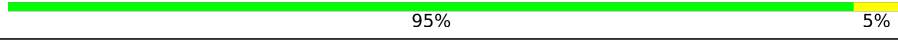
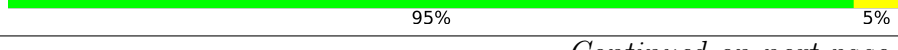
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	2M	604	77% 94% 6%
1	2m	604	77% 94% 6%
2	2N	259	24% 95% 5%
2	2n	259	23% 95% 5%

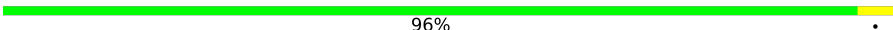
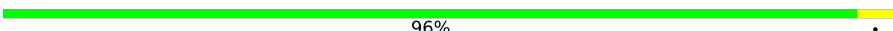
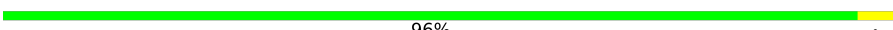
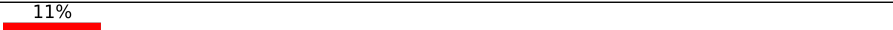
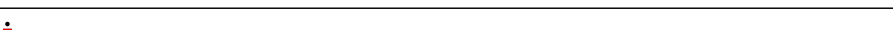
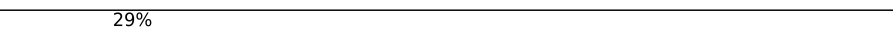
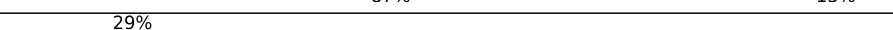
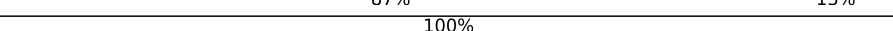
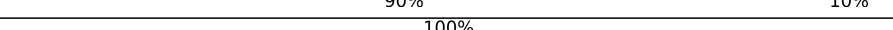
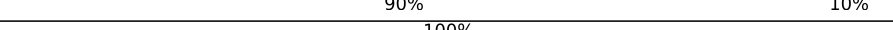
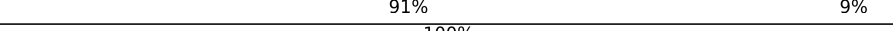
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Mol	Chain	Length	Quality of chain
3	2O	160	
3	2o	160	
4	2P	158	
4	2p	158	
5	2Q	69	
5	2q	69	
6	2R	117	
6	2r	117	
7	2S	165	
7	2s	165	
8	2T	82	
8	2t	82	
9	2U	48	
9	2u	48	
10	2V	87	
10	2v	87	
11	3A	454	
11	3a	454	
12	3B	496	
12	3b	496	
13	3C	241	
13	3c	241	
14	3D	95	
14	3d	95	
15	3E	92	

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Mol	Chain	Length	Quality of chain
15	3e	92	 96% .
16	3F	84	 96% .
16	3f	84	 96% .
17	3G	354	 90% 10%
17	3g	354	 90% 10%
18	3H	326	 30% 87% 13%
18	3h	326	 30% 87% 13%
19	3I	176	 95% 5%
19	3i	176	 95% 5%
20	3J	92	 11% 99% .
20	3j	92	 11% 99% .
21	3K	79	 . 97% .
21	3k	79	 . 95% 5%
22	3L	69	 29% 87% 13%
22	3l	69	 29% 87% 13%
23	40	230	 100% 90% 10%
23	41	230	 100% 90% 10%
24	4A	100	 100% 91% 9%
24	4a	100	 100% 91% 9%
25	4B	93	 98% 91% 8% .
25	4b	93	 98% 91% 8% .
26	4C	75	 96% 88% 11% .
26	4c	75	 96% 88% 11% .
27	4D	90	 99% 92% 8%
27	4d	90	 100% 93% 7%

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Mol	Chain	Length	Quality of chain	
28	4E	152	100%	5%
28	4e	152	100%	5%
29	4F	73	99%	.
29	4f	73	99%	.
30	4G	100	99%	.
30	4g	100	98%	.
31	4H	141	100%	.
31	4h	141	95%	5%
32	4I	196	100%	5%
32	4i	196	94%	6%
33	4J	186	100%	8%
33	4j	186	91%	9%
34	4K	93	100%	5%
34	4k	93	100%	5%
35	4L	122	100%	.
35	4l	122	96%	.
36	4M	98	100%	7%
36	4m	98	93%	7%
37	4N	131	100%	5%
37	4n	131	95%	5%
38	4O	47	100%	9%
38	4o	47	91%	9%
39	4P	180	100%	.
39	4p	180	96%	.
40	4Q	459	100%	12%

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Mol	Chain	Length	Quality of chain
40	4q	459	100% 88%12%
41	4R	103	100% 97%
41	4r	103	100% 96%
42	4S	65	100% 97%
42	4s	65	100% 100%
43	4T	121	100% 93%7%
43	4t	121	100% 93%7%
44	4U	91	100% 88%12%
44	4u	91	100% 89%11%
45	4V	185	100% 93%7%
45	4v	185	100% 93%7%
46	4W	141	100% 96%
46	4w	141	100% 96%
47	4X	226	100% 91%9%
47	4x	226	100% 90%10%
48	4Y	107	100% 95%5%
48	4y	107	100% 95%5%
49	4Z	186	100% 98%
49	4z	186	100% 98%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	AJP	40	304	X	-	-	-
61	AJP	41	304	X	-	-	-

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 142424 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2M	604	Total	C	N	O	S	0	0
			4610	2880	831	873	26		
1	2m	604	Total	C	N	O	S	0	0
			4610	2880	831	873	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2N	259	Total	C	N	O	S	0	0
			2068	1309	355	378	26		
2	2n	259	Total	C	N	O	S	0	0
			2068	1309	355	378	26		

- Molecule 3 is a protein called SDHG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2O	160	Total	C	N	O	S	0	0
			1254	806	229	213	6		
3	2o	160	Total	C	N	O	S	0	0
			1254	806	229	213	6		

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2P	158	Total	C	N	O	S	0	0
			1309	846	246	211	6		
4	2p	158	Total	C	N	O	S	0	0
			1309	846	246	211	6		

- Molecule 5 is a protein called Kinesin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2Q	69	Total	C	N	O	S	0	0
			564	367	100	94	3		
5	2q	69	Total	C	N	O	S	0	0
			564	367	100	94	3		

- Molecule 6 is a protein called SDHH.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2R	117	Total	C	N	O	S	0	0
			950	621	166	157	6		
6	2r	117	Total	C	N	O	S	0	0
			950	621	166	157	6		

- Molecule 7 is a protein called DUF6827 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2S	165	Total	C	N	O	S	0	0
			1323	832	223	257	11		
7	2s	165	Total	C	N	O	S	0	0
			1323	832	223	257	11		

- Molecule 8 is a protein called Rab-GAP TBC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2T	82	Total	C	N	O	S	0	0
			695	446	117	128	4		
8	2t	82	Total	C	N	O	S	0	0
			695	446	117	128	4		

- Molecule 9 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2U	48	Total	C	N	O	S	0	0
			390	246	68	75	1		
9	2u	48	Total	C	N	O	S	0	0
			390	246	68	75	1		

- Molecule 10 is a protein called SDHI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2V	87	Total	C	N	O	S	0	0
			709	457	119	126	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2v	87	Total	C	N	O	S	0	0
			709	457	119	126	7		

- Molecule 11 is a protein called Mitochondrial processing peptidase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3A	454	Total	C	N	O	S	0	0
			3622	2285	621	698	18		
11	3a	454	Total	C	N	O	S	0	0
			3622	2285	621	698	18		

- Molecule 12 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3B	496	Total	C	N	O	S	0	0
			3884	2459	669	734	22		
12	3b	496	Total	C	N	O	S	0	0
			3884	2459	669	734	22		

- Molecule 13 is a protein called Iso-1-cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3C	241	Total	C	N	O	S	0	0
			1921	1225	334	349	13		
13	3c	241	Total	C	N	O	S	0	0
			1921	1225	334	349	13		

- Molecule 14 is a protein called QCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3D	95	Total	C	N	O	S	0	0
			836	551	146	135	4		
14	3d	95	Total	C	N	O	S	0	0
			836	551	146	135	4		

- Molecule 15 is a protein called QCR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3E	92	Total	C	N	O	S	0	0
			813	545	138	127	3		
15	3e	92	Total	C	N	O	S	0	0
			813	545	138	127	3		

- Molecule 16 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3F	84	Total	C	N	O	S	0	0
			734	493	123	114	4		
16	3f	84	Total	C	N	O	S	0	0
			734	493	123	114	4		

- Molecule 17 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3G	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		
17	3g	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		

- Molecule 18 is a protein called Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3H	326	Total	C	N	O	S	0	0
			2628	1669	478	466	15		
18	3h	326	Total	C	N	O	S	0	0
			2628	1669	478	466	15		

- Molecule 19 is a protein called Ubiquinol-cytochrome C reductase complex 14kD subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3I	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		
19	3i	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		

- Molecule 20 is a protein called Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3J	92	Total	C	N	O	S	0	0
			755	471	134	139	11		
20	3j	92	Total	C	N	O	S	0	0
			755	471	134	139	11		

- Molecule 21 is a protein called Cu-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3K	79	Total	C	N	O	S	0	0
			608	391	110	103	4		
21	3k	79	Total	C	N	O	S	0	0
			608	391	110	103	4		

- Molecule 22 is a protein called Aurora kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3L	69	Total	C	N	O	S	0	0
			509	327	91	89	2		
22	3l	69	Total	C	N	O	S	0	0
			509	327	91	89	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	40	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		
23	41	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4A	100	Total	C	N	O	S	0	0
			841	518	157	157	9		
24	4a	100	Total	C	N	O	S	0	0
			841	518	157	157	9		

- Molecule 25 is a protein called Peptidase M14 carboxypeptidase A domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4B	93	Total	C	N	O	S	0	0
			732	479	116	129	8		
25	4b	93	Total	C	N	O	S	0	0
			732	479	116	129	8		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4C	75	Total	C	N	O	S	0	0
			626	414	95	113	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	4c	75	Total	C	N	O	S	0	0
			626	414	95	113	4		

- Molecule 27 is a protein called Cytochrome c oxidase subunit 34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4D	90	Total	C	N	O	S	0	0
			787	525	128	131	3		
27	4d	90	Total	C	N	O	S	0	0
			787	525	128	131	3		

- Molecule 28 is a protein called Merozoite surface protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4E	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		
28	4e	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		

- Molecule 29 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4F	73	Total	C	N	O	S	0	0
			613	406	108	97	2		
29	4f	73	Total	C	N	O	S	0	0
			613	406	108	97	2		

- Molecule 30 is a protein called Cytochrome c oxidase subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4G	100	Total	C	N	O	S	0	0
			854	550	156	144	4		
30	4g	100	Total	C	N	O	S	0	0
			854	550	156	144	4		

- Molecule 31 is a protein called Cytochrome c oxidase subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4H	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		
31	4h	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		

- Molecule 32 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4I	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		
32	4i	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		

- Molecule 33 is a protein called Cytochrome c oxidase subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4J	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		
33	4j	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		

- Molecule 34 is a protein called Cytochrome c oxidase subunit 37.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4K	93	Total	C	N	O	S	0	0
			722	473	129	118	2		
34	4k	93	Total	C	N	O	S	0	0
			722	473	129	118	2		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4L	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		
35	4l	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4M	98	Total	C	N	O	S	0	0
			773	498	147	127	1		
36	4m	98	Total	C	N	O	S	0	0
			773	498	147	127	1		

- Molecule 37 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4N	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		
37	4n	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		

- Molecule 38 is a protein called GINS subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4O	47	Total	C	N	O	S	0	0
			383	257	60	63	3		
38	4o	47	Total	C	N	O	S	0	0
			383	257	60	63	3		

- Molecule 39 is a protein called Cytochrome c oxidase subunit 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4P	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		
39	4p	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		

- Molecule 40 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4Q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		
40	4q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

- Molecule 41 is a protein called Cytochrome c oxidase subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	4R	103	Total	C	N	O	S	0	0
			916	609	156	145	6		
41	4r	103	Total	C	N	O	S	0	0
			916	609	156	145	6		

- Molecule 42 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4S	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	4s	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4T	121	Total	C	N	O	S	0	0
			983	634	170	167	12		
43	4t	121	Total	C	N	O	S	0	0
			983	634	170	167	12		

- Molecule 44 is a protein called Amino acid transporter transmembrane domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	4U	91	Total	C	N	O	S	0	0
			758	503	125	127	3		
44	4u	91	Total	C	N	O	S	0	0
			758	503	125	127	3		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4V	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		
45	4v	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4W	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		
46	4w	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		

- Molecule 47 is a protein called Cytochrome Coxidase subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4X	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
47	4x	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

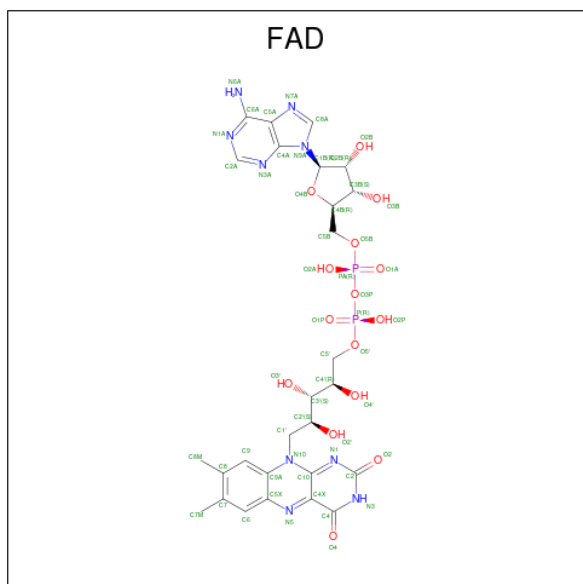
- Molecule 48 is a protein called Cytochrome c oxidase subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4Y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		
48	4y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		

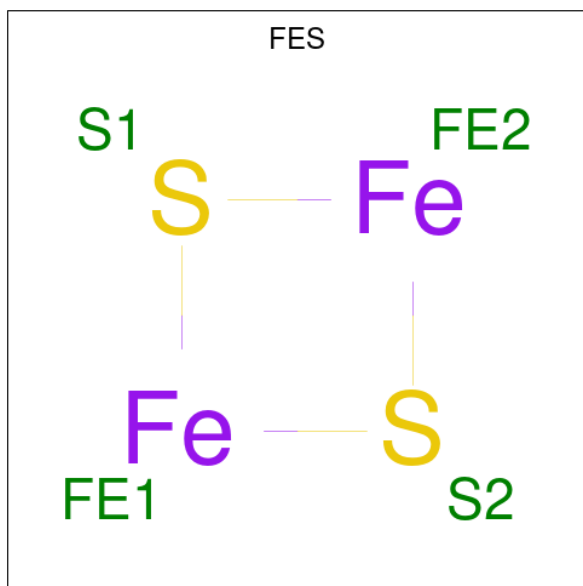
- Molecule 49 is a protein called Cytochrome c oxidase subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	4Z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		
49	4z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		

- Molecule 50 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

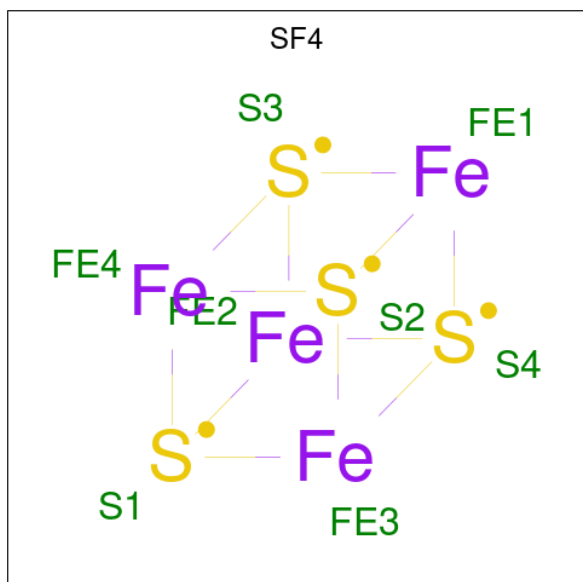


- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



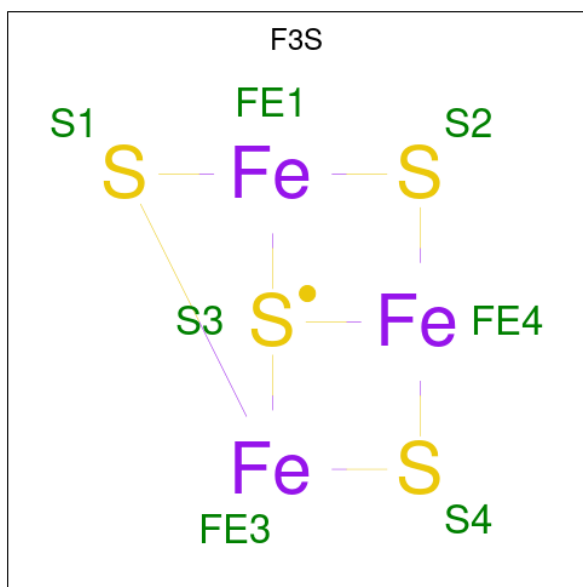
Mol	Chain	Residues	Atoms			AltConf
51	2N	1	Total	Fe	S	0
			4	2	2	
51	3H	1	Total	Fe	S	0
			4	2	2	
51	2n	1	Total	Fe	S	0
			4	2	2	
51	3h	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
52	2N	1	Total	Fe	S	0
			8	4	4	
52	2n	1	Total	Fe	S	0
			8	4	4	

- Molecule 53 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

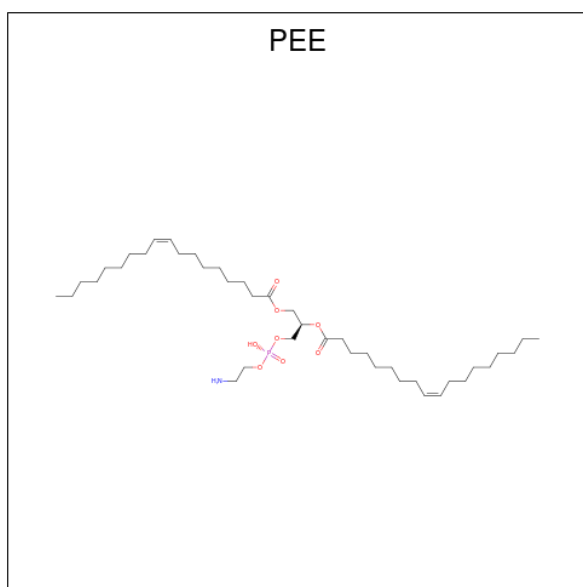


Mol	Chain	Residues	Atoms			AltConf
53	2N	1	Total	Fe	S	0
			7	3	4	
53	2n	1	Total	Fe	S	0
			7	3	4	

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
54	2N	1	Total	K	0
			1	1	
54	4Q	1	Total	K	0
			1	1	
54	2n	1	Total	K	0
			1	1	
54	4q	1	Total	K	0
			1	1	

- Molecule 55 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



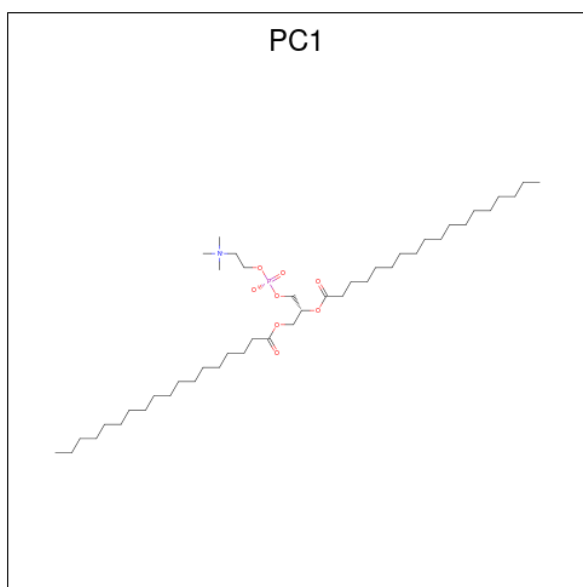
Mol	Chain	Residues	Atoms					AltConf
55	2O	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2P	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2P	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2R	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3F	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	40	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	40	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	40	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4D	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4R	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4S	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
55	4W	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2o	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2p	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2p	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2r	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3c	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3f	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4l	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4l	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4l	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4d	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4r	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4s	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4w	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4z	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 56 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



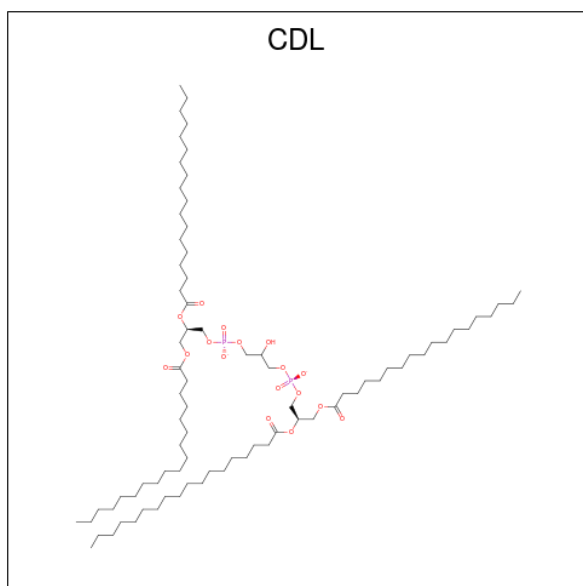
Mol	Chain	Residues	Atoms					AltConf
56	2O	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2O	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2P	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2R	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2T	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3A	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3A	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3H	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	4E	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2o	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2o	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2p	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2r	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2t	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
56	3a	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3a	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3h	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	4e	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 57 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	2O	1	Total	C	O	P	0
			100	81	17	2	
57	2P	1	Total	C	O	P	0
			100	81	17	2	
57	2Q	1	Total	C	O	P	0
			100	81	17	2	
57	2U	1	Total	C	O	P	0
			100	81	17	2	
57	3D	1	Total	C	O	P	0
			100	81	17	2	
57	3D	1	Total	C	O	P	0
			100	81	17	2	
57	3E	1	Total	C	O	P	0
			100	81	17	2	

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Mol	Chain	Residues	Atoms				AltConf
57	3E	1	Total 100	C 81	O 17	P 2	0
57	3E	1	Total 100	C 81	O 17	P 2	0
57	3G	1	Total 100	C 81	O 17	P 2	0
57	3H	1	Total 100	C 81	O 17	P 2	0
57	3I	1	Total 100	C 81	O 17	P 2	0
57	3I	1	Total 100	C 81	O 17	P 2	0
57	3I	1	Total 100	C 81	O 17	P 2	0
57	3L	1	Total 100	C 81	O 17	P 2	0
57	3L	1	Total 100	C 81	O 17	P 2	0
57	4E	1	Total 100	C 81	O 17	P 2	0
57	4J	1	Total 100	C 81	O 17	P 2	0
57	4K	1	Total 100	C 81	O 17	P 2	0
57	4K	1	Total 100	C 81	O 17	P 2	0
57	4L	1	Total 100	C 81	O 17	P 2	0
57	4M	1	Total 100	C 81	O 17	P 2	0
57	4Q	1	Total 100	C 81	O 17	P 2	0
57	4Q	1	Total 100	C 81	O 17	P 2	0
57	4S	1	Total 100	C 81	O 17	P 2	0
57	4T	1	Total 100	C 81	O 17	P 2	0
57	4U	1	Total 100	C 81	O 17	P 2	0
57	4W	1	Total 100	C 81	O 17	P 2	0

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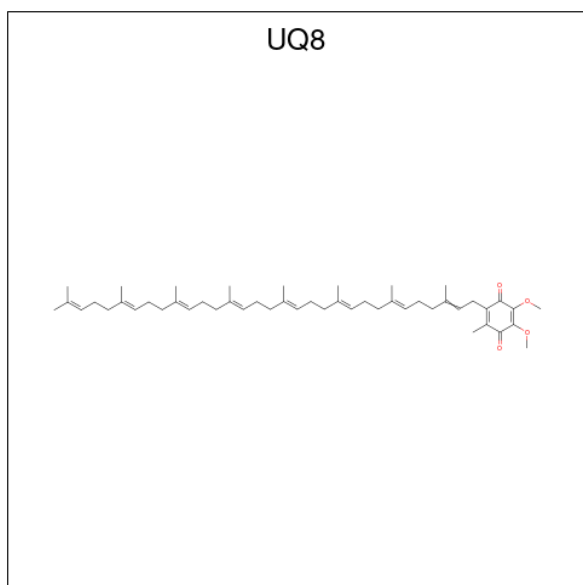
Mol	Chain	Residues	Atoms				AltConf
57	4W	1	Total 100	C 81	O 17	P 2	0
57	4Z	1	Total 100	C 81	O 17	P 2	0
57	2o	1	Total 100	C 81	O 17	P 2	0
57	2p	1	Total 100	C 81	O 17	P 2	0
57	2q	1	Total 100	C 81	O 17	P 2	0
57	2u	1	Total 100	C 81	O 17	P 2	0
57	3d	1	Total 100	C 81	O 17	P 2	0
57	3d	1	Total 100	C 81	O 17	P 2	0
57	3e	1	Total 100	C 81	O 17	P 2	0
57	3e	1	Total 100	C 81	O 17	P 2	0
57	3e	1	Total 100	C 81	O 17	P 2	0
57	3g	1	Total 100	C 81	O 17	P 2	0
57	3h	1	Total 100	C 81	O 17	P 2	0
57	3i	1	Total 100	C 81	O 17	P 2	0
57	3i	1	Total 100	C 81	O 17	P 2	0
57	3i	1	Total 100	C 81	O 17	P 2	0
57	3l	1	Total 100	C 81	O 17	P 2	0
57	3l	1	Total 100	C 81	O 17	P 2	0
57	4e	1	Total 100	C 81	O 17	P 2	0
57	4j	1	Total 100	C 81	O 17	P 2	0
57	4k	1	Total 100	C 81	O 17	P 2	0

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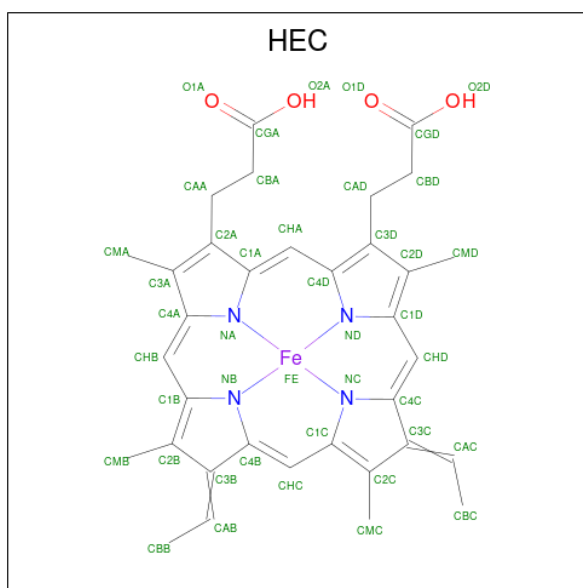
Mol	Chain	Residues	Atoms				AltConf
57	4k	1	Total 100	C 81	O 17	P 2	0
57	4l	1	Total 100	C 81	O 17	P 2	0
57	4m	1	Total 100	C 81	O 17	P 2	0
57	4q	1	Total 100	C 81	O 17	P 2	0
57	4q	1	Total 100	C 81	O 17	P 2	0
57	4s	1	Total 100	C 81	O 17	P 2	0
57	4t	1	Total 100	C 81	O 17	P 2	0
57	4u	1	Total 100	C 81	O 17	P 2	0
57	4w	1	Total 100	C 81	O 17	P 2	0
57	4w	1	Total 100	C 81	O 17	P 2	0
57	4z	1	Total 100	C 81	O 17	P 2	0

- Molecule 58 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



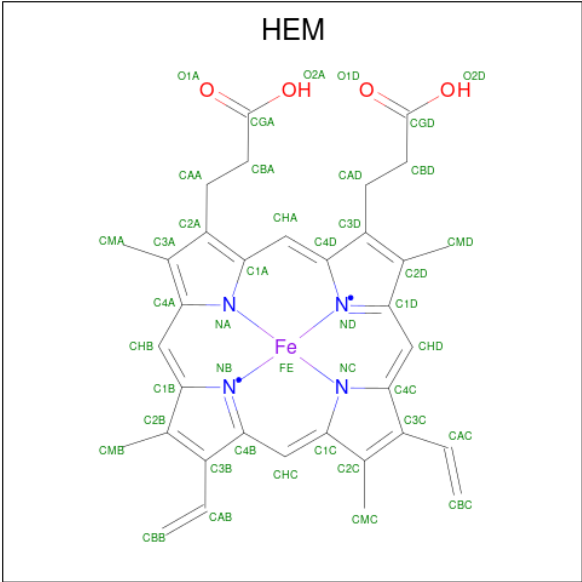
Mol	Chain	Residues	Atoms			AltConf
58	2S	1	Total	C	O	0
			53	49	4	
58	3D	1	Total	C	O	0
			53	49	4	
58	3G	1	Total	C	O	0
			53	49	4	
58	3G	1	Total	C	O	0
			53	49	4	
58	2s	1	Total	C	O	0
			53	49	4	
58	3d	1	Total	C	O	0
			53	49	4	
58	3g	1	Total	C	O	0
			53	49	4	
58	3g	1	Total	C	O	0
			53	49	4	

- Molecule 59 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



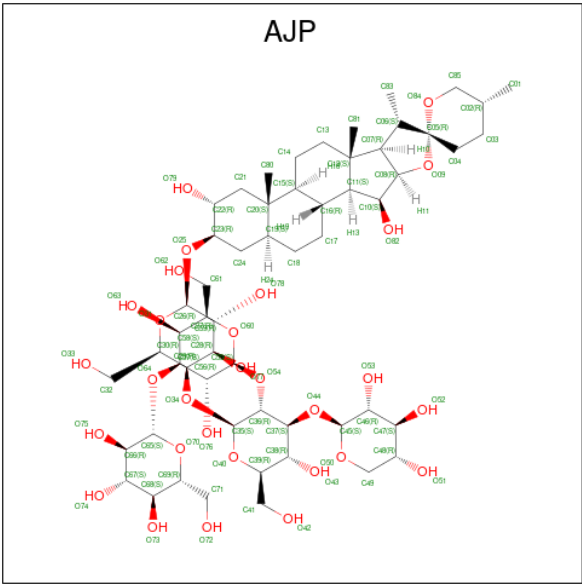
Mol	Chain	Residues	Atoms					AltConf
59	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
59	3c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 60 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



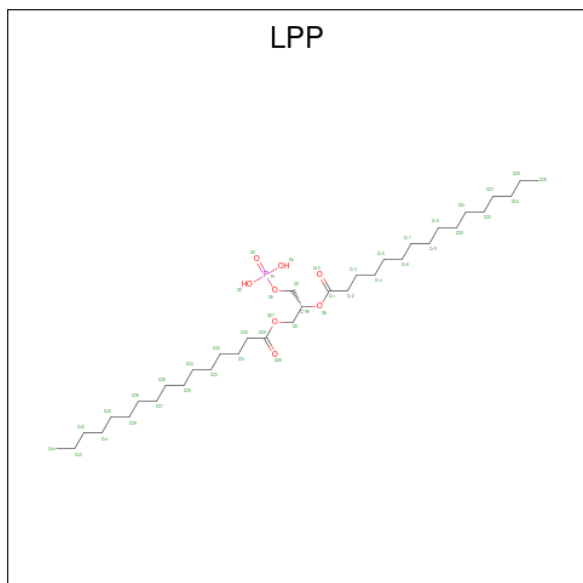
Mol	Chain	Residues	Atoms					AltConf
60	3G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
60	3G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
60	3g	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
60	3g	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 61 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



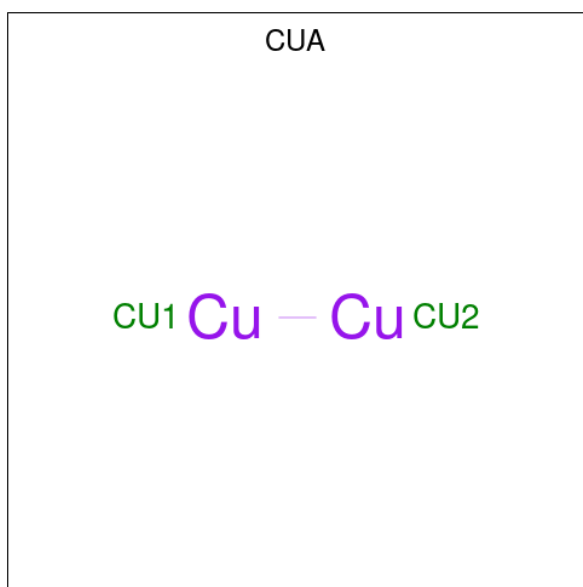
Mol	Chain	Residues	Atoms			AltConf
61	40	1	Total	C	O	0
			43	33	10	
61	41	1	Total	C	O	0
			43	33	10	

- Molecule 62 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
62	4C	1	Total	C	O	P	0
			44	35	8	1	
62	4D	1	Total	C	O	P	0
			44	35	8	1	
62	4c	1	Total	C	O	P	0
			44	35	8	1	
62	4d	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 63 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
63	4N	1	Total 2	Cu 2	0
63	4n	1	Total 2	Cu 2	0

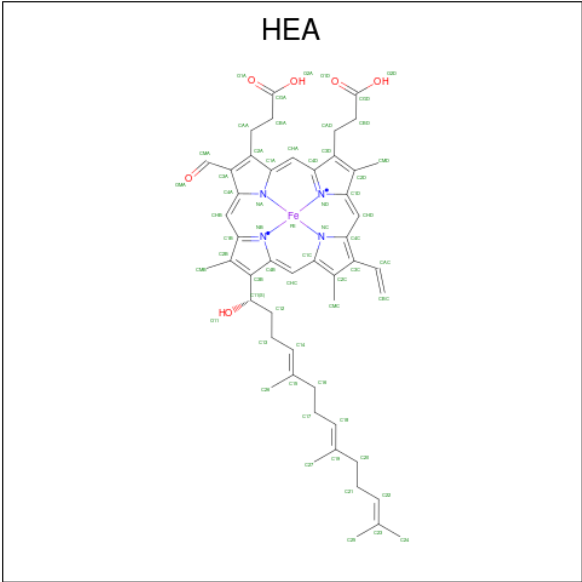
- Molecule 64 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
64	4Q	1	Total 1	Cu 1	0
64	4q	1	Total 1	Cu 1	0

- Molecule 65 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

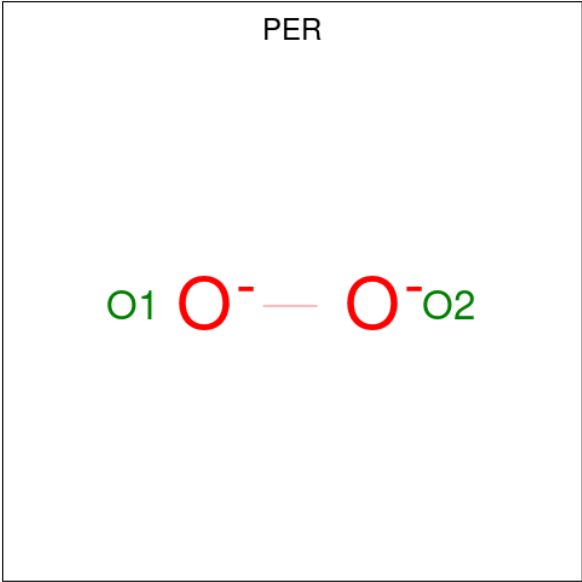
Mol	Chain	Residues	Atoms		AltConf
65	4Q	1	Total 1	Mg 1	0
65	4q	1	Total 1	Mg 1	0

- Molecule 66 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
66	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
66	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
66	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
66	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 67 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		AltConf
67	4Q	1	Total	O	0
			2	2	
67	4q	1	Total	O	0
			2	2	

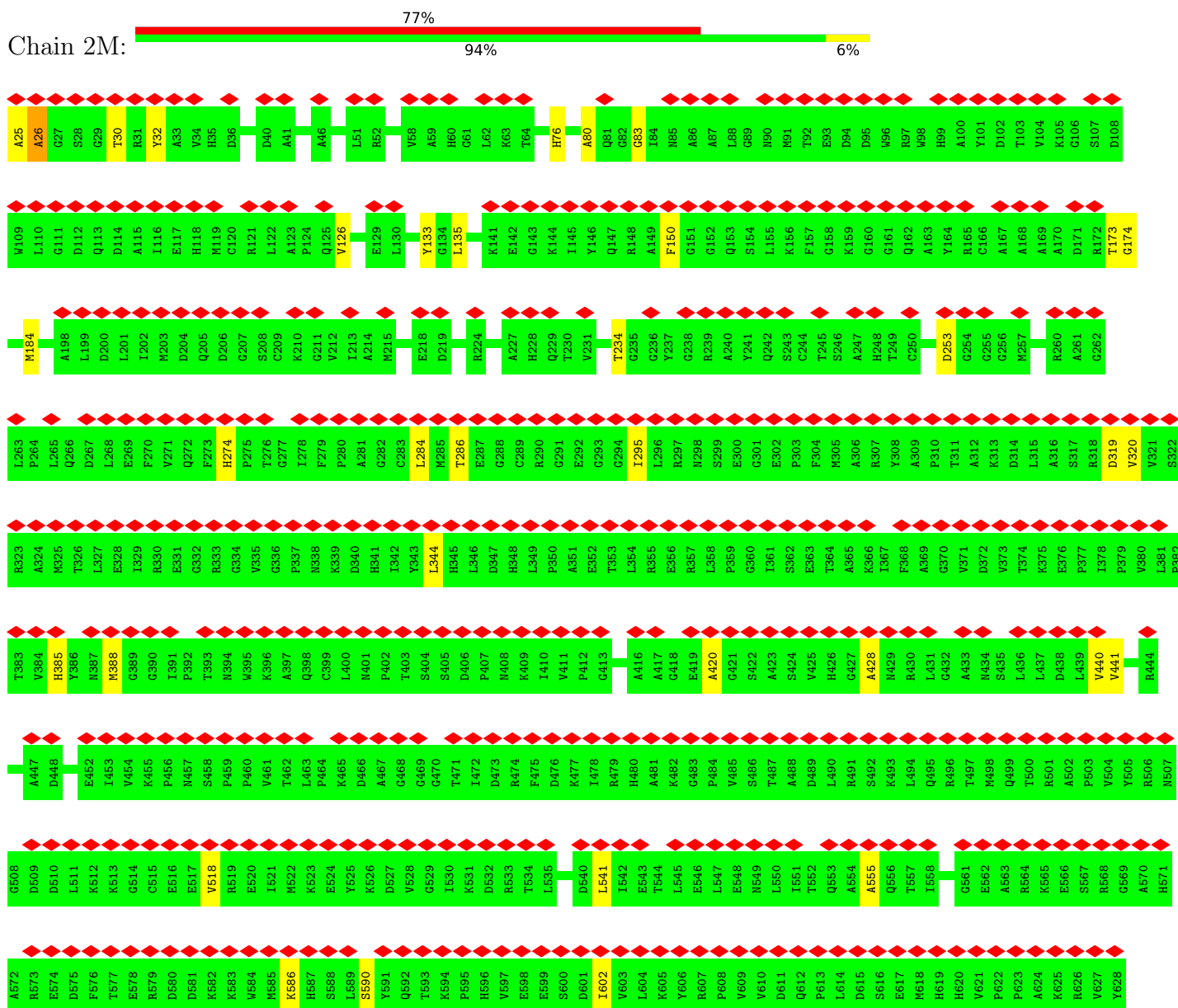
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	4T	2	Total	Zn	0
			2	2	
68	4X	1	Total	Zn	0
			1	1	
68	4t	2	Total	Zn	0
			2	2	
68	4x	1	Total	Zn	0
			1	1	

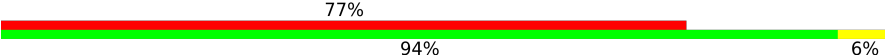
3 Residue-property plots

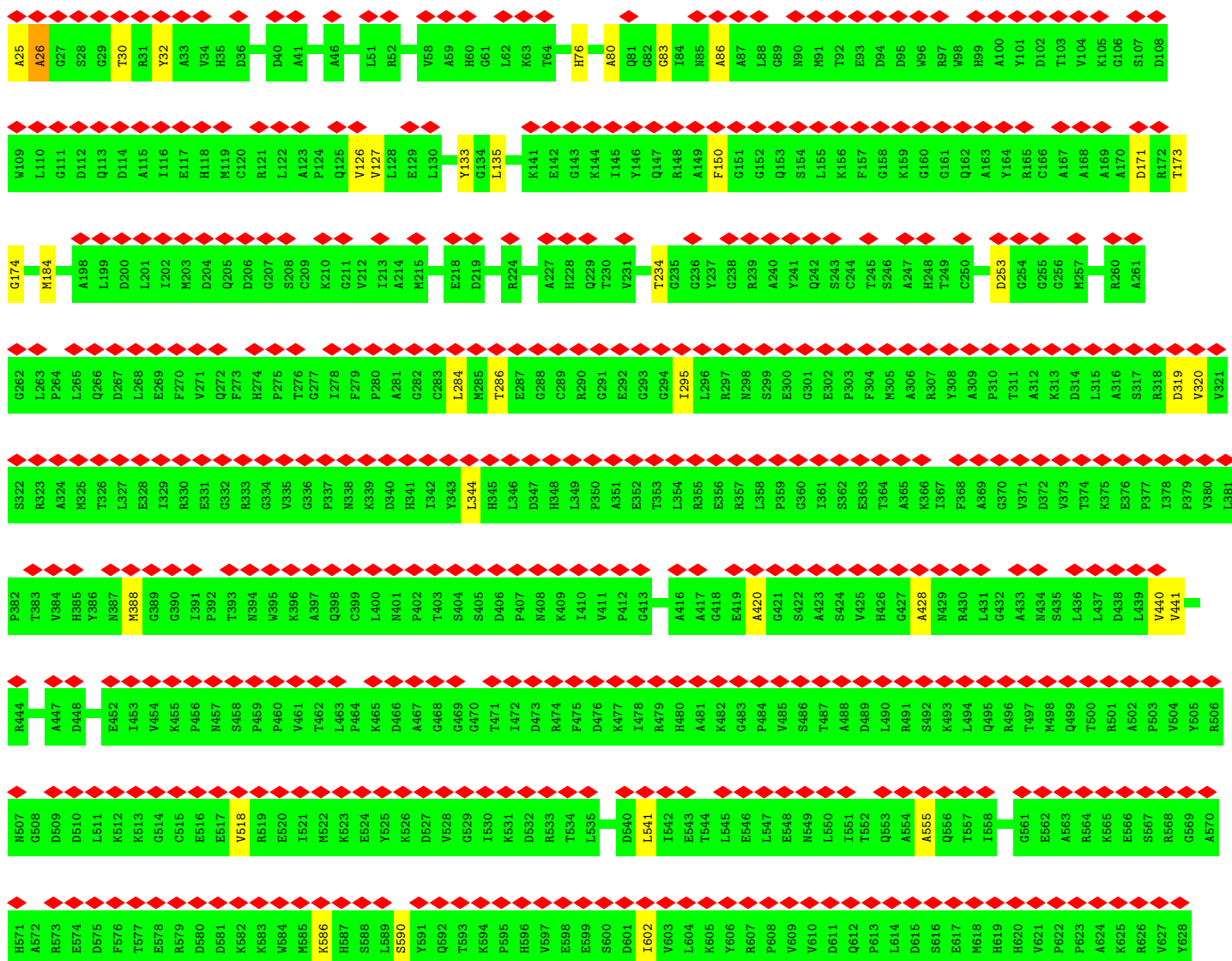
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

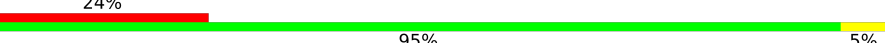


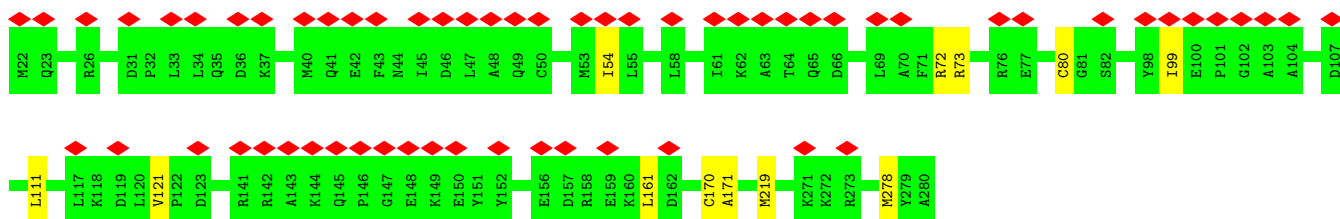
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain 2m: 

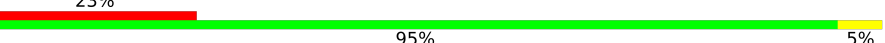


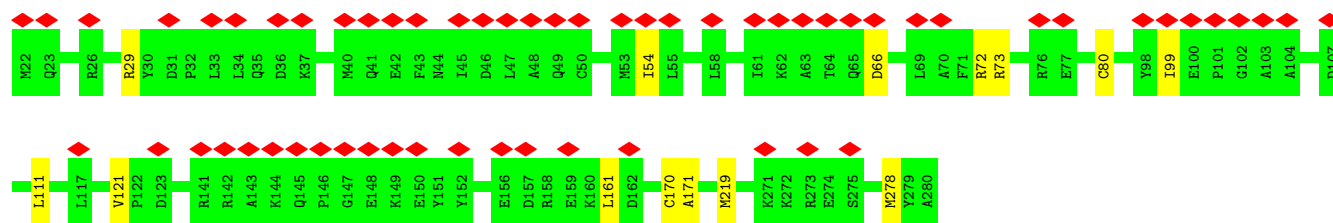
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain 2N: 



- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain 2n: 



- Molecule 3: SDHG



- Molecule 3: SDHG



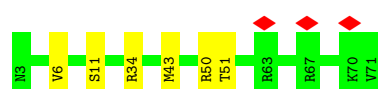
- Molecule 4: Transmembrane protein



- Molecule 4: Transmembrane protein



- Molecule 5: Kinesin-like protein

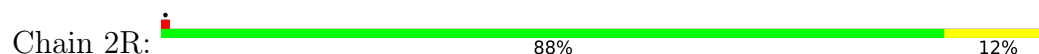


- Molecule 5: Kinesin-like protein





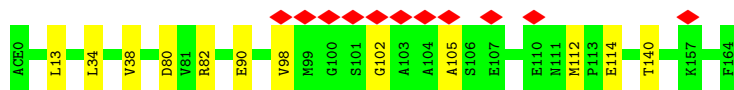
- Molecule 6: SDHH



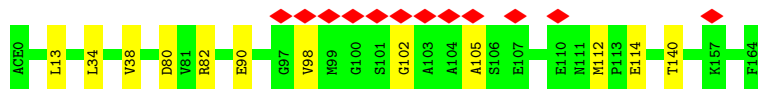
- Molecule 6: SDHH



- Molecule 7: DUF6827 domain-containing protein



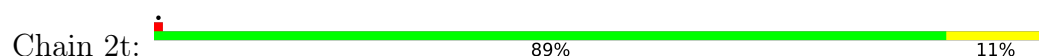
- Molecule 7: DUF6827 domain-containing protein



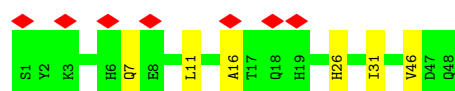
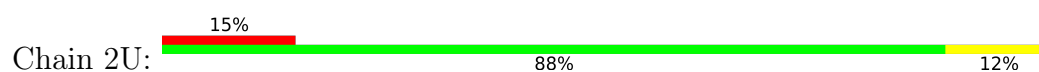
- Molecule 8: Rab-GAP TBC domain-containing protein



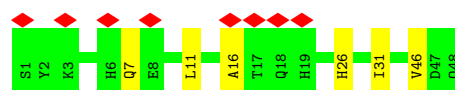
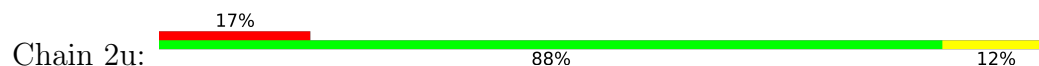
- Molecule 8: Rab-GAP TBC domain-containing protein



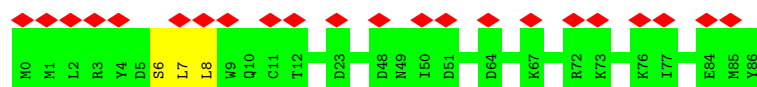
- Molecule 9: Syntaxin-1A



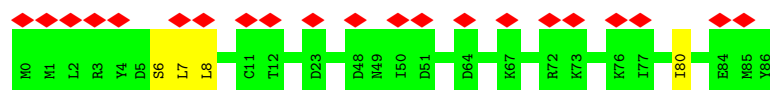
• Molecule 9: Syntaxin-1A



• Molecule 10: SDHI



• Molecule 10: SDHI



• Molecule 11: Mitochondrial processing peptidase beta subunit



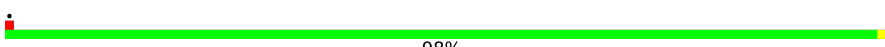
• Molecule 11: Mitochondrial processing peptidase beta subunit

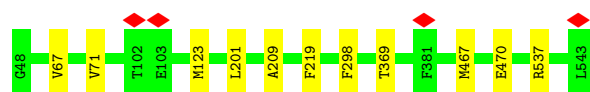


• Molecule 12: Alpha-MPP



- Molecule 12: Alpha-MPP

Chain 3b:  98%

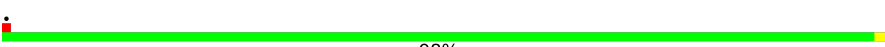


- Molecule 13: Iso-1-cytochrome c

Chain 3C:  97%

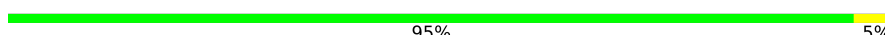


- Molecule 13: Iso-1-cytochrome c

Chain 3c:  98%

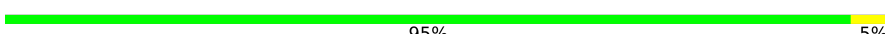


- Molecule 14: QCR8

Chain 3D:  95%

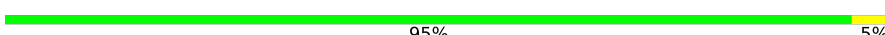


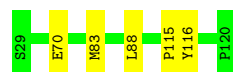
- Molecule 14: QCR8

Chain 3d:  95%

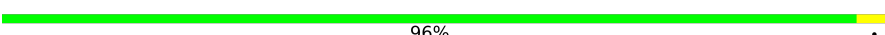


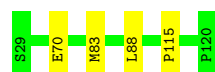
- Molecule 15: QCR9

Chain 3E:  95%

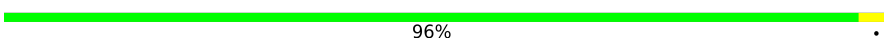


- Molecule 15: QCR9

Chain 3e:  96%

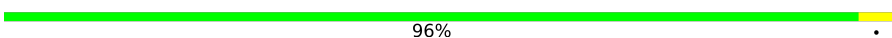


- Molecule 16: QCR10

Chain 3F:  96%

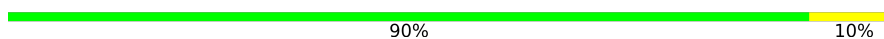


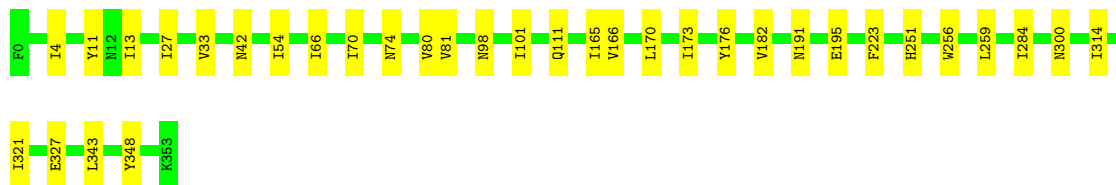
- Molecule 16: QCR10

Chain 3f:  96%



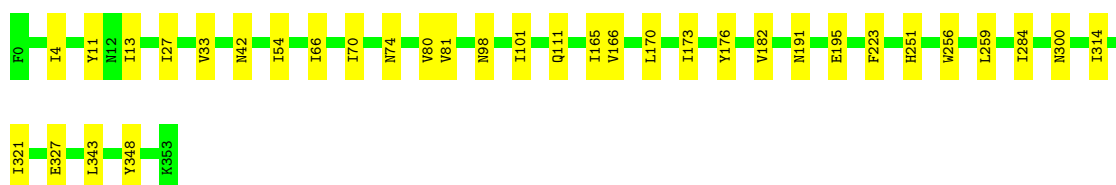
- Molecule 17: Cytochrome b

Chain 3G:  90% 10%

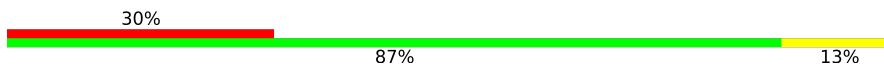


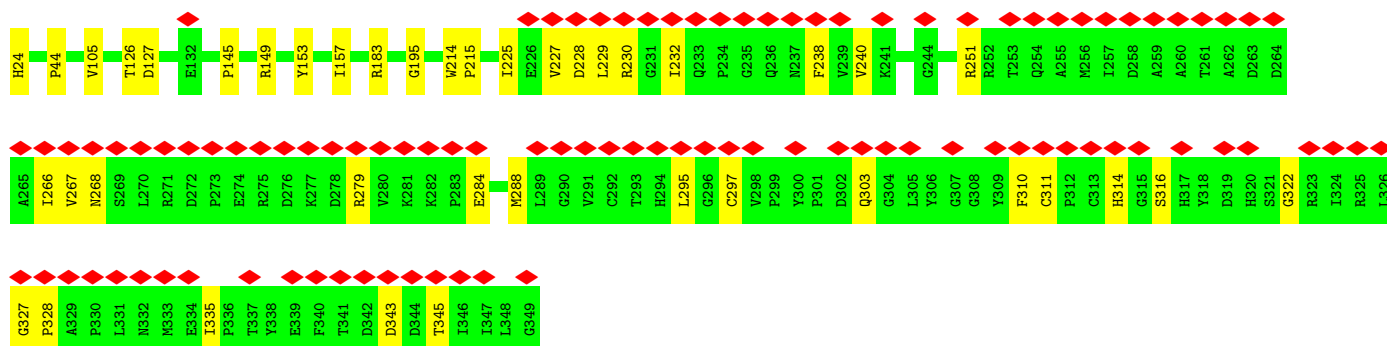
- Molecule 17: Cytochrome b

Chain 3g:  90% 10%

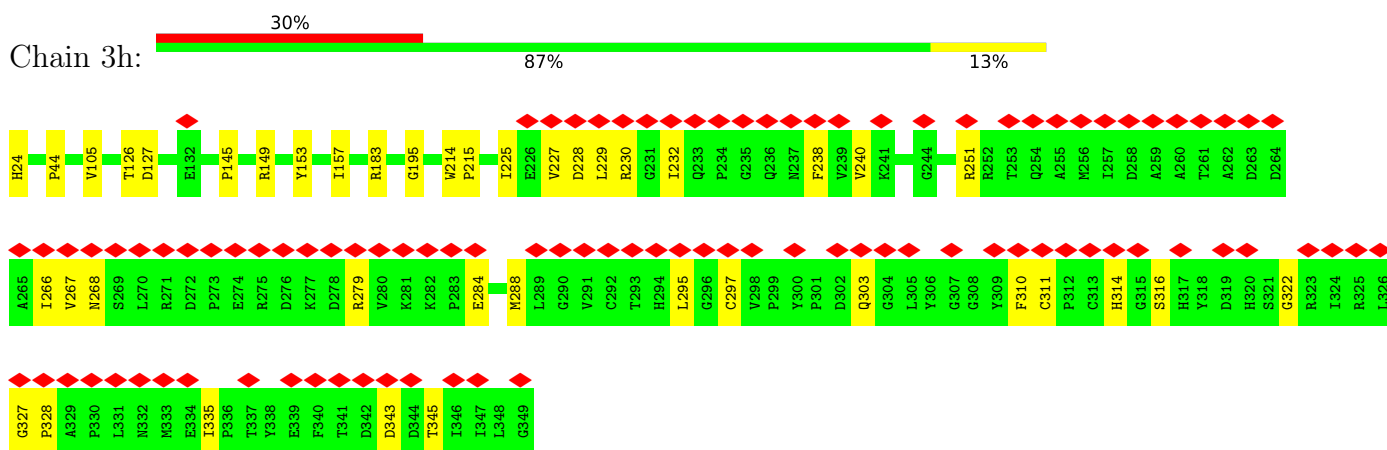


- Molecule 18: Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative

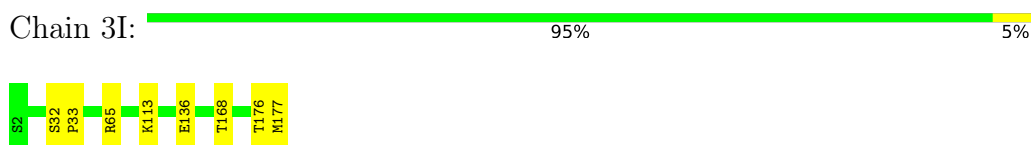
Chain 3H:  30% 87% 13%



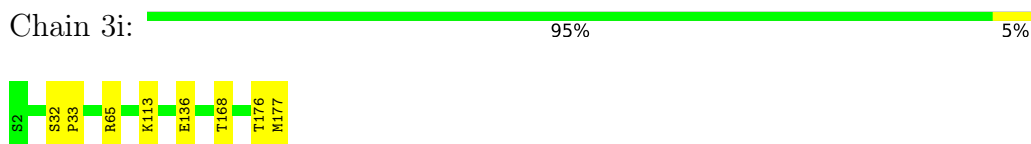
- Molecule 18: Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative



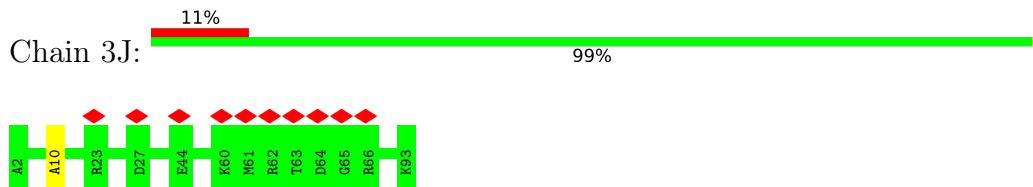
- Molecule 19: Ubiquinol-cytochrome C reductase complex 14kD subunit, putative



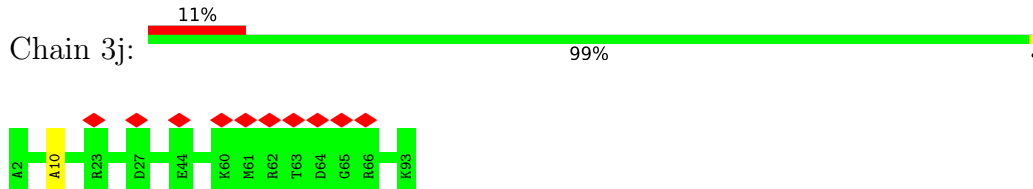
- Molecule 19: Ubiquinol-cytochrome C reductase complex 14kD subunit, putative



