



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2026 – 09:11 pm BST

PDB ID : 8BPX / pdb_00008bpx
EMDB ID : EMD-16168
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (Complete composition)
Authors : Klusch, N.; Kuehlbrandt, W.
Deposited on : 2022-11-18
Resolution : 2.09 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:

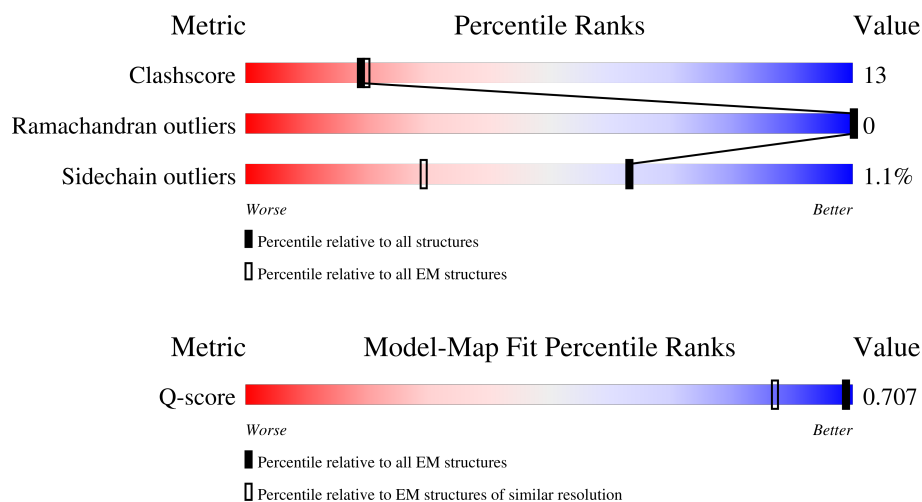
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.09 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	2022 (1.60 - 2.59)

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	A	119	
2	B	218	
3	C	190	
4	D	394	

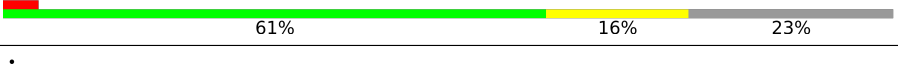
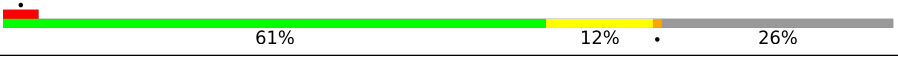
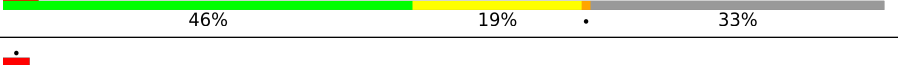
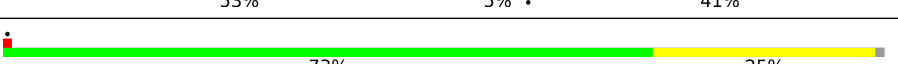
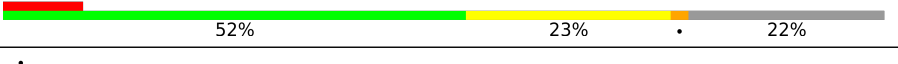
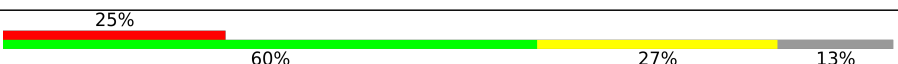
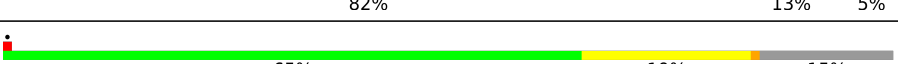
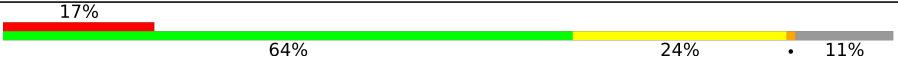
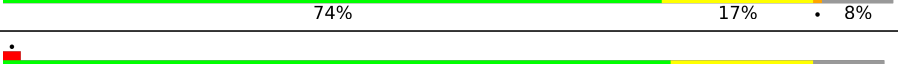
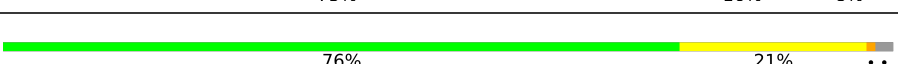
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Y	159	
26	Z	143	
27	a	65	
28	b	65	
29	c	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	d	81	
31	e	83	
32	f	106	
33	g	114	
34	i	98	
35	j	69	
36	k	72	
37	l	125	
38	m	71	
39	n	117	
40	o	103	
41	p	106	
42	q	159	
43	u	63	
44	v	113	
45	x	256	
46	y	278	
47	z	275	
48	AA	503	
48	BA	503	
49	AB	531	
49	BB	531	
50	AC	393	
50	BC	393	
51	AD	272	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
51	BD	272	
52	AE	307	
52	BE	307	
53	AF	122	
53	BF	122	
54	AG	72	
54	BG	72	
55	AH	69	
55	BH	69	
56	AI	72	
56	BI	72	
57	AJ	57	
57	BJ	57	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	SF4	I	500	-	-	X	-
73	COO	y	302	X	-	-	-

2 Entry composition

There are 76 unique types of molecules in this entry. The entry contains 104814 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	94	Total	C	N	O	S	0	0
			802	565	110	123	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1244	797	218	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	181	Total	C	N	O	S	0	0
			1545	997	266	276	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3079	1957	542	556	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5243	3285	919	1000	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	126	ARG	TRP	conflict	UNP P92558

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1349	849	229	261	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1399	949	213	228	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	155	SER	PRO	conflict	UNP P60497

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			784	525	121	131	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	665	Total	C	N	O	S	0	0
			5222	3474	808	901	39		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	variant	UNP P29388
L	288	PHE	SER	variant	UNP P29388
L	537	LEU	PRO	variant	UNP P29388

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	494	Total	C	N	O	S	1	0
			3952	2668	610	649	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	variant	UNP P93313
M	326	LEU	PRO	variant	UNP P93313
M	383	PHE	SER	variant	UNP P93313

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	2	0
			3839	2587	580	644	28		

- Molecule 15 is a protein called 2Fe-2S ferredoxin-like superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	123	Total	C	N	O	S	0	0
			963	603	170	186	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	316	Total	C	N	O	S	0	0
			2453	1580	414	444	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	105	Total	C	N	O	S	0	0
			837	536	144	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	73	Total	C	N	O	S	0	0
			571	359	101	105	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			659	417	104	135	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	87	Total	C	N	O	S	0	0
			677	427	110	139	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			904	578	161	162	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	98	Total	C	N	O	S	0	0
			776	486	134	144	12		

- Molecule 25 is a protein called Outer envelope pore protein 16-3, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	125	Total	C	N	O	S	0	0
			928	596	162	167	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	125	Total	C	N	O	S	0	0
			997	640	175	177	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 28 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	43	Total	C	N	O	S	0	0
			315	206	51	55	3		

- Molecule 29 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 30 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 32 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	101	Total	C	N	O	S	0	0
			765	491	126	143	5		

- Molecule 33 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	79	Total	C	N	O	S	0	0
			641	412	111	115	3		

- Molecule 34 is a protein called At1g67350.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	83	Total	C	N	O	S	0	0
			721	458	132	126	5		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	48	Total	C	N	O	S	0	0
			382	244	72	63	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	74	Total	C	N	O	S	0	0
			562	367	91	103	1		

- Molecule 38 is a protein called AT2G31490 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	70	Total	C	N	O	S	0	0
			577	370	107	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	90	Total	C	N	O	S	0	0
			757	479	141	133	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	80	Total	C	N	O	S	1	0
			669	427	120	120	2		

- Molecule 43 is a protein called Uncharacterized protein At1g67785.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	55	Total	C	N	O	S	0	0
			463	298	84	78	3		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	29	Total	C	N	O	S	0	0
			219	142	38	39			

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	210	Total	C	N	O	S	0	0
			1629	1043	280	301	5		

- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	265	Total	C	N	O	S	0	0
			2013	1258	359	388	8		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 48 is a protein called Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	450	Total	C	N	O	S	0	0
			3431	2178	573	663	17		
48	BA	451	Total	C	N	O	S	0	0
			3436	2181	574	664	17		

- Molecule 49 is a protein called Probable mitochondrial-processing peptidase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		
49	BB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		

- Molecule 50 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
50	BC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	40	SER	PRO	variant	UNP P42792
BC	40	SER	PRO	variant	UNP P42792

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AD	196	Total	C	N	O	S	0	0
			1528	978	264	281	5		
51	BD	195	Total	C	N	O	S	0	0
			1519	973	263	278	5		

- Molecule 52 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
52	BE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		
53	BF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	69	Total	C	N	O	S	0	0
			581	387	95	98	1		
54	BG	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AH	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
55	BH	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
56	BI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

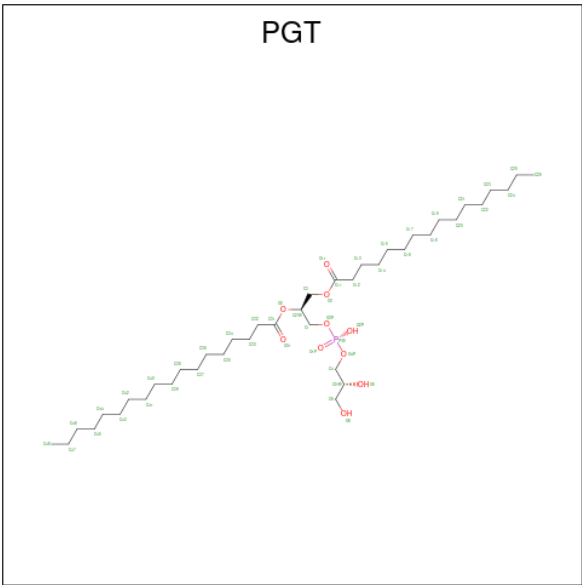
Mol	Chain	Residues	Atoms				AltConf	Trace
57	AJ	28	Total	C	N	O	0	0
			203	137	33	33		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	BJ	28	205	139	34	32	0	0

- Molecule 58 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSP HORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



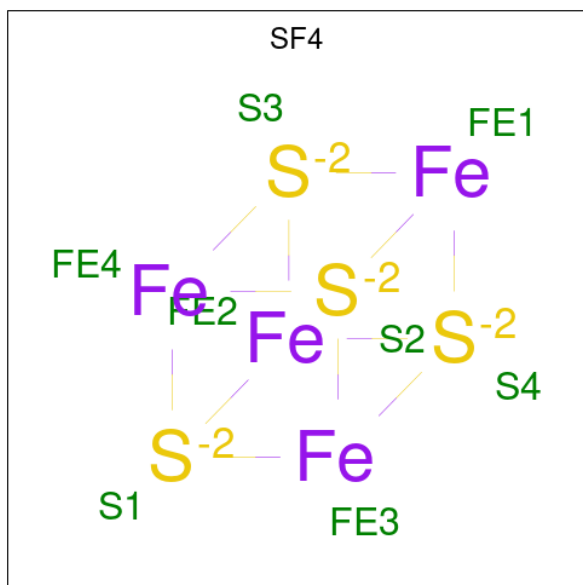
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
58	A	1	51	40	10	1	0
58	L	1	36	25	10	1	0
58	L	1	51	40	10	1	0
58	L	1	45	34	10	1	0
58	M	1	29	18	10	1	0
58	y	1	41	30	10	1	0
58	AC	1	41	30	10	1	0
58	AC	1	51	40	10	1	0
58	AF	1	51	40	10	1	0

Continued on next page...

Continued from previous page...

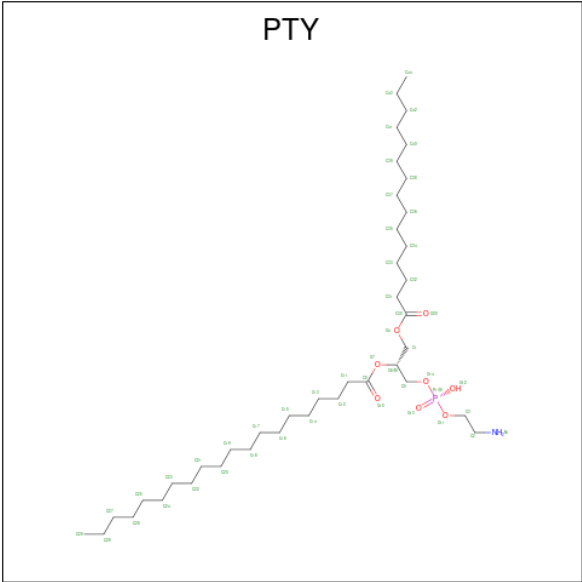
Mol	Chain	Residues	Atoms				AltConf
58	BC	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



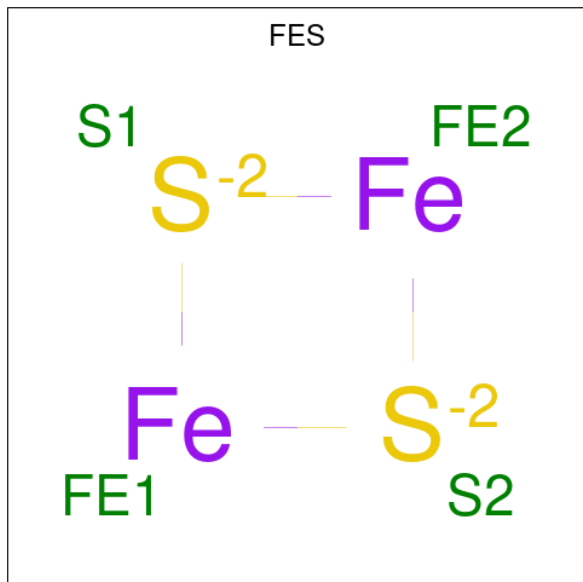
Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total	Fe	S	0
			8	4	4	
59	F	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 60 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $\text{C}_{40}\text{H}_{80}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



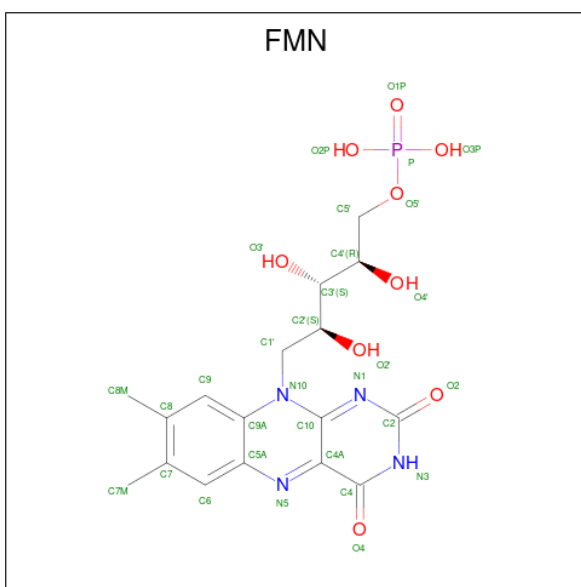
Mol	Chain	Residues	Atoms					AltConf
60	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
60	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
60	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	N	1	Total	C	N	O	P	0
			45	35	1	8	1	
60	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
60	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
60	m	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	z	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	AB	1	Total	C	N	O	P	0
			41	31	1	8	1	
60	BB	1	Total	C	N	O	P	0
			29	19	1	8	1	
60	BF	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



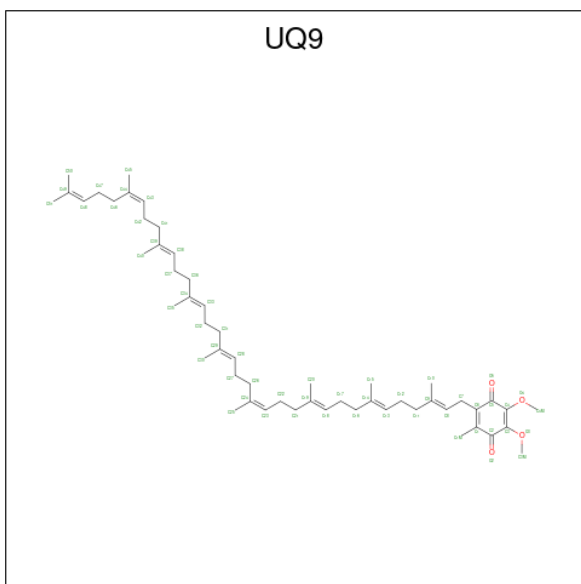
Mol	Chain	Residues	Atoms			AltConf
61	E	1	Total	Fe	S	0
			4	2	2	
61	G	1	Total	Fe	S	0
			4	2	2	
61	AD	1	Total	Fe	S	0
			4	2	2	
61	BD	1	Total	Fe	S	0
			4	2	2	

- Molecule 62 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 63 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).

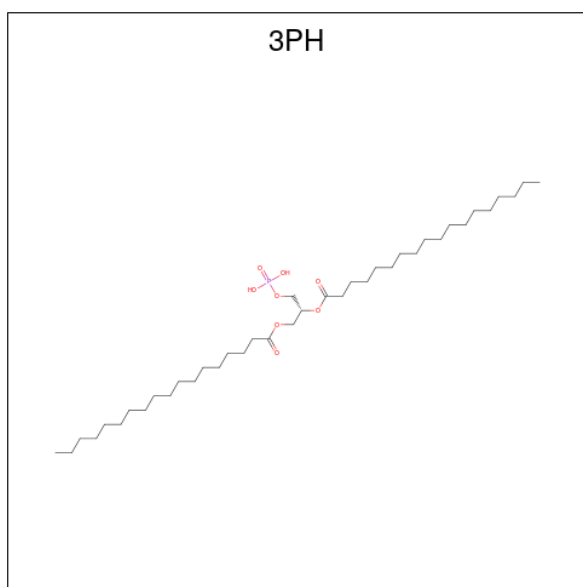


Mol	Chain	Residues	Atoms			AltConf
63	H	1	Total	C	O	0
			35	31	4	

- Molecule 64 is 2-{[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl}-4-{[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-alpha

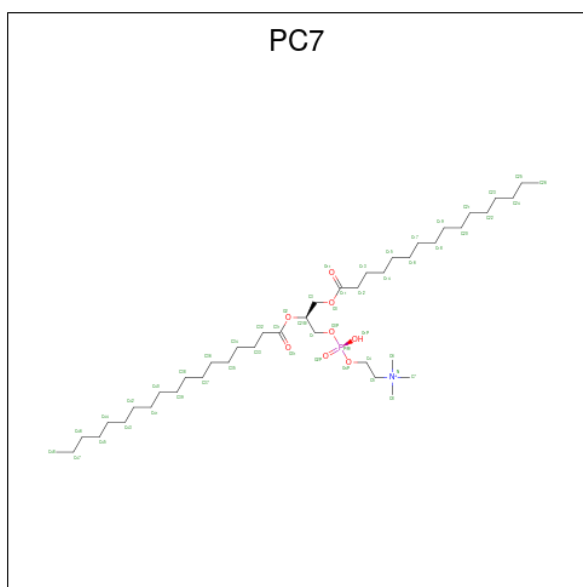
Mol	Chain	Residues	Atoms			AltConf
64	H	1	Total 81	C 56	O 25	0
64	K	1	Total 81	C 56	O 25	0
64	M	1	Total 39	C 34	O 5	0
64	a	1	Total 39	C 34	O 5	0
64	BC	1	Total 39	C 34	O 5	0
64	BC	1	Total 39	C 34	O 5	0

- Molecule 65 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



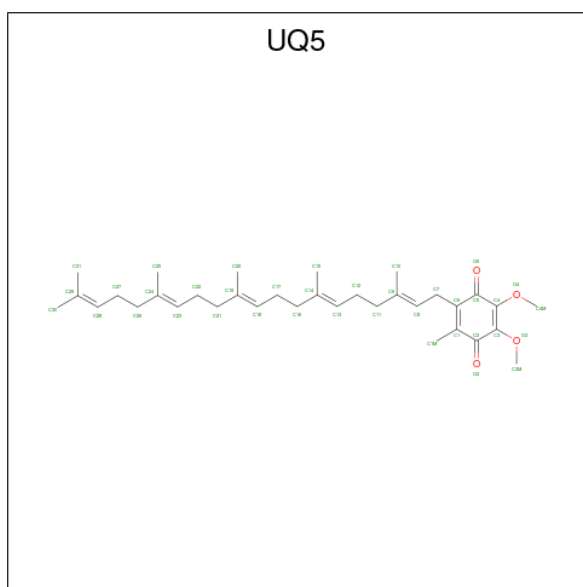
Mol	Chain	Residues	Atoms				AltConf
65	L	1	Total	C	O	P	0
			37	28	8	1	
65	M	1	Total	C	O	P	0
			41	32	8	1	
65	Y	1	Total	C	O	P	0
			33	24	8	1	
65	f	1	Total	C	O	P	0
			41	32	8	1	
65	f	1	Total	C	O	P	0
			43	34	8	1	
65	l	1	Total	C	O	P	0
			37	28	8	1	
65	AC	1	Total	C	O	P	0
			33	24	8	1	
65	AI	1	Total	C	O	P	0
			32	23	8	1	
65	BC	1	Total	C	O	P	0
			44	35	8	1	
65	BJ	1	Total	C	O	P	0
			41	32	8	1	
65	BJ	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 66 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
66	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
66	d	1	Total	C	N	O	P	0
			52	42	1	8	1	
66	f	1	Total	C	N	O	P	0
			48	38	1	8	1	
66	v	1	Total	C	N	O	P	0
			52	42	1	8	1	
66	AB	1	Total	C	N	O	P	0
			34	24	1	8	1	
66	AC	1	Total	C	N	O	P	0
			51	41	1	8	1	
66	AG	1	Total	C	N	O	P	0
			52	42	1	8	1	
66	BC	1	Total	C	N	O	P	0
			41	31	1	8	1	
66	BD	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 67 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄) (labeled as "Ligand of Interest" by depositor).

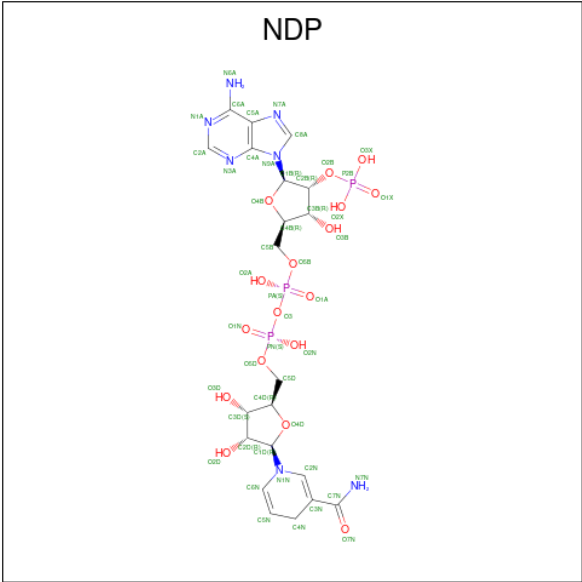


Mol	Chain	Residues	Atoms			AltConf
67	L	1	Total	C	O	0
			38	34	4	
67	AC	1	Total	C	O	0
			38	34	4	
67	AC	1	Total	C	O	0
			38	34	4	
67	BC	1	Total	C	O	0
			38	34	4	

- Molecule 68 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
68	O	1	Total	Fe	0
			1	1	

- Molecule 69 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

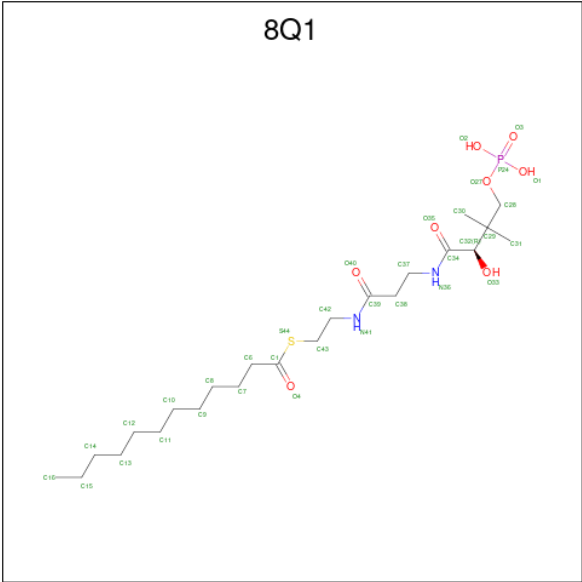


Mol	Chain	Residues	Atoms					AltConf
69	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

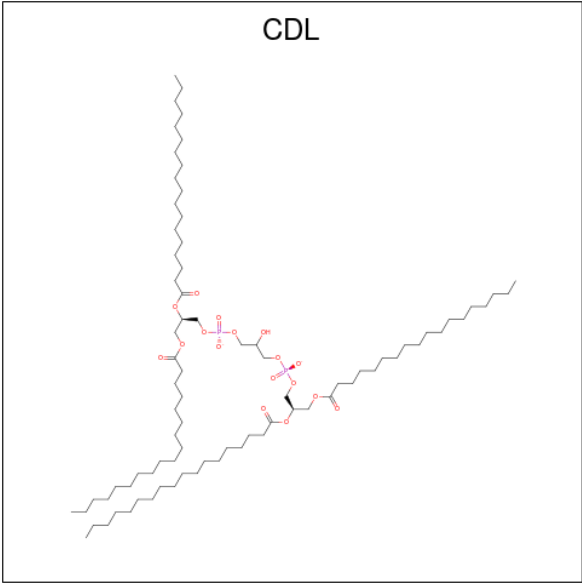
Mol	Chain	Residues	Atoms		AltConf
70	R	1	Total	Zn	0
			1	1	
70	y	1	Total	Zn	0
			1	1	
70	AB	1	Total	Zn	0
			1	1	
70	BB	1	Total	Zn	0
			1	1	

- Molecule 71 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
71	T	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
71	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



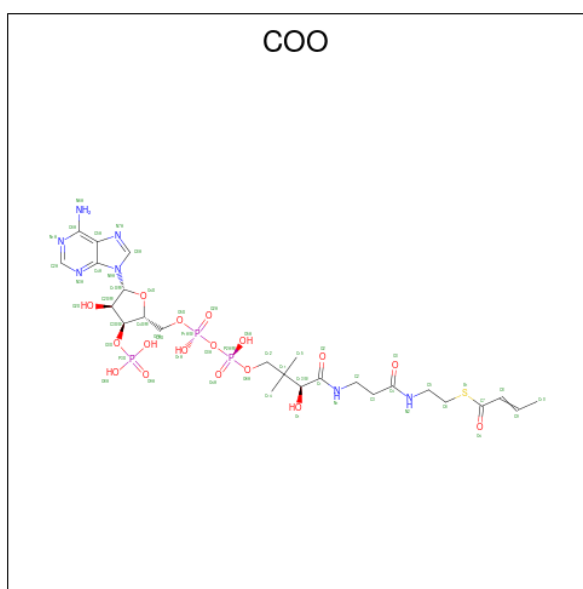
Mol	Chain	Residues	Atoms				AltConf
72	u	1	Total	C	O	P	0
			100	81	17	2	

Continued on next page...

Continued from previous page...

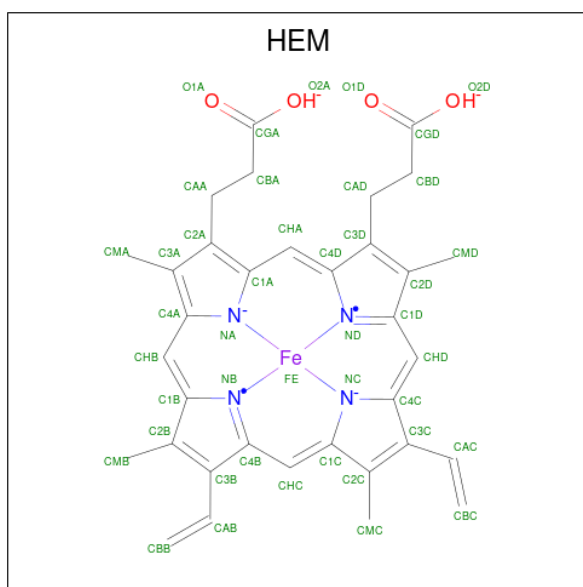
Mol	Chain	Residues	Atoms				AltConf
72	u	1	Total	C	O	P	0
			100	81	17	2	
72	AC	1	Total	C	O	P	0
			81	62	17	2	
72	AC	1	Total	C	O	P	0
			85	66	17	2	
72	AE	1	Total	C	O	P	0
			85	66	17	2	
72	BC	1	Total	C	O	P	0
			81	62	17	2	
72	BC	1	Total	C	O	P	0
			77	58	17	2	
72	BE	1	Total	C	O	P	0
			88	69	17	2	
72	BG	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 73 is CROTONYL COENZYME A (CCD ID: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



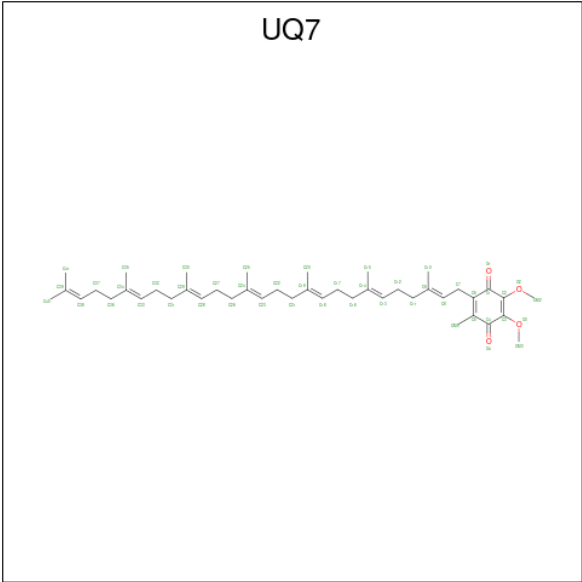
Mol	Chain	Residues	Atoms						AltConf
73	y	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

- Molecule 74 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
74	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	AC	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	AE	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	BC	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	BC	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	BE	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 75 is UBIQUINONE-7 (CCD ID: UQ7) (formula: $C_{44}H_{66}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
75	BC	1	Total	C	O	0
			48	44	4	

- Molecule 76 is water.

Mol	Chain	Residues	Atoms		AltConf
76	A	20	Total	O	0
			20	20	
76	B	84	Total	O	0
			84	84	
76	C	104	Total	O	0
			104	104	
76	D	226	Total	O	0
			226	226	
76	E	89	Total	O	0
			89	89	
76	F	152	Total	O	0
			152	152	
76	G	313	Total	O	0
			313	313	
76	H	129	Total	O	0
			129	129	
76	I	102	Total	O	0
			102	102	
76	J	64	Total	O	0
			64	64	
76	K	49	Total	O	0
			49	49	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
76	L	213	Total 213	O 213	0
76	M	158	Total 158	O 158	0
76	N	201	Total 201	O 201	0
76	O	88	Total 88	O 88	0
76	P	44	Total 44	O 44	0
76	Q	22	Total 22	O 22	0
76	R	44	Total 44	O 44	0
76	S	17	Total 17	O 17	0
76	T	13	Total 13	O 13	0
76	U	3	Total 3	O 3	0
76	V	31	Total 31	O 31	0
76	W	10	Total 10	O 10	0
76	X	19	Total 19	O 19	0
76	Y	5	Total 5	O 5	0
76	Z	53	Total 53	O 53	0
76	a	19	Total 19	O 19	0
76	b	2	Total 2	O 2	0
76	c	30	Total 30	O 30	0
76	d	21	Total 21	O 21	0
76	e	30	Total 30	O 30	0
76	f	49	Total 49	O 49	0

Continued on next page...

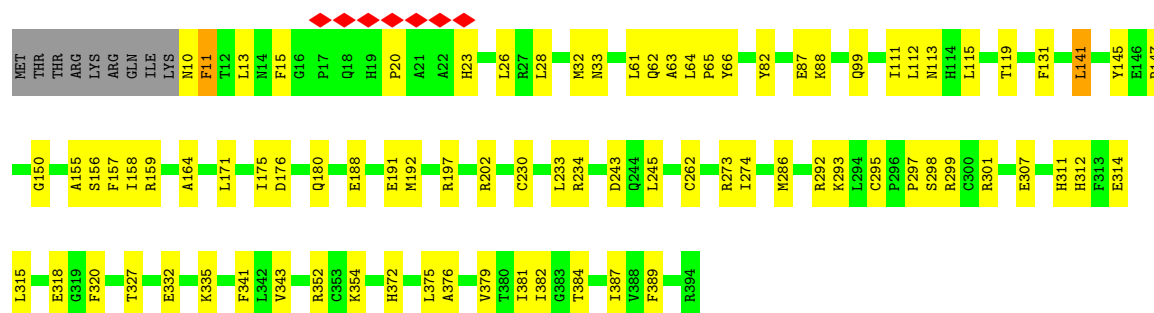
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
76	g	29	Total 29	O 29	0
76	i	26	Total 26	O 26	0
76	j	3	Total 3	O 3	0
76	k	10	Total 10	O 10	0
76	l	25	Total 25	O 25	0
76	m	24	Total 24	O 24	0
76	n	52	Total 52	O 52	0
76	o	50	Total 50	O 50	0
76	p	52	Total 52	O 52	0
76	q	31	Total 31	O 31	0
76	u	10	Total 10	O 10	0
76	v	10	Total 10	O 10	0
76	x	180	Total 180	O 180	0
76	y	167	Total 167	O 167	0
76	z	121	Total 121	O 121	0
76	AA	43	Total 43	O 43	0
76	AB	259	Total 259	O 259	0
76	AC	187	Total 187	O 187	0
76	AD	60	Total 60	O 60	0
76	AE	171	Total 171	O 171	0
76	AF	109	Total 109	O 109	0

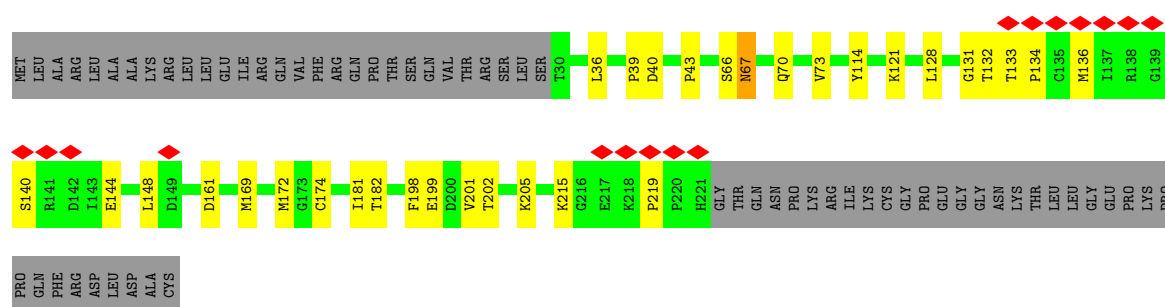
Continued on next page...

Continued from previous page...

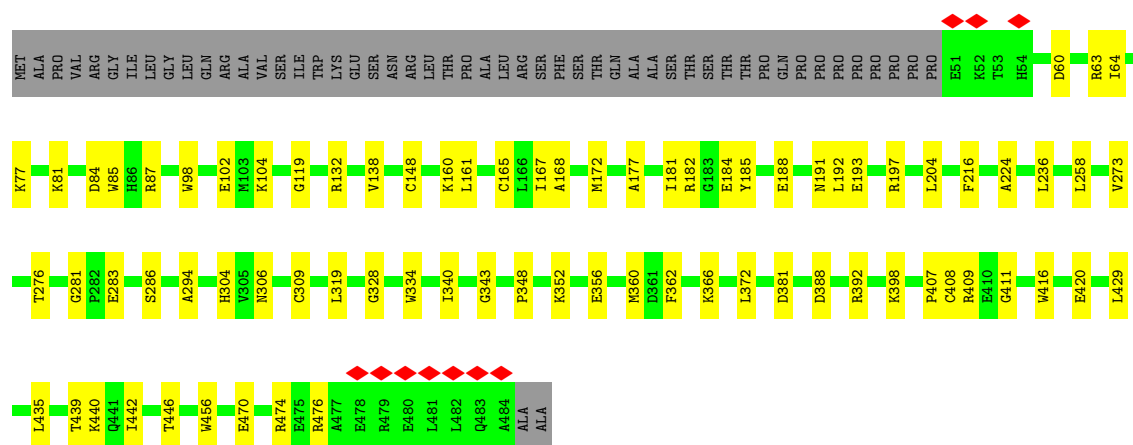
Mol	Chain	Residues	Atoms		AltConf
76	AG	25	Total 25	O 25	0
76	AH	13	Total 13	O 13	0
76	AI	20	Total 20	O 20	0
76	BA	77	Total 77	O 77	0
76	BB	260	Total 260	O 260	0
76	BC	148	Total 148	O 148	0
76	BD	43	Total 43	O 43	0
76	BE	118	Total 118	O 118	0
76	BF	71	Total 71	O 71	0
76	BG	19	Total 19	O 19	0
76	BH	2	Total 2	O 2	0
76	BI	14	Total 14	O 14	0
76	BJ	1	Total 1	O 1	0



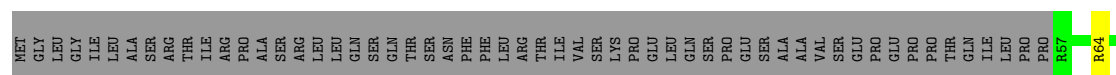
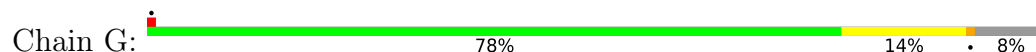
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

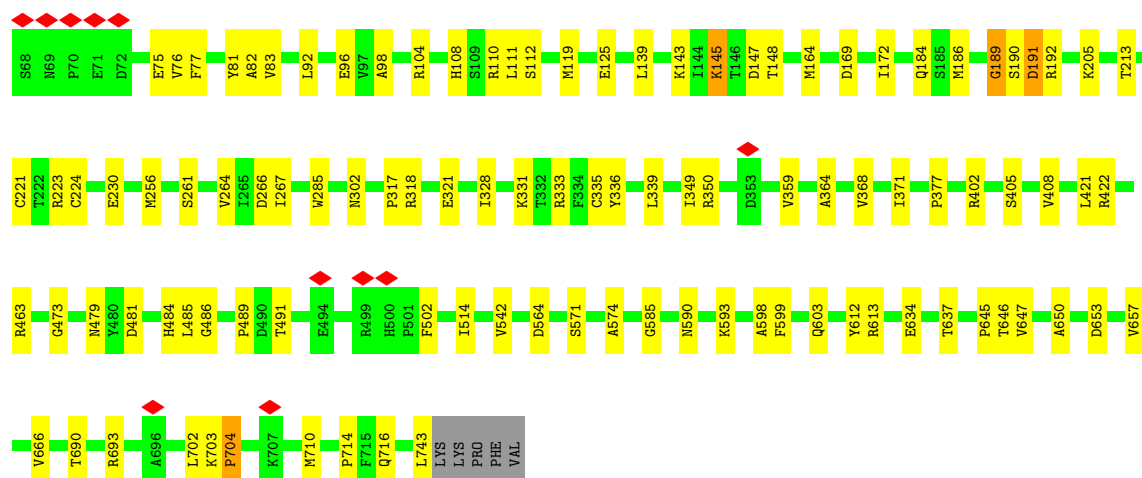


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



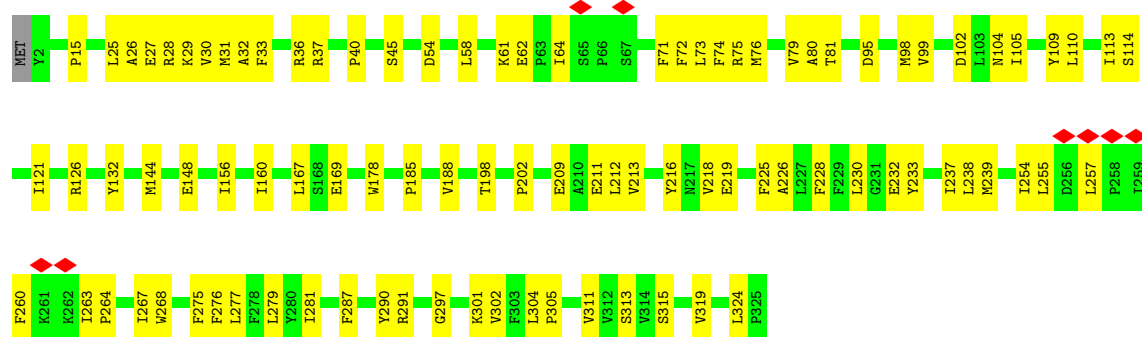
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial





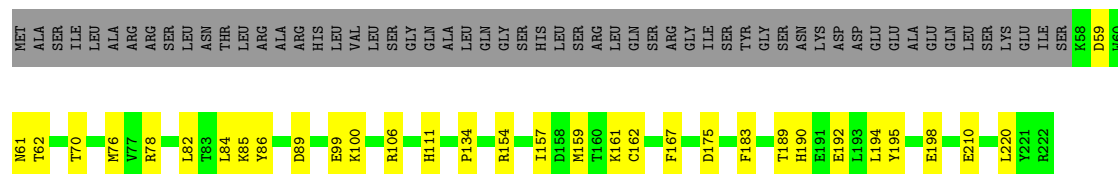
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 71% 29%



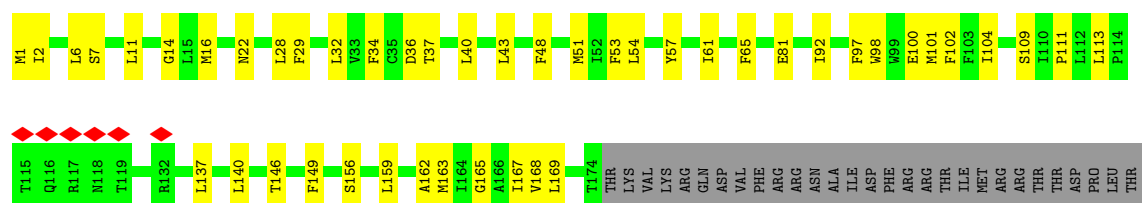
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I: 60% 14% 26%



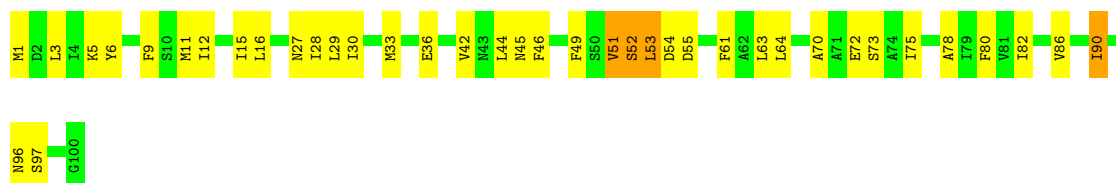
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 62% 22% 15%

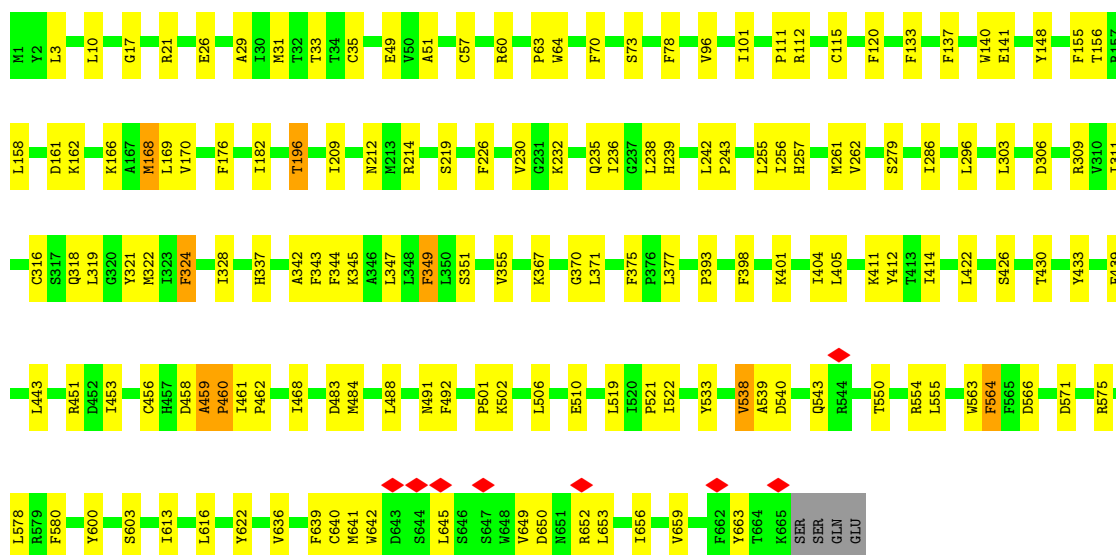


TYR

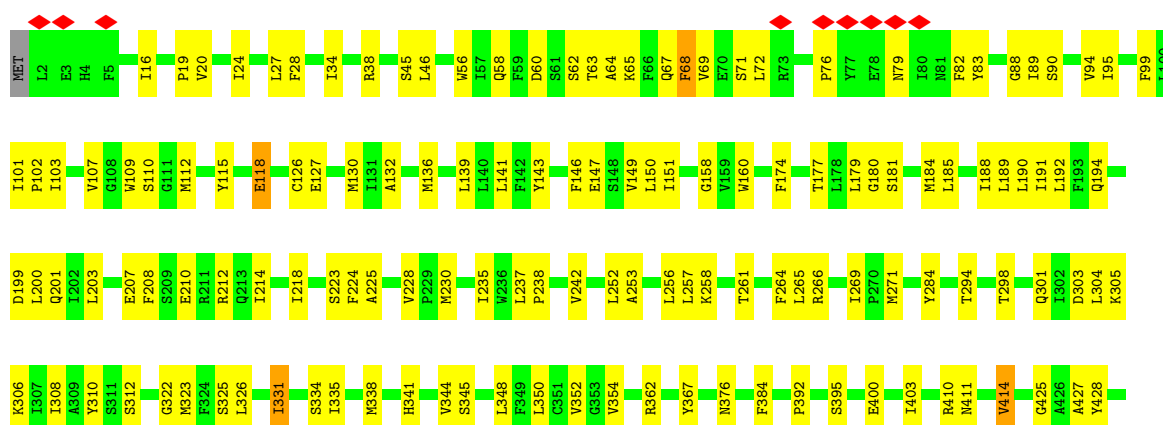
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

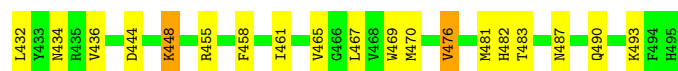
Chain K:  61% 35%

- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

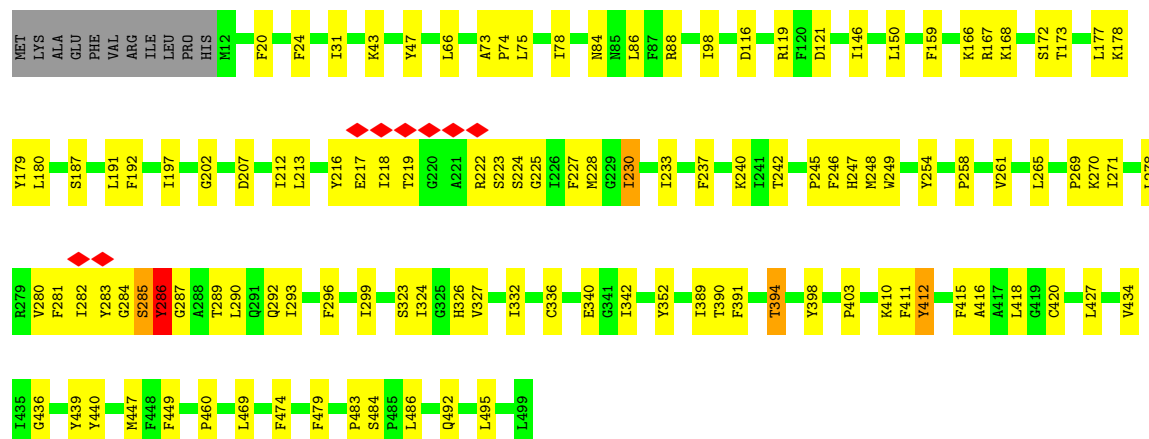
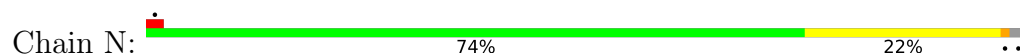
Chain L:  76% 22%

- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

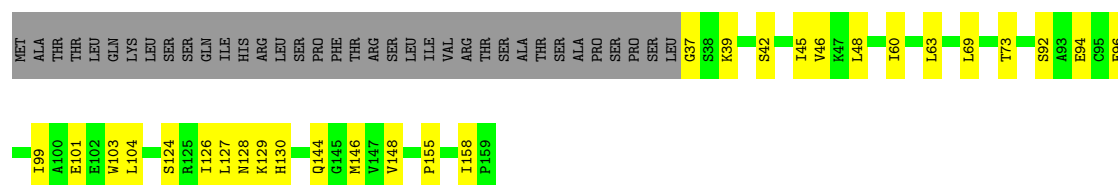
Chain M:  68% 31%



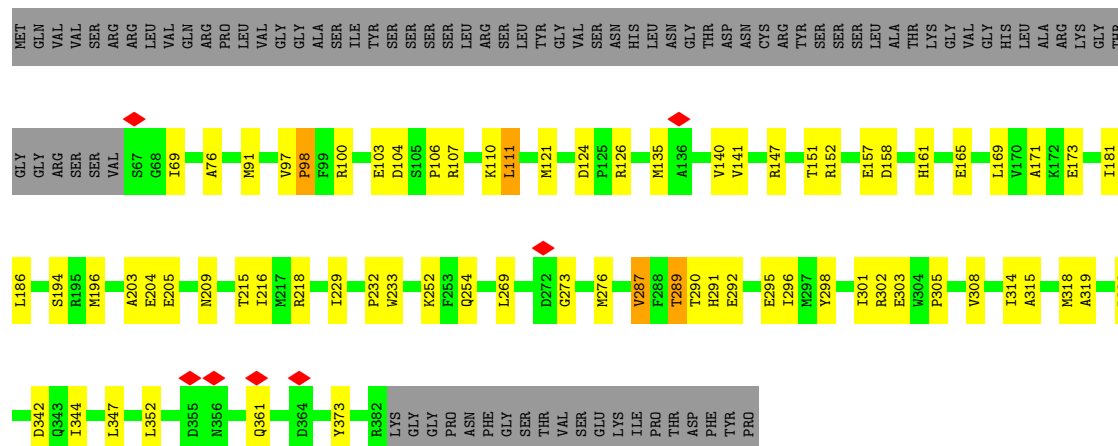
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



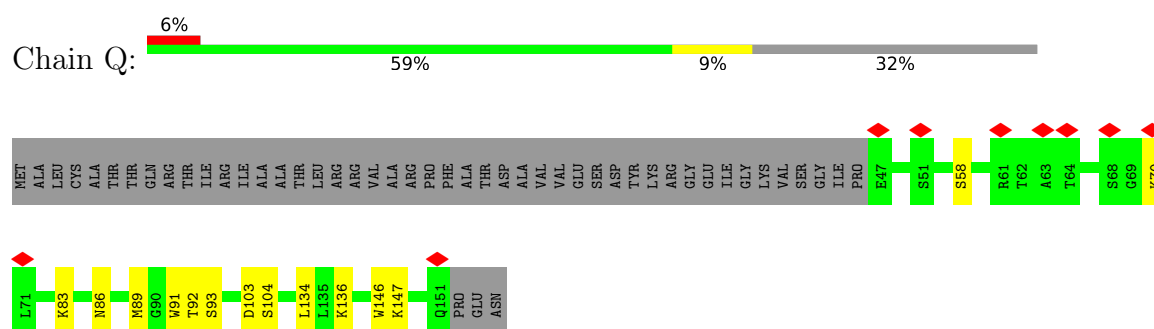
• Molecule 15: 2Fe-2S ferredoxin-like superfamily protein



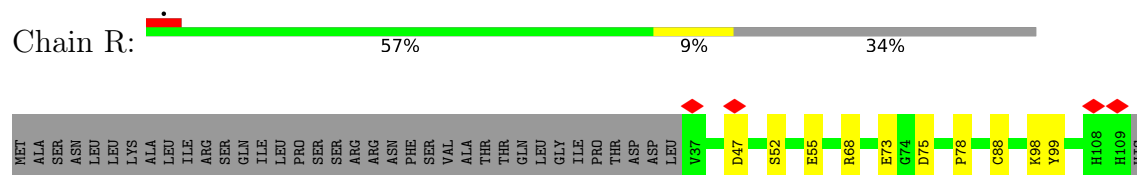
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



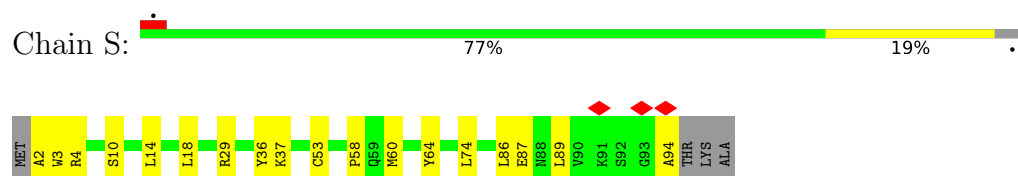
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



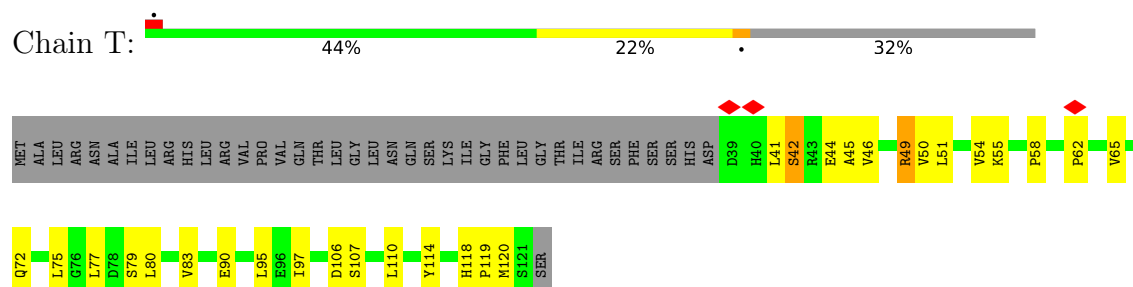
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



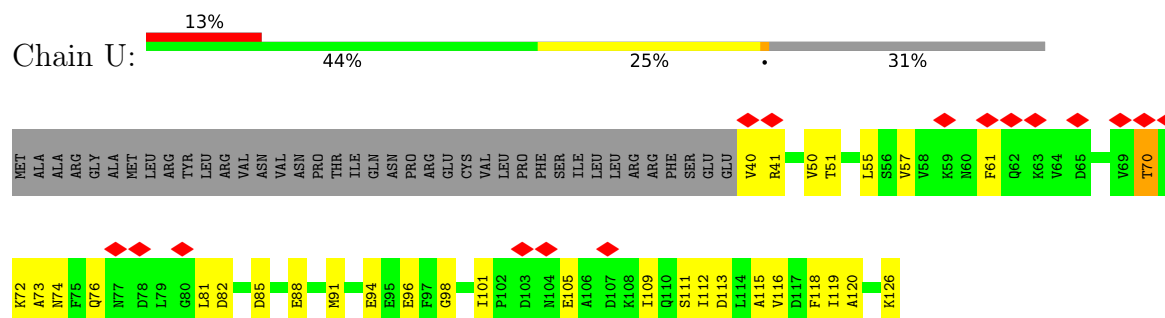
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: Acyl carrier protein 1, mitochondrial



- Molecule 21: Acyl carrier protein 2, mitochondrial

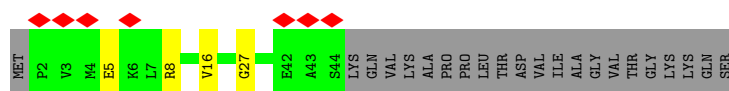


- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial





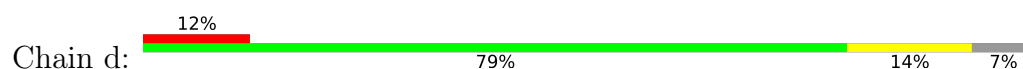
- Molecule 28: At2g46540/F11C10.23



- Molecule 29: Transmembrane protein



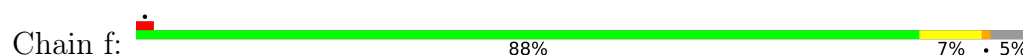
- Molecule 30: Excitatory amino acid transporter



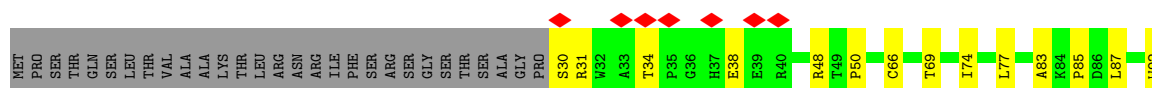
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



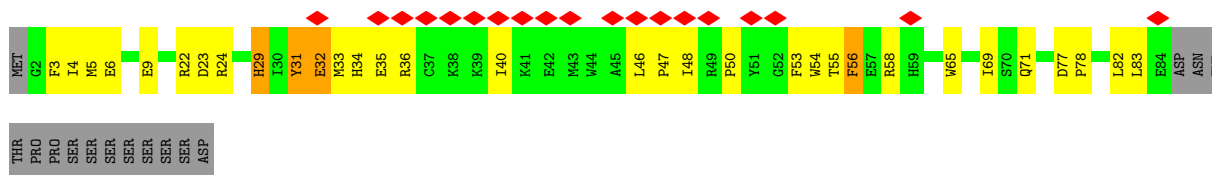
- Molecule 32: At4g16450



- Molecule 33: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



- Molecule 34: At1g67350



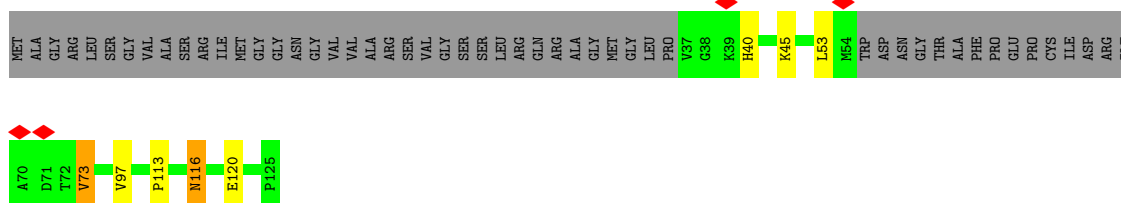
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2



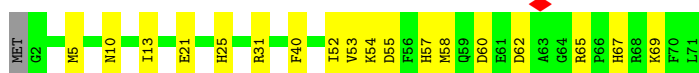
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



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



- Molecule 38: AT2G31490 protein

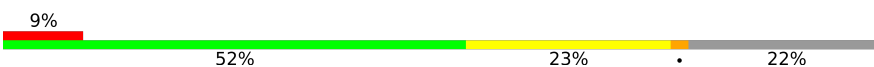


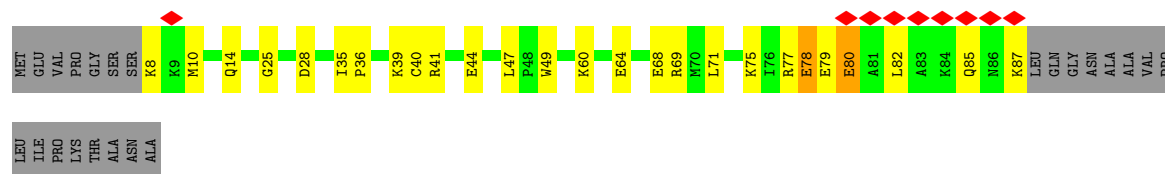
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 



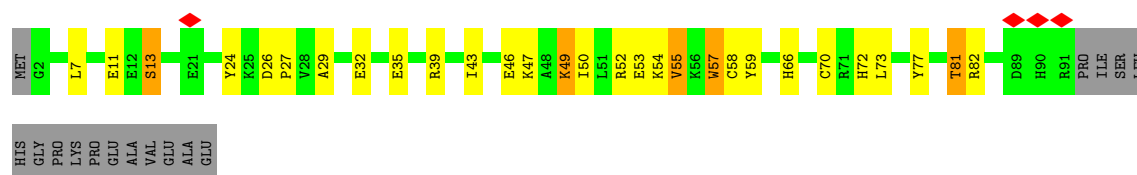
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 

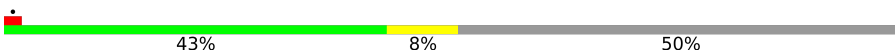


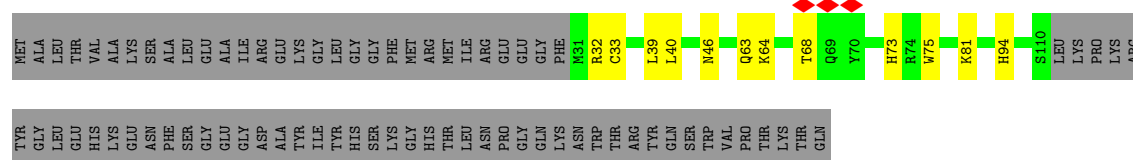
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

Chain p: 



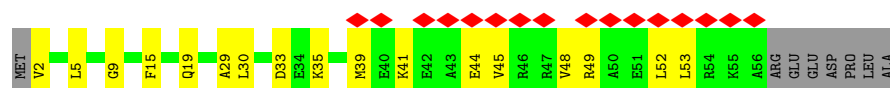
- Molecule 42: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 



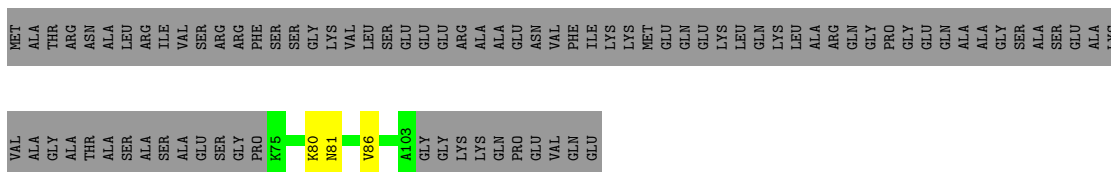
- Molecule 43: Uncharacterized protein At1g67785

Chain u: 



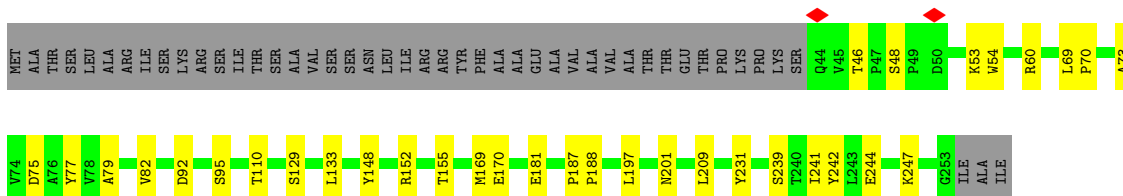
- Molecule 44: Uncharacterized protein At2g27730, mitochondrial

Chain v:  23% 74%



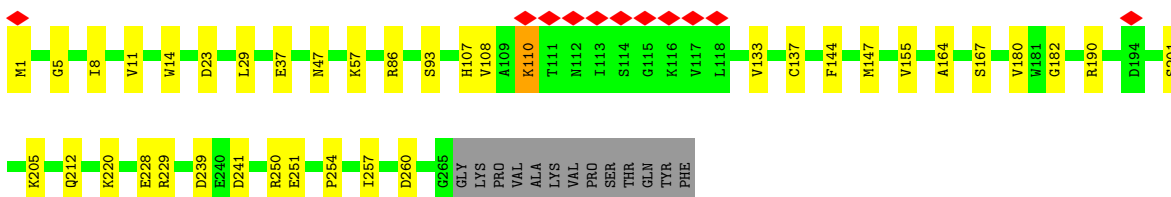
- Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial

Chain x:  69% 13% 18%



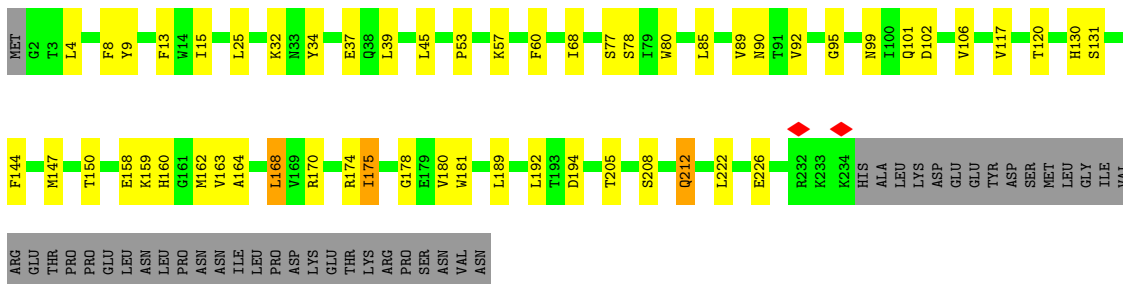
- Molecule 46: Gamma carbonic anhydrase 2, mitochondrial

Chain y:  82% 13% 5%



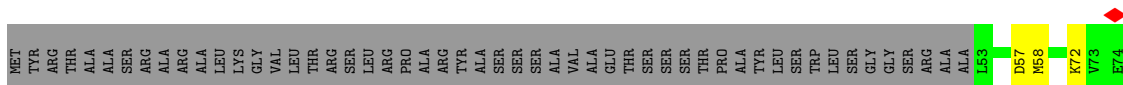
- Molecule 47: Gamma carbonic anhydrase 1, mitochondrial

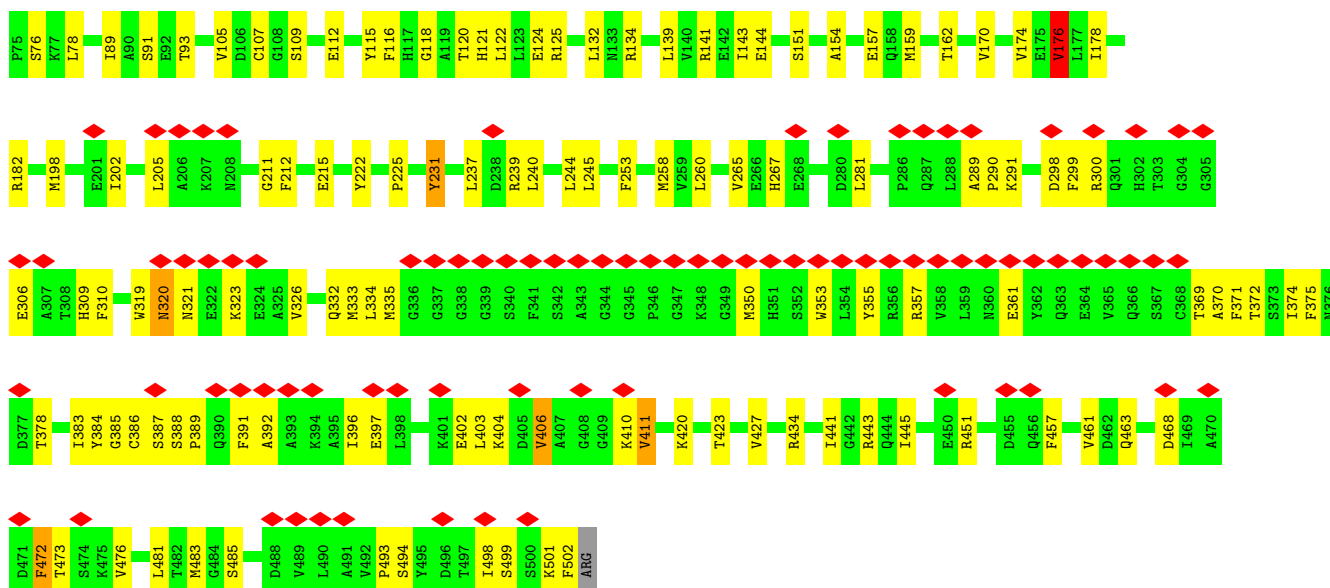
Chain z:  65% 19% 15%



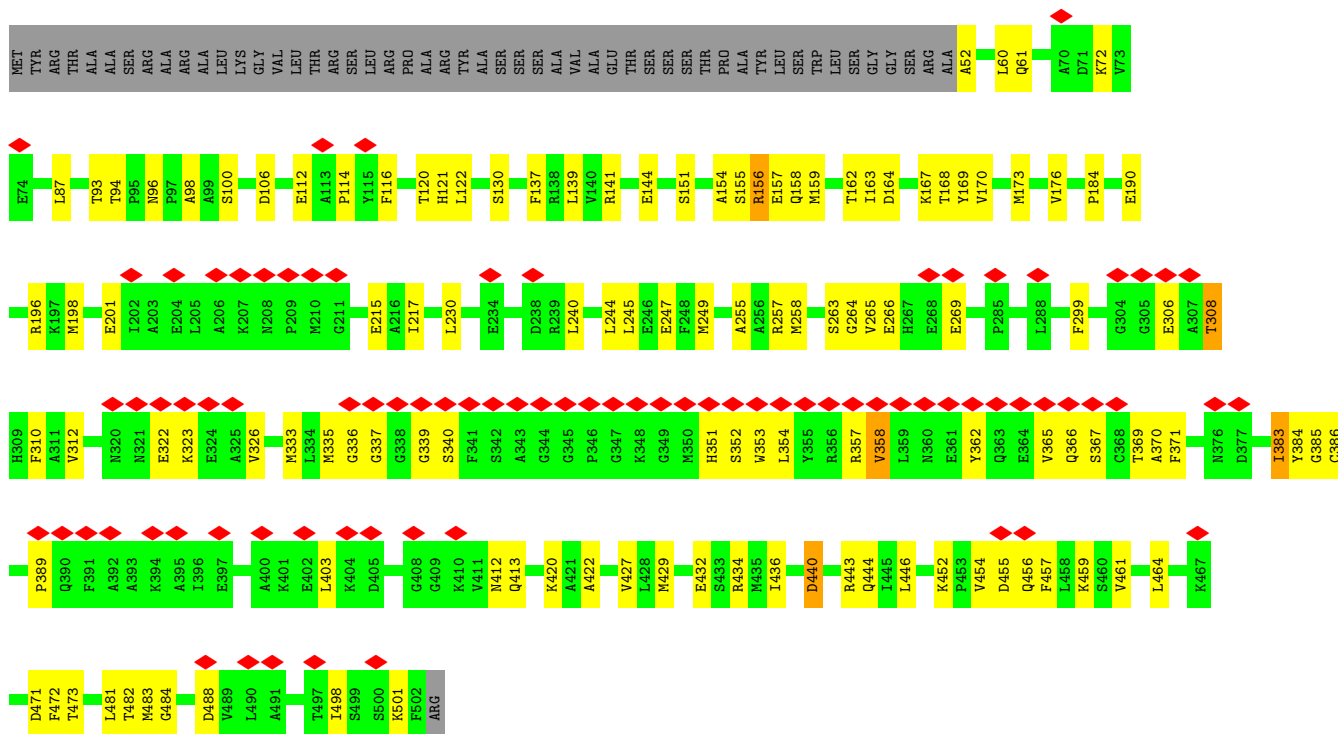
- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial

Chain AA:  17% 64% 24% 11%

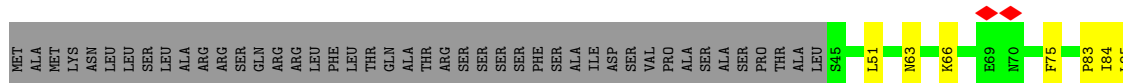
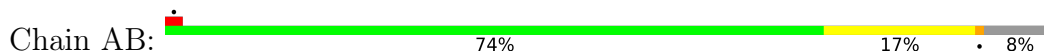


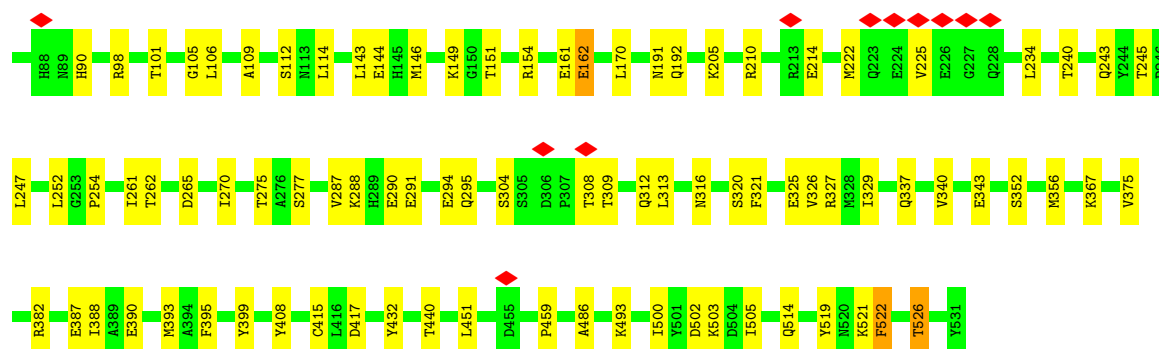


- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial



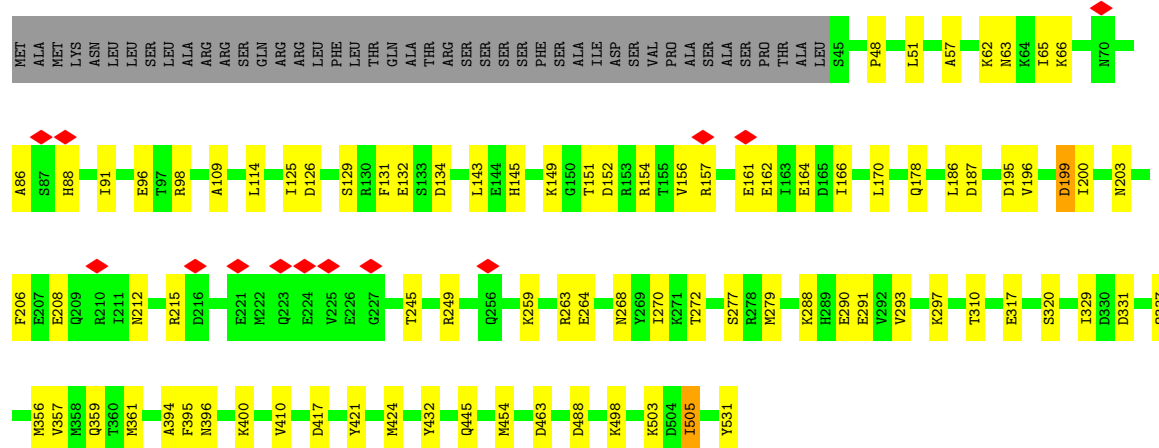
- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial





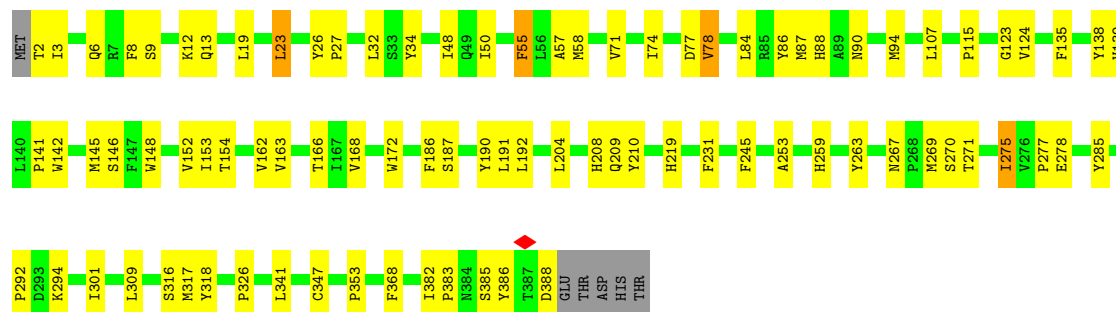
- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

Chain BB: 75% 16% 8%



- Molecule 50: Cytochrome b

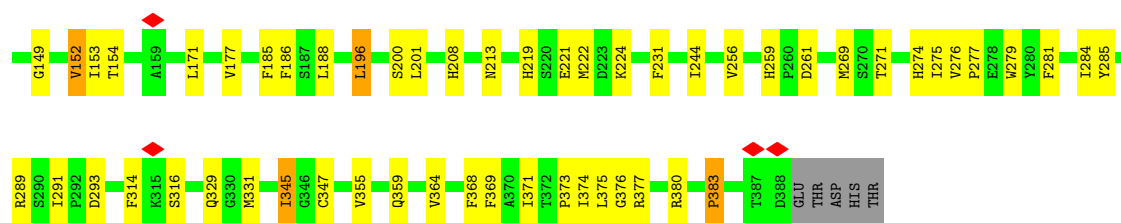
Chain AC: 76% 21% 3%



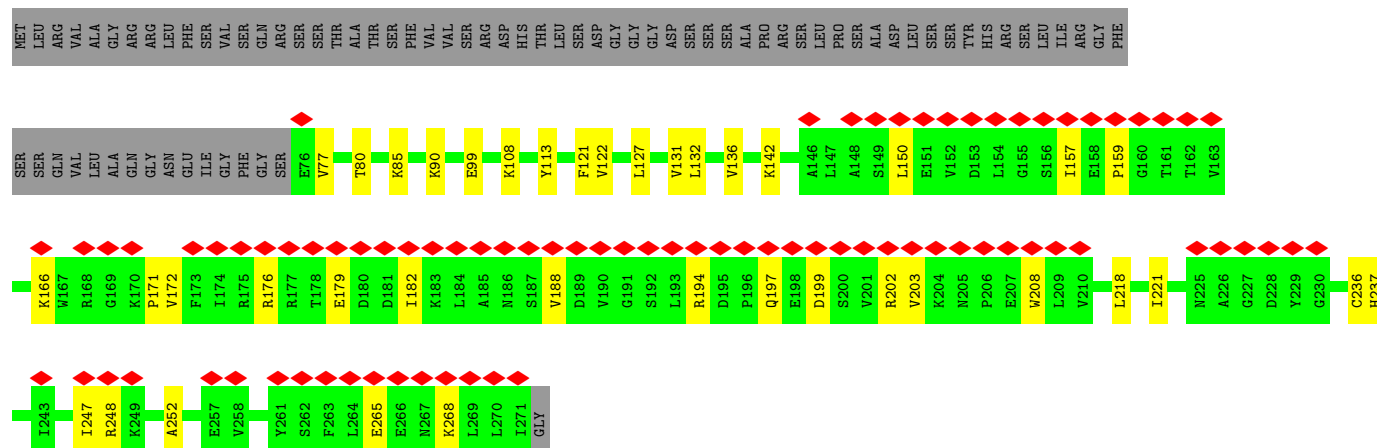
- Molecule 50: Cytochrome b

Chain BC: 76% 22% 2%

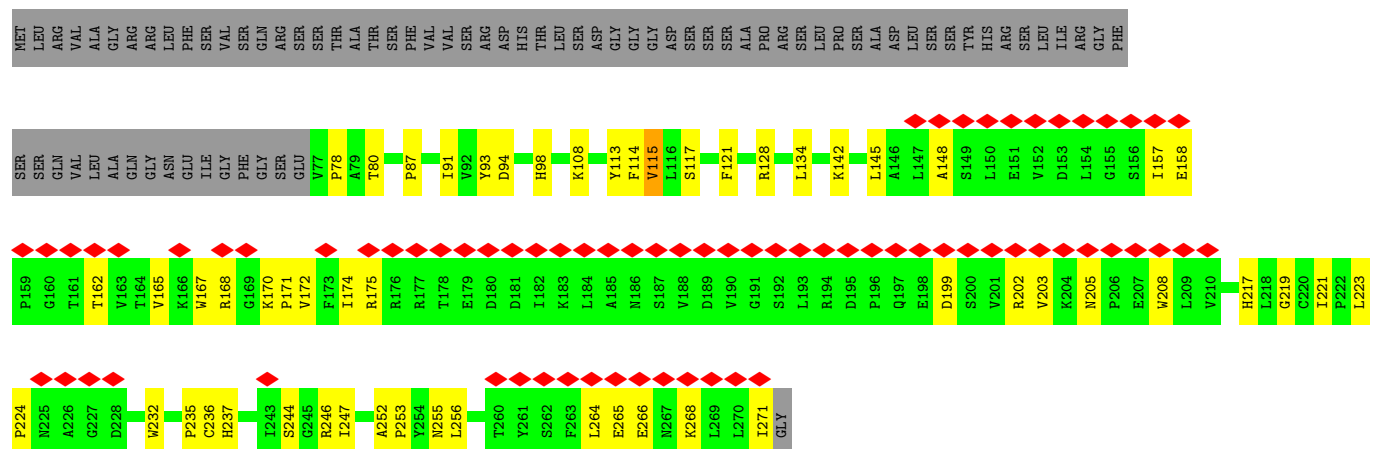




- Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

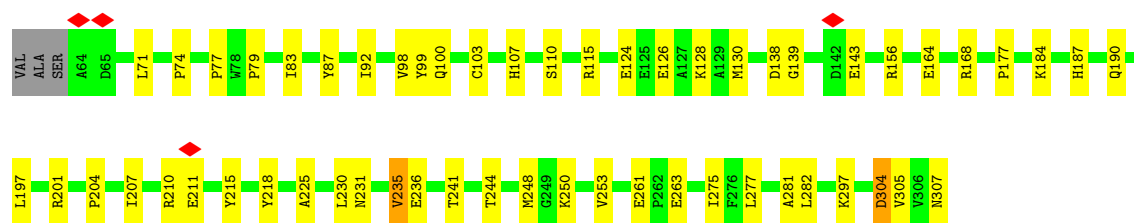


- Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial



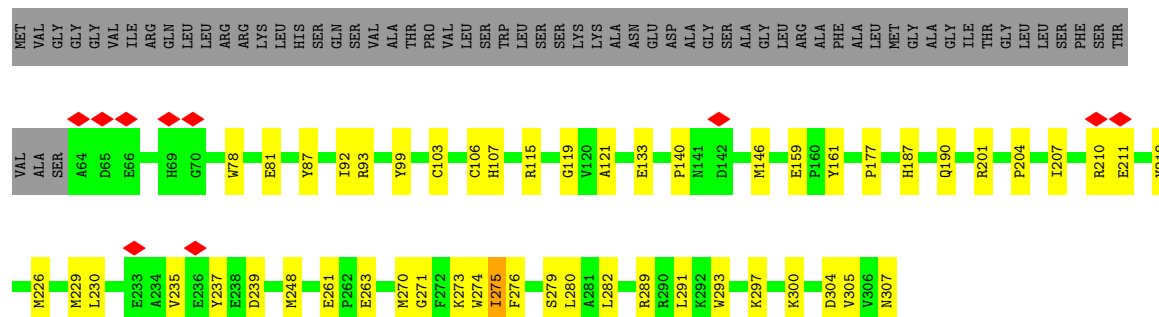
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial





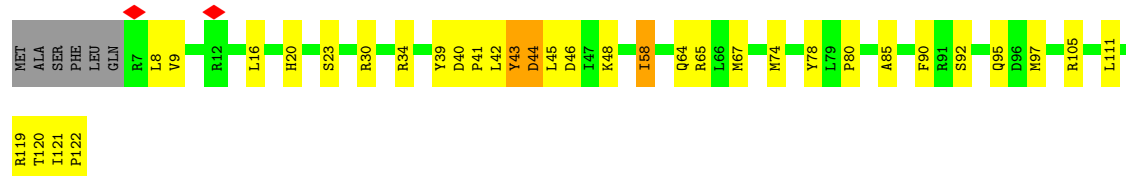
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial

Chain BE: 63% 17% 21%



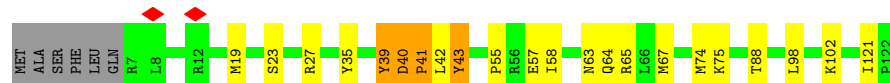
- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

Chain AF: 67% 25% 5%



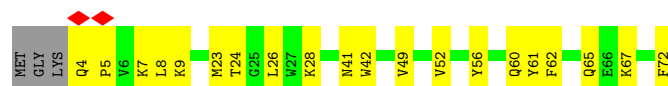
- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

Chain BF: 77% 15% 5%



- Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial

Chain AG: 68% 28% 0%



- Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial

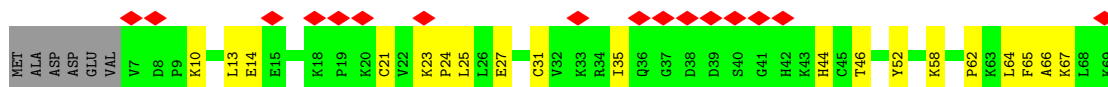
Chain BG: 76% 18% 6%



- Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial



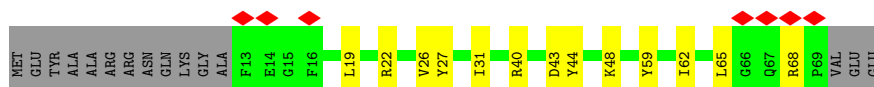
- Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial



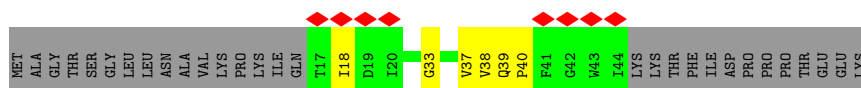
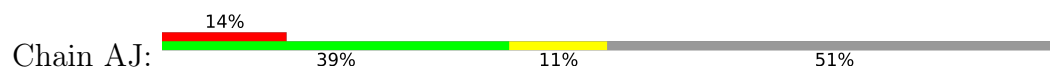
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



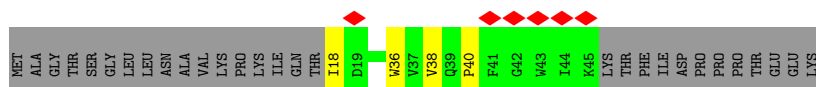
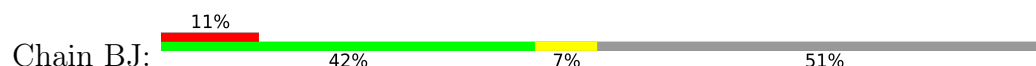
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	24.801	Depositor
Minimum map value	-12.512	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	429.75, 429.75, 429.75	wwPDB
Map dimensions	750, 750, 750	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, COO, UQ7, 8Q1, 3PH, Q7G, FES, FE, FMN, PGT, SF4, PTY, NDP, UQ9, UQ5, PC7, FME, CDL, HEM

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	A	0.19	0/820	0.41	0/1113
2	B	0.90	6/1279 (0.5%)	0.83	0/1734
3	C	0.68	0/1590	0.75	3/2152 (0.1%)
4	D	0.75	13/3149 (0.4%)	0.73	1/4259 (0.0%)
5	E	0.79	6/1535 (0.4%)	0.78	0/2084
6	F	0.14	0/3441	0.29	0/4641
7	G	0.35	1/5338 (0.0%)	0.53	10/7231 (0.1%)
8	H	0.22	0/2609	0.41	0/3553
9	I	0.67	3/1378 (0.2%)	0.69	2/1862 (0.1%)
10	J	0.61	0/1435	0.72	0/1957
11	K	1.09	9/785 (1.1%)	1.07	5/1062 (0.5%)
12	L	0.77	13/5368 (0.2%)	0.98	15/7291 (0.2%)
13	M	0.57	2/4066 (0.0%)	0.74	5/5525 (0.1%)
14	N	0.71	9/3948 (0.2%)	0.84	7/5360 (0.1%)
15	O	0.54	1/979 (0.1%)	0.61	0/1326
16	P	0.62	2/2509 (0.1%)	0.79	3/3401 (0.1%)
17	Q	0.08	0/862	0.24	0/1166
18	R	0.43	0/585	0.59	0/793
19	S	0.51	0/739	0.61	0/996
20	T	0.77	1/671 (0.1%)	1.04	1/911 (0.1%)
21	U	0.19	0/687	0.41	0/929
22	V	0.70	2/1146 (0.2%)	0.79	0/1555
23	W	0.47	0/923	0.68	2/1249 (0.2%)
24	X	0.15	0/790	0.36	0/1060
25	Y	0.62	2/944 (0.2%)	0.70	0/1277
26	Z	0.38	0/1027	0.55	0/1392
27	a	0.22	0/481	0.38	0/646
28	b	0.16	0/320	0.39	0/434
29	c	0.48	0/637	0.60	1/860 (0.1%)
30	d	0.66	1/605 (0.2%)	0.77	0/815
31	e	0.69	0/559	0.70	0/745

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.16	0/771	0.31	0/1042
33	g	0.41	0/661	0.66	2/899 (0.2%)
34	i	0.79	3/741 (0.4%)	1.16	10/997 (1.0%)
35	j	0.60	0/433	0.90	2/592 (0.3%)
36	k	0.66	0/392	0.87	2/526 (0.4%)
37	l	0.54	0/575	0.75	1/781 (0.1%)
38	m	0.71	2/592 (0.3%)	1.03	0/793
39	n	1.00	2/938 (0.2%)	1.13	8/1273 (0.6%)
40	o	0.78	1/666 (0.2%)	1.19	5/886 (0.6%)
41	p	0.93	2/777 (0.3%)	1.23	8/1043 (0.8%)
42	q	0.25	0/690	0.38	0/936
43	u	0.13	0/472	0.22	0/632
44	v	0.13	0/222	0.29	0/300
45	x	0.67	3/1669 (0.2%)	0.62	1/2279 (0.0%)
46	y	0.52	0/2046	0.62	1/2772 (0.0%)
47	z	0.59	3/1804 (0.2%)	0.71	3/2441 (0.1%)
48	AA	0.47	1/3503 (0.0%)	0.73	7/4752 (0.1%)
48	BA	0.57	2/3508 (0.1%)	0.72	5/4759 (0.1%)
49	AB	0.46	2/3908 (0.1%)	0.61	5/5305 (0.1%)
49	BB	0.35	0/3908	0.53	2/5305 (0.0%)
50	AC	0.67	9/3208 (0.3%)	0.79	8/4395 (0.2%)
50	BC	0.67	7/3208 (0.2%)	0.83	5/4395 (0.1%)
51	AD	0.42	0/1567	0.59	0/2135
51	BD	0.49	0/1558	0.68	4/2123 (0.2%)
52	AE	0.40	0/1968	0.58	2/2672 (0.1%)
52	BE	0.45	0/1968	0.55	2/2672 (0.1%)
53	AF	0.82	5/993 (0.5%)	0.89	3/1336 (0.2%)
53	BF	0.64	3/993 (0.3%)	0.73	1/1336 (0.1%)
54	AG	0.66	1/600 (0.2%)	0.81	1/815 (0.1%)
54	BG	0.48	0/591	0.85	0/802
55	AH	0.26	0/531	0.43	0/713
55	BH	0.64	2/524 (0.4%)	0.80	1/703 (0.1%)
56	AI	0.99	4/488 (0.8%)	1.01	0/655
56	BI	0.51	0/488	0.84	2/655 (0.3%)
57	AJ	0.65	0/210	1.11	4/290 (1.4%)
57	BJ	0.23	0/212	0.39	0/291
All	All	0.58	123/98588 (0.1%)	0.72	150/133680 (0.1%)

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
1	A	0	1
14	N	0	2
All	All	0	3

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	51	LYS	C-O	16.00	1.42	1.24
50	AC	88	HIS	C-O	-9.50	1.13	1.24
50	AC	192	LEU	C-O	-9.23	1.15	1.24
25	Y	125	ALA	C-O	-9.15	1.13	1.24
22	V	107	ASP	C-O	-8.98	1.19	1.23

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	191	ASP	CB-CA-C	-12.13	89.52	109.53
34	i	32	GLU	CA-C-N	-11.27	101.92	122.09
34	i	32	GLU	C-N-CA	-11.27	101.92	122.09
12	L	70	PHE	CB-CA-C	10.93	125.90	110.16
40	o	79	GLU	N-CA-C	-10.50	101.52	114.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	FME	Mainchain
14	N	411	PHE	Mainchain
14	N	412[B]	TYR	Mainchain

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	A	802	0	817	34	0
2	B	1244	0	1231	45	0
3	C	1545	0	1501	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3079	0	3049	93	0
5	E	1500	0	1473	24	0
6	F	3368	0	3355	72	0
7	G	5243	0	5228	79	0
8	H	2536	0	2641	124	0
9	I	1349	0	1293	38	0
10	J	1399	0	1472	46	0
11	K	784	0	843	36	0
12	L	5222	0	5251	145	0
13	M	3952	0	4092	180	0
14	N	3839	0	3941	111	0
15	O	963	0	975	22	0
16	P	2453	0	2493	53	0
17	Q	837	0	818	26	0
18	R	571	0	559	12	0
19	S	727	0	759	21	0
20	T	659	0	644	37	0
21	U	677	0	665	27	0
22	V	1123	0	1112	19	0
23	W	904	0	901	22	0
24	X	776	0	775	13	0
25	Y	928	0	960	62	0
26	Z	997	0	979	18	0
27	a	469	0	472	11	0
28	b	315	0	338	3	0
29	c	617	0	619	18	0
30	d	592	0	610	13	0
31	e	546	0	510	11	0
32	f	765	0	766	8	0
33	g	641	0	632	24	0
34	i	721	0	695	53	0
35	j	415	0	406	7	0
36	k	382	0	380	16	0
37	l	562	0	567	11	0
38	m	577	0	564	16	0
39	n	911	0	879	46	0
40	o	657	0	669	25	0
41	p	757	0	745	39	0
42	q	669	0	630	11	0
43	u	463	0	471	73	0
44	v	219	0	227	8	0
45	x	1629	0	1636	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	y	2013	0	2024	47	0
47	z	1772	0	1771	59	0
48	AA	3431	0	3416	101	0
48	BA	3436	0	3421	89	0
49	AB	3834	0	3797	97	0
49	BB	3834	0	3797	93	0
50	AC	3093	0	3074	92	0
50	BC	3093	0	3074	115	0
51	AD	1528	0	1529	35	0
51	BD	1519	0	1523	50	0
52	AE	1917	0	1844	52	0
52	BE	1917	0	1844	51	0
53	AF	976	0	1001	40	0
53	BF	976	0	1001	41	0
54	AG	581	0	588	25	0
54	BG	572	0	582	28	0
55	AH	518	0	518	100	0
55	BH	511	0	511	11	0
56	AI	476	0	469	13	0
56	BI	476	0	469	14	0
57	AJ	203	0	197	13	0
57	BJ	205	0	203	12	0
58	A	51	0	78	7	0
58	AC	92	0	133	8	0
58	AF	51	0	78	9	0
58	BC	37	0	47	2	0
58	L	132	0	183	7	0
58	M	29	0	28	1	0
58	y	41	0	52	8	0
59	B	8	0	0	1	0
59	F	8	0	0	1	0
59	G	16	0	0	0	0
59	I	16	0	0	2	0
60	AB	41	0	58	0	0
60	BB	29	0	31	1	0
60	BF	40	0	56	16	0
60	D	50	0	79	13	0
60	L	42	0	60	2	0
60	M	87	0	126	4	0
60	N	135	0	201	9	0
60	Y	31	0	35	0	0
60	d	39	0	51	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	m	50	0	79	0	0
60	z	50	0	79	12	0
61	AD	4	0	0	0	0
61	BD	4	0	0	1	0
61	E	4	0	0	1	0
61	G	4	0	0	1	0
62	F	31	0	19	0	0
63	H	35	0	43	6	0
64	BC	78	0	0	0	0
64	H	81	0	0	3	0
64	K	81	0	0	1	0
64	M	39	0	0	0	0
64	a	39	0	0	0	0
65	AC	33	0	39	2	0
65	AI	32	0	37	3	0
65	BC	44	0	64	6	0
65	BJ	89	0	133	2	0
65	L	37	0	47	4	0
65	M	41	0	58	15	0
65	Y	33	0	39	2	0
65	f	84	0	120	5	0
65	l	37	0	47	0	0
66	AB	34	0	42	1	0
66	AC	51	0	79	3	0
66	AG	52	0	84	6	0
66	BC	41	0	56	3	0
66	BD	39	0	52	3	0
66	L	40	0	54	6	0
66	d	52	0	84	8	0
66	f	48	0	73	1	0
66	v	52	0	84	7	0
67	AC	76	0	100	10	0
67	BC	38	0	50	8	0
67	L	38	0	50	7	0
68	O	1	0	0	0	0
69	P	48	0	26	0	0
70	AB	1	0	0	0	0
70	BB	1	0	0	0	0
70	R	1	0	0	0	0
70	y	1	0	0	0	0
71	T	35	0	0	0	0
71	W	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	AC	166	0	232	15	0
72	AE	85	0	120	4	0
72	BC	158	0	210	9	0
72	BE	88	0	123	6	0
72	BG	70	0	87	6	0
72	u	200	0	312	25	0
73	y	53	0	37	5	0
74	AC	86	0	60	3	0
74	AE	43	0	30	4	0
74	BC	86	0	60	1	0
74	BE	43	0	30	6	0
75	BC	48	0	66	11	0
76	A	20	0	0	3	0
76	AA	43	0	0	2	0
76	AB	259	0	0	11	0
76	AC	187	0	0	25	0
76	AD	60	0	0	1	0
76	AE	171	0	0	13	0
76	AF	109	0	0	8	0
76	AG	25	0	0	7	0
76	AH	13	0	0	1	0
76	AI	20	0	0	2	0
76	B	84	0	0	6	0
76	BA	77	0	0	5	0
76	BB	260	0	0	17	0
76	BC	148	0	0	21	0
76	BD	43	0	0	5	0
76	BE	118	0	0	8	0
76	BF	71	0	0	5	0
76	BG	19	0	0	2	0
76	BH	2	0	0	2	0
76	BI	14	0	0	6	0
76	BJ	1	0	0	0	0
76	C	104	0	0	6	0
76	D	226	0	0	24	0
76	E	89	0	0	3	0
76	F	152	0	0	18	0
76	G	313	0	0	8	0
76	H	129	0	0	35	0
76	I	102	0	0	11	0
76	J	64	0	0	14	0
76	K	49	0	0	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	L	213	0	0	23	0
76	M	158	0	0	29	0
76	N	201	0	0	25	0
76	O	88	0	0	2	0
76	P	44	0	0	7	0
76	Q	22	0	0	1	0
76	R	44	0	0	4	0
76	S	17	0	0	8	0
76	T	13	0	0	2	0
76	U	3	0	0	1	0
76	V	31	0	0	4	0
76	W	10	0	0	1	0
76	X	19	0	0	1	0
76	Y	5	0	0	2	0
76	Z	53	0	0	2	0
76	a	19	0	0	2	0
76	b	2	0	0	0	0
76	c	30	0	0	3	0
76	d	21	0	0	3	0
76	e	30	0	0	2	0
76	f	49	0	0	2	0
76	g	29	0	0	7	0
76	i	26	0	0	8	0
76	j	3	0	0	1	0
76	k	10	0	0	0	0
76	l	25	0	0	0	0
76	m	24	0	0	2	0
76	n	52	0	0	17	0
76	o	50	0	0	6	0
76	p	52	0	0	11	0
76	q	31	0	0	2	0
76	u	10	0	0	0	0
76	v	10	0	0	3	0
76	x	180	0	0	13	0
76	y	167	0	0	11	0
76	z	121	0	0	20	0
All	All	104814	0	100597	2566	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 13.