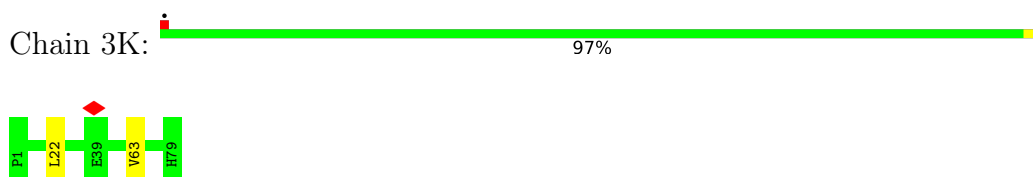
- Molecule 20: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative



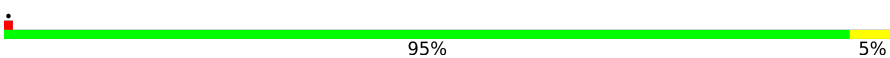
- Molecule 20: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative

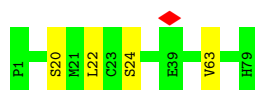


- Molecule 21: Cu-binding protein



- Molecule 21: Cu-binding protein

Chain 3k:  95% 5%



- Molecule 22: Aurora kinase

Chain 3L:  29% 87% 13%



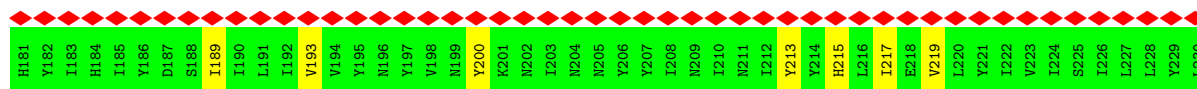
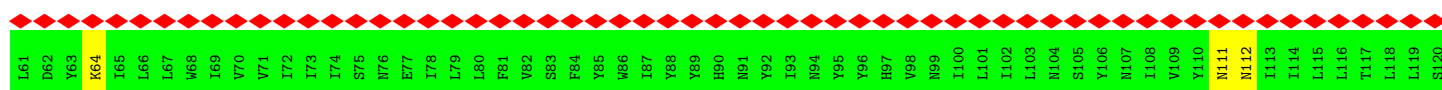
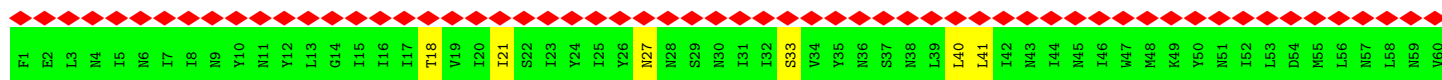
- Molecule 22: Aurora kinase

Chain 3l:  29% 87% 13%



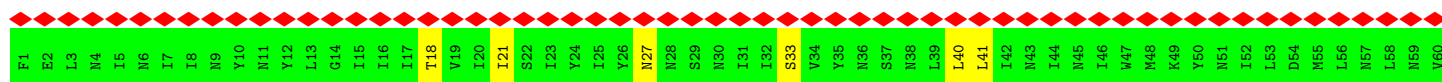
- Molecule 23: Cytochrome c oxidase subunit 3

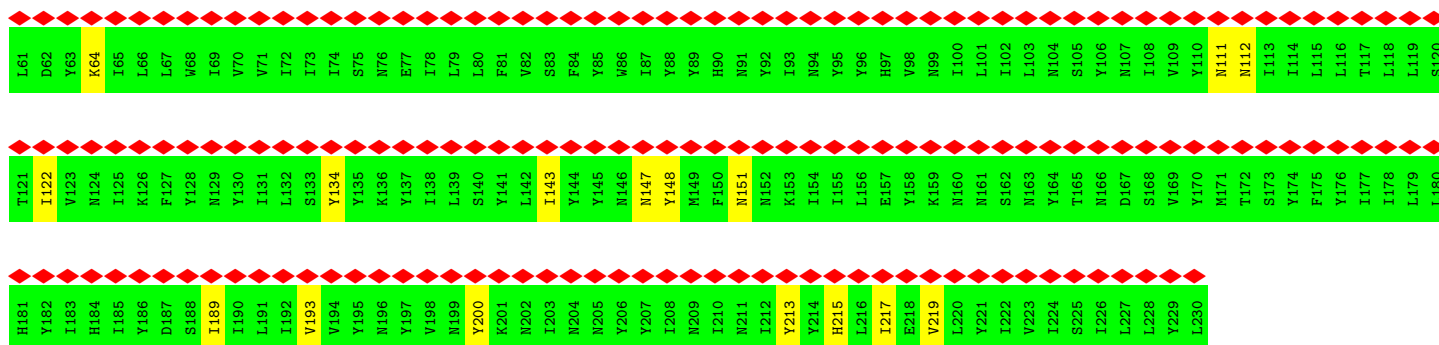
Chain 40:  100% 90% 10%



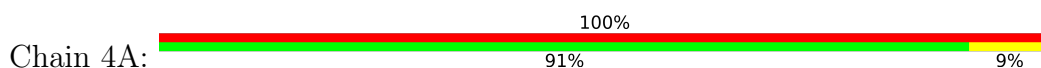
- Molecule 23: Cytochrome c oxidase subunit 3

Chain 41:  100% 90% 10%

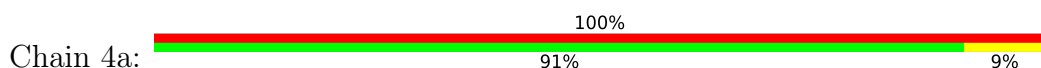




• Molecule 24: Cytochrome c oxidase subunit 6B



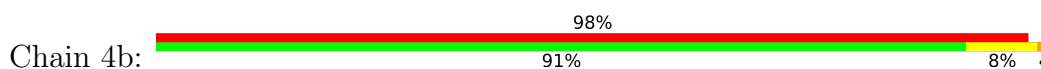
• Molecule 24: Cytochrome c oxidase subunit 6B

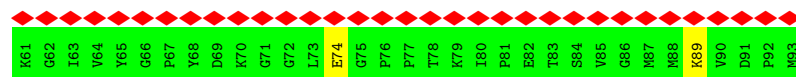


• Molecule 25: Peptidase M14 carboxypeptidase A domain-containing protein

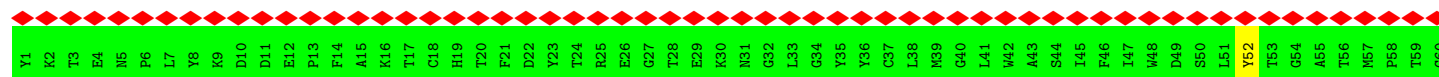


• Molecule 25: Peptidase M14 carboxypeptidase A domain-containing protein

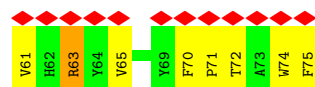
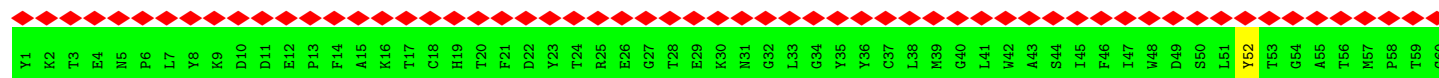
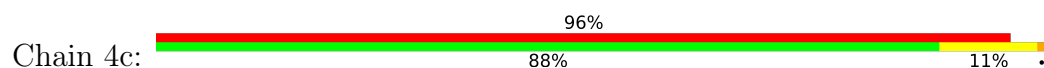




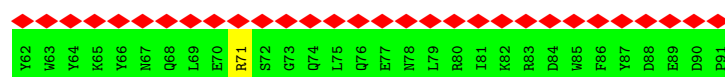
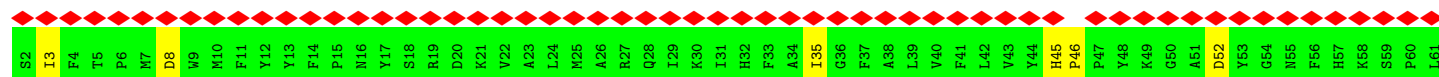
• Molecule 26: Cytochrome c oxidase subunit 40



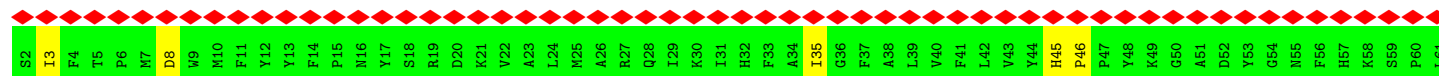
• Molecule 26: Cytochrome c oxidase subunit 40



• Molecule 27: Cytochrome c oxidase subunit 34



• Molecule 27: Cytochrome c oxidase subunit 34

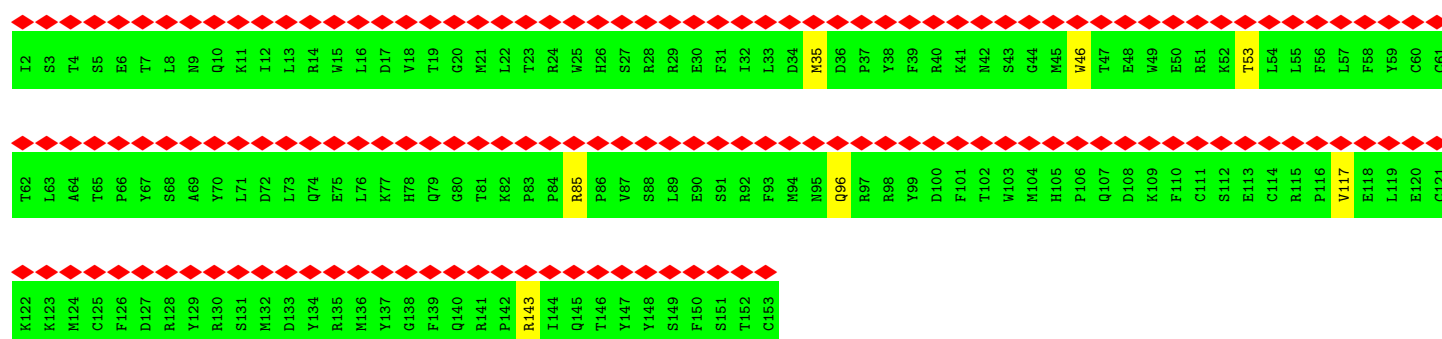


• Molecule 28: Merozoite surface protein, putative

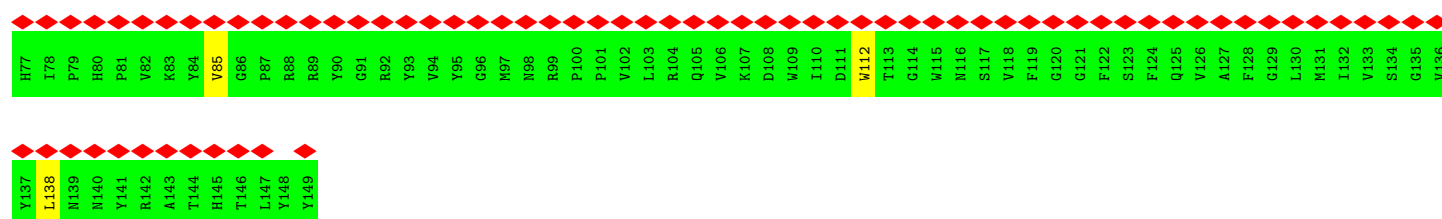




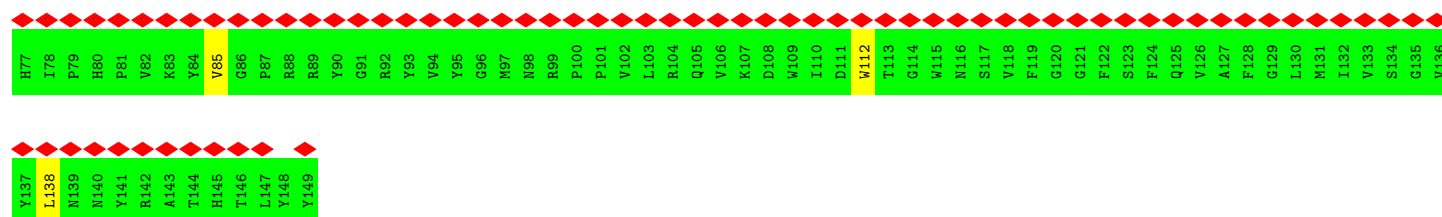
• Molecule 28: Merozoite surface protein, putative



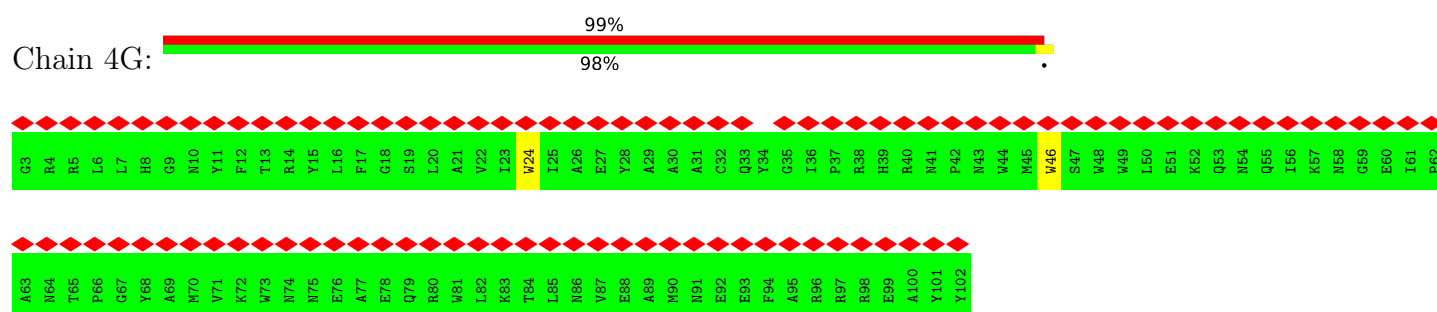
• Molecule 29: Ubiquitin, putative



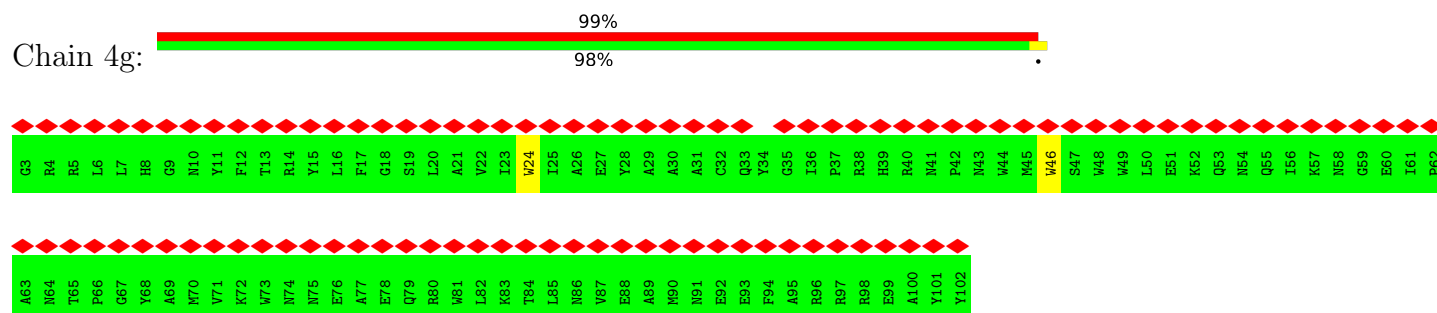
• Molecule 29: Ubiquitin, putative



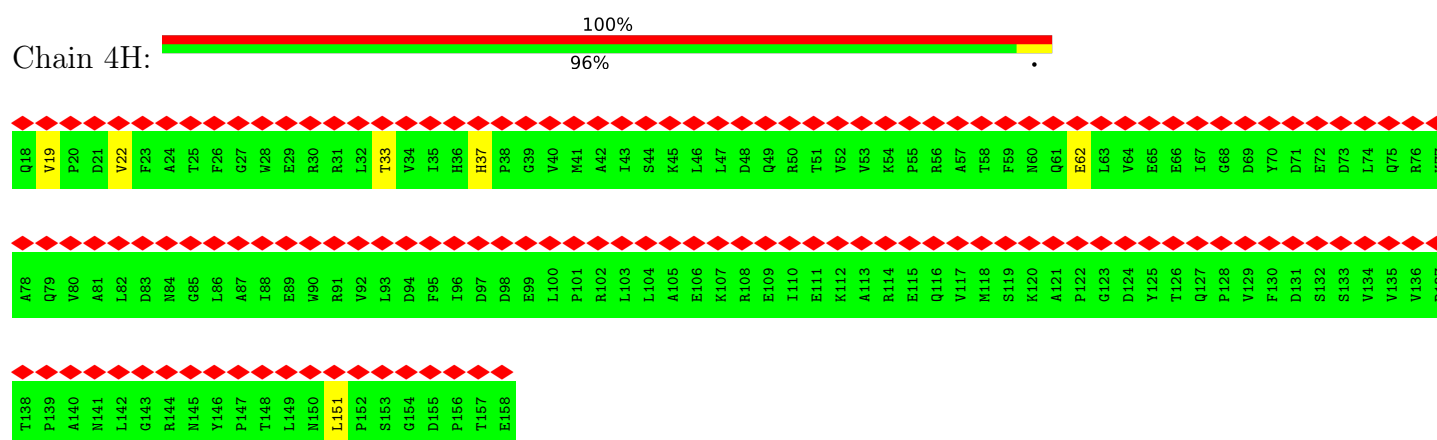
• Molecule 30: Cytochrome c oxidase subunit 33



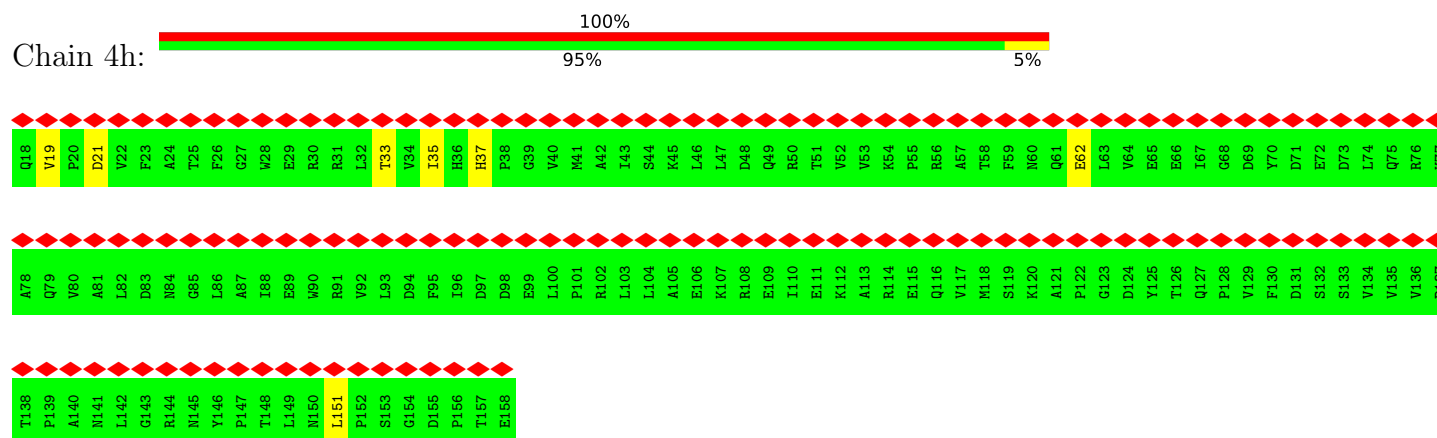
• Molecule 30: Cytochrome c oxidase subunit 33



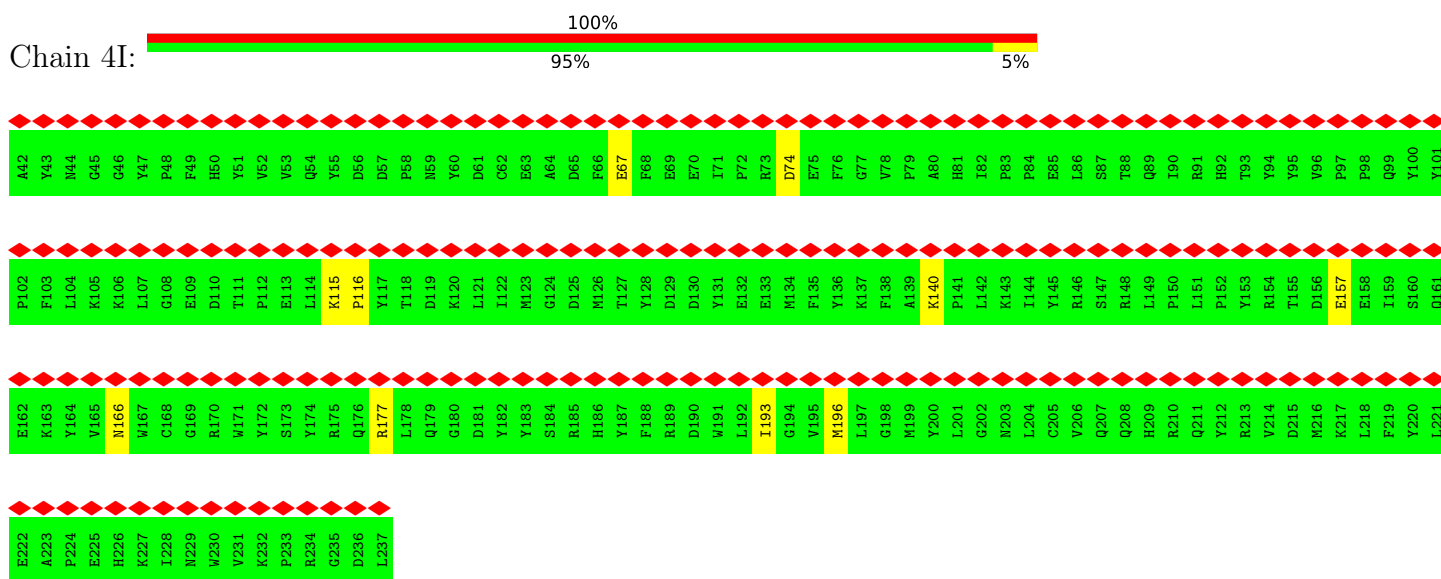
• Molecule 31: Cytochrome c oxidase subunit 30



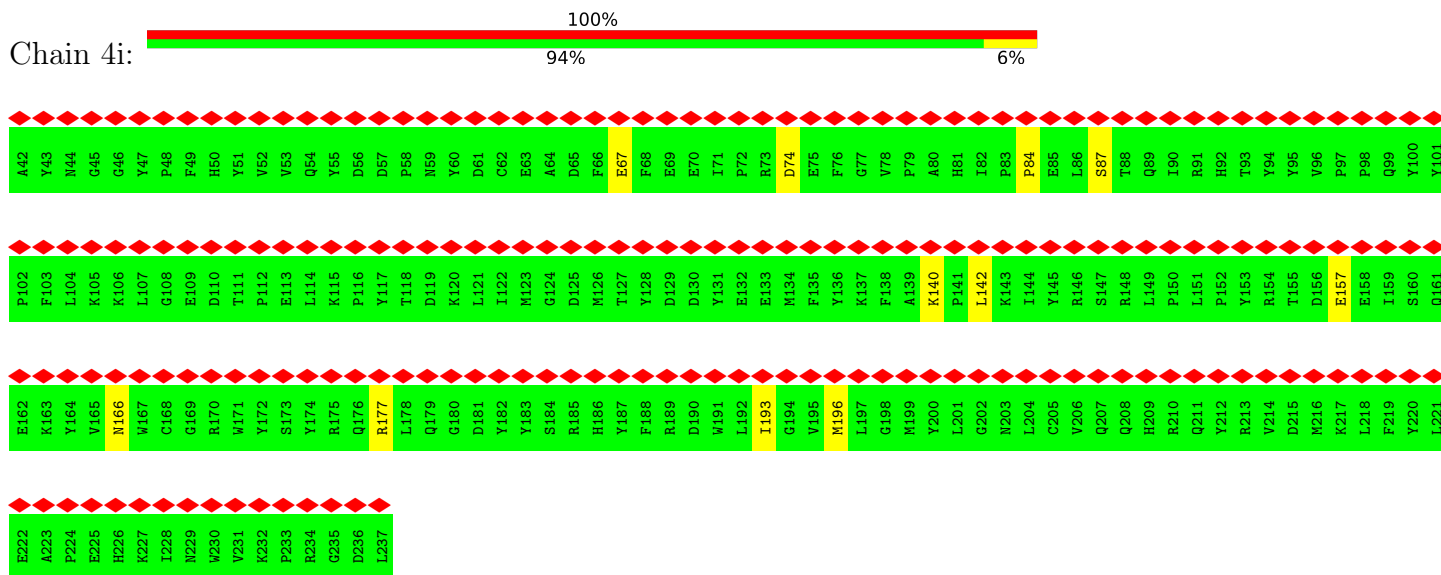
• Molecule 31: Cytochrome c oxidase subunit 30



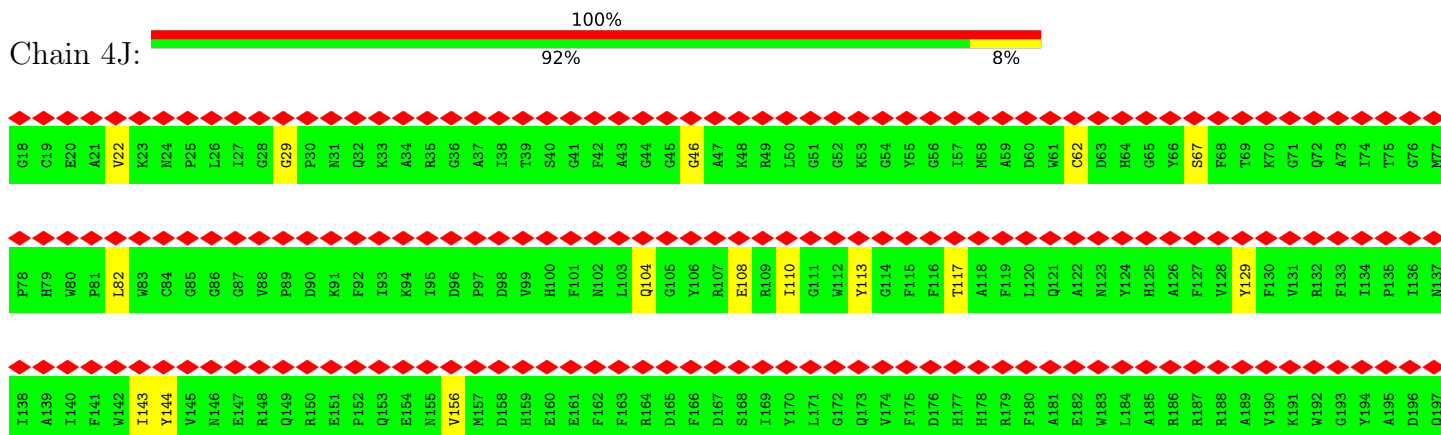
• Molecule 32: Cytochrome c oxidase subunit 6C

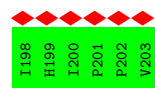


- Molecule 32: Cytochrome c oxidase subunit 6C

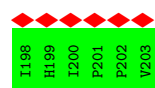
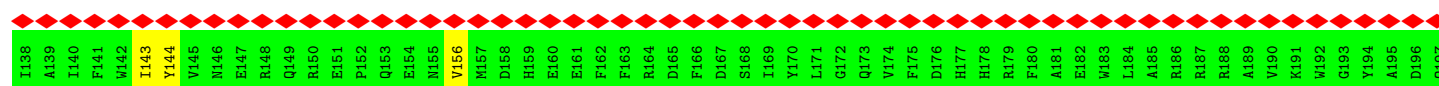
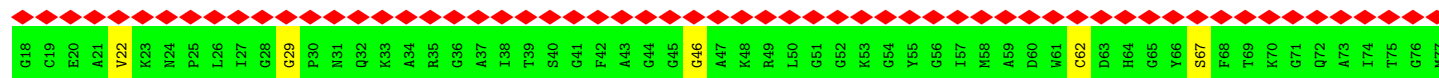
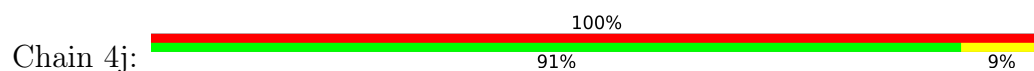


- Molecule 33: Cytochrome c oxidase subunit 24

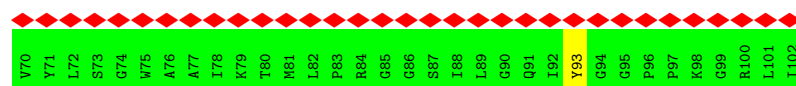
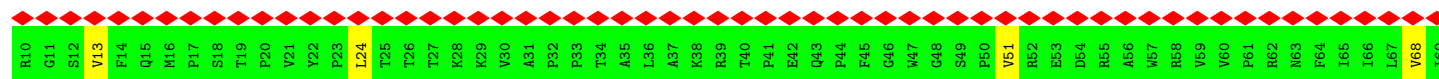




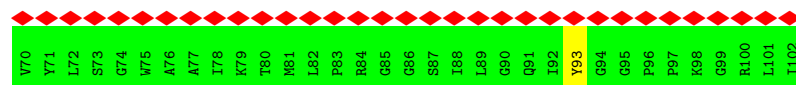
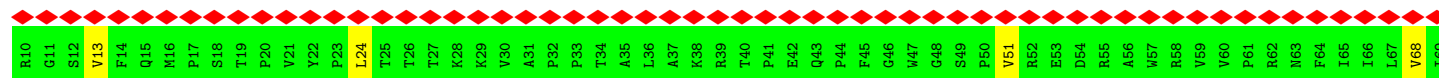
• Molecule 33: Cytochrome c oxidase subunit 24



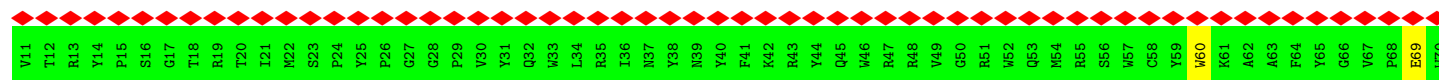
• Molecule 34: Cytochrome c oxidase subunit 37



• Molecule 34: Cytochrome c oxidase subunit 37



• Molecule 35: Cytochrome c oxidase subunit 7A





• Molecule 35: Cytochrome c oxidase subunit 7A



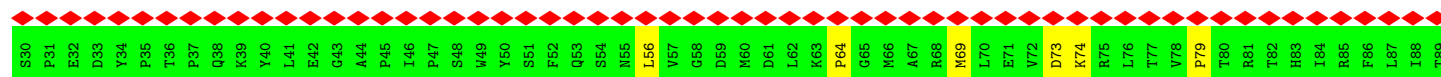
• Molecule 36: Cytochrome c oxidase subunit 35

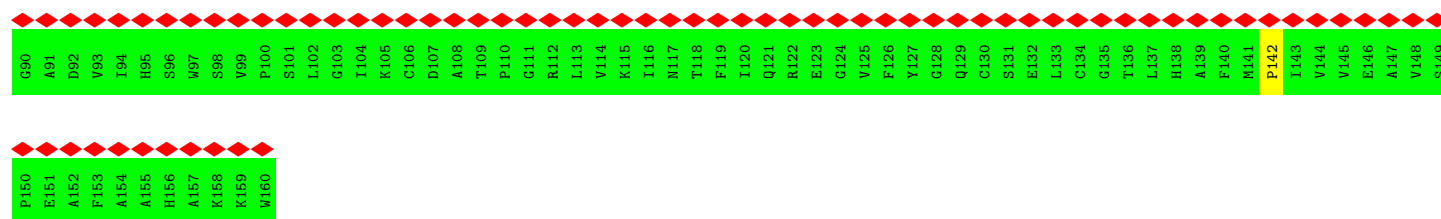


• Molecule 36: Cytochrome c oxidase subunit 35

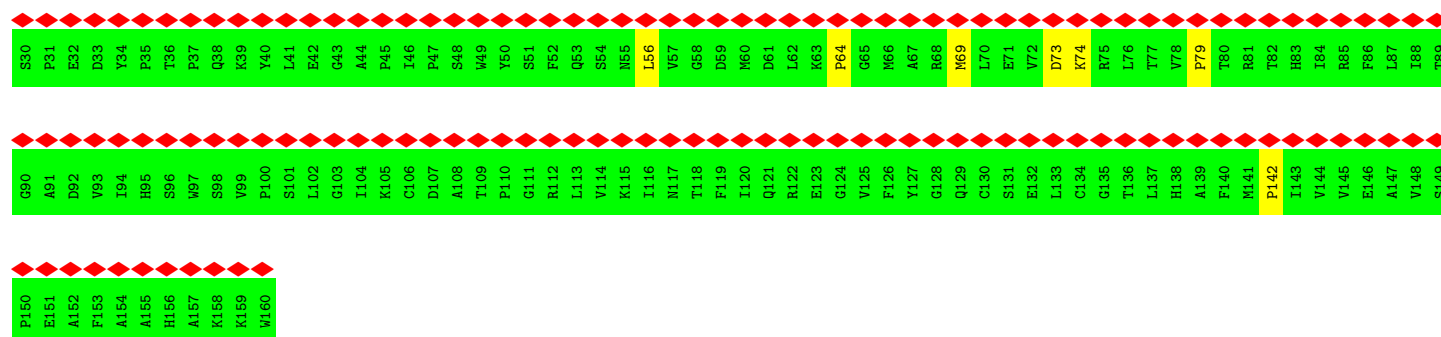


• Molecule 37: Cytochrome c oxidase polypeptide II

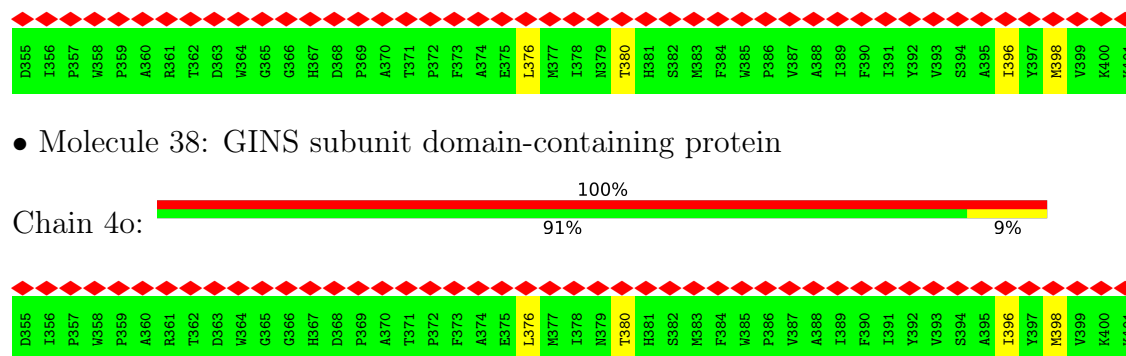




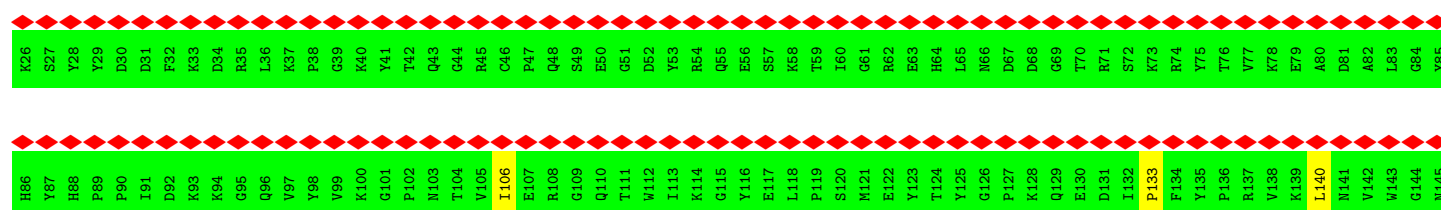
• Molecule 37: Cytochrome c oxidase polypeptide II



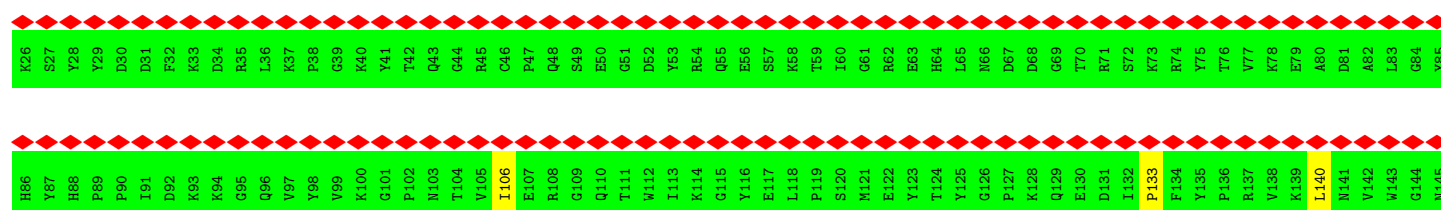
• Molecule 38: GINS subunit domain-containing protein



• Molecule 38: GINS subunit domain-containing protein

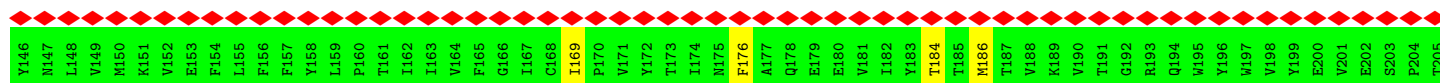
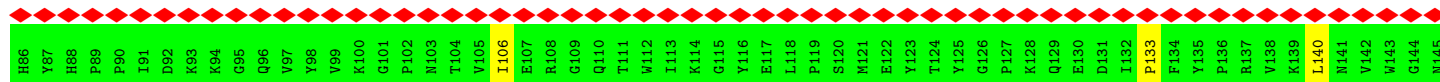


• Molecule 39: Cytochrome c oxidase subunit 2A

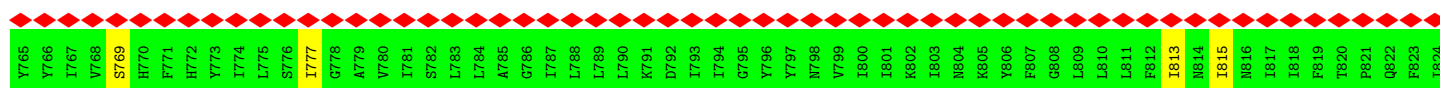
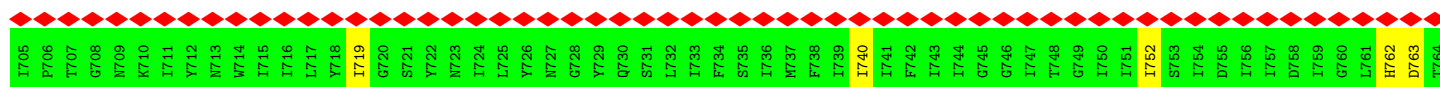
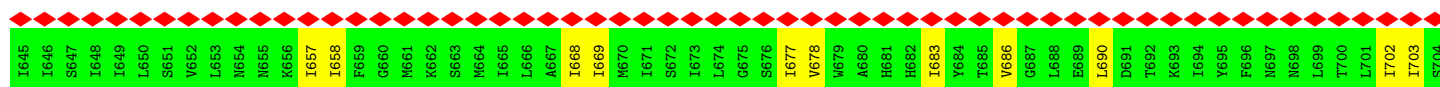
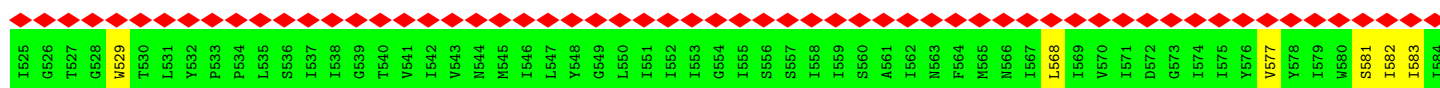
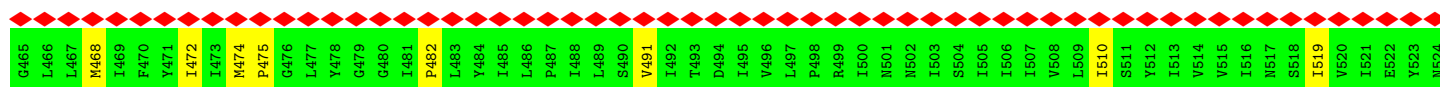
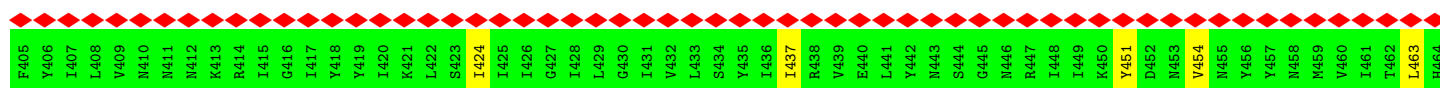
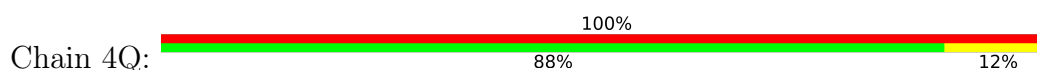


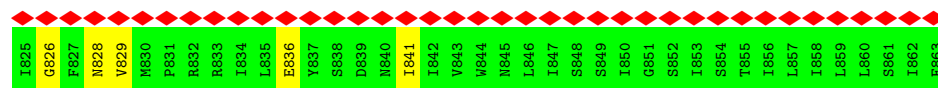


• Molecule 39: Cytochrome c oxidase subunit 2A

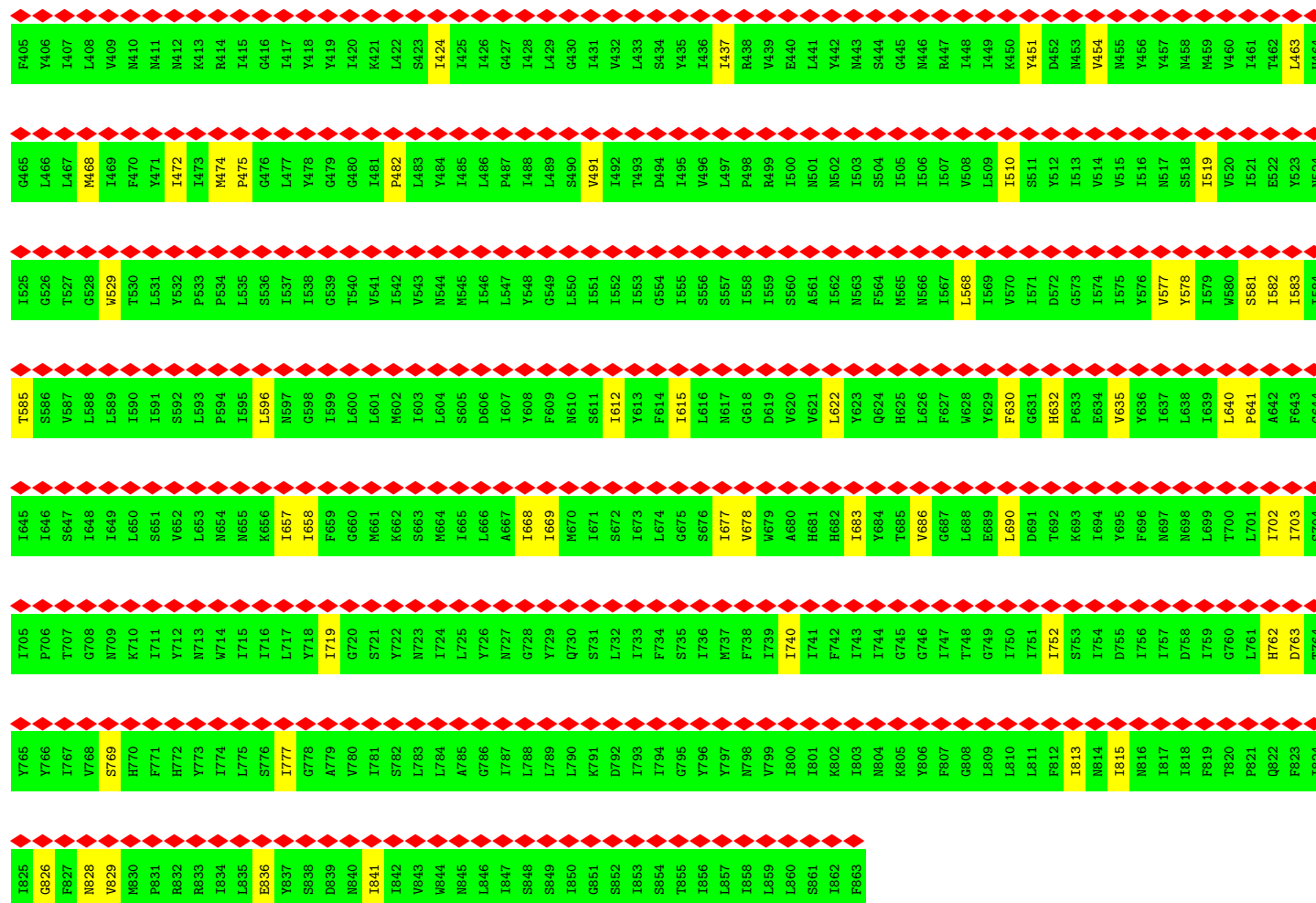
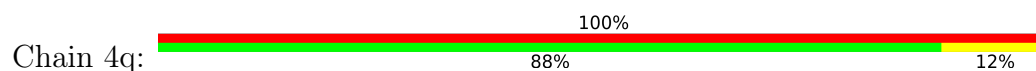


• Molecule 40: Cytochrome c oxidase subunit 1





• Molecule 40: Cytochrome c oxidase subunit 1



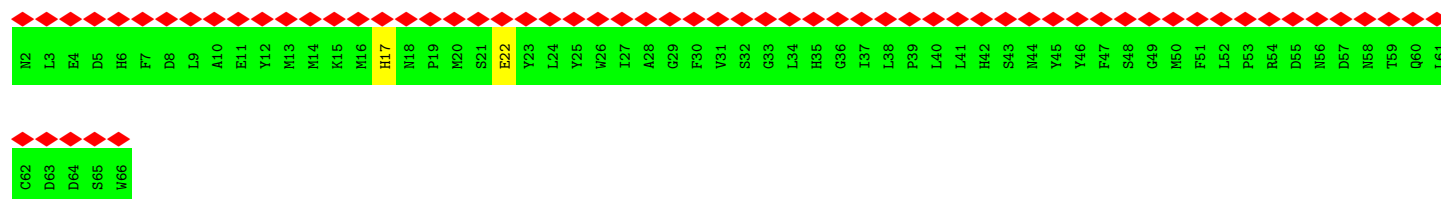
• Molecule 41: Cytochrome c oxidase subunit 32



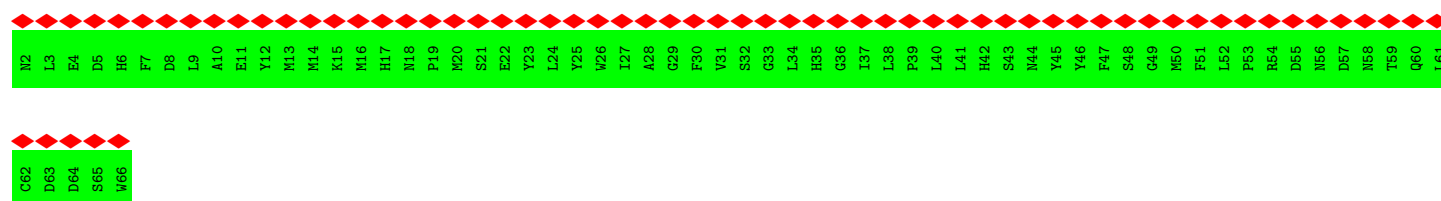
• Molecule 41: Cytochrome c oxidase subunit 32



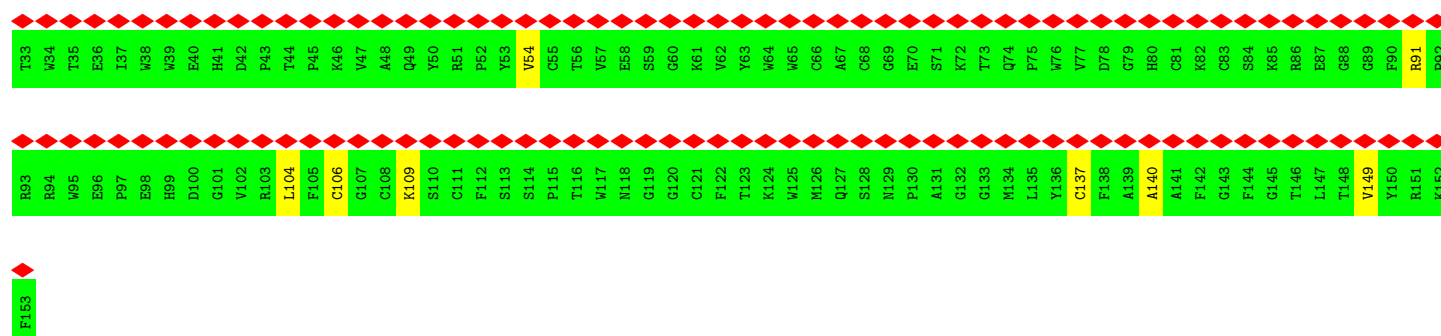
• Molecule 42: Cytochrome c oxidase subunit 7C



• Molecule 42: Cytochrome c oxidase subunit 7C

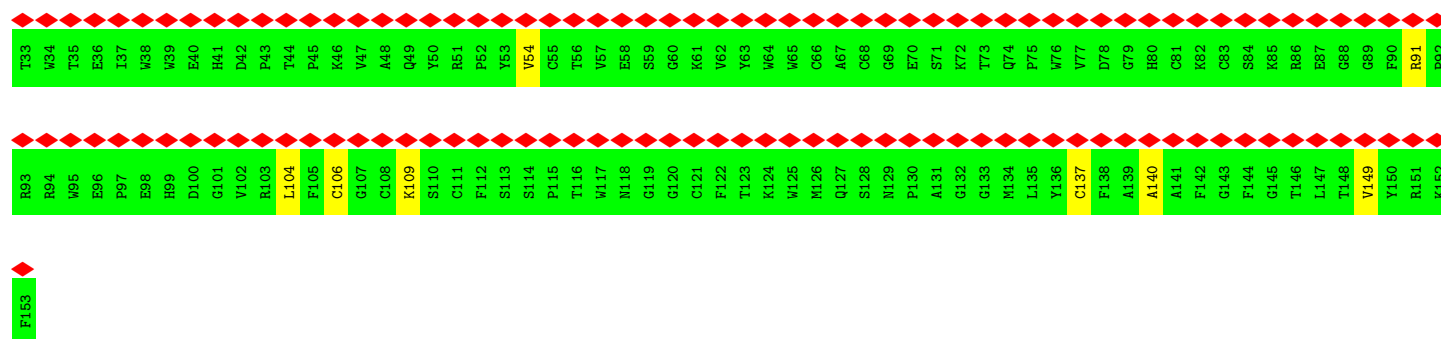


• Molecule 43: Cytochrome c oxidase subunit 13

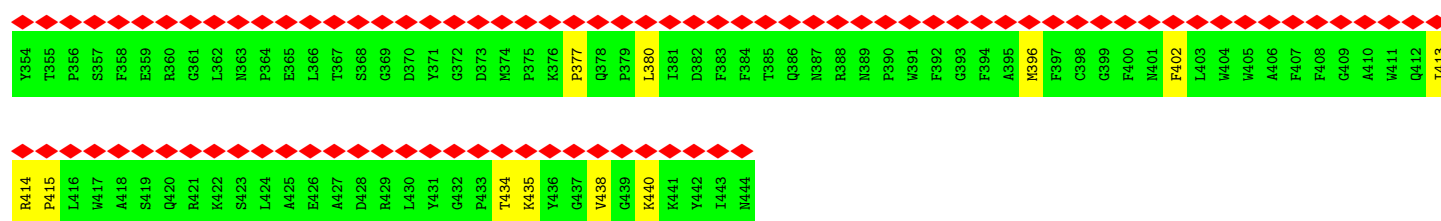
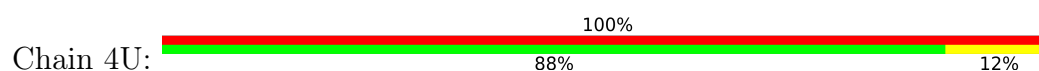


• Molecule 43: Cytochrome c oxidase subunit 13

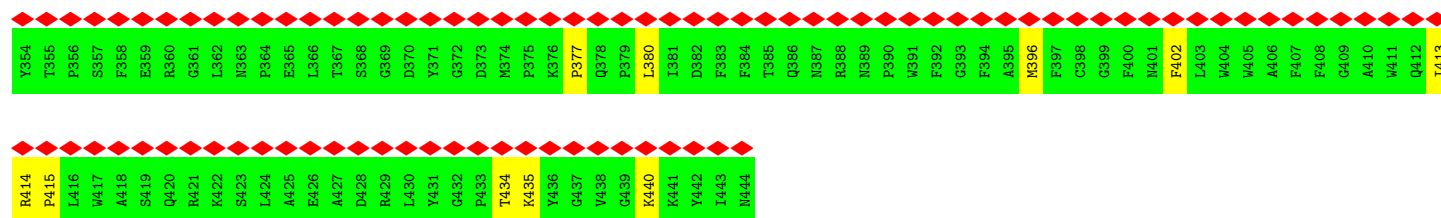
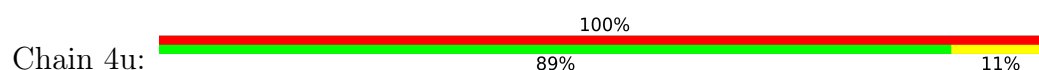




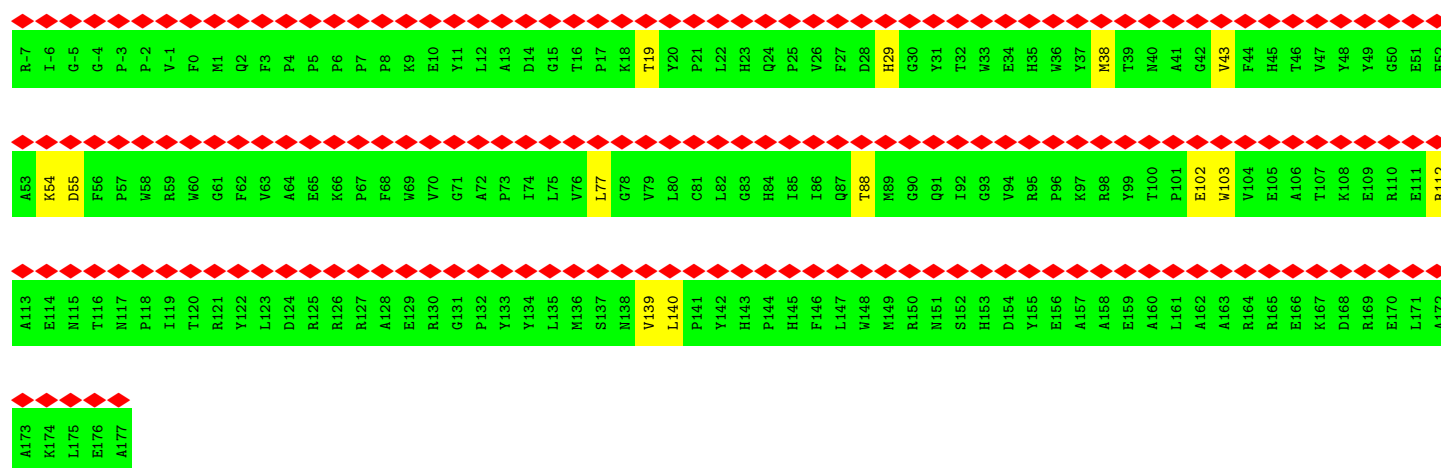
• Molecule 44: Amino acid transporter transmembrane domain-containing protein



• Molecule 44: Amino acid transporter transmembrane domain-containing protein

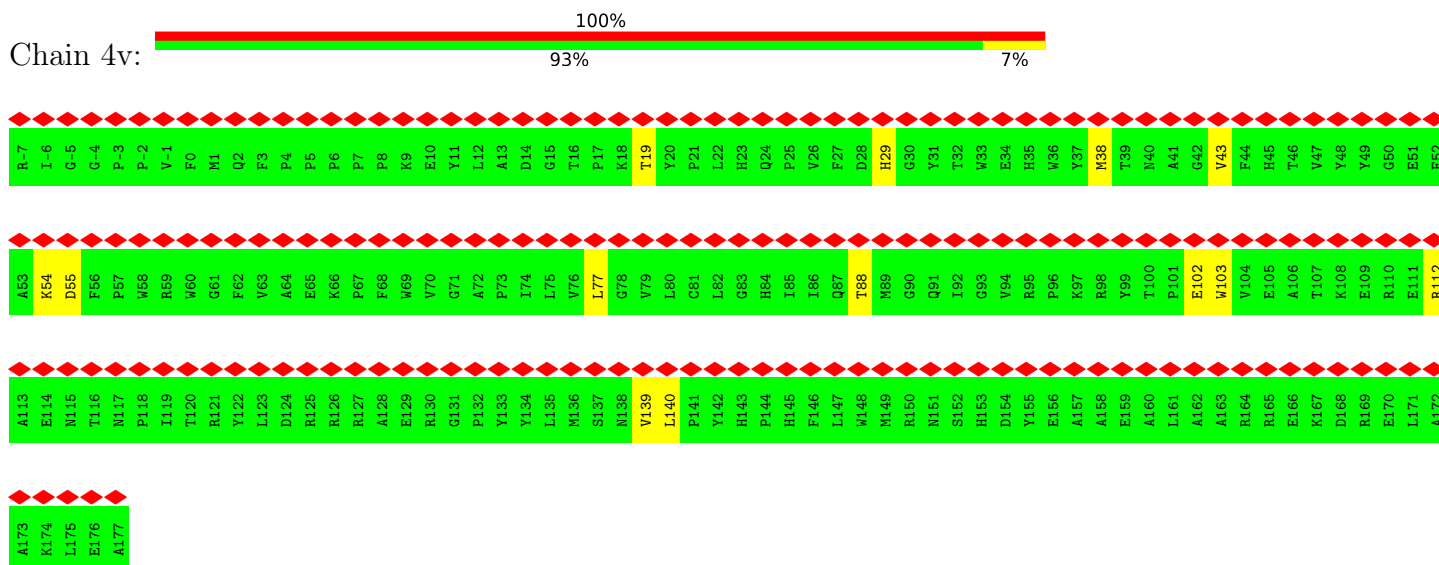


• Molecule 45: Cytochrome c oxidase subunit 4



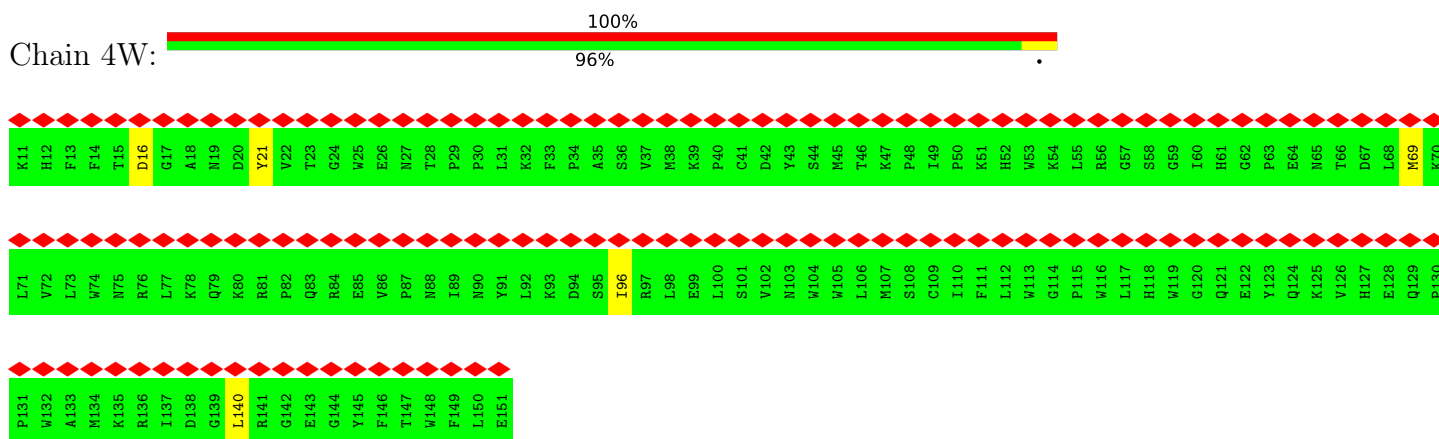
- Molecule 45: Cytochrome c oxidase subunit 4

Chain 4v:



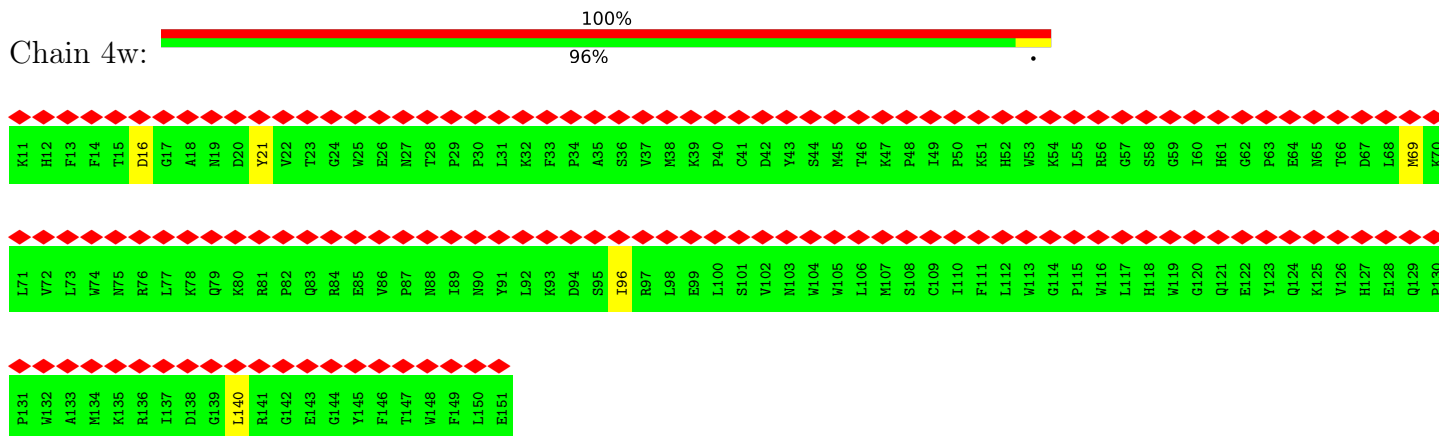
- Molecule 46: Cytochrome c oxidase subunit 19

Chain 4W:



- Molecule 46: Cytochrome c oxidase subunit 19

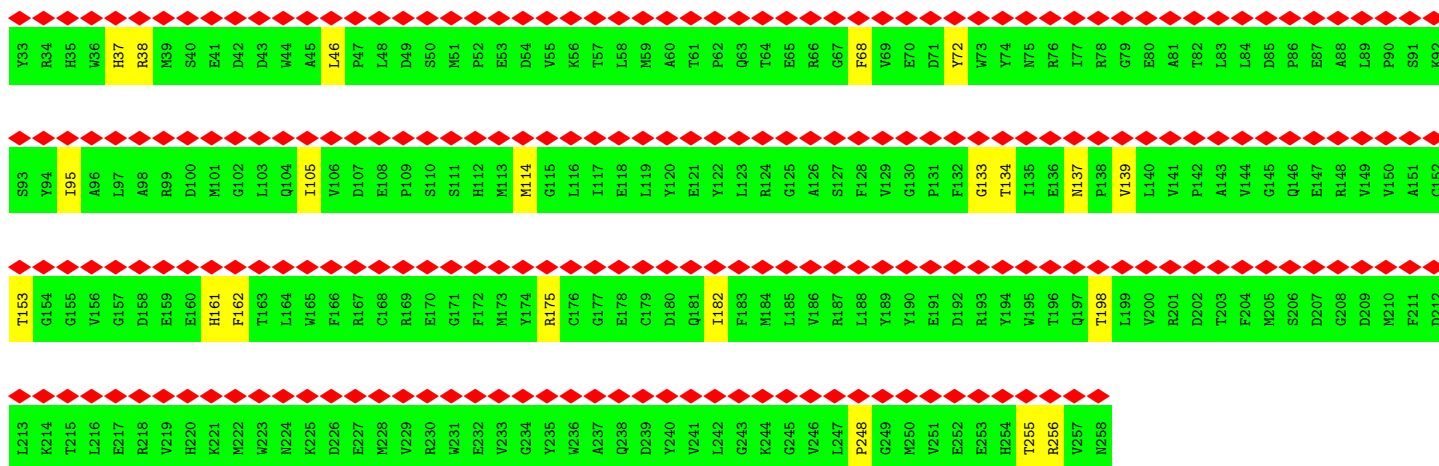
Chain 4w:



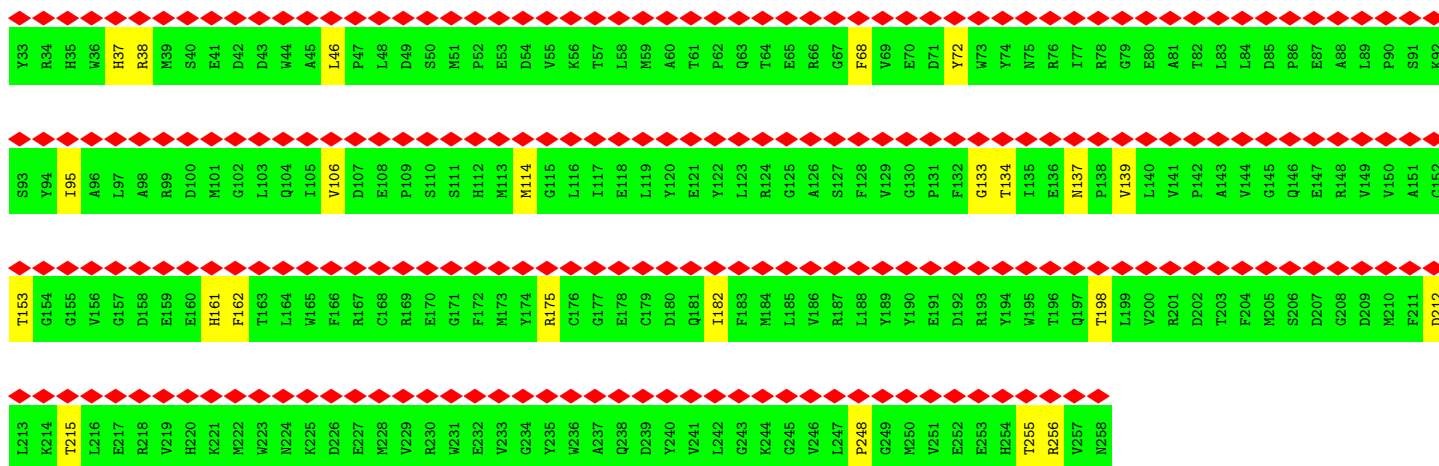
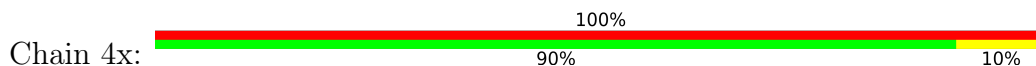
- Molecule 47: Cytochrome Coxidase subunit, putative

Chain 4X:

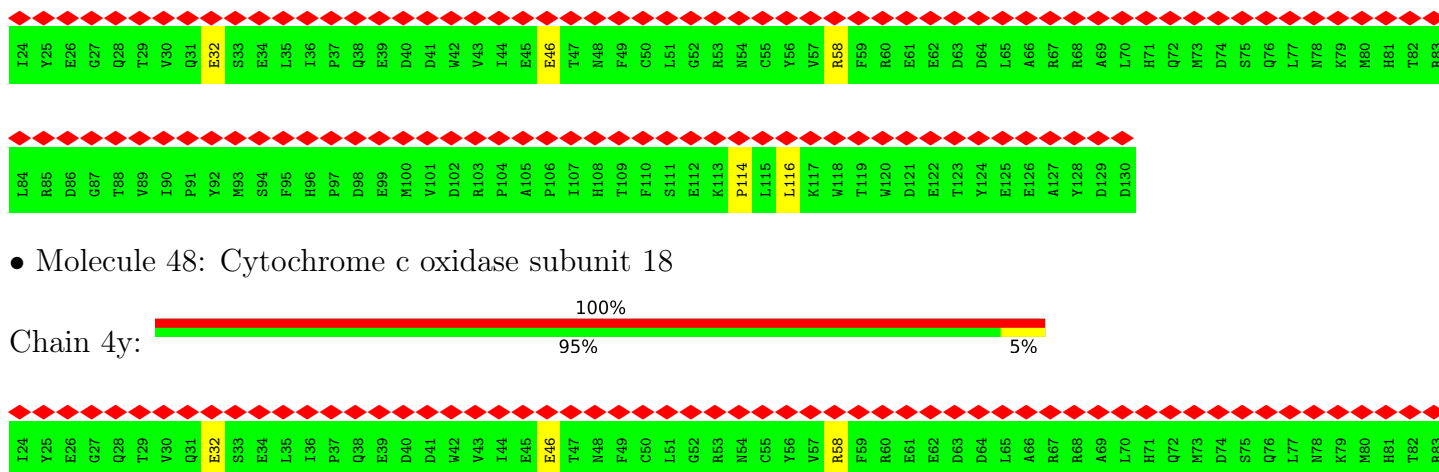




• Molecule 47: Cytochrome Oxidase subunit, putative

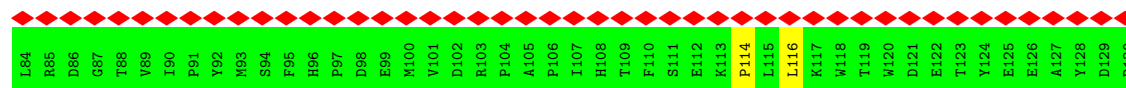


• Molecule 48: Cytochrome c oxidase subunit 18

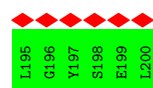
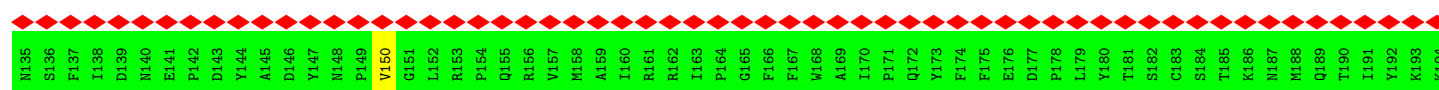
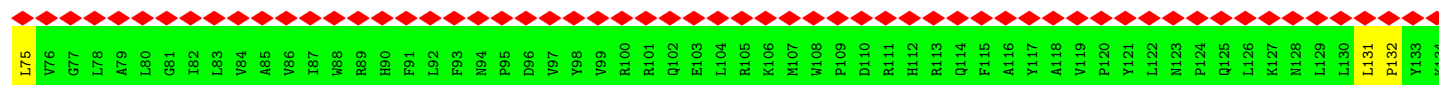
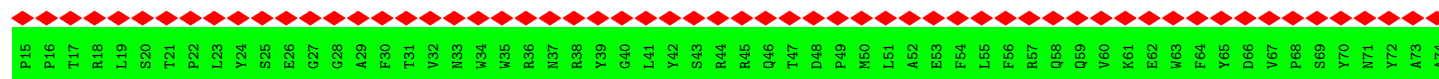


• Molecule 48: Cytochrome c oxidase subunit 18

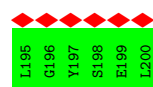
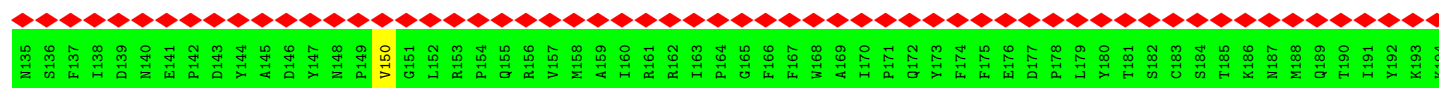




• Molecule 49: Cytochrome c oxidase subunit 31



• Molecule 49: Cytochrome c oxidase subunit 31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296890	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0203	Depositor
Map size ($\text{\AA}$)	423.2, 423.2, 423.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, UQ8, HEM, AJP, F3S, CDL, PER, HEA, K, ACE, HEC, MG, PEE, PC1, FAD, SF4, CU, ZN, CUA, FES

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	2M	0.16	0/4709	0.29	0/6372
1	2m	0.16	0/4709	0.29	0/6372
2	2N	0.20	0/2118	0.27	0/2863
2	2n	0.20	0/2118	0.27	0/2863
3	2O	0.24	0/1292	0.25	0/1759
3	2o	0.24	0/1292	0.25	0/1759
4	2P	0.23	0/1342	0.25	0/1812
4	2p	0.23	0/1342	0.25	0/1812
5	2Q	0.22	0/580	0.31	0/788
5	2q	0.22	0/580	0.31	0/788
6	2R	0.25	0/985	0.26	0/1336
6	2r	0.25	0/985	0.26	0/1336
7	2S	0.24	0/1350	0.23	0/1828
7	2s	0.24	0/1350	0.23	0/1828
8	2T	0.27	0/714	0.24	0/971
8	2t	0.27	0/714	0.24	0/971
9	2U	0.23	0/400	0.22	0/547
9	2u	0.23	0/400	0.22	0/547
10	2V	0.19	0/724	0.21	0/975
10	2v	0.19	0/724	0.21	0/975
11	3A	0.25	0/3701	0.32	0/5025
11	3a	0.25	0/3701	0.32	0/5025
12	3B	0.26	0/3967	0.26	0/5371
12	3b	0.26	0/3967	0.26	0/5371
13	3C	0.39	0/1988	0.44	0/2712
13	3c	0.39	0/1988	0.44	0/2712
14	3D	0.30	0/872	0.28	0/1182
14	3d	0.30	0/872	0.28	0/1182
15	3E	0.31	0/848	0.25	0/1148
15	3e	0.31	0/848	0.25	0/1148
16	3F	0.31	0/767	0.30	0/1042

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	3f	0.31	0/767	0.30	0/1042
17	3G	0.31	0/3098	0.30	0/4231
17	3g	0.31	0/3098	0.30	0/4231
18	3H	0.22	0/2713	0.32	0/3693
18	3h	0.22	0/2713	0.32	0/3693
19	3I	0.28	0/1514	0.33	0/2045
19	3i	0.28	0/1514	0.33	0/2045
20	3J	0.20	0/776	0.29	0/1045
20	3j	0.20	0/776	0.29	0/1045
21	3K	0.23	0/627	0.28	0/847
21	3k	0.23	0/627	0.28	0/847
22	3L	0.26	0/521	0.50	2/713 (0.3%)
22	3l	0.26	0/521	0.50	2/713 (0.3%)
23	40	0.20	0/2060	0.27	0/2822
23	41	0.20	0/2060	0.27	0/2822
24	4A	0.18	0/863	0.25	0/1166
24	4a	0.18	0/863	0.25	0/1166
25	4B	0.20	0/751	0.31	0/1013
25	4b	0.20	0/751	0.31	0/1013
26	4C	0.18	0/653	0.31	0/891
26	4c	0.18	0/653	0.31	0/891
27	4D	0.19	0/819	0.24	0/1110
27	4d	0.19	0/819	0.23	0/1110
28	4E	0.20	0/1353	0.27	0/1824
28	4e	0.20	0/1353	0.27	0/1824
29	4F	0.18	0/638	0.26	0/870
29	4f	0.18	0/638	0.26	0/870
30	4G	0.18	0/883	0.22	0/1199
30	4g	0.18	0/883	0.22	0/1199
31	4H	0.18	0/1149	0.22	0/1565
31	4h	0.18	0/1149	0.22	0/1565
32	4I	0.21	0/1757	0.24	0/2386
32	4i	0.21	0/1757	0.24	0/2386
33	4J	0.20	0/1573	0.24	0/2131
33	4j	0.20	0/1573	0.24	0/2131
34	4K	0.17	0/745	0.22	0/1017
34	4k	0.17	0/745	0.22	0/1017
35	4L	0.21	0/1131	0.26	0/1537
35	4l	0.21	0/1131	0.26	0/1537
36	4M	0.18	0/800	0.22	0/1097
36	4m	0.18	0/800	0.22	0/1097
37	4N	0.19	0/1055	0.27	0/1436
37	4n	0.19	0/1055	0.27	0/1436

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	4O	0.20	0/400	0.24	0/549
38	4o	0.20	0/400	0.24	0/549
39	4P	0.19	0/1551	0.25	0/2106
39	4p	0.19	0/1551	0.25	0/2106
40	4Q	0.19	0/3774	0.30	0/5155
40	4q	0.19	0/3774	0.30	0/5155
41	4R	0.18	0/958	0.20	0/1301
41	4r	0.18	0/958	0.20	0/1301
42	4S	0.18	0/560	0.23	0/760
42	4s	0.18	0/560	0.23	0/760
43	4T	0.20	0/1024	0.27	0/1391
43	4t	0.20	0/1024	0.27	0/1391
44	4U	0.16	0/790	0.31	0/1073
44	4u	0.16	0/790	0.31	0/1073
45	4V	0.19	0/1600	0.24	0/2183
45	4v	0.19	0/1600	0.24	0/2183
46	4W	0.19	0/1240	0.29	0/1686
46	4w	0.19	0/1240	0.29	0/1686
47	4X	0.19	0/1912	0.23	0/2592
47	4x	0.19	0/1912	0.23	0/2592
48	4Y	0.19	0/929	0.24	0/1261
48	4y	0.19	0/929	0.24	0/1261
49	4Z	0.22	0/1639	0.24	0/2233
49	4z	0.22	0/1639	0.24	0/2233
All	All	0.23	0/136426	0.28	4/185318 (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
2	2N	0	1
2	2n	0	1
4	2P	0	1
4	2p	0	1
6	2R	0	1
6	2r	0	1
11	3A	0	1
11	3a	0	1
13	3C	0	1
13	3c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	3H	0	2
18	3h	0	2
26	4C	0	1
26	4c	0	1
28	4E	0	1
28	4e	0	1
All	All	0	18

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	609	PRO	N-CA-CB	7.75	110.20	103.31
22	3l	609	PRO	N-CA-CB	7.74	110.19	103.31
22	3L	605	PRO	N-CA-CB	6.97	109.94	103.46
22	3l	605	PRO	N-CA-CB	6.95	109.92	103.46

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2N	73	ARG	Sidechain
4	2P	41	ARG	Sidechain
6	2R	5	ARG	Sidechain
11	3A	71	ARG	Sidechain
13	3C	180	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2M	4610	0	4538	28	0
1	2m	4610	0	4538	29	0
2	2N	2068	0	2025	6	0
2	2n	2068	0	2025	7	0
3	2O	1254	0	1263	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2o	1254	0	1263	7	0
4	2P	1309	0	1367	11	0
4	2p	1309	0	1367	11	0
5	2Q	564	0	567	6	0
5	2q	564	0	567	6	0
6	2R	950	0	935	12	0
6	2r	950	0	935	10	0
7	2S	1323	0	1261	9	0
7	2s	1323	0	1261	9	0
8	2T	695	0	672	9	0
8	2t	695	0	672	9	0
9	2U	390	0	369	7	0
9	2u	390	0	369	6	0
10	2V	709	0	723	3	0
10	2v	709	0	723	4	0
11	3A	3622	0	3508	8	0
11	3a	3622	0	3508	8	0
12	3B	3884	0	3842	10	0
12	3b	3884	0	3842	9	0
13	3C	1921	0	1816	8	0
13	3c	1921	0	1816	6	0
14	3D	836	0	798	5	0
14	3d	836	0	798	5	0
15	3E	813	0	776	5	0
15	3e	813	0	776	4	0
16	3F	734	0	704	2	0
16	3f	734	0	704	2	0
17	3G	3016	0	3162	28	0
17	3g	3016	0	3162	28	0
18	3H	2628	0	2541	26	0
18	3h	2628	0	2541	26	0
19	3I	1472	0	1436	7	0
19	3i	1472	0	1436	7	0
20	3J	755	0	693	1	0
20	3j	755	0	693	1	0
21	3K	608	0	617	2	0
21	3k	608	0	617	3	0
22	3L	509	0	475	5	0
22	3l	509	0	475	5	0
23	40	2004	0	2032	17	0
23	41	2004	0	2032	17	0
24	4A	841	0	766	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4a	841	0	766	9	0
25	4B	732	0	746	6	0
25	4b	732	0	746	6	0
26	4C	626	0	575	10	0
26	4c	626	0	575	10	0
27	4D	787	0	745	6	0
27	4d	787	0	745	5	0
28	4E	1313	0	1269	7	0
28	4e	1313	0	1269	7	0
29	4F	613	0	591	3	0
29	4f	613	0	591	3	0
30	4G	854	0	811	1	0
30	4g	854	0	811	1	0
31	4H	1125	0	1112	6	0
31	4h	1125	0	1112	7	0
32	4I	1695	0	1593	7	0
32	4i	1695	0	1593	8	0
33	4J	1517	0	1435	10	0
33	4j	1517	0	1435	11	0
34	4K	722	0	760	5	0
34	4k	722	0	760	5	0
35	4L	1083	0	1027	5	0
35	4l	1083	0	1027	5	0
36	4M	773	0	797	7	0
36	4m	773	0	797	7	0
37	4N	1025	0	1018	6	0
37	4n	1025	0	1018	6	0
38	4O	383	0	368	3	0
38	4o	383	0	368	3	0
39	4P	1504	0	1461	8	0
39	4p	1504	0	1461	9	0
40	4Q	3687	0	3955	41	0
40	4q	3687	0	3955	42	0
41	4R	916	0	854	2	0
41	4r	916	0	854	3	0
42	4S	541	0	489	1	0
42	4s	541	0	489	0	0
43	4T	983	0	902	9	0
43	4t	983	0	902	9	0
44	4U	758	0	713	10	0
44	4u	758	0	713	9	0
45	4V	1539	0	1482	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	4v	1539	0	1482	11	0
46	4W	1193	0	1164	6	0
46	4w	1193	0	1164	6	0
47	4X	1860	0	1764	16	0
47	4x	1860	0	1764	17	0
48	4Y	905	0	835	5	0
48	4y	905	0	835	5	0
49	4Z	1582	0	1548	4	0
49	4z	1582	0	1548	4	0
50	2M	53	0	31	11	0
50	2m	53	0	31	11	0
51	2N	4	0	0	0	0
51	2n	4	0	0	0	0
51	3H	4	0	0	1	0
51	3h	4	0	0	1	0
52	2N	8	0	0	0	0
52	2n	8	0	0	0	0
53	2N	7	0	0	0	0
53	2n	7	0	0	0	0
54	2N	1	0	0	0	0
54	2n	1	0	0	0	0
54	4Q	1	0	0	0	0
54	4q	1	0	0	0	0
55	2O	51	0	82	0	0
55	2P	102	0	164	0	0
55	2R	51	0	82	0	0
55	2o	51	0	82	0	0
55	2p	102	0	164	0	0
55	2r	51	0	82	0	0
55	3C	51	0	82	1	0
55	3F	51	0	82	1	0
55	3c	51	0	82	1	0
55	3f	51	0	82	1	0
55	40	153	0	246	1	0
55	41	153	0	246	1	0
55	4D	51	0	82	0	0
55	4Q	102	0	164	2	0
55	4R	51	0	82	0	0
55	4S	51	0	82	0	0
55	4W	51	0	82	0	0
55	4Z	51	0	82	0	0
55	4d	51	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	4q	102	0	164	2	0
55	4r	51	0	82	0	0
55	4s	51	0	82	0	0
55	4w	51	0	82	0	0
55	4z	51	0	82	0	0
56	2O	108	0	176	5	0
56	2P	54	0	88	2	0
56	2R	54	0	88	1	0
56	2T	54	0	88	1	0
56	2o	108	0	176	5	0
56	2p	54	0	88	2	0
56	2r	54	0	88	1	0
56	2t	54	0	88	1	0
56	3A	108	0	176	2	0
56	3H	54	0	88	0	0
56	3a	108	0	176	2	0
56	3h	54	0	88	0	0
56	4E	54	0	88	2	0
56	4e	54	0	88	2	0
57	2O	100	0	156	1	0
57	2P	100	0	156	3	0
57	2Q	100	0	156	2	0
57	2U	100	0	156	2	0
57	2o	100	0	156	1	0
57	2p	100	0	156	3	0
57	2q	100	0	156	2	0
57	2u	100	0	156	2	0
57	3D	200	0	312	0	0
57	3E	300	0	468	0	0
57	3G	100	0	156	5	0
57	3H	100	0	156	1	0
57	3I	300	0	468	3	0
57	3L	200	0	312	1	0
57	3d	200	0	312	0	0
57	3e	300	0	468	0	0
57	3g	100	0	156	4	0
57	3h	100	0	156	1	0
57	3i	300	0	468	3	0
57	3l	200	0	312	1	0
57	4E	100	0	156	0	0
57	4J	100	0	156	1	0
57	4K	200	0	312	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	4L	100	0	156	0	0
57	4M	100	0	156	0	0
57	4Q	200	0	312	3	0
57	4S	100	0	156	0	0
57	4T	100	0	156	3	0
57	4U	100	0	156	2	0
57	4W	200	0	312	1	0
57	4Z	100	0	156	0	0
57	4e	100	0	156	0	0
57	4j	100	0	156	1	0
57	4k	200	0	312	3	0
57	4l	100	0	156	0	0
57	4m	100	0	156	0	0
57	4q	200	0	312	3	0
57	4s	100	0	156	1	0
57	4t	100	0	156	3	0
57	4u	100	0	156	2	0
57	4w	200	0	312	1	0
57	4z	100	0	156	0	0
58	2S	53	0	74	2	0
58	2s	53	0	74	2	0
58	3D	53	0	74	12	0
58	3G	106	0	148	15	0
58	3d	53	0	74	12	0
58	3g	106	0	148	15	0
59	3C	43	0	31	6	0
59	3c	43	0	31	5	0
60	3G	86	0	60	5	0
60	3g	86	0	60	5	0
61	40	43	0	0	1	0
61	41	43	0	0	1	0
62	4C	44	0	67	0	0
62	4D	44	0	67	1	0
62	4c	44	0	67	0	0
62	4d	44	0	67	1	0
63	4N	2	0	0	0	0
63	4n	2	0	0	0	0
64	4Q	1	0	0	0	0
64	4q	1	0	0	0	0
65	4Q	1	0	0	0	0
65	4q	1	0	0	0	0
66	4Q	120	0	108	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	4q	120	0	108	6	0
67	4Q	2	0	0	0	0
67	4q	2	0	0	0	0
68	4T	2	0	0	0	0
68	4X	1	0	0	0	0
68	4t	2	0	0	0	0
68	4x	1	0	0	0	0
All	All	142424	0	144688	735	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 735 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2M:76:HIS:CE1	50:2M:701:FAD:HM82	1.21	1.70
1:2m:76:HIS:CE1	50:2m:701:FAD:HM82	1.21	1.65
1:2m:76:HIS:NE2	50:2m:701:FAD:C8M	1.75	1.46
1:2M:76:HIS:NE2	50:2M:701:FAD:C8M	1.75	1.45
13:3C:76:CYS:SG	59:3C:301:HEC:HAC	1.67	1.34

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2M	602/604 (100%)	586 (97%)	15 (2%)	1 (0%)	43	51
1	2m	602/604 (100%)	586 (97%)	15 (2%)	1 (0%)	43	51
2	2N	257/259 (99%)	250 (97%)	7 (3%)	0	100	100
2	2n	257/259 (99%)	250 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2O	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
3	2o	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
4	2P	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	2p	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
5	2Q	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
5	2q	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
6	2R	115/117 (98%)	115 (100%)	0	0	100	100
6	2r	115/117 (98%)	115 (100%)	0	0	100	100
7	2S	163/165 (99%)	162 (99%)	1 (1%)	0	100	100
7	2s	163/165 (99%)	162 (99%)	1 (1%)	0	100	100
8	2T	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
8	2t	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
9	2U	46/48 (96%)	46 (100%)	0	0	100	100
9	2u	46/48 (96%)	46 (100%)	0	0	100	100
10	2V	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
10	2v	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
11	3A	452/454 (100%)	447 (99%)	5 (1%)	0	100	100
11	3a	452/454 (100%)	447 (99%)	5 (1%)	0	100	100
12	3B	494/496 (100%)	489 (99%)	5 (1%)	0	100	100
12	3b	494/496 (100%)	489 (99%)	5 (1%)	0	100	100
13	3C	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
13	3c	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
14	3D	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
14	3d	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
15	3E	90/92 (98%)	90 (100%)	0	0	100	100
15	3e	90/92 (98%)	90 (100%)	0	0	100	100
16	3F	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
16	3f	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
17	3G	352/354 (99%)	340 (97%)	12 (3%)	0	100	100
17	3g	352/354 (99%)	340 (97%)	12 (3%)	0	100	100
18	3H	324/326 (99%)	314 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	3h	324/326 (99%)	314 (97%)	10 (3%)	0	100	100
19	3I	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
19	3i	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
20	3J	90/92 (98%)	90 (100%)	0	0	100	100
20	3j	90/92 (98%)	90 (100%)	0	0	100	100
21	3K	77/79 (98%)	77 (100%)	0	0	100	100
21	3k	77/79 (98%)	77 (100%)	0	0	100	100
22	3L	67/69 (97%)	64 (96%)	2 (3%)	1 (2%)	8	6
22	3l	67/69 (97%)	64 (96%)	2 (3%)	1 (2%)	8	6
23	40	228/230 (99%)	226 (99%)	2 (1%)	0	100	100
23	41	228/230 (99%)	226 (99%)	2 (1%)	0	100	100
24	4A	98/100 (98%)	98 (100%)	0	0	100	100
24	4a	98/100 (98%)	98 (100%)	0	0	100	100
25	4B	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
25	4b	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
26	4C	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
26	4c	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
27	4D	88/90 (98%)	88 (100%)	0	0	100	100
27	4d	88/90 (98%)	88 (100%)	0	0	100	100
28	4E	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
28	4e	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
29	4F	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
29	4f	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
30	4G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
30	4g	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
31	4H	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
31	4h	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
32	4I	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
32	4i	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
33	4J	184/186 (99%)	178 (97%)	6 (3%)	0	100	100
33	4j	184/186 (99%)	178 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	4K	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
34	4k	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
35	4L	120/122 (98%)	120 (100%)	0	0	100	100
35	4l	120/122 (98%)	120 (100%)	0	0	100	100
36	4M	96/98 (98%)	96 (100%)	0	0	100	100
36	4m	96/98 (98%)	96 (100%)	0	0	100	100
37	4N	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
37	4n	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
38	4O	45/47 (96%)	45 (100%)	0	0	100	100
38	4o	45/47 (96%)	45 (100%)	0	0	100	100
39	4P	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
39	4p	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
40	4Q	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
40	4q	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
41	4R	101/103 (98%)	101 (100%)	0	0	100	100
41	4r	101/103 (98%)	101 (100%)	0	0	100	100
42	4S	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
42	4s	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
43	4T	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
43	4t	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
44	4U	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
44	4u	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
45	4V	183/185 (99%)	182 (100%)	1 (0%)	0	100	100
45	4v	183/185 (99%)	182 (100%)	1 (0%)	0	100	100
46	4W	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
46	4w	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
47	4X	224/226 (99%)	221 (99%)	3 (1%)	0	100	100
47	4x	224/226 (99%)	221 (99%)	3 (1%)	0	100	100
48	4Y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
48	4y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
49	4Z	184/186 (99%)	181 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	4z	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
All	All	16000/16196 (99%)	15719 (98%)	277 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	3L	604	PHE
22	3l	604	PHE
1	2M	26	ALA
1	2m	26	ALA

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	2M	481/481 (100%)	478 (99%)	3 (1%)	78	89
1	2m	481/481 (100%)	478 (99%)	3 (1%)	78	89
2	2N	221/221 (100%)	219 (99%)	2 (1%)	70	84
2	2n	221/221 (100%)	219 (99%)	2 (1%)	70	84
3	2O	130/130 (100%)	130 (100%)	0	100	100
3	2o	130/130 (100%)	130 (100%)	0	100	100
4	2P	139/139 (100%)	139 (100%)	0	100	100
4	2p	139/139 (100%)	139 (100%)	0	100	100
5	2Q	60/60 (100%)	60 (100%)	0	100	100
5	2q	60/60 (100%)	60 (100%)	0	100	100
6	2R	100/100 (100%)	100 (100%)	0	100	100
6	2r	100/100 (100%)	100 (100%)	0	100	100
7	2S	144/144 (100%)	144 (100%)	0	100	100
7	2s	144/144 (100%)	144 (100%)	0	100	100
8	2T	73/73 (100%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2t	73/73 (100%)	73 (100%)	0	100	100
9	2U	43/43 (100%)	43 (100%)	0	100	100
9	2u	43/43 (100%)	43 (100%)	0	100	100
10	2V	76/76 (100%)	76 (100%)	0	100	100
10	2v	76/76 (100%)	76 (100%)	0	100	100
11	3A	386/386 (100%)	386 (100%)	0	100	100
11	3a	386/386 (100%)	386 (100%)	0	100	100
12	3B	423/423 (100%)	422 (100%)	1 (0%)	87	94
12	3b	423/423 (100%)	422 (100%)	1 (0%)	87	94
13	3C	204/204 (100%)	203 (100%)	1 (0%)	81	90
13	3c	204/204 (100%)	203 (100%)	1 (0%)	81	90
14	3D	88/88 (100%)	88 (100%)	0	100	100
14	3d	88/88 (100%)	88 (100%)	0	100	100
15	3E	81/81 (100%)	81 (100%)	0	100	100
15	3e	81/81 (100%)	81 (100%)	0	100	100
16	3F	72/72 (100%)	72 (100%)	0	100	100
16	3f	72/72 (100%)	72 (100%)	0	100	100
17	3G	336/336 (100%)	334 (99%)	2 (1%)	78	89
17	3g	336/336 (100%)	334 (99%)	2 (1%)	78	89
18	3H	280/280 (100%)	280 (100%)	0	100	100
18	3h	280/280 (100%)	280 (100%)	0	100	100
19	3I	154/154 (100%)	153 (99%)	1 (1%)	78	89
19	3i	154/154 (100%)	153 (99%)	1 (1%)	78	89
20	3J	79/79 (100%)	79 (100%)	0	100	100
20	3j	79/79 (100%)	79 (100%)	0	100	100
21	3K	67/67 (100%)	67 (100%)	0	100	100
21	3k	67/67 (100%)	67 (100%)	0	100	100
22	3L	48/60 (80%)	48 (100%)	0	100	100
22	3l	48/60 (80%)	48 (100%)	0	100	100
23	40	229/229 (100%)	229 (100%)	0	100	100
23	41	229/229 (100%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	4A	91/91 (100%)	90 (99%)	1 (1%)	65	79
24	4a	91/91 (100%)	90 (99%)	1 (1%)	65	79
25	4B	77/77 (100%)	75 (97%)	2 (3%)	40	55
25	4b	77/77 (100%)	75 (97%)	2 (3%)	40	55
26	4C	64/64 (100%)	64 (100%)	0	100	100
26	4c	64/64 (100%)	64 (100%)	0	100	100
27	4D	81/81 (100%)	81 (100%)	0	100	100
27	4d	81/81 (100%)	81 (100%)	0	100	100
28	4E	146/146 (100%)	146 (100%)	0	100	100
28	4e	146/146 (100%)	146 (100%)	0	100	100
29	4F	63/63 (100%)	63 (100%)	0	100	100
29	4f	63/63 (100%)	63 (100%)	0	100	100
30	4G	83/83 (100%)	82 (99%)	1 (1%)	63	78
30	4g	83/83 (100%)	82 (99%)	1 (1%)	63	78
31	4H	124/124 (100%)	124 (100%)	0	100	100
31	4h	124/124 (100%)	124 (100%)	0	100	100
32	4I	180/180 (100%)	178 (99%)	2 (1%)	65	79
32	4i	180/180 (100%)	178 (99%)	2 (1%)	65	79
33	4J	148/148 (100%)	145 (98%)	3 (2%)	48	64
33	4j	148/148 (100%)	145 (98%)	3 (2%)	48	64
34	4K	77/77 (100%)	77 (100%)	0	100	100
34	4k	77/77 (100%)	77 (100%)	0	100	100
35	4L	108/108 (100%)	108 (100%)	0	100	100
35	4l	108/108 (100%)	108 (100%)	0	100	100
36	4M	85/85 (100%)	85 (100%)	0	100	100
36	4m	85/85 (100%)	85 (100%)	0	100	100
37	4N	112/112 (100%)	112 (100%)	0	100	100
37	4n	112/112 (100%)	112 (100%)	0	100	100
38	4O	40/40 (100%)	40 (100%)	0	100	100
38	4o	40/40 (100%)	40 (100%)	0	100	100
39	4P	163/163 (100%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	4p	163/163 (100%)	163 (100%)	0	100	100
40	4Q	419/419 (100%)	417 (100%)	2 (0%)	81	90
40	4q	419/419 (100%)	417 (100%)	2 (0%)	81	90
41	4R	92/92 (100%)	92 (100%)	0	100	100
41	4r	92/92 (100%)	92 (100%)	0	100	100
42	4S	59/59 (100%)	59 (100%)	0	100	100
42	4s	59/59 (100%)	59 (100%)	0	100	100
43	4T	102/102 (100%)	102 (100%)	0	100	100
43	4t	102/102 (100%)	102 (100%)	0	100	100
44	4U	76/76 (100%)	75 (99%)	1 (1%)	61	76
44	4u	76/76 (100%)	75 (99%)	1 (1%)	61	76
45	4V	156/156 (100%)	154 (99%)	2 (1%)	61	76
45	4v	156/156 (100%)	154 (99%)	2 (1%)	61	76
46	4W	128/128 (100%)	128 (100%)	0	100	100
46	4w	128/128 (100%)	128 (100%)	0	100	100
47	4X	198/198 (100%)	197 (100%)	1 (0%)	81	90
47	4x	198/198 (100%)	197 (100%)	1 (0%)	81	90
48	4Y	100/100 (100%)	100 (100%)	0	100	100
48	4y	100/100 (100%)	100 (100%)	0	100	100
49	4Z	167/167 (100%)	167 (100%)	0	100	100
49	4z	167/167 (100%)	167 (100%)	0	100	100
All	All	14106/14130 (100%)	14056 (100%)	50 (0%)	81	92

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2n	80	CYS
24	4a	26	ASP
47	4x	37	HIS
2	2n	278	MET
17	3g	251	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
33	4j	64	HIS
35	4l	96	ASN
46	4w	61	HIS
33	4J	64	HIS
32	4I	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 162 ligands modelled in this entry, 14 are monoatomic - leaving 148 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	$\# Z > 2$
57	CDL	4S	101	-	99,99,99	0.28	0	105,111,111	0.39	0
57	CDL	4q	907	-	99,99,99	0.29	0	105,111,111	0.48	1 (0%)
57	CDL	4k	201	-	99,99,99	0.28	0	105,111,111	0.33	0
57	CDL	4K	201	-	99,99,99	0.28	0	105,111,111	0.33	0
57	CDL	2u	101	-	99,99,99	0.29	0	105,111,111	0.31	0
62	LPP	4C	101	-	43,43,43	0.26	0	46,48,48	0.34	0
56	PC1	2T	101	-	53,53,53	0.29	0	59,61,61	0.35	0
57	CDL	3e	202	-	99,99,99	0.29	0	105,111,111	0.37	0
55	PEE	4r	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	4l	201	-	99,99,99	0.28	0	105,111,111	0.34	0
57	CDL	3H	402	-	99,99,99	0.30	0	105,111,111	0.41	0
51	FES	2N	301	2	0,4,4	-	-	-		
66	HEA	4q	904	40	67,67,67	1.37	7 (10%)	81,103,103	2.08	25 (30%)
58	UQ8	3G	405	-	53,53,53	1.86	6 (11%)	66,67,67	1.53	15 (22%)
55	PEE	4W	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
61	AJP	4l	304	-	49,49,95	1.08	3 (6%)	75,80,149	1.56	13 (17%)
55	PEE	4Z	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.54	0
57	CDL	2U	101	-	99,99,99	0.29	0	105,111,111	0.31	0
51	FES	2n	301	2	0,4,4	-	-	-		
55	PEE	4l	303	-	50,50,50	0.79	2 (4%)	53,55,55	0.53	0
57	CDL	3l	702	-	99,99,99	0.30	0	105,111,111	0.32	0
55	PEE	2R	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.50	0
55	PEE	2o	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.66	0
55	PEE	4Q	910	-	50,50,50	0.79	2 (4%)	53,55,55	0.61	1 (1%)
57	CDL	4s	101	-	99,99,99	0.28	0	105,111,111	0.39	0
63	CUA	4n	201	37	0,1,1	-	-	-		
57	CDL	4j	301	-	99,99,99	0.29	0	105,111,111	0.43	0
60	HEM	3g	402	17	50,50,50	1.47	7 (14%)	67,82,82	1.32	7 (10%)
57	CDL	4Q	907	-	99,99,99	0.29	0	105,111,111	0.48	1 (0%)
56	PC1	2t	101	-	53,53,53	0.29	0	59,61,61	0.35	0
57	CDL	2p	201	-	99,99,99	0.29	0	105,111,111	0.33	0
58	UQ8	3g	405	-	53,53,53	1.87	6 (11%)	66,67,67	1.53	15 (22%)
55	PEE	40	301	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
56	PC1	3A	502	-	53,53,53	0.30	0	59,61,61	0.41	0
55	PEE	2r	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.50	0
50	FAD	2M	701	-	58,58,58	0.70	3 (5%)	85,89,89	0.97	4 (4%)
57	CDL	3D	201	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
55	PEE	4d	101	-	50,50,50	0.77	2 (4%)	53,55,55	0.48	0
55	PEE	2P	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.57	0
58	UQ8	3G	404	-	53,53,53	1.83	6 (11%)	66,67,67	1.72	17 (25%)
57	CDL	4M	201	-	99,99,99	0.28	0	105,111,111	0.30	0
57	CDL	4q	908	-	99,99,99	0.29	0	105,111,111	0.33	0
57	CDL	4w	201	-	99,99,99	0.28	0	105,111,111	0.34	0
50	FAD	2m	701	-	58,58,58	0.70	3 (5%)	85,89,89	0.97	4 (4%)
57	CDL	2P	201	-	99,99,99	0.29	0	105,111,111	0.33	0
57	CDL	3d	201	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
57	CDL	3i	203	-	99,99,99	0.29	0	105,111,111	0.46	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	PER	4Q	906	64,66	1,1,1	0.18	0	-		
55	PEE	2P	202	-	50,50,50	0.77	2 (4%)	53,55,55	0.52	0
56	PC1	2O	203	-	53,53,53	0.28	0	59,61,61	0.57	1 (1%)
55	PEE	2O	201	-	50,50,50	0.78	2 (4%)	53,55,55	0.66	0
57	CDL	3e	201	-	99,99,99	0.30	0	105,111,111	0.44	0
57	CDL	2q	101	-	99,99,99	0.29	0	105,111,111	0.37	1 (0%)
57	CDL	3h	402	-	99,99,99	0.30	0	105,111,111	0.41	0
57	CDL	4k	202	-	99,99,99	0.28	0	105,111,111	0.41	0
56	PC1	2O	202	-	53,53,53	0.28	0	59,61,61	0.42	0
55	PEE	2p	202	-	50,50,50	0.77	2 (4%)	53,55,55	0.52	0
60	HEM	3G	401	17	50,50,50	1.50	7 (14%)	67,82,82	1.26	5 (7%)
57	CDL	4J	301	-	99,99,99	0.29	0	105,111,111	0.43	0
55	PEE	40	303	-	50,50,50	0.79	2 (4%)	53,55,55	0.53	0
55	PEE	4R	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.58	0
57	CDL	4L	201	-	99,99,99	0.29	0	105,111,111	0.34	0
57	CDL	4z	301	-	99,99,99	0.28	0	105,111,111	0.43	1 (0%)
57	CDL	4m	201	-	99,99,99	0.28	0	105,111,111	0.30	0
57	CDL	3E	202	-	99,99,99	0.29	0	105,111,111	0.37	0
58	UQ8	2S	201	-	53,53,53	1.84	7 (13%)	66,67,67	1.62	16 (24%)
57	CDL	3D	202	-	99,99,99	0.32	0	105,111,111	0.47	0
57	CDL	4Q	908	-	99,99,99	0.29	0	105,111,111	0.33	0
57	CDL	2o	201	-	99,99,99	0.29	0	105,111,111	0.32	0
57	CDL	2Q	101	-	99,99,99	0.29	0	105,111,111	0.37	1 (0%)
55	PEE	4q	909	-	50,50,50	0.77	2 (4%)	53,55,55	0.65	1 (1%)
57	CDL	3I	203	-	99,99,99	0.30	0	105,111,111	0.39	0
56	PC1	3a	501	-	53,53,53	0.30	0	59,61,61	0.55	1 (1%)
59	HEC	3c	301	13	46,50,50	1.96	6 (13%)	58,82,82	1.78	5 (8%)
60	HEM	3G	402	17	50,50,50	1.47	7 (14%)	67,82,82	1.32	7 (10%)
62	LPP	4d	102	-	43,43,43	0.21	0	46,48,48	0.31	0
56	PC1	2r	202	-	53,53,53	0.29	0	59,61,61	0.46	0
58	UQ8	3D	203	-	53,53,53	1.90	5 (9%)	66,67,67	1.66	12 (18%)
57	CDL	3G	403	-	99,99,99	0.30	0	105,111,111	0.40	1 (0%)
57	CDL	4e	201	-	99,99,99	0.28	0	105,111,111	0.40	0
57	CDL	4W	201	-	99,99,99	0.28	0	105,111,111	0.34	0
58	UQ8	3d	203	-	53,53,53	1.90	5 (9%)	66,67,67	1.66	12 (18%)
56	PC1	4e	202	-	53,53,53	0.29	0	59,61,61	0.46	0
57	CDL	4T	203	-	99,99,99	0.29	0	105,111,111	0.29	0
55	PEE	4Q	909	-	50,50,50	0.76	2 (4%)	53,55,55	0.65	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	CDL	3i	201	-	99,99,99	0.30	0	105,111,111	0.39	0
63	CUA	4N	201	37	0,1,1	-	-	-		
55	PEE	3C	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.68	1 (1%)
56	PC1	3a	502	-	53,53,53	0.30	0	59,61,61	0.41	0
53	F3S	2N	303	2	0,9,9	-	-	-		
52	SF4	2n	302	2	0,12,12	-	-	-		
55	PEE	4D	101	-	50,50,50	0.77	2 (4%)	53,55,55	0.48	0
55	PEE	3c	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.68	1 (1%)
57	CDL	4U	501	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
57	CDL	3e	203	-	99,99,99	0.28	0	105,111,111	0.40	1 (0%)
62	LPP	4D	102	-	43,43,43	0.21	0	46,48,48	0.31	0
56	PC1	4E	202	-	53,53,53	0.29	0	59,61,61	0.46	0
57	CDL	2O	204	-	99,99,99	0.29	0	105,111,111	0.32	0
51	FES	3h	401	18	0,4,4	-	-	-		
57	CDL	3g	403	-	99,99,99	0.31	0	105,111,111	0.40	1 (0%)
61	AJP	40	304	-	49,49,95	1.08	3 (6%)	75,80,149	1.56	13 (17%)
59	HEC	3C	301	13	46,50,50	1.95	6 (13%)	58,82,82	1.78	6 (10%)
53	F3S	2n	303	2	0,9,9	-	-	-		
66	HEA	4Q	905	67,40	67,67,67	1.36	9 (13%)	81,103,103	2.05	24 (29%)
51	FES	3H	401	18	0,4,4	-	-	-		
56	PC1	2p	204	-	53,53,53	0.28	0	59,61,61	0.36	0
66	HEA	4Q	904	40	67,67,67	1.37	7 (10%)	81,103,103	2.08	25 (30%)
57	CDL	3I	202	-	99,99,99	0.29	0	105,111,111	0.46	1 (0%)
57	CDL	3d	202	-	99,99,99	0.31	0	105,111,111	0.47	0
55	PEE	4I	301	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
56	PC1	2o	203	-	53,53,53	0.28	0	59,61,61	0.42	0
57	CDL	3i	202	-	99,99,99	0.29	0	105,111,111	0.47	1 (0%)
57	CDL	4t	203	-	99,99,99	0.29	0	105,111,111	0.29	0
57	CDL	4w	202	-	99,99,99	0.28	0	105,111,111	0.33	0
55	PEE	40	302	-	50,50,50	0.76	2 (4%)	53,55,55	0.51	0
55	PEE	4S	102	-	50,50,50	0.78	2 (4%)	53,55,55	0.55	0
60	HEM	3g	401	17	50,50,50	1.50	8 (16%)	67,82,82	1.26	5 (7%)
56	PC1	3H	403	-	53,53,53	0.30	0	59,61,61	0.42	0
57	CDL	3I	701	-	99,99,99	0.30	0	105,111,111	0.37	0
52	SF4	2N	302	2	0,12,12	-	-	-		
55	PEE	3F	101	-	50,50,50	0.78	2 (4%)	53,55,55	0.58	0
55	PEE	4I	302	-	50,50,50	0.76	2 (4%)	53,55,55	0.51	0
57	CDL	4Z	301	-	99,99,99	0.28	0	105,111,111	0.43	1 (0%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PC1	2o	204	-	53,53,53	0.28	0	59,61,61	0.57	1 (1%)
57	CDL	3E	203	-	99,99,99	0.29	0	105,111,111	0.40	1 (0%)
67	PER	4q	906	64,66	1,1,1	0.18	0	-		
57	CDL	3I	201	-	99,99,99	0.29	0	105,111,111	0.47	1 (0%)
57	CDL	4W	202	-	99,99,99	0.28	0	105,111,111	0.33	0
58	UQ8	2s	201	-	53,53,53	1.84	7 (13%)	66,67,67	1.62	16 (24%)
57	CDL	4E	201	-	99,99,99	0.28	0	105,111,111	0.41	0
57	CDL	4K	202	-	99,99,99	0.28	0	105,111,111	0.41	0
62	LPP	4c	101	-	43,43,43	0.26	0	46,48,48	0.34	0
57	CDL	3L	702	-	99,99,99	0.30	0	105,111,111	0.32	0
55	PEE	2p	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.57	0
55	PEE	3f	101	-	50,50,50	0.78	2 (4%)	53,55,55	0.58	0
57	CDL	4u	501	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
55	PEE	4s	102	-	50,50,50	0.78	2 (4%)	53,55,55	0.55	0
66	HEA	4q	905	67,40	67,67,67	1.36	9 (13%)	81,103,103	2.04	24 (29%)
55	PEE	4q	910	-	50,50,50	0.79	2 (4%)	53,55,55	0.61	1 (1%)
57	CDL	3E	201	-	99,99,99	0.30	0	105,111,111	0.44	0
56	PC1	2P	204	-	53,53,53	0.28	0	59,61,61	0.36	0
55	PEE	4z	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.54	0
56	PC1	2R	202	-	53,53,53	0.29	0	59,61,61	0.46	0
56	PC1	3A	501	-	53,53,53	0.29	0	59,61,61	0.55	1 (1%)
55	PEE	4w	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
56	PC1	3h	403	-	53,53,53	0.29	0	59,61,61	0.42	0
58	UQ8	3g	404	-	53,53,53	1.83	7 (13%)	66,67,67	1.72	17 (25%)
57	CDL	3L	701	-	99,99,99	0.30	0	105,111,111	0.37	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
57	CDL	4S	101	-	-	20/110/110/110	-
57	CDL	4q	907	-	-	38/110/110/110	-
57	CDL	4k	201	-	-	28/110/110/110	-
57	CDL	4K	201	-	-	28/110/110/110	-
57	CDL	2u	101	-	-	18/110/110/110	-
62	LPP	4C	101	-	-	13/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PC1	2T	101	-	-	13/57/57/57	-
57	CDL	3e	202	-	-	26/110/110/110	-
55	PEE	4r	201	-	-	16/54/54/54	-
57	CDL	4l	201	-	-	14/110/110/110	-
57	CDL	3H	402	-	-	13/110/110/110	-
51	FES	2N	301	2	-	-	0/1/1/1
66	HEA	4q	904	40	-	7/36/76/76	-
58	UQ8	3G	405	-	-	6/51/75/75	0/1/1/1
55	PEE	4W	203	-	-	11/54/54/54	-
61	AJP	4i	304	-	3/3/19/38	3/6/121/220	0/7/7/11
55	PEE	4Z	302	-	-	24/54/54/54	-
57	CDL	2U	101	-	-	18/110/110/110	-
51	FES	2n	301	2	-	-	0/1/1/1
55	PEE	4i	303	-	-	19/54/54/54	-
57	CDL	3l	702	-	-	22/110/110/110	-
55	PEE	2R	201	-	-	18/54/54/54	-
55	PEE	2o	202	-	-	16/54/54/54	-
55	PEE	4Q	910	-	-	13/54/54/54	-
57	CDL	4s	101	-	-	20/110/110/110	-
57	CDL	4j	301	-	-	32/110/110/110	-
60	HEM	3g	402	17	-	4/14/54/54	-
57	CDL	4Q	907	-	-	38/110/110/110	-
56	PC1	2t	101	-	-	13/57/57/57	-
57	CDL	2p	201	-	-	21/110/110/110	-
58	UQ8	3g	405	-	-	6/51/75/75	0/1/1/1
55	PEE	40	301	-	-	13/54/54/54	-
56	PC1	3A	502	-	-	15/57/57/57	-
55	PEE	2r	201	-	-	18/54/54/54	-
50	FAD	2M	701	-	-	4/34/50/50	0/6/6/6
57	CDL	3D	201	-	-	38/110/110/110	-
55	PEE	4d	101	-	-	15/54/54/54	-
55	PEE	2P	203	-	-	17/54/54/54	-
58	UQ8	3G	404	-	-	14/51/75/75	0/1/1/1
57	CDL	4M	201	-	-	16/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	4q	908	-	-	19/110/110/110	-
57	CDL	4w	201	-	-	16/110/110/110	-
50	FAD	2m	701	-	-	4/34/50/50	0/6/6/6
57	CDL	2P	201	-	-	21/110/110/110	-
57	CDL	3d	201	-	-	38/110/110/110	-
57	CDL	3i	203	-	-	37/110/110/110	-
55	PEE	2P	202	-	-	18/54/54/54	-
56	PC1	2O	203	-	-	14/57/57/57	-
55	PEE	2O	201	-	-	16/54/54/54	-
57	CDL	3e	201	-	-	28/110/110/110	-
57	CDL	2q	101	-	-	31/110/110/110	-
57	CDL	3h	402	-	-	12/110/110/110	-
57	CDL	4k	202	-	-	29/110/110/110	-
56	PC1	2O	202	-	-	9/57/57/57	-
55	PEE	2p	202	-	-	18/54/54/54	-
60	HEM	3G	401	17	-	5/14/54/54	-
57	CDL	4J	301	-	-	32/110/110/110	-
55	PEE	40	303	-	-	19/54/54/54	-
55	PEE	4R	201	-	-	16/54/54/54	-
57	CDL	4L	201	-	-	14/110/110/110	-
57	CDL	4z	301	-	-	16/110/110/110	-
57	CDL	4m	201	-	-	16/110/110/110	-
57	CDL	3E	202	-	-	26/110/110/110	-
58	UQ8	2S	201	-	-	8/51/75/75	0/1/1/1
57	CDL	3D	202	-	-	56/110/110/110	-
57	CDL	4Q	908	-	-	19/110/110/110	-
57	CDL	2o	201	-	-	21/110/110/110	-
57	CDL	2Q	101	-	-	31/110/110/110	-
55	PEE	4q	909	-	-	21/54/54/54	-
57	CDL	3I	203	-	-	22/110/110/110	-
56	PC1	3a	501	-	-	19/57/57/57	-
59	HEC	3c	301	13	-	9/14/54/54	-
60	HEM	3G	402	17	-	4/14/54/54	-
62	LPP	4d	102	-	-	5/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PC1	2r	202	-	-	16/57/57/57	-
58	UQ8	3D	203	-	-	12/51/75/75	0/1/1/1
57	CDL	3G	403	-	-	22/110/110/110	-
57	CDL	4e	201	-	-	29/110/110/110	-
57	CDL	4W	201	-	-	16/110/110/110	-
58	UQ8	3d	203	-	-	12/51/75/75	0/1/1/1
56	PC1	4e	202	-	-	10/57/57/57	-
57	CDL	4T	203	-	-	23/110/110/110	-
55	PEE	4Q	909	-	-	21/54/54/54	-
57	CDL	3i	201	-	-	22/110/110/110	-
55	PEE	3C	302	-	-	14/54/54/54	-
56	PC1	3a	502	-	-	14/57/57/57	-
53	F3S	2N	303	2	-	-	0/3/3/3
52	SF4	2n	302	2	-	-	0/6/5/5
55	PEE	4D	101	-	-	15/54/54/54	-
55	PEE	3c	302	-	-	14/54/54/54	-
57	CDL	4U	501	-	-	33/110/110/110	-
57	CDL	3e	203	-	-	36/110/110/110	-
62	LPP	4D	102	-	-	5/45/45/45	-
56	PC1	4E	202	-	-	10/57/57/57	-
57	CDL	2O	204	-	-	21/110/110/110	-
51	FES	3h	401	18	-	-	0/1/1/1
61	AJP	40	304	-	3/3/19/38	3/6/121/220	0/7/7/11
57	CDL	3g	403	-	-	22/110/110/110	-
59	HEC	3C	301	13	-	9/14/54/54	-
53	F3S	2n	303	2	-	-	0/3/3/3
66	HEA	4Q	905	67,40	-	9/36/76/76	-
51	FES	3H	401	18	-	-	0/1/1/1
56	PC1	2p	204	-	-	4/57/57/57	-
66	HEA	4Q	904	40	-	7/36/76/76	-
57	CDL	3I	202	-	-	37/110/110/110	-
57	CDL	3d	202	-	-	56/110/110/110	-
55	PEE	4I	301	-	-	13/54/54/54	-
56	PC1	2o	203	-	-	9/57/57/57	-
57	CDL	3i	202	-	-	25/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	4t	203	-	-	23/110/110/110	-
57	CDL	4w	202	-	-	28/110/110/110	-
55	PEE	40	302	-	-	5/54/54/54	-
55	PEE	4S	102	-	-	10/54/54/54	-
60	HEM	3g	401	17	-	5/14/54/54	-
56	PC1	3H	403	-	-	16/57/57/57	-
57	CDL	3l	701	-	-	31/110/110/110	-
52	SF4	2N	302	2	-	-	0/6/5/5
55	PEE	3F	101	-	-	16/54/54/54	-
55	PEE	41	302	-	-	5/54/54/54	-
57	CDL	4Z	301	-	-	16/110/110/110	-
56	PC1	2o	204	-	-	14/57/57/57	-
57	CDL	3E	203	-	-	36/110/110/110	-
57	CDL	3I	201	-	-	25/110/110/110	-
57	CDL	4W	202	-	-	28/110/110/110	-
58	UQ8	2s	201	-	-	8/51/75/75	0/1/1/1
57	CDL	4E	201	-	-	29/110/110/110	-
57	CDL	4K	202	-	-	29/110/110/110	-
62	LPP	4c	101	-	-	12/45/45/45	-
57	CDL	3L	702	-	-	21/110/110/110	-
55	PEE	2p	203	-	-	17/54/54/54	-
55	PEE	3f	101	-	-	16/54/54/54	-
57	CDL	4u	501	-	-	35/110/110/110	-
55	PEE	4s	102	-	-	10/54/54/54	-
66	HEA	4q	905	67,40	-	9/36/76/76	-
55	PEE	4q	910	-	-	13/54/54/54	-
57	CDL	3E	201	-	-	29/110/110/110	-
56	PC1	2P	204	-	-	4/57/57/57	-
55	PEE	4z	302	-	-	24/54/54/54	-
56	PC1	2R	202	-	-	16/57/57/57	-
56	PC1	3A	501	-	-	19/57/57/57	-
55	PEE	4w	203	-	-	11/54/54/54	-
56	PC1	3h	403	-	-	16/57/57/57	-
58	UQ8	3g	404	-	-	14/51/75/75	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	3L	701	-	-	30/110/110/110	-

The worst 5 of 198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	3D	203	UQ8	C6-C1	10.42	1.53	1.35
58	3d	203	UQ8	C6-C1	10.40	1.53	1.35
58	3G	405	UQ8	C6-C1	9.95	1.53	1.35
58	3g	405	UQ8	C6-C1	9.94	1.53	1.35
58	2s	201	UQ8	C6-C1	9.92	1.53	1.35

The worst 5 of 315 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	3C	301	HEC	CBB-CAB-C3B	-8.15	111.15	127.43
59	3c	301	HEC	CBB-CAB-C3B	-8.14	111.17	127.43
66	4Q	904	HEA	C3A-C2A-C1A	-6.64	100.77	107.05
66	4q	904	HEA	C3A-C2A-C1A	-6.64	100.77	107.05
59	3C	301	HEC	CBC-CAC-C3C	-6.47	114.50	127.43

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
61	40	304	AJP	C30
61	40	304	AJP	C28
61	40	304	AJP	C29
61	41	304	AJP	C30
61	41	304	AJP	C28

5 of 2496 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	2M	701	FAD	C5B-O5B-PA-O3P
50	2M	701	FAD	N10-C1'-C2'-O2'
50	2m	701	FAD	C5B-O5B-PA-O3P
50	2m	701	FAD	N10-C1'-C2'-O2'
55	2O	201	PEE	C11-C10-O2-C2

There are no ring outliers.