The worst 5 of 2566 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)
4:D:15:PHE:CD2	8:H:212:LEU:HD13	1.18	1.68
46:y:133:VAL:HG11	47:z:147:MET:CE	1.14	1.57
25:Y:9:LEU:CD1	55:AH:20:LYS:HB2	1.10	1.55
43:u:53:LEU:CD2	55:AH:19:PRO:HG3	1.38	1.54
34:i:34:HIS:CE1	41:p:27:PRO:CG	1.93	1.51

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	A	90/119 (76%)	89 (99%)	1 (1%)	0	100	100
2	B	155/218 (71%)	149 (96%)	6 (4%)	0	100	100
3	C	179/190 (94%)	176 (98%)	3 (2%)	0	100	100
4	D	383/394 (97%)	366 (96%)	17 (4%)	0	100	100
5	E	190/255 (74%)	178 (94%)	12 (6%)	0	100	100
6	F	432/486 (89%)	421 (98%)	11 (2%)	0	100	100
7	G	685/748 (92%)	668 (98%)	17 (2%)	0	100	100
8	H	322/325 (99%)	314 (98%)	8 (2%)	0	100	100
9	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
10	J	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
11	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
12	L	663/669 (99%)	637 (96%)	26 (4%)	0	100	100
13	M	493/495 (100%)	487 (99%)	6 (1%)	0	100	100
14	N	488/499 (98%)	474 (97%)	14 (3%)	0	100	100
15	O	121/159 (76%)	117 (97%)	4 (3%)	0	100	100
16	P	314/402 (78%)	301 (96%)	13 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	103/154 (67%)	100 (97%)	3 (3%)	0	100	100
18	R	71/110 (64%)	70 (99%)	1 (1%)	0	100	100
19	S	91/97 (94%)	89 (98%)	2 (2%)	0	100	100
20	T	81/122 (66%)	78 (96%)	3 (4%)	0	100	100
21	U	85/126 (68%)	77 (91%)	8 (9%)	0	100	100
22	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
23	W	108/133 (81%)	99 (92%)	9 (8%)	0	100	100
24	X	96/106 (91%)	95 (99%)	1 (1%)	0	100	100
25	Y	123/159 (77%)	117 (95%)	6 (5%)	0	100	100
26	Z	123/143 (86%)	122 (99%)	1 (1%)	0	100	100
27	a	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
28	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
29	c	74/88 (84%)	73 (99%)	1 (1%)	0	100	100
30	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
31	e	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
32	f	99/106 (93%)	98 (99%)	1 (1%)	0	100	100
33	g	77/114 (68%)	77 (100%)	0	0	100	100
34	i	81/98 (83%)	79 (98%)	2 (2%)	0	100	100
35	j	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
36	k	46/72 (64%)	45 (98%)	1 (2%)	0	100	100
37	l	70/125 (56%)	69 (99%)	1 (1%)	0	100	100
38	m	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
39	n	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
40	o	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
41	p	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
42	q	79/159 (50%)	75 (95%)	4 (5%)	0	100	100
43	u	53/63 (84%)	53 (100%)	0	0	100	100
44	v	27/113 (24%)	27 (100%)	0	0	100	100
45	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
46	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
47	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	AA	448/503 (89%)	431 (96%)	17 (4%)	0	100	100
48	BA	449/503 (89%)	431 (96%)	18 (4%)	0	100	100
49	AB	485/531 (91%)	475 (98%)	10 (2%)	0	100	100
49	BB	485/531 (91%)	476 (98%)	9 (2%)	0	100	100
50	AC	385/393 (98%)	375 (97%)	10 (3%)	0	100	100
50	BC	385/393 (98%)	374 (97%)	11 (3%)	0	100	100
51	AD	194/272 (71%)	182 (94%)	12 (6%)	0	100	100
51	BD	193/272 (71%)	181 (94%)	12 (6%)	0	100	100
52	AE	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
52	BE	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
53	AF	114/122 (93%)	114 (100%)	0	0	100	100
53	BF	114/122 (93%)	114 (100%)	0	0	100	100
54	AG	67/72 (93%)	67 (100%)	0	0	100	100
54	BG	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
55	AH	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
55	BH	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
56	AI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
56	BI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
57	AJ	26/57 (46%)	25 (96%)	1 (4%)	0	100	100
57	BJ	26/57 (46%)	23 (88%)	3 (12%)	0	100	100
All	All	12051/14108 (85%)	11717 (97%)	334 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	85/105 (81%)	83 (98%)	2 (2%)	43	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	132/184 (72%)	131 (99%)	1 (1%)	73	81
3	C	171/179 (96%)	171 (100%)	0	100	100
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	164 (99%)	2 (1%)	63	72
6	F	353/396 (89%)	352 (100%)	1 (0%)	86	91
7	G	570/625 (91%)	568 (100%)	2 (0%)	84	89
8	H	271/272 (100%)	271 (100%)	0	100	100
9	I	147/195 (75%)	145 (99%)	2 (1%)	59	67
10	J	156/186 (84%)	153 (98%)	3 (2%)	50	58
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	72
12	L	564/568 (99%)	558 (99%)	6 (1%)	65	74
13	M	434/434 (100%)	428 (99%)	6 (1%)	59	67
14	N	408/416 (98%)	402 (98%)	6 (2%)	57	65
15	O	108/141 (77%)	107 (99%)	1 (1%)	70	78
16	P	263/334 (79%)	257 (98%)	6 (2%)	44	51
17	Q	89/128 (70%)	89 (100%)	0	100	100
18	R	64/97 (66%)	64 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100
20	T	78/112 (70%)	76 (97%)	2 (3%)	40	46
21	U	78/113 (69%)	77 (99%)	1 (1%)	61	69
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	98/114 (86%)	98 (100%)	0	100	100
24	X	88/94 (94%)	88 (100%)	0	100	100
25	Y	92/120 (77%)	91 (99%)	1 (1%)	65	74
26	Z	100/115 (87%)	99 (99%)	1 (1%)	68	76
27	a	48/53 (91%)	47 (98%)	1 (2%)	47	54
28	b	35/53 (66%)	35 (100%)	0	100	100
29	c	66/71 (93%)	66 (100%)	0	100	100
30	d	60/66 (91%)	59 (98%)	1 (2%)	53	62
31	e	59/73 (81%)	59 (100%)	0	100	100
32	f	80/83 (96%)	80 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	g	68/96 (71%)	66 (97%)	2 (3%)	37	42
34	i	75/90 (83%)	74 (99%)	1 (1%)	61	69
35	j	42/51 (82%)	40 (95%)	2 (5%)	23	23
36	k	39/60 (65%)	39 (100%)	0	100	100
37	l	60/97 (62%)	58 (97%)	2 (3%)	33	37
38	m	58/59 (98%)	58 (100%)	0	100	100
39	n	92/99 (93%)	92 (100%)	0	100	100
40	o	70/87 (80%)	66 (94%)	4 (6%)	18	17
41	p	80/93 (86%)	79 (99%)	1 (1%)	61	69
42	q	69/133 (52%)	69 (100%)	0	100	100
43	u	47/54 (87%)	46 (98%)	1 (2%)	47	54
44	v	22/84 (26%)	22 (100%)	0	100	100
45	x	179/216 (83%)	178 (99%)	1 (1%)	78	86
46	y	221/232 (95%)	220 (100%)	1 (0%)	81	88
47	z	188/228 (82%)	185 (98%)	3 (2%)	55	64
48	AA	369/408 (90%)	362 (98%)	7 (2%)	50	58
48	BA	369/408 (90%)	364 (99%)	5 (1%)	59	67
49	AB	415/452 (92%)	408 (98%)	7 (2%)	53	62
49	BB	415/452 (92%)	411 (99%)	4 (1%)	68	76
50	AC	330/336 (98%)	326 (99%)	4 (1%)	63	72
50	BC	330/336 (98%)	323 (98%)	7 (2%)	47	54
51	AD	170/232 (73%)	166 (98%)	4 (2%)	43	49
51	BD	169/232 (73%)	168 (99%)	1 (1%)	78	86
52	AE	200/247 (81%)	199 (100%)	1 (0%)	81	88
52	BE	200/247 (81%)	198 (99%)	2 (1%)	68	76
53	AF	105/110 (96%)	104 (99%)	1 (1%)	68	76
53	BF	105/110 (96%)	105 (100%)	0	100	100
54	AG	63/65 (97%)	63 (100%)	0	100	100
54	BG	62/65 (95%)	62 (100%)	0	100	100
55	AH	58/62 (94%)	58 (100%)	0	100	100
55	BH	57/62 (92%)	56 (98%)	1 (2%)	51	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	AI	48/59 (81%)	47 (98%)	1 (2%)	47	54
56	BI	48/59 (81%)	48 (100%)	0	100	100
57	AJ	16/41 (39%)	16 (100%)	0	100	100
57	BJ	16/41 (39%)	16 (100%)	0	100	100
All	All	10339/11908 (87%)	10230 (99%)	109 (1%)	63	74

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	p	49	LYS
49	AB	154	ARG
50	BC	98	VAL
45	x	148	TYR
48	AA	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
48	AA	133	ASN
53	AF	20	HIS
49	AB	113	ASN
50	AC	13	GLN
48	BA	149	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FME	K	1	11	8,9,10	0.82	0	7,9,11	2.07	3 (42%)
32	FME	f	1	32	8,9,10	1.70	1 (12%)	7,9,11	1.55	1 (14%)
1	FME	A	1	1	8,9,10	1.70	1 (12%)	7,9,11	1.61	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	K	1	11	-	5/7/9/11	-
32	FME	f	1	32	-	5/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	1	FME	O-C	4.12	1.36	1.19
1	A	1	FME	O-C	4.09	1.36	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-3.69	115.10	124.78
11	K	1	FME	C-CA-N	3.58	116.19	109.73
32	f	1	FME	O-C-CA	-3.39	115.89	124.78
11	K	1	FME	O-C-CA	-2.97	116.99	124.78
11	K	1	FME	CG-CB-CA	-2.40	106.29	112.95

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	N-CA-CB-CG
32	f	1	FME	O1-CN-N-CA
32	f	1	FME	C-CA-CB-CG
32	f	1	FME	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	f	1	FME	3	0
1	A	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 5 are monoatomic - leaving 86 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	$\# Z > 2$
69	NDP	P	500	-	49,52,52	0.61	0	66,80,80	0.71	0
72	CDL	BG	101	-	69,69,99	1.04	8 (11%)	75,81,111	1.16	5 (6%)
60	PTY	N	503	-	49,49,49	0.27	0	52,54,54	0.36	0
59	SF4	B	500	2	0,12,12	-	-	-	-	-
75	UQ7	BC	404	-	48,48,48	0.66	2 (4%)	58,61,61	0.77	3 (5%)
65	3PH	M	501	-	40,40,47	0.70	1 (2%)	44,45,52	0.66	1 (2%)
67	UQ5	L	707	-	38,38,38	0.76	2 (5%)	46,49,49	0.84	3 (6%)
66	PC7	L	706	-	39,39,51	1.08	3 (7%)	45,47,59	1.10	3 (6%)
60	PTY	m	101	-	49,49,49	0.26	0	52,54,54	0.35	0
72	CDL	BC	407	-	80,80,99	0.30	0	86,92,111	0.38	0
61	FES	AD	301	51	0,4,4	-	-	-	-	-
64	Q7G	K	201	-	90,90,90	0.78	2 (2%)	136,138,138	1.33	19 (13%)
60	PTY	Y	202	-	30,30,49	0.35	0	33,35,54	0.37	0
74	HEM	AC	401	50	50,50,50	1.46	7 (14%)	66,82,82	1.29	6 (9%)
58	PGT	L	702	-	35,35,50	0.31	0	38,41,56	0.40	0
72	CDL	AE	402	-	84,84,99	0.29	0	90,96,111	0.36	0
74	HEM	BE	401	52	50,50,50	2.03	16 (32%)	66,82,82	2.10	21 (31%)
65	3PH	Y	201	-	32,32,47	0.35	0	36,37,52	0.34	0
60	PTY	M	503	-	36,36,49	0.31	0	39,41,54	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	PTY	L	705	-	41,41,49	0.96	4 (9%)	44,46,54	1.07	2 (4%)
72	CDL	AC	409	-	84,84,99	0.31	0	90,96,111	0.36	0
60	PTY	BF	201	-	39,39,49	0.97	4 (10%)	42,44,54	1.06	2 (4%)
65	3PH	L	701	-	36,36,47	0.54	0	40,41,52	0.73	2 (5%)
60	PTY	z	301	-	49,49,49	0.86	3 (6%)	52,54,54	1.17	3 (5%)
62	FMN	F	500	-	33,33,33	0.61	0	48,50,50	0.67	1 (2%)
59	SF4	I	500	9	0,12,12	-	-	-	-	-
58	PGT	AC	406	-	40,40,50	0.32	0	43,46,56	0.33	0
64	Q7G	H	402	-	90,90,90	0.70	3 (3%)	136,138,138	1.17	10 (7%)
63	UQ9	H	401	-	35,35,58	2.48	11 (31%)	42,45,73	2.16	13 (30%)
58	PGT	AF	201	-	50,50,50	1.07	3 (6%)	53,56,56	1.06	2 (3%)
74	HEM	AE	401	52	50,50,50	1.43	6 (12%)	66,82,82	1.28	10 (15%)
66	PC7	AG	101	-	51,51,51	0.97	4 (7%)	57,59,59	1.01	2 (3%)
65	3PH	l	201	-	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
58	PGT	L	704	-	44,44,50	1.13	4 (9%)	47,50,56	1.06	2 (4%)
67	UQ5	AC	403	-	38,38,38	0.77	2 (5%)	46,49,49	0.51	0
59	SF4	I	501	9	0,12,12	-	-	-	-	-
66	PC7	BC	409	-	40,40,51	0.34	0	46,48,59	0.51	0
74	HEM	BC	401	50	50,50,50	2.01	18 (36%)	66,82,82	1.83	19 (28%)
61	FES	G	801	7	0,4,4	-	-	-	-	-
64	Q7G	a	101	-	44,44,90	0.66	0	66,68,138	1.32	9 (13%)
65	3PH	f	202	-	42,42,47	0.67	1 (2%)	46,47,52	0.64	2 (4%)
72	CDL	AC	408	-	80,80,99	0.30	0	86,92,111	0.35	0
58	PGT	L	703	-	50,50,50	0.29	0	53,56,56	0.31	0
64	Q7G	BC	411	-	44,44,90	0.76	1 (2%)	66,68,138	1.37	13 (19%)
67	UQ5	BC	403	-	38,38,38	0.48	0	46,49,49	0.62	1 (2%)
58	PGT	BC	406	-	36,36,50	0.33	0	39,42,56	0.45	0
60	PTY	d	101	-	38,38,49	0.31	0	41,43,54	0.40	0
66	PC7	d	102	-	51,51,51	0.41	0	57,59,59	0.52	0
58	PGT	y	303	-	40,40,50	1.17	4 (10%)	43,46,56	1.11	2 (4%)
60	PTY	N	501	-	39,39,49	0.30	0	42,44,54	0.35	0
72	CDL	BE	402	-	87,87,99	0.93	8 (9%)	93,99,111	1.11	4 (4%)
61	FES	E	500	5	0,4,4	-	-	-	-	-
60	PTY	D	401	-	49,49,49	0.88	4 (8%)	52,54,54	1.03	2 (3%)
60	PTY	AB	602	-	40,40,49	0.30	0	43,45,54	0.32	0
74	HEM	AC	402	50	50,50,50	1.98	14 (28%)	66,82,82	1.71	11 (16%)
60	PTY	BB	602	-	28,28,49	0.36	0	31,33,54	0.52	0
59	SF4	G	803	7	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	3PH	BC	405	-	43,43,47	0.65	1 (2%)	47,48,52	0.62	1 (2%)
72	CDL	u	101	-	99,99,99	0.88	7 (7%)	105,111,111	1.07	5 (4%)
60	PTY	M	504	-	49,49,49	0.29	0	52,54,54	0.40	0
66	PC7	AC	410	-	50,50,51	0.35	0	56,58,59	0.47	0
65	3PH	f	201	-	40,40,47	0.67	1 (2%)	44,45,52	0.73	2 (4%)
60	PTY	N	502	-	44,44,49	0.29	0	47,49,54	0.41	0
66	PC7	f	203	-	47,47,51	0.28	0	53,55,59	0.31	0
58	PGT	AC	407	-	50,50,50	1.09	3 (6%)	53,56,56	1.04	2 (3%)
64	Q7G	M	505	-	44,44,90	0.85	1 (2%)	66,68,138	1.75	17 (25%)
59	SF4	F	501	6	0,12,12	-	-	-	-	-
65	3PH	AI	101	-	31,31,47	0.76	1 (3%)	35,36,52	0.76	2 (5%)
66	PC7	AB	603	-	33,33,51	0.38	0	39,41,59	0.43	0
71	8Q1	T	200	-	31,34,34	0.38	0	40,43,43	1.14	3 (7%)
58	PGT	A	201	-	50,50,50	1.08	4 (8%)	53,56,56	1.08	3 (5%)
65	3PH	BJ	101	-	40,40,47	0.68	1 (2%)	44,45,52	0.65	1 (2%)
66	PC7	v	201	-	51,51,51	0.97	4 (7%)	57,59,59	1.13	3 (5%)
65	3PH	AC	405	-	32,32,47	0.33	0	36,37,52	0.41	0
59	SF4	G	802	7	0,12,12	-	-	-	-	-
71	8Q1	W	200	-	31,34,34	0.32	0	40,43,43	0.46	0
74	HEM	BC	402	50	50,50,50	2.08	13 (26%)	66,82,82	1.80	16 (24%)
65	3PH	BJ	102	-	47,47,47	0.63	1 (2%)	51,52,52	0.59	1 (1%)
67	UQ5	AC	404	-	38,38,38	0.45	0	46,49,49	0.82	1 (2%)
58	PGT	M	502	-	28,28,50	0.34	0	31,34,56	0.38	0
64	Q7G	BC	410	-	44,44,90	0.75	1 (2%)	66,68,138	1.44	10 (15%)
72	CDL	BC	408	-	76,76,99	0.31	0	82,88,111	0.33	0
66	PC7	BD	302	-	38,38,51	0.34	0	44,46,59	0.46	0
73	COO	y	302	-	48,55,55	4.11	15 (31%)	68,81,81	4.17	21 (30%)
72	CDL	u	102	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
61	FES	BD	301	51	0,4,4	-	-	-	-	-

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
69	NDP	P	500	-	-	7/34/77/77	0/5/5/5
72	CDL	BG	101	-	-	38/80/80/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PTY	N	503	-	-	17/53/53/53	-
59	SF4	B	500	2	-	-	0/6/5/5
65	3PH	M	501	-	-	19/42/42/49	-
67	UQ5	L	707	-	-	16/33/57/57	0/1/1/1
66	PC7	L	706	-	-	17/43/43/55	-
60	PTY	m	101	-	-	17/53/53/53	-
72	CDL	BC	407	-	-	47/91/91/110	-
61	FES	AD	301	51	-	-	0/1/1/1
64	Q7G	K	201	-	-	6/32/200/200	0/10/10/10
60	PTY	Y	202	-	-	6/34/34/53	-
74	HEM	AC	401	50	-	2/14/54/54	-
58	PGT	L	702	-	-	20/40/40/55	-
72	CDL	AE	402	-	-	41/95/95/110	-
74	HEM	BE	401	52	-	4/14/54/54	-
65	3PH	Y	201	-	-	18/34/34/49	-
60	PTY	M	503	-	-	22/40/40/53	-
60	PTY	L	705	-	-	20/45/45/53	-
72	CDL	AC	409	-	-	52/95/95/110	-
60	PTY	BF	201	-	-	18/43/43/53	-
65	3PH	L	701	-	-	14/38/38/49	-
73	COO	y	302	-	1/1/12/16	11/54/70/70	0/3/3/3
60	PTY	z	301	-	-	27/53/53/53	-
62	FMN	F	500	-	-	2/18/18/18	0/3/3/3
59	SF4	I	500	9	-	-	0/6/5/5
58	PGT	AC	406	-	-	20/45/45/55	-
64	Q7G	H	402	-	-	12/32/200/200	0/10/10/10
63	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
58	PGT	AF	201	-	-	37/55/55/55	-
61	FES	BD	301	51	-	-	0/1/1/1
74	HEM	AE	401	52	-	2/14/54/54	-
66	PC7	AG	101	-	-	20/55/55/55	-
65	3PH	l	201	-	-	11/38/38/49	-
58	PGT	L	704	-	-	29/49/49/55	-
67	UQ5	AC	403	-	-	16/33/57/57	0/1/1/1
66	PC7	BC	409	-	-	25/44/44/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	I	501	9	-	-	0/6/5/5
74	HEM	BC	401	50	-	2/14/54/54	-
61	FES	G	801	7	-	-	0/1/1/1
64	Q7G	a	101	-	-	4/12/100/200	0/6/6/10
65	3PH	f	202	-	-	18/44/44/49	-
72	CDL	AC	408	-	-	50/91/91/110	-
58	PGT	L	703	-	-	13/55/55/55	-
64	Q7G	BC	411	-	-	4/12/100/200	0/6/6/10
67	UQ5	BC	403	-	-	9/33/57/57	0/1/1/1
58	PGT	BC	406	-	-	26/41/41/55	-
60	PTY	d	101	-	-	25/42/42/53	-
66	PC7	d	102	-	-	27/55/55/55	-
58	PGT	y	303	-	-	28/45/45/55	-
60	PTY	N	501	-	-	13/43/43/53	-
72	CDL	BE	402	-	-	35/98/98/110	-
61	FES	E	500	5	-	-	0/1/1/1
60	PTY	D	401	-	-	19/53/53/53	-
60	PTY	AB	602	-	-	24/44/44/53	-
74	HEM	AC	402	50	-	6/14/54/54	-
60	PTY	BB	602	-	-	16/32/32/53	-
59	SF4	G	803	7	-	-	0/6/5/5
65	3PH	BC	405	-	-	20/45/45/49	-
72	CDL	u	101	-	-	49/110/110/110	-
66	PC7	AC	410	-	-	20/54/54/55	-
65	3PH	f	201	-	-	14/42/42/49	-
60	PTY	N	502	-	-	29/48/48/53	-
66	PC7	f	203	-	-	25/51/51/55	-
58	PGT	AC	407	-	-	22/55/55/55	-
64	Q7G	M	505	-	-	6/12/100/200	0/6/6/10
59	SF4	F	501	6	-	-	0/6/5/5
65	3PH	AI	101	-	-	15/33/33/49	-
66	PC7	AB	603	-	-	18/37/37/55	-
71	8Q1	T	200	-	-	24/41/41/41	-
58	PGT	A	201	-	-	26/55/55/55	-
65	3PH	BJ	101	-	-	14/42/42/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	PC7	v	201	-	-	25/55/55/55	-
65	3PH	AC	405	-	-	23/34/34/49	-
59	SF4	G	802	7	-	-	0/6/5/5
71	8Q1	W	200	-	-	11/41/41/41	-
74	HEM	BC	402	50	-	4/14/54/54	-
65	3PH	BJ	102	-	-	13/49/49/49	-
67	UQ5	AC	404	-	-	13/33/57/57	0/1/1/1
58	PGT	M	502	-	-	18/33/33/55	-
64	Q7G	BC	410	-	-	6/12/100/200	0/6/6/10
72	CDL	BC	408	-	-	36/87/87/110	-
66	PC7	BD	302	-	-	18/42/42/55	-
75	UQ7	BC	404	-	-	19/45/69/69	0/1/1/1
72	CDL	u	102	-	-	44/110/110/110	-
60	PTY	M	504	-	-	34/53/53/53	-

The worst 5 of 197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	y	302	COO	C2A-N1A	-15.18	1.05	1.33
73	y	302	COO	C5A-C4A	12.62	1.62	1.39
63	H	401	UQ9	C6-C1	9.79	1.53	1.35
73	y	302	COO	C2A-N3A	-8.54	1.18	1.33
73	y	302	COO	C6A-N1A	-7.68	1.13	1.35

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	y	302	COO	C5A-C4A-N3A	-15.13	107.00	126.75
73	y	302	COO	C6A-C5A-N7A	14.40	158.86	132.02
73	y	302	COO	C4A-C5A-N7A	-12.97	94.83	110.62
73	y	302	COO	C4A-N9A-C8A	-10.36	94.50	105.73
73	y	302	COO	C6A-C5A-C4A	-8.09	106.30	117.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
73	y	302	COO	C13

5 of 1487 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	A	201	PGT	C32-C31-O2-C2
58	A	201	PGT	O4P-C4-C5-O5
58	L	702	PGT	C32-C31-O2-C2
58	L	702	PGT	O31-C31-O2-C2
58	L	704	PGT	C32-C31-O2-C2

There are no ring outliers.

68 monomers are involved in 299 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	BG	101	CDL	6	0
60	N	503	PTY	1	0
59	B	500	SF4	1	0
75	BC	404	UQ7	11	0
65	M	501	3PH	15	0
67	L	707	UQ5	7	0
66	L	706	PC7	6	0
72	BC	407	CDL	3	0
64	K	201	Q7G	1	0
74	AC	401	HEM	2	0
72	AE	402	CDL	4	0
74	BE	401	HEM	6	0
65	Y	201	3PH	2	0
60	M	503	PTY	2	0
60	L	705	PTY	2	0
72	AC	409	CDL	7	0
60	BF	201	PTY	16	0
65	L	701	3PH	4	0
60	z	301	PTY	12	0
59	I	500	SF4	2	0
58	AC	406	PGT	4	0
64	H	402	Q7G	3	0
63	H	401	UQ9	6	0
58	AF	201	PGT	9	0
74	AE	401	HEM	4	0
66	AG	101	PC7	6	0
58	L	704	PGT	5	0
67	AC	403	UQ5	4	0
66	BC	409	PC7	3	0
61	G	801	FES	1	0
65	f	202	3PH	3	0
72	AC	408	CDL	8	0
58	L	703	PGT	2	0

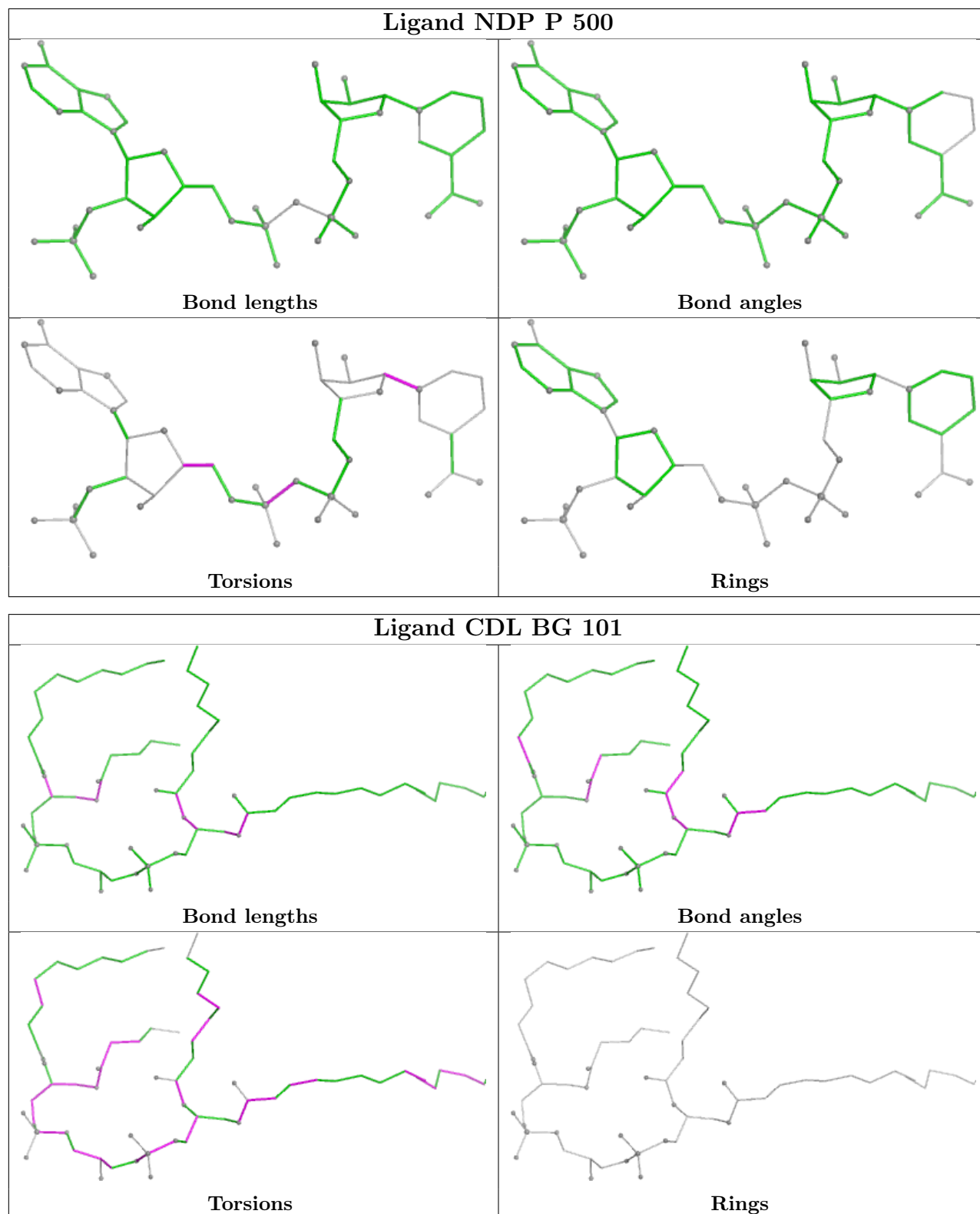
Continued on next page...

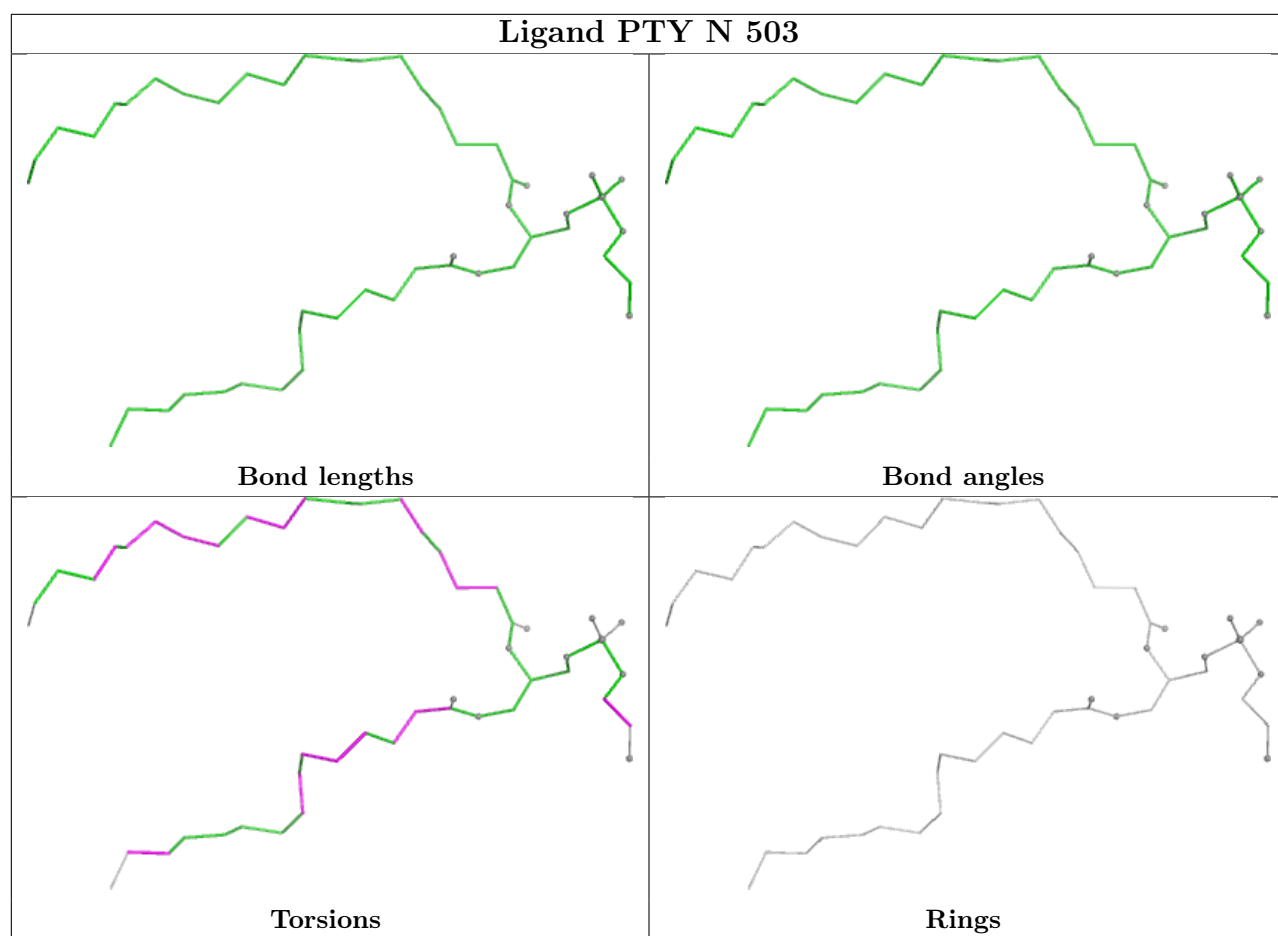
Continued from previous page...

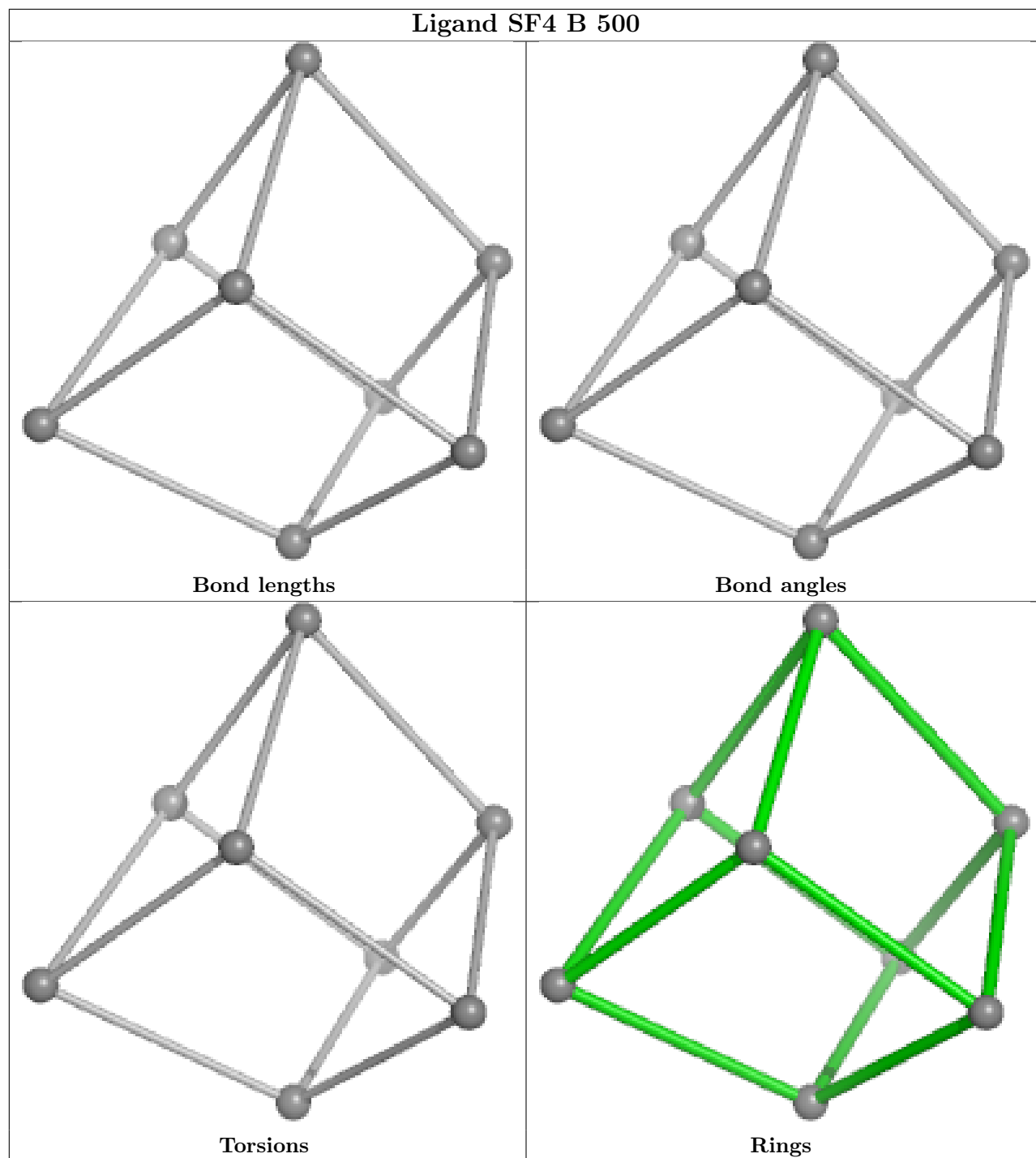
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	BC	403	UQ5	8	0
58	BC	406	PGT	2	0
60	d	101	PTY	3	0
66	d	102	PC7	8	0
58	y	303	PGT	8	0
60	N	501	PTY	6	0
72	BE	402	CDL	6	0
61	E	500	FES	1	0
60	D	401	PTY	13	0
74	AC	402	HEM	1	0
60	BB	602	PTY	1	0
65	BC	405	3PH	6	0
72	u	101	CDL	12	0
60	M	504	PTY	2	0
66	AC	410	PC7	3	0
65	f	201	3PH	2	0
60	N	502	PTY	2	0
66	f	203	PC7	1	0
58	AC	407	PGT	4	0
59	F	501	SF4	1	0
65	AI	101	3PH	3	0
66	AB	603	PC7	1	0
58	A	201	PGT	7	0
65	BJ	101	3PH	2	0
66	v	201	PC7	7	0
65	AC	405	3PH	2	0
74	BC	402	HEM	1	0
65	BJ	102	3PH	1	0
67	AC	404	UQ5	6	0
58	M	502	PGT	1	0
72	BC	408	CDL	6	0
66	BD	302	PC7	3	0
73	y	302	COO	5	0
72	u	102	CDL	13	0
61	BD	301	FES	1	0

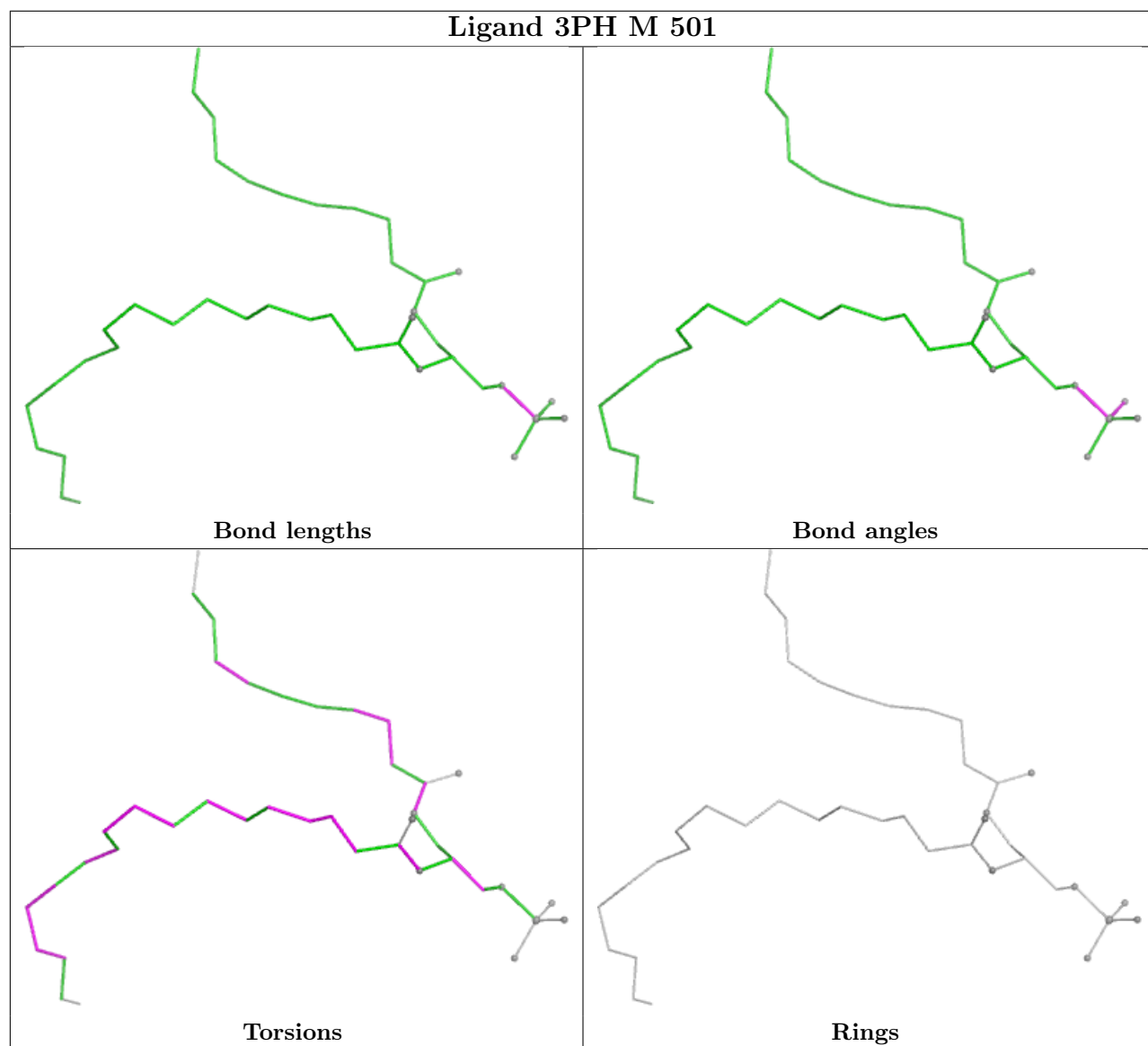
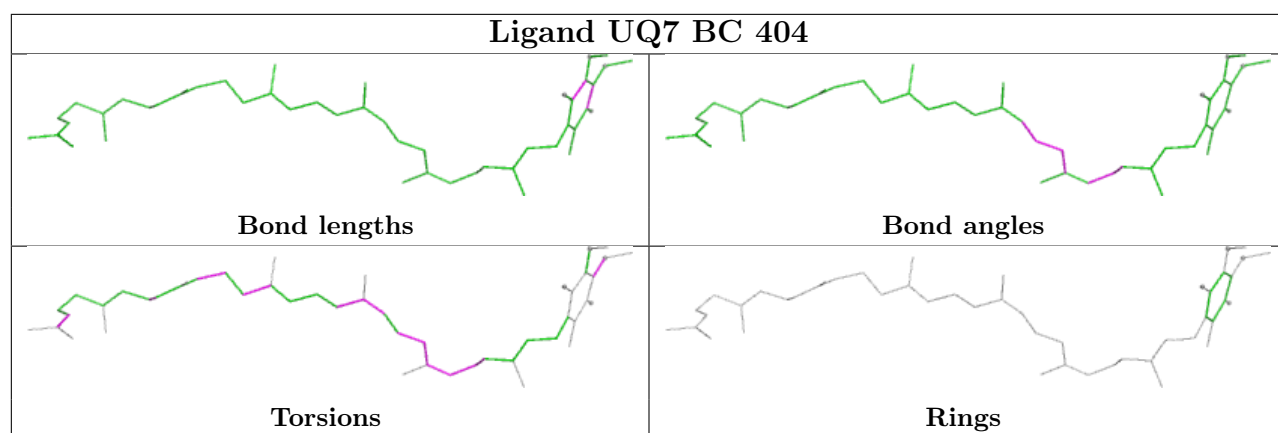
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