83 monomers are involved in 209 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	4q	907	CDL	1	0
57	4k	201	CDL	1	0
57	4K	201	CDL	1	0
57	2u	101	CDL	2	0
56	2T	101	PC1	1	0
57	3H	402	CDL	1	0
66	4q	904	HEA	4	0
58	3G	405	UQ8	5	0
61	4l	304	AJP	1	0
57	2U	101	CDL	2	0
55	4Q	910	PEE	1	0
57	4s	101	CDL	1	0
57	4j	301	CDL	1	0
60	3g	402	HEM	1	0
57	4Q	907	CDL	1	0
56	2t	101	PC1	1	0
57	2p	201	CDL	3	0
58	3g	405	UQ8	4	0
50	2M	701	FAD	11	0
58	3G	404	UQ8	10	0
57	4q	908	CDL	2	0
50	2m	701	FAD	11	0
57	2P	201	CDL	3	0
56	2O	203	PC1	3	0
57	2q	101	CDL	2	0
57	3h	402	CDL	1	0
57	4k	202	CDL	2	0
56	2O	202	PC1	2	0
60	3G	401	HEM	4	0
57	4J	301	CDL	1	0
58	2S	201	UQ8	2	0
57	4Q	908	CDL	2	0
57	2o	201	CDL	1	0
57	2Q	101	CDL	2	0
55	4q	909	PEE	1	0
56	3a	501	PC1	2	0
59	3c	301	HEC	5	0
60	3G	402	HEM	1	0
62	4d	102	LPP	1	0
56	2r	202	PC1	1	0
58	3D	203	UQ8	12	0
57	3G	403	CDL	5	0
58	3d	203	UQ8	12	0

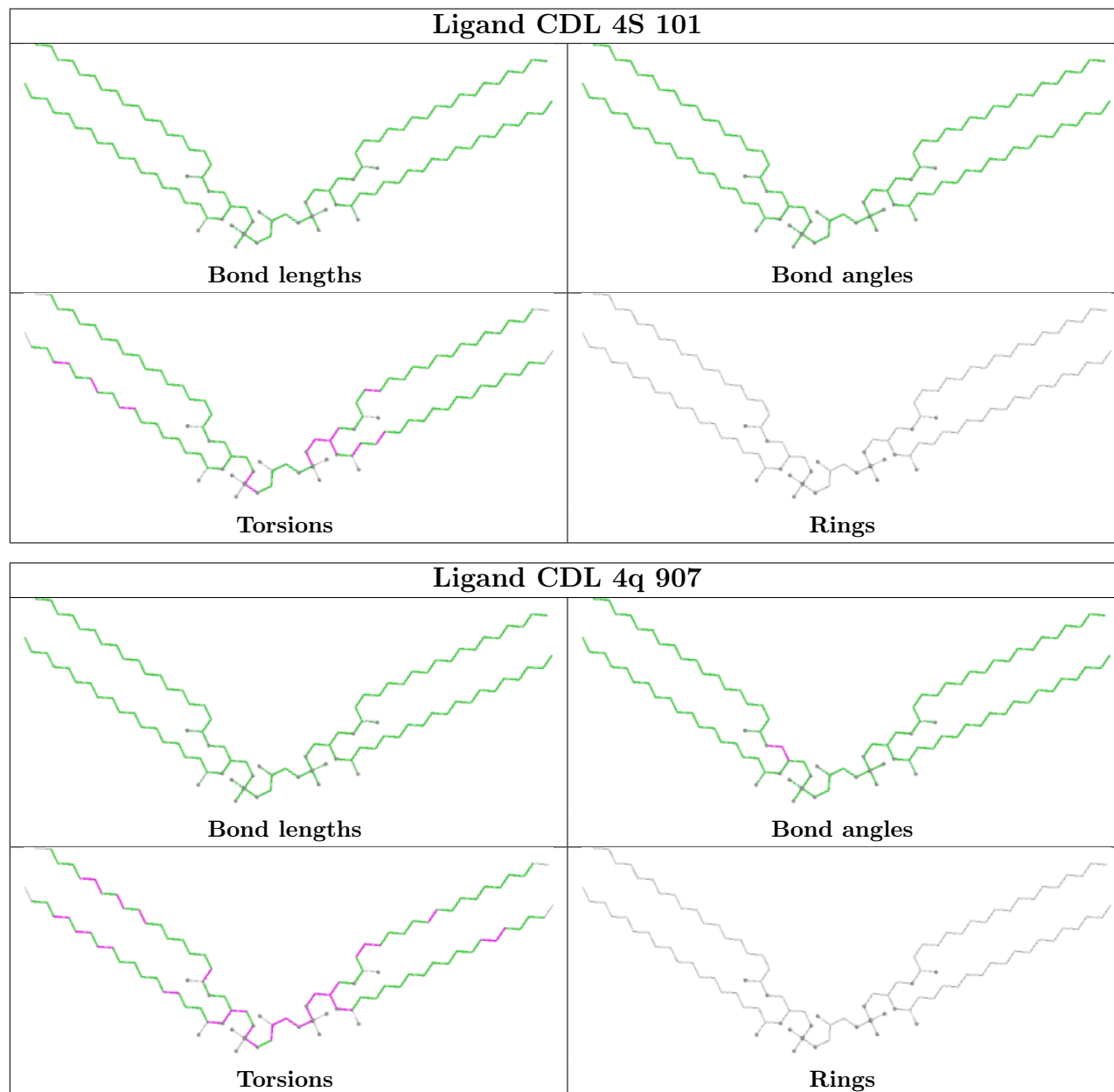
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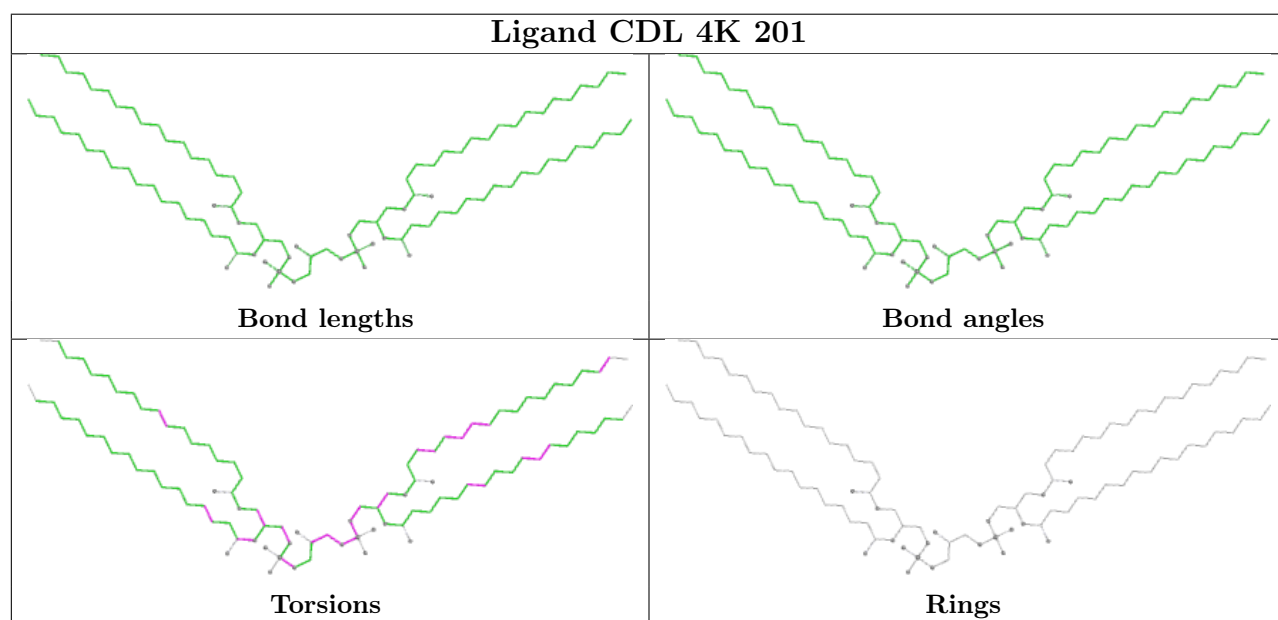
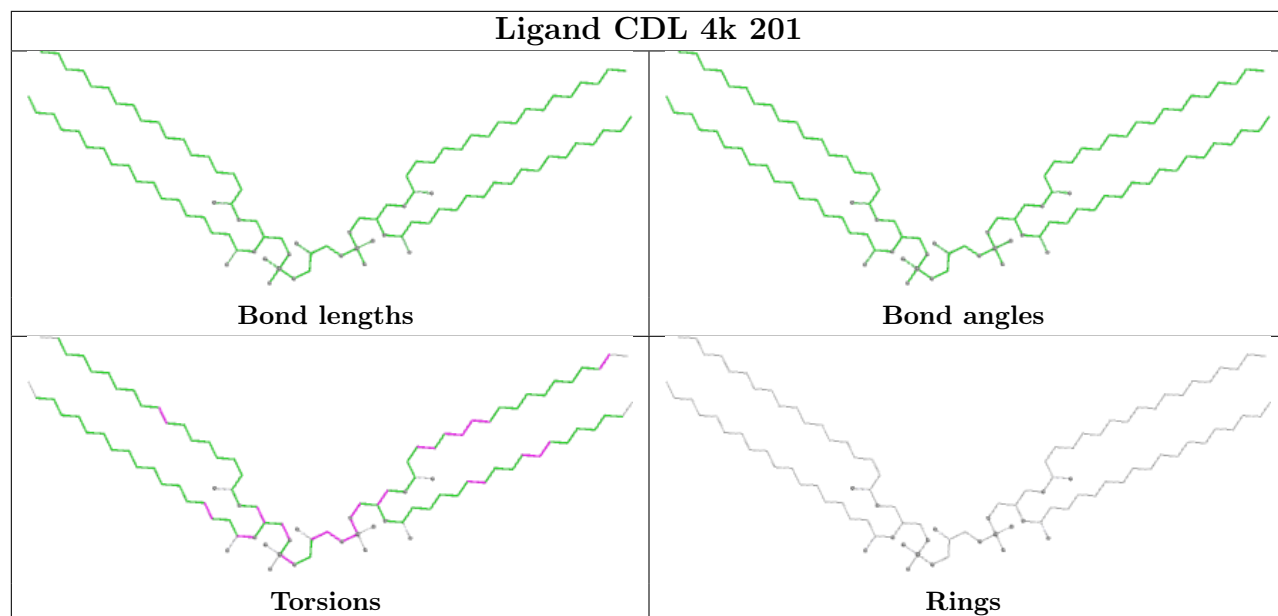
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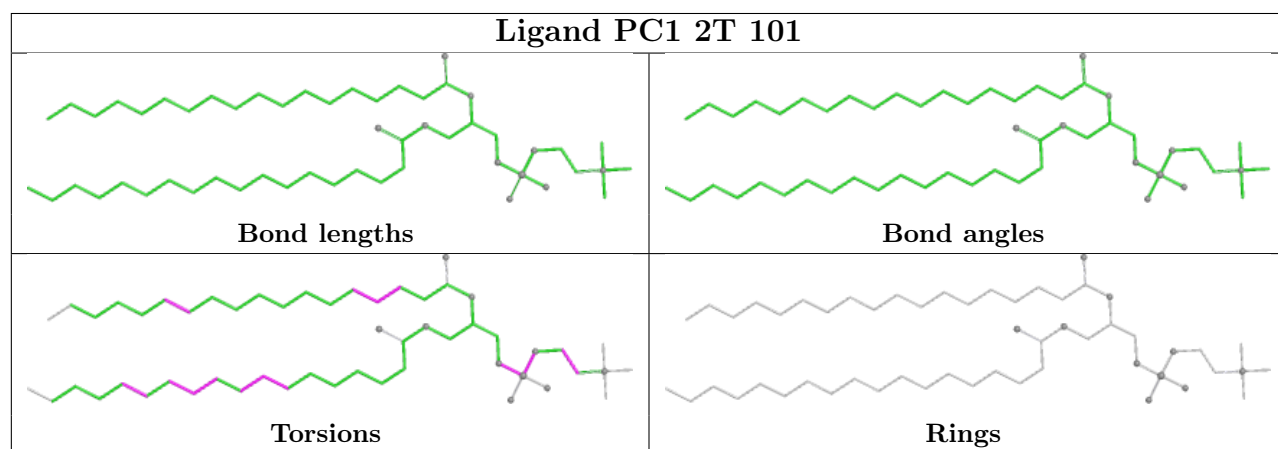
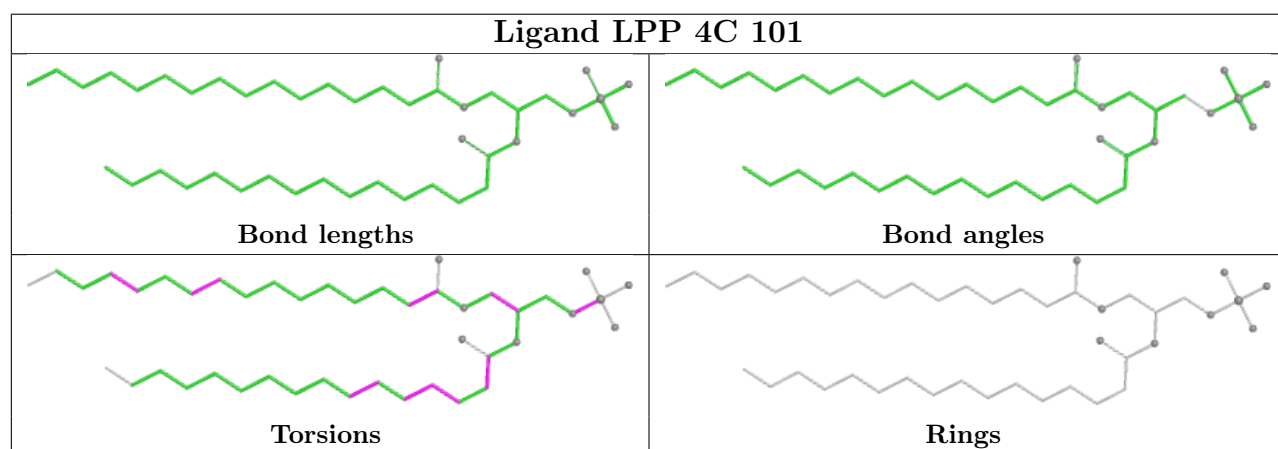
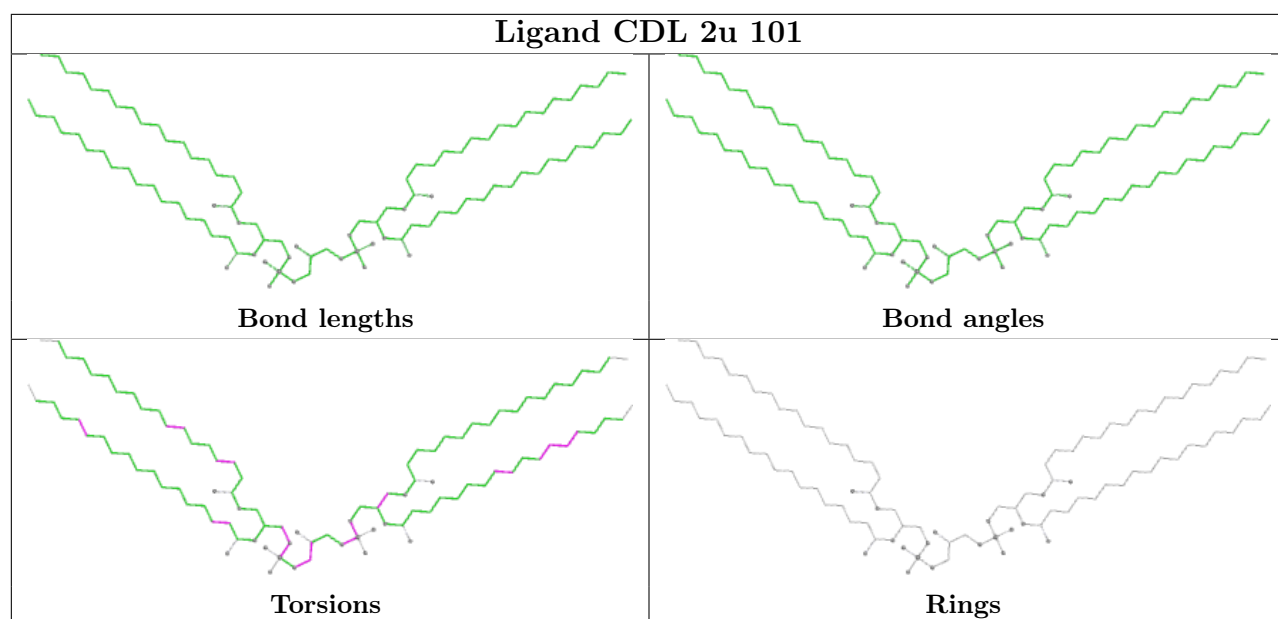
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	4e	202	PC1	2	0
57	4T	203	CDL	3	0
55	4Q	909	PEE	1	0
55	3C	302	PEE	1	0
55	3c	302	PEE	1	0
57	4U	501	CDL	2	0
62	4D	102	LPP	1	0
56	4E	202	PC1	2	0
57	2O	204	CDL	1	0
51	3h	401	FES	1	0
57	3g	403	CDL	4	0
61	40	304	AJP	1	0
59	3C	301	HEC	6	0
66	4Q	905	HEA	2	0
51	3H	401	FES	1	0
56	2p	204	PC1	2	0
66	4Q	904	HEA	4	0
56	2o	203	PC1	2	0
57	3i	202	CDL	3	0
57	4t	203	CDL	3	0
57	4w	202	CDL	1	0
55	40	302	PEE	1	0
60	3g	401	HEM	4	0
57	3l	701	CDL	1	0
55	3F	101	PEE	1	0
55	41	302	PEE	1	0
56	2o	204	PC1	3	0
57	3I	201	CDL	3	0
57	4W	202	CDL	1	0
58	2s	201	UQ8	2	0
57	4K	202	CDL	1	0
55	3f	101	PEE	1	0
57	4u	501	CDL	2	0
66	4q	905	HEA	2	0
55	4q	910	PEE	1	0
56	2P	204	PC1	2	0
56	2R	202	PC1	1	0
56	3A	501	PC1	2	0
58	3g	404	UQ8	11	0
57	3L	701	CDL	1	0

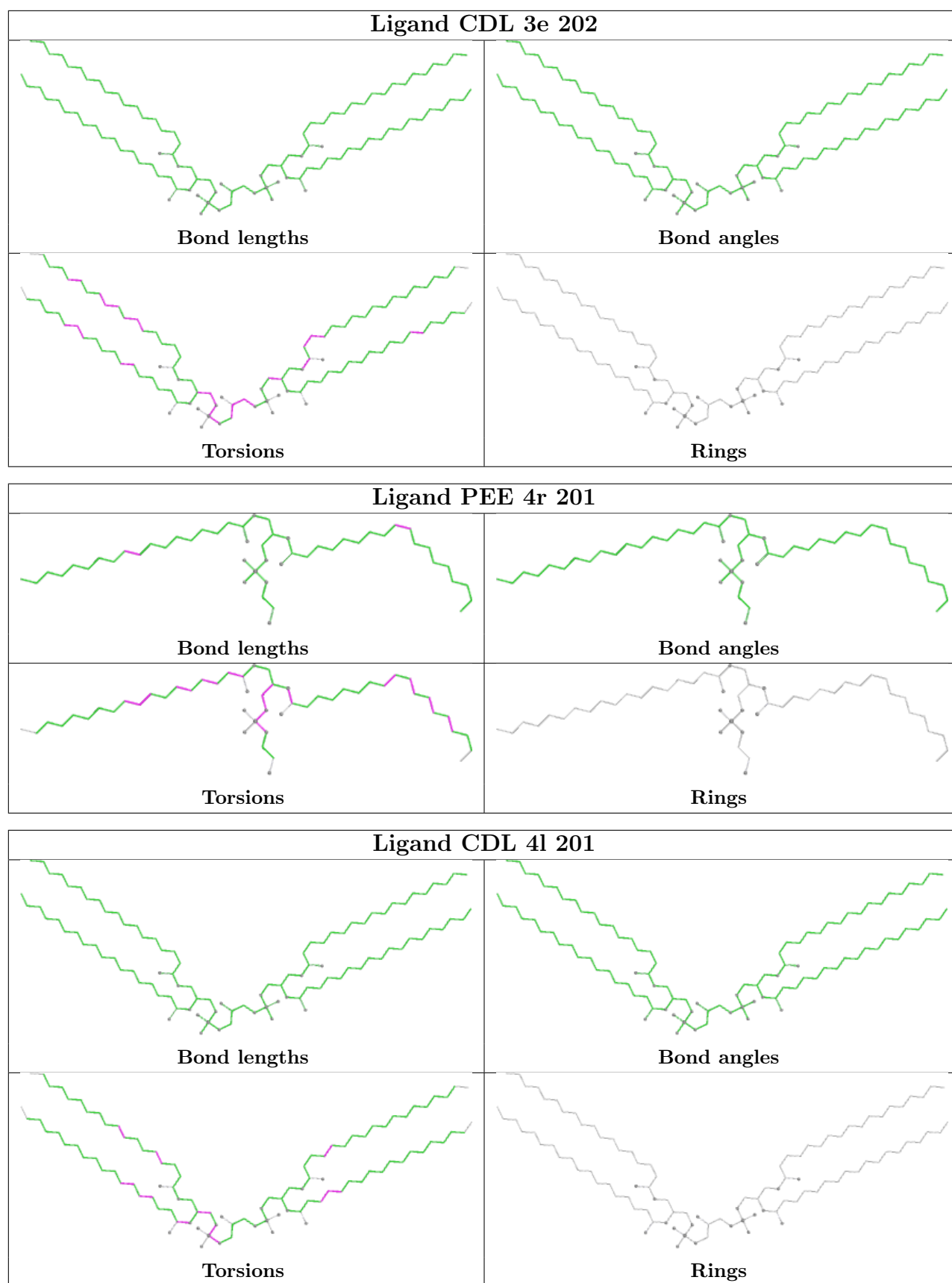
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

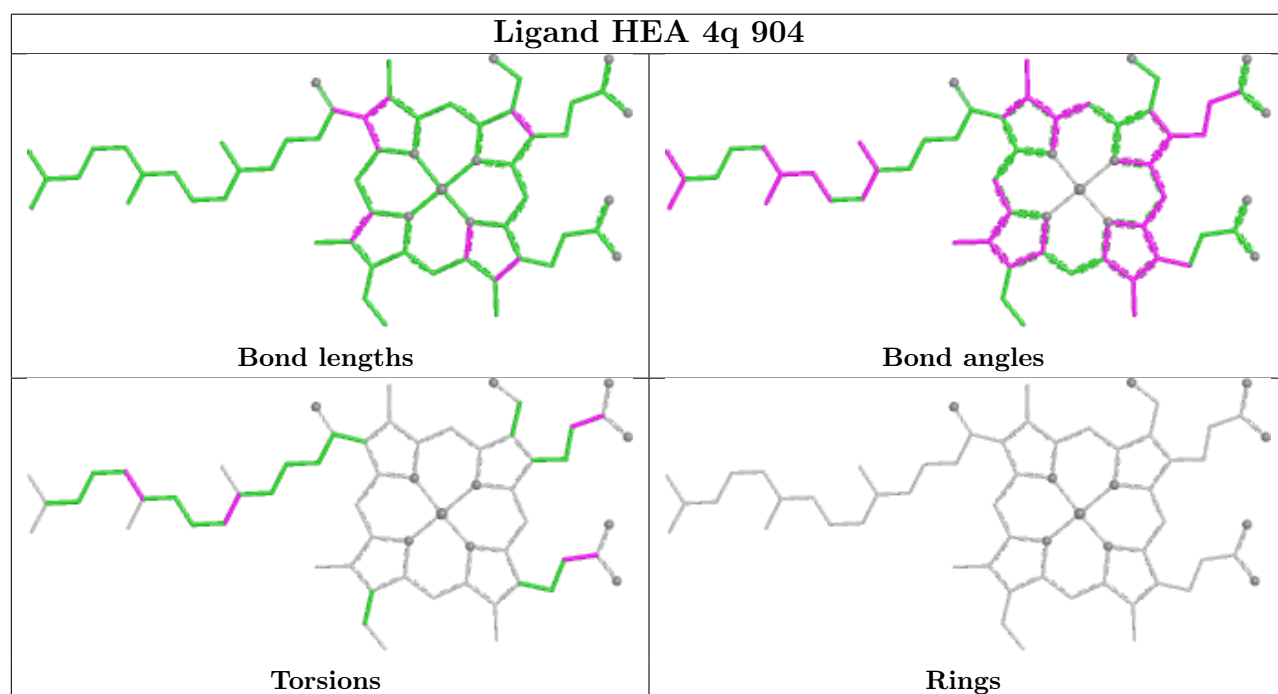
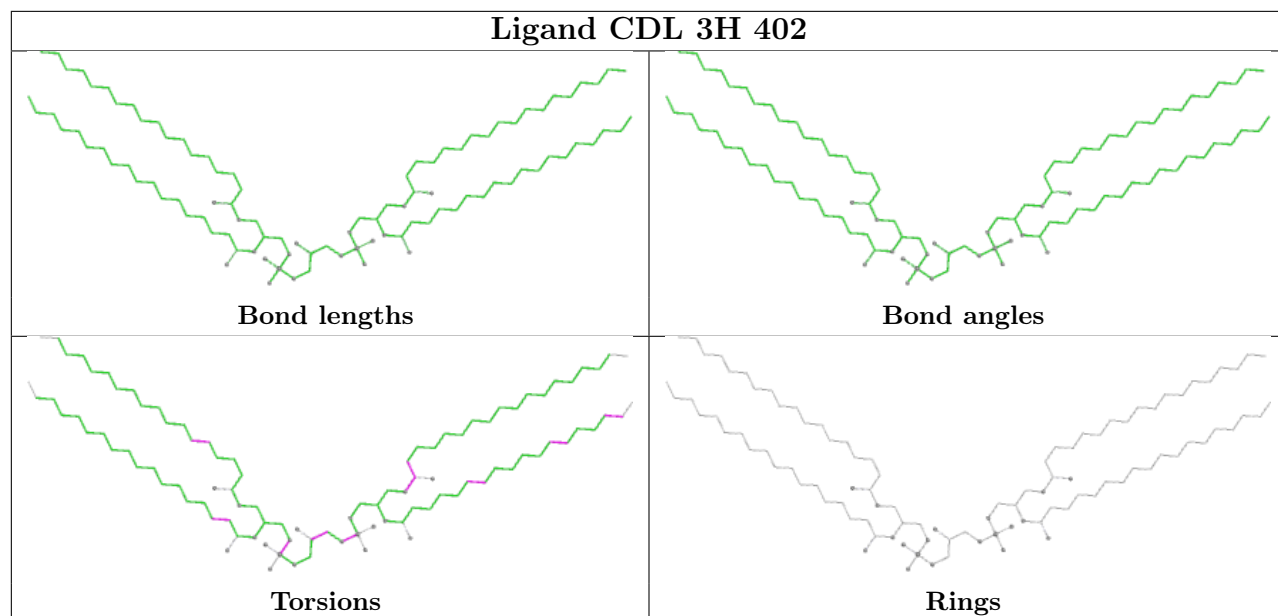
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

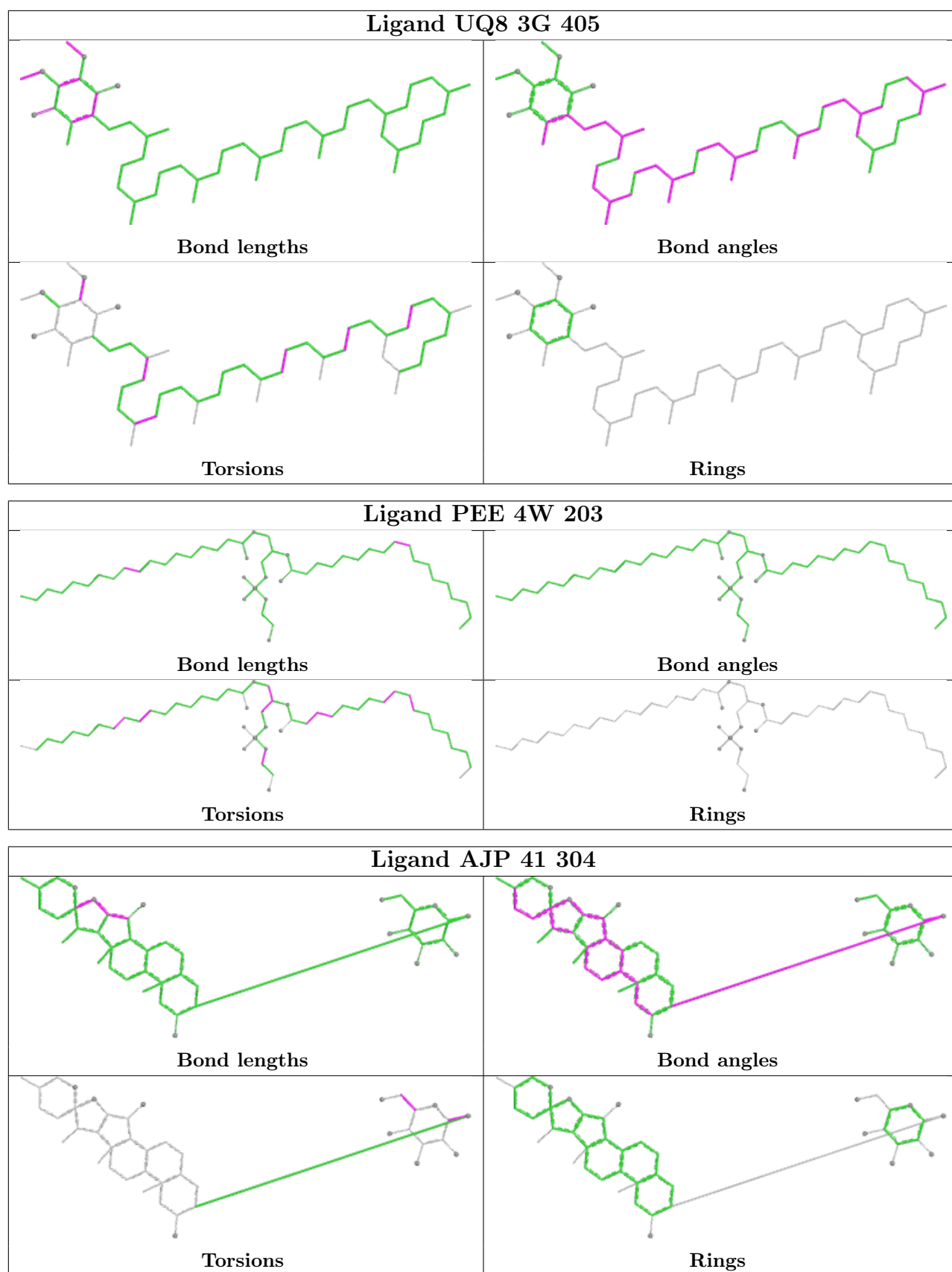


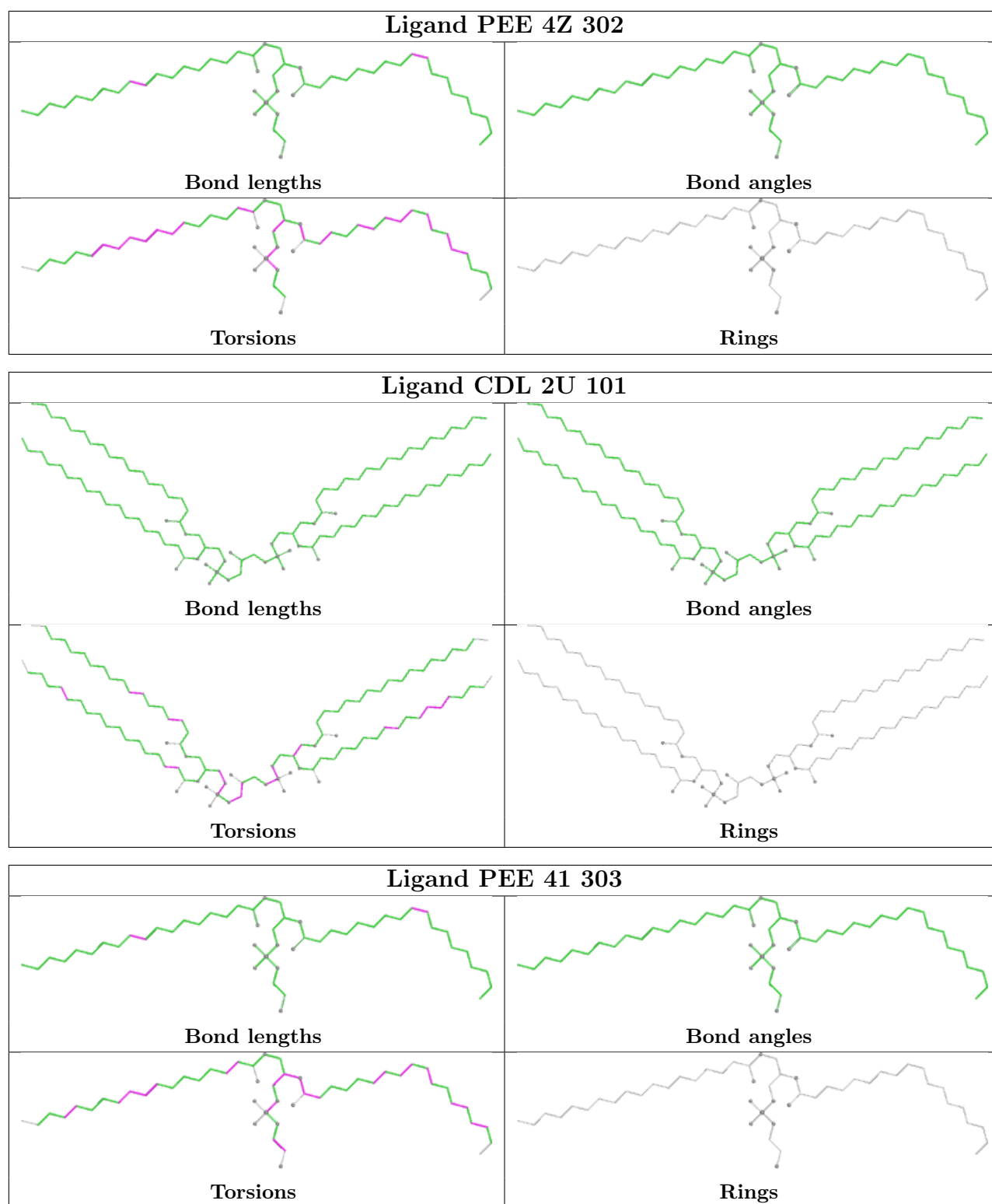


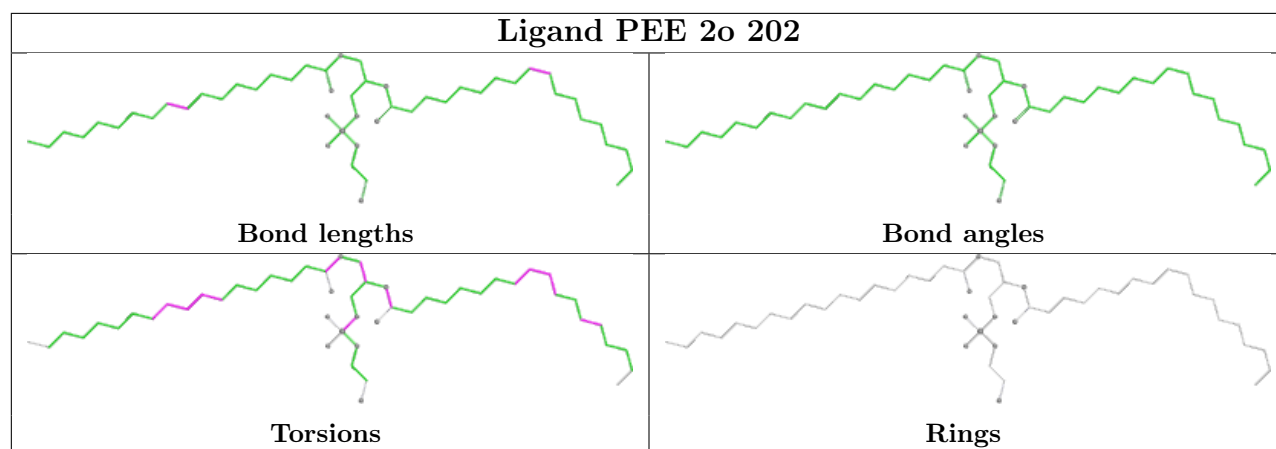
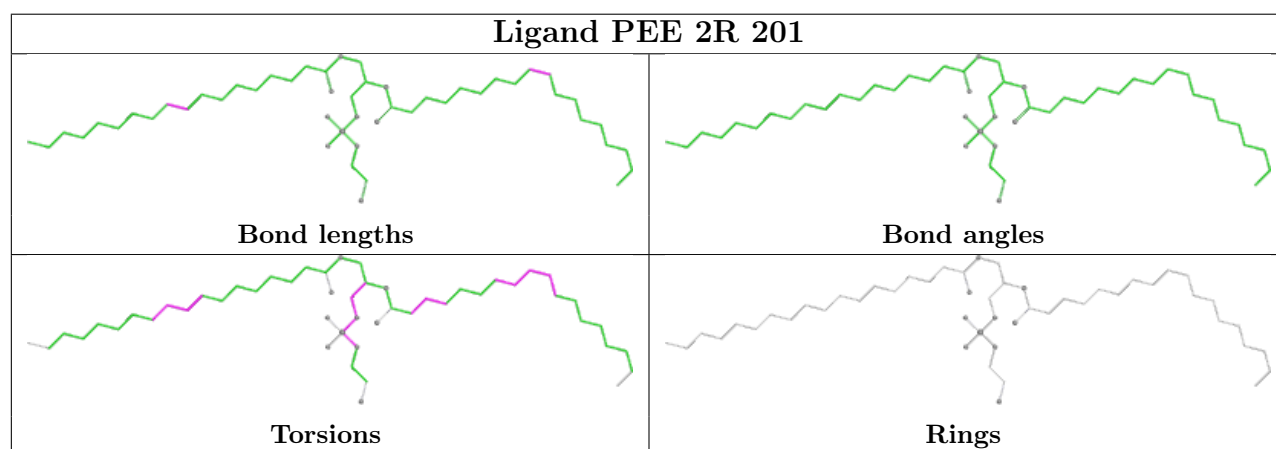
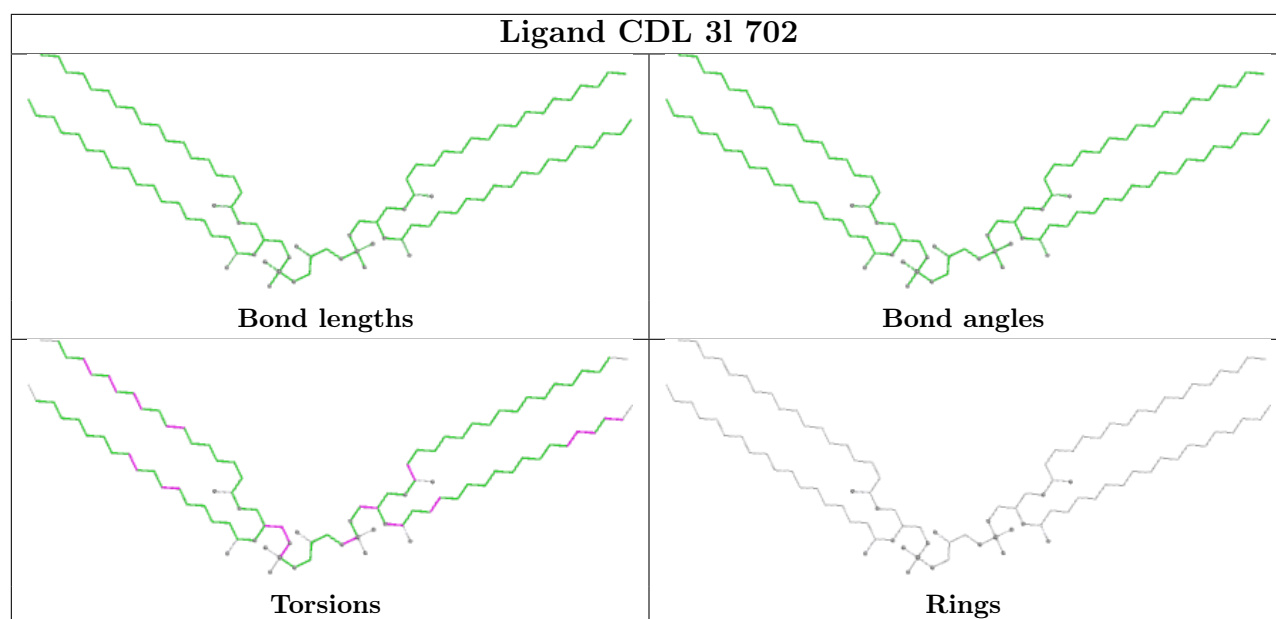


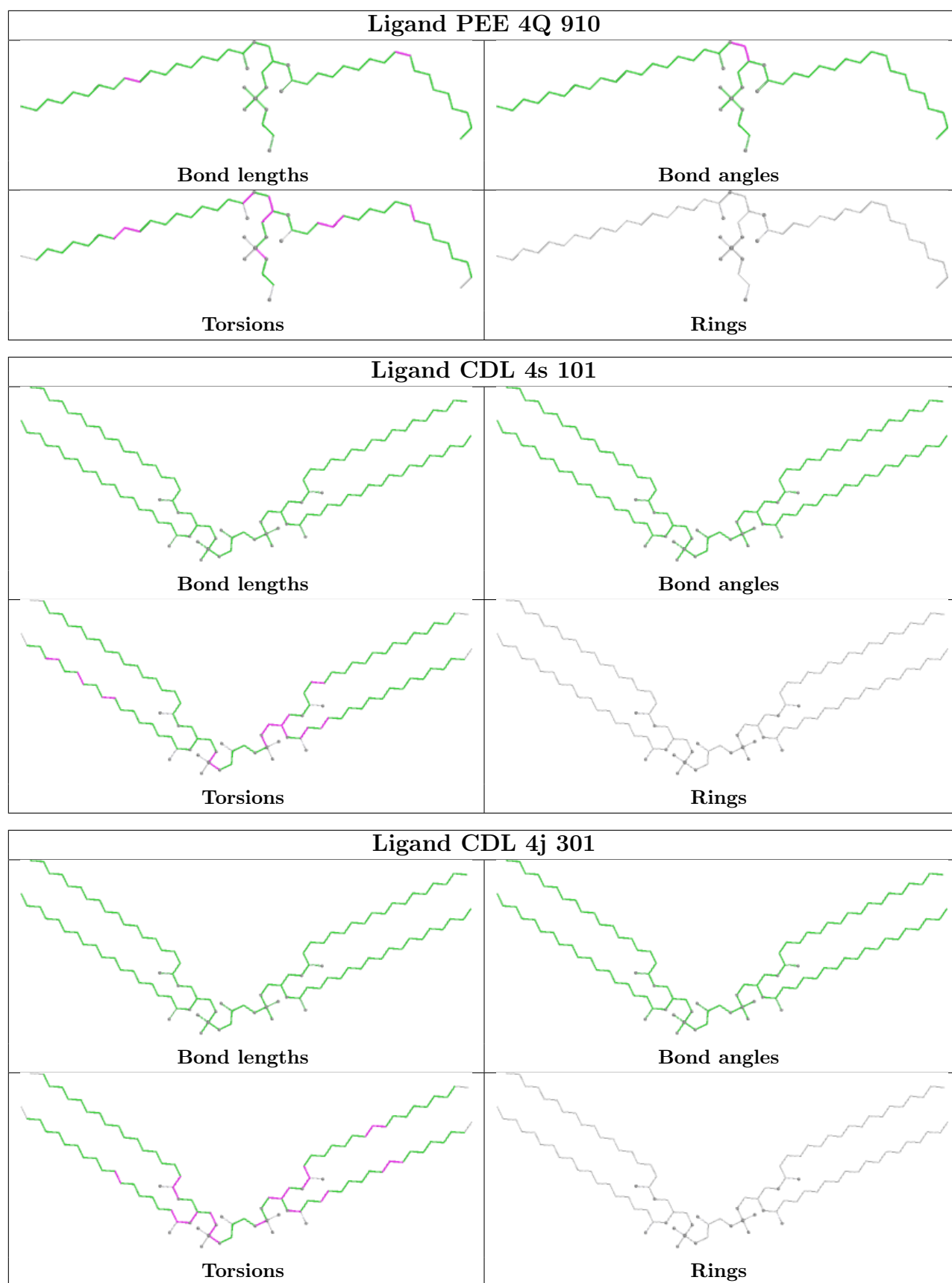


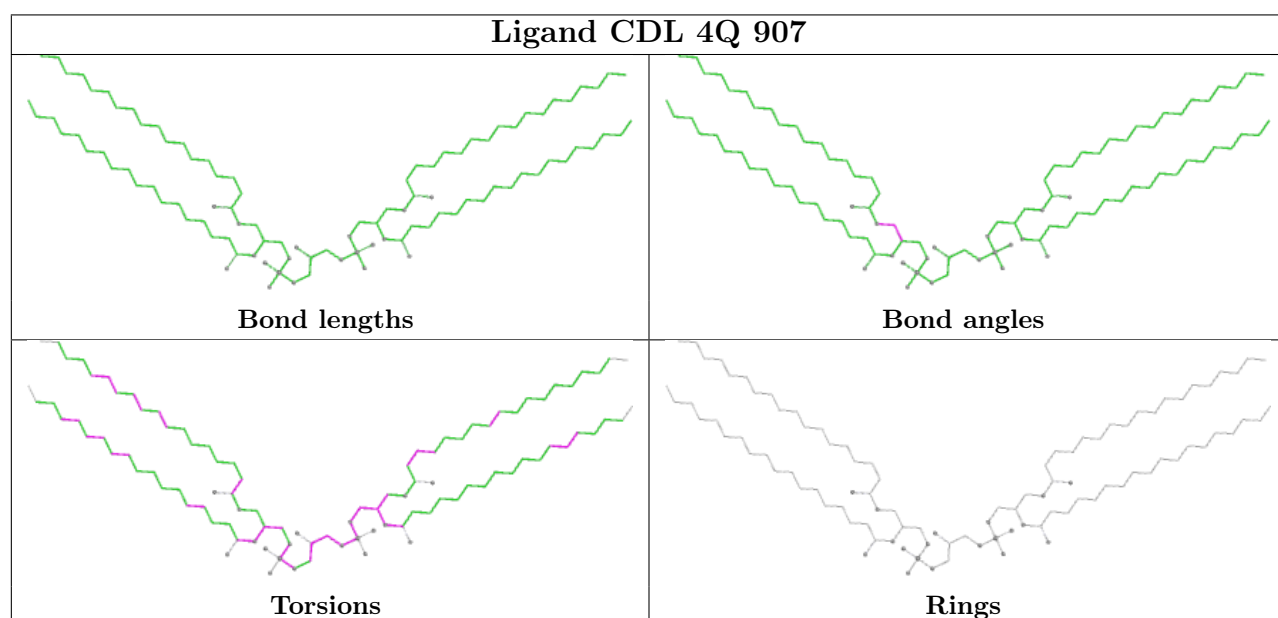
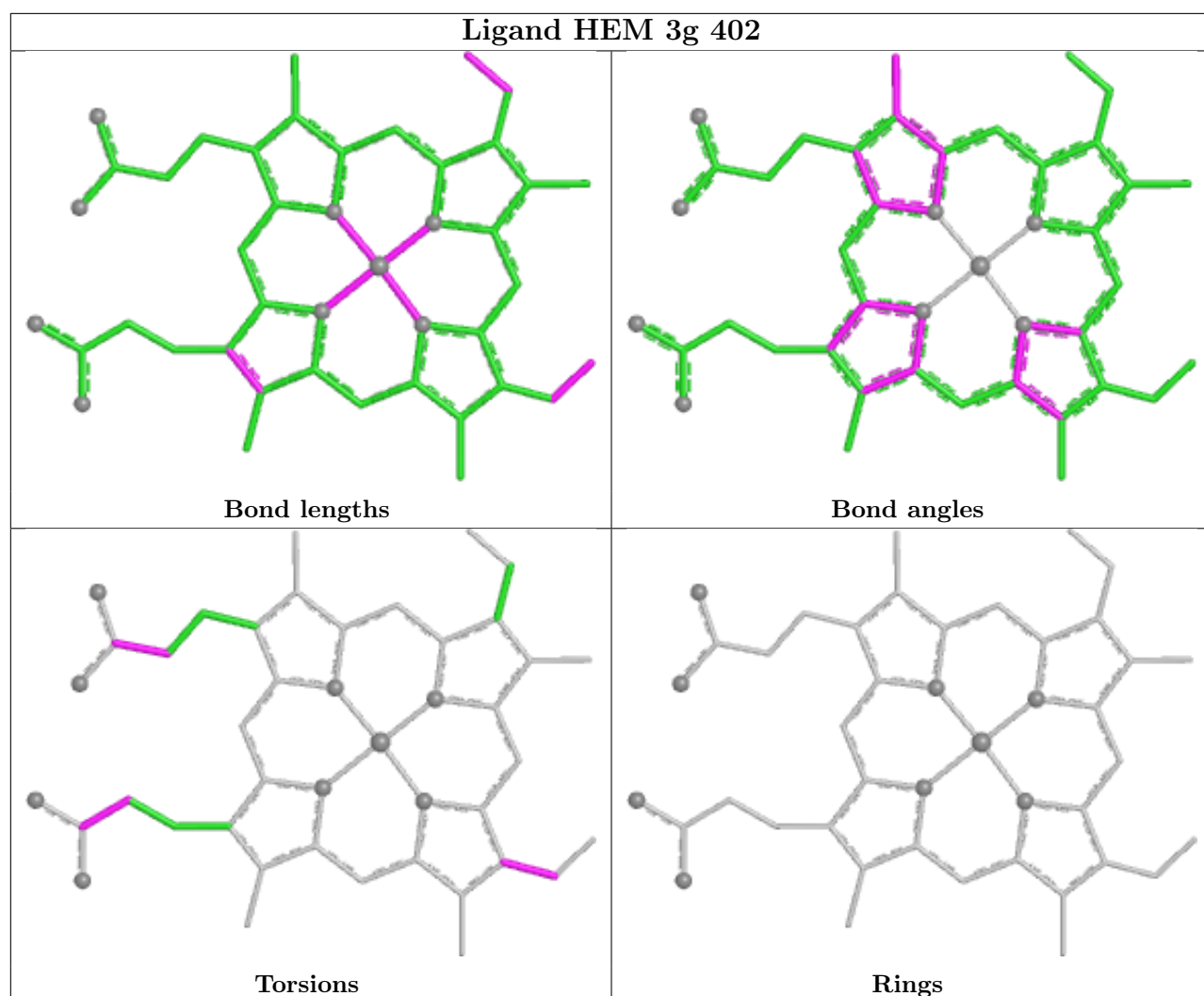


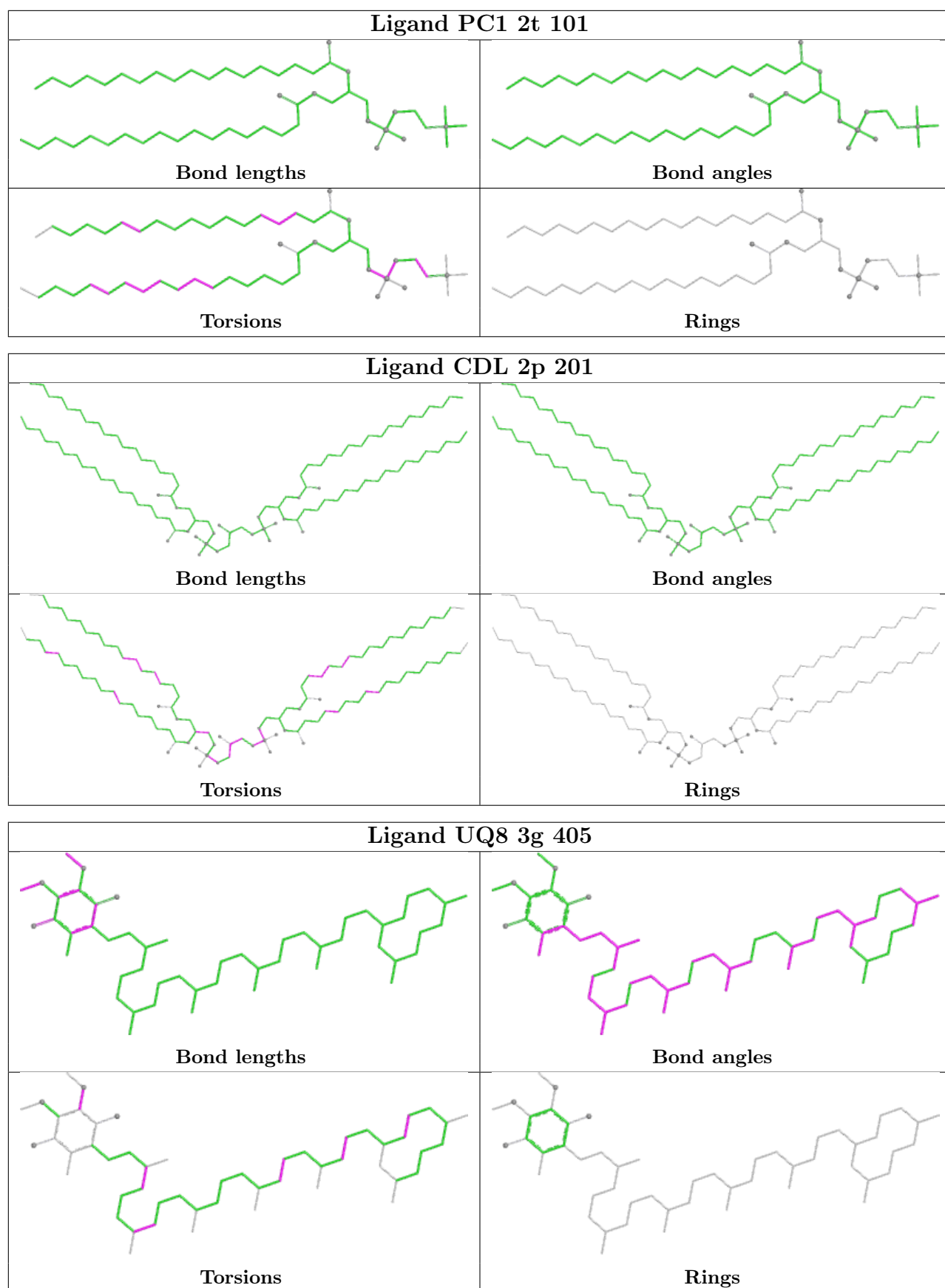


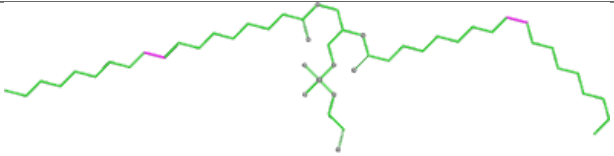
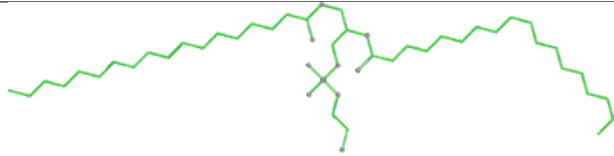
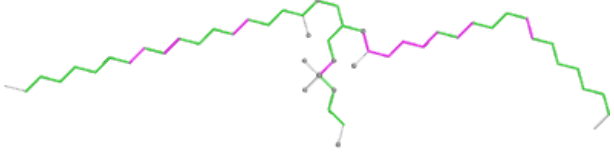
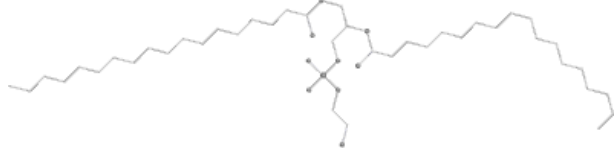


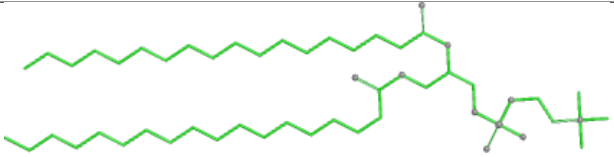
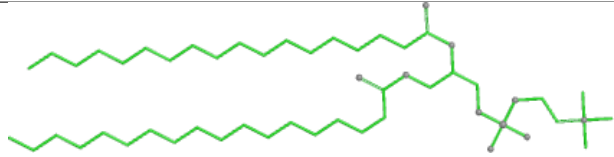
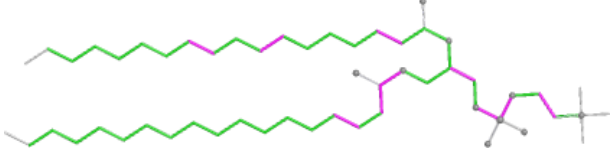
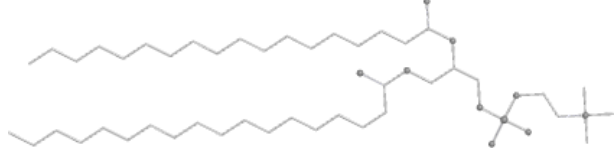