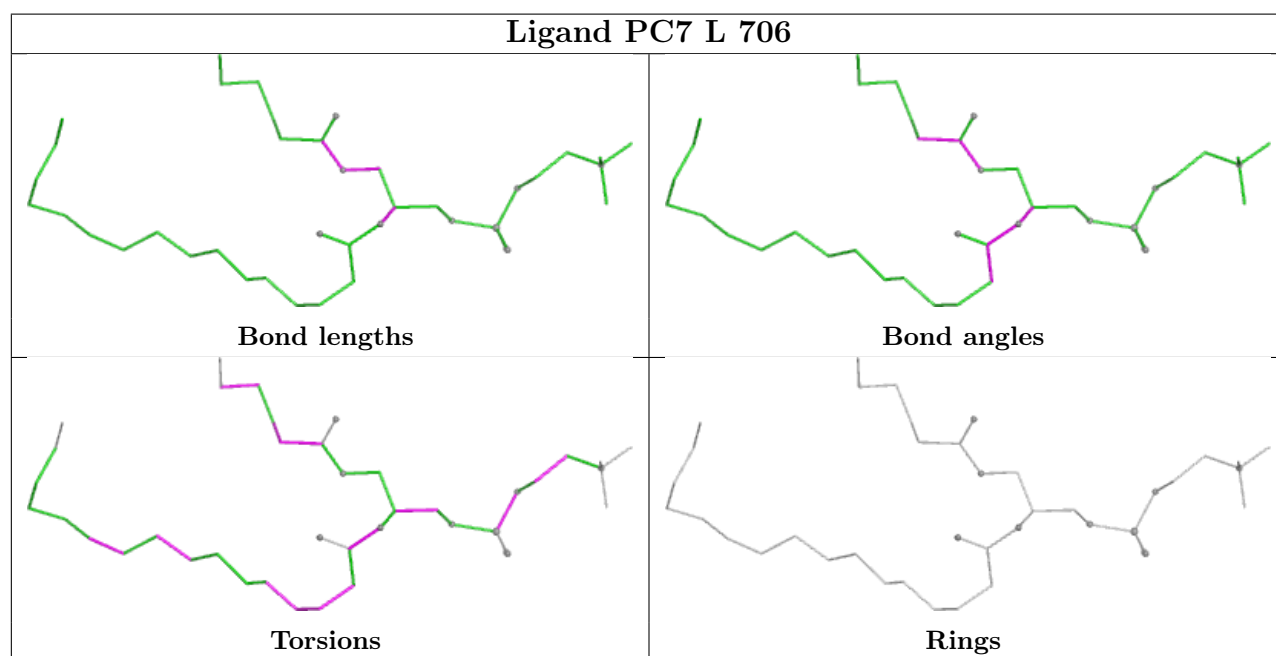
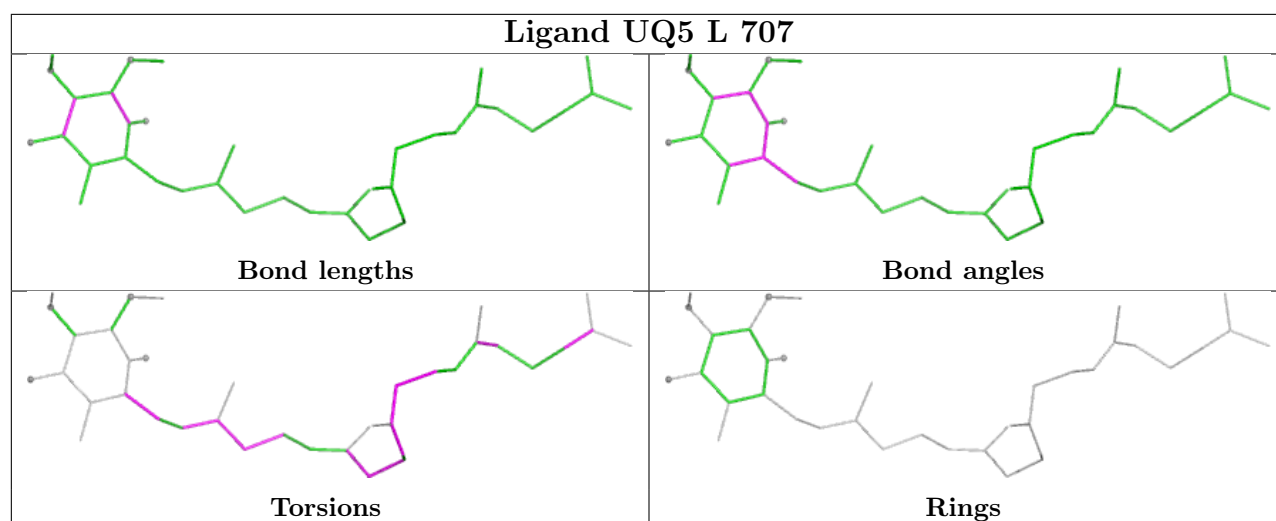
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

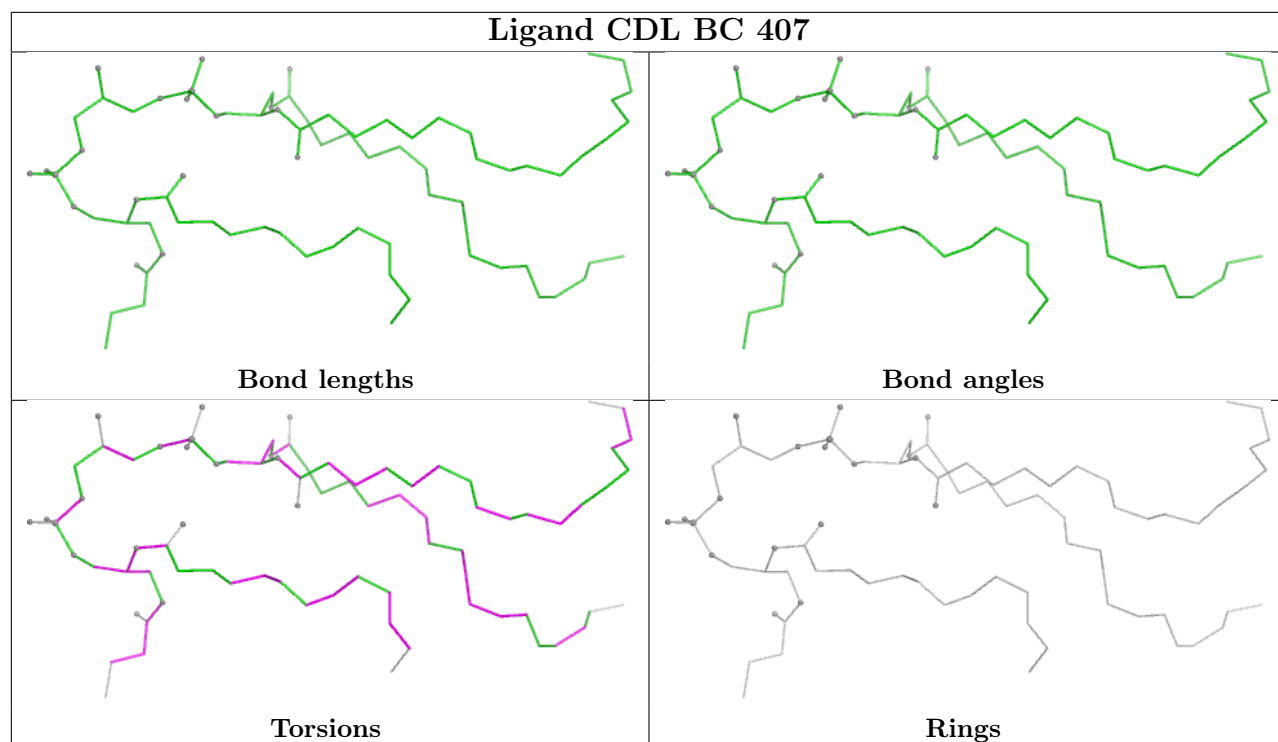
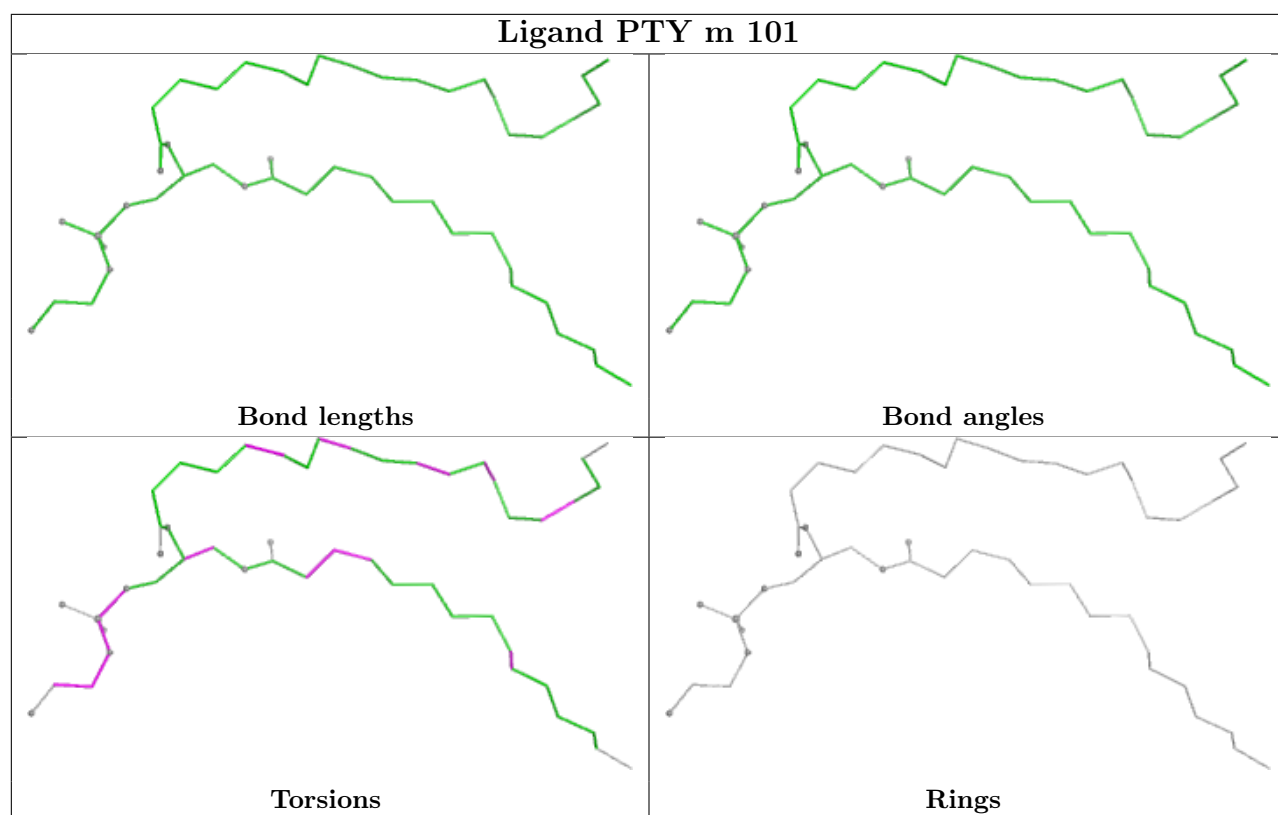


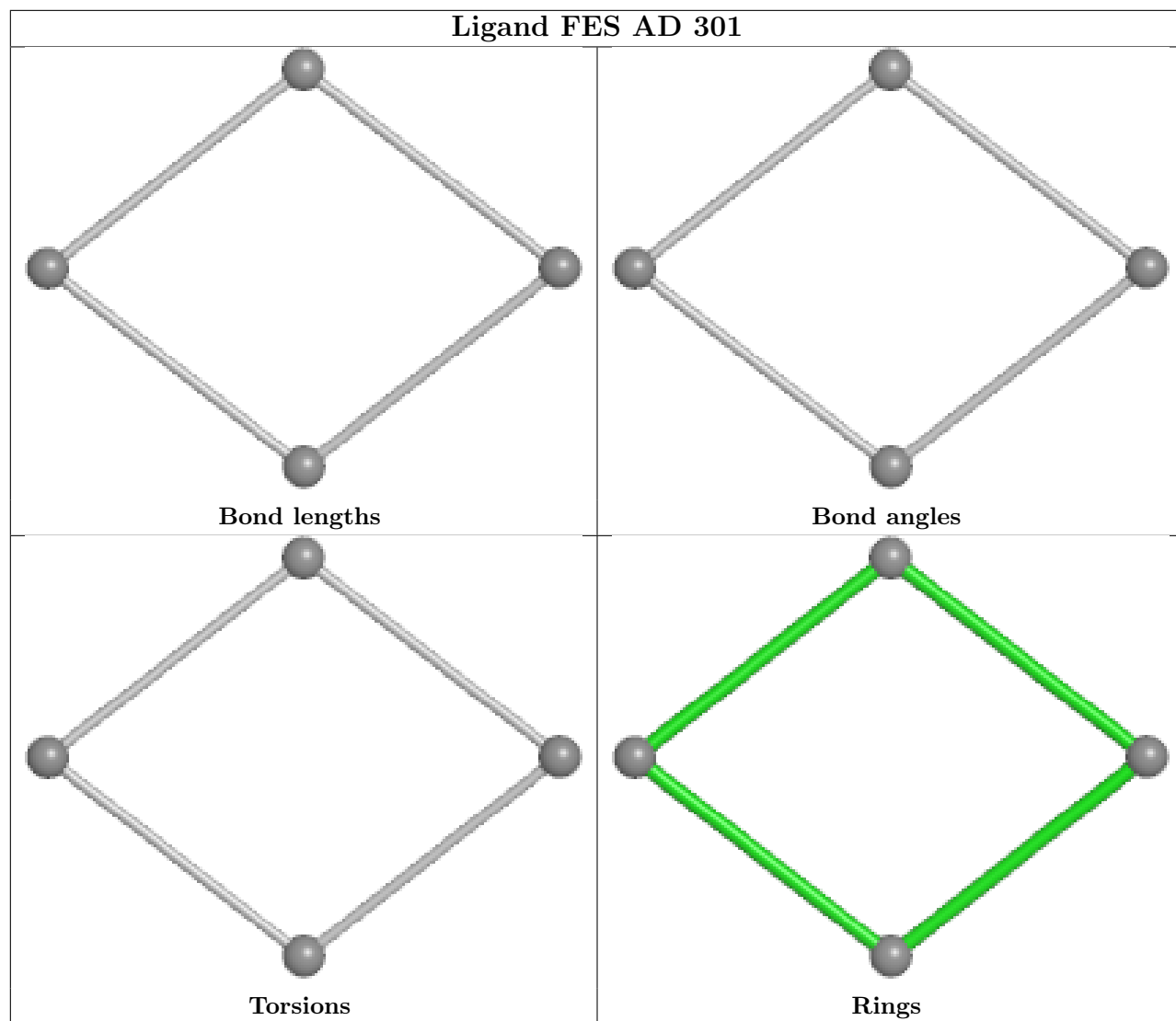


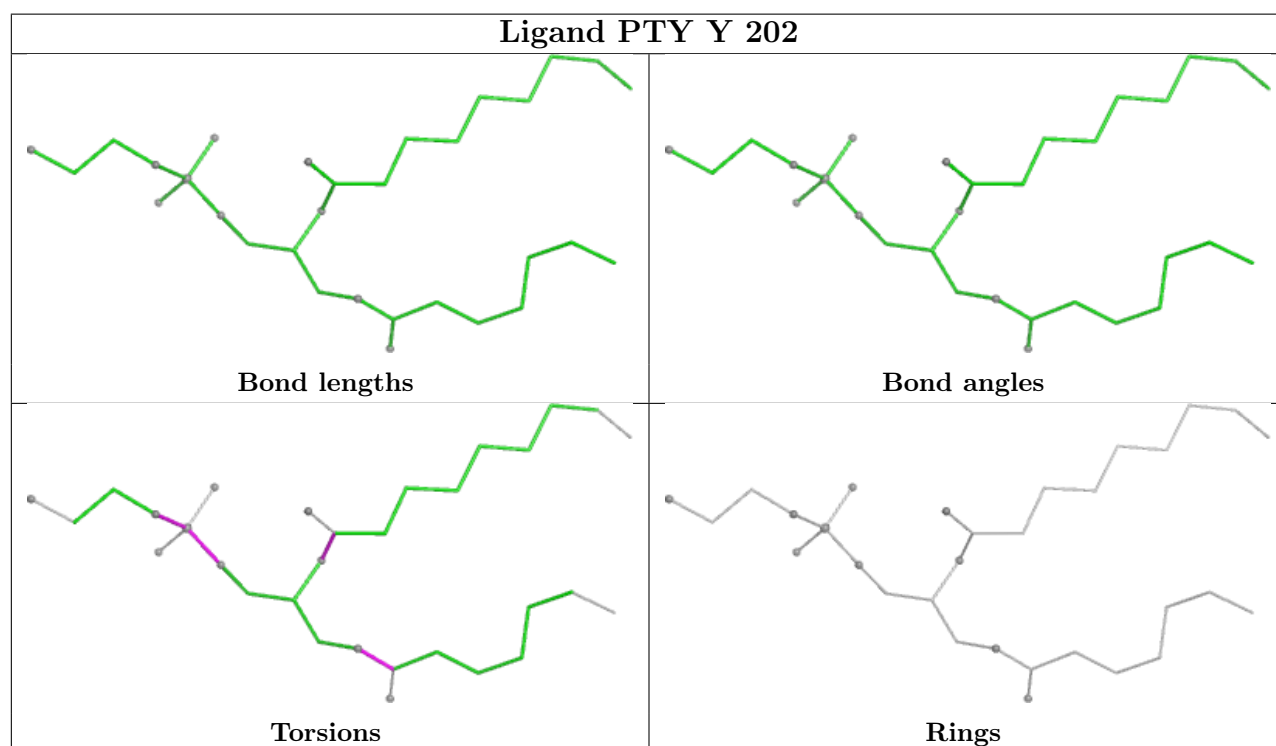
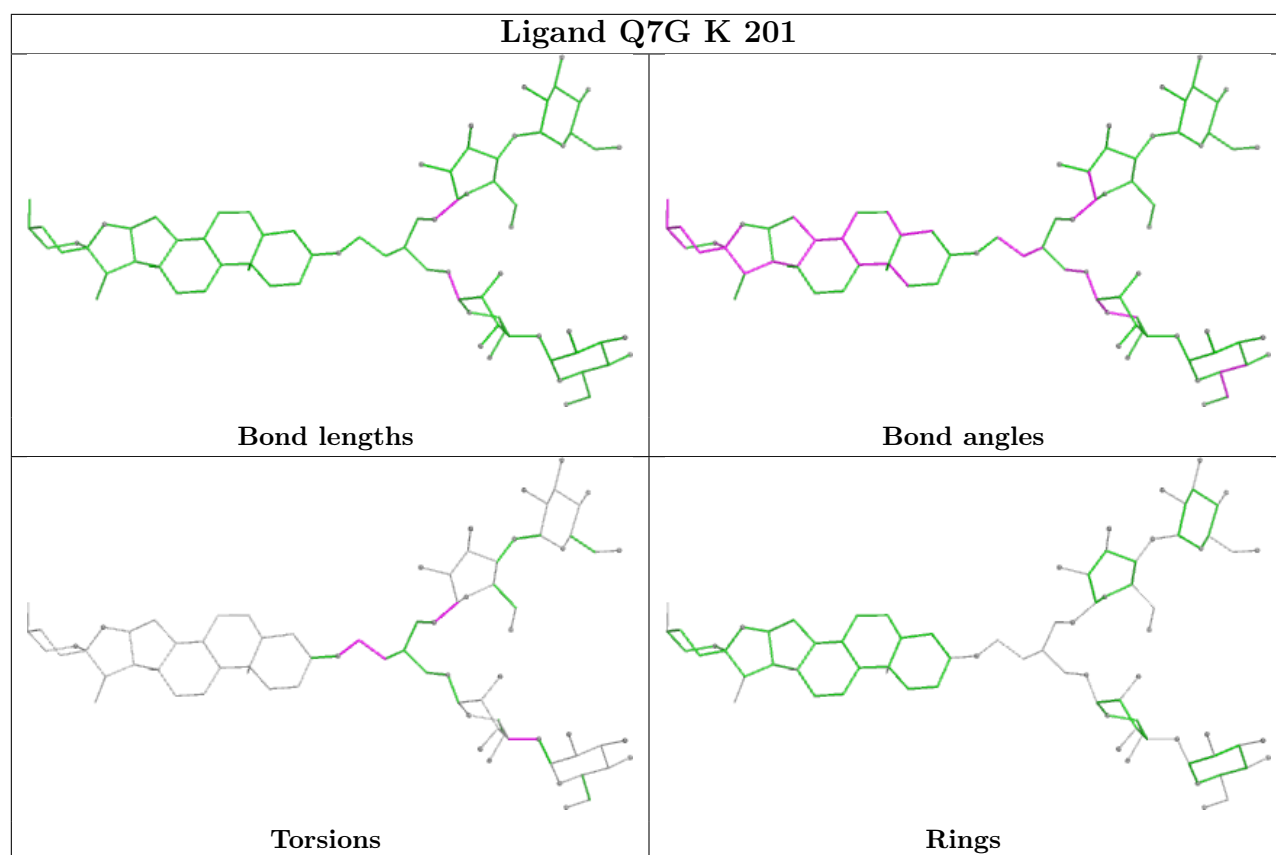




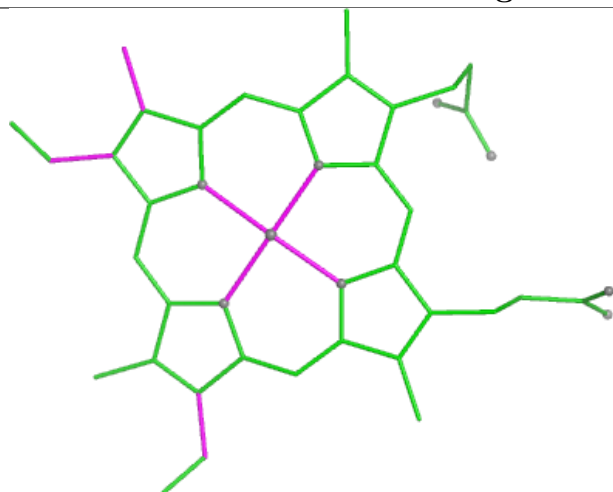




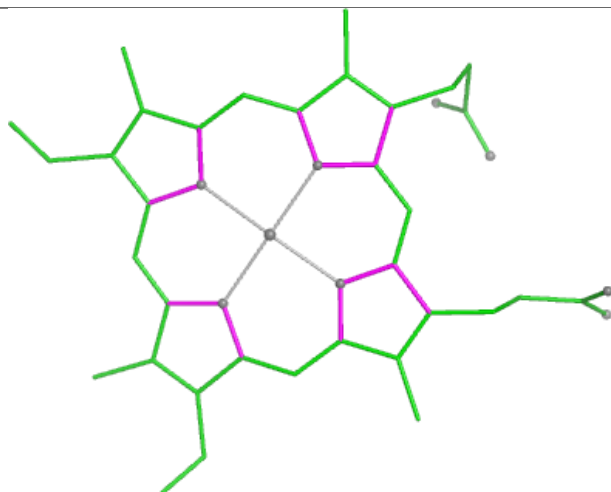




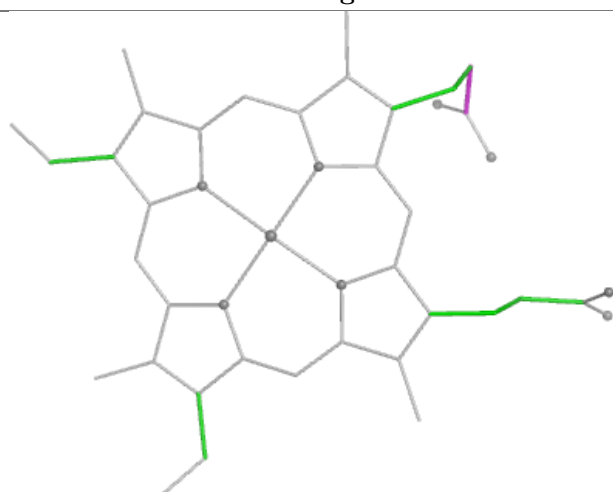
Ligand HEM AC 401



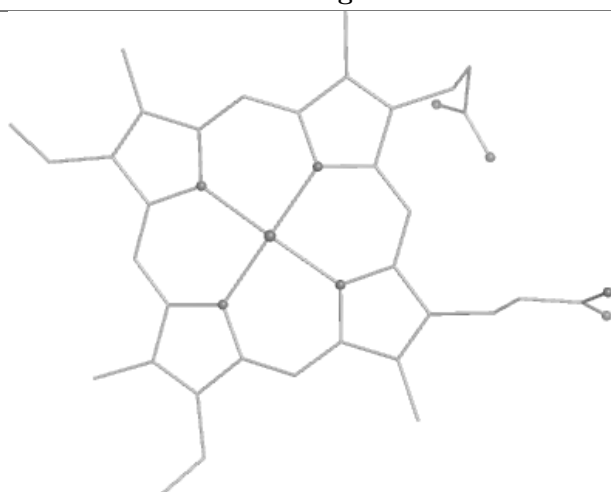
Bond lengths



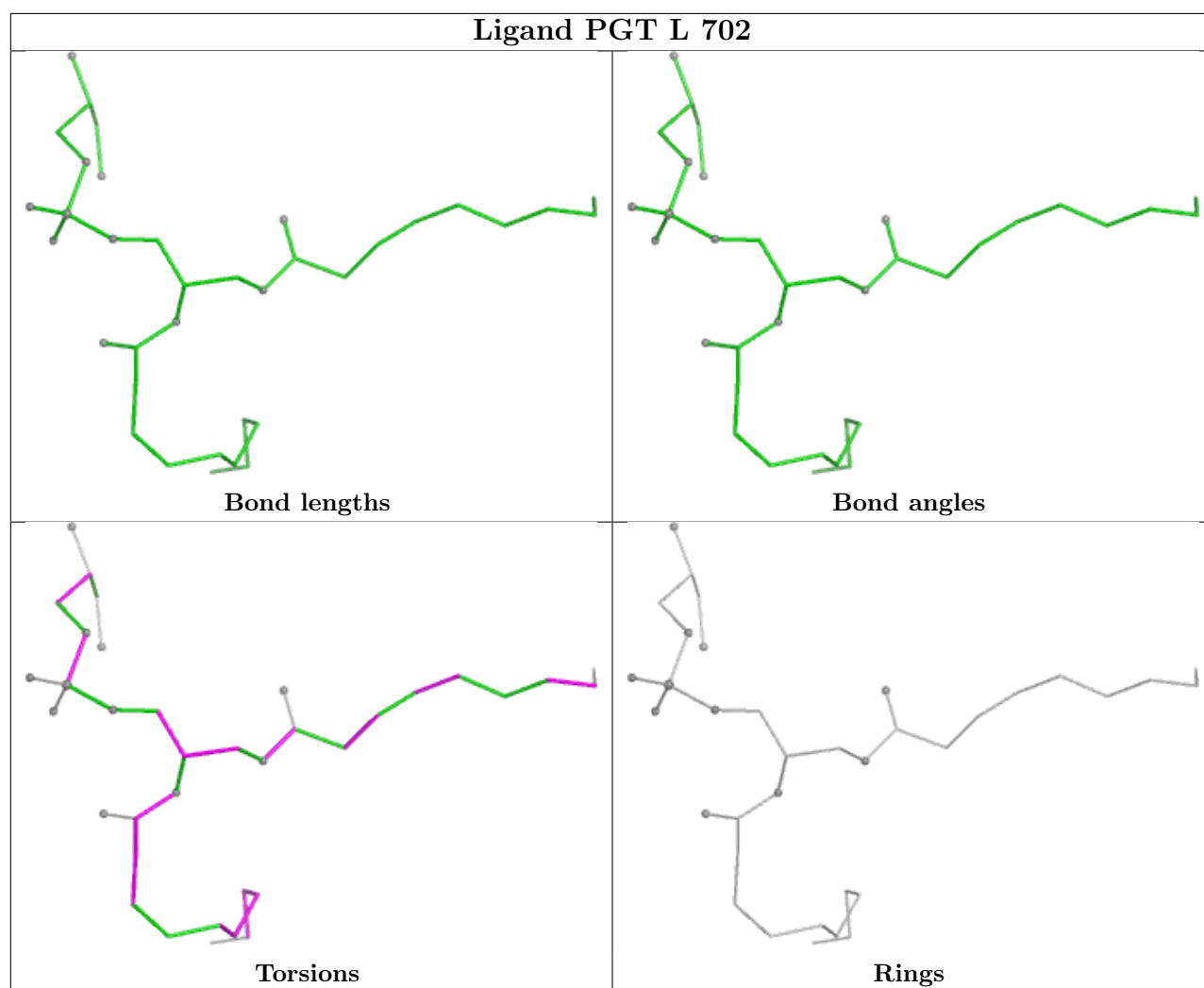
Bond angles

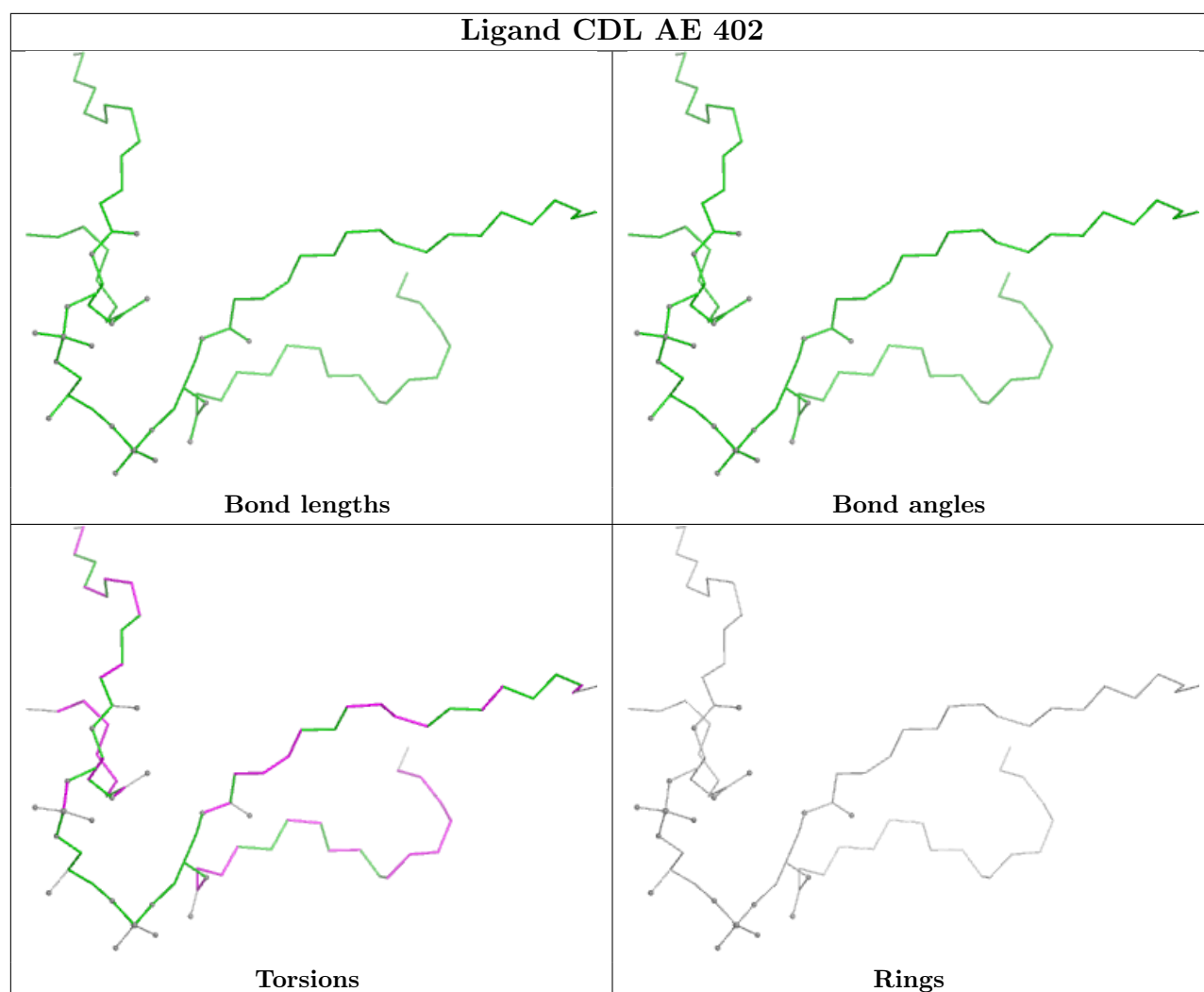


Torsions

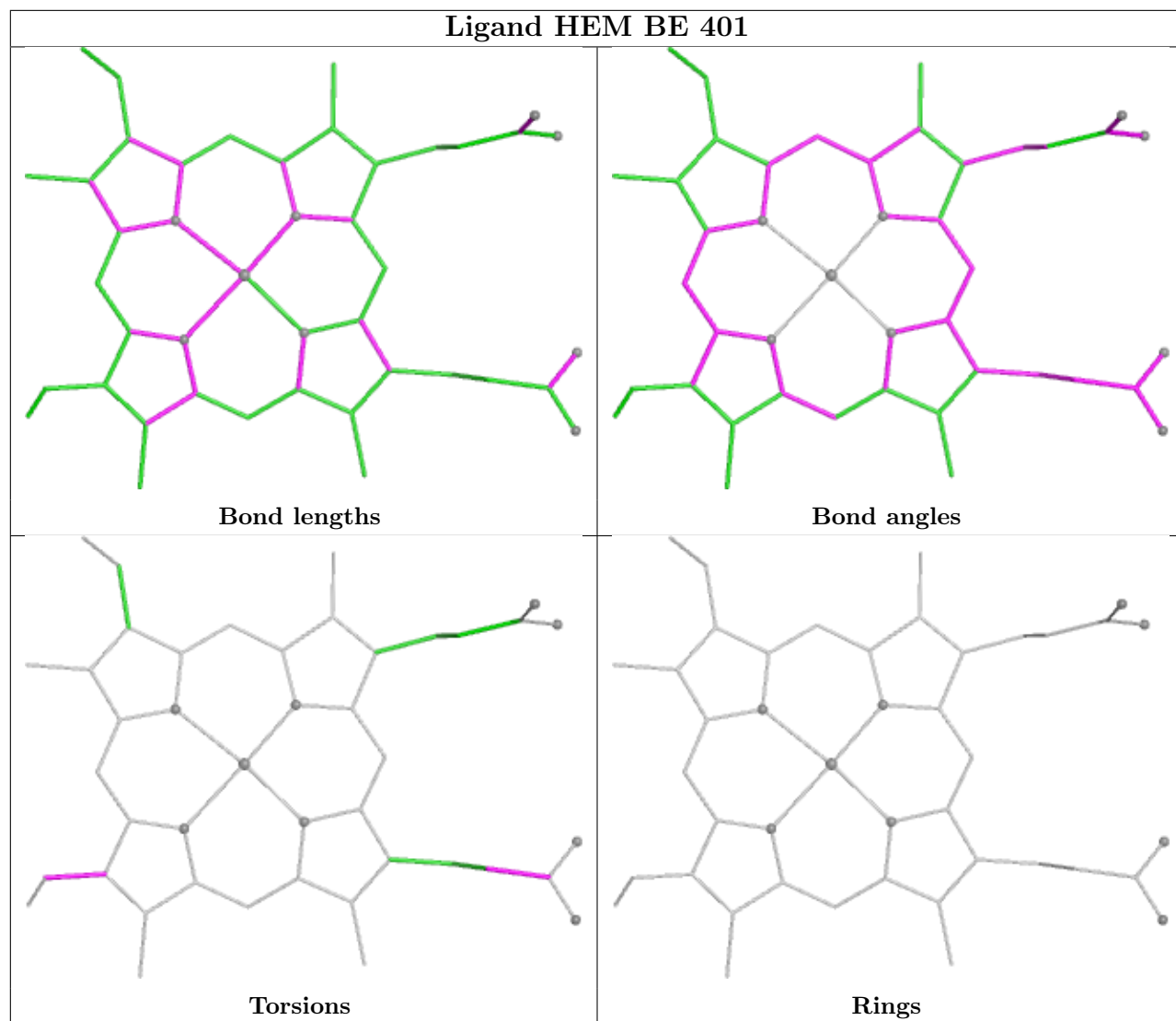


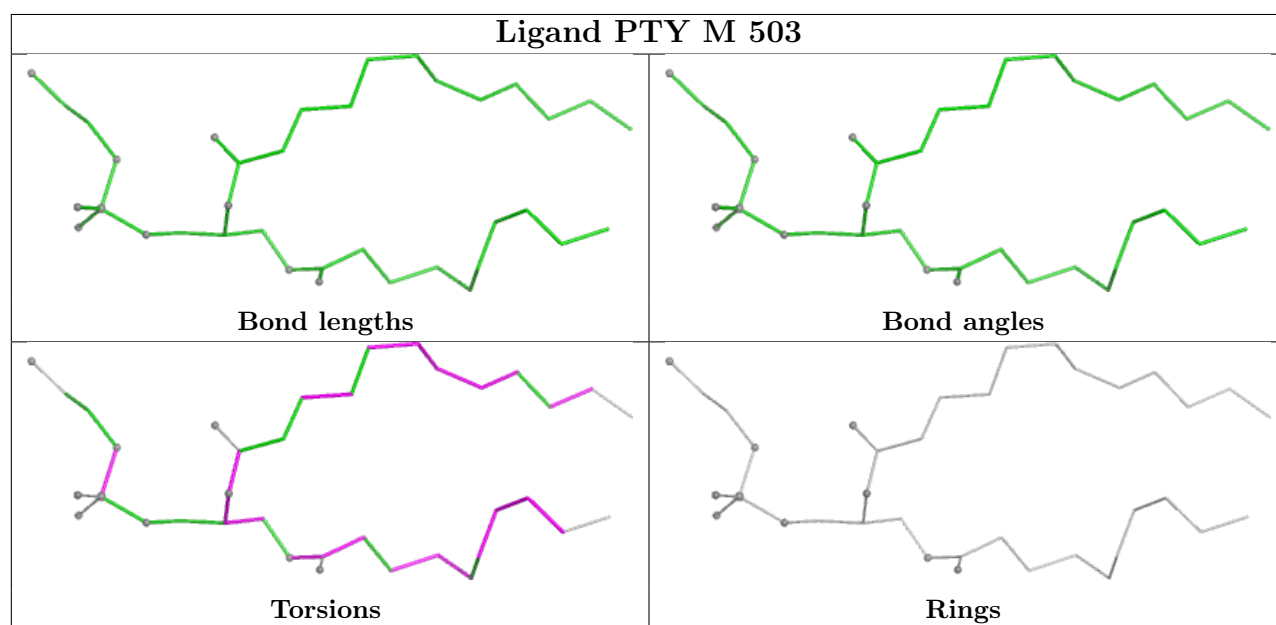
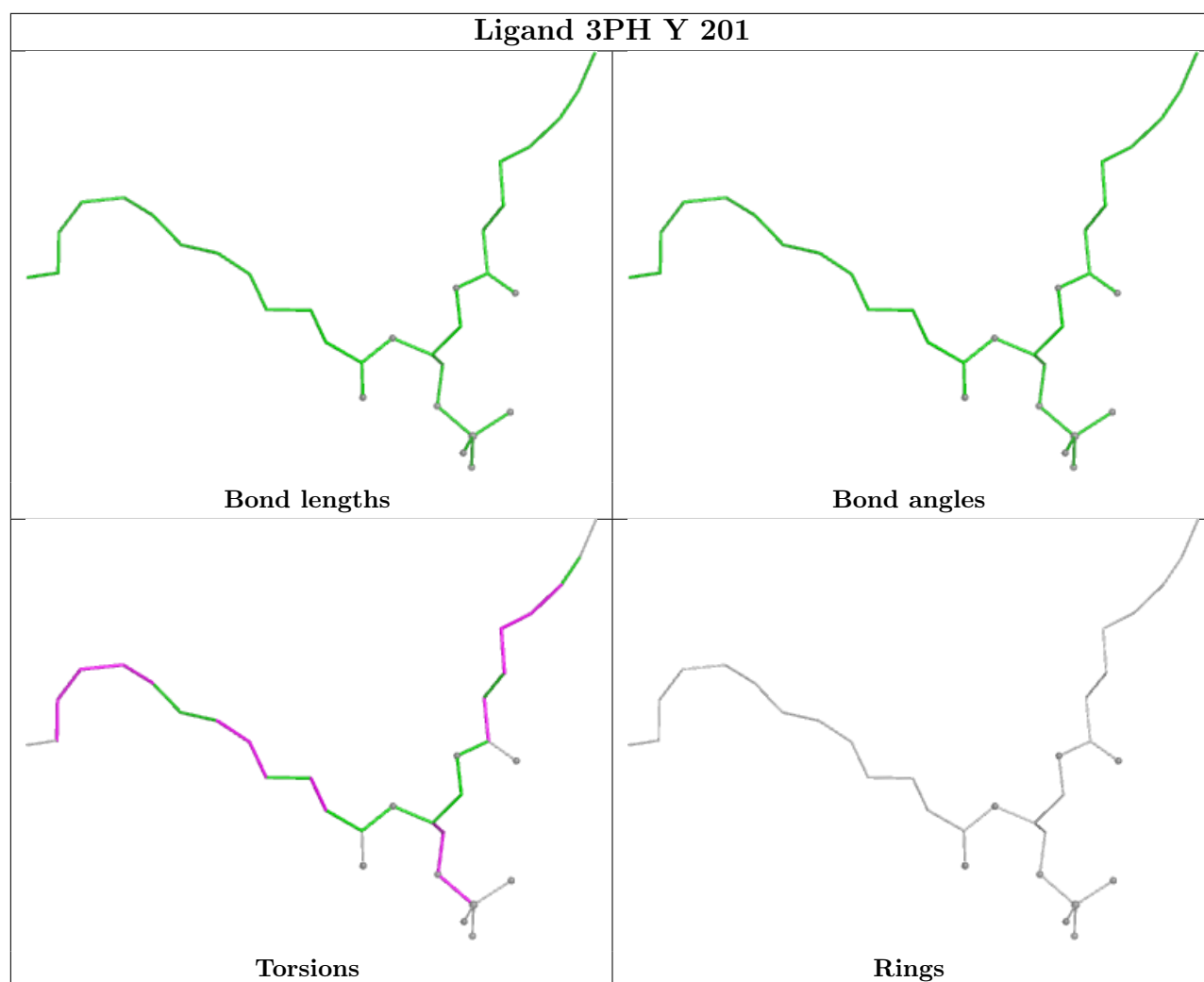
Rings