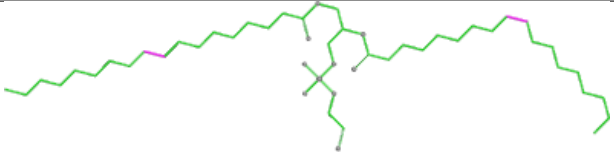
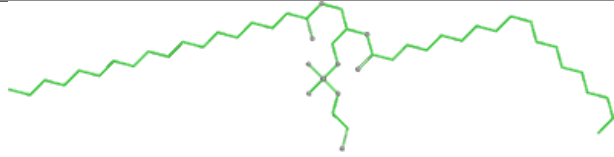
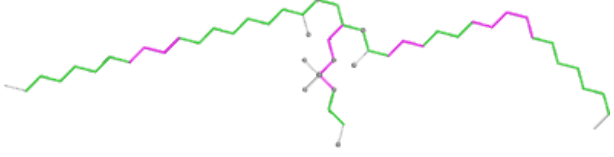
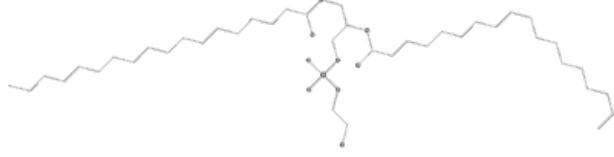


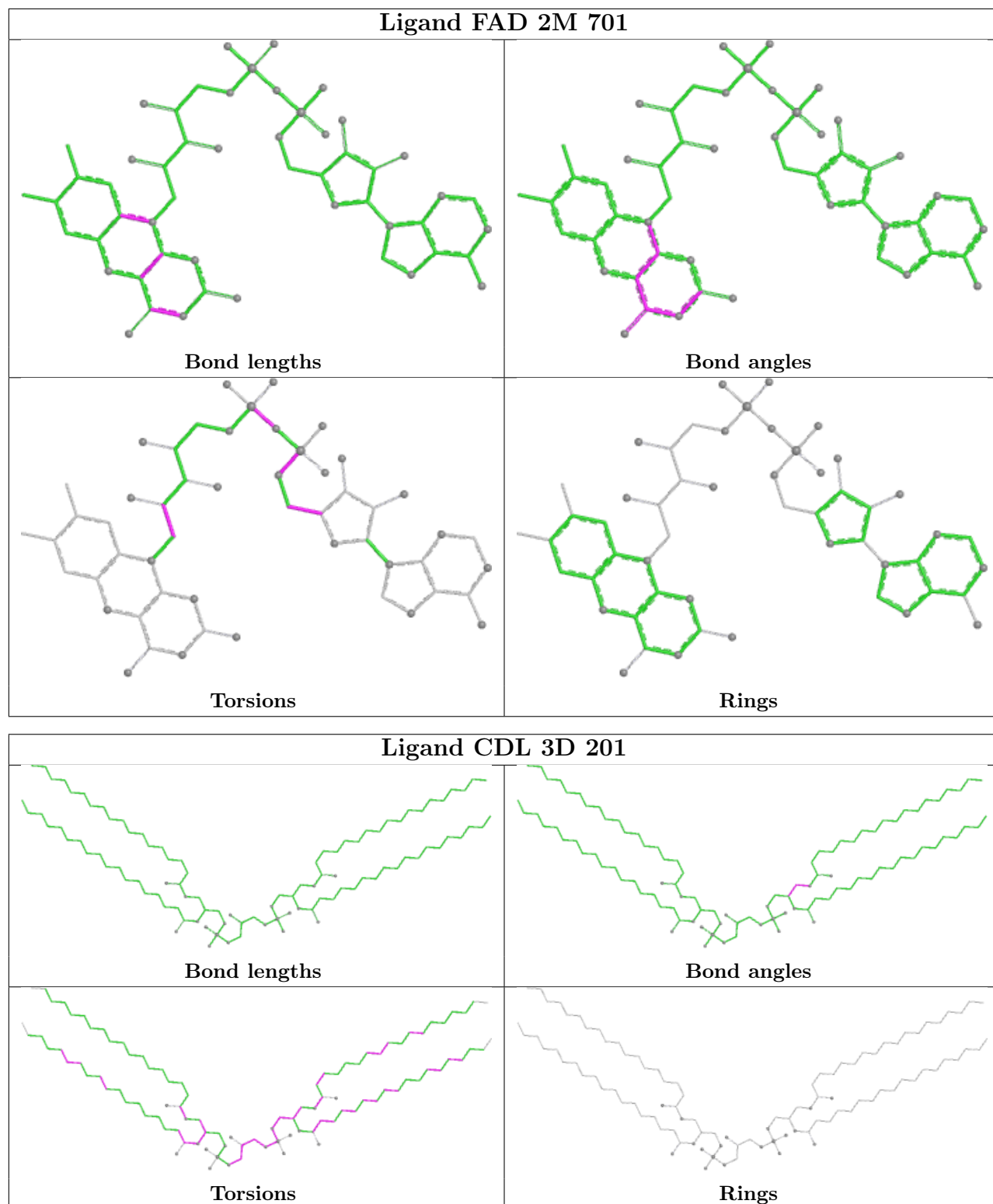


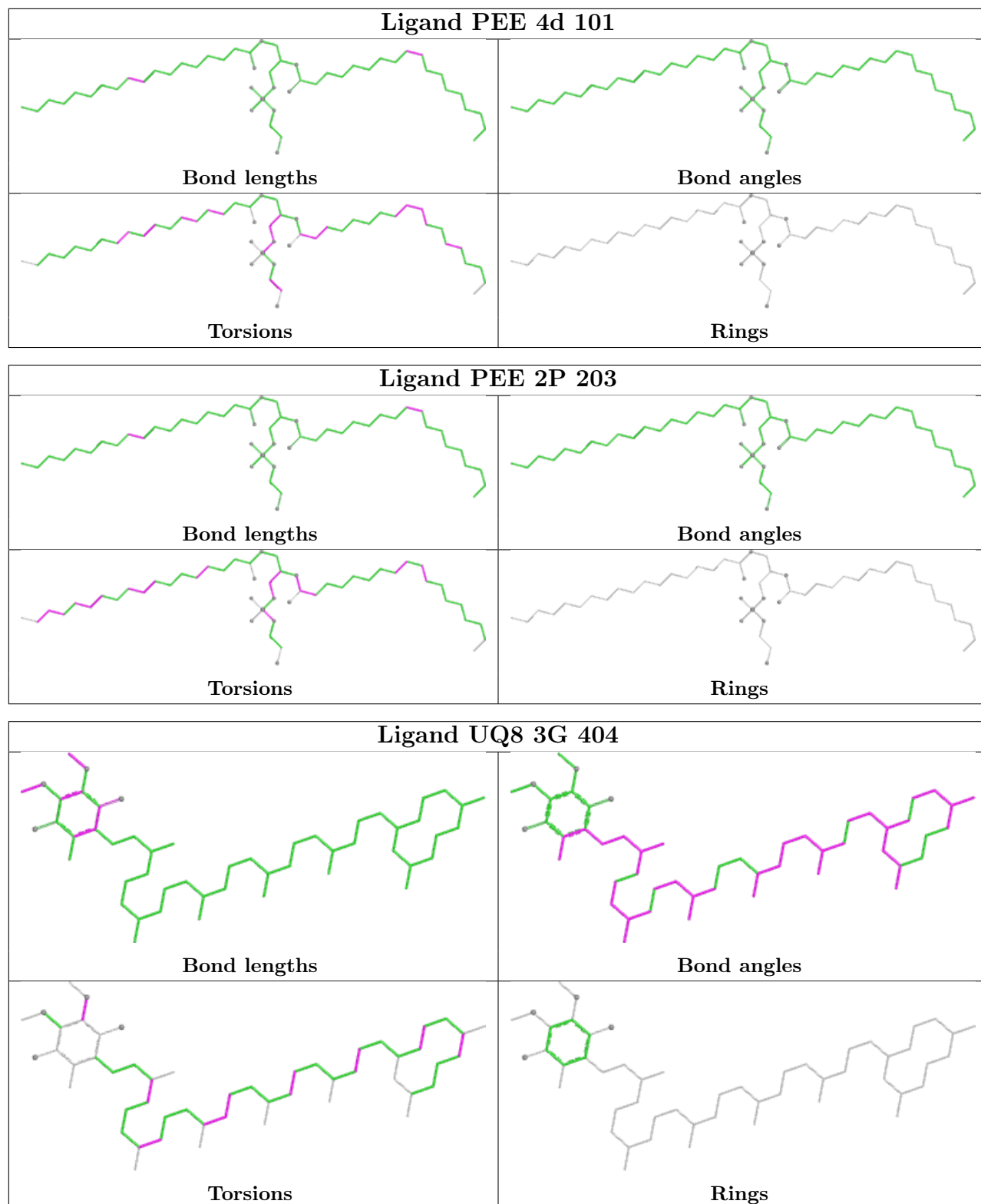


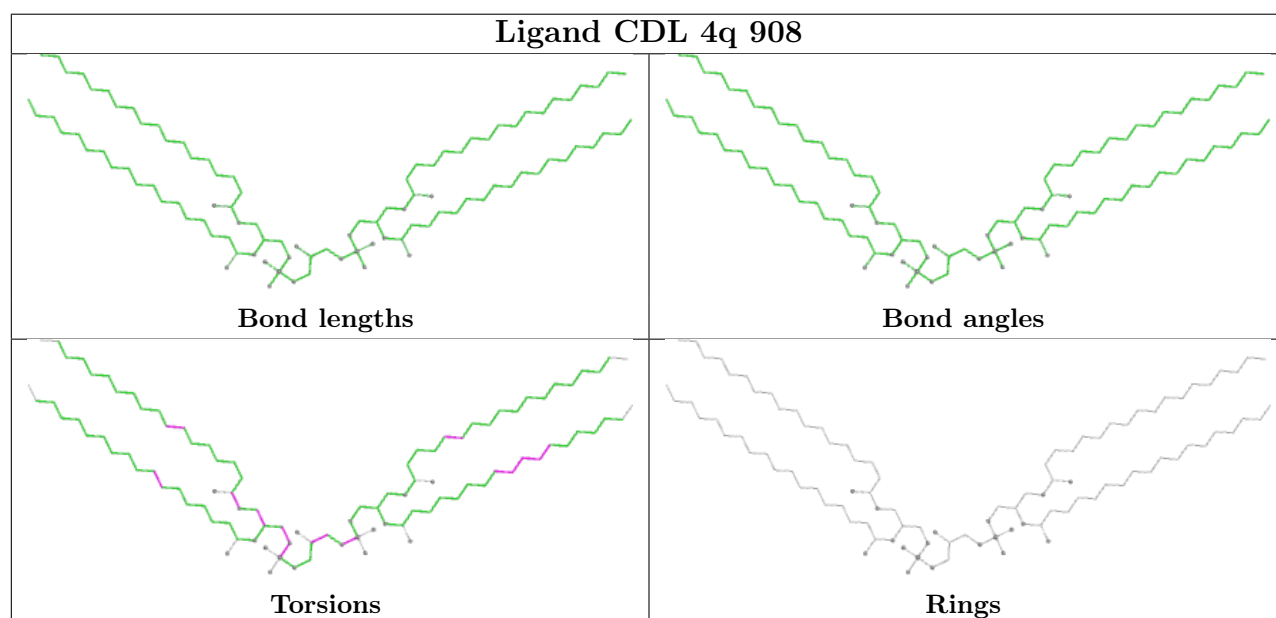
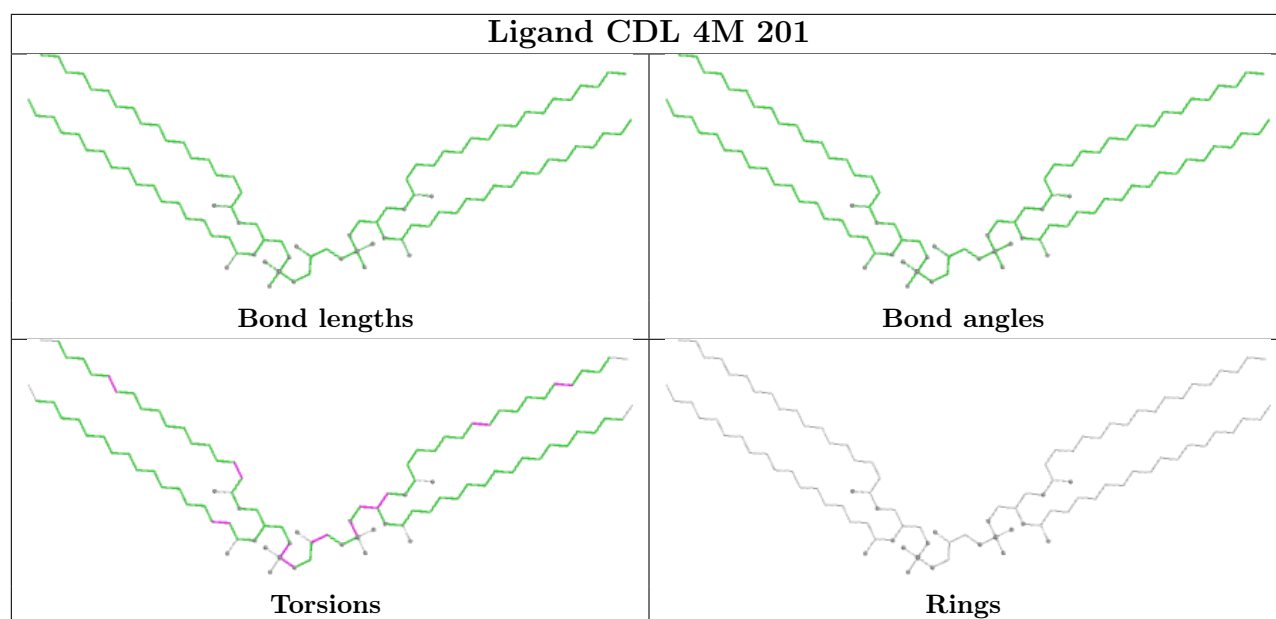
Ligand PEE 40 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

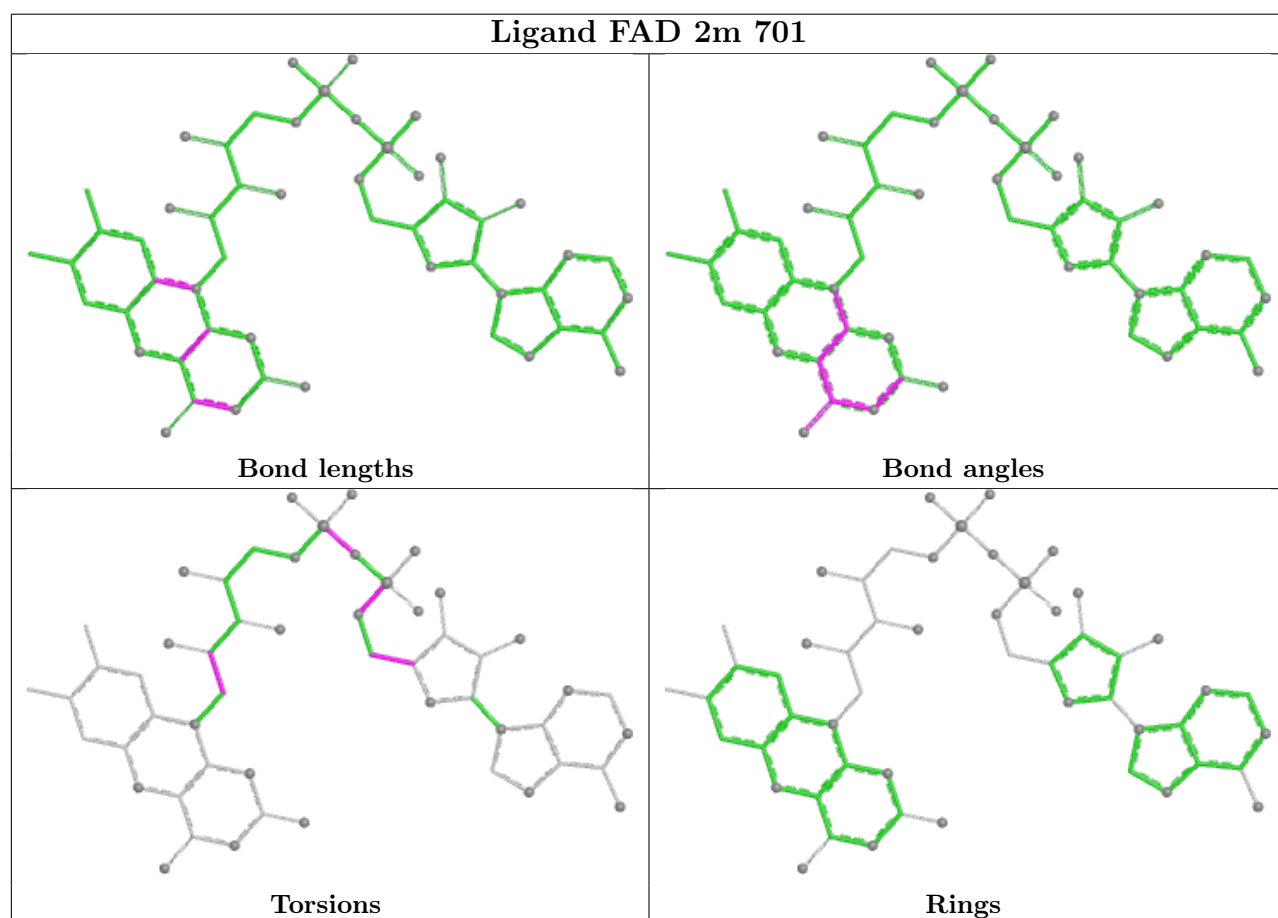
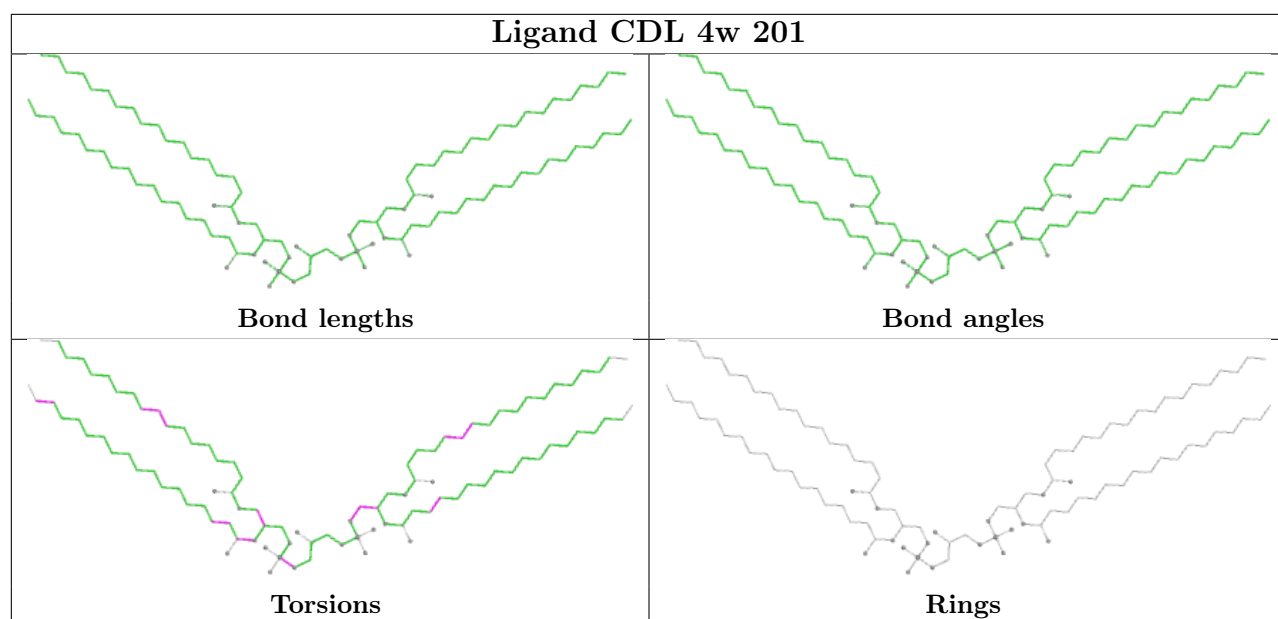
Ligand PC1 3A 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

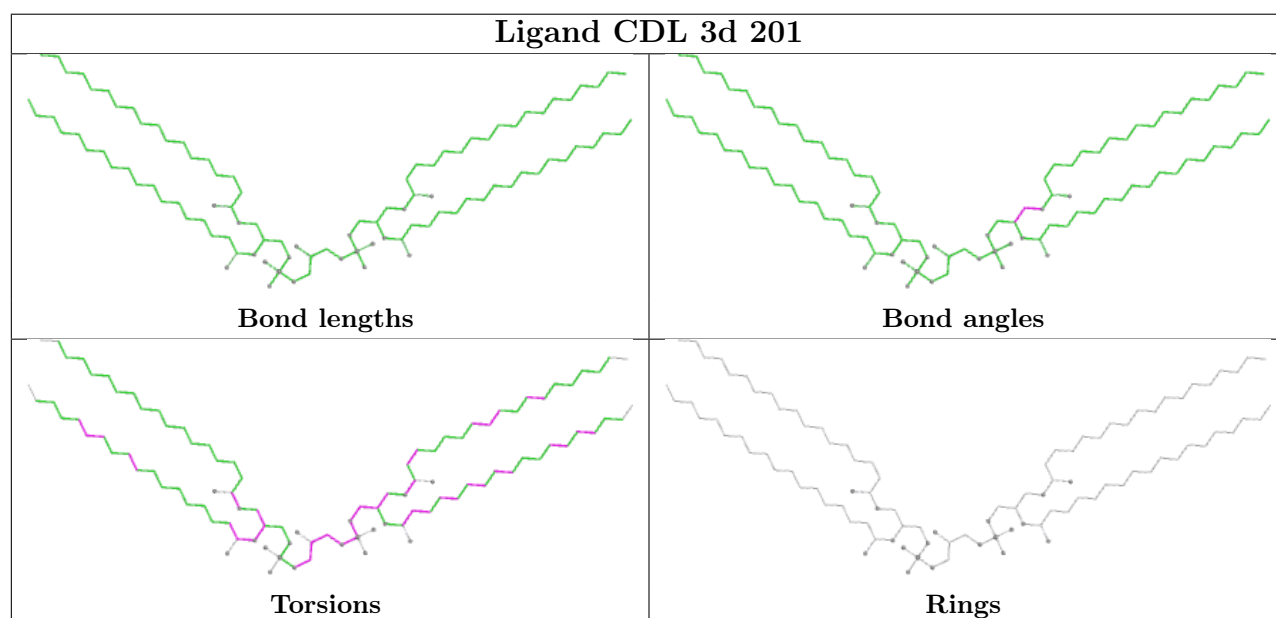
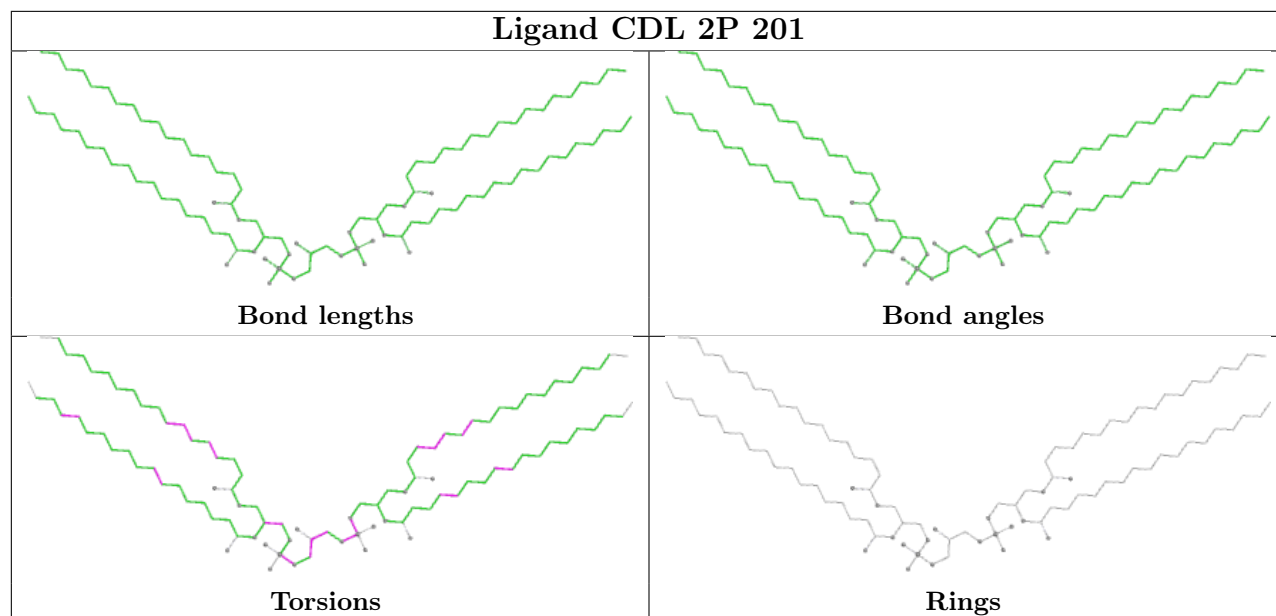
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Bond lengths	Bond angles
	
Torsions	Rings

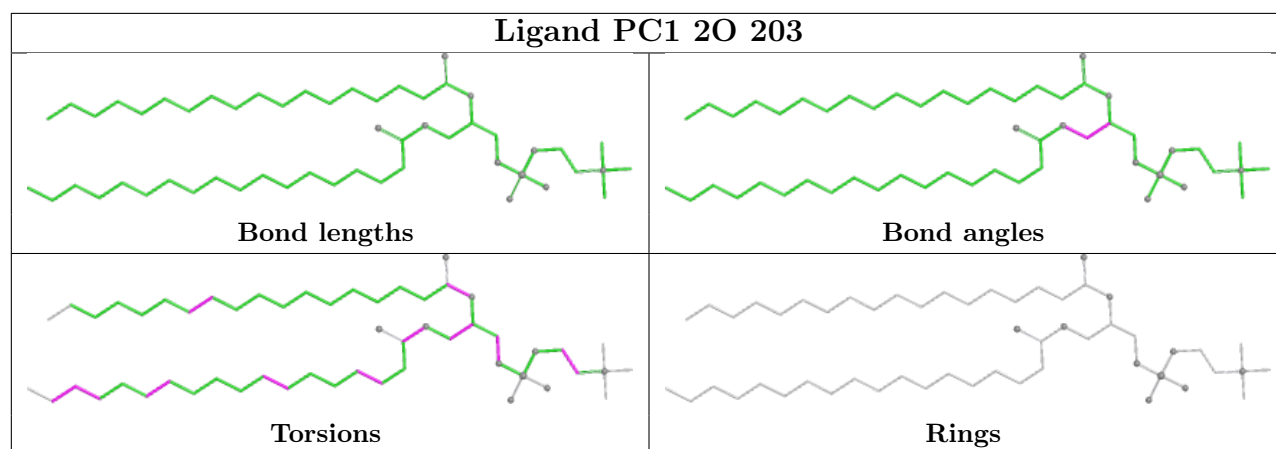
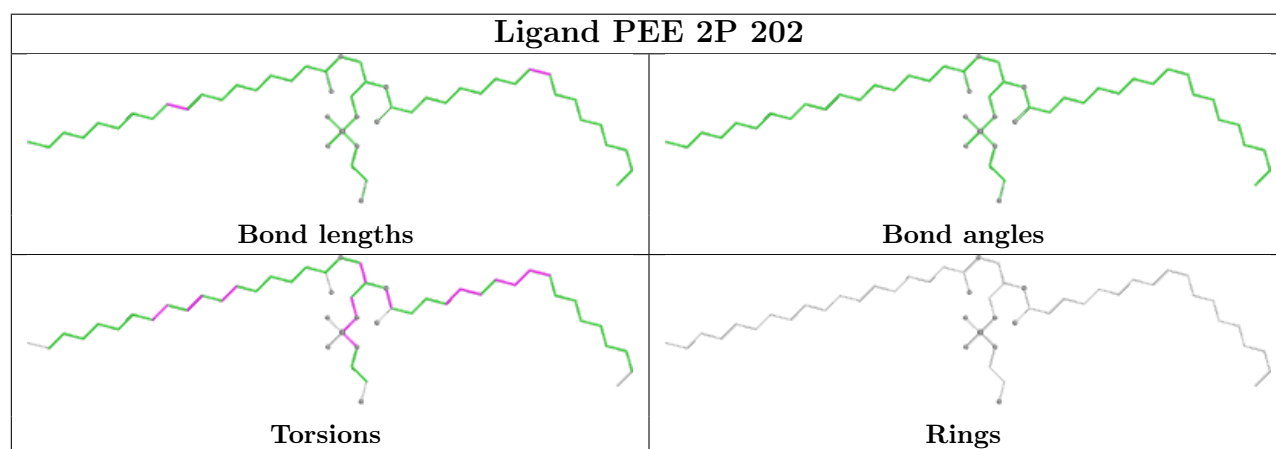
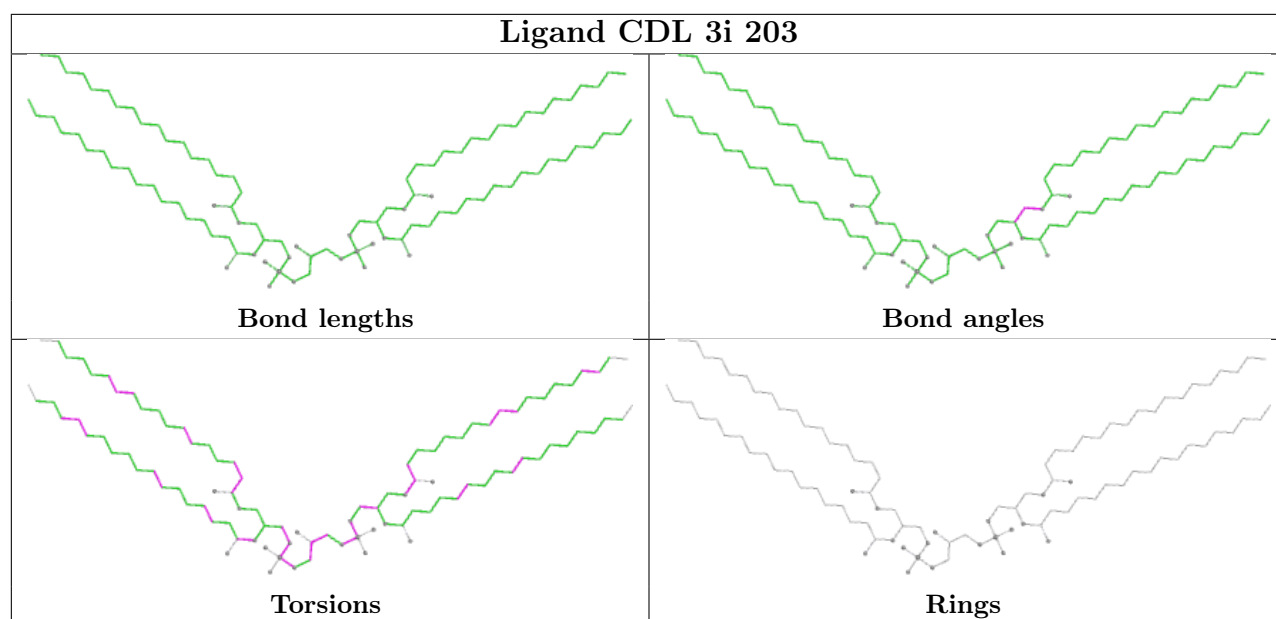


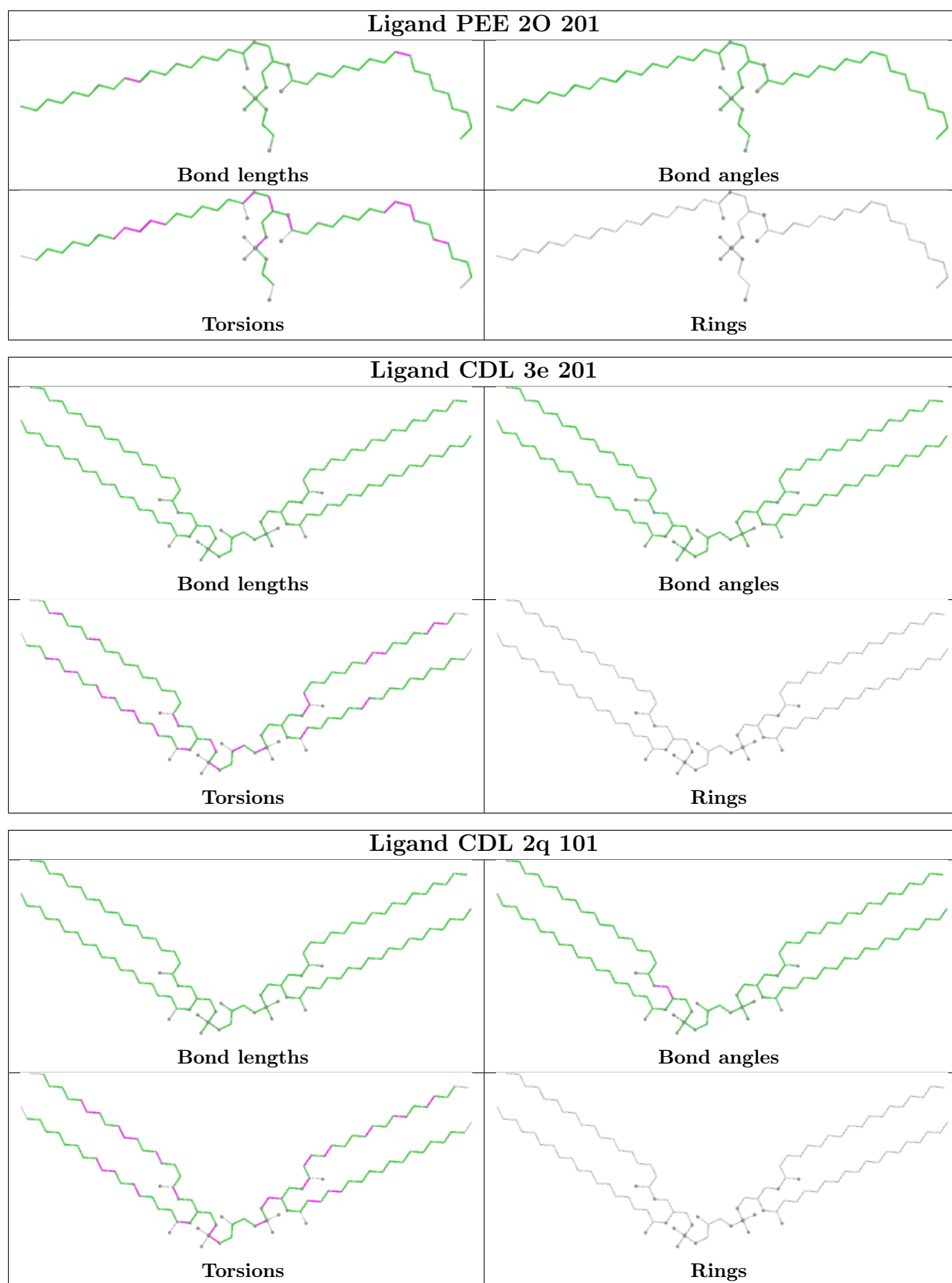


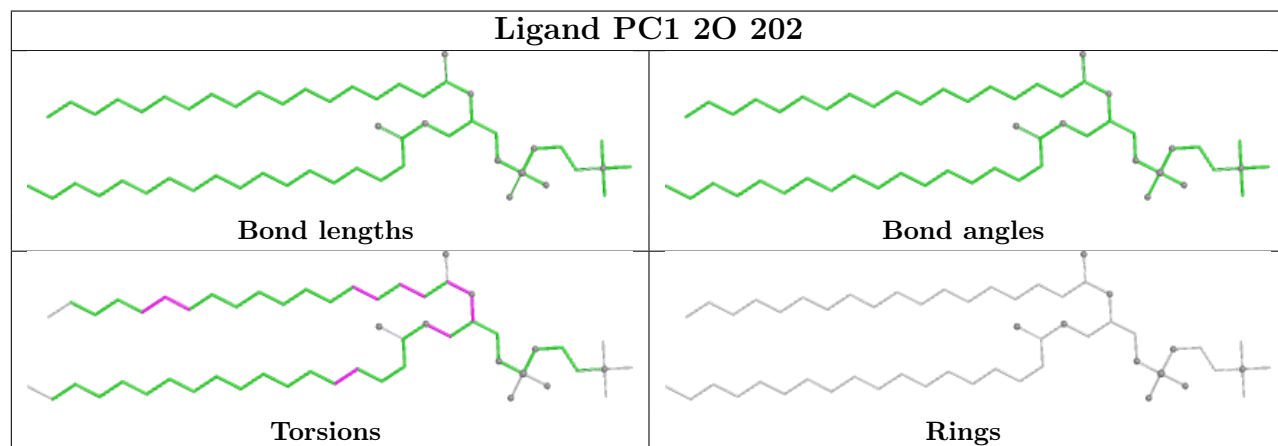
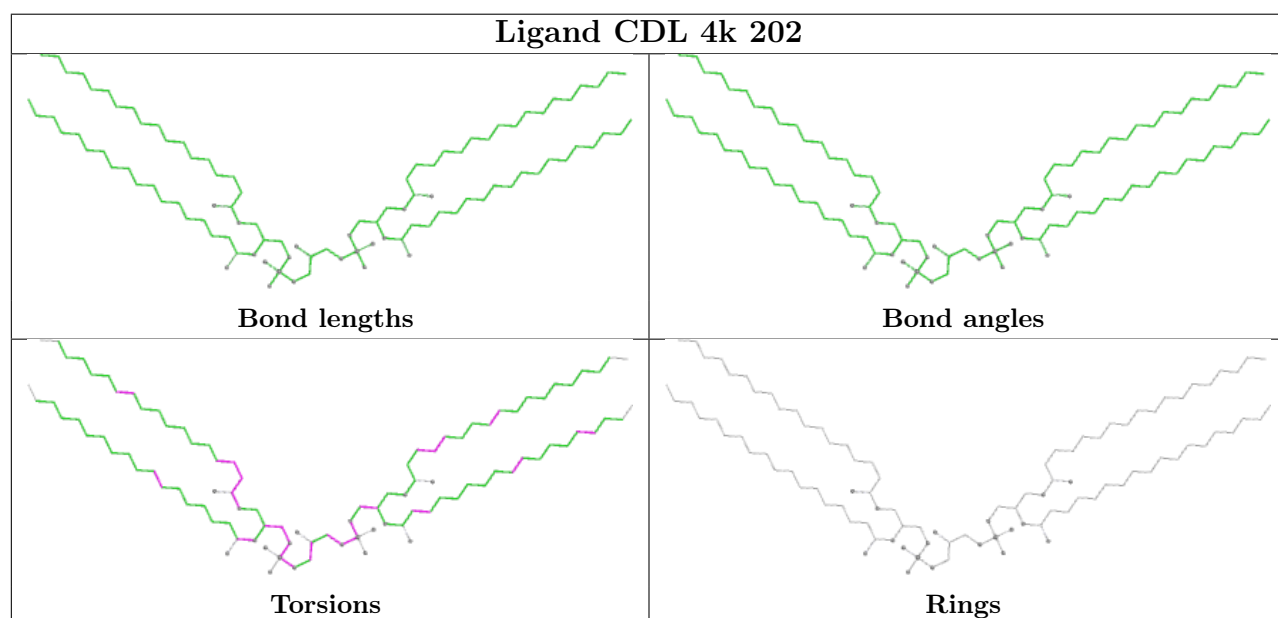
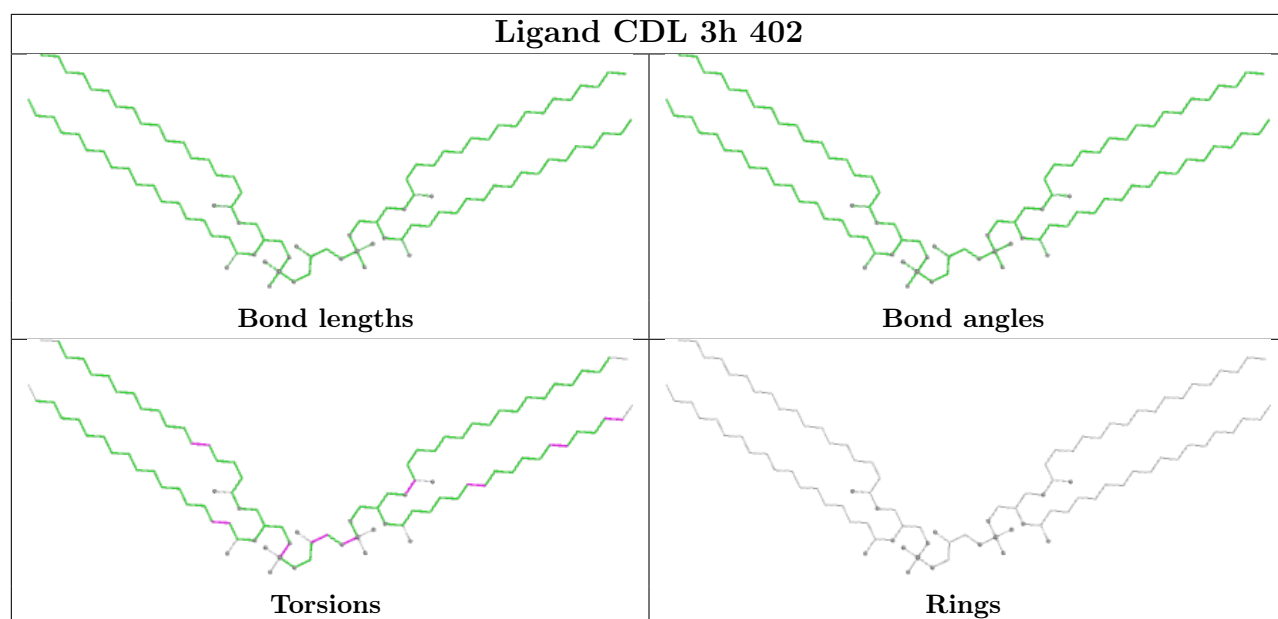


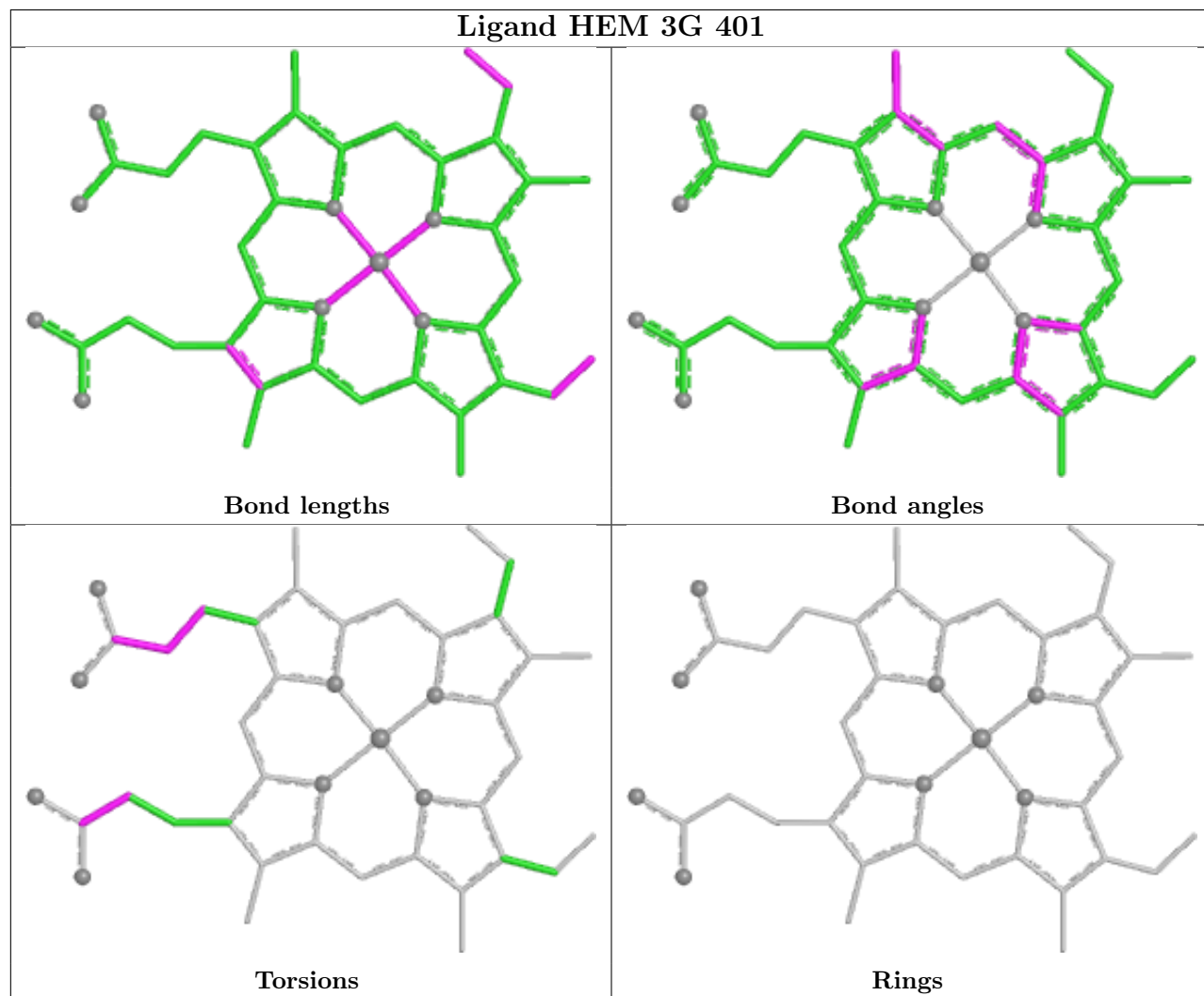
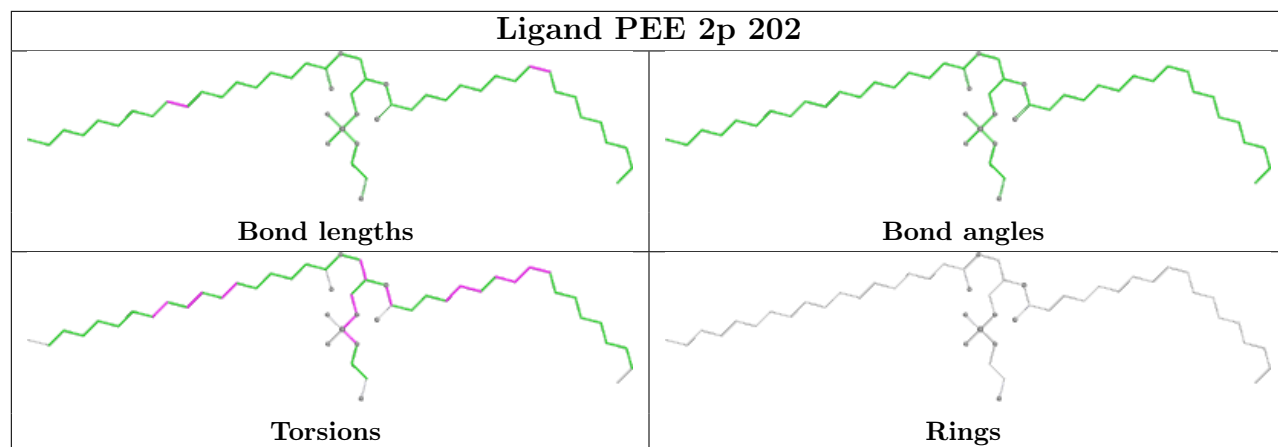


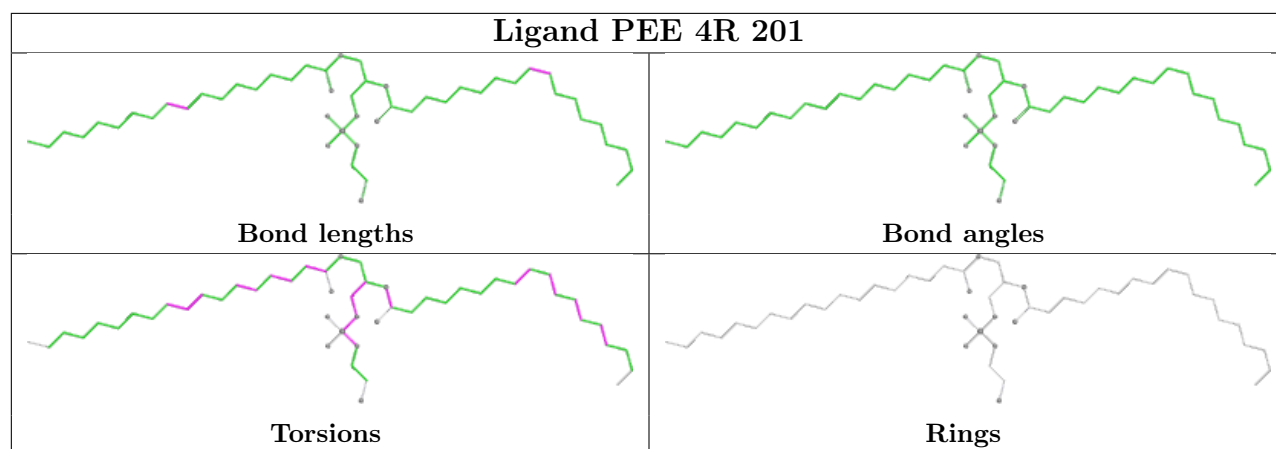
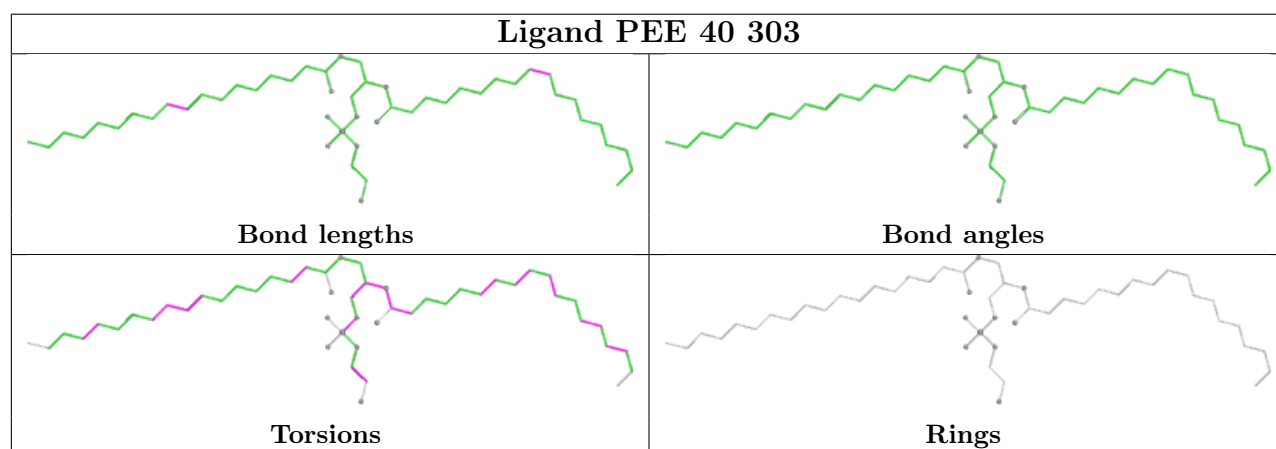
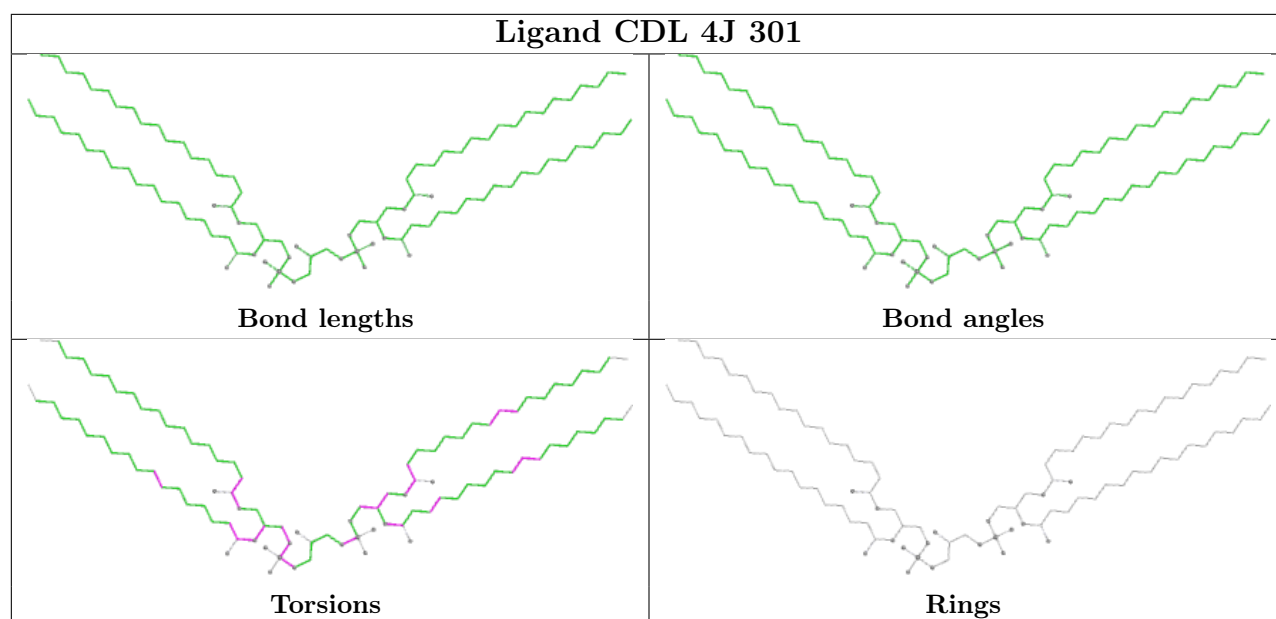


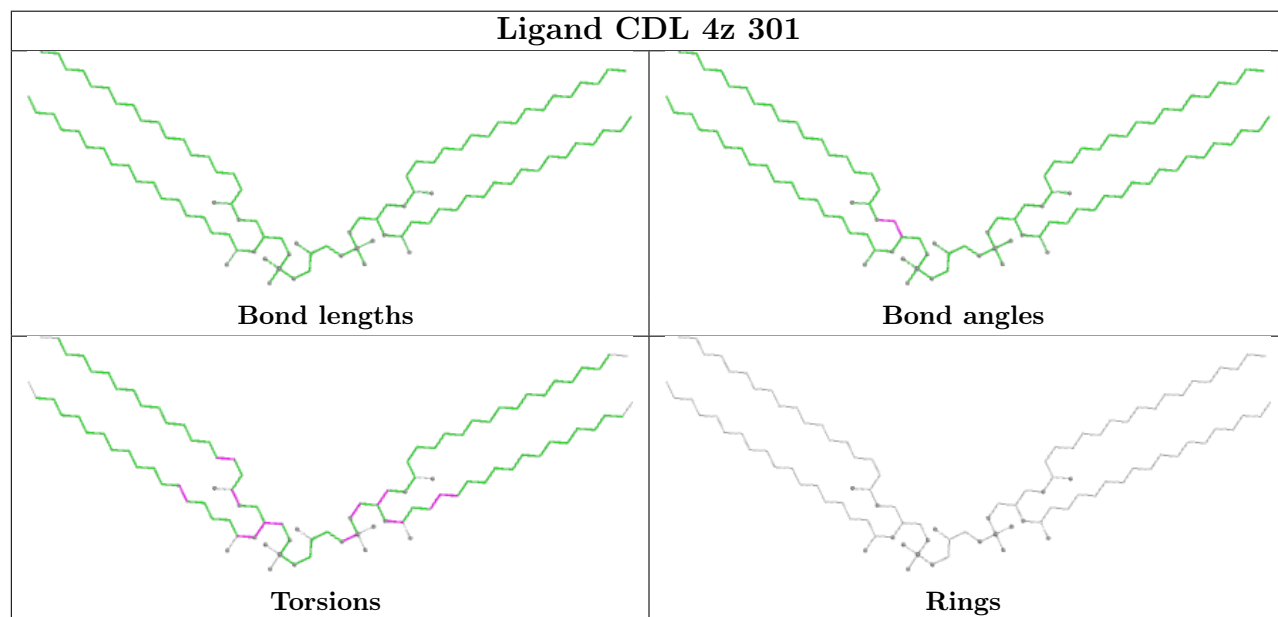
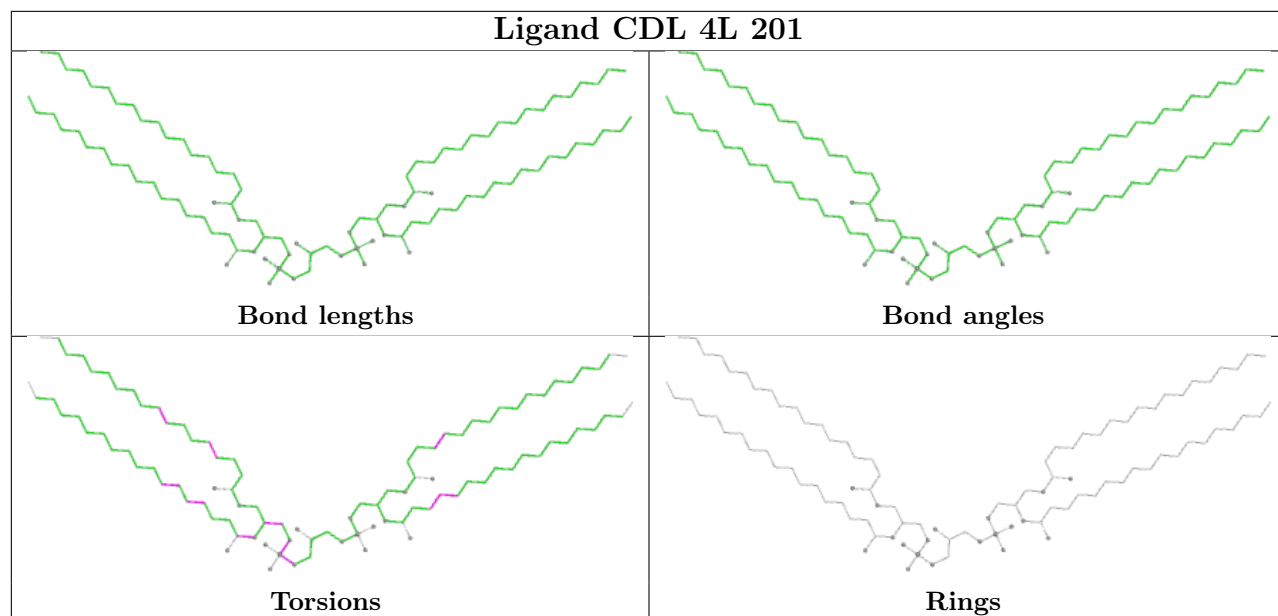


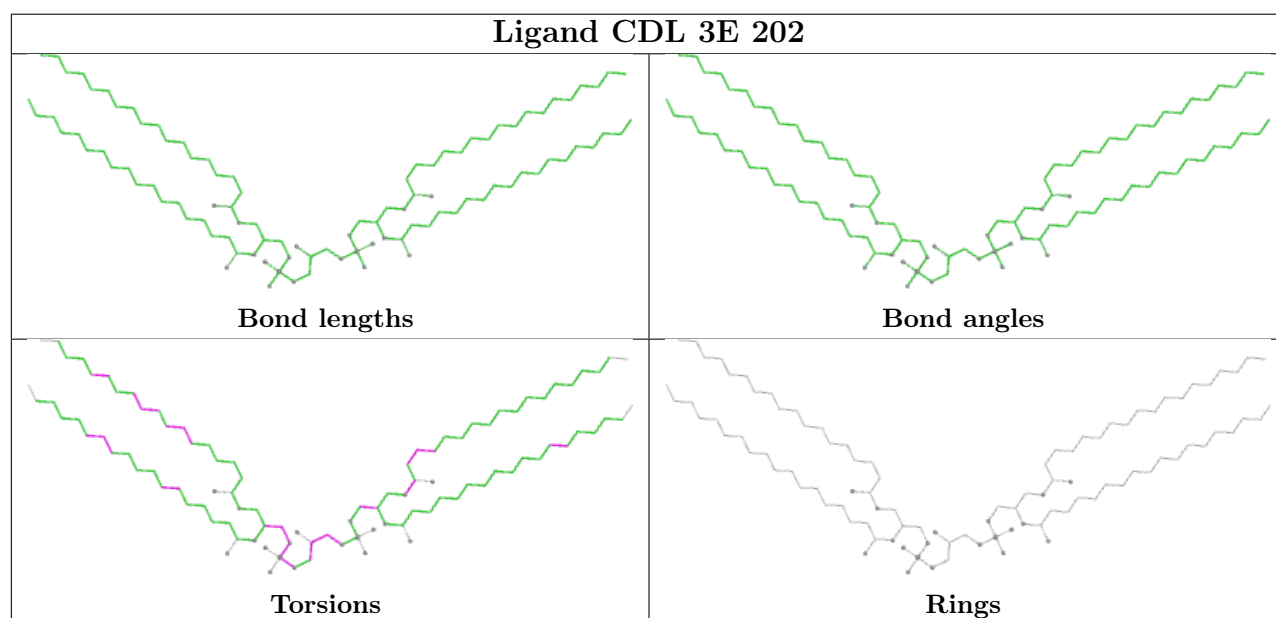
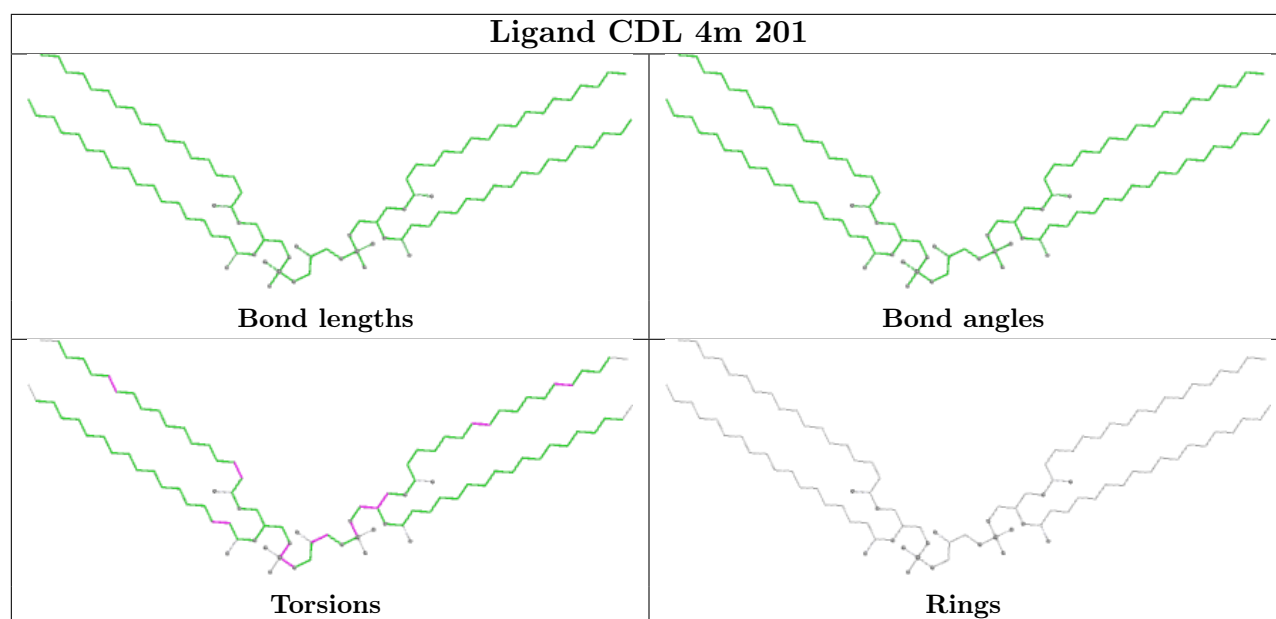


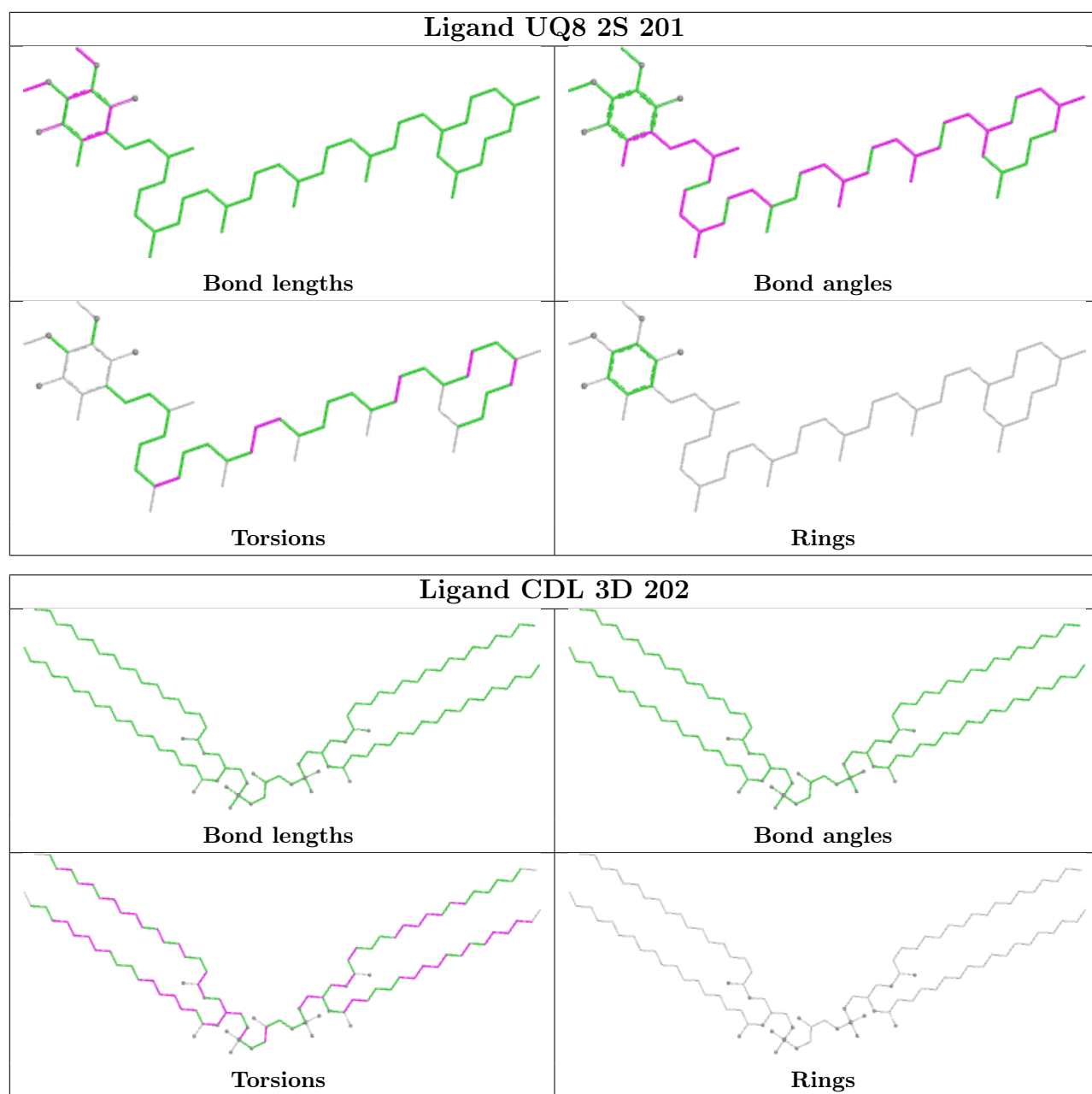


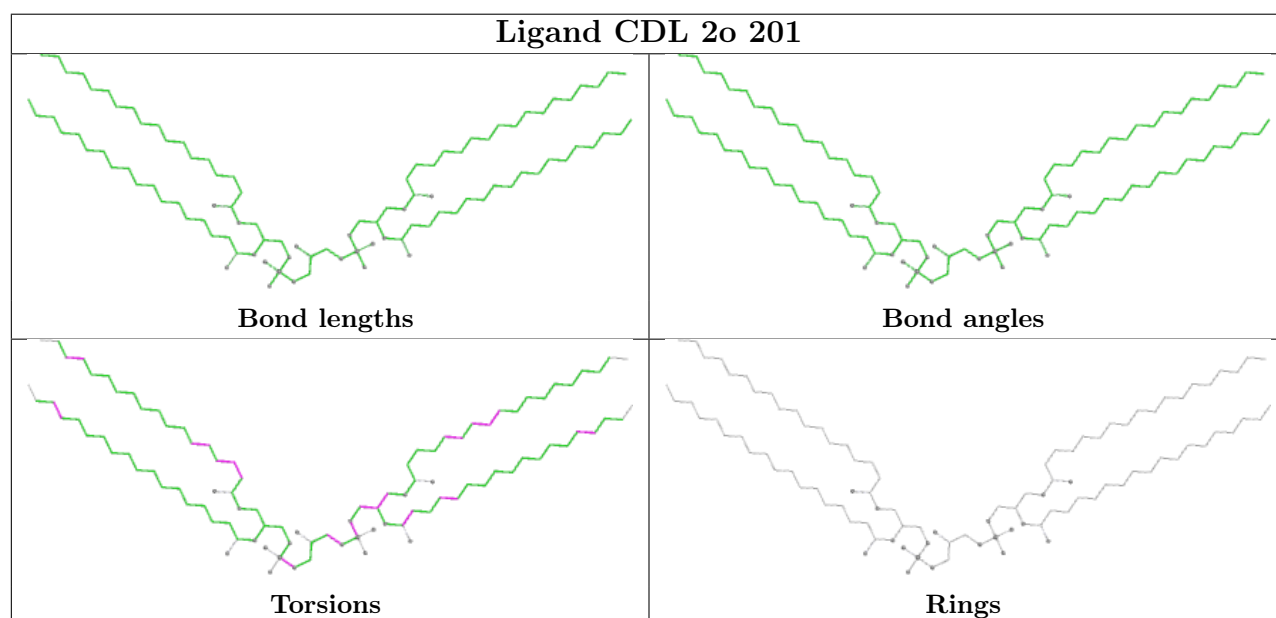
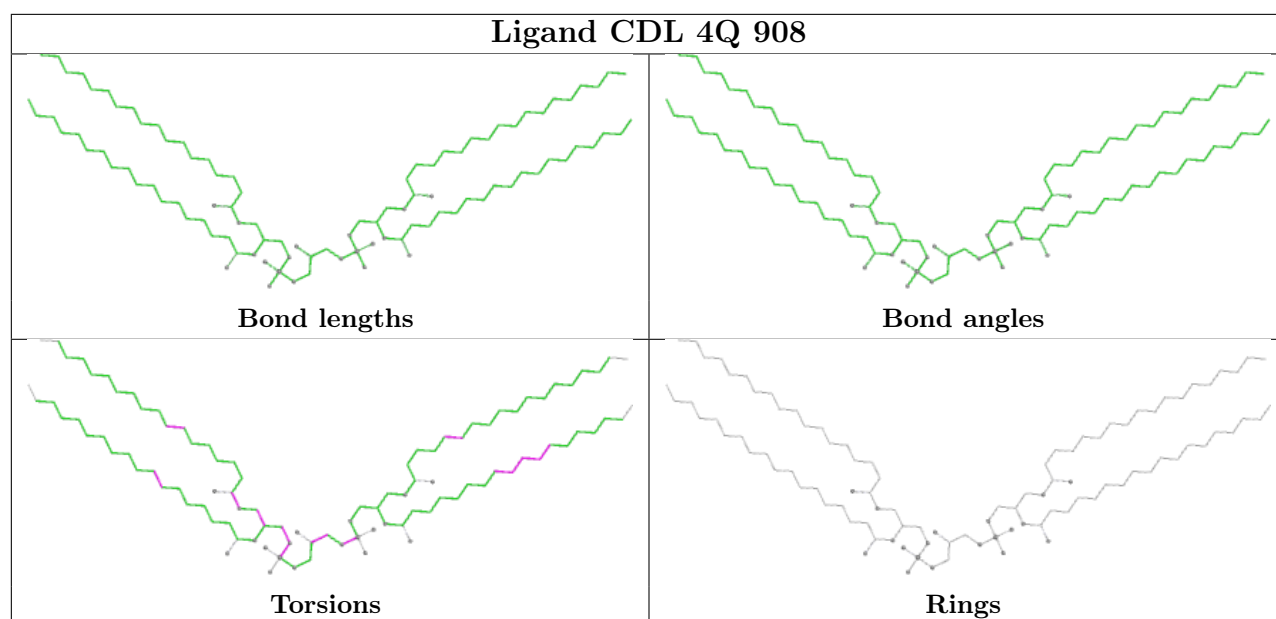


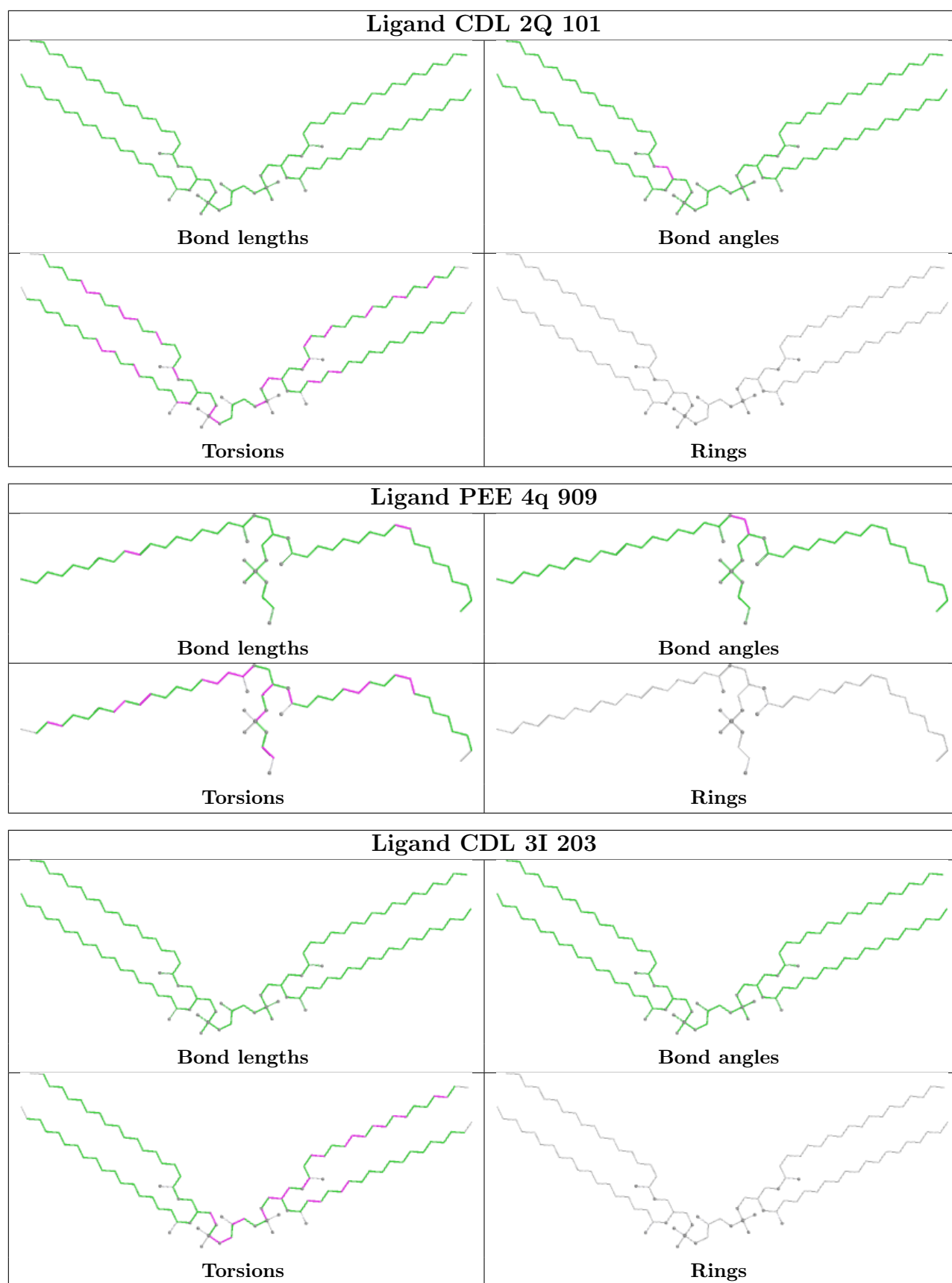


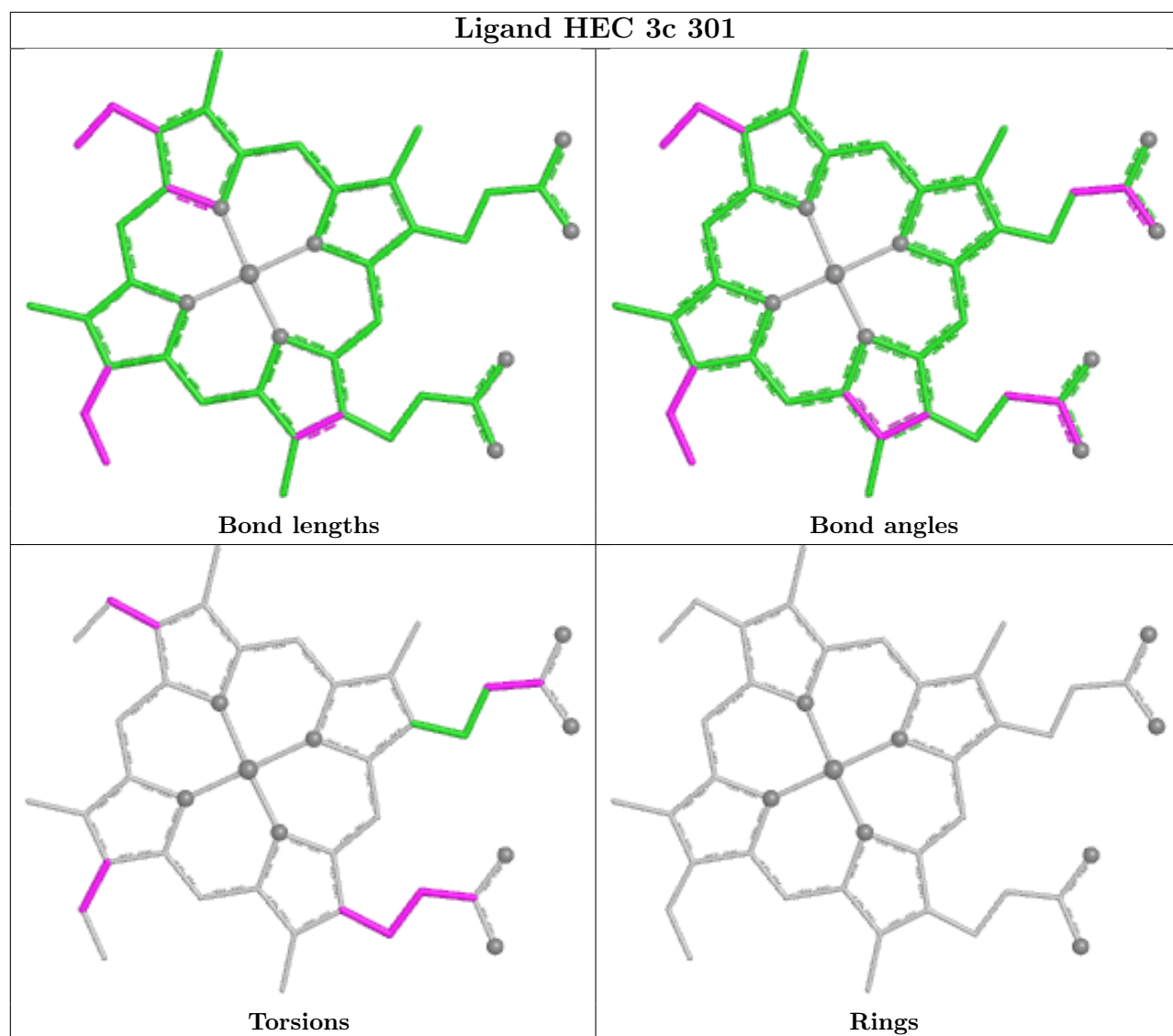
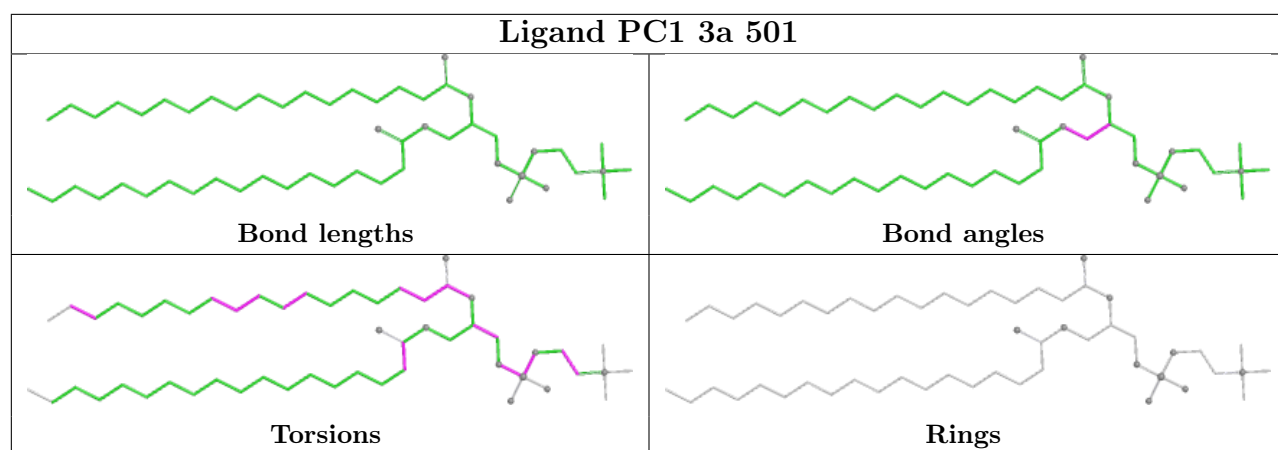




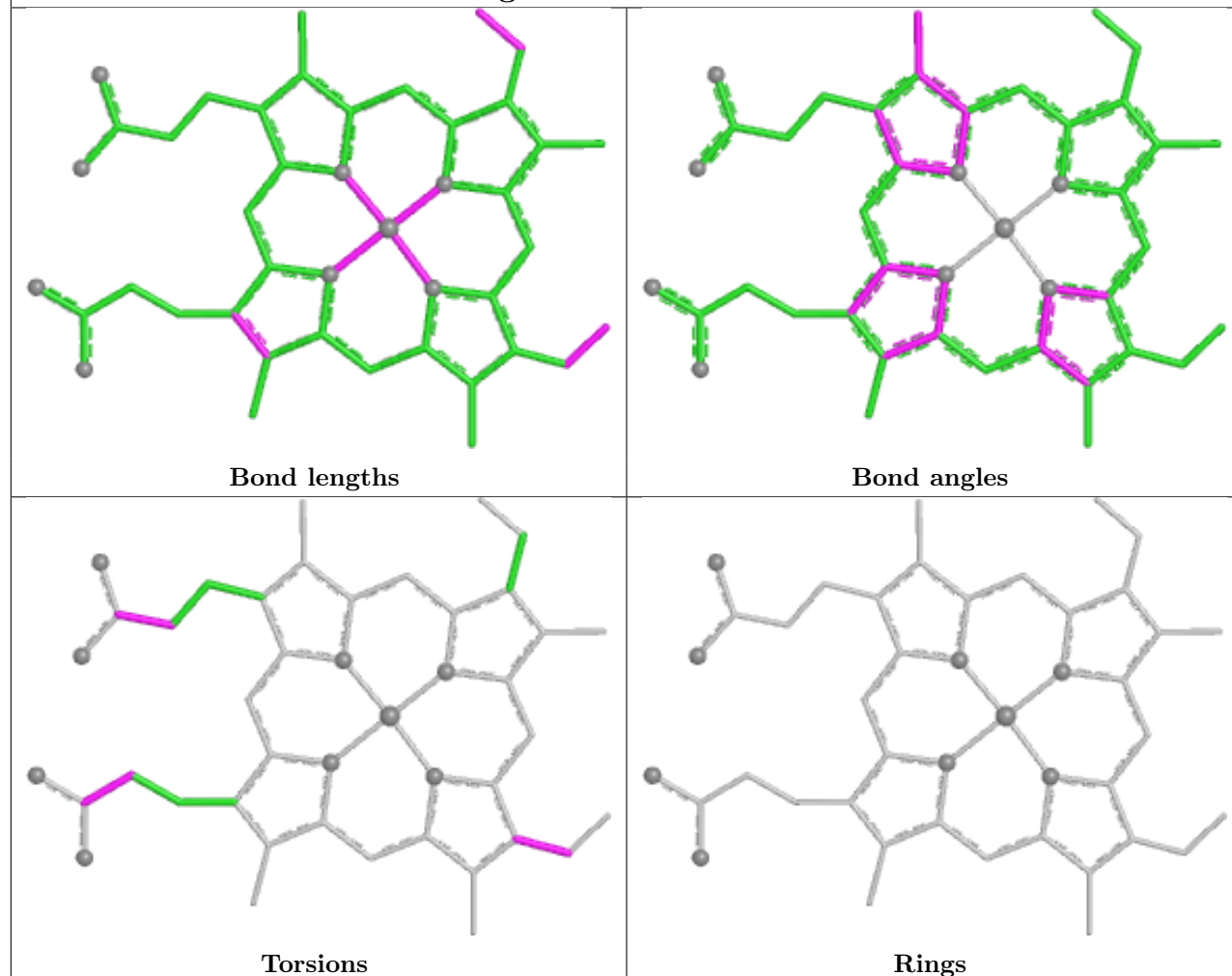




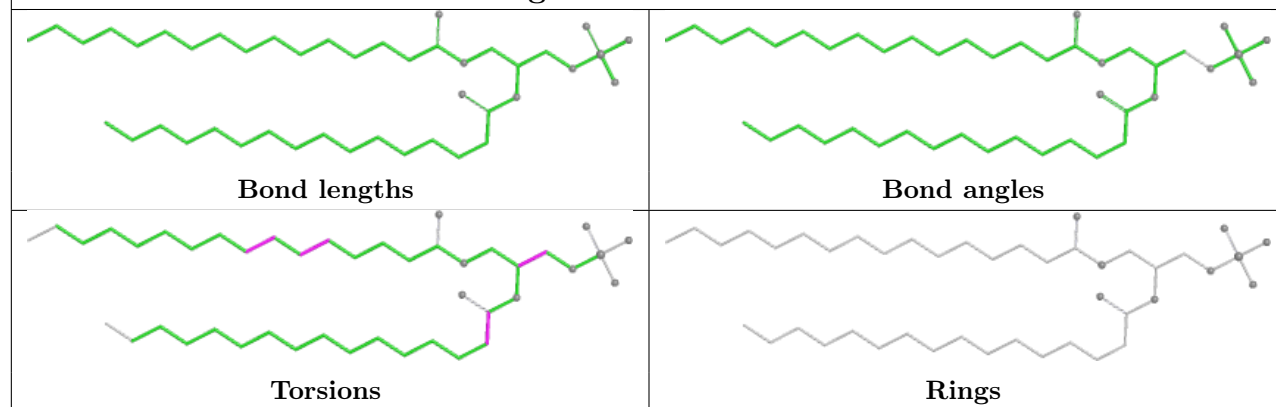


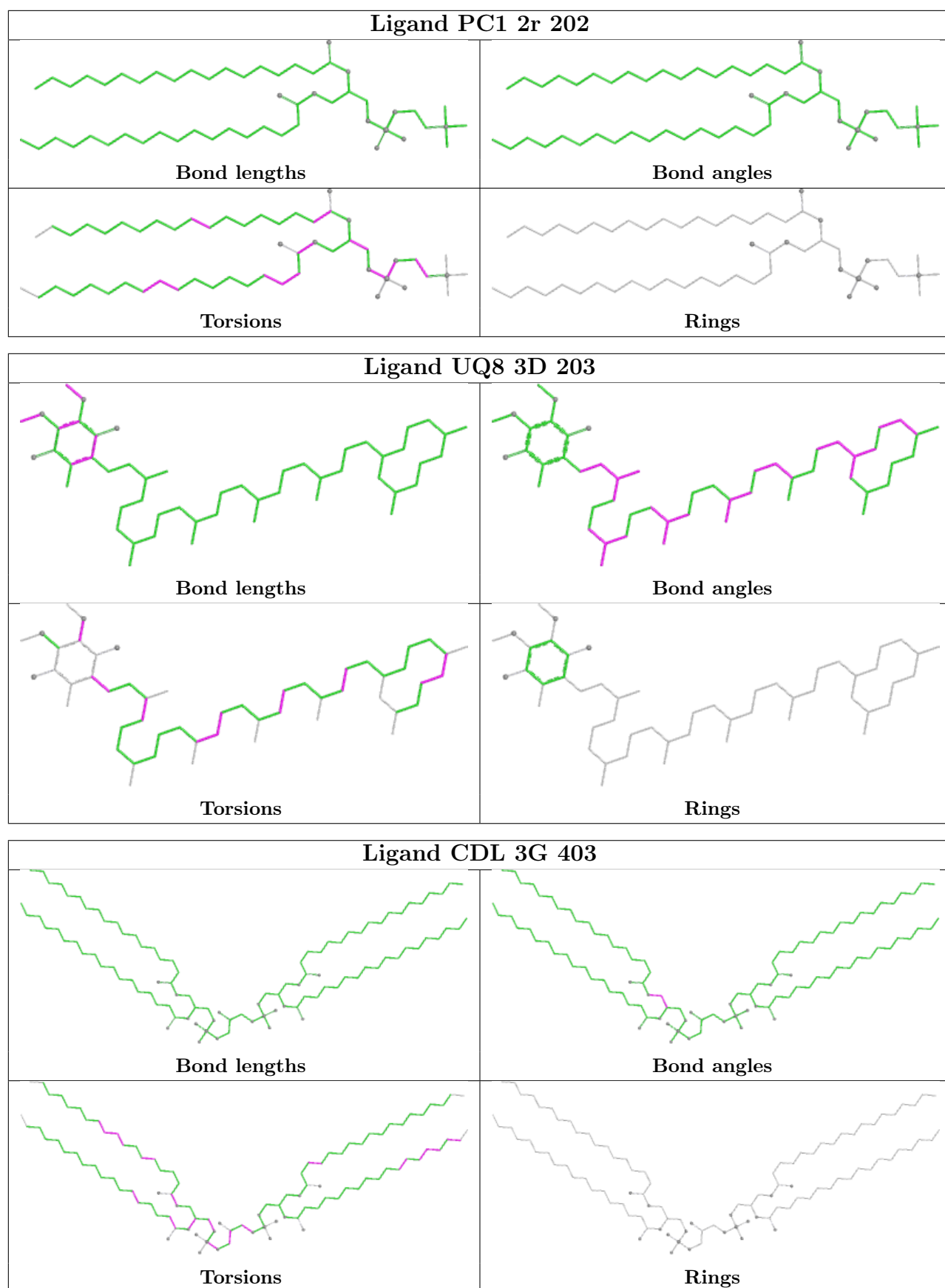


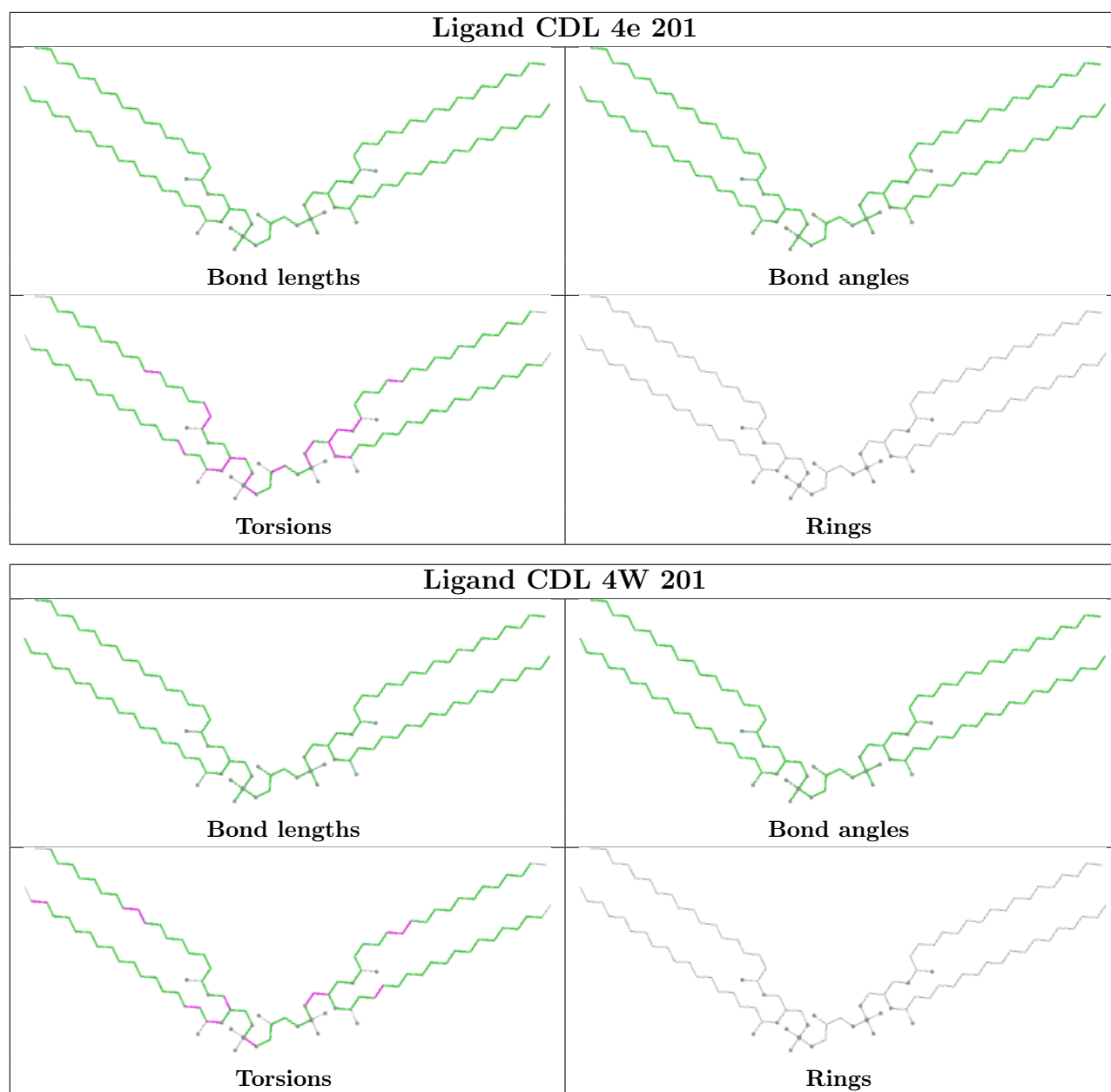
Ligand HEM 3G 402

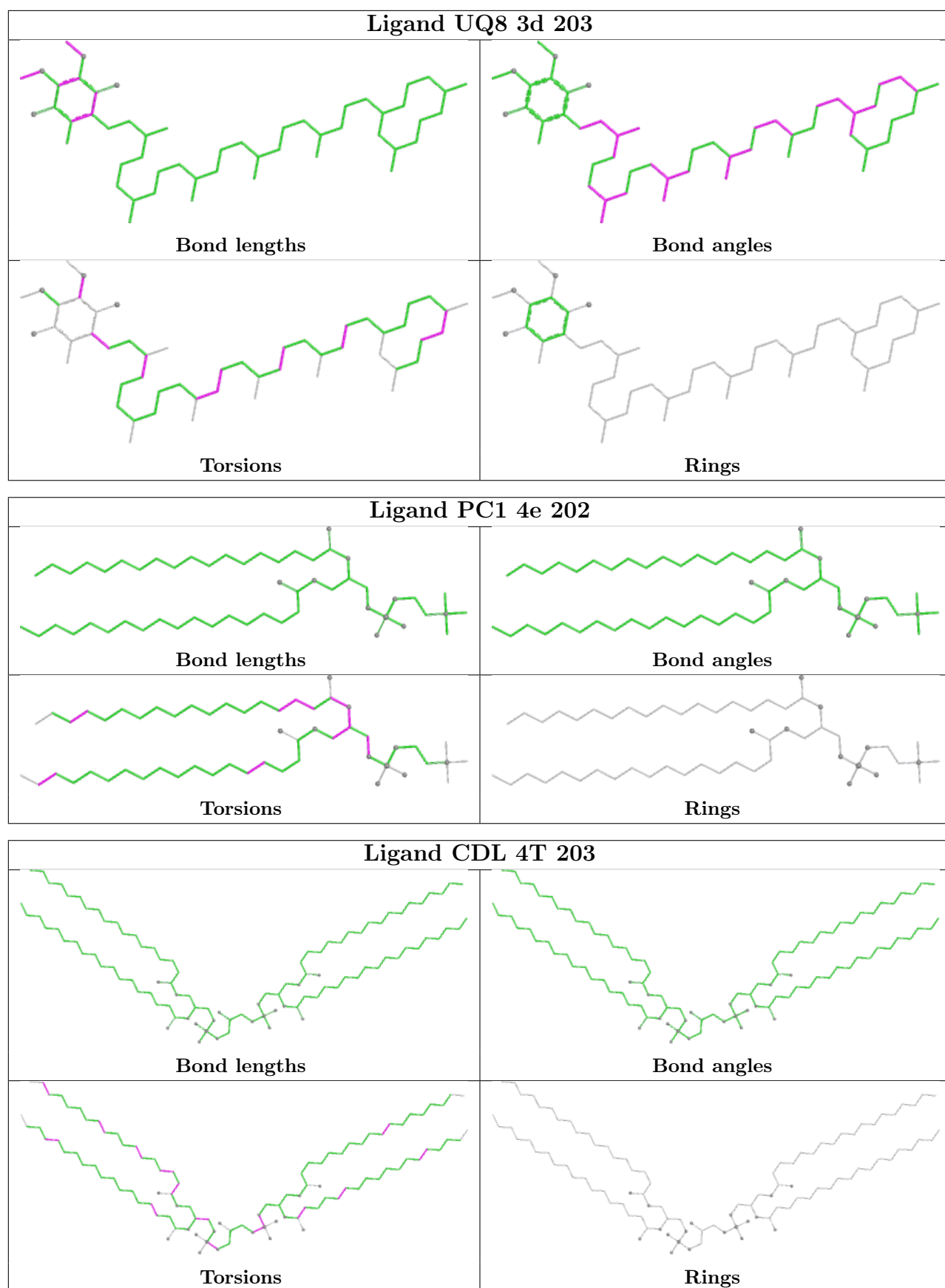


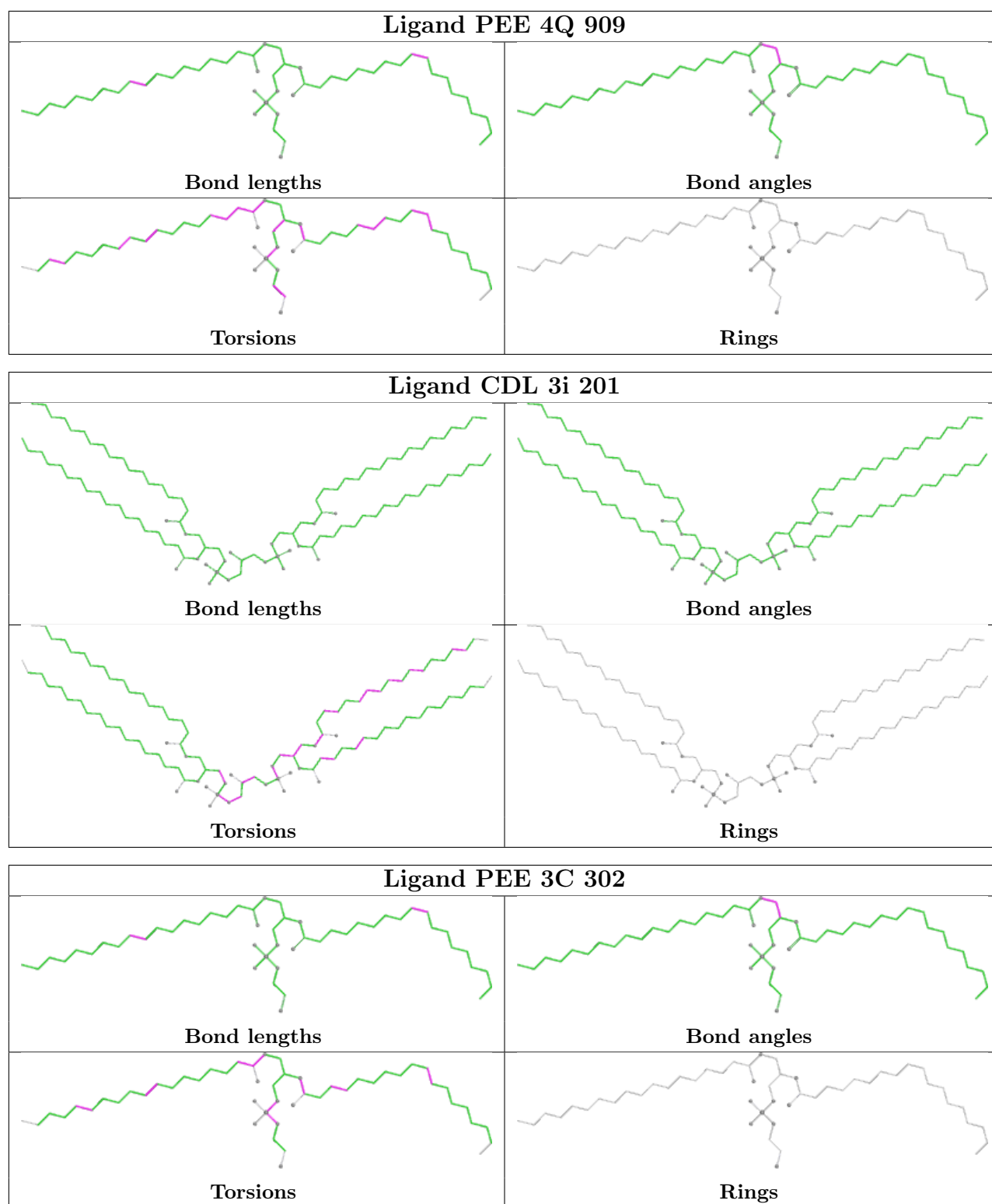
Ligand LPP 4d 102

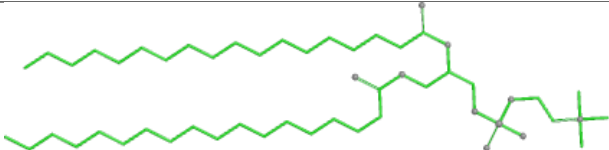
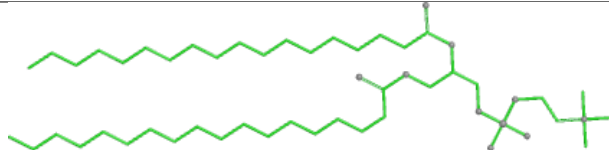
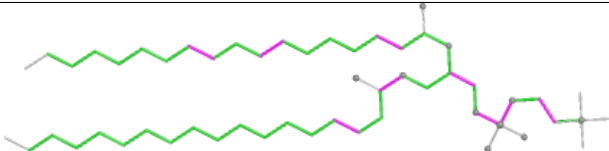
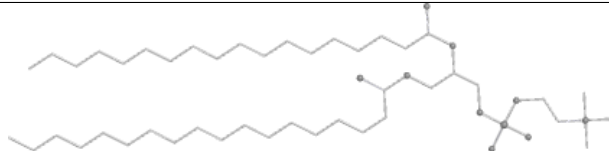


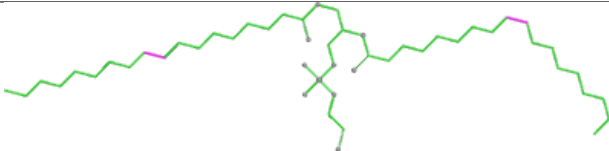
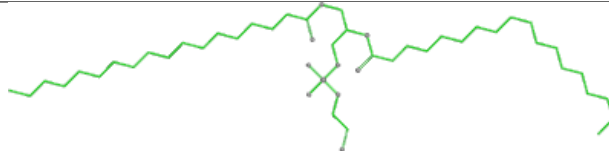
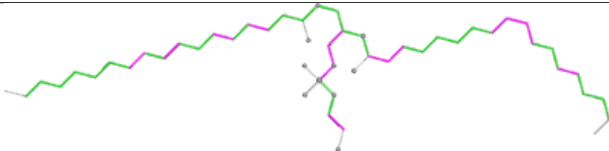
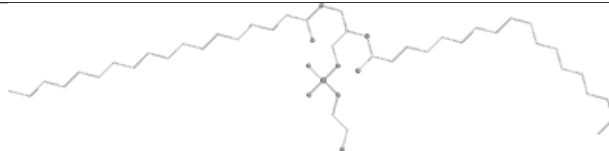


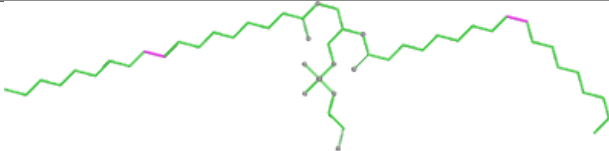
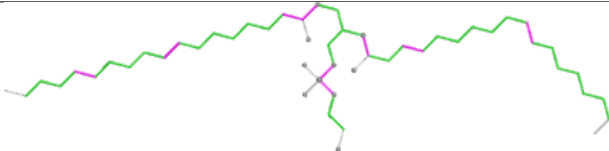
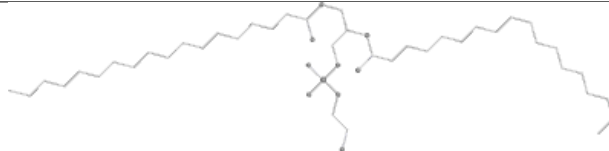


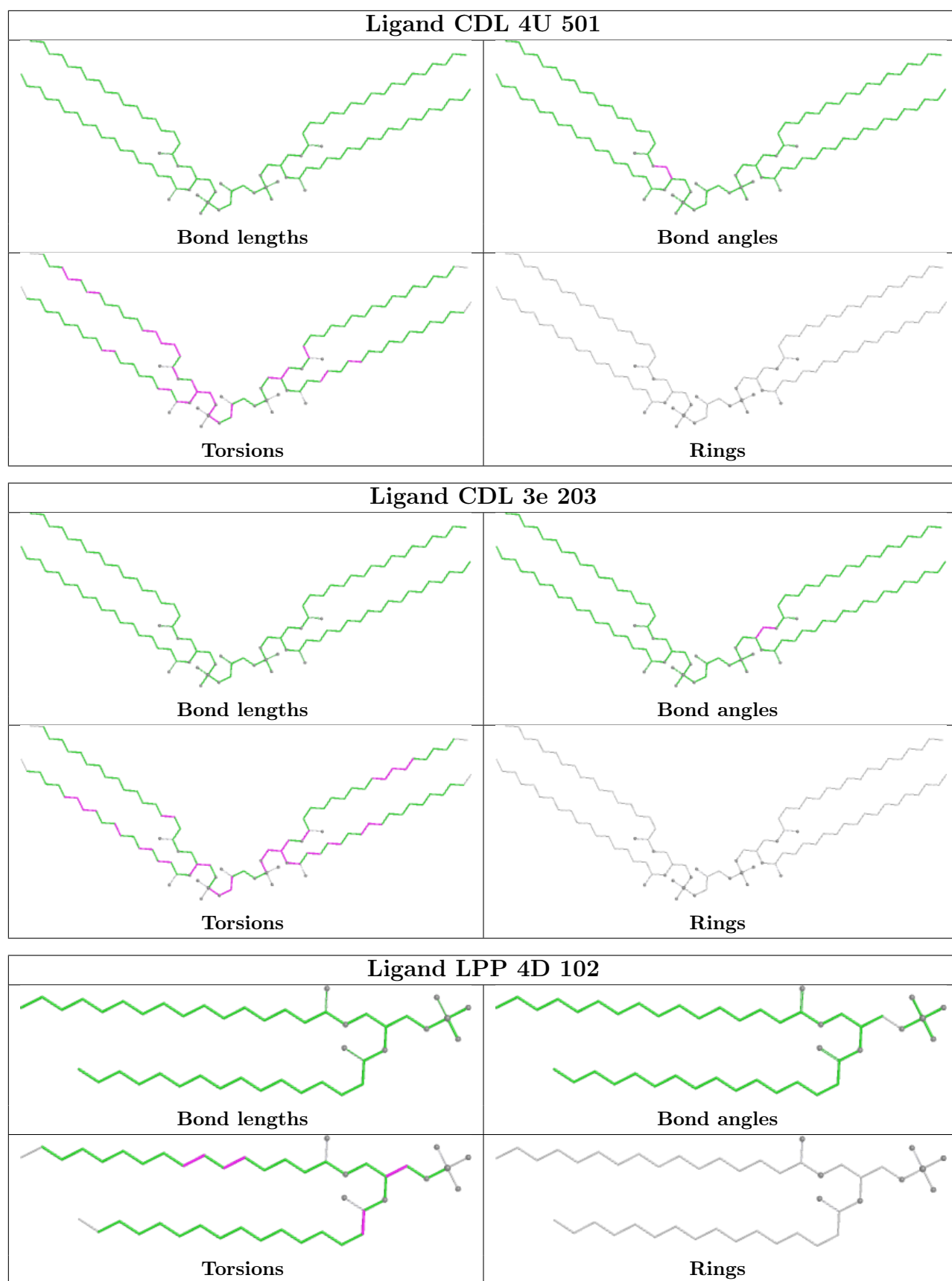


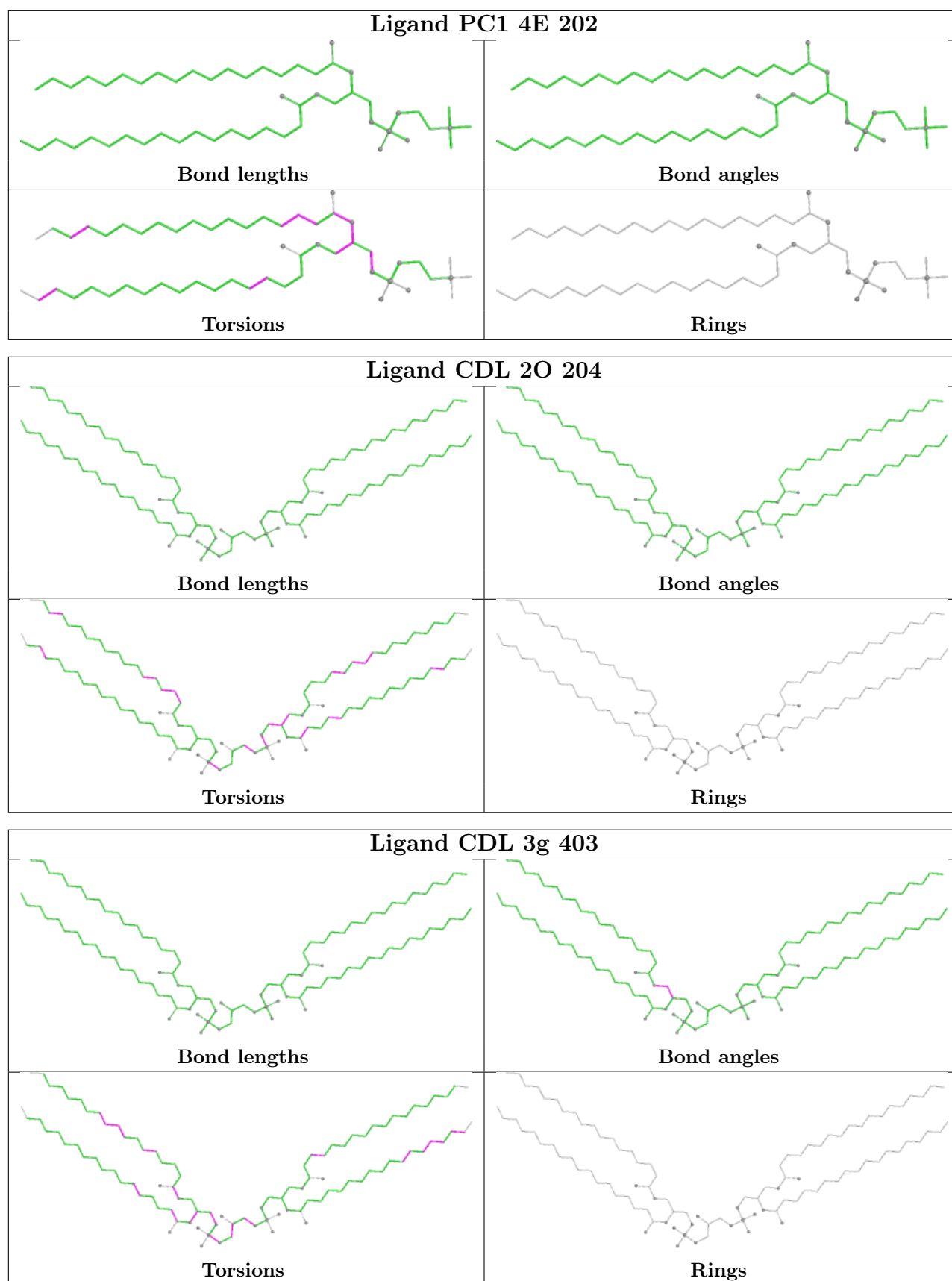


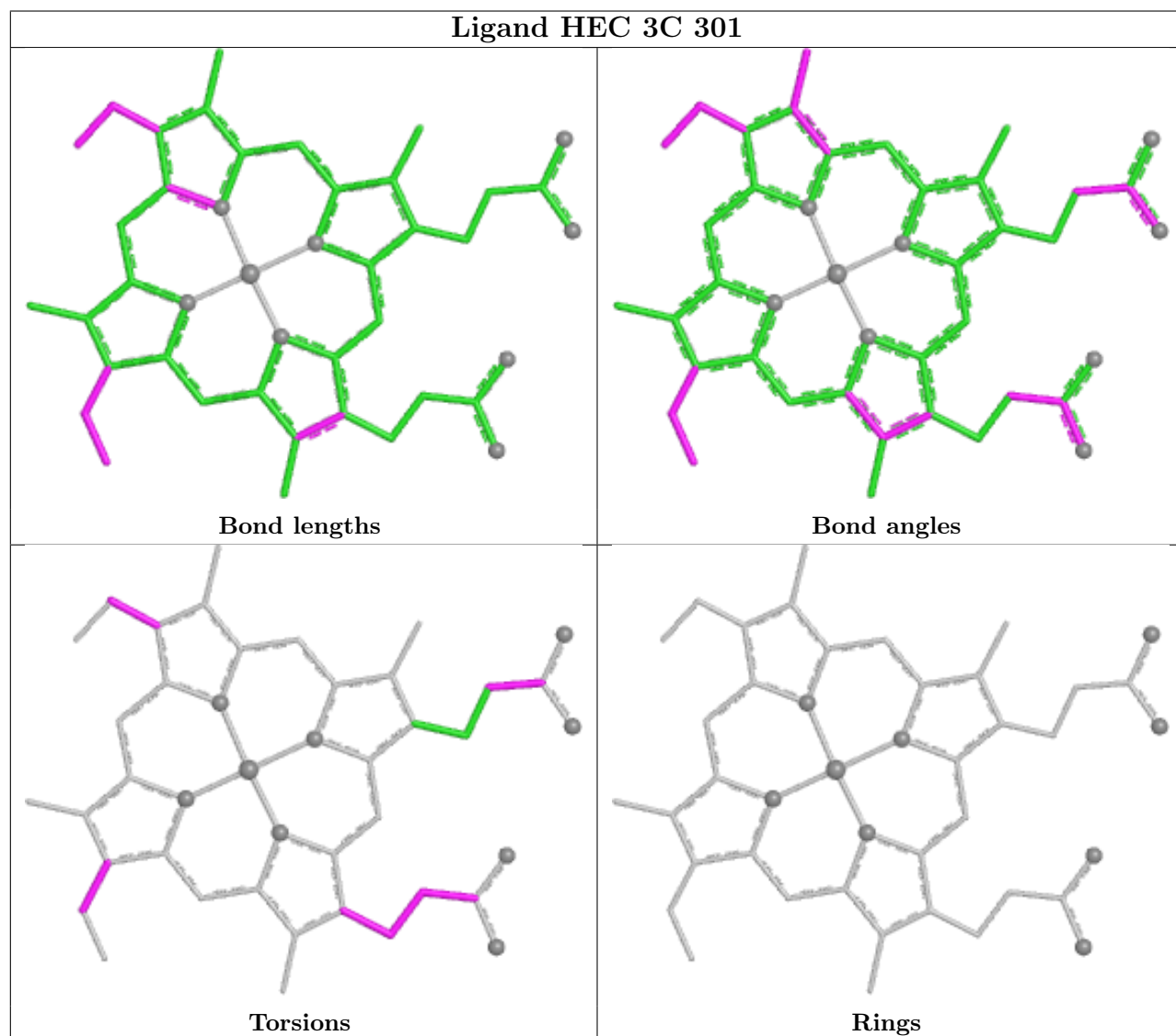
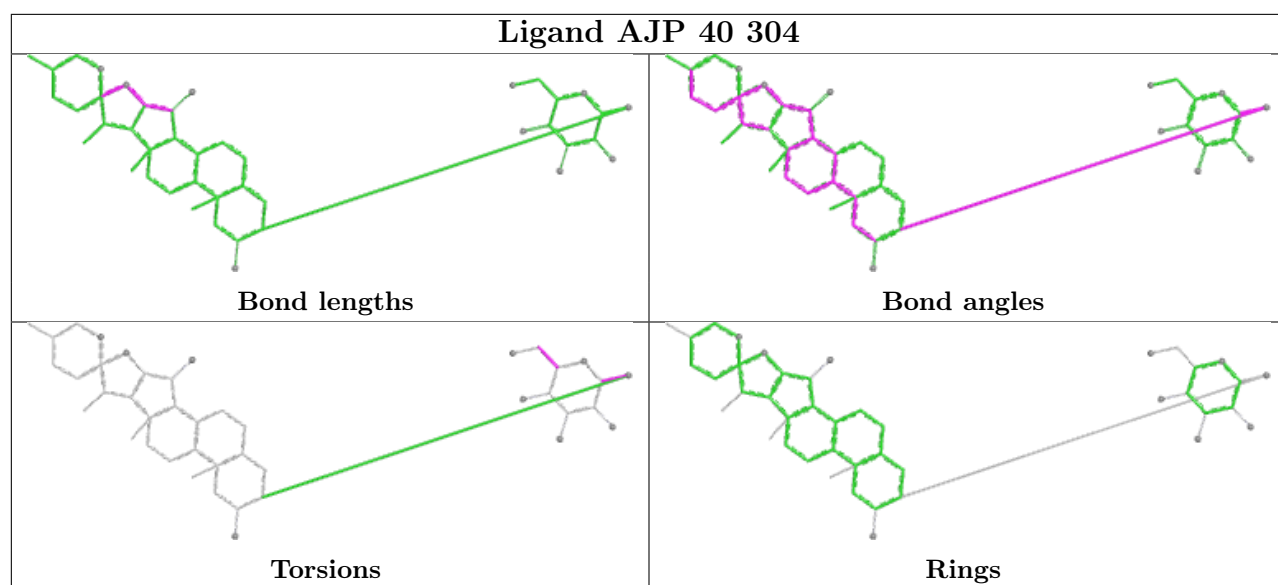
Ligand PC1 3a 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