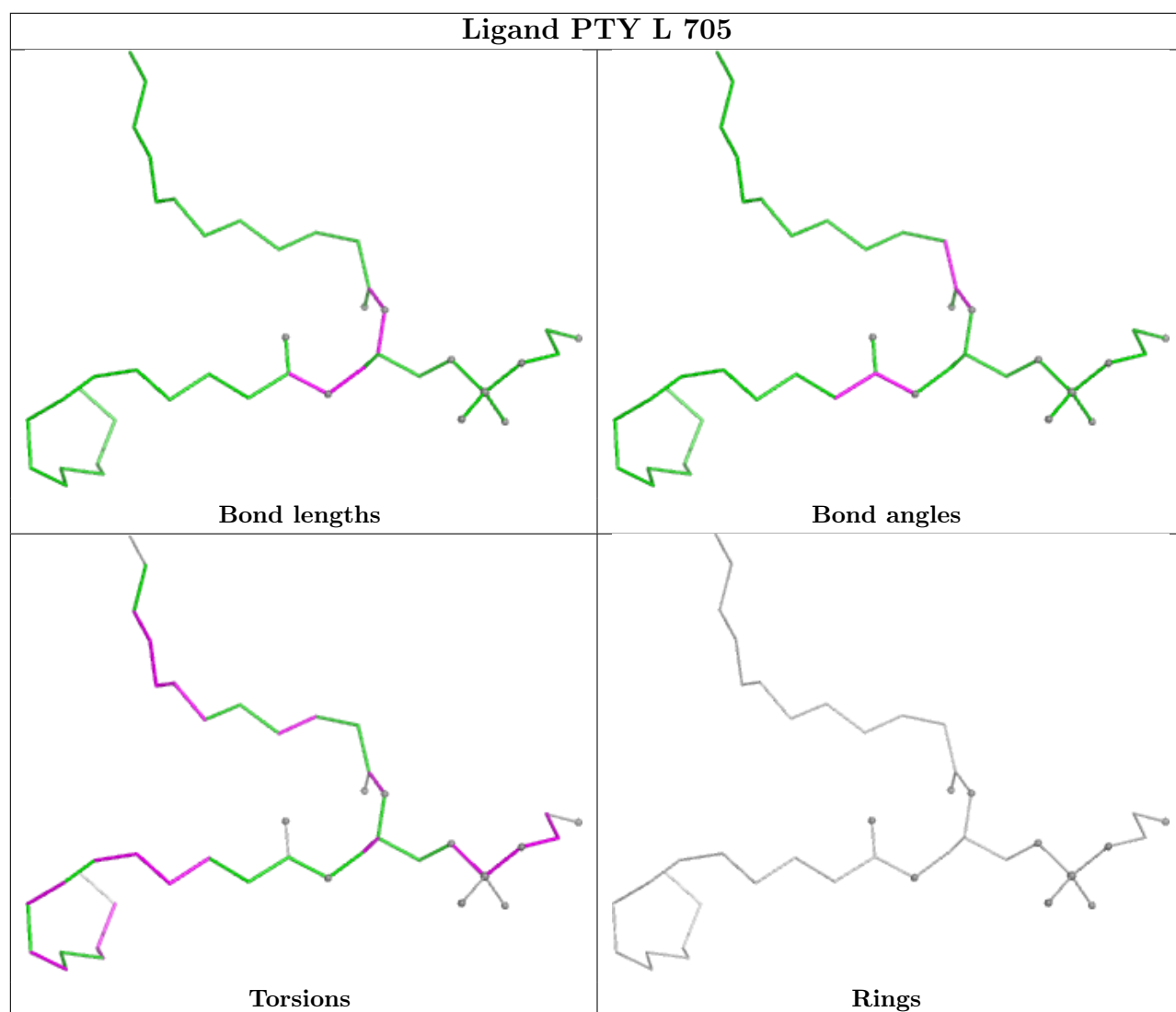


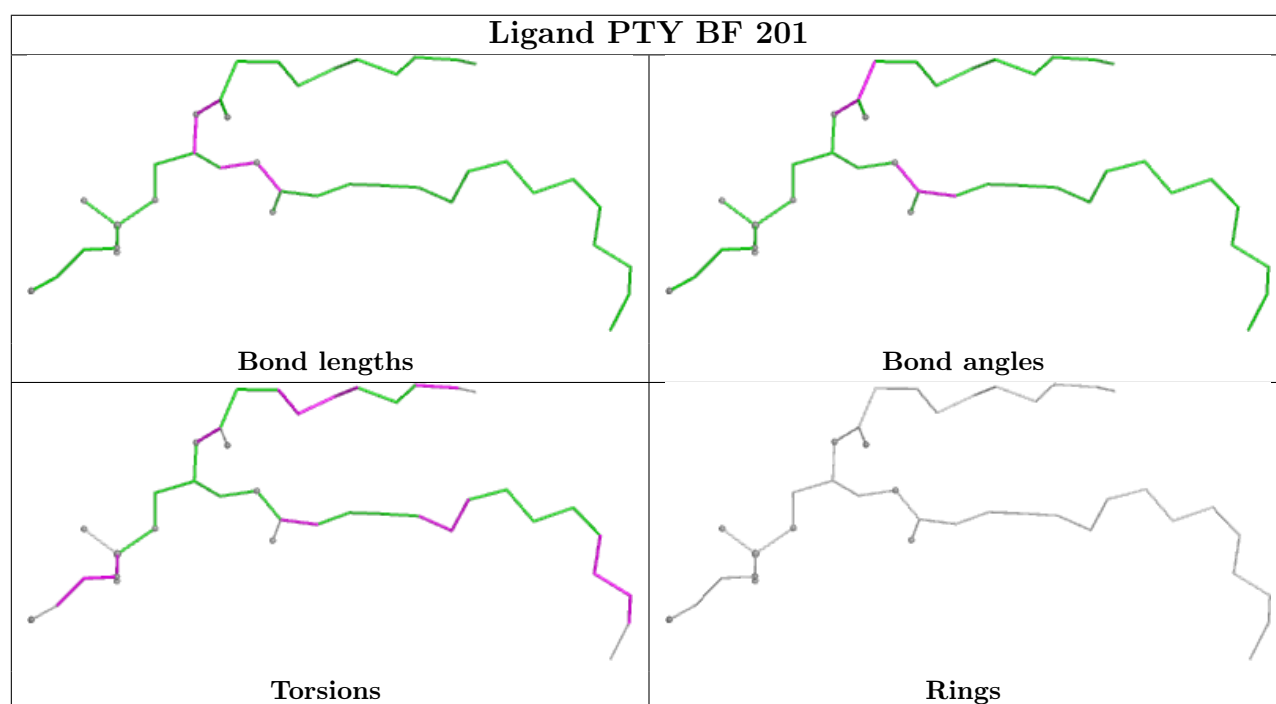
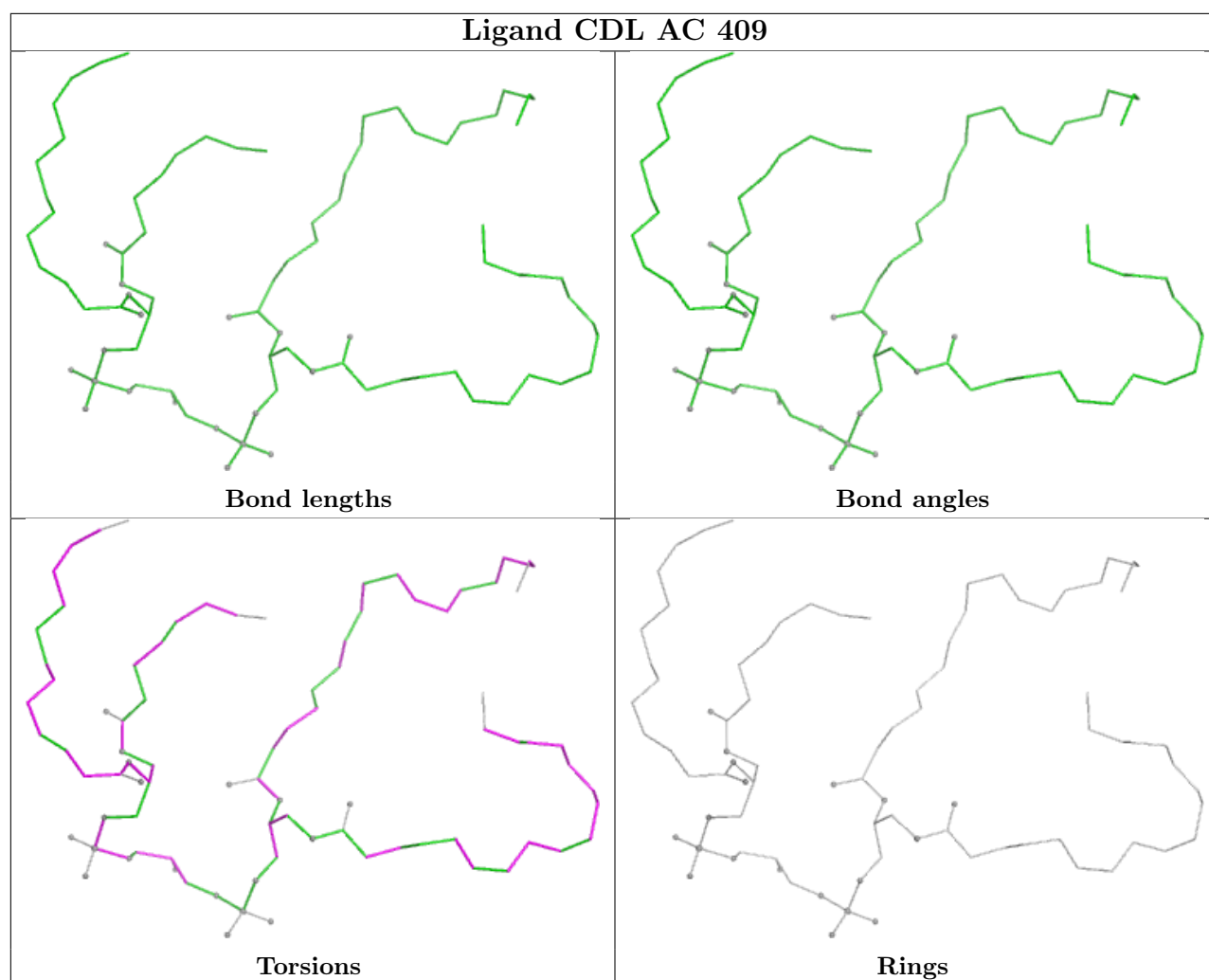


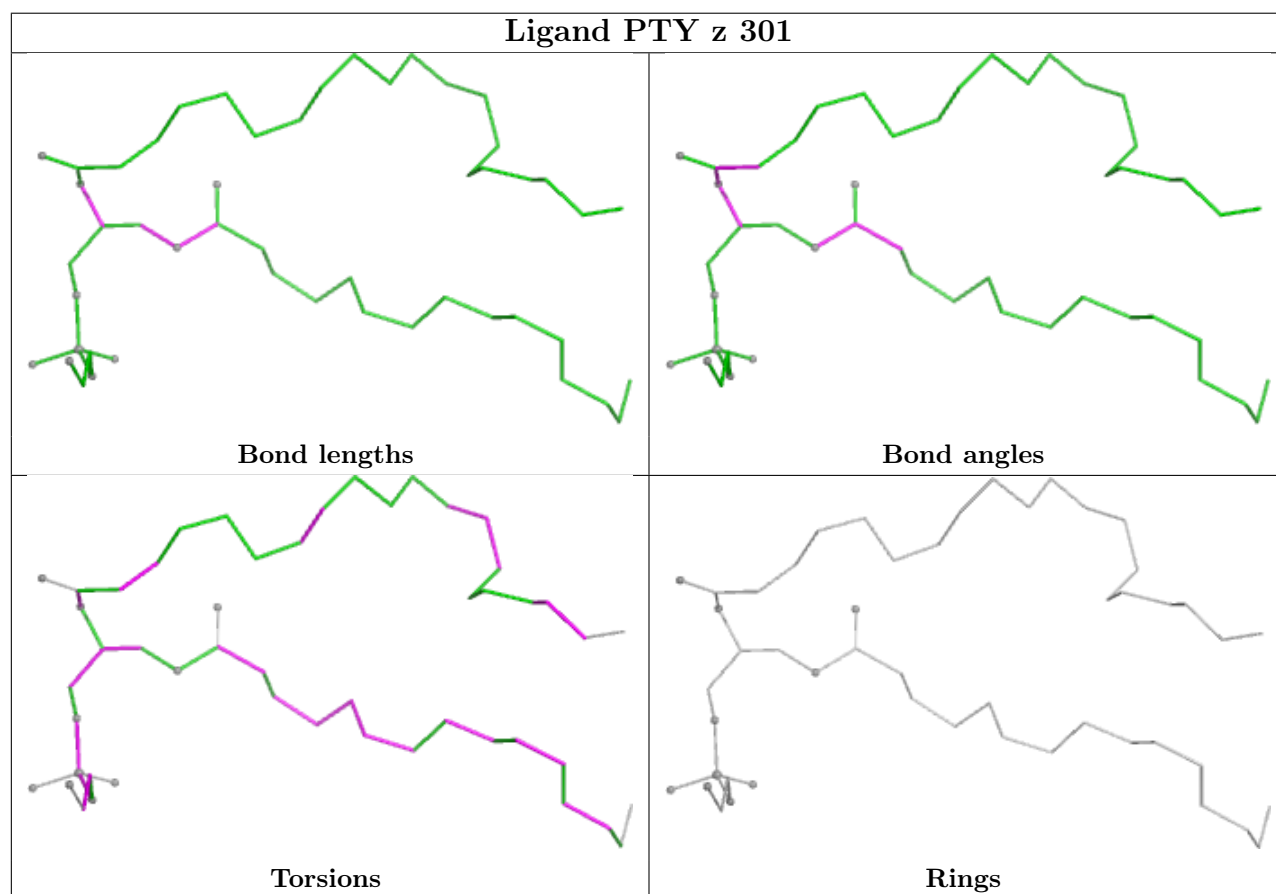
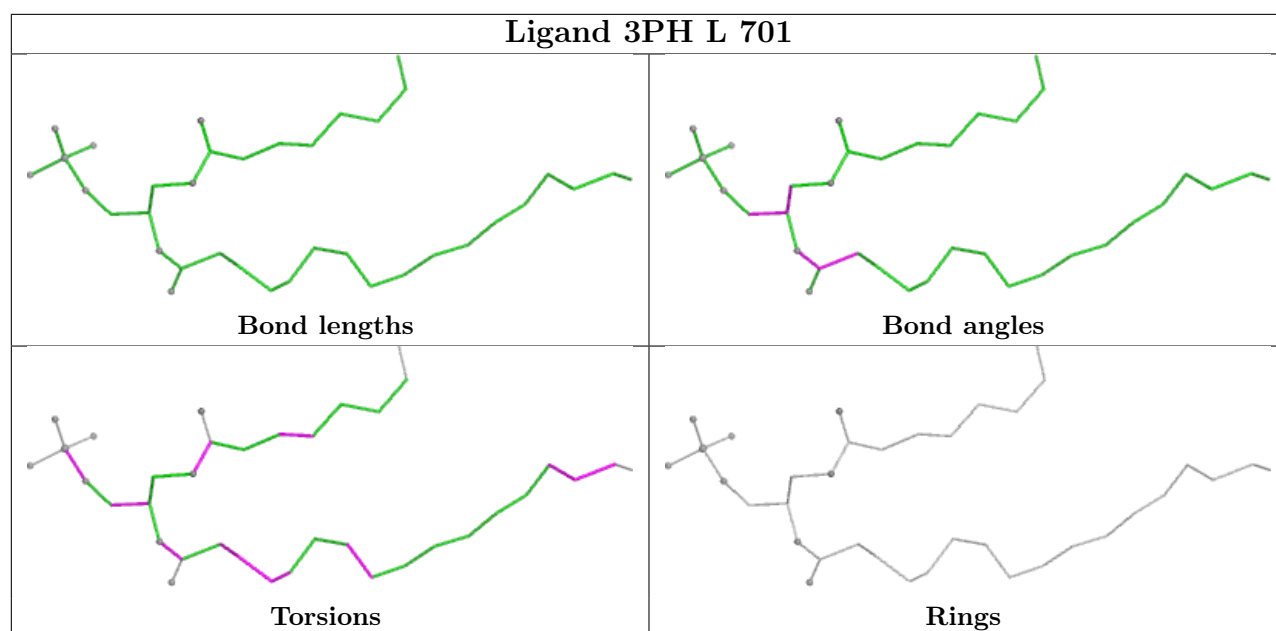
Ligand HEM BE 401

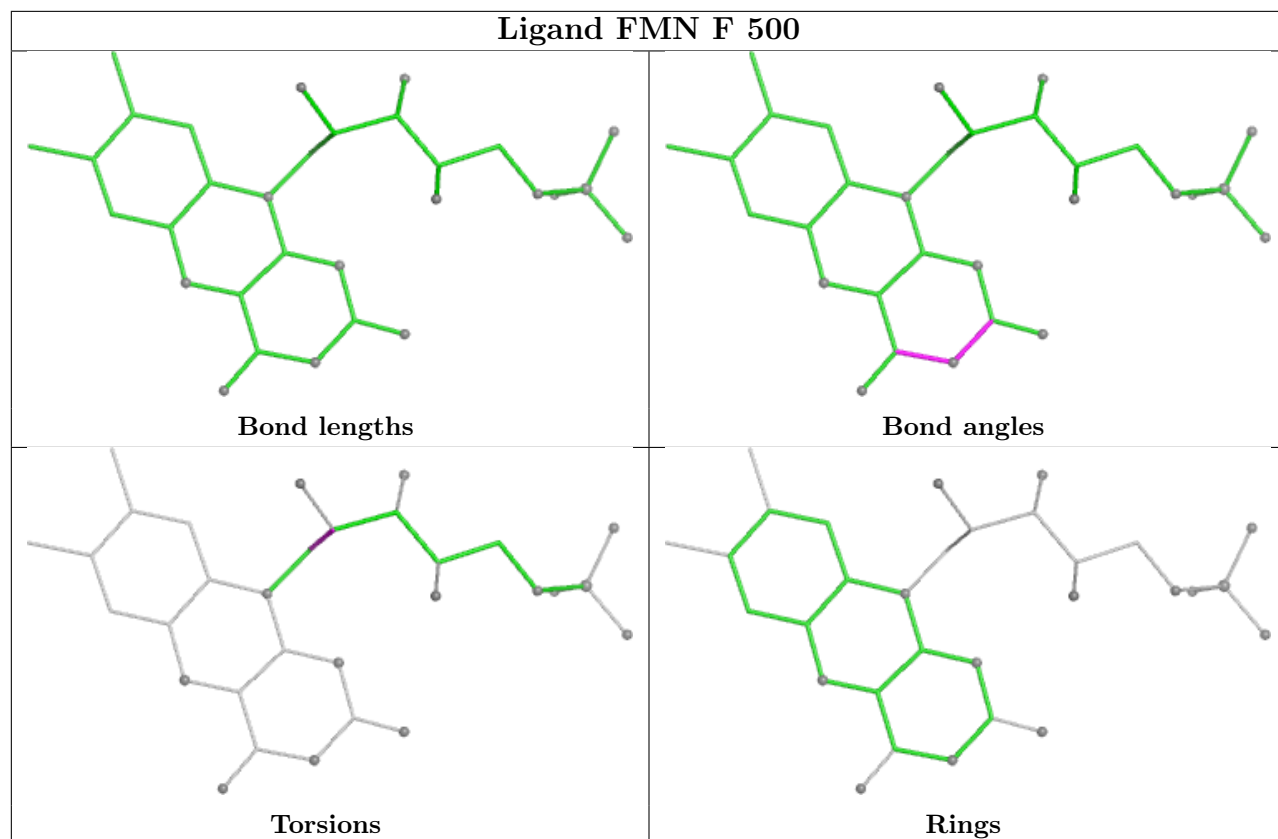


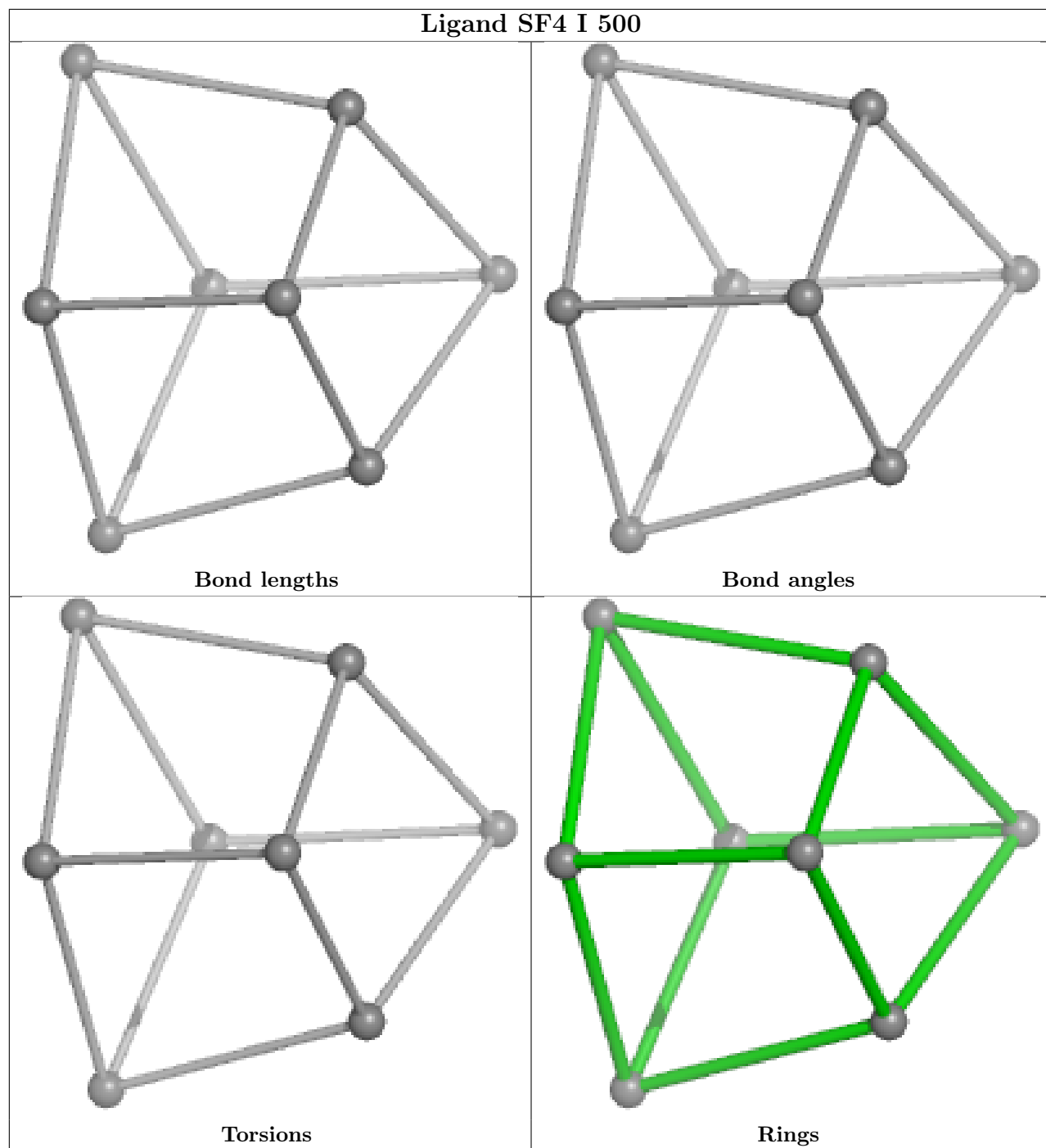


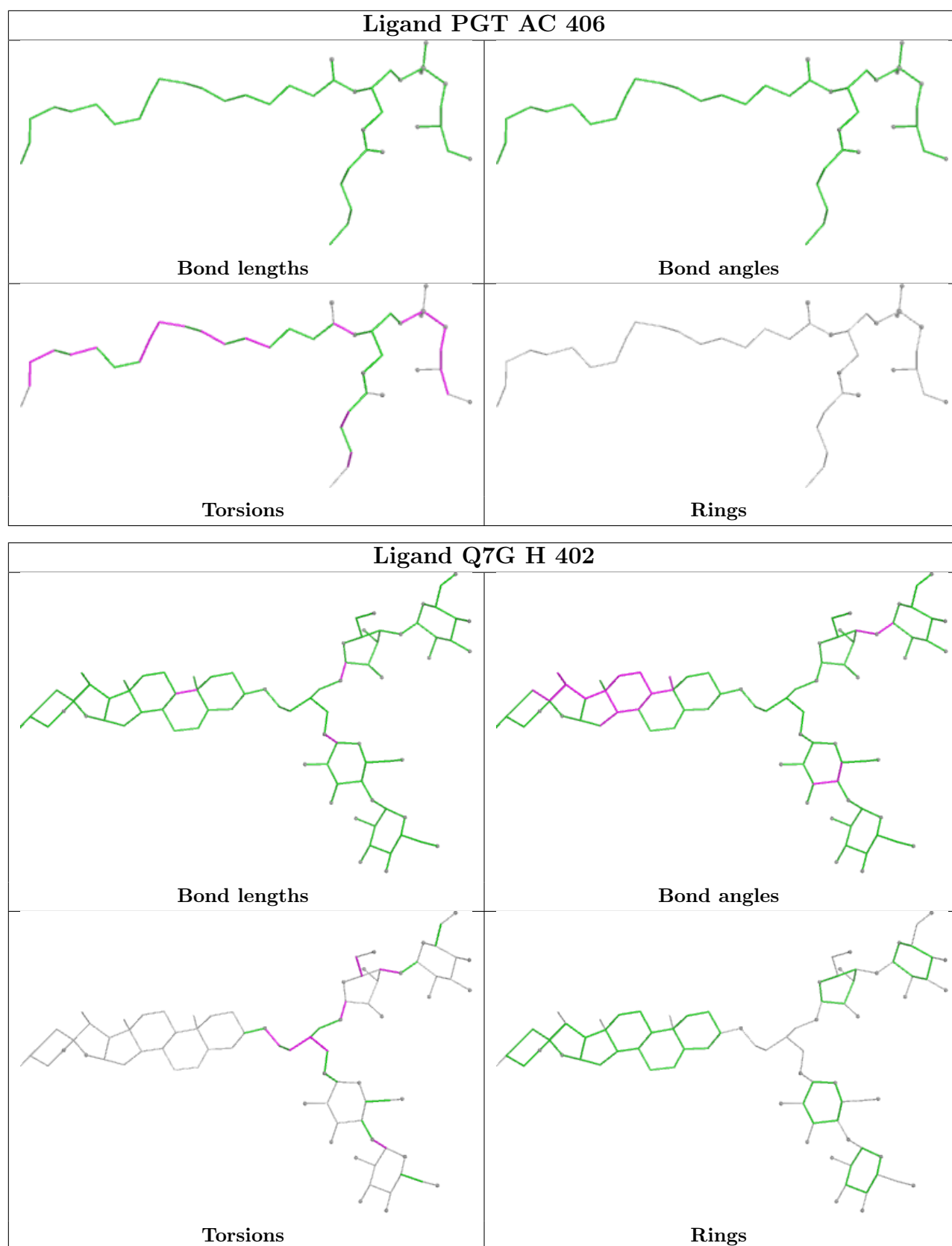


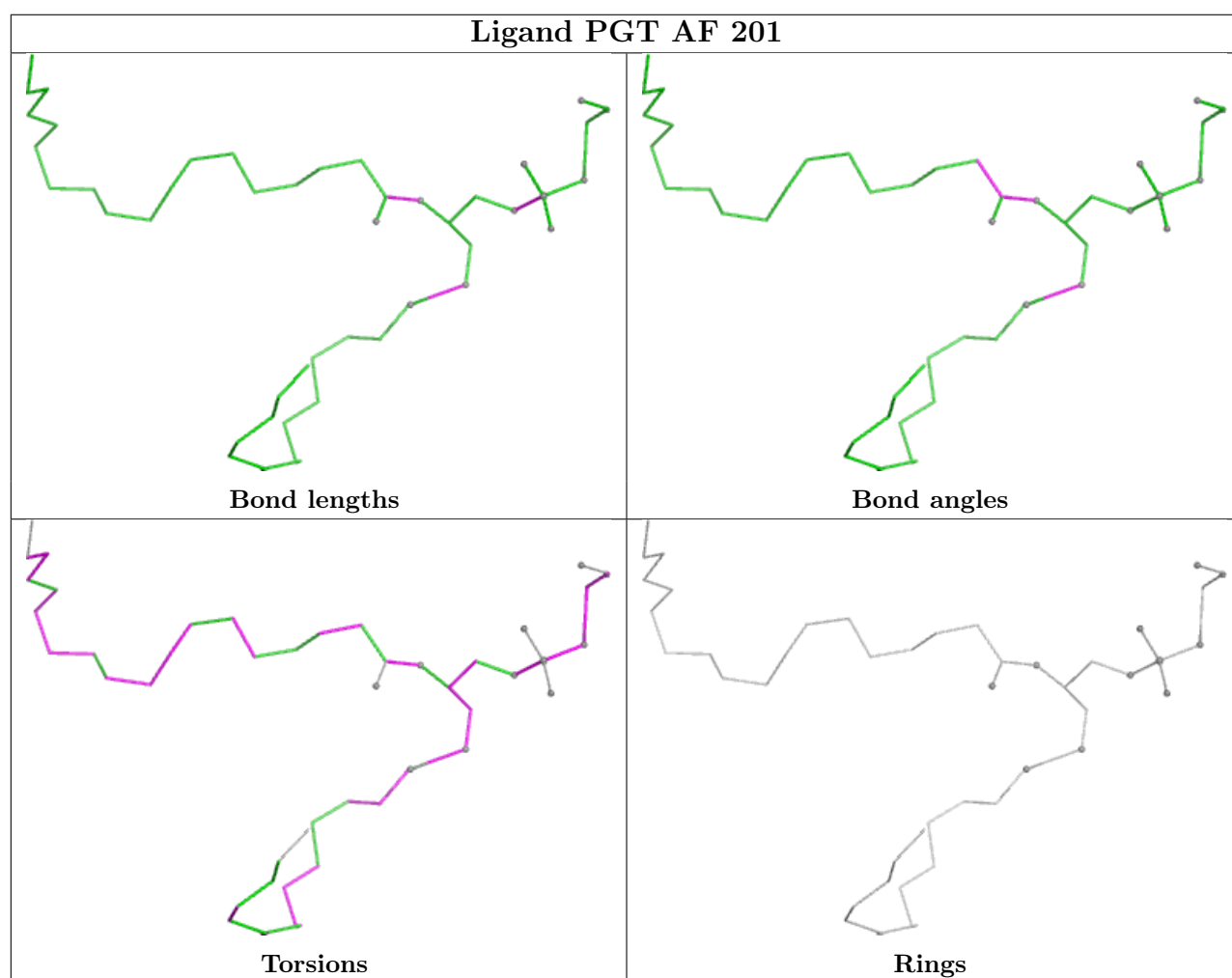
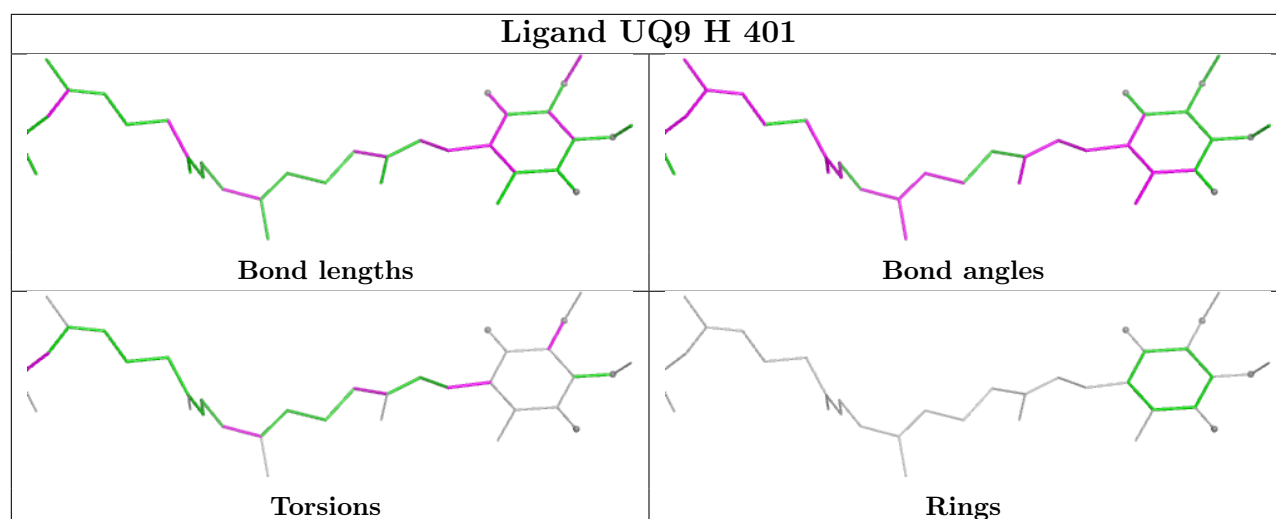




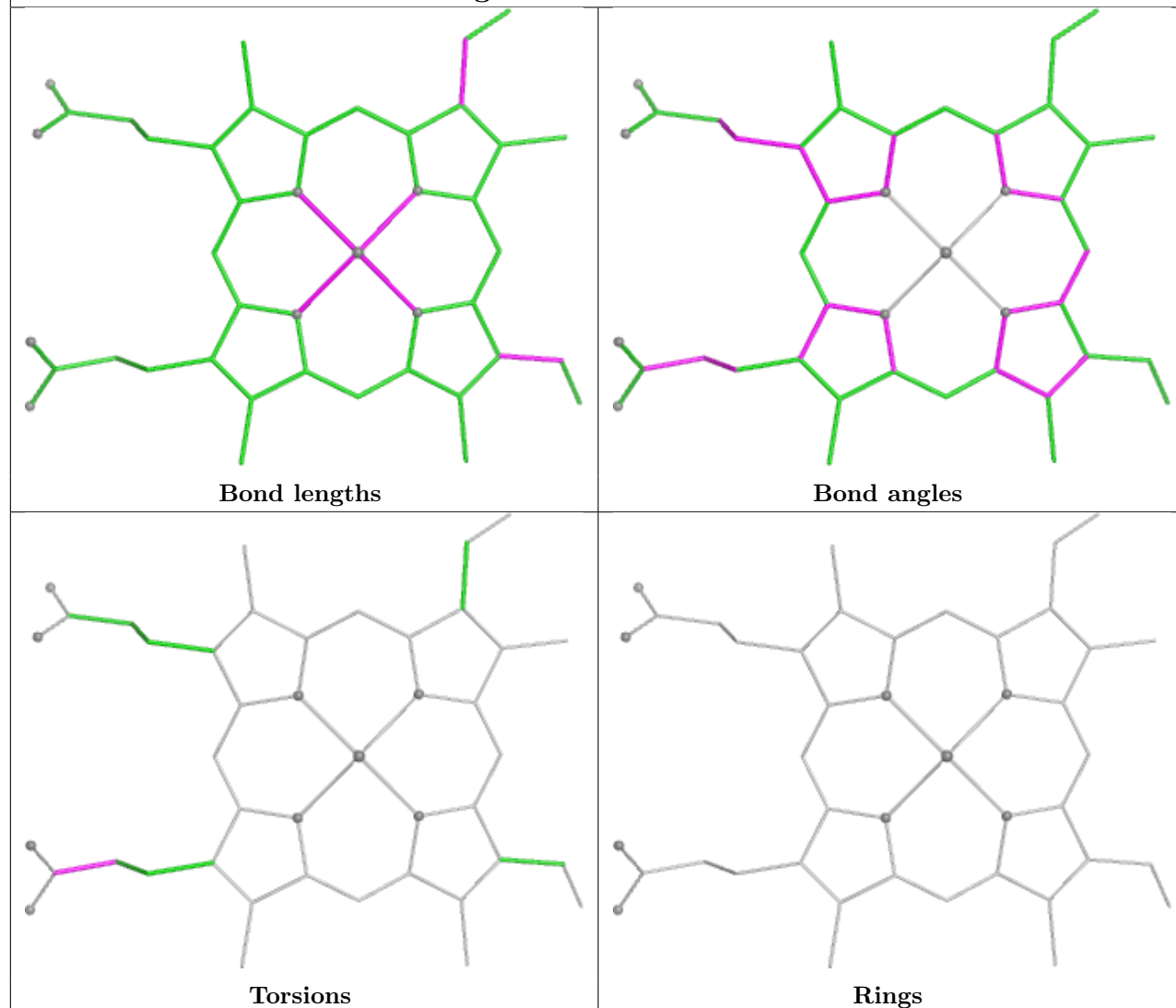


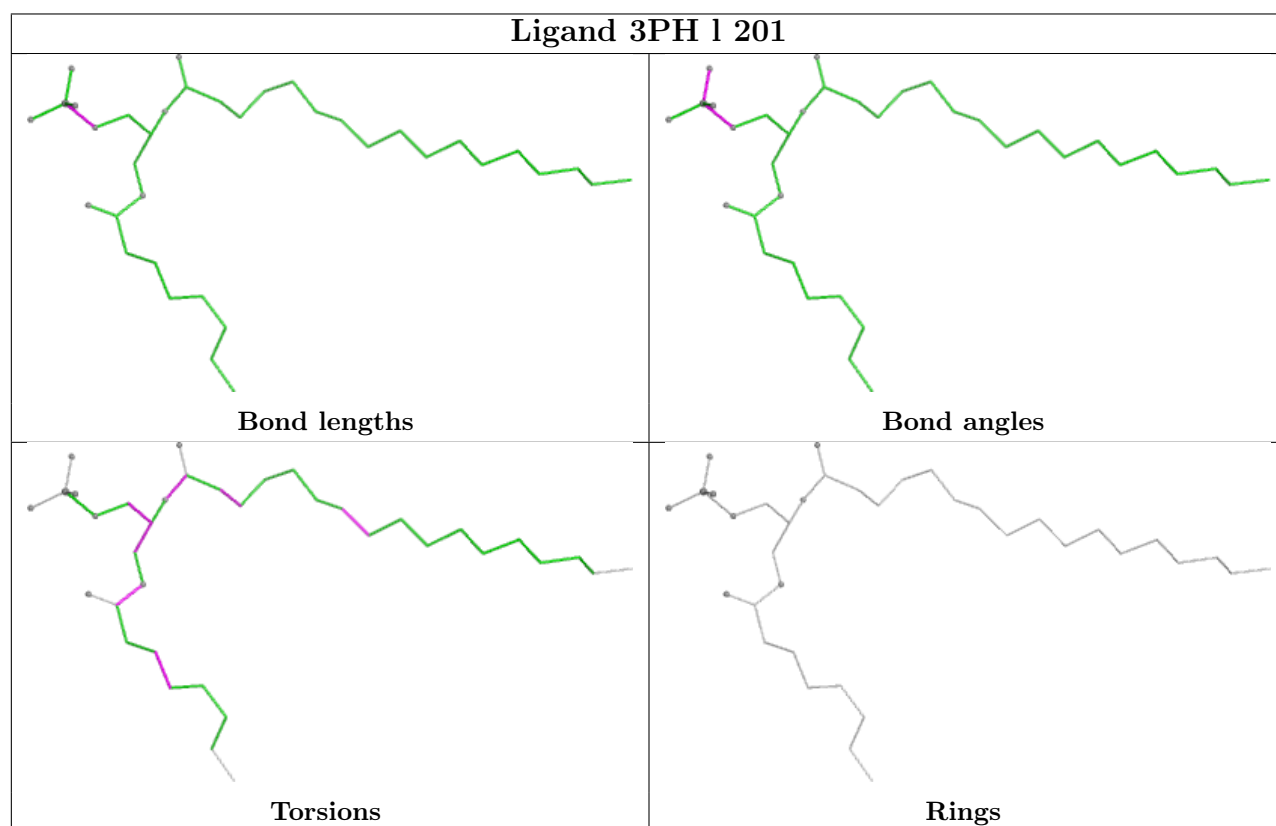
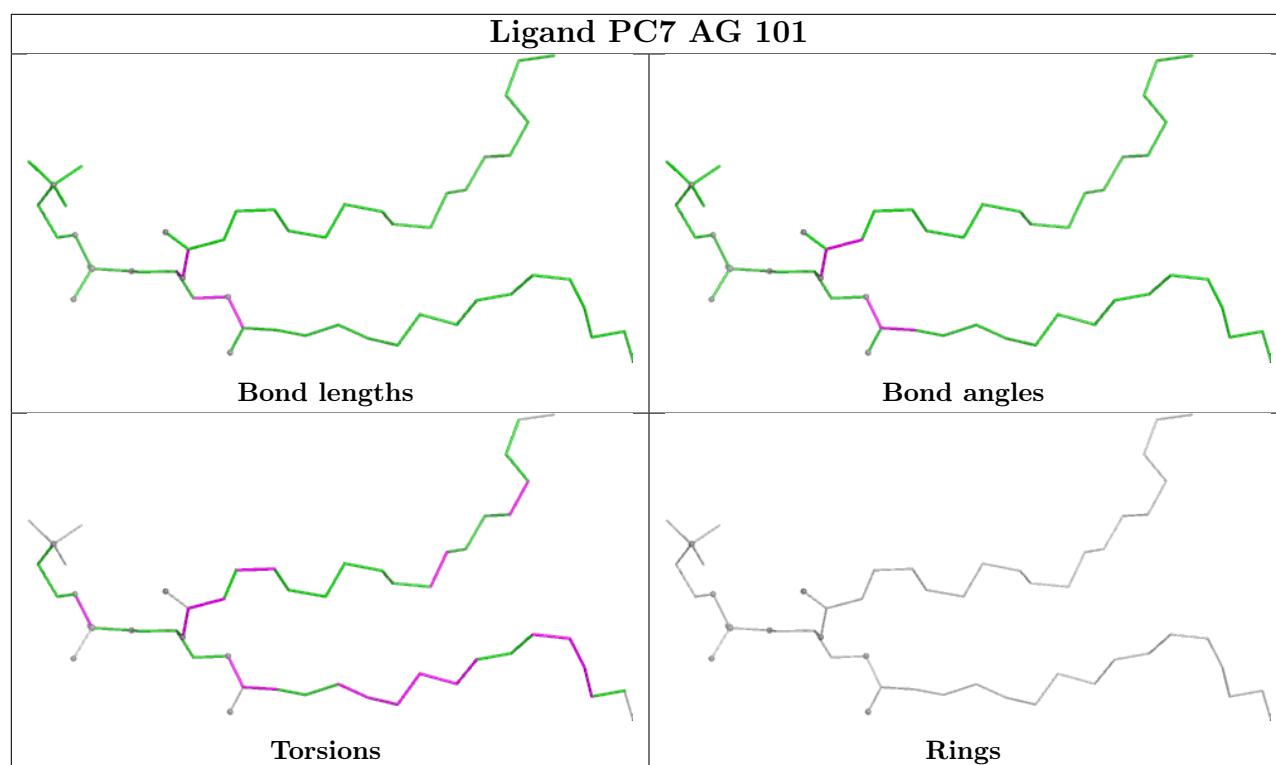


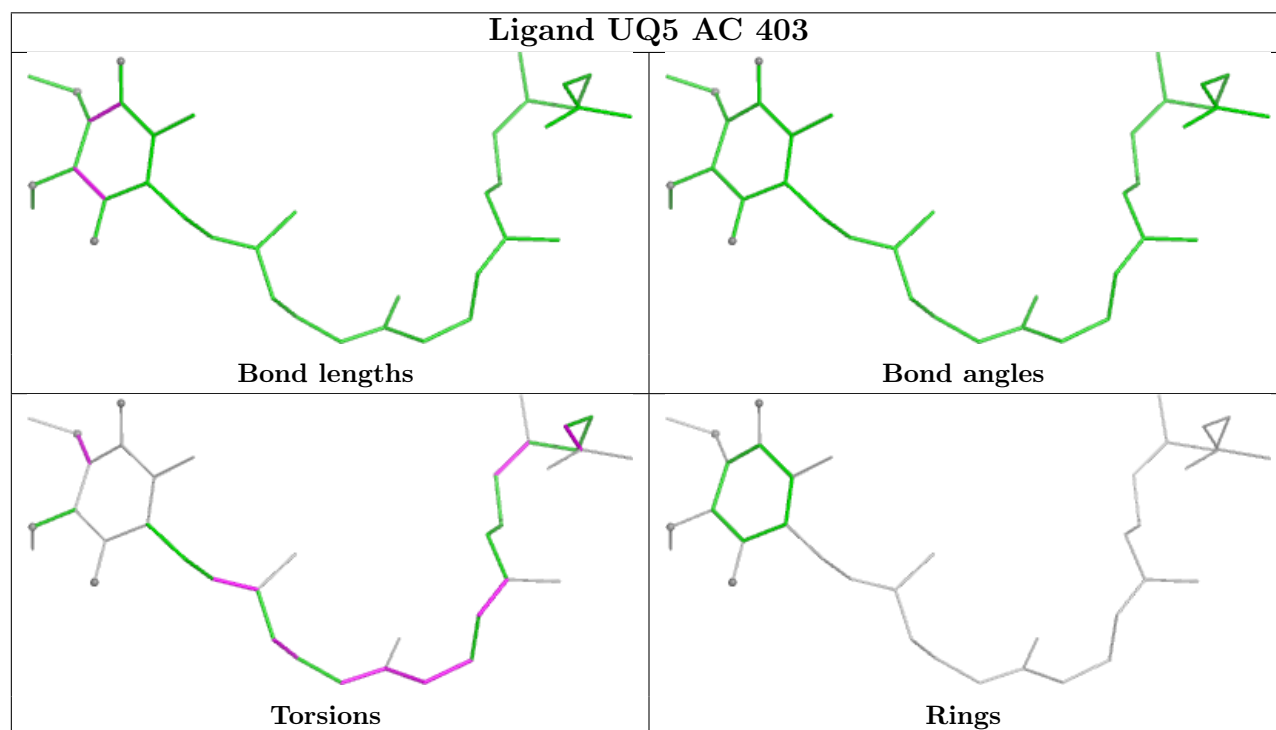
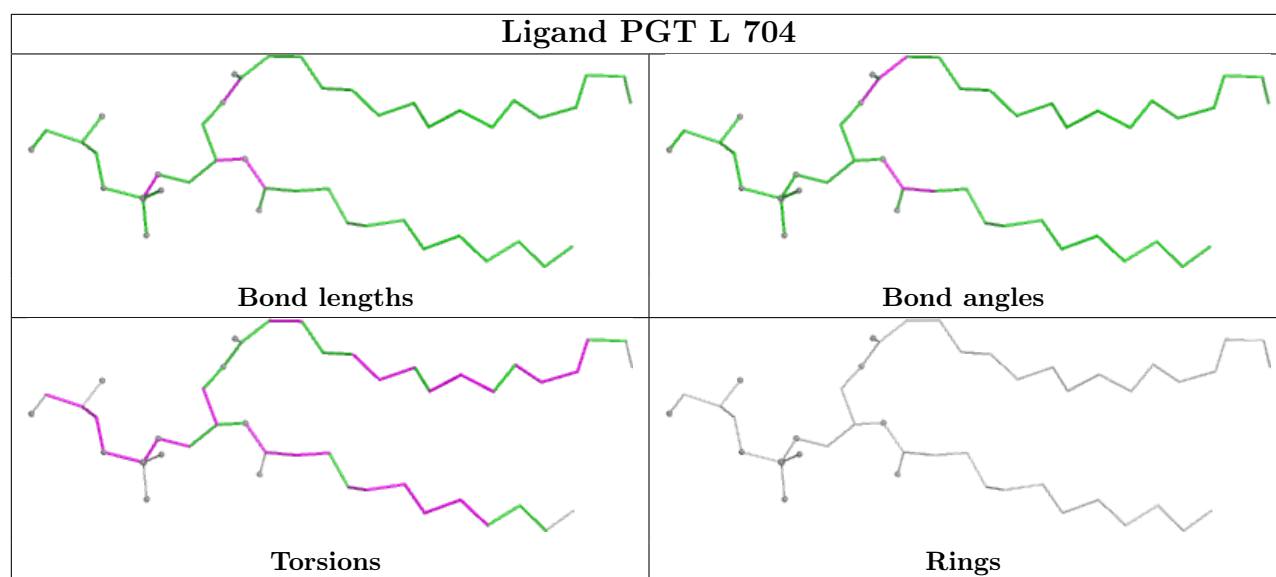


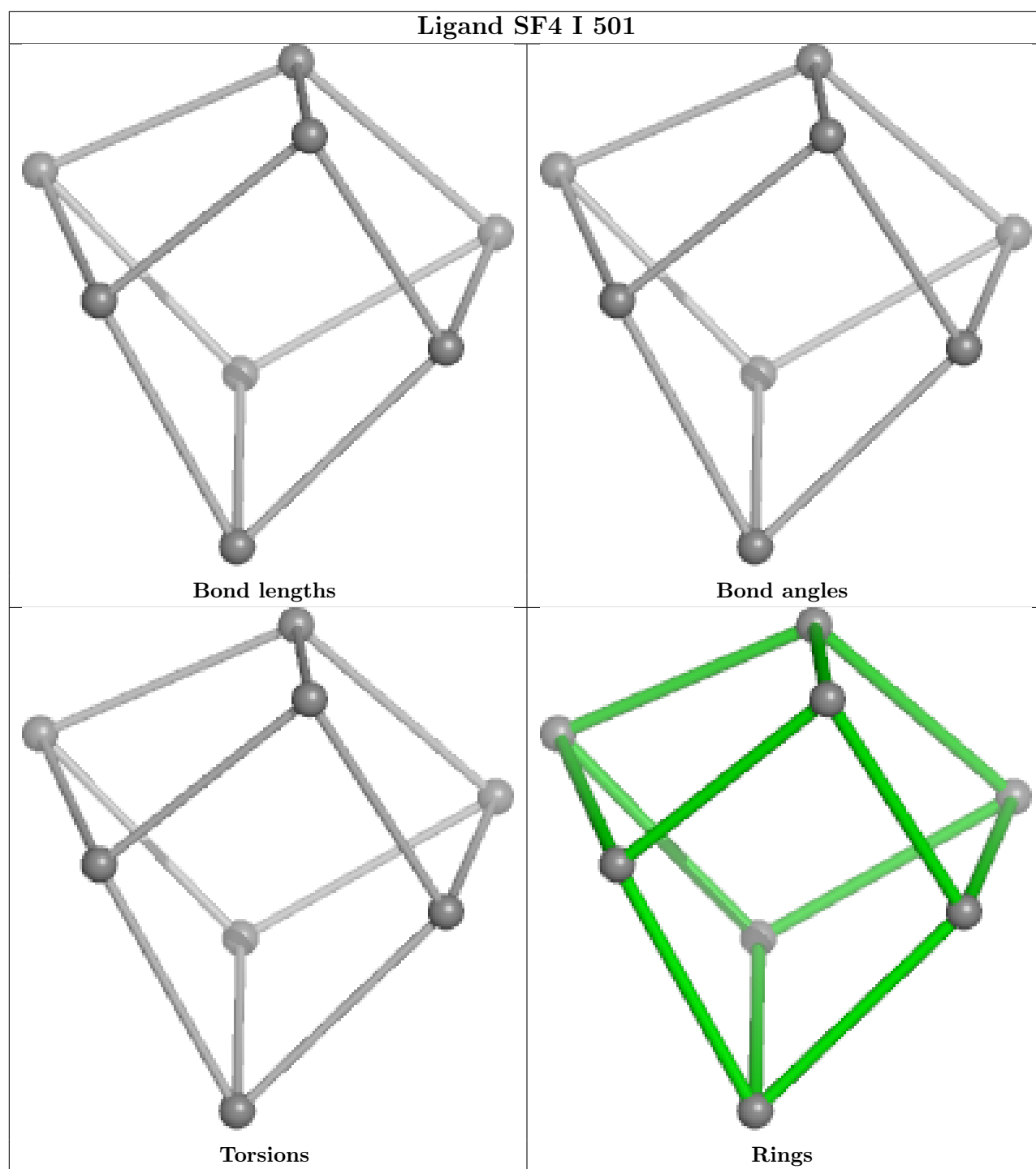


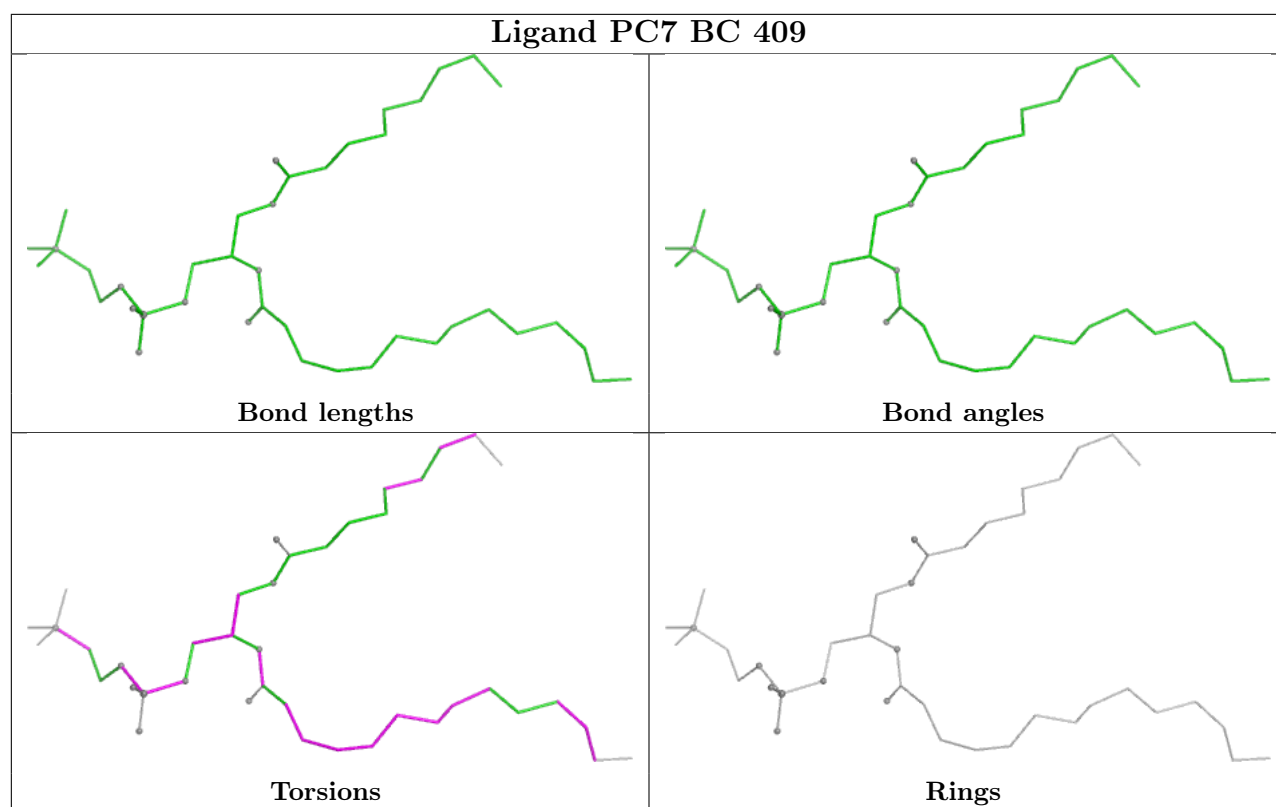
Ligand HEM AE 401

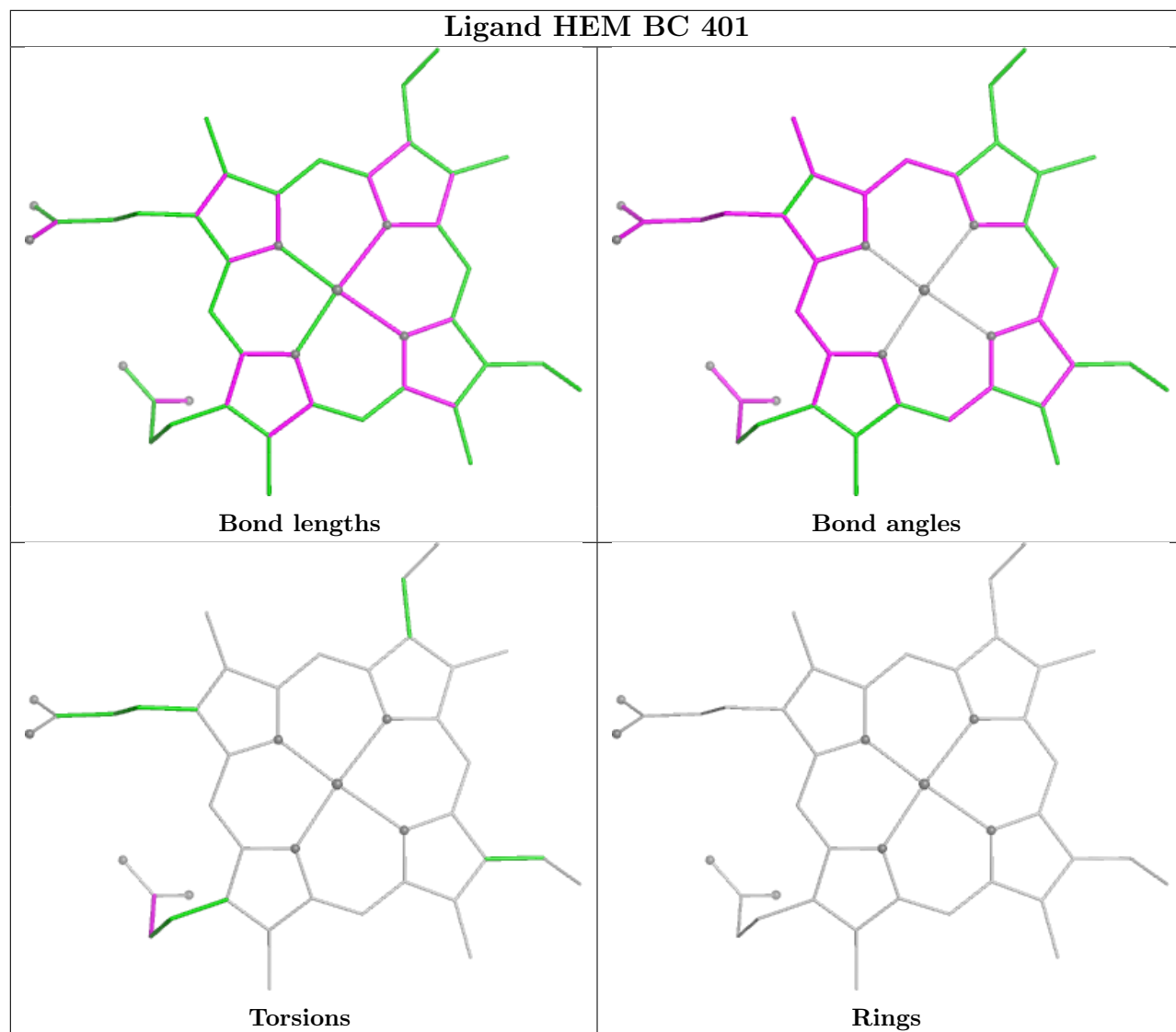


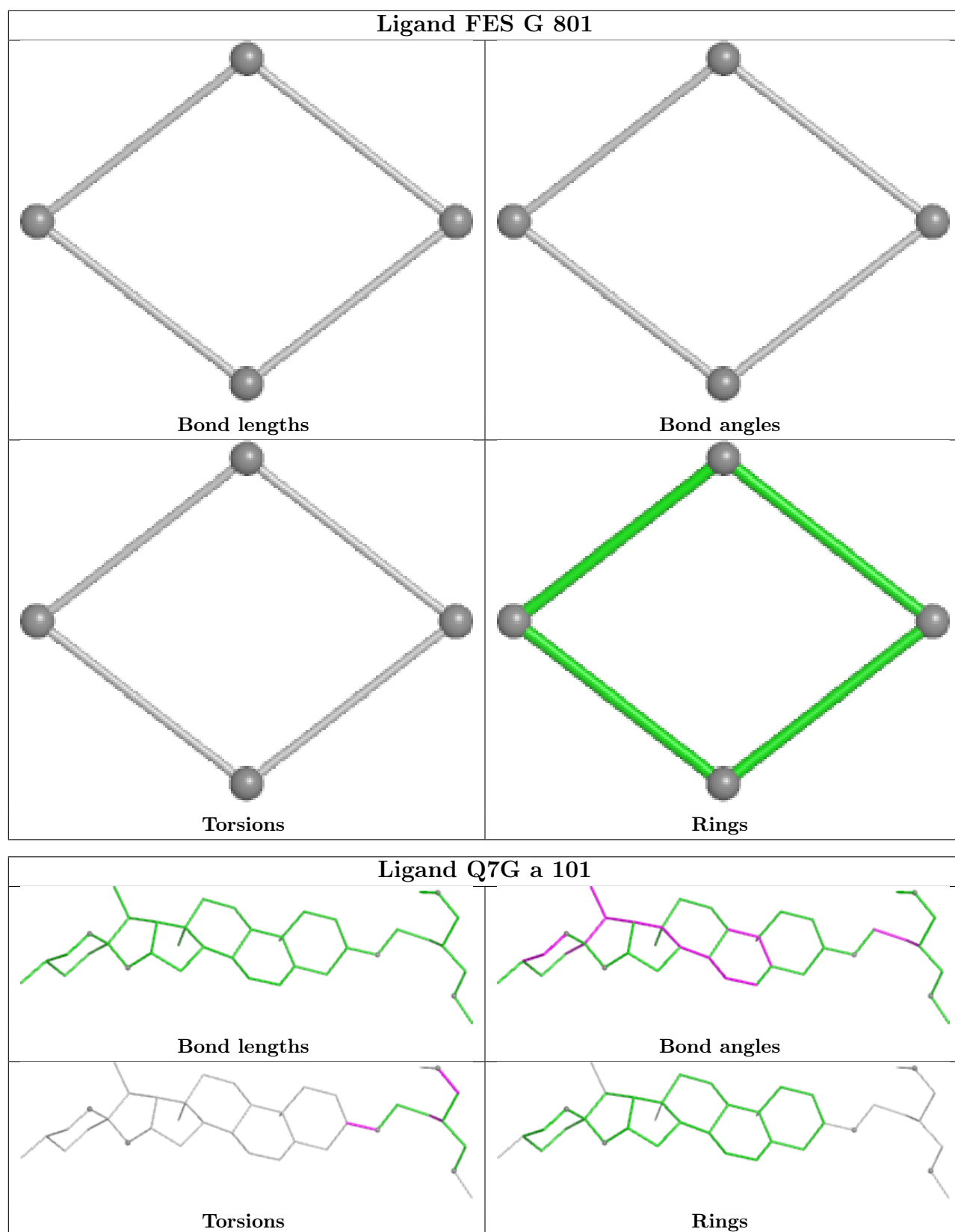


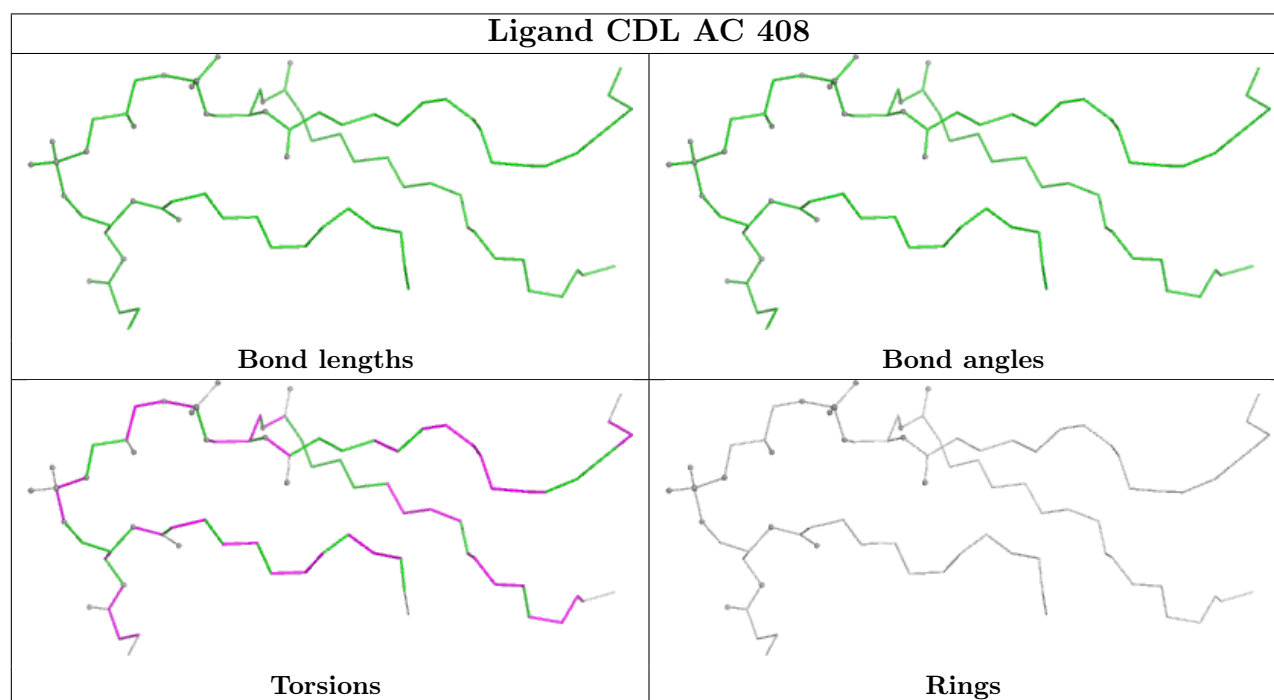
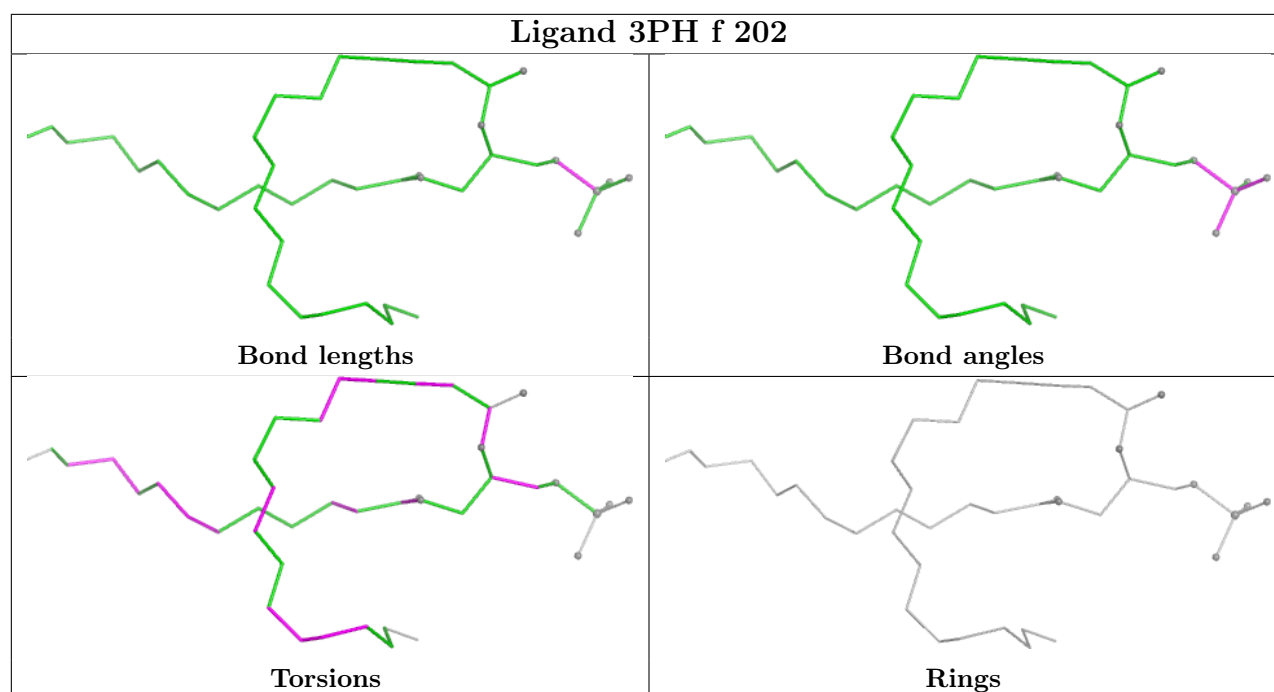


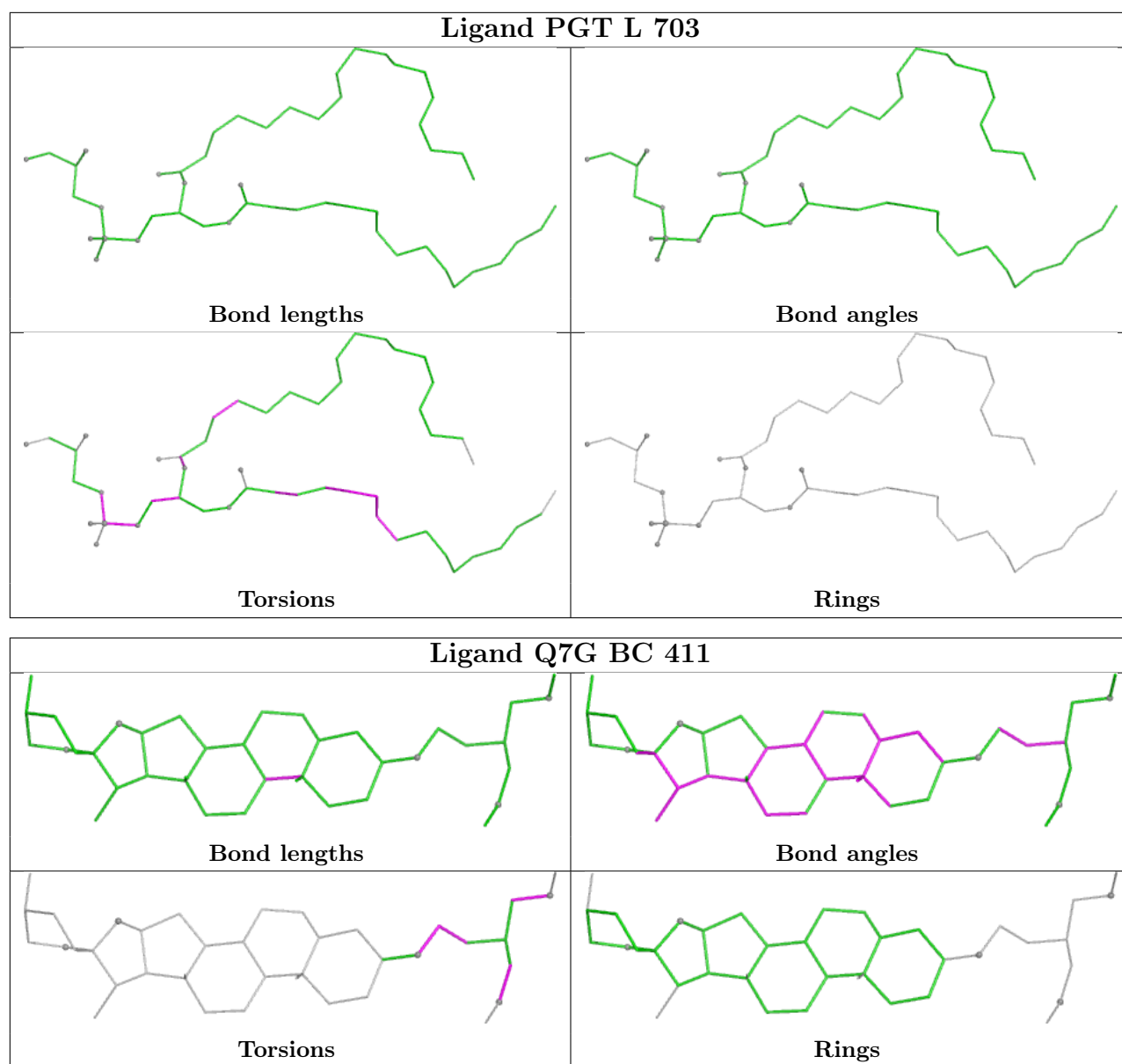


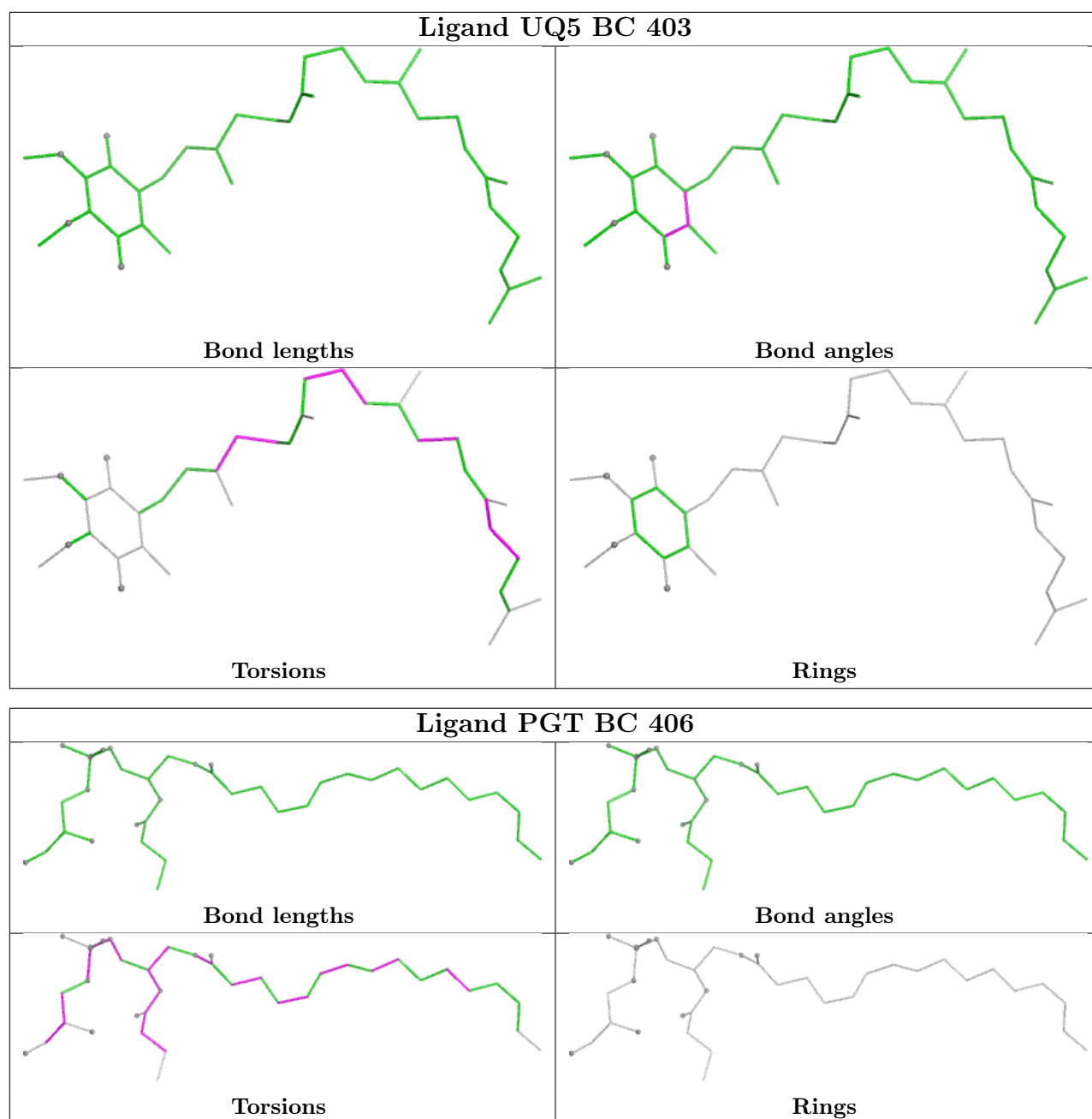


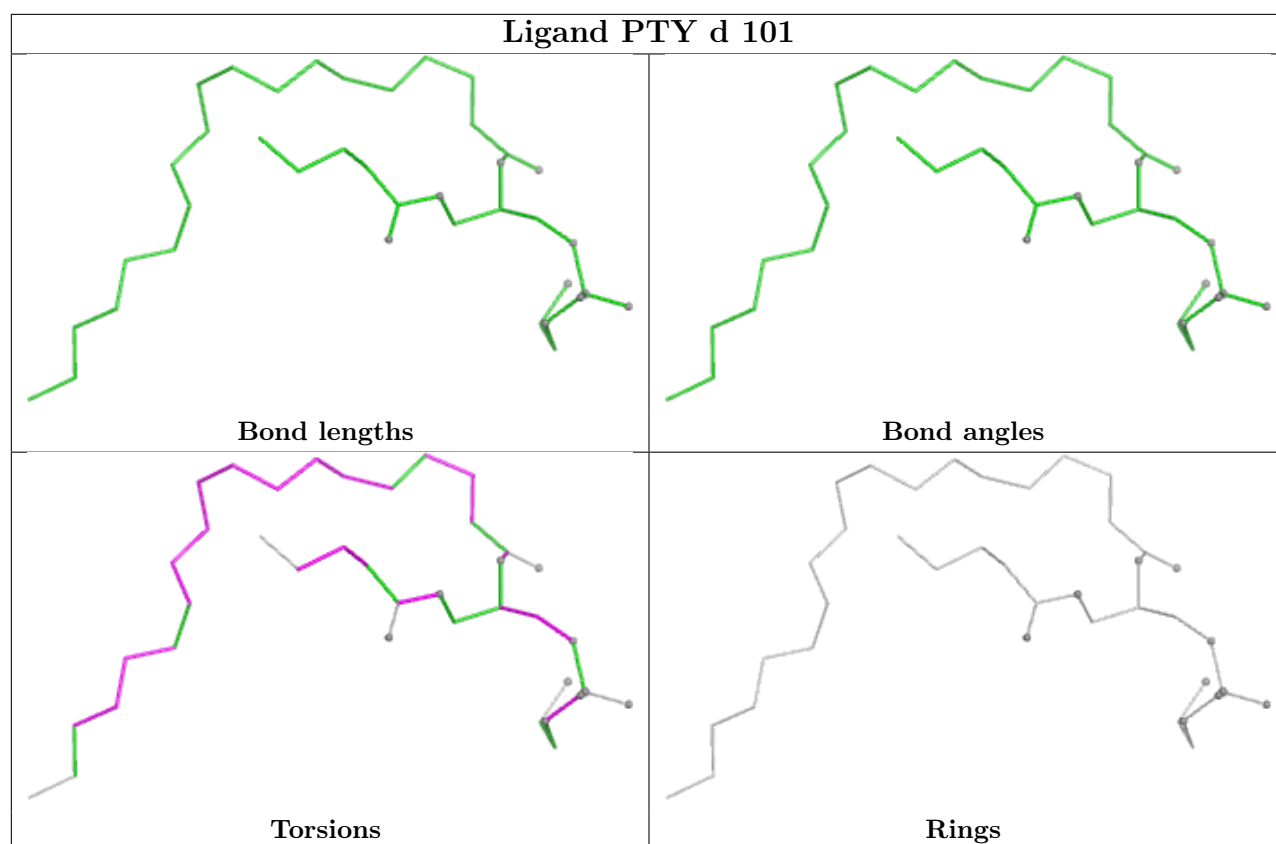


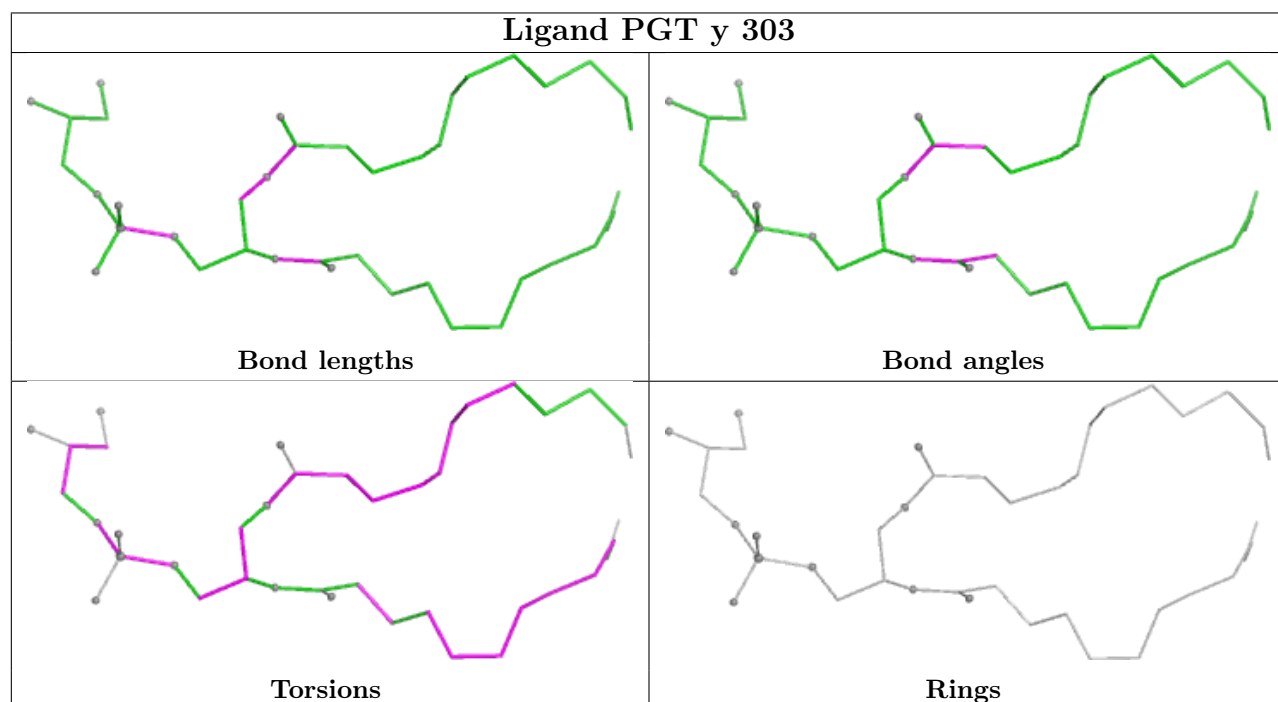
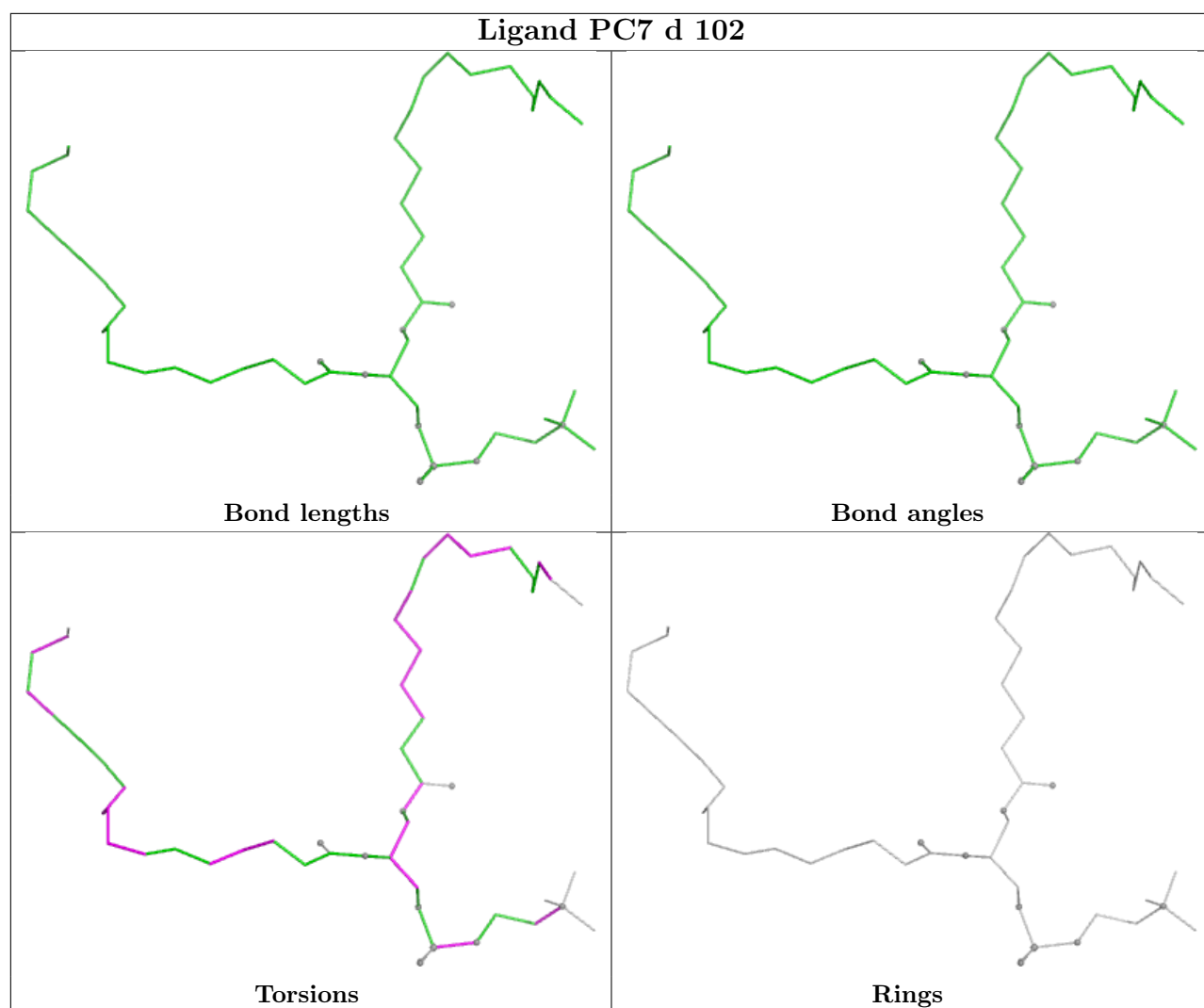


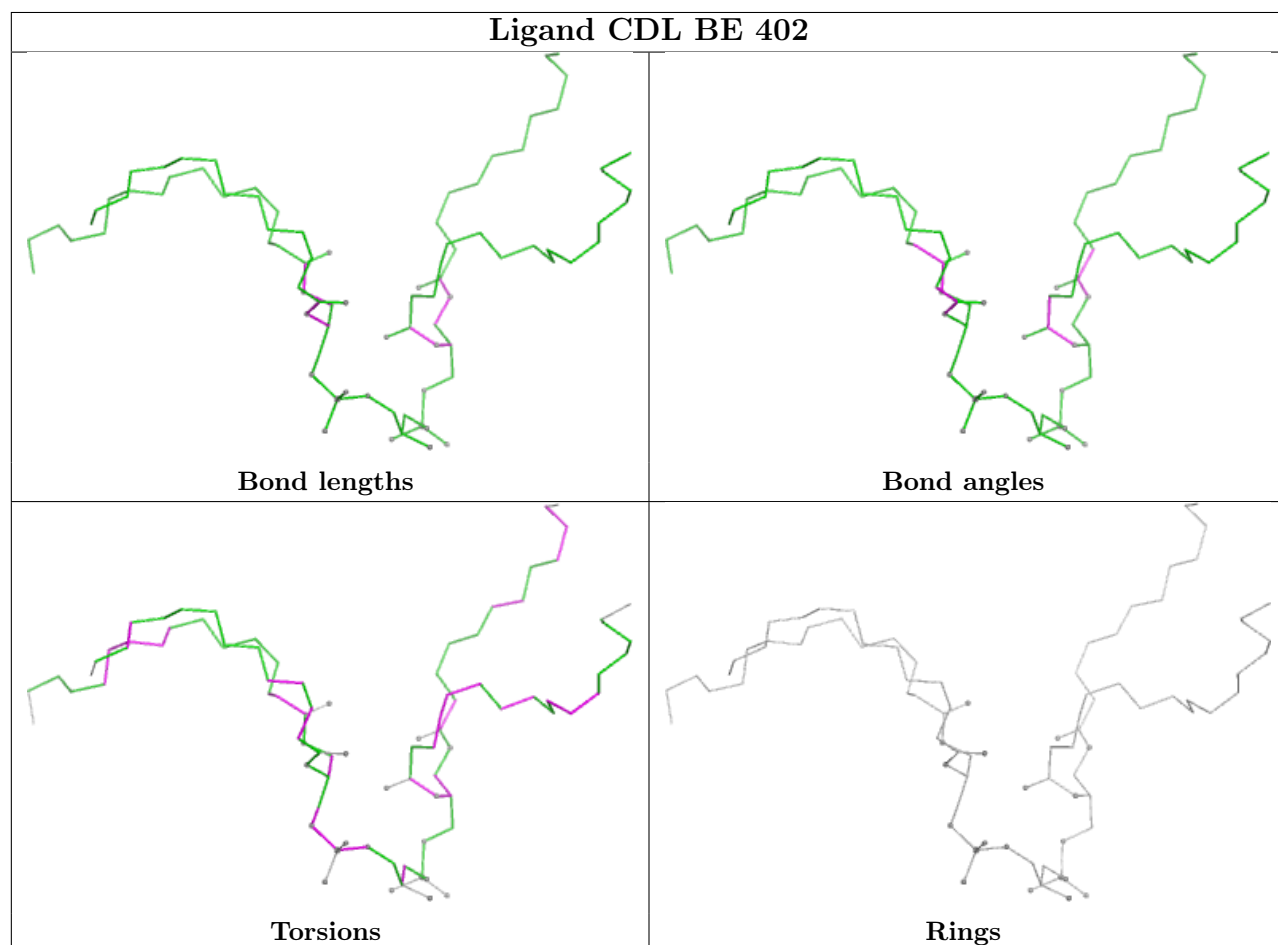
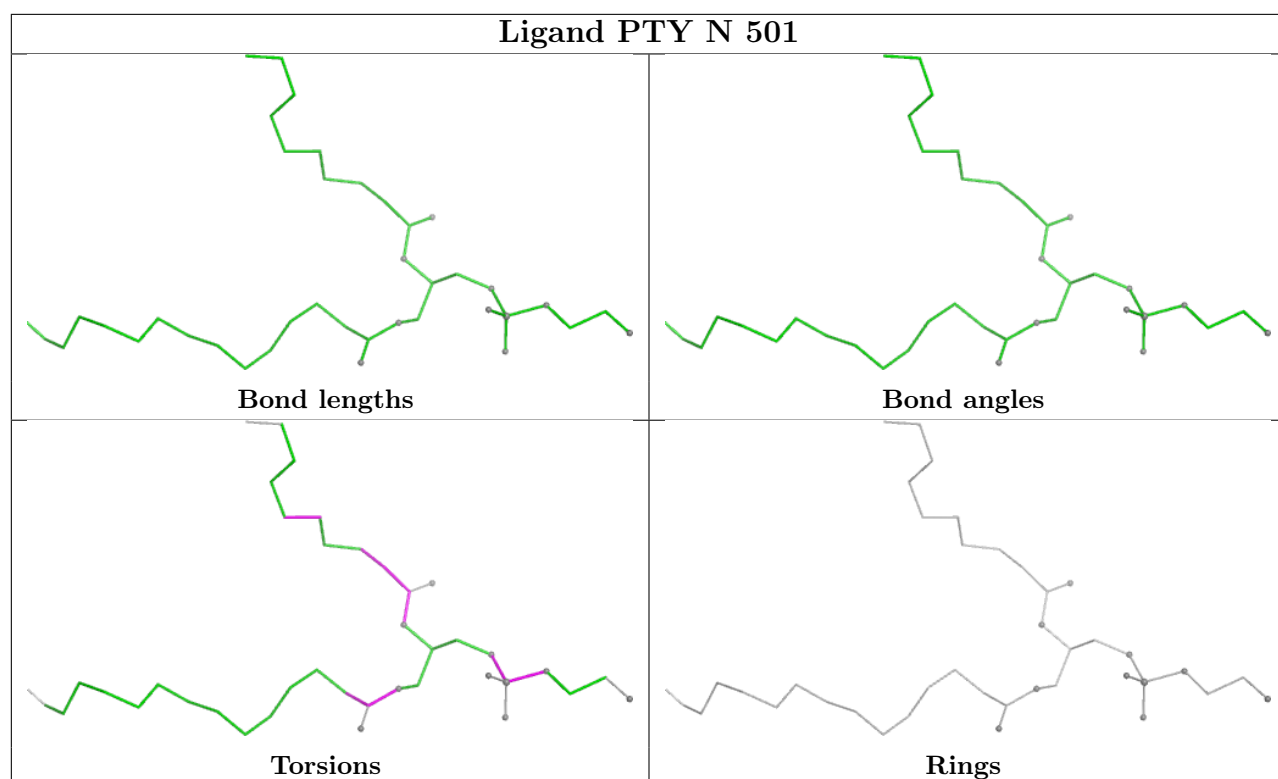


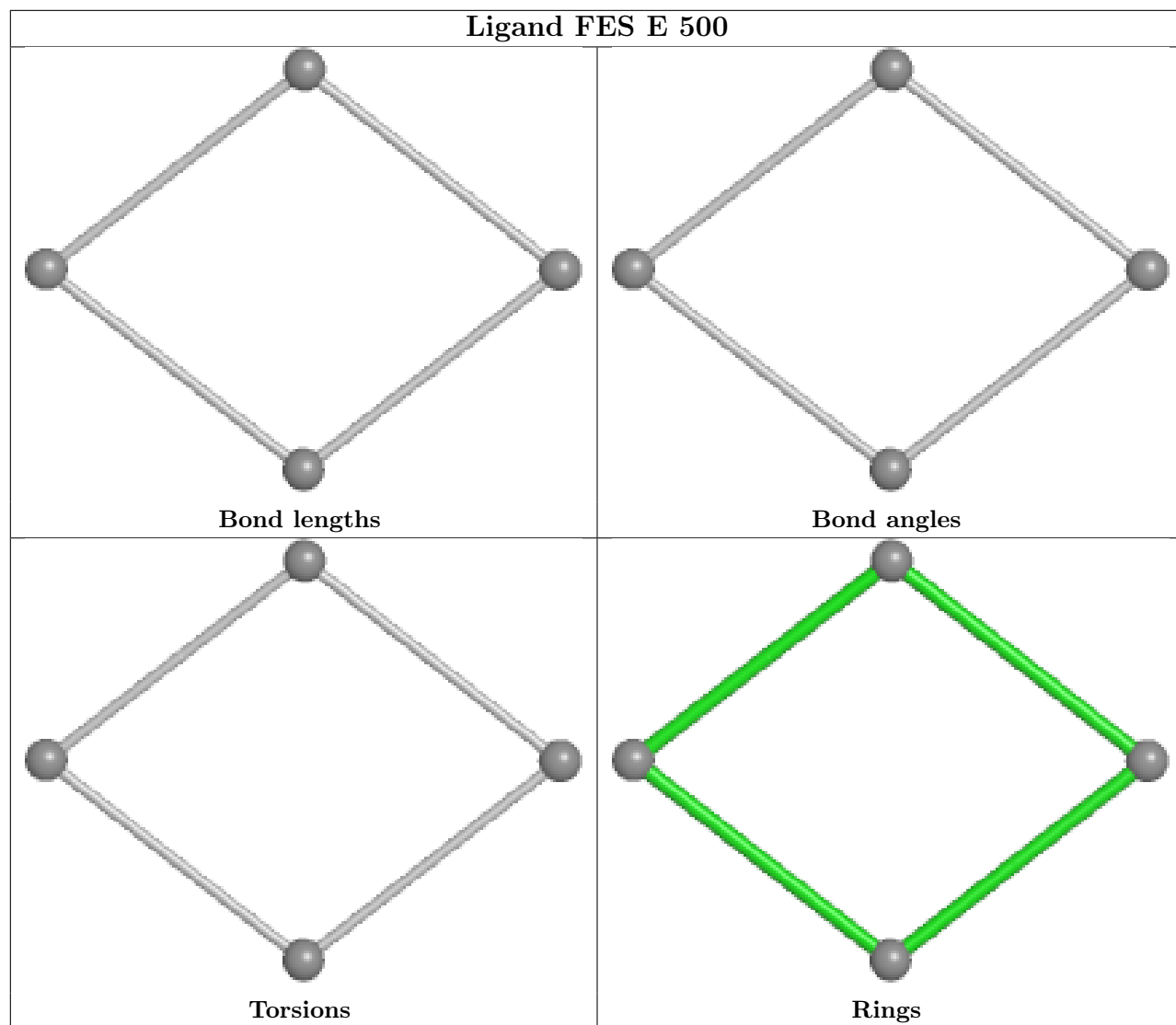


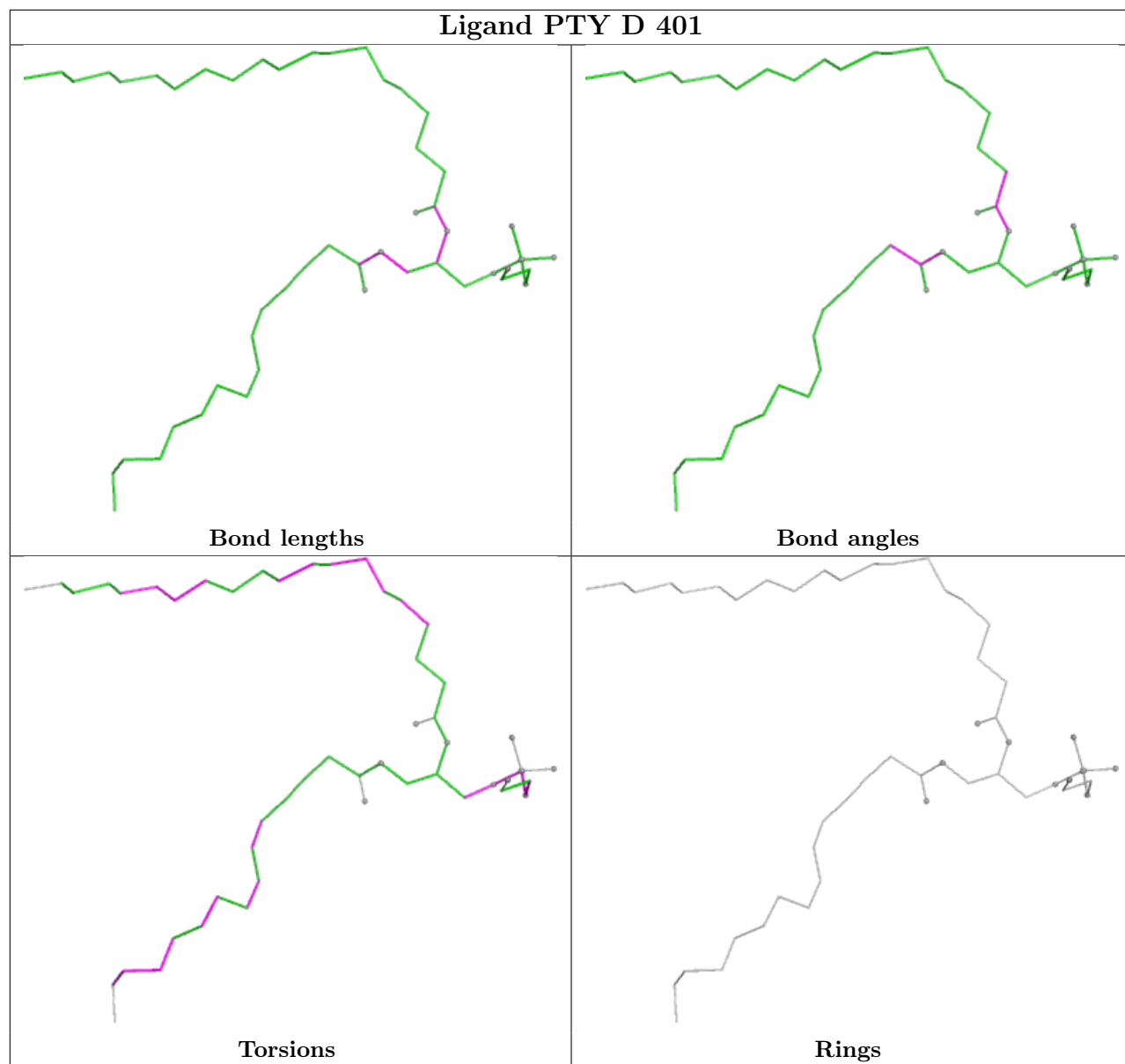


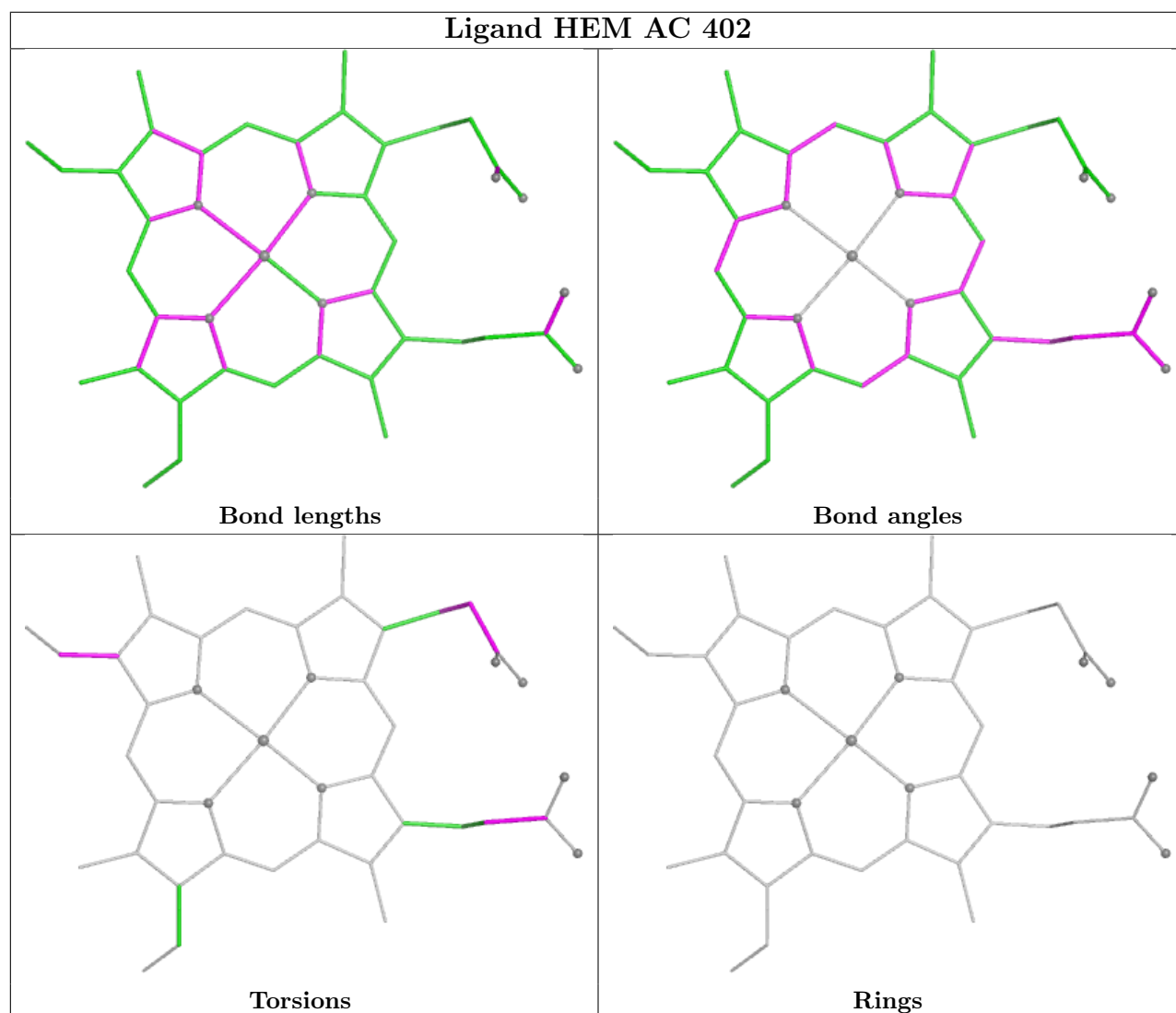
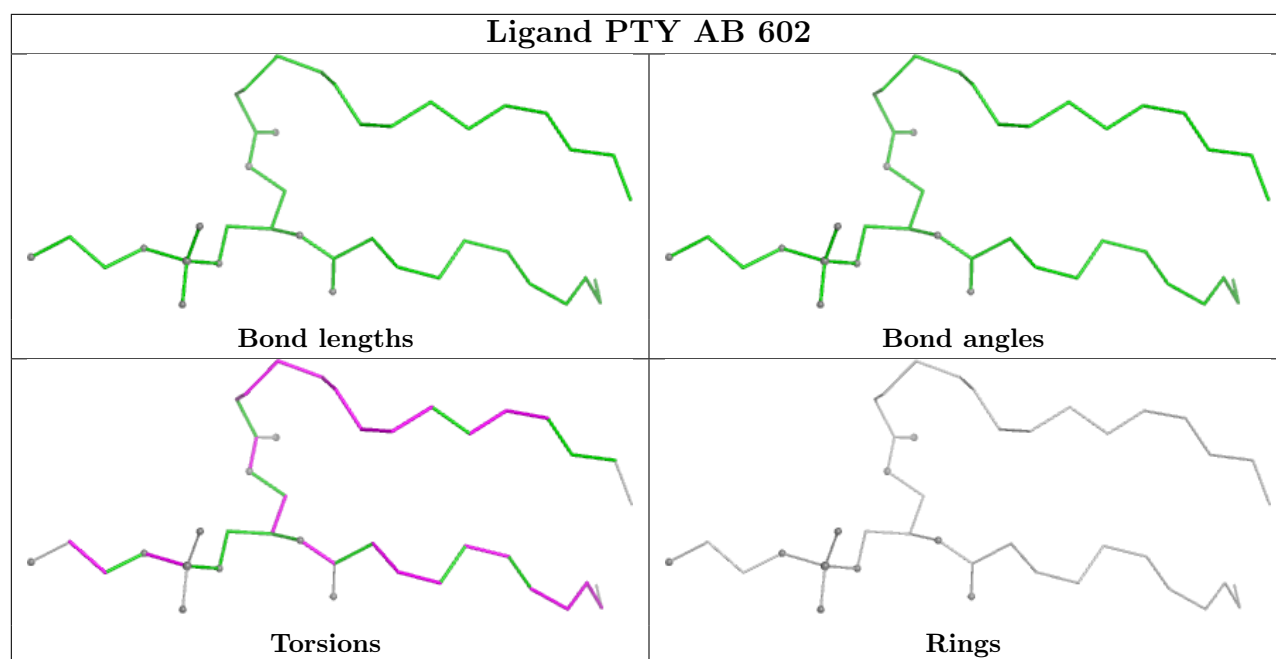


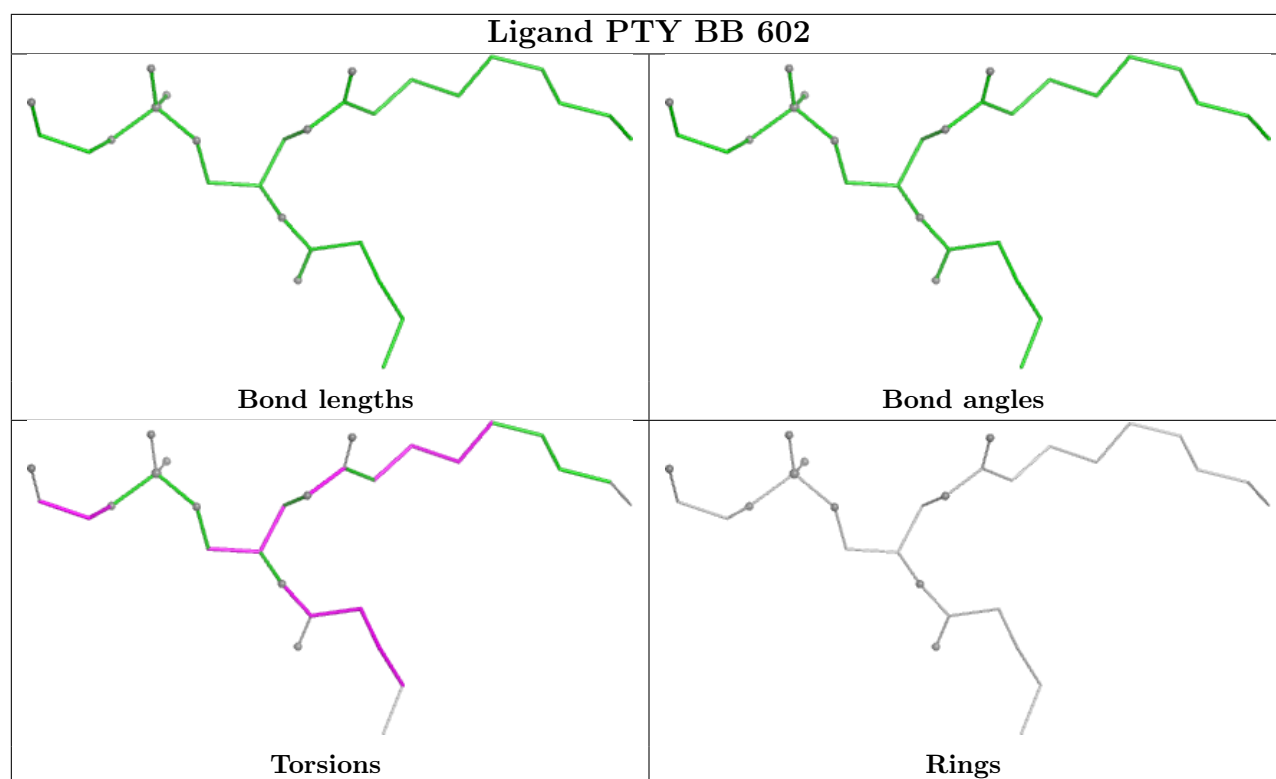


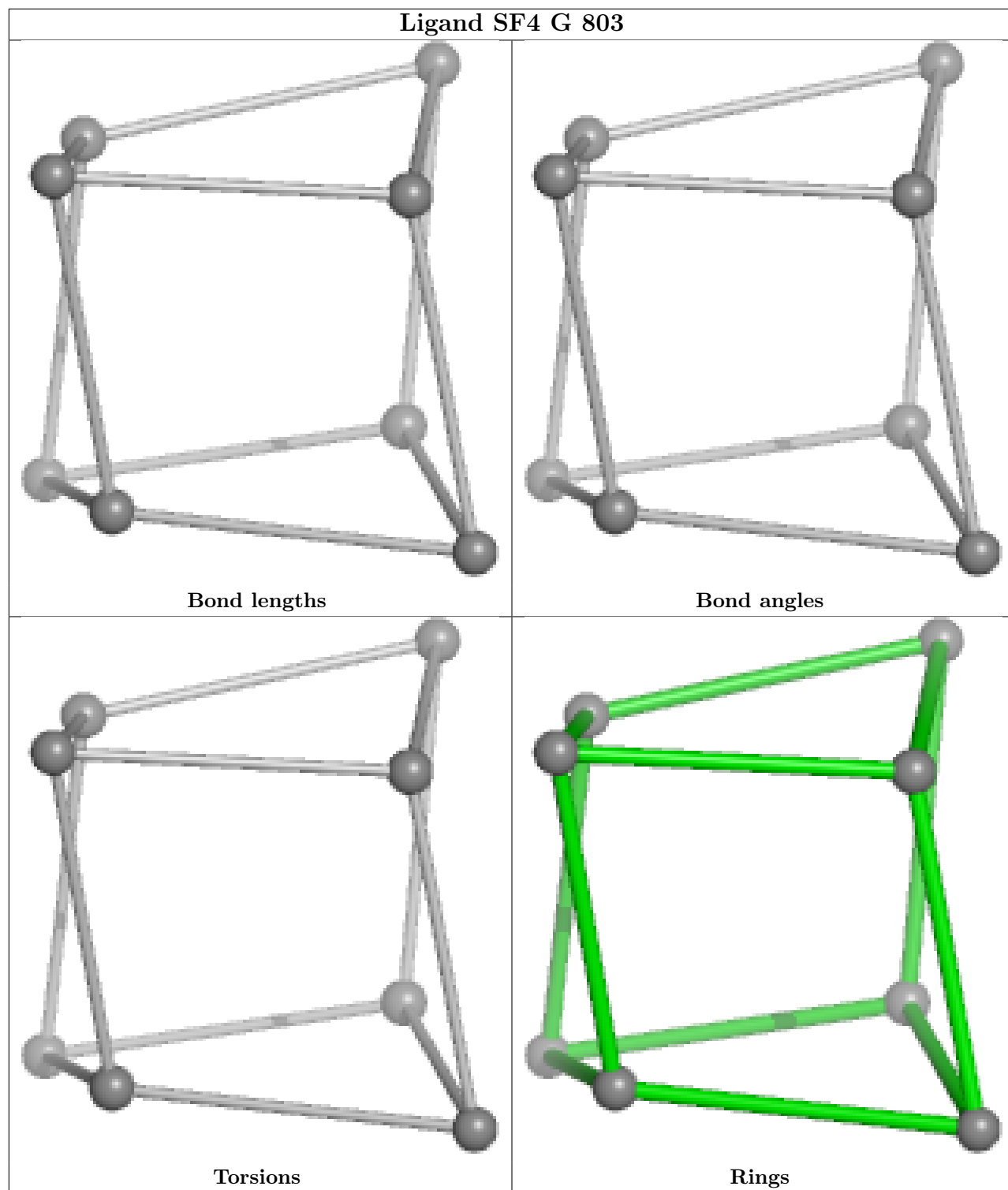


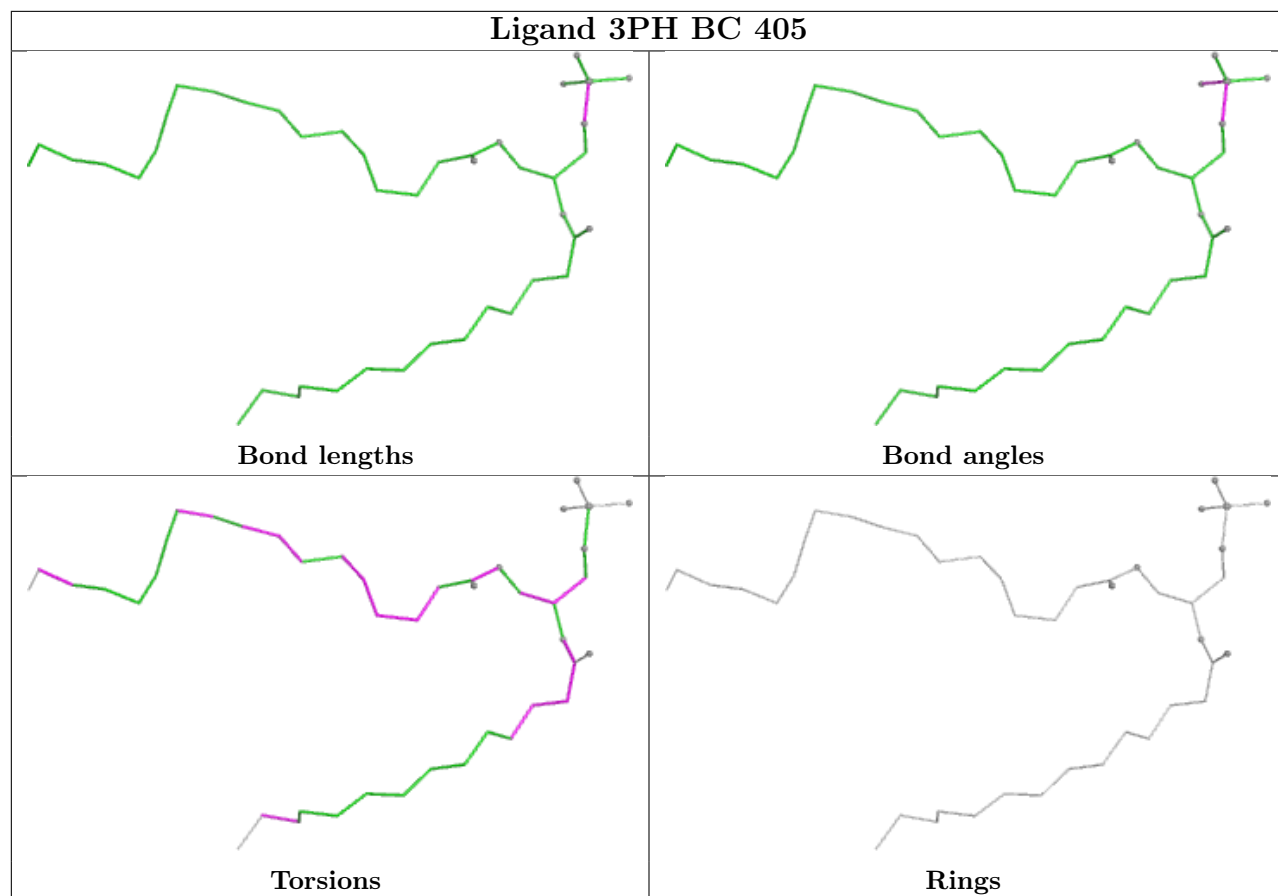


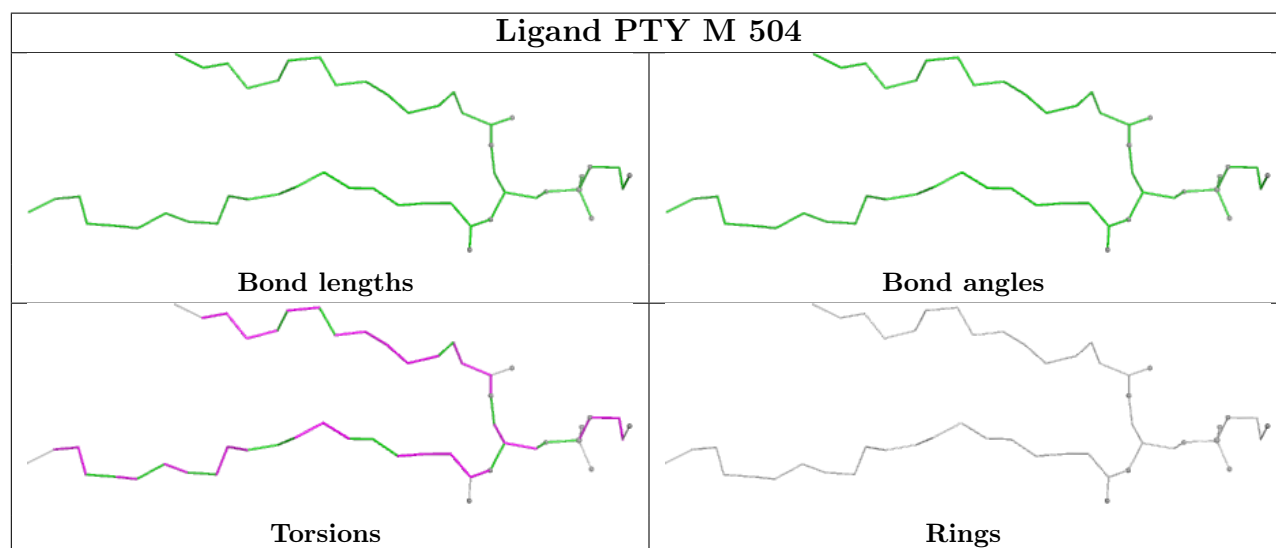
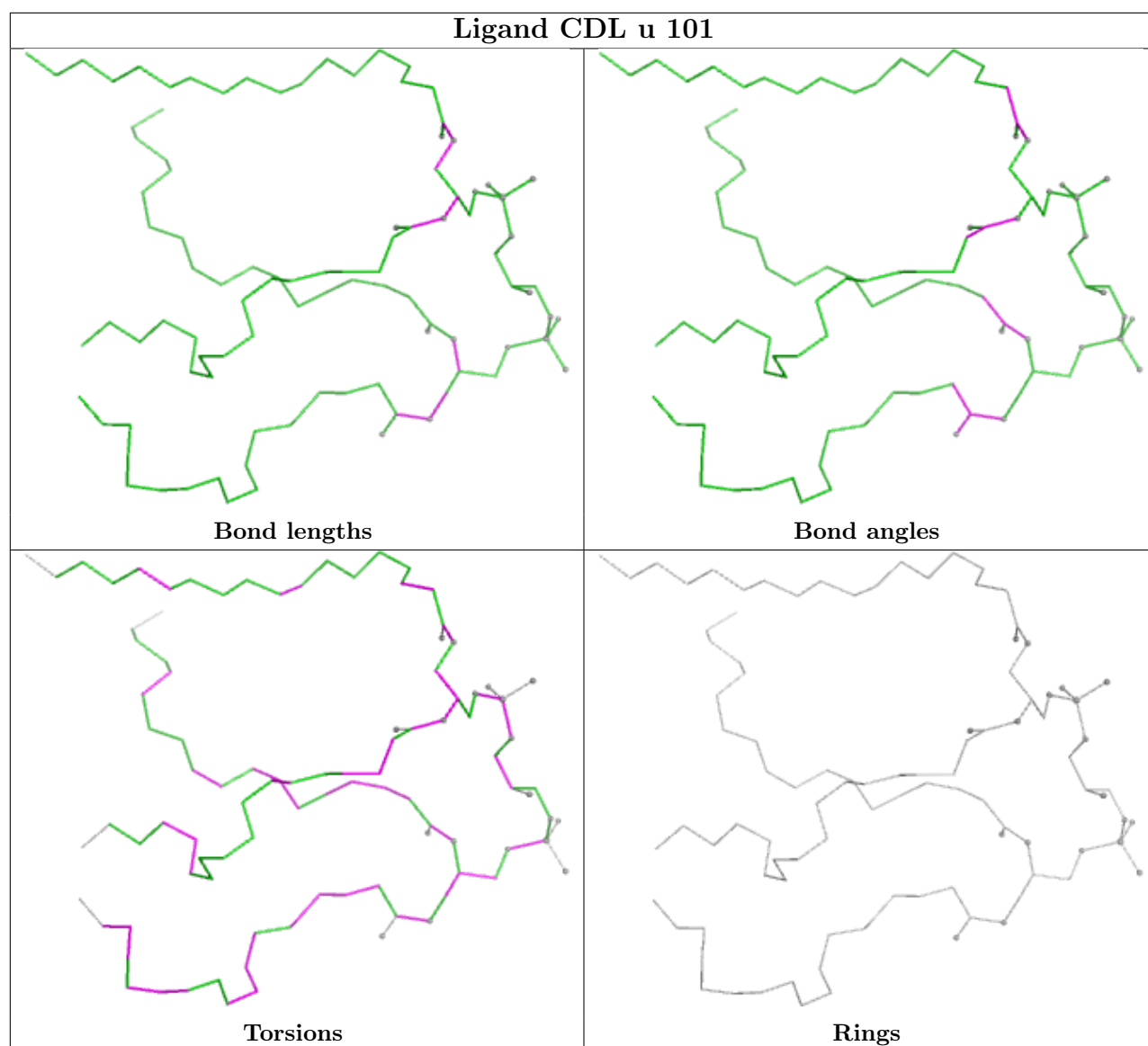


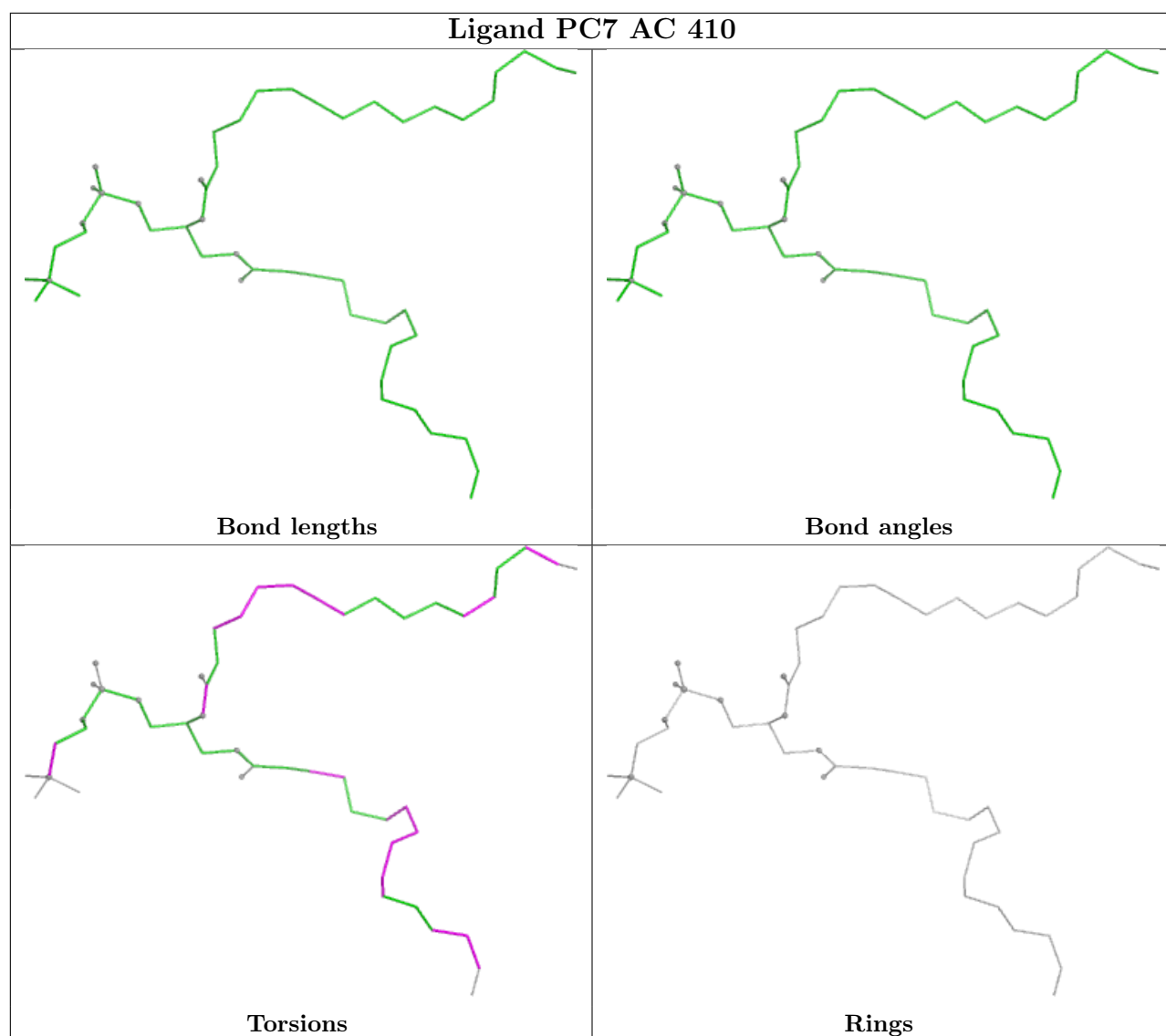


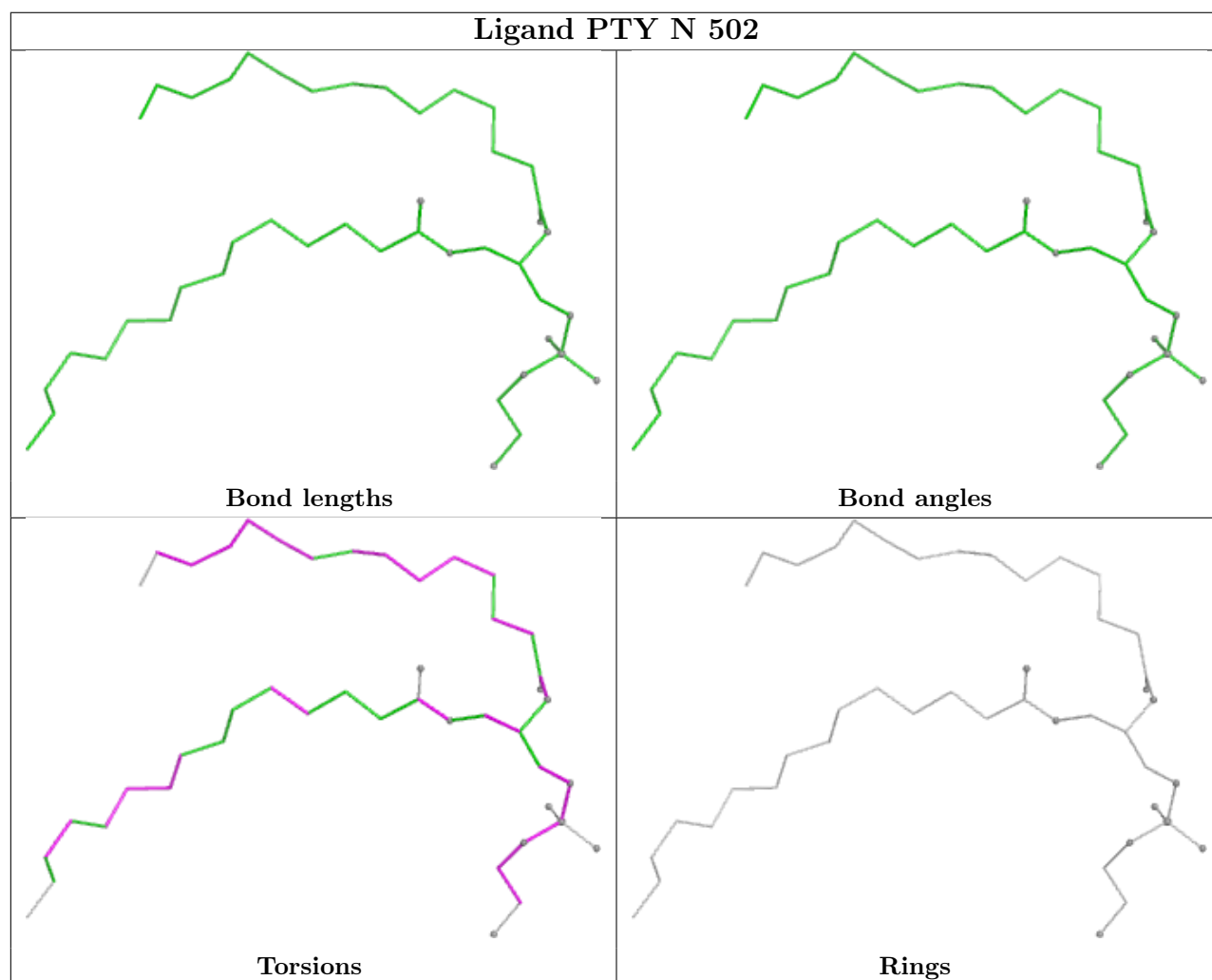
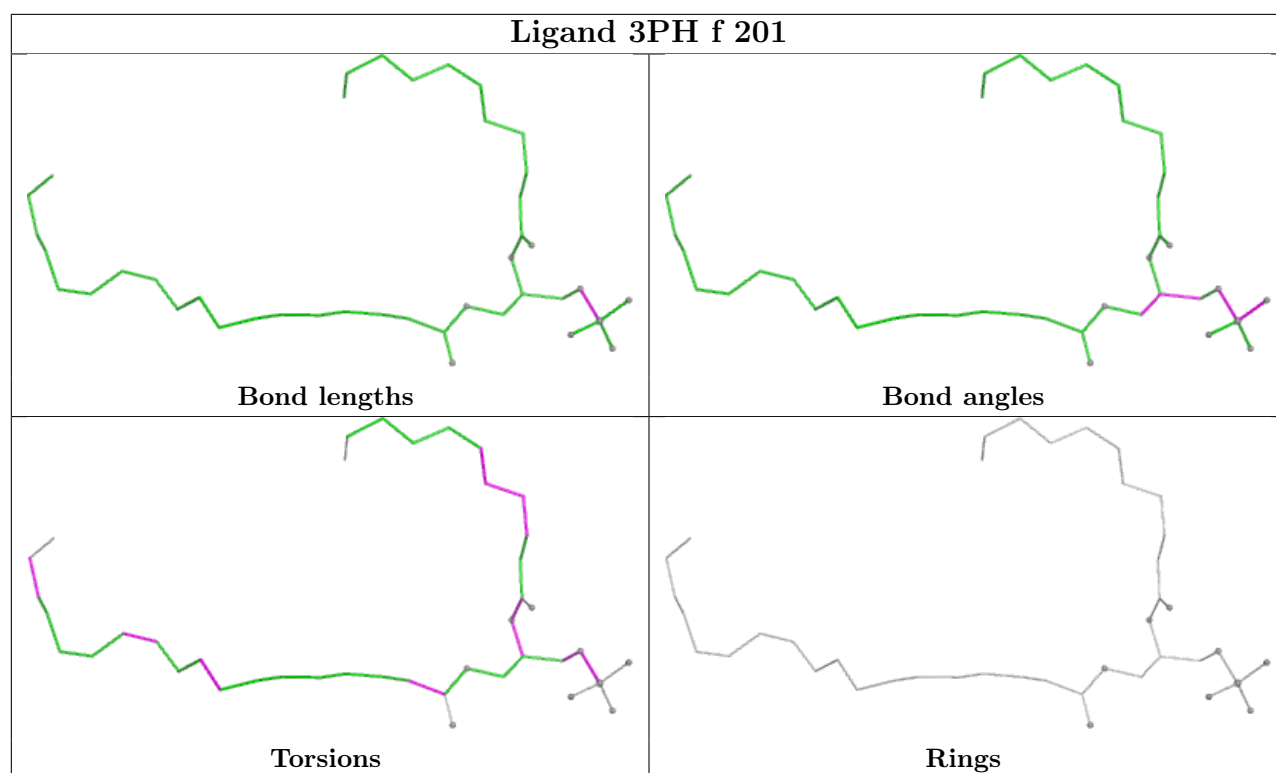


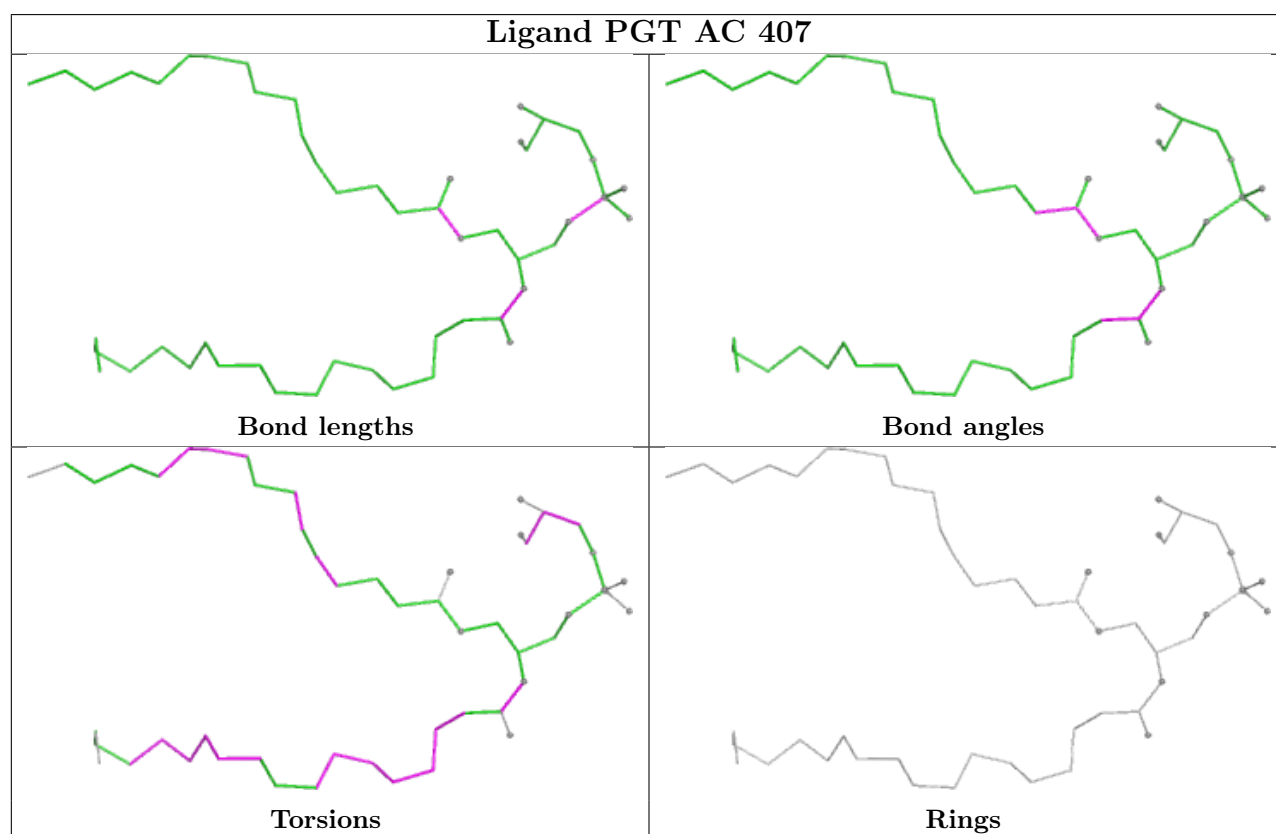
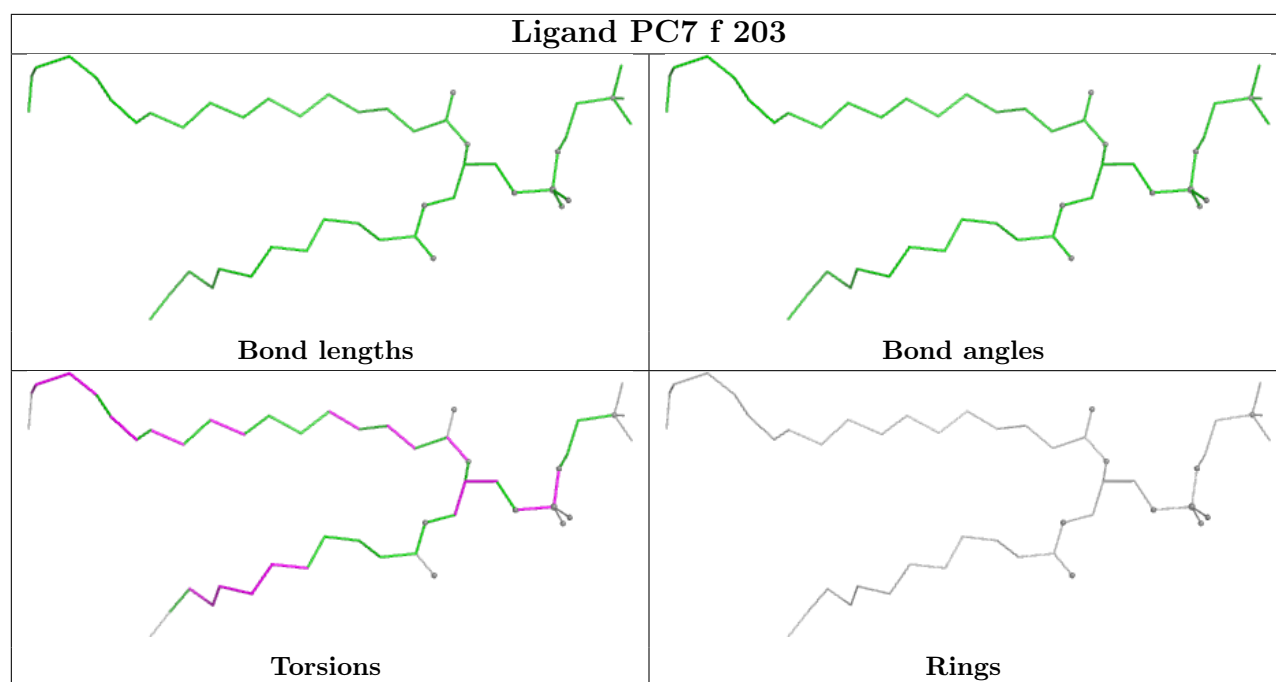


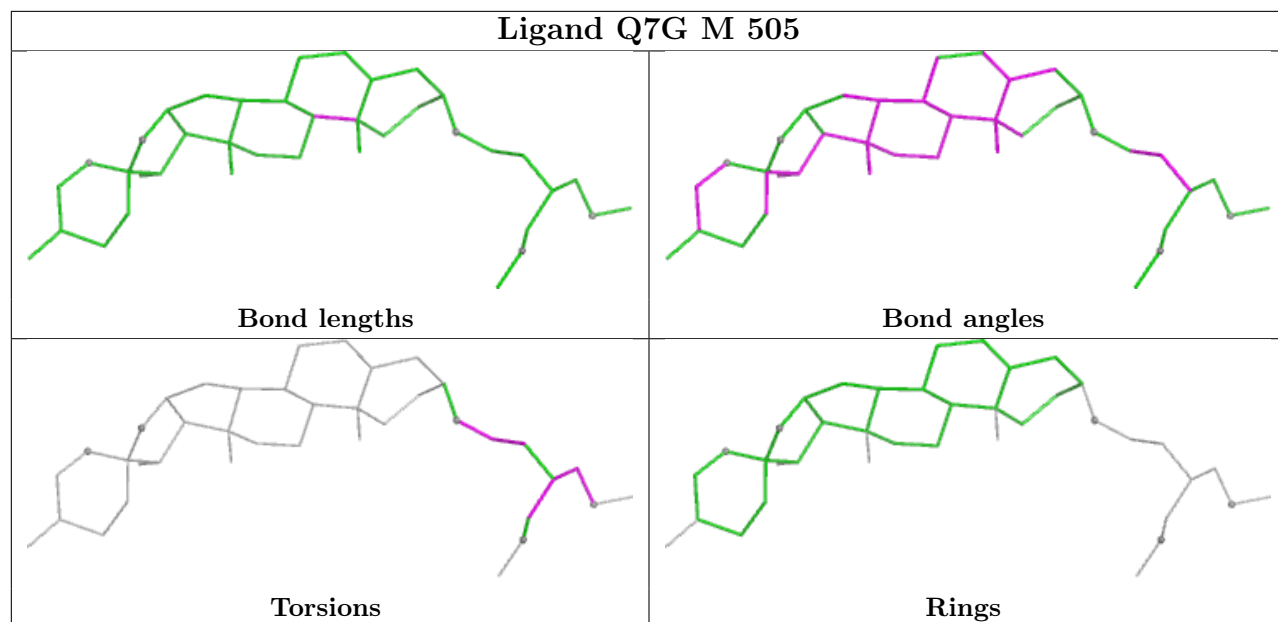




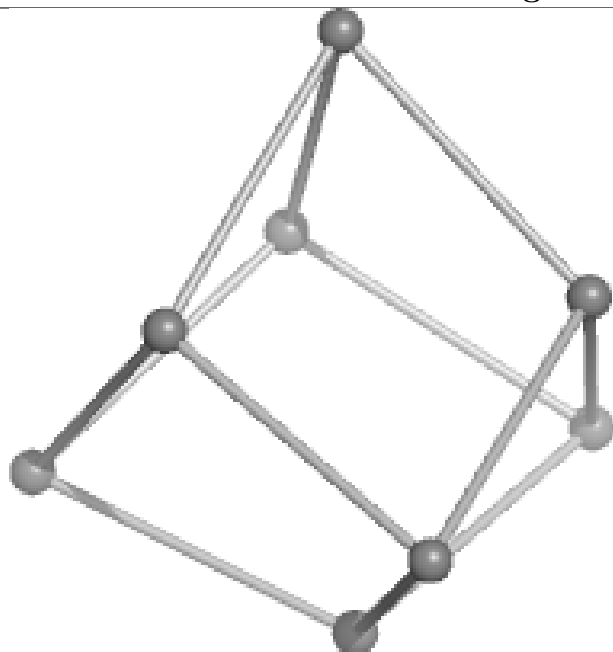




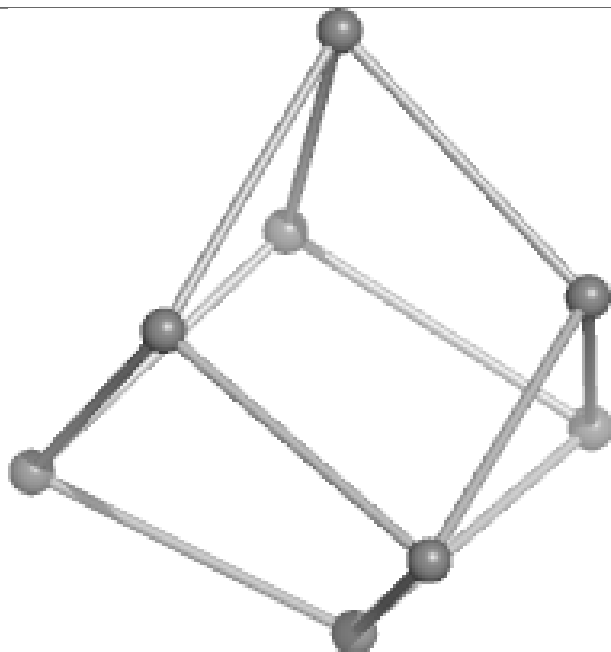




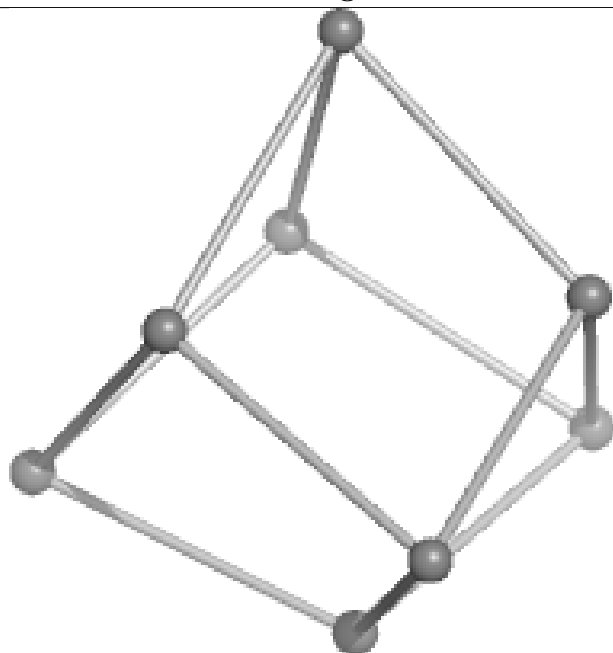
Ligand SF4 F 501



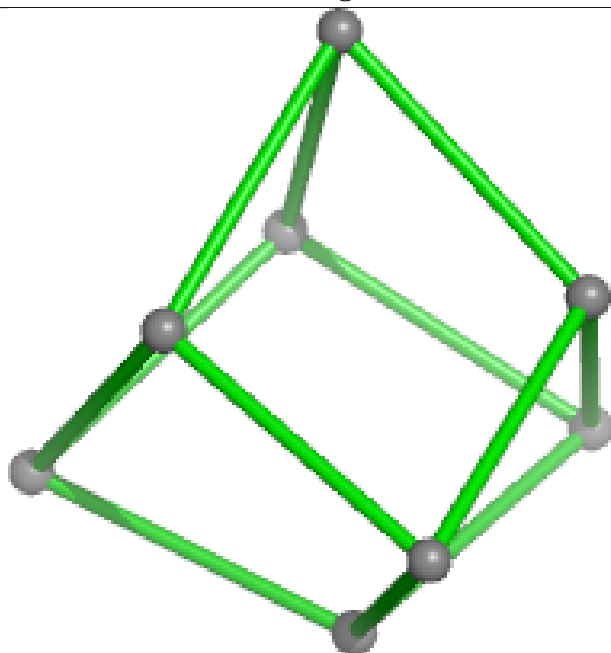
Bond lengths



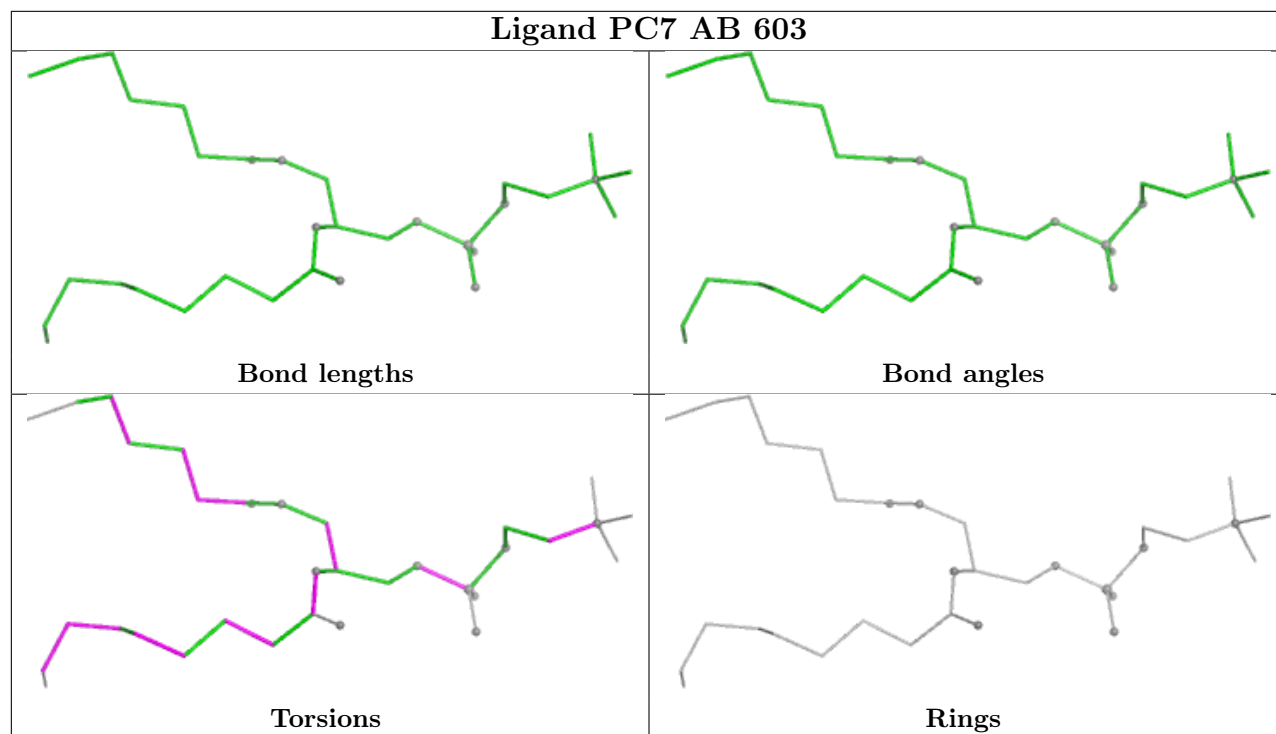
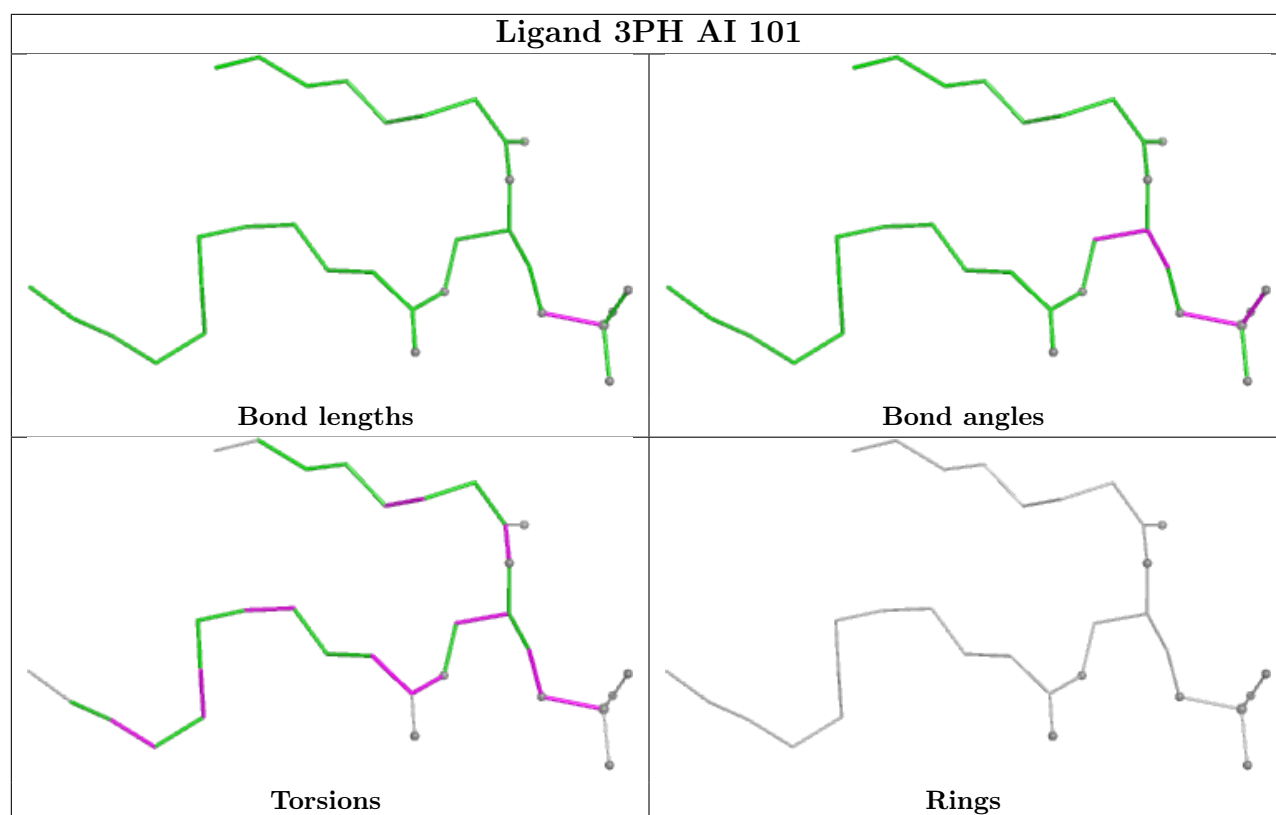
Bond angles

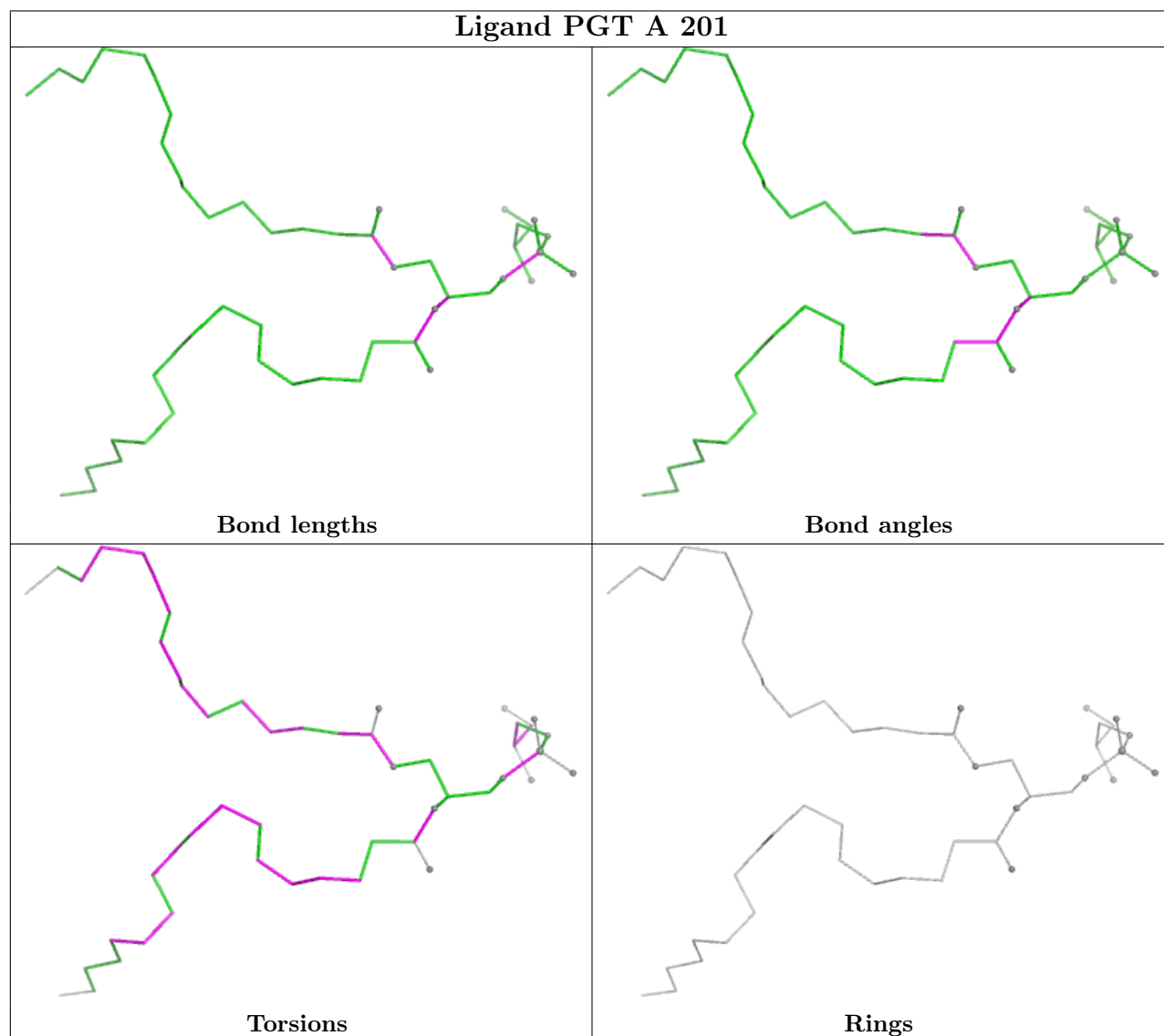
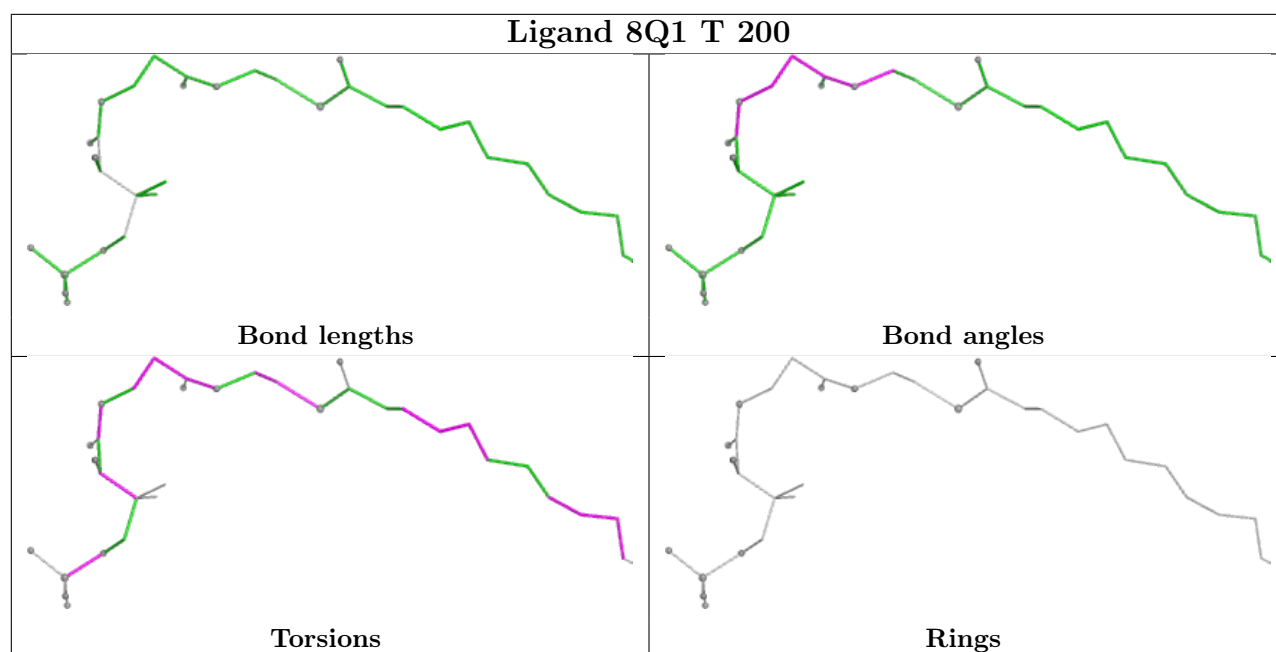


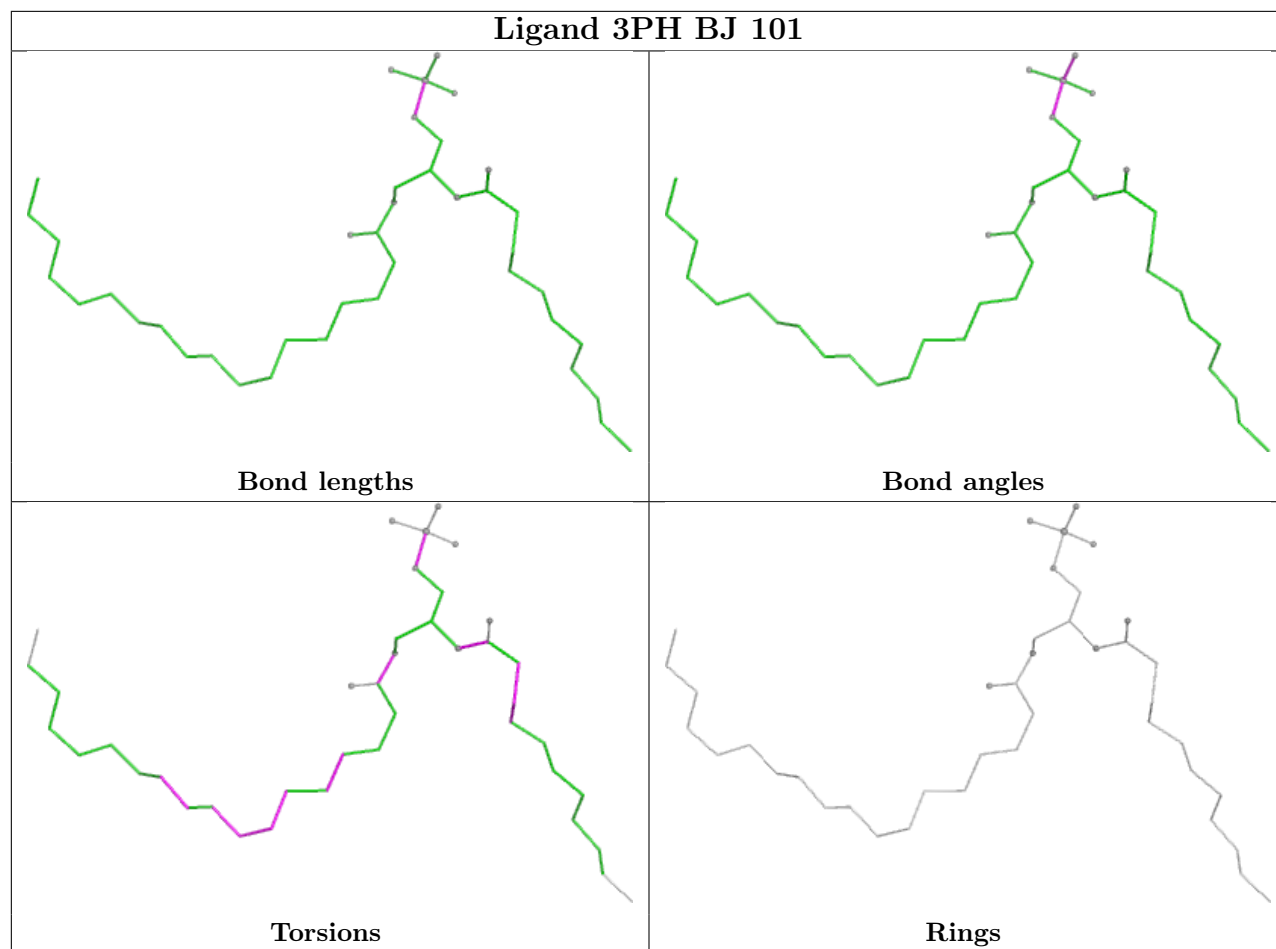
Torsions

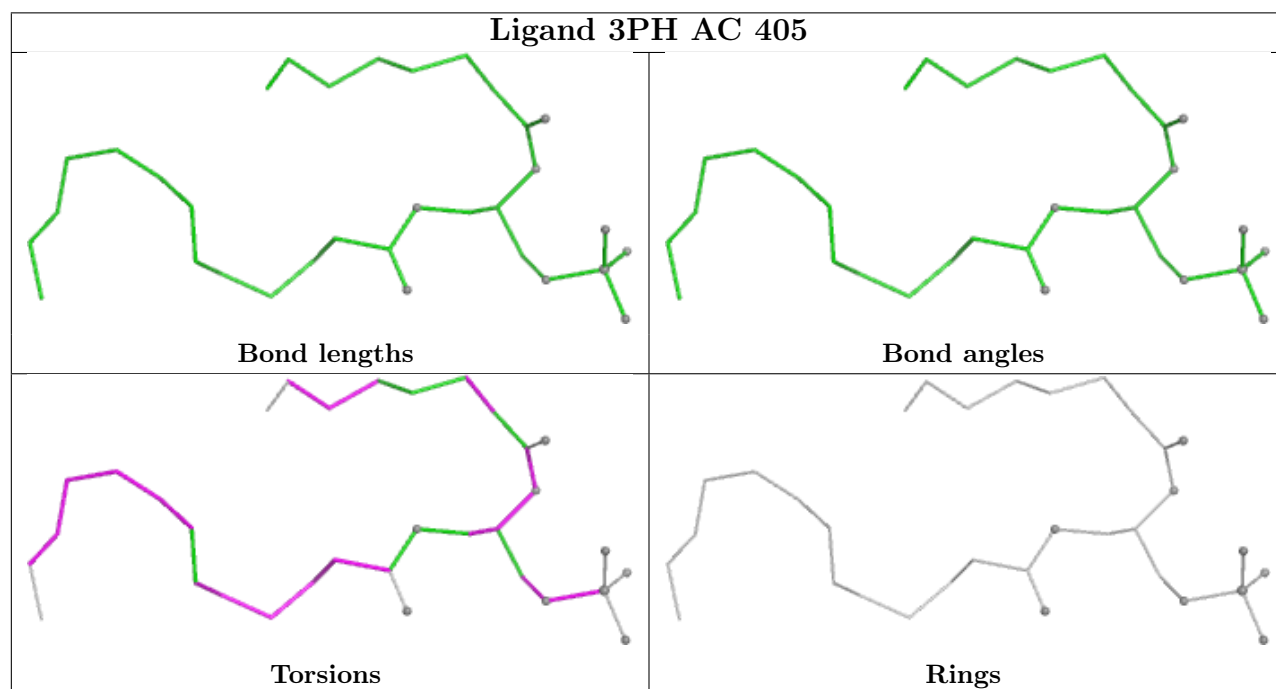
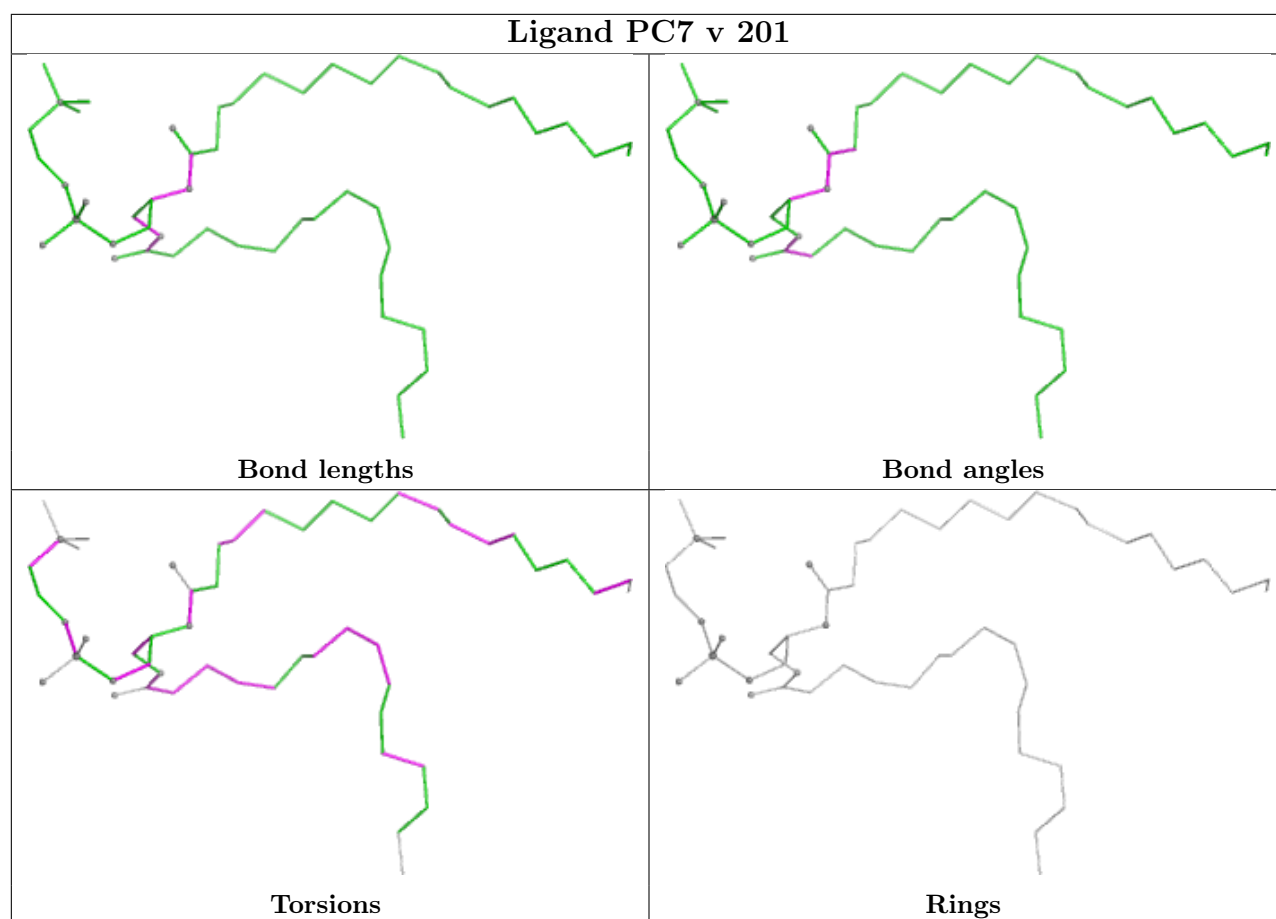


Rings

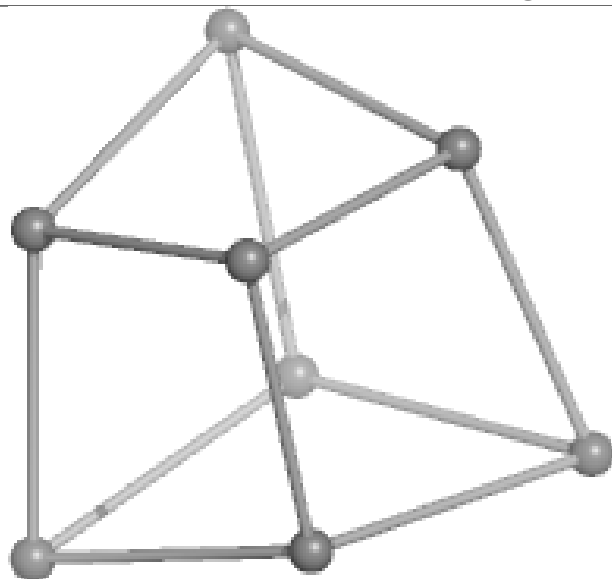




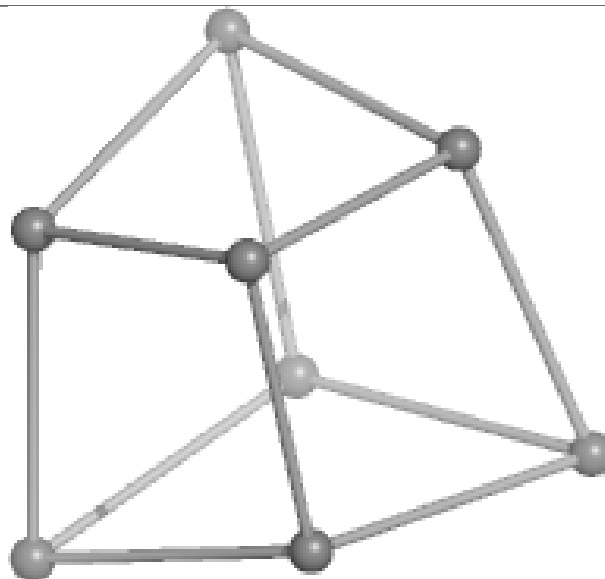




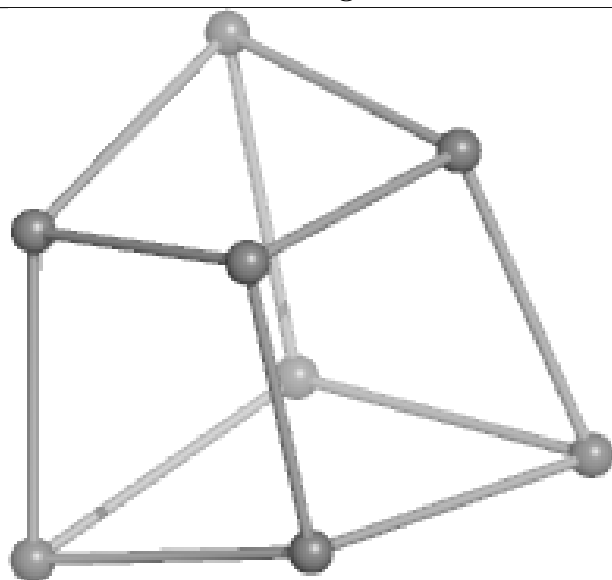
Ligand SF4 G 802



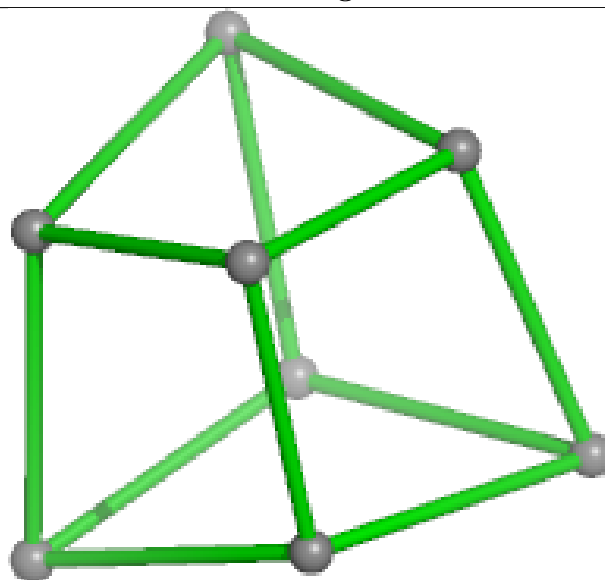
Bond lengths



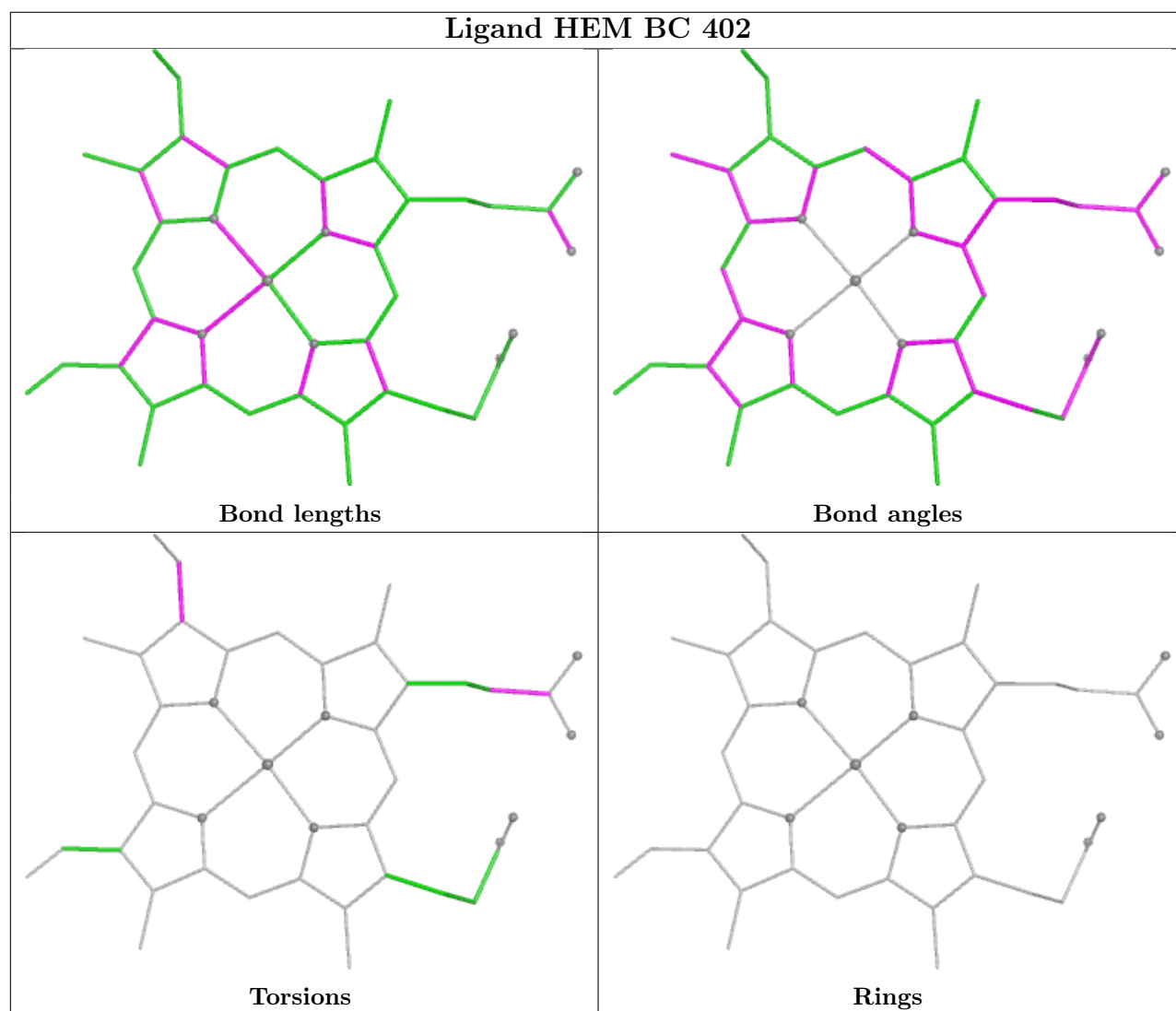
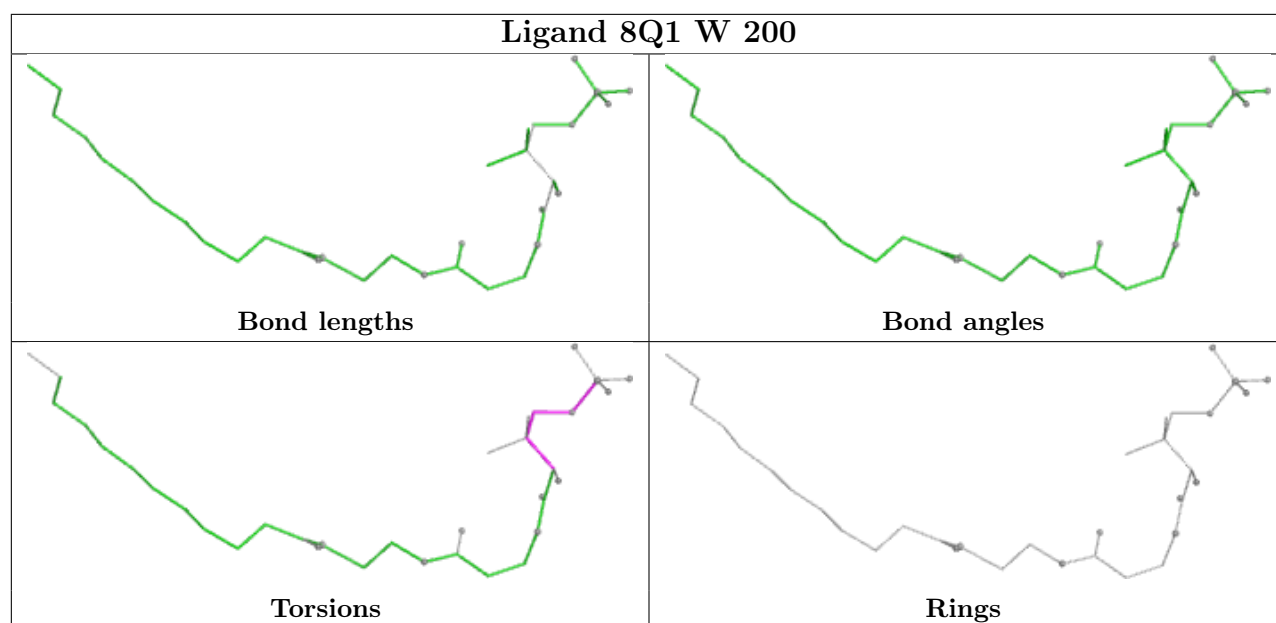
Bond angles

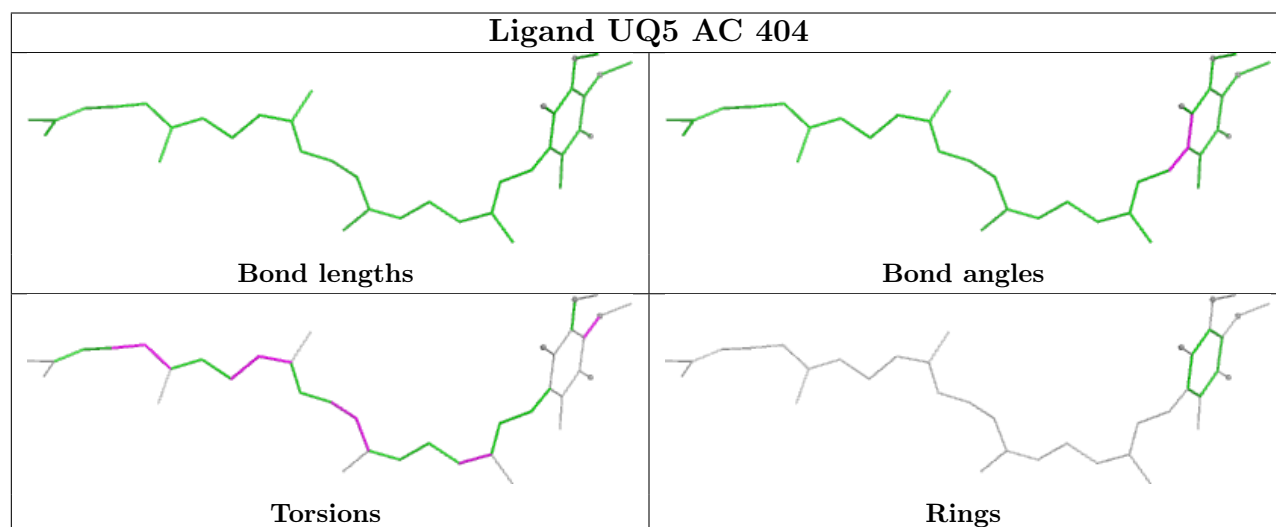
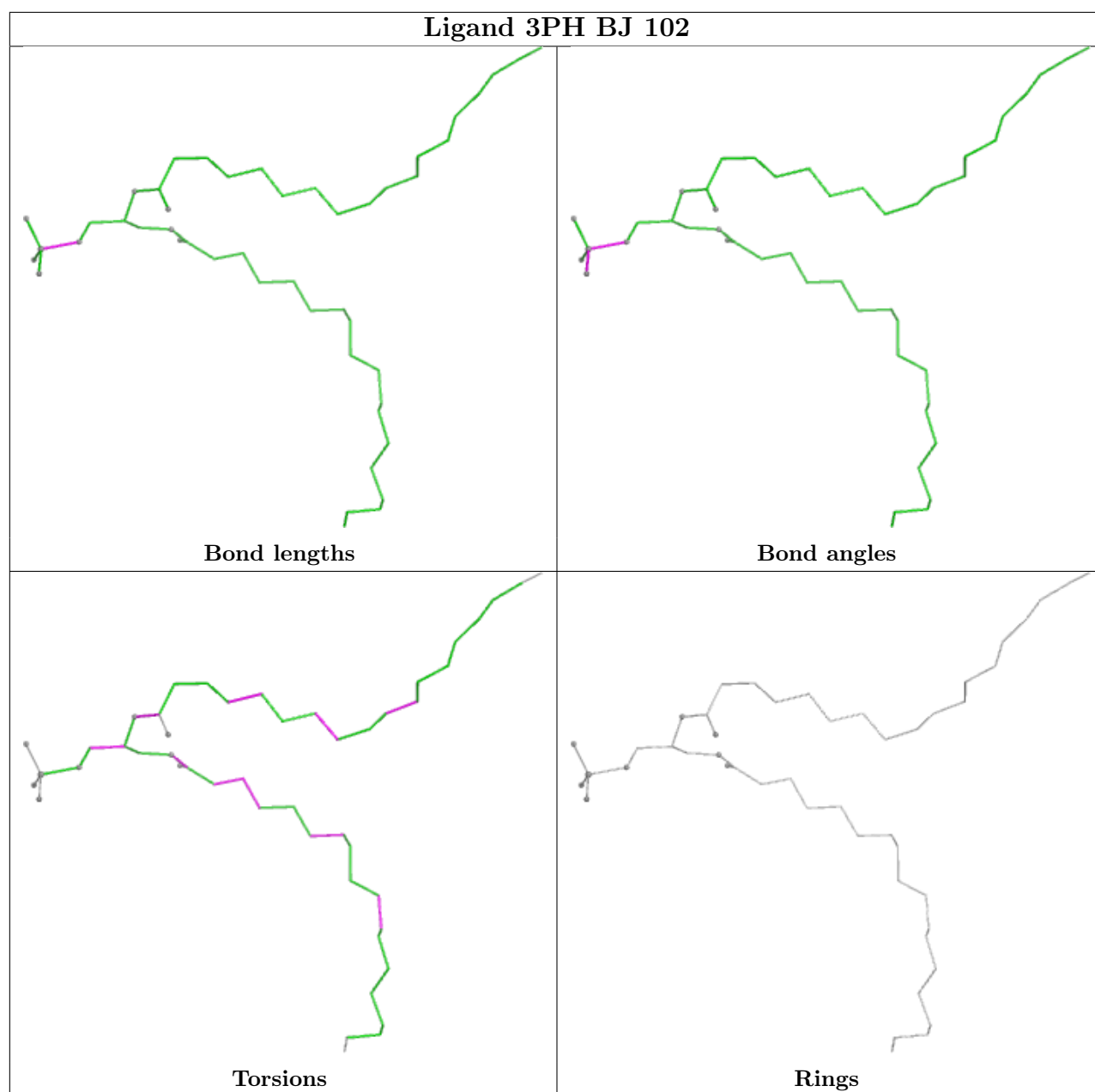


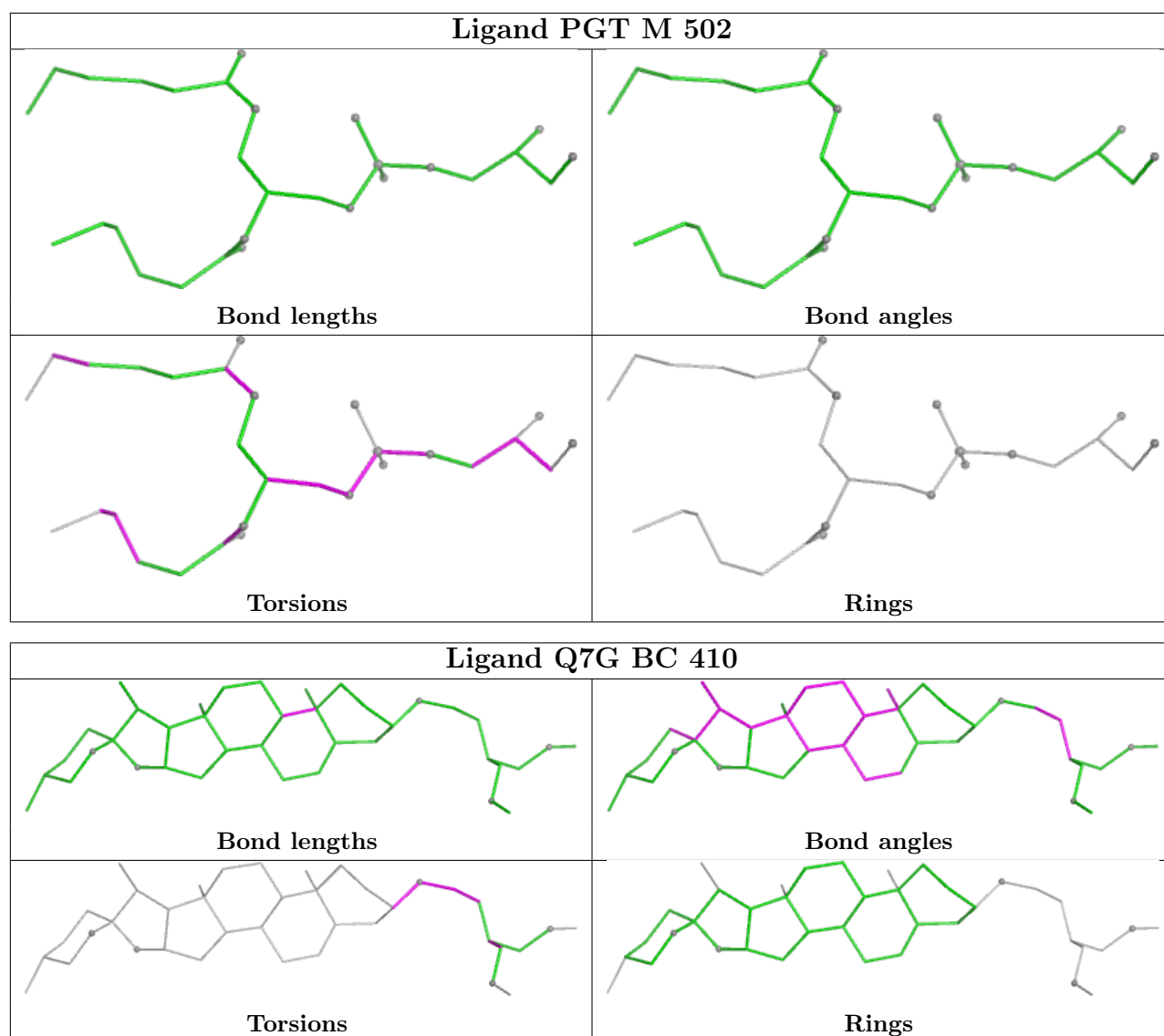
Torsions

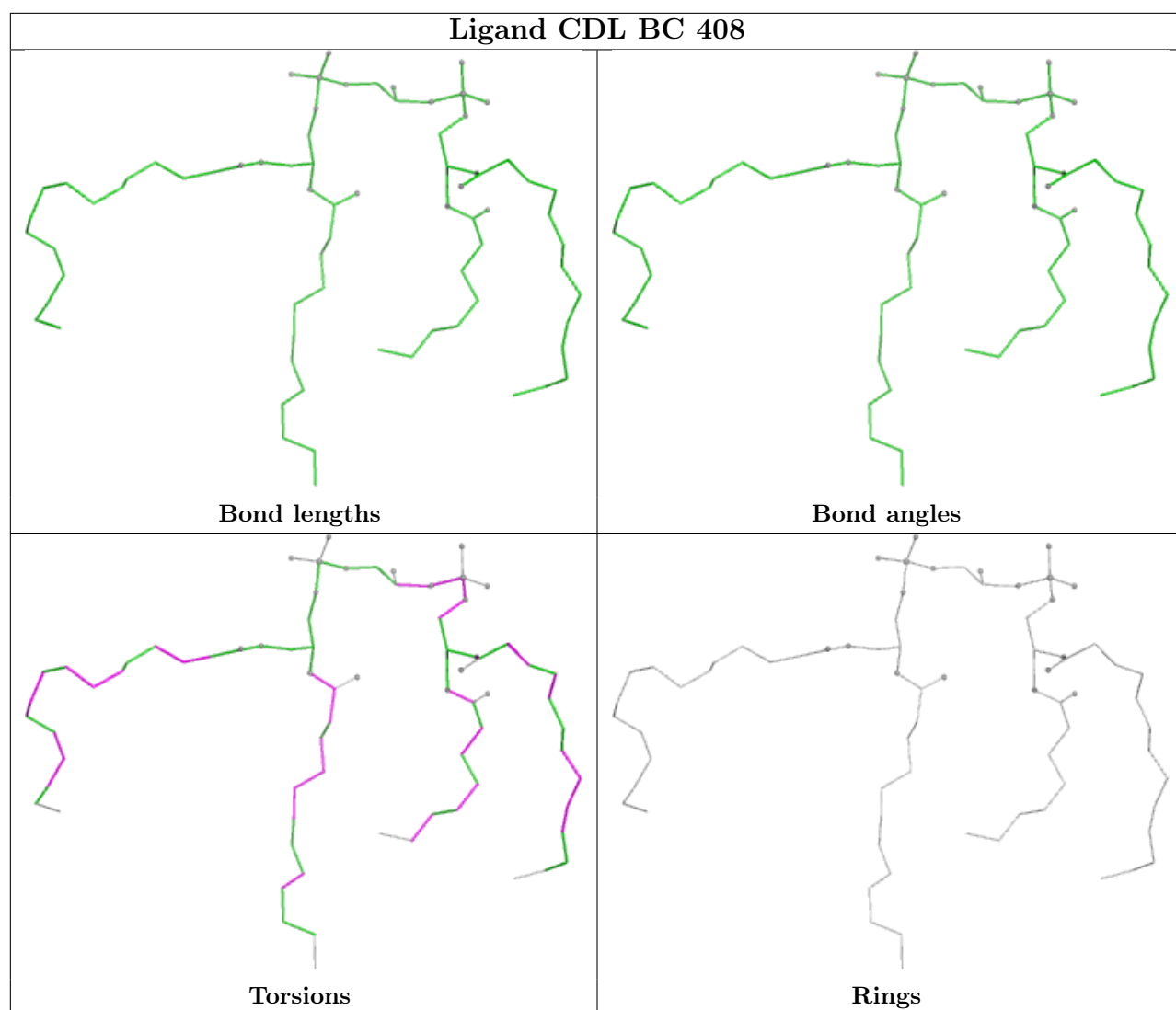