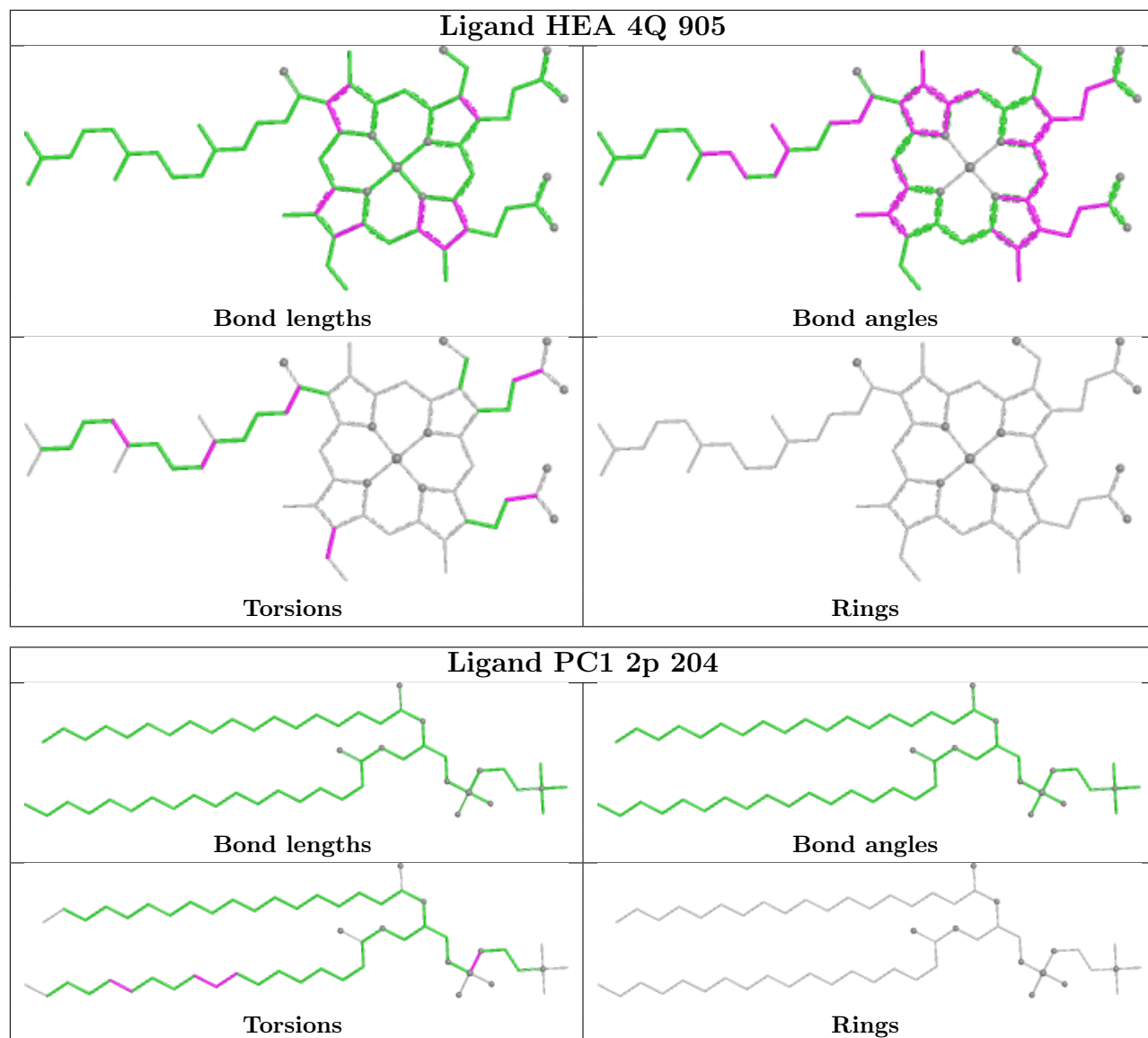
Ligand PEE 4D 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

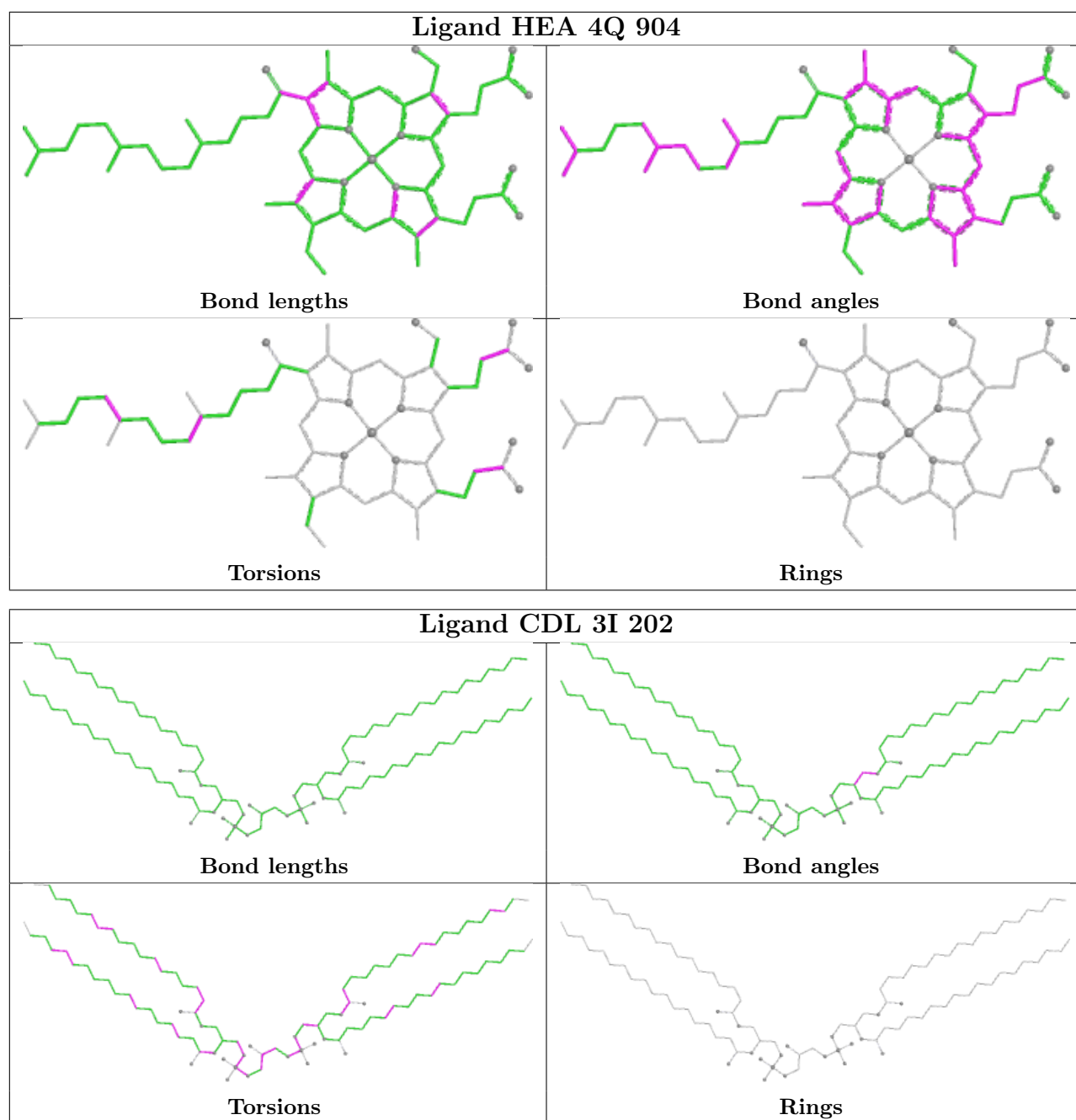
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Bond lengths	Bond angles
	
Torsions	Rings

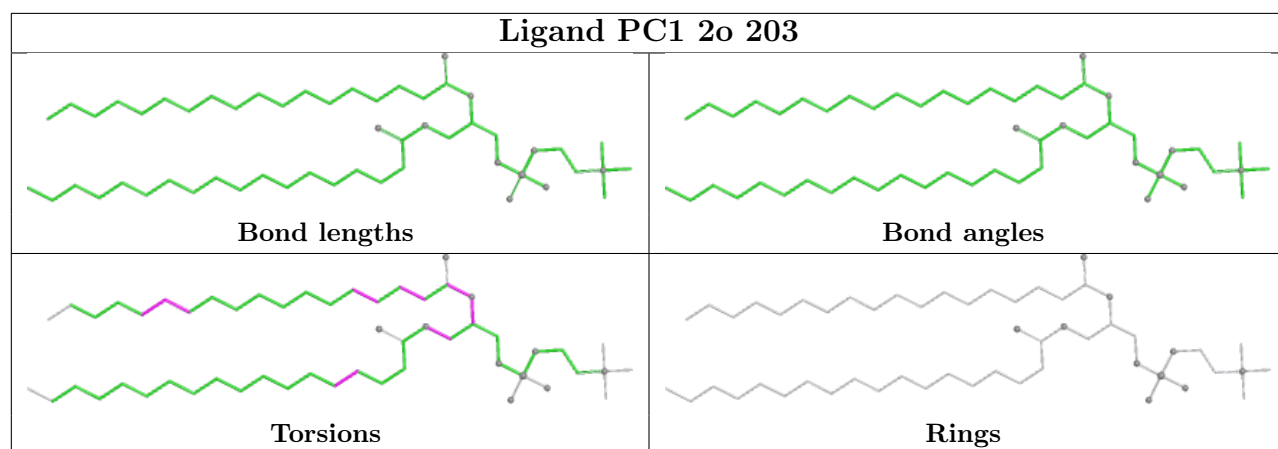
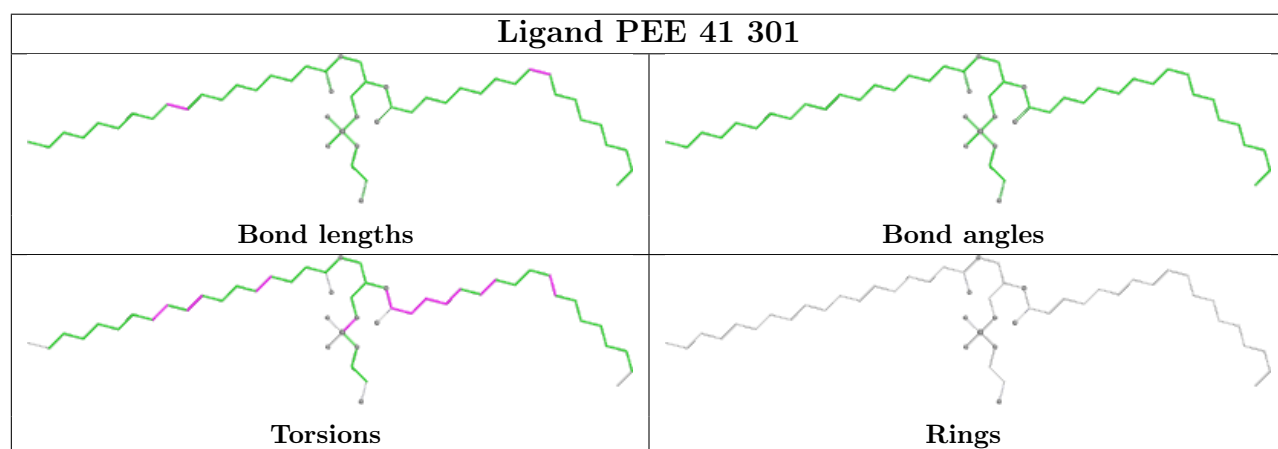
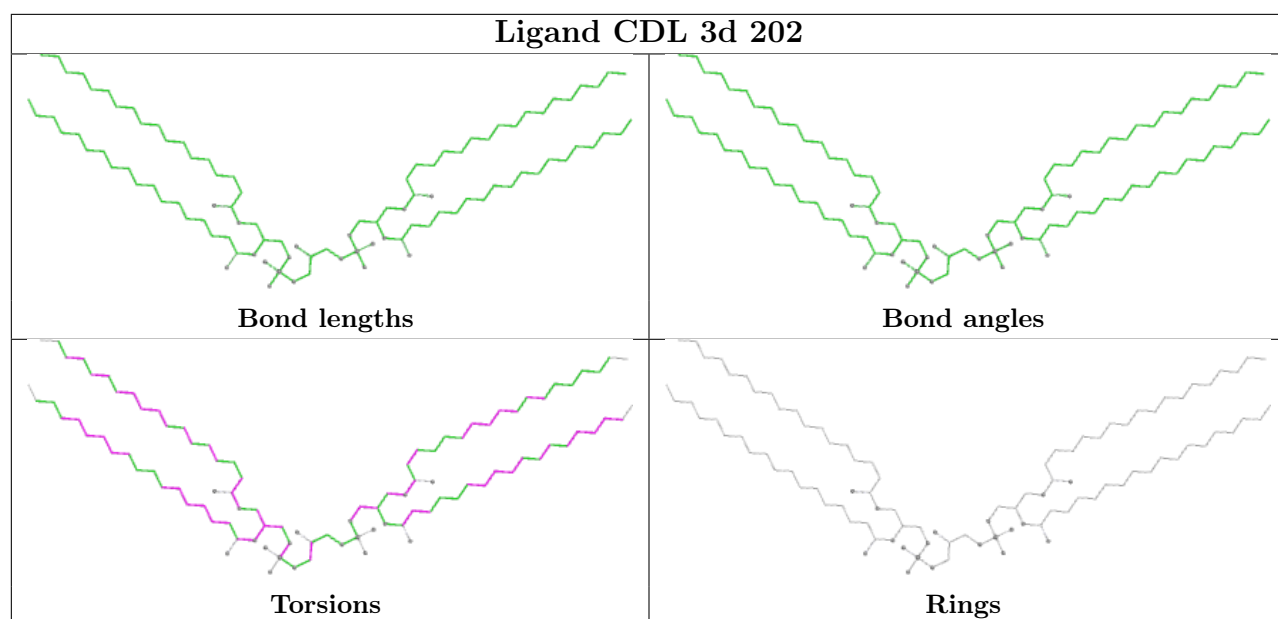


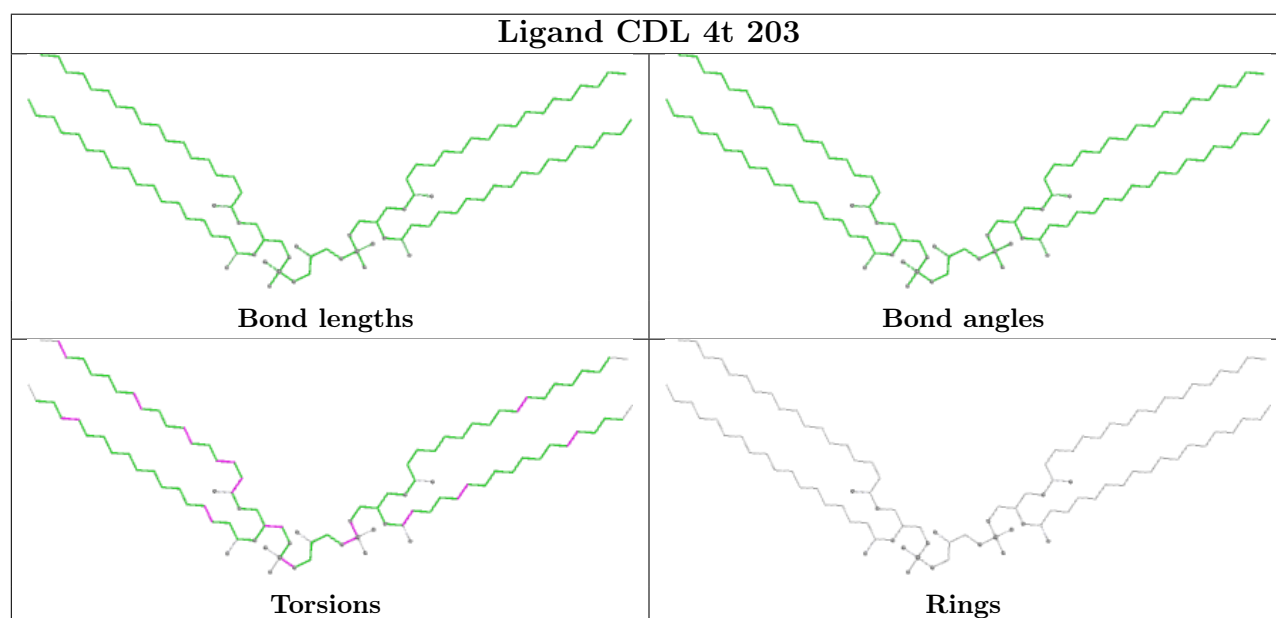
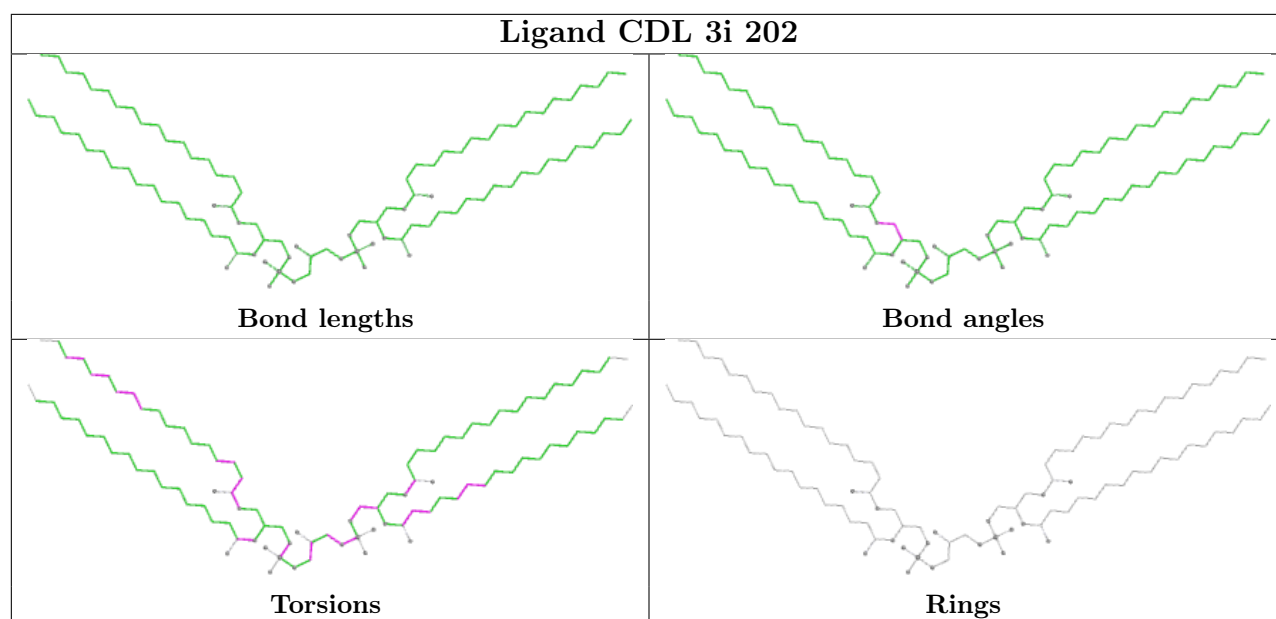


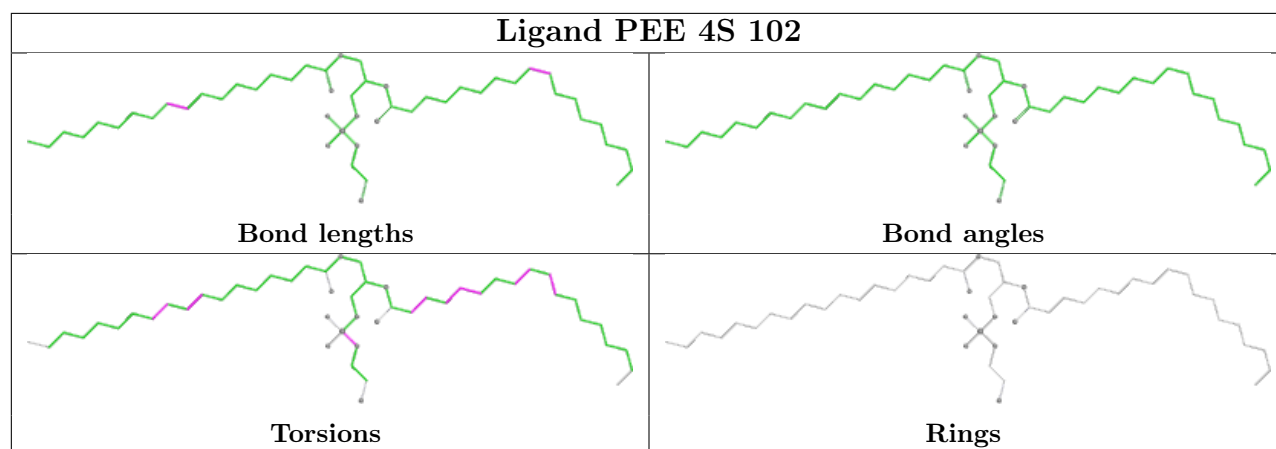
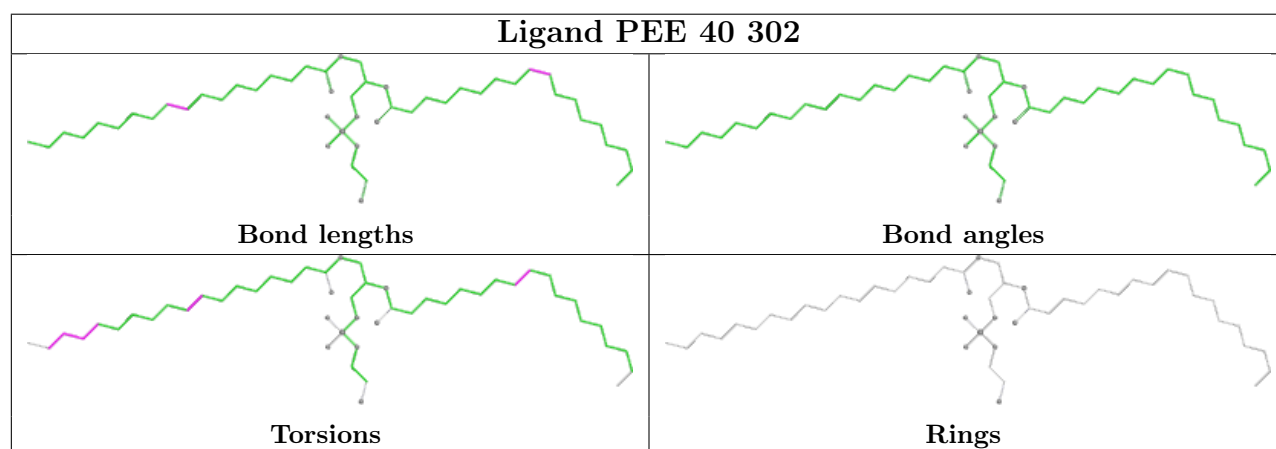
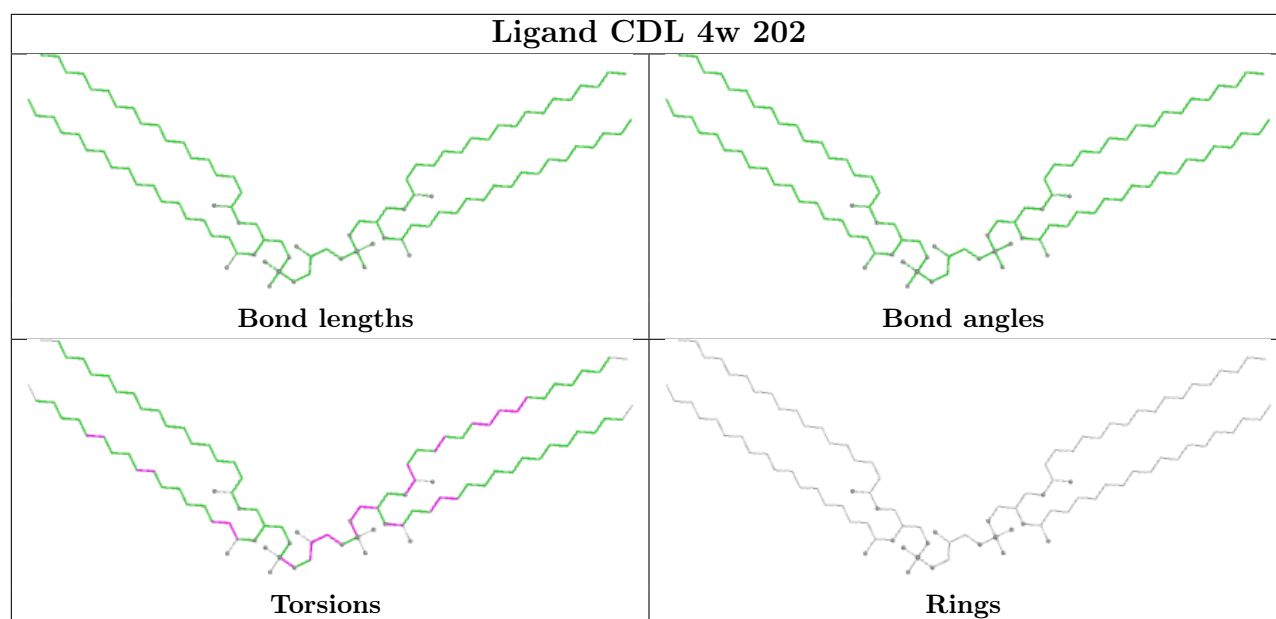




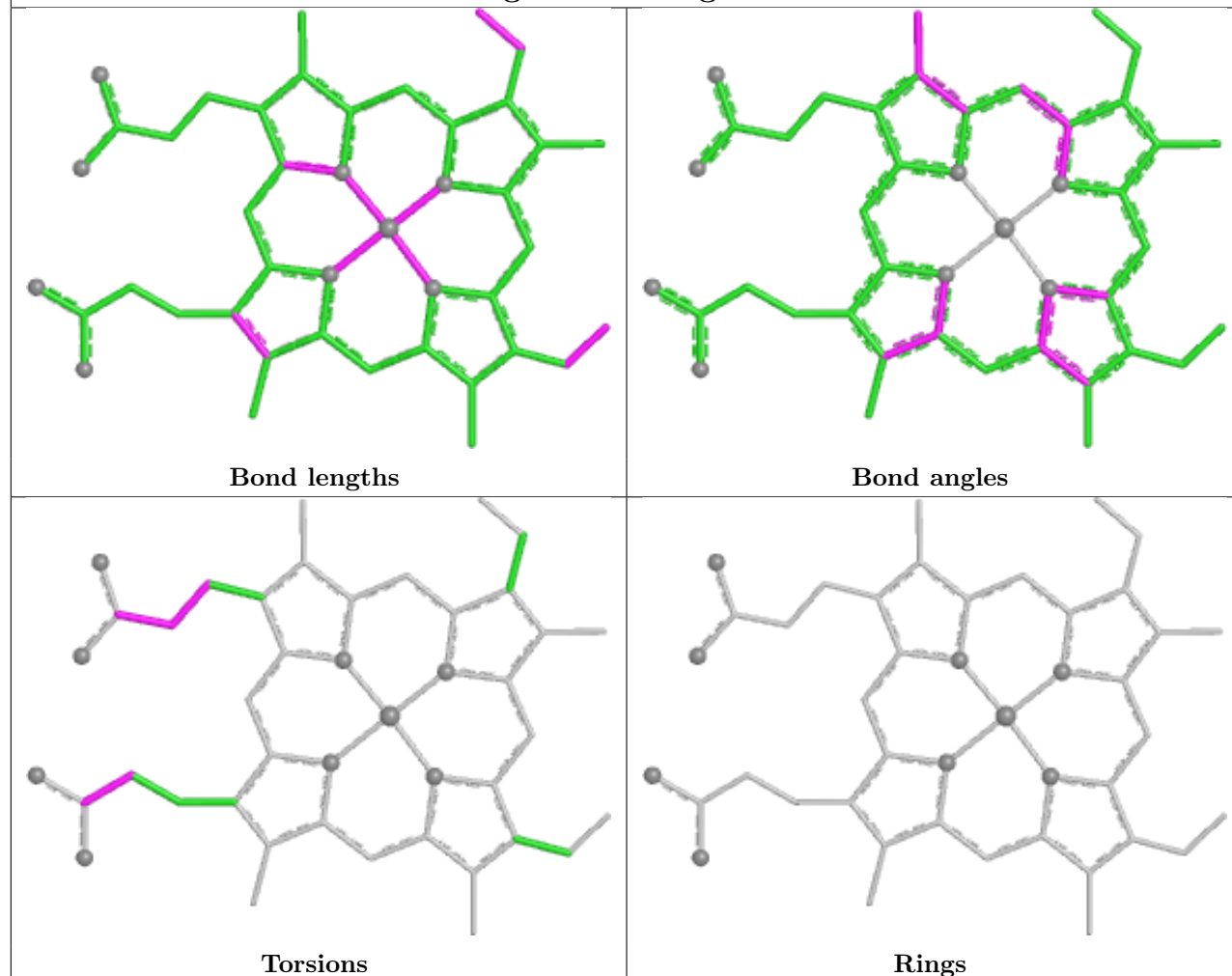




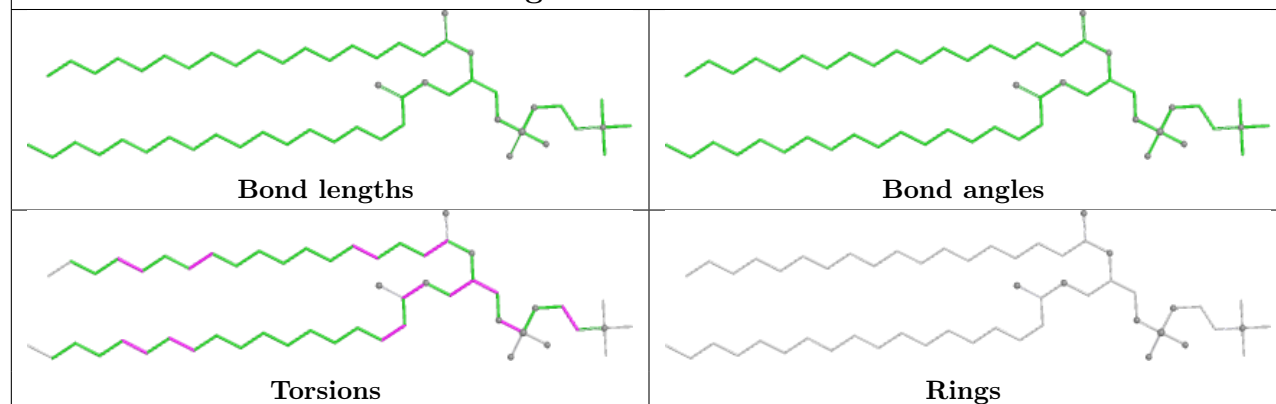


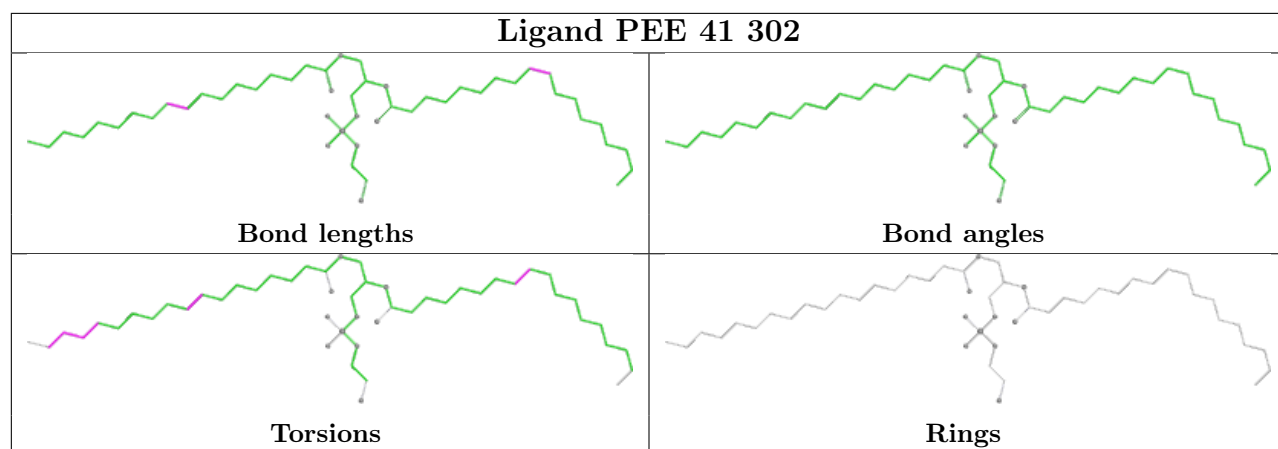
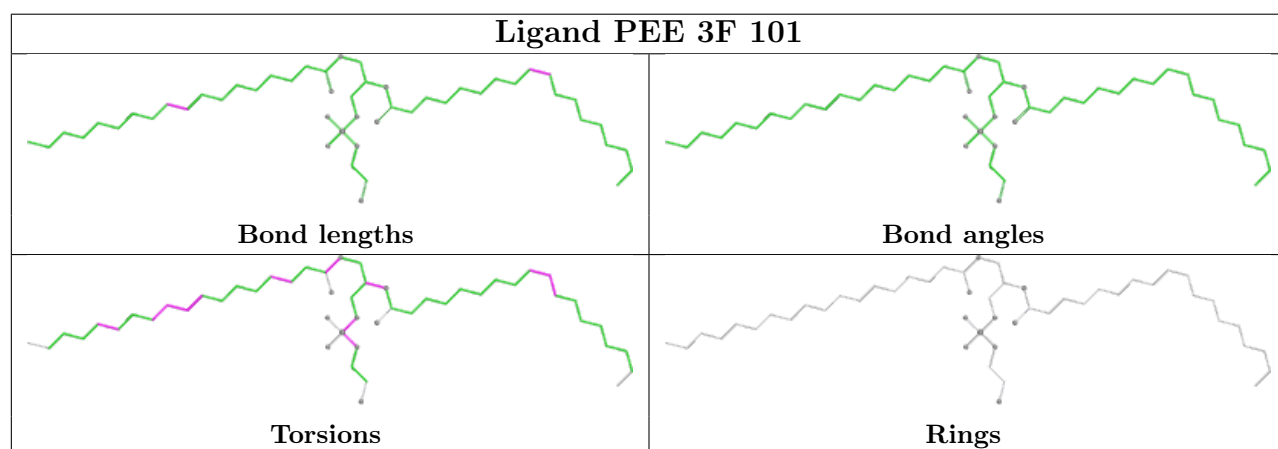
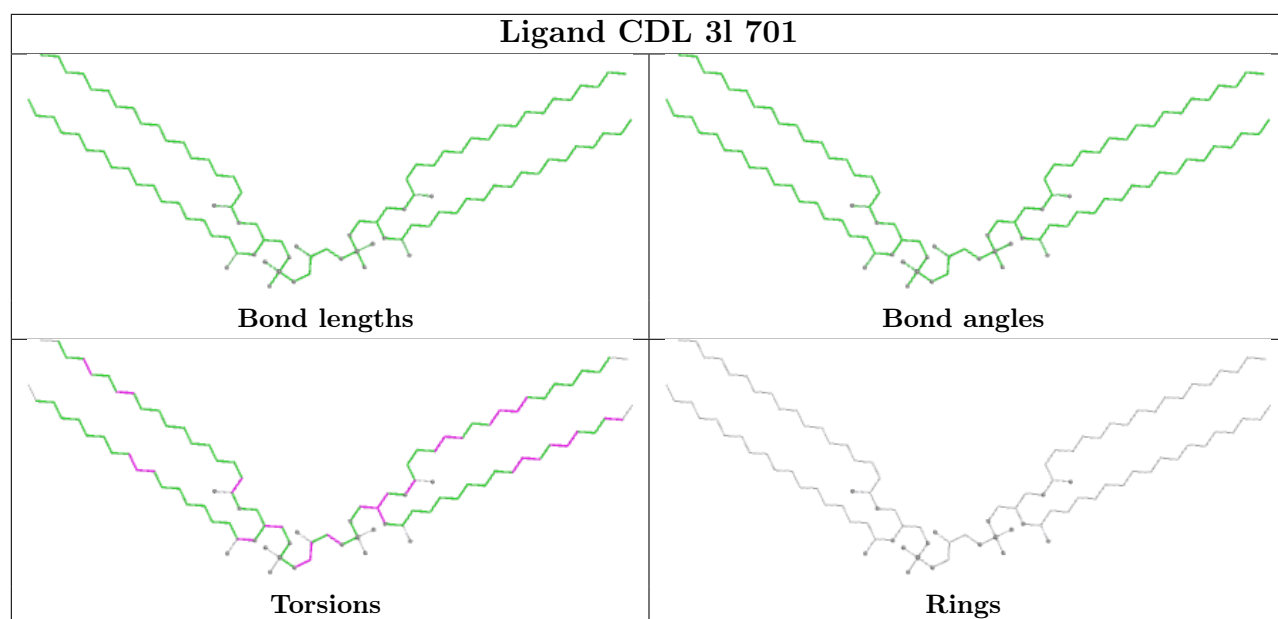


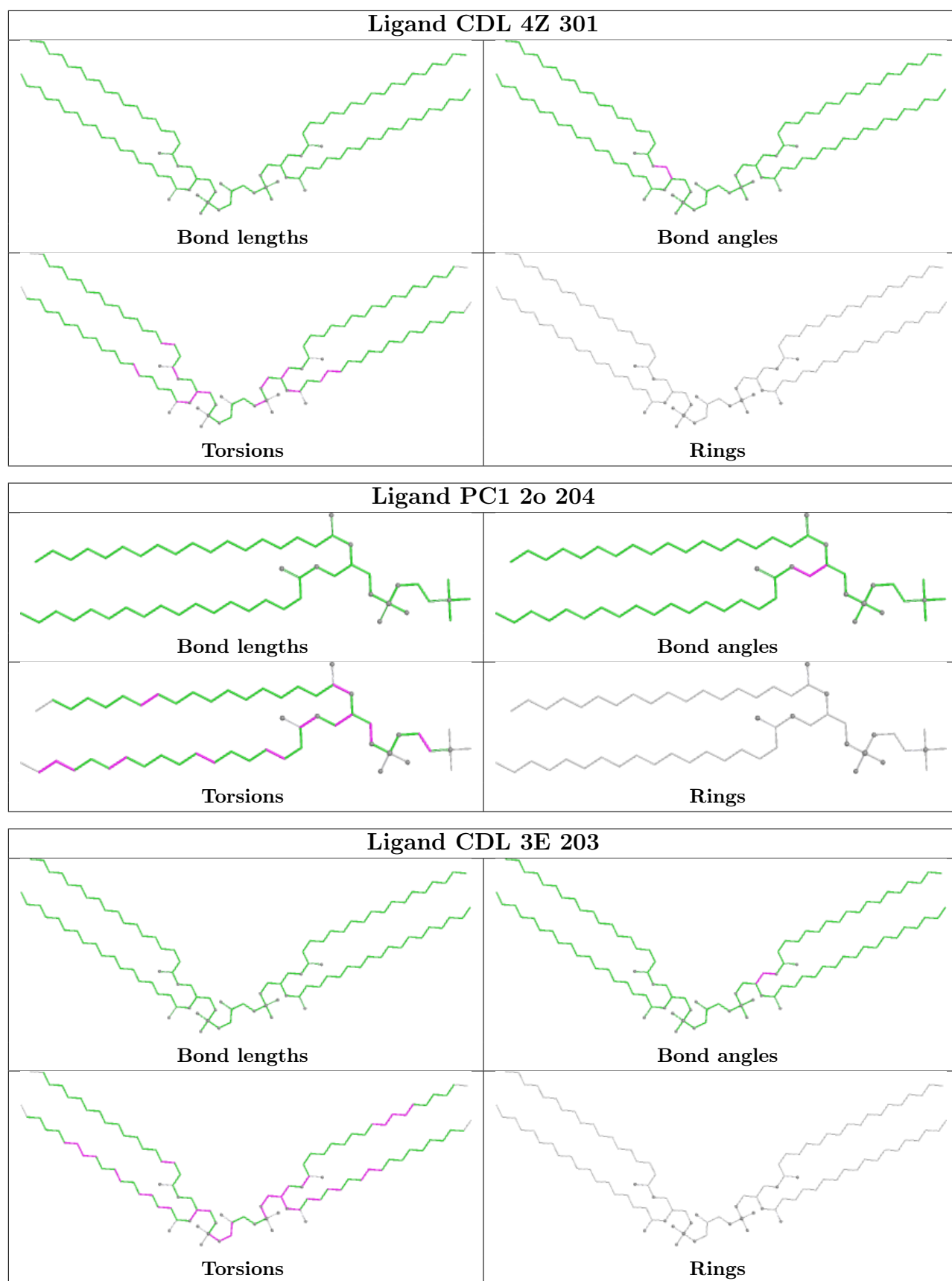
Ligand HEM 3g 401

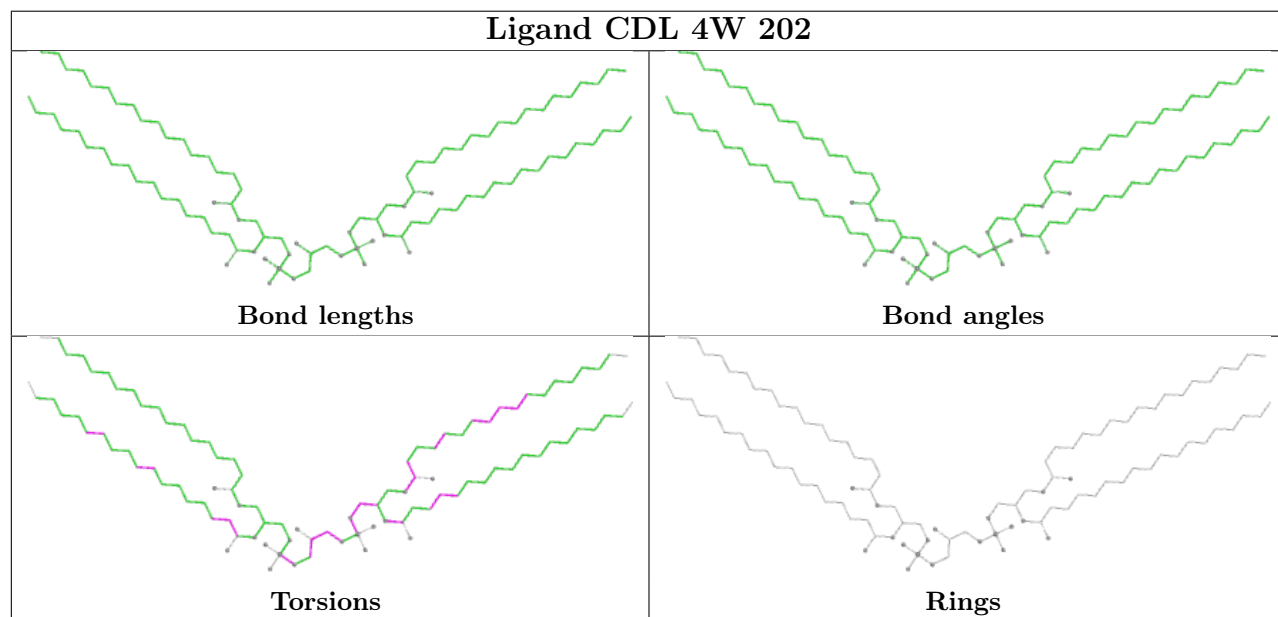
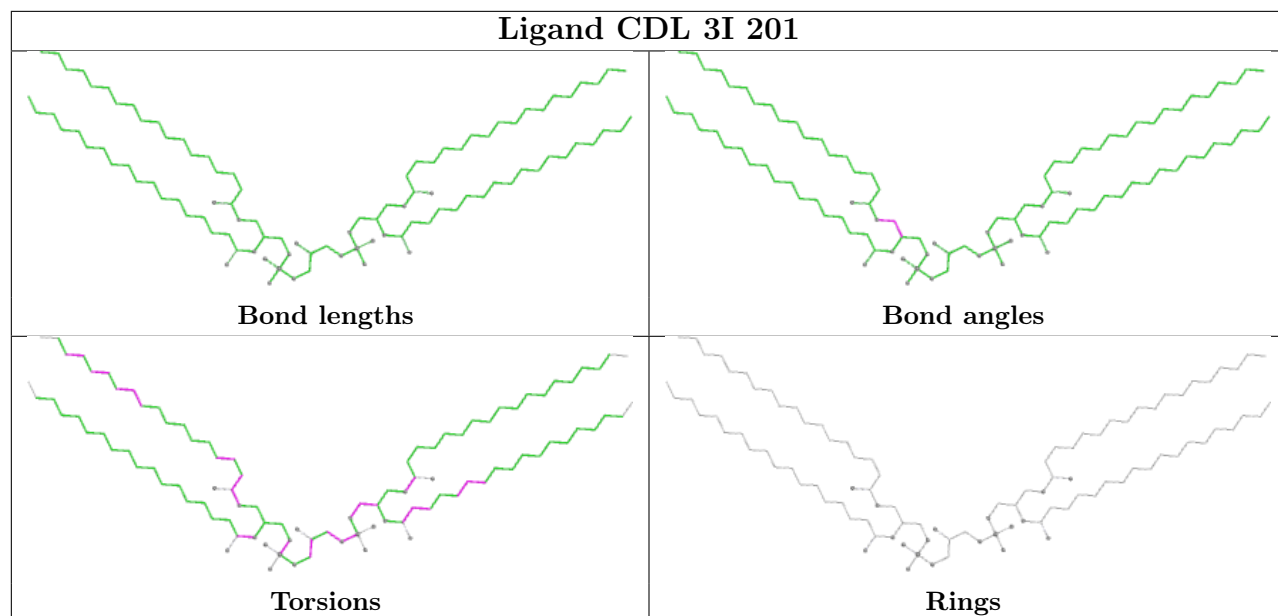


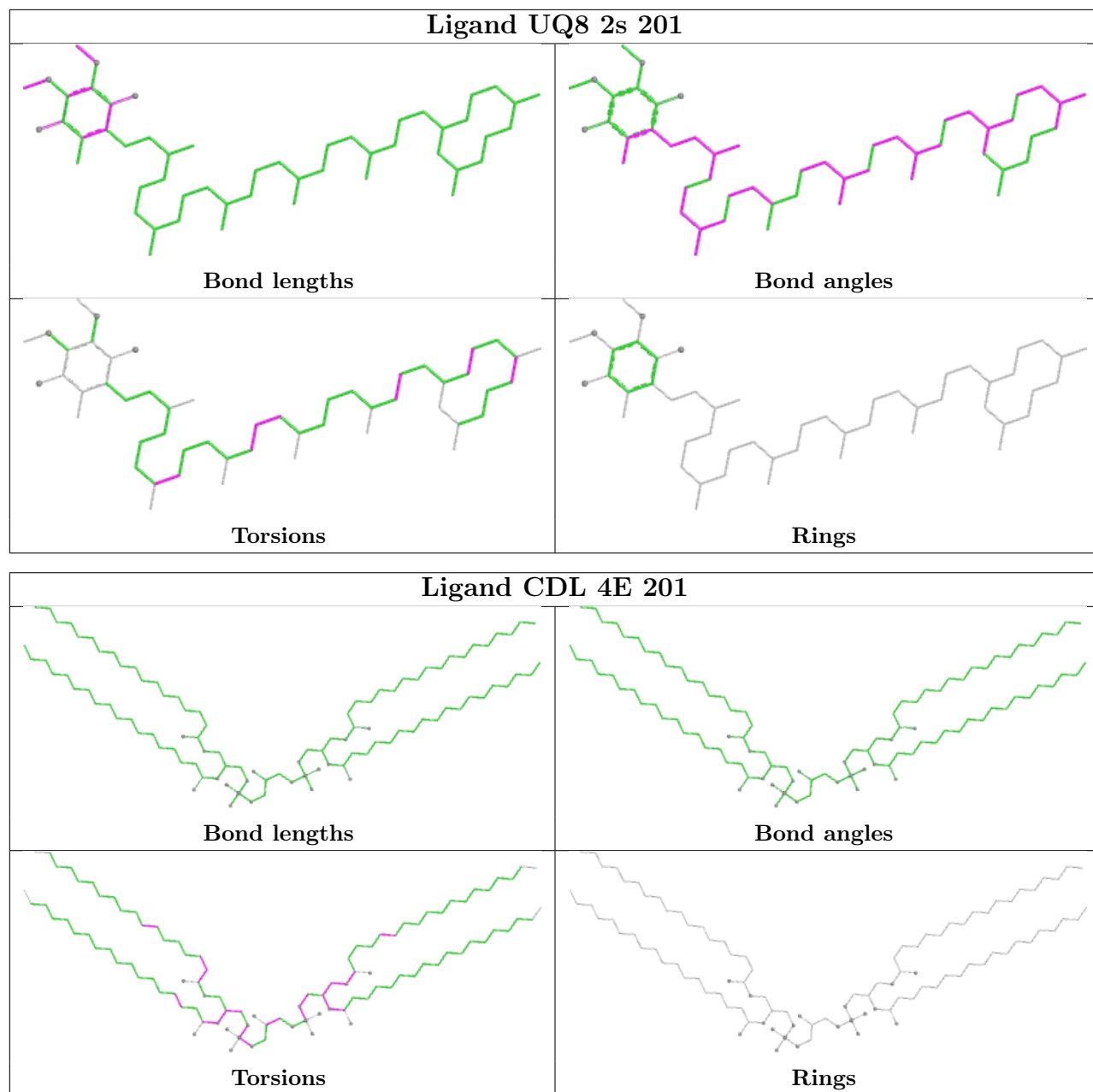
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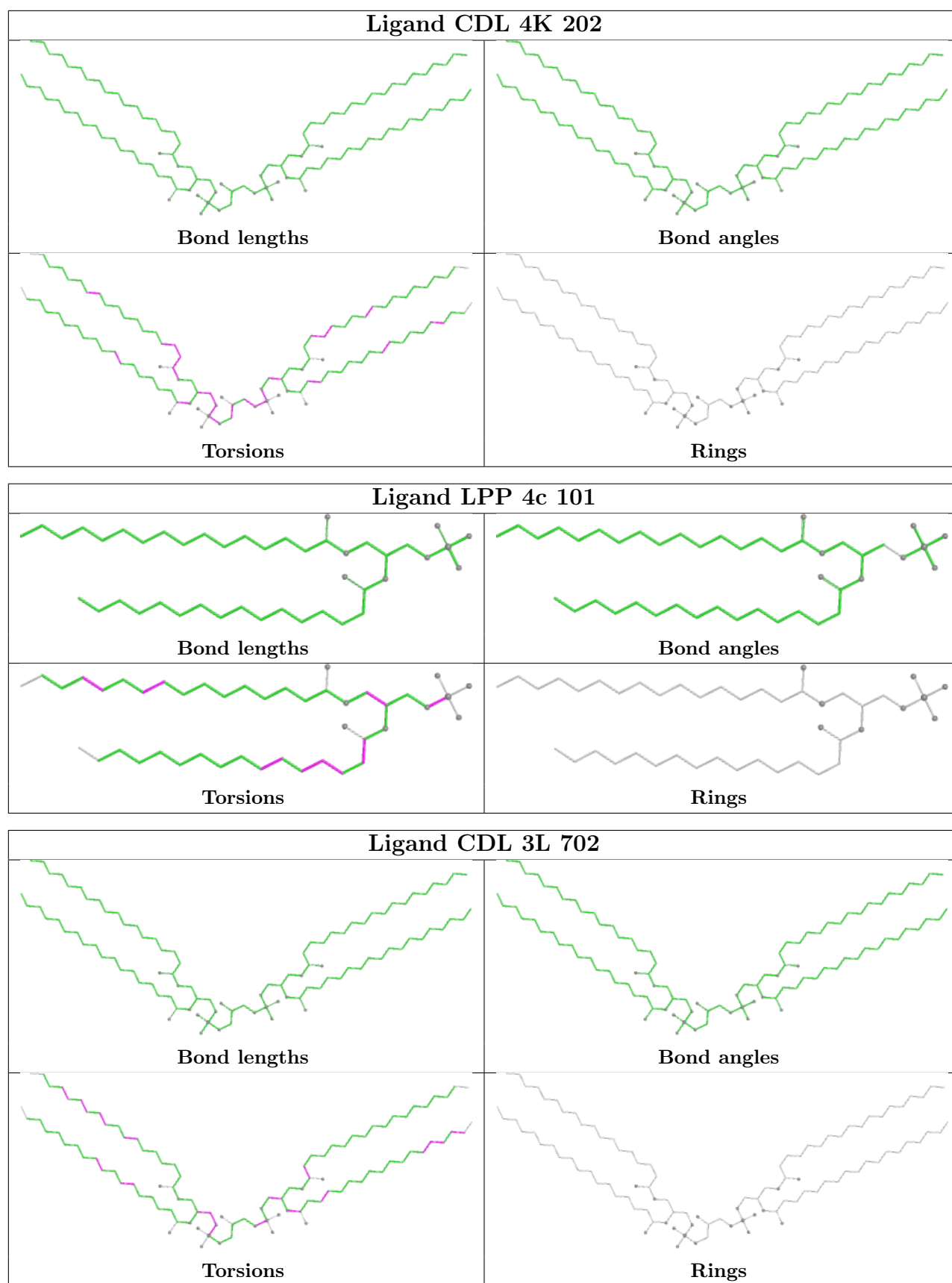


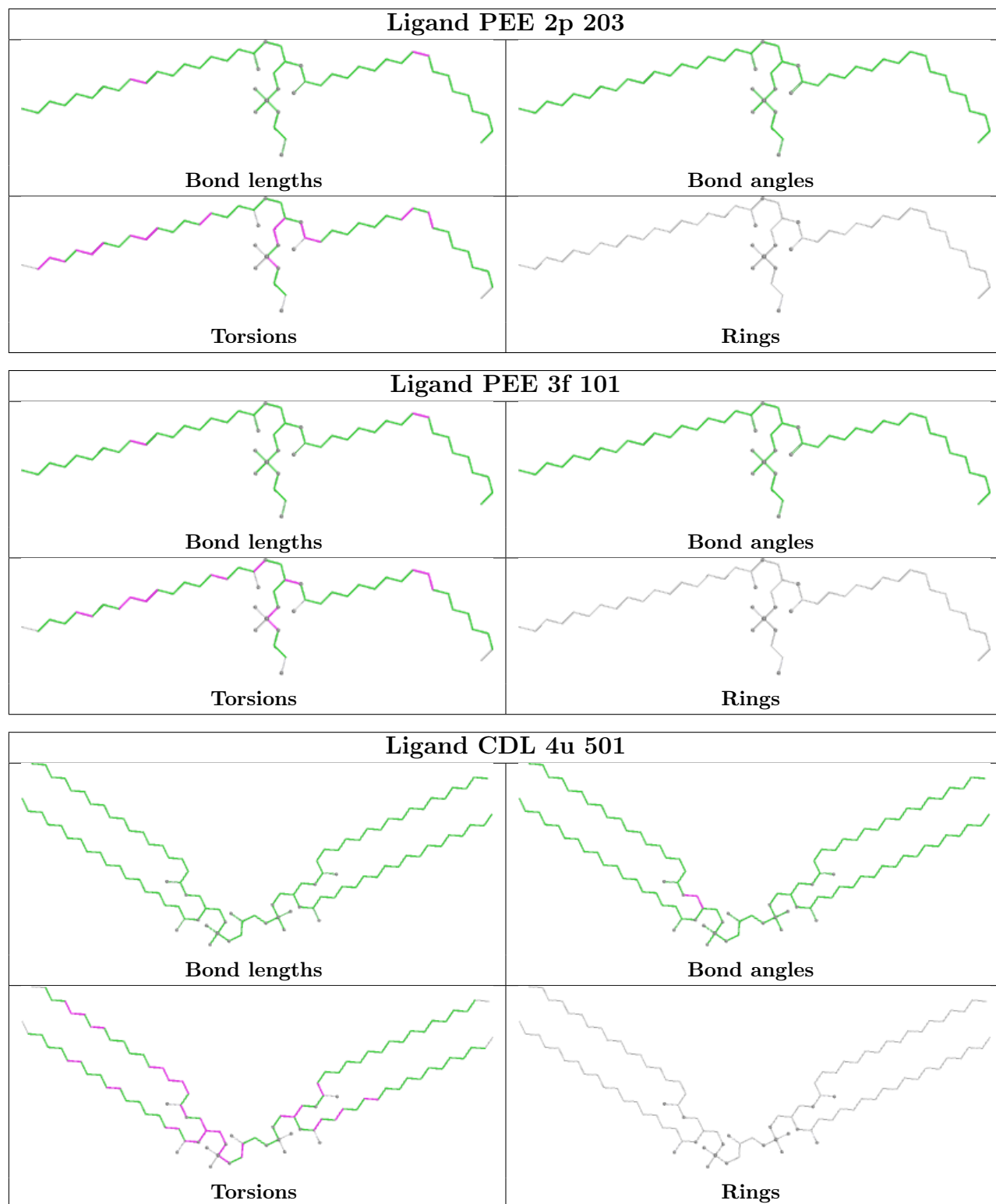


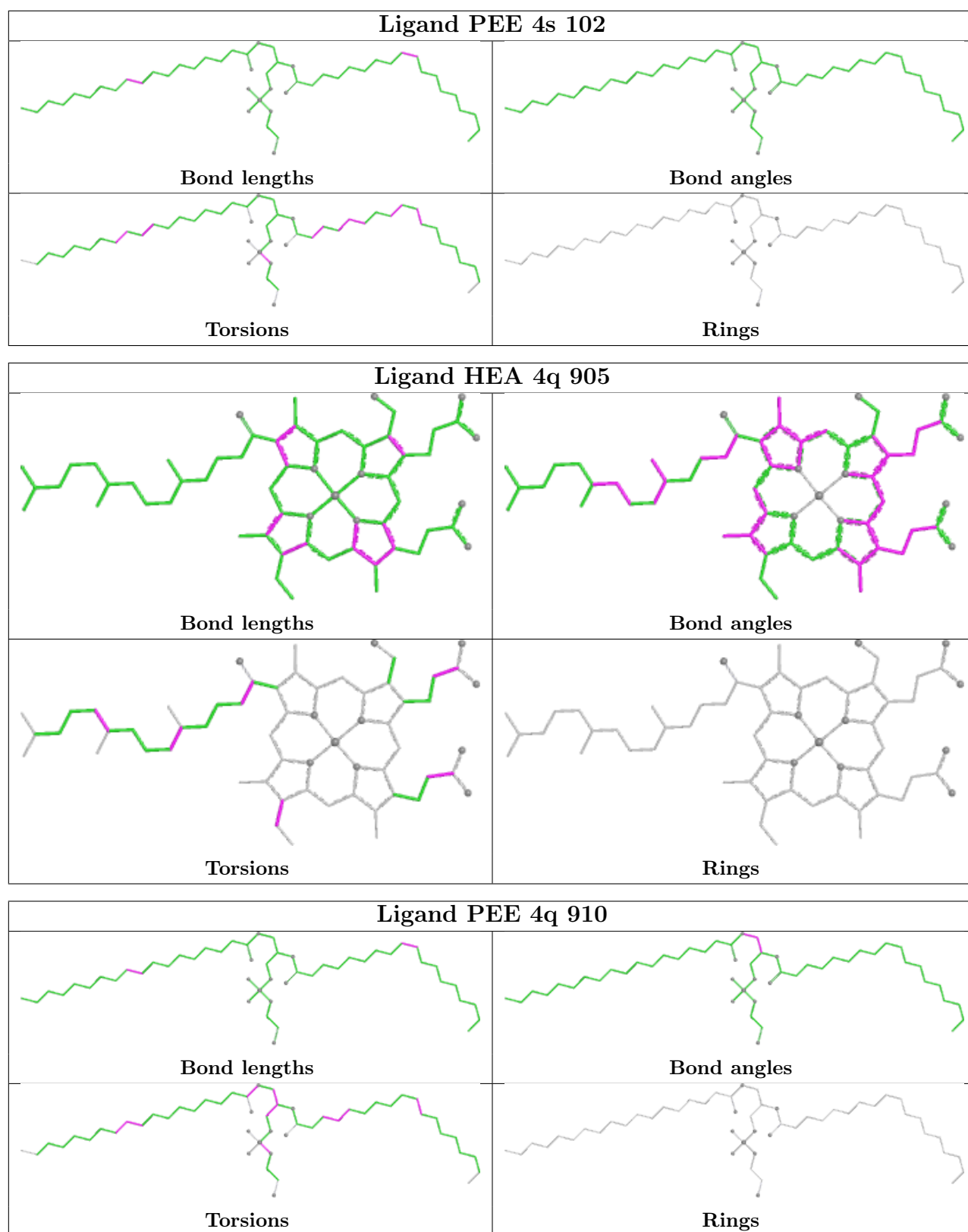


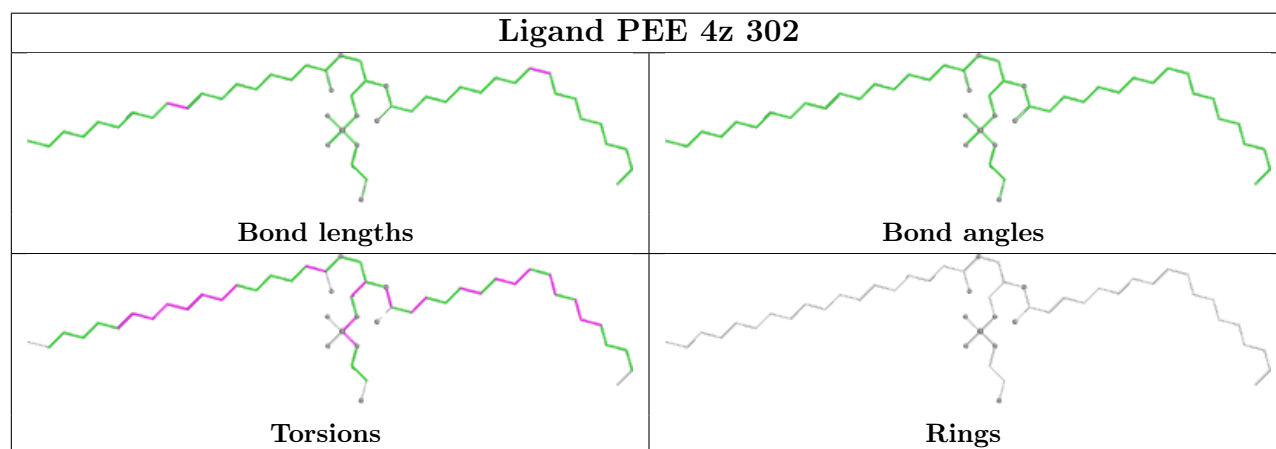
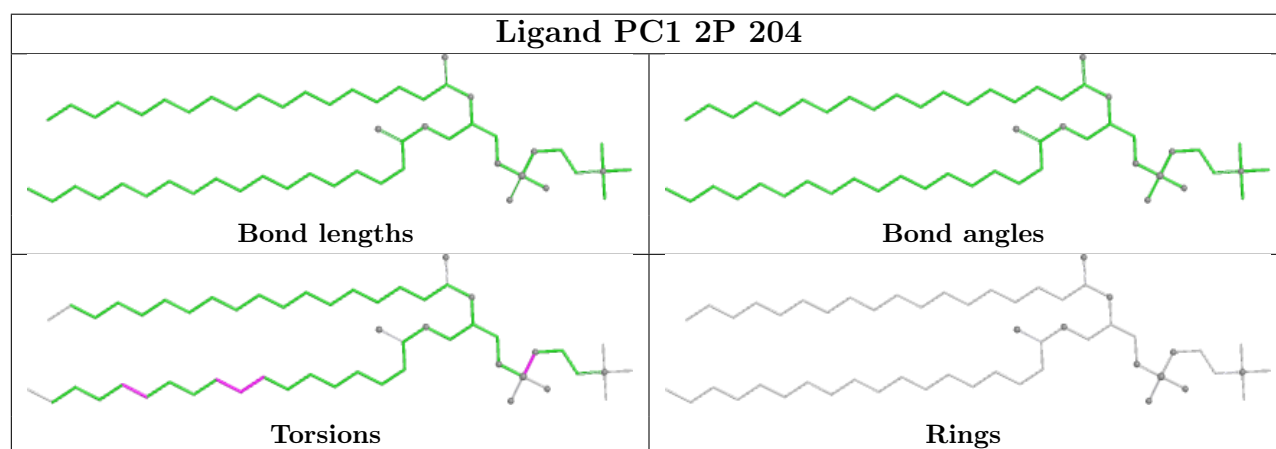
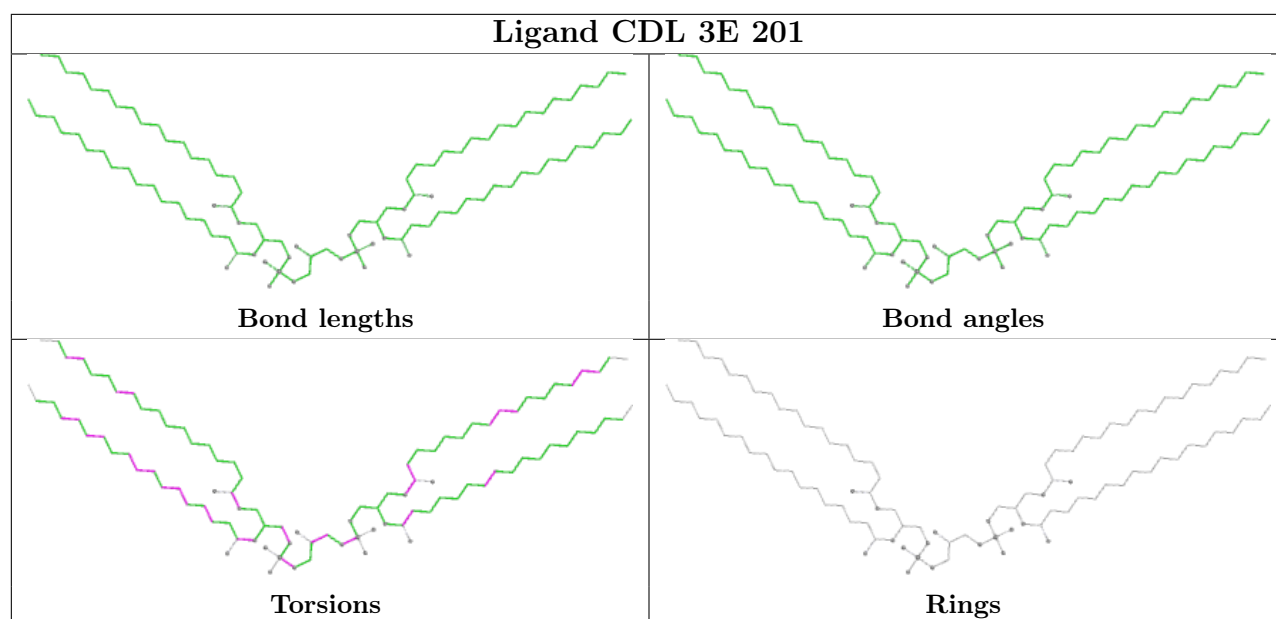


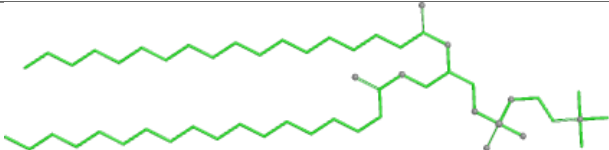
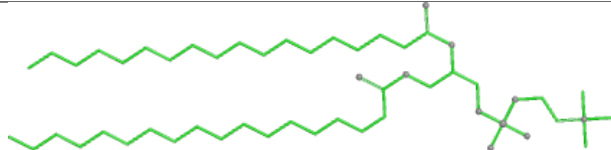
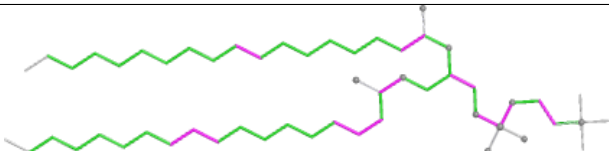
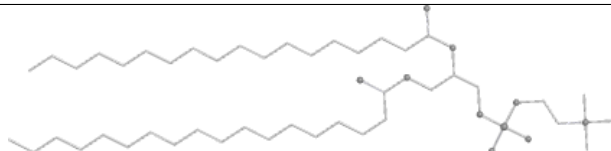


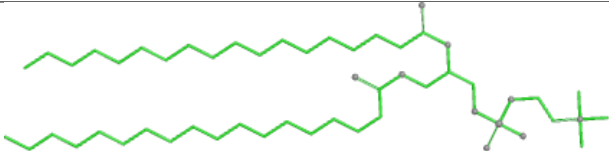
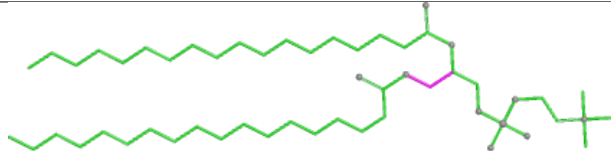
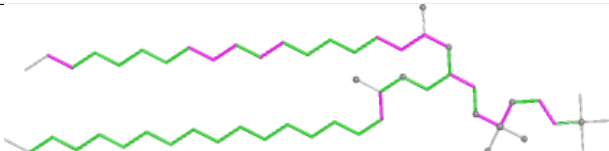


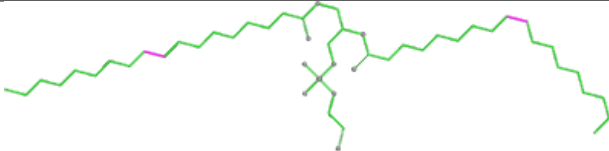
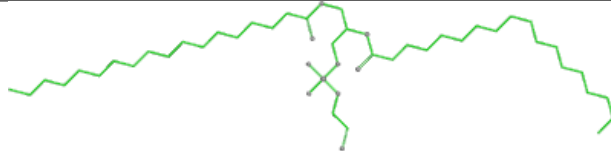
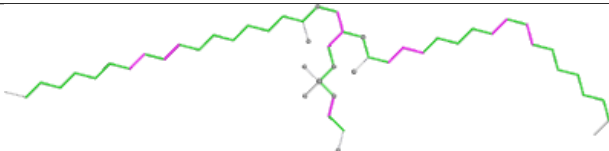
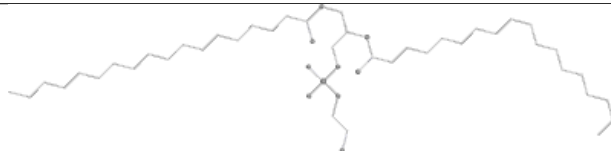


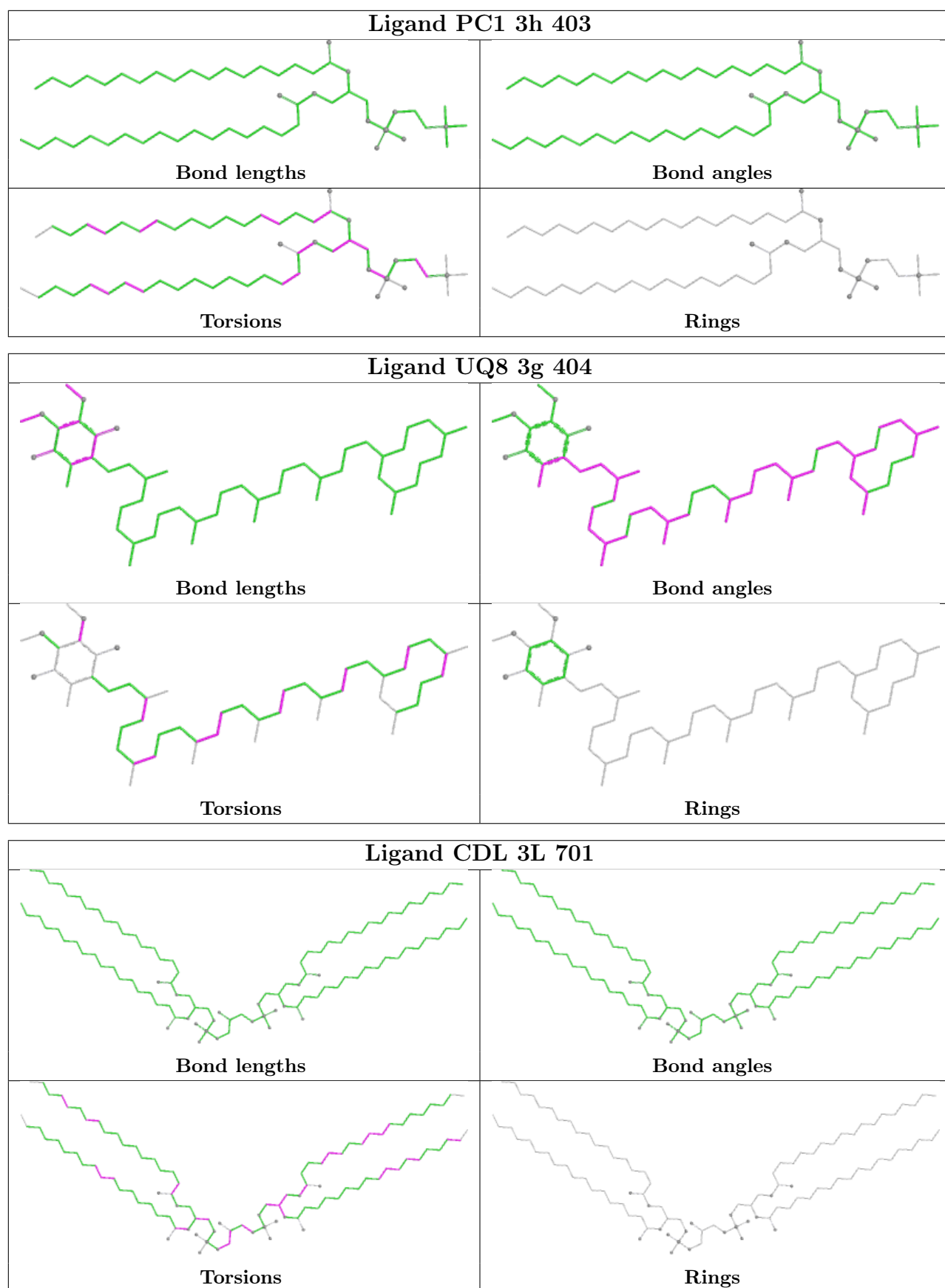




Ligand PC1 2R 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 3A 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE 4w 203	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

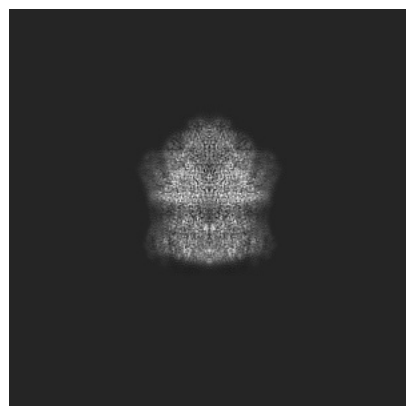
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50491. These allow visual inspection of the internal detail of the map and identification of artifacts.

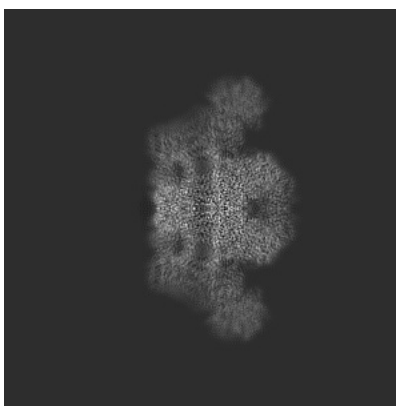
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

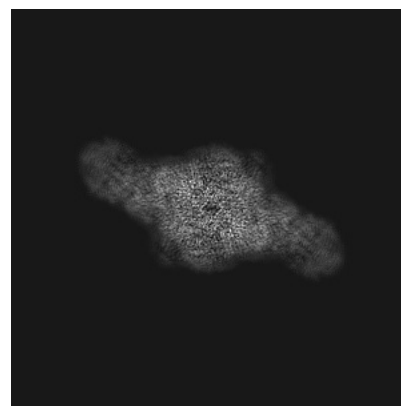
6.1.1 Primary map



X

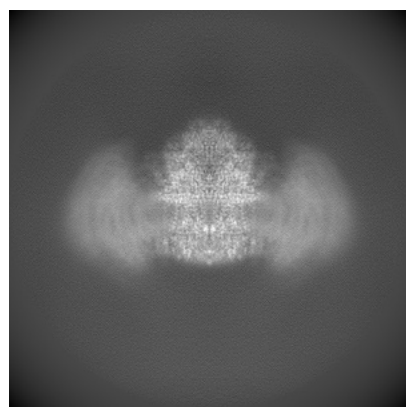


Y

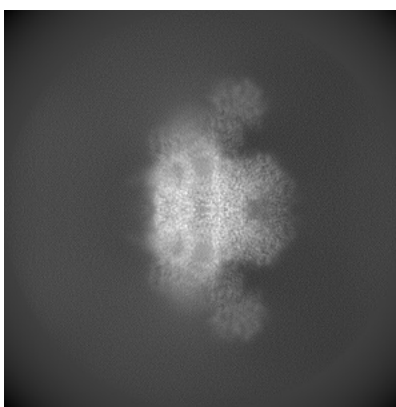


Z

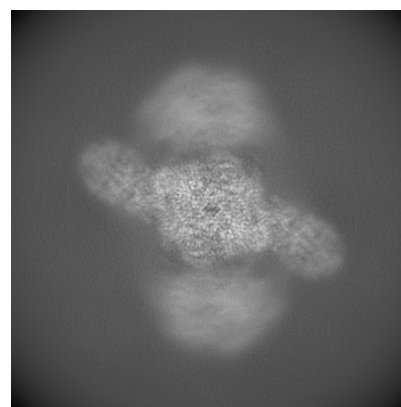
6.1.2 Raw map



X



Y



Z

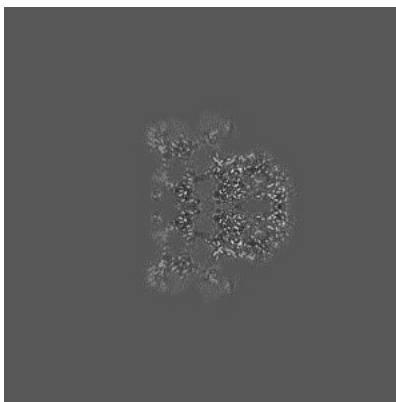
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

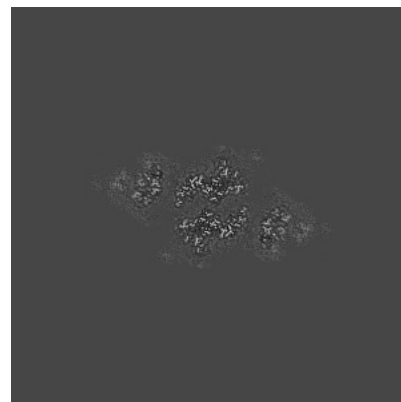
6.2.1 Primary map



X Index: 250

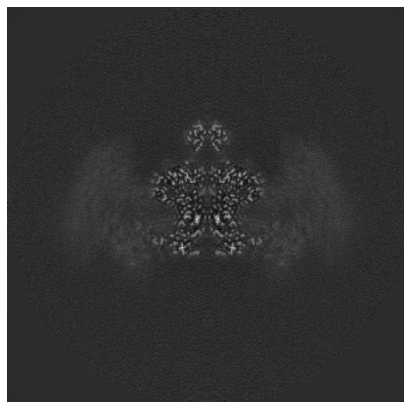


Y Index: 250

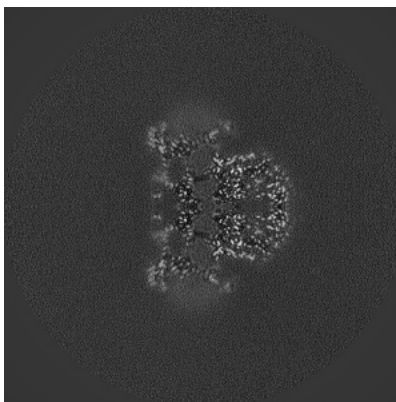


Z Index: 250

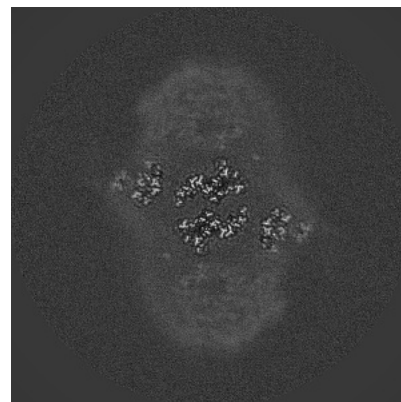
6.2.2 Raw map



X Index: 250



Y Index: 250

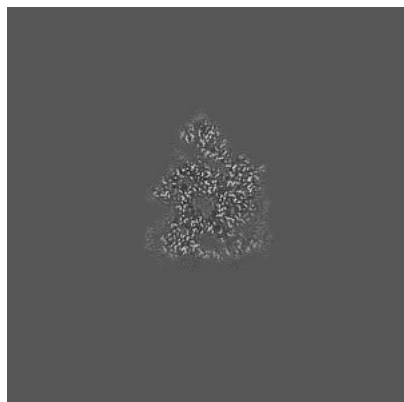


Z Index: 250

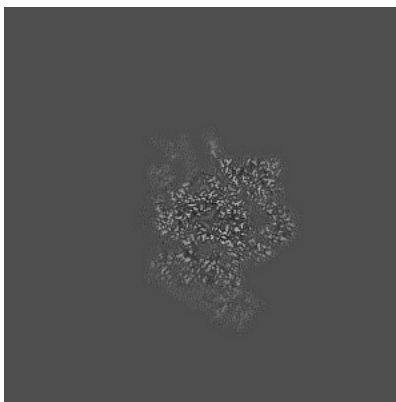
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

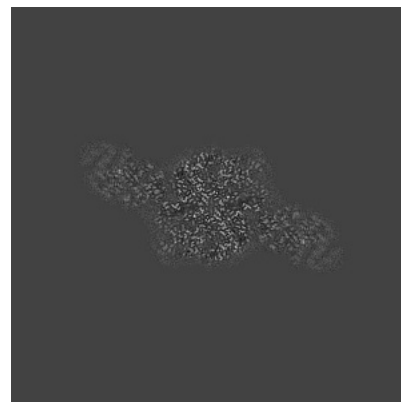
6.3.1 Primary map



X Index: 263

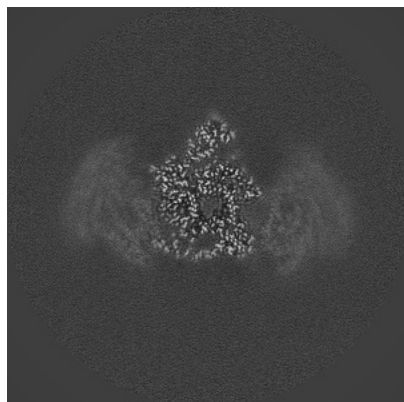


Y Index: 267

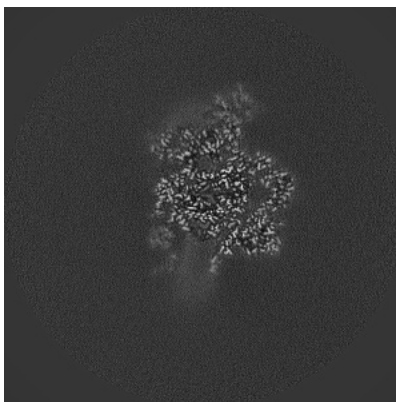


Z Index: 268

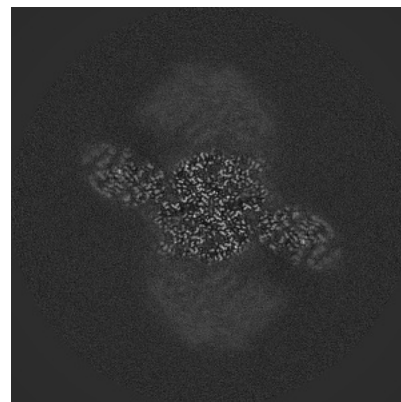
6.3.2 Raw map



X Index: 237



Y Index: 233

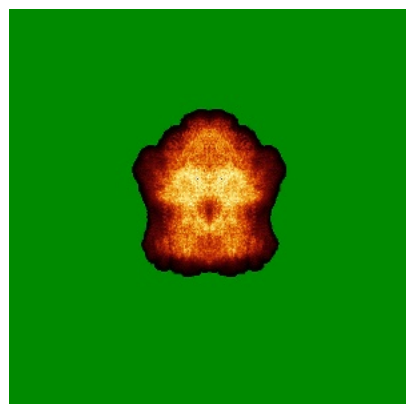


Z Index: 268

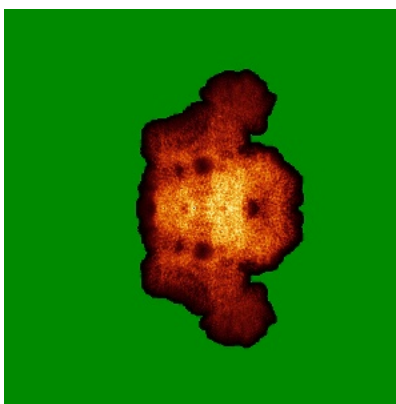
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

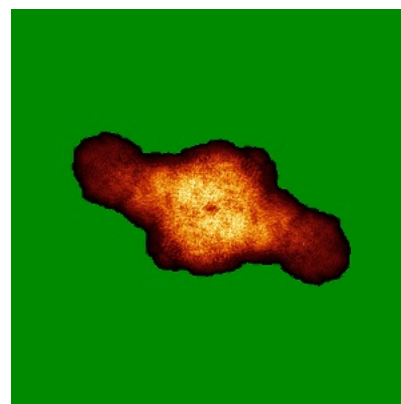
6.4.1 Primary map



X

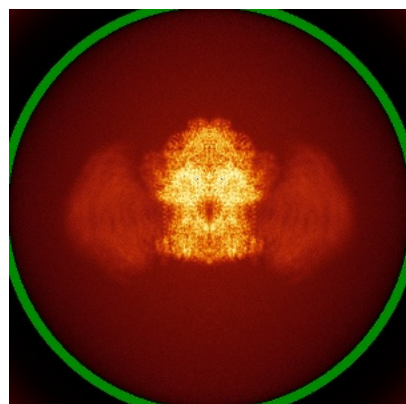


Y

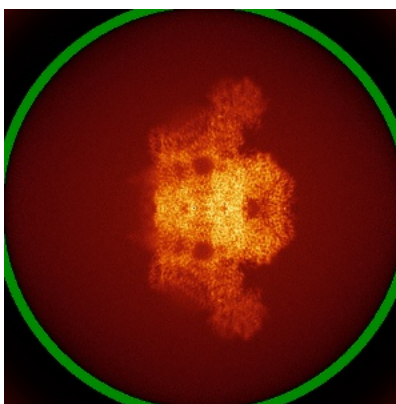


Z

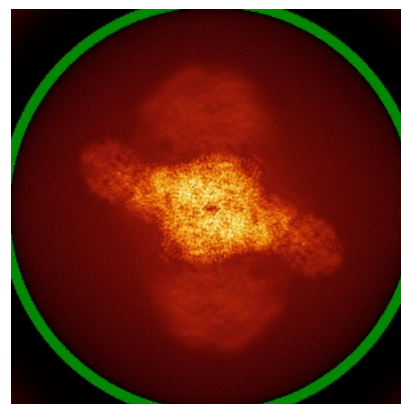
6.4.2 Raw map



X



Y

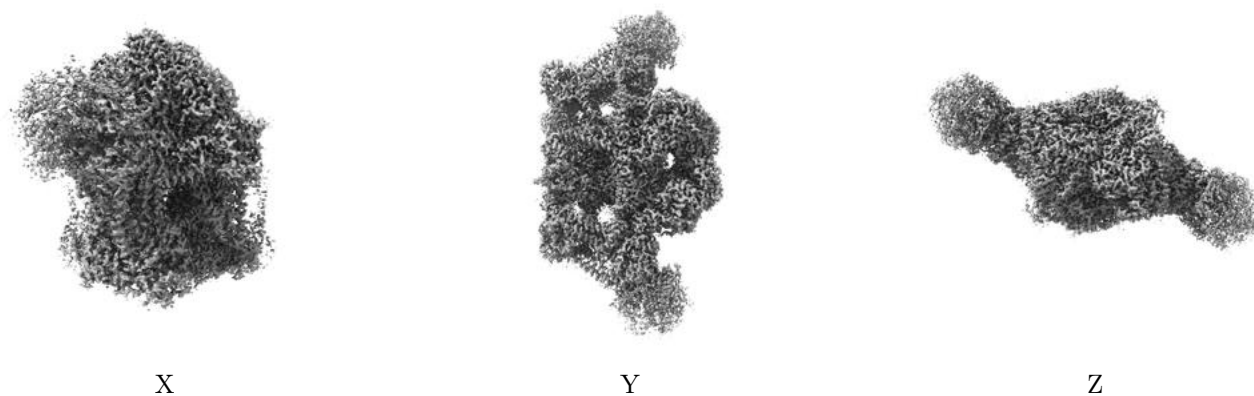


Z

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.

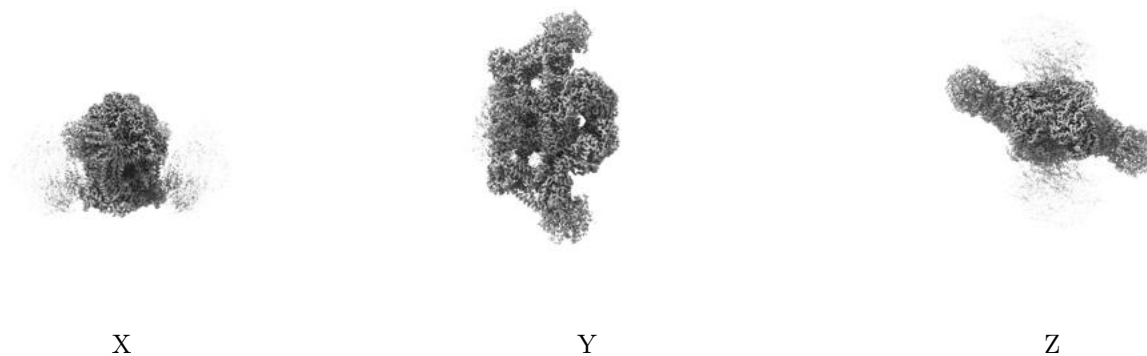
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0203. 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.

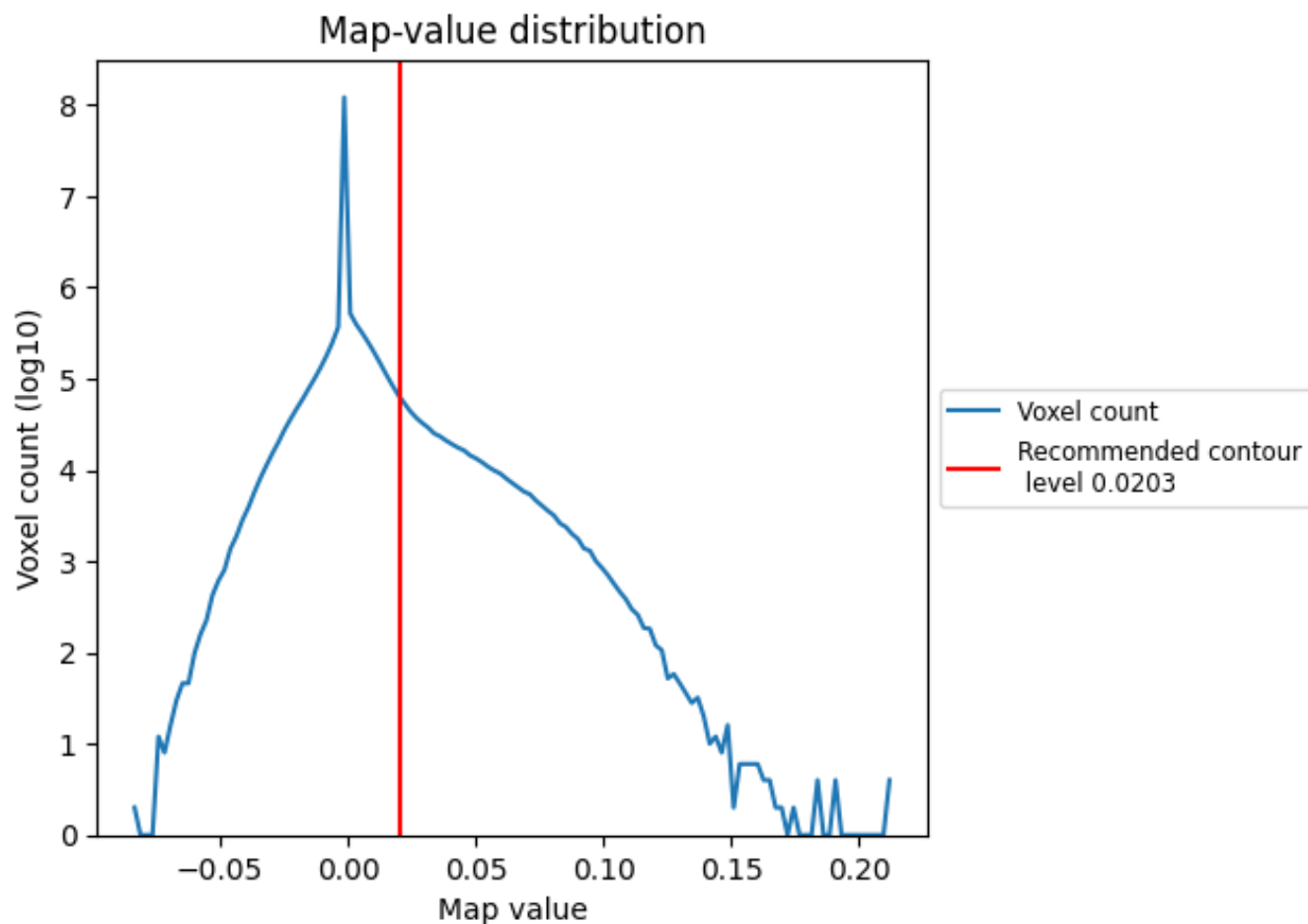
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

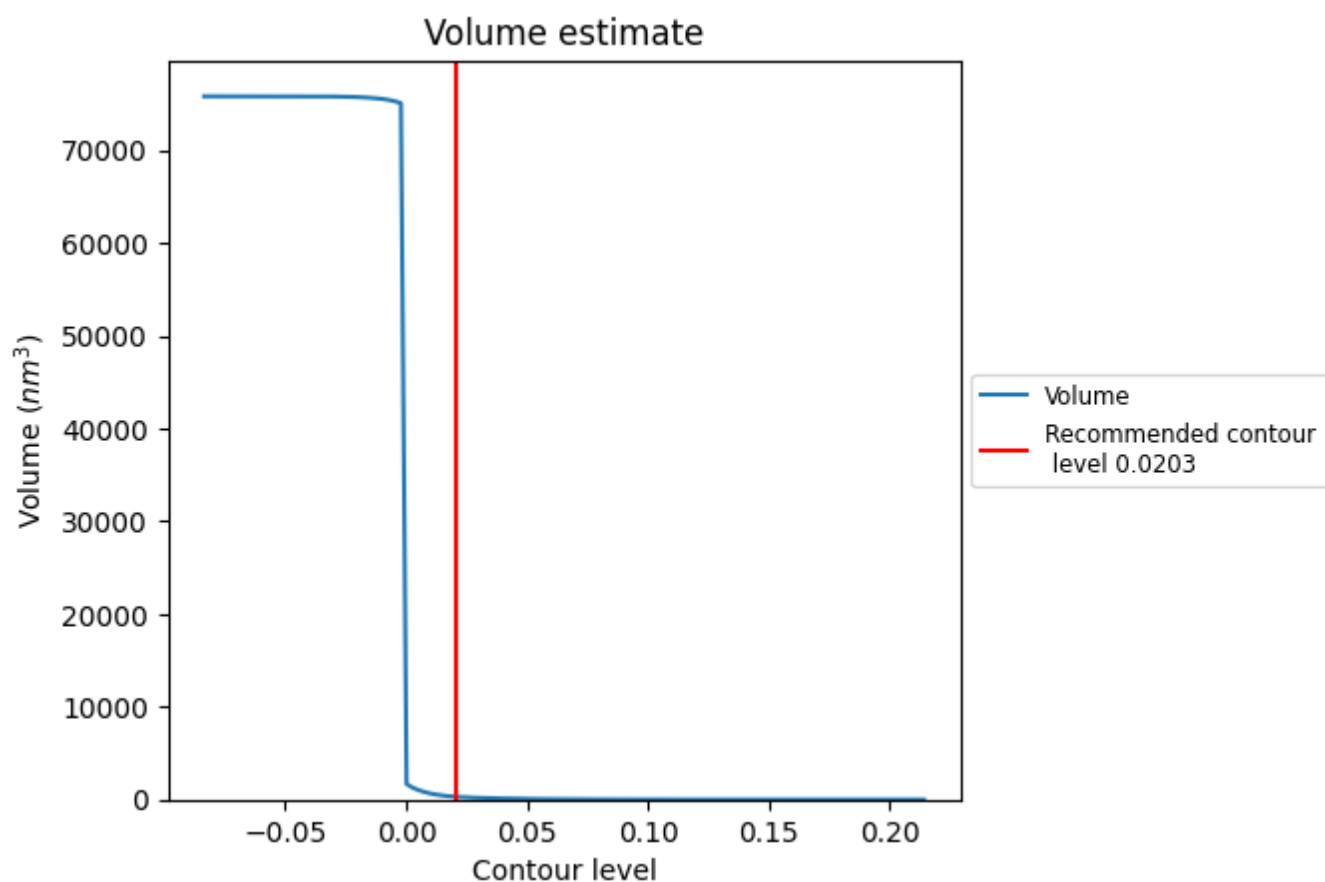
This section contains the results of statistical analysis of the map.

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.

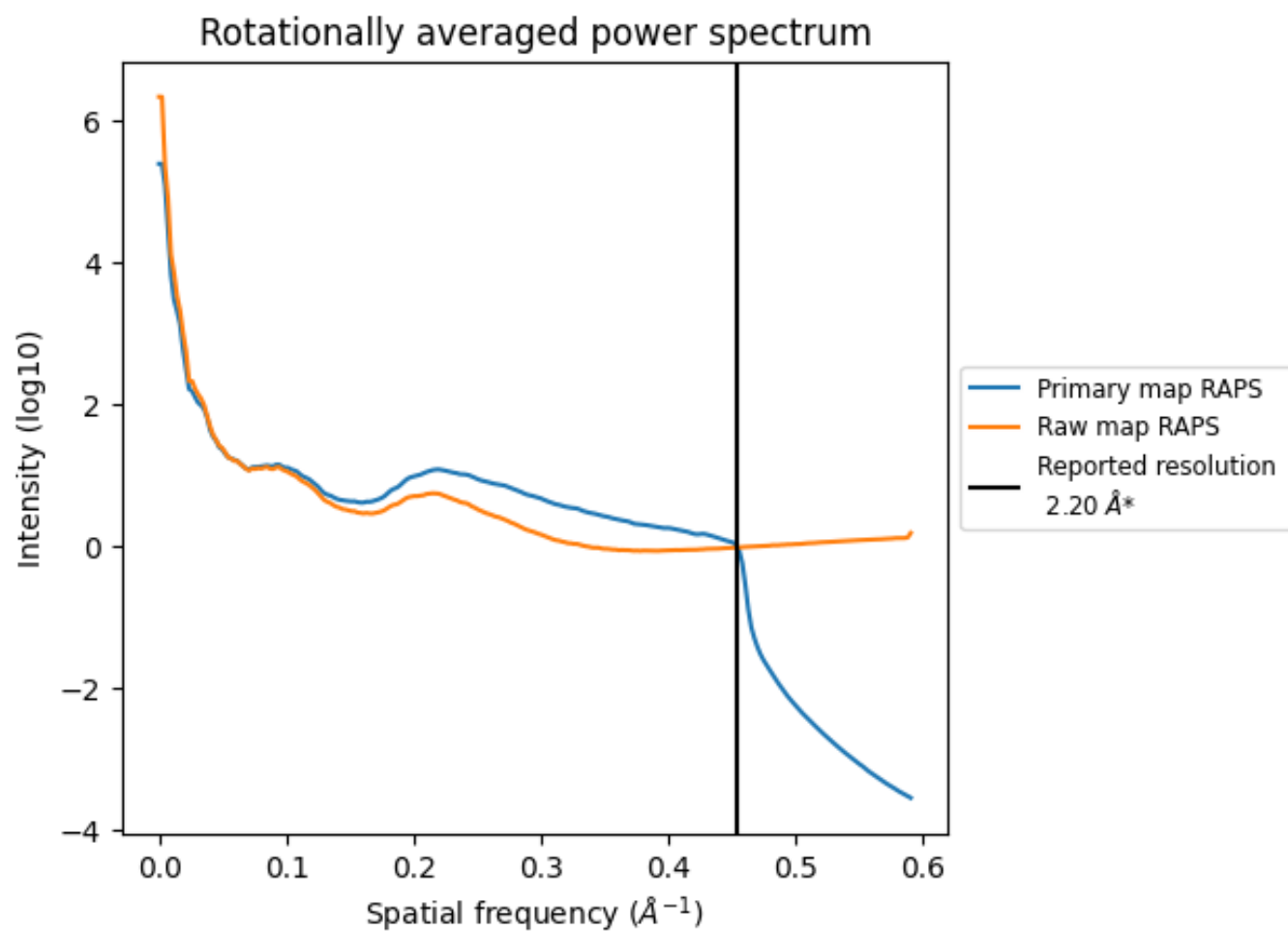
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm³; this corresponds to an approximate mass of 276 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 ⓘ

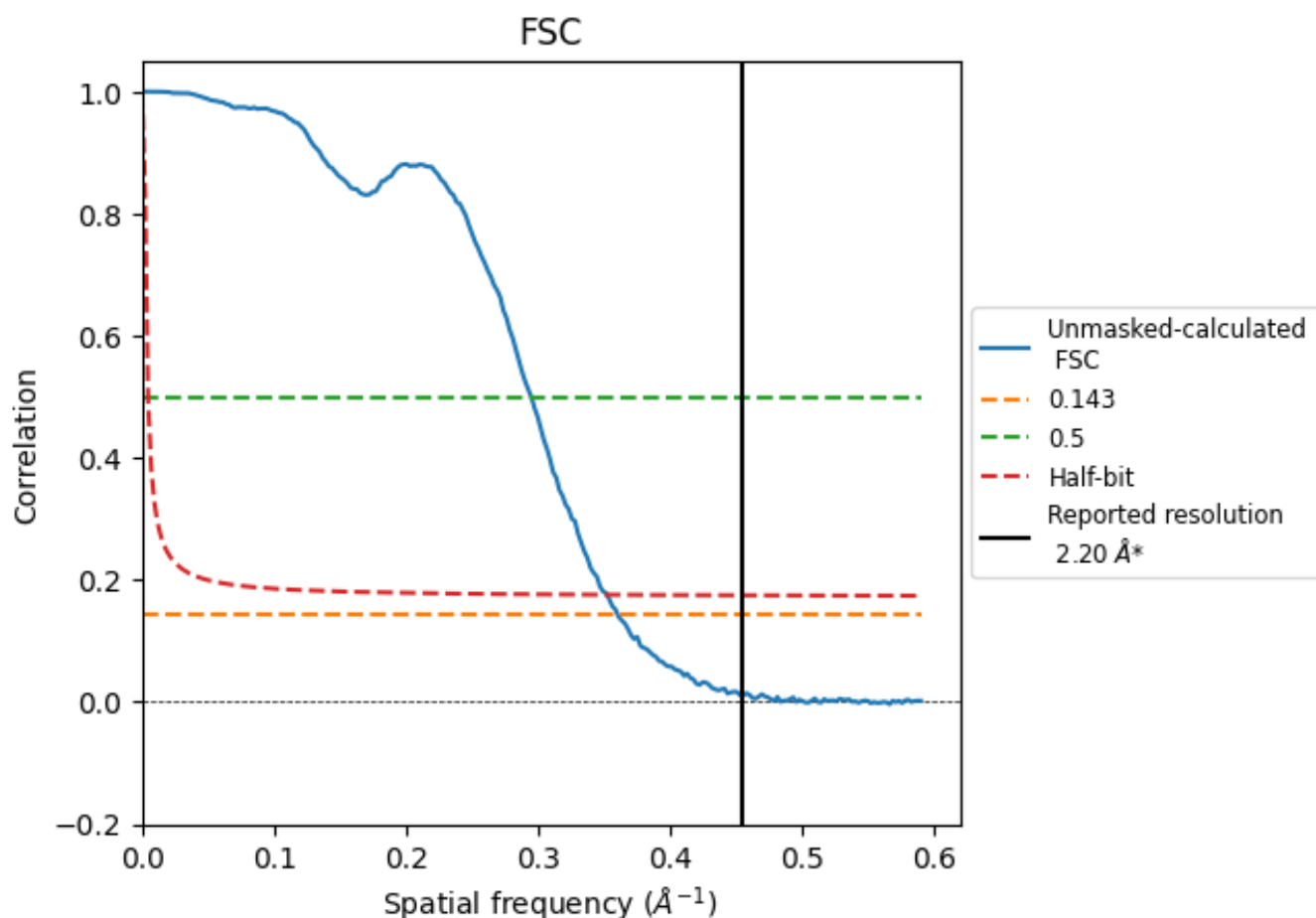


*Reported resolution corresponds to spatial frequency of $0.455 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

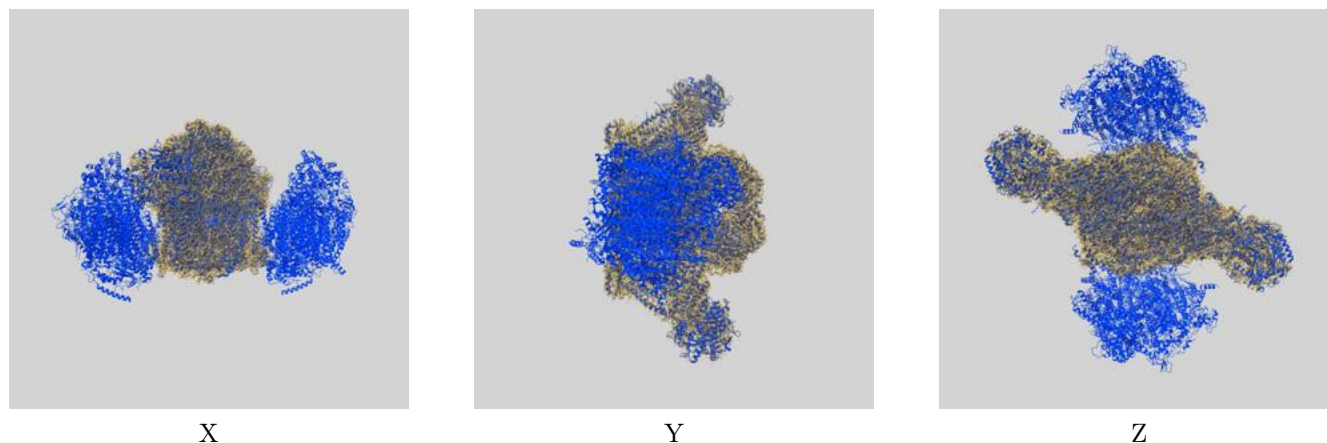
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.77	3.39	2.84

*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 2.77 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

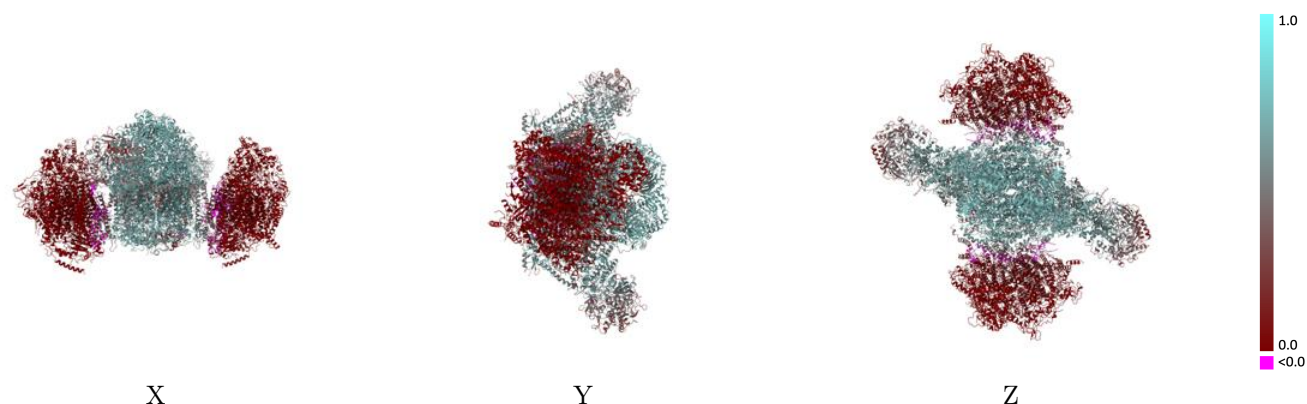
This section contains information regarding the fit between EMDB map EMD-50491 and PDB model 9FZL. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



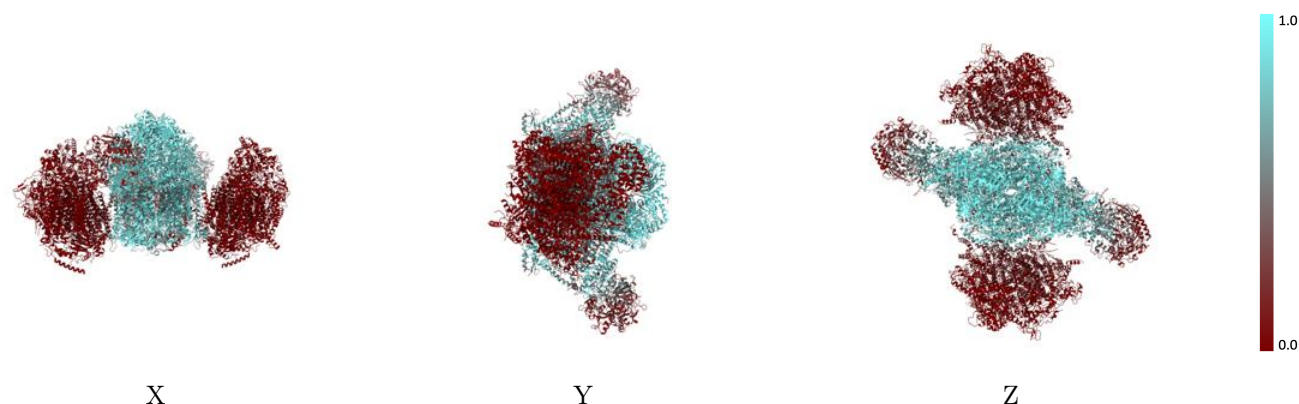
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



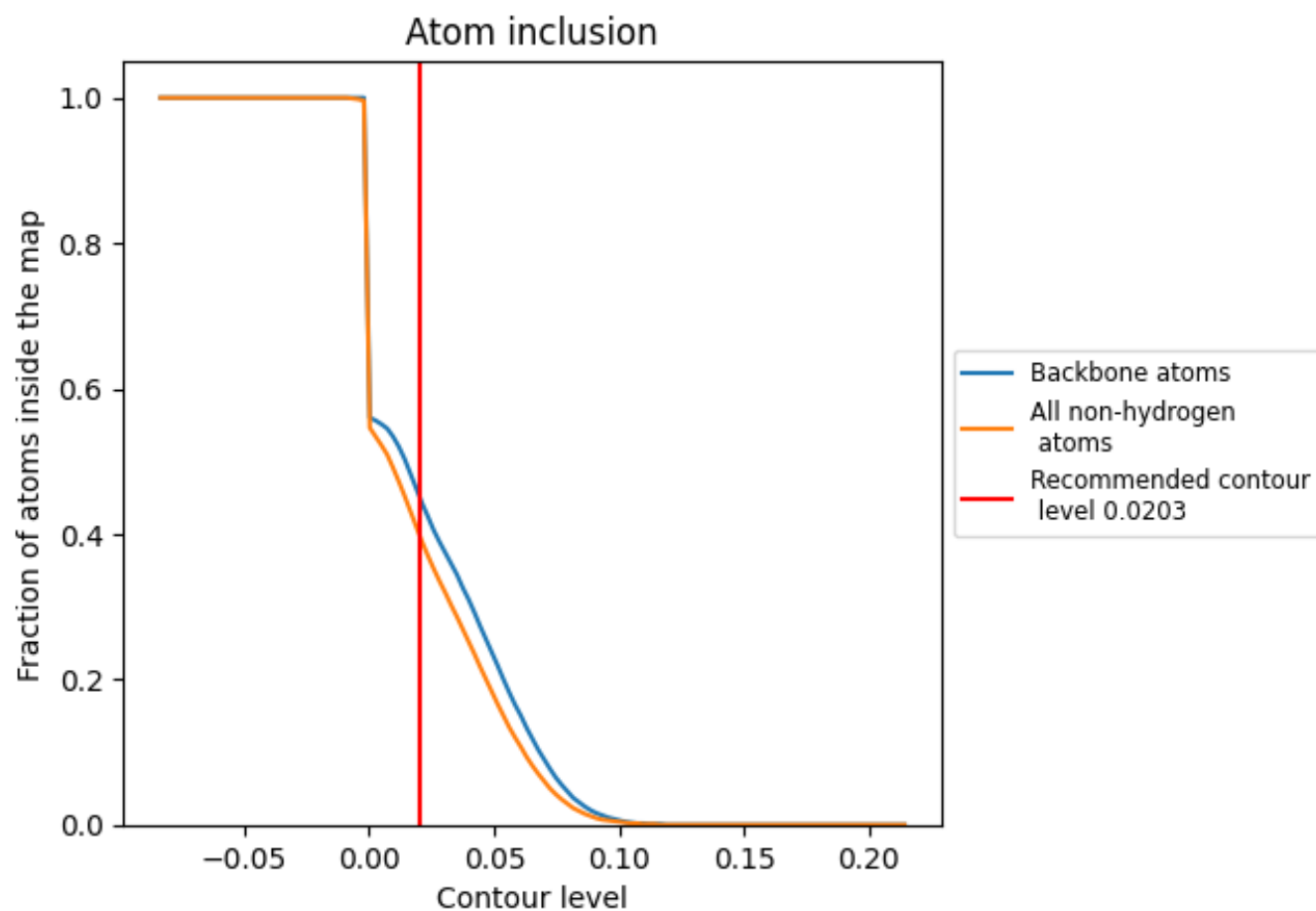
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 40% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3970	 0.3250
2M	 0.2660	 0.4070
2N	 0.6330	 0.5480
2O	 0.7970	 0.6040
2P	 0.7940	 0.5970
2Q	 0.7560	 0.5850
2R	 0.7950	 0.6090
2S	 0.8110	 0.6220
2T	 0.8780	 0.6560
2U	 0.5740	 0.5030
2V	 0.5780	 0.4910
2m	 0.2670	 0.4070
2n	 0.6360	 0.5480
2o	 0.7970	 0.6040
2p	 0.7940	 0.5950
2q	 0.7540	 0.5860
2r	 0.7950	 0.6140
2s	 0.8090	 0.6250
2t	 0.8780	 0.6580
2u	 0.5700	 0.5020
2v	 0.5730	 0.4930
3A	 0.9080	 0.6830
3B	 0.9090	 0.6720
3C	 0.9180	 0.6900
3D	 0.7940	 0.6250
3E	 0.8240	 0.6350
3F	 0.9370	 0.6950
3G	 0.9190	 0.6920
3H	 0.6570	 0.5320
3I	 0.8470	 0.6510
3J	 0.7730	 0.5920
3K	 0.9210	 0.6950
3L	 0.6370	 0.5310
3a	 0.9070	 0.6850
3b	 0.9100	 0.6730



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Chain	Atom inclusion	Q-score
3c	 0.9180	 0.6880
3d	 0.7950	 0.6260
3e	 0.8250	 0.6350
3f	 0.9370	 0.6940
3g	 0.9190	 0.6920
3h	 0.6570	 0.5330
3i	 0.8480	 0.6520
3j	 0.7750	 0.5900
3k	 0.9210	 0.6930
3l	 0.6370	 0.5320
40	 0.0000	 0.0000
41	 0.0000	 -0.0000
4A	 0.0050	 0.0700
4B	 0.0530	 0.1050
4C	 0.0720	 0.2140
4D	 0.0270	 0.1230
4E	 0.0000	 0.0000
4F	 0.0140	 0.0510
4G	 0.0220	 0.0640
4H	 0.0000	 0.0000
4I	 0.0000	 0.0000
4J	 0.0000	 0.0000
4K	 0.0000	 0.0000
4L	 0.0000	 0.0000
4M	 0.0000	 0.0000
4N	 0.0000	 0.0140
4O	 0.0000	 0.0000
4P	 0.0000	 0.0050
4Q	 0.0000	 0.0000
4R	 0.0000	 0.0000
4S	 0.0000	 0.0000
4T	 0.0000	 0.0000
4U	 0.0000	 0.0000
4V	 0.0000	 0.0000
4W	 0.0000	 -0.0030
4X	 0.0000	 0.0000
4Y	 0.0000	 0.0000
4Z	 0.0110	 0.0760
4a	 0.0050	 0.0750
4b	 0.0520	 0.1020
4c	 0.0690	 0.2070
4d	 0.0280	 0.1150

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Chain	Atom inclusion	Q-score
4e	 0.0000	 0.0000
4f	 0.0140	 0.0520
4g	 0.0230	 0.0700
4h	 0.0000	 0.0000
4i	 0.0000	 0.0000
4j	 0.0000	 0.0000
4k	 0.0000	 0.0000
4l	 0.0000	 0.0000
4m	 0.0000	 0.0000
4n	 0.0000	 0.0130
4o	 0.0000	 0.0000
4p	 0.0000	 0.0030
4q	 0.0000	 -0.0000
4r	 0.0000	 0.0000
4s	 0.0000	 0.0000
4t	 0.0000	 0.0000
4u	 0.0000	 0.0000
4v	 0.0000	 0.0000
4w	 0.0000	 -0.0040
4x	 0.0000	 0.0000
4y	 0.0000	 0.0000
4z	 0.0100	 0.0760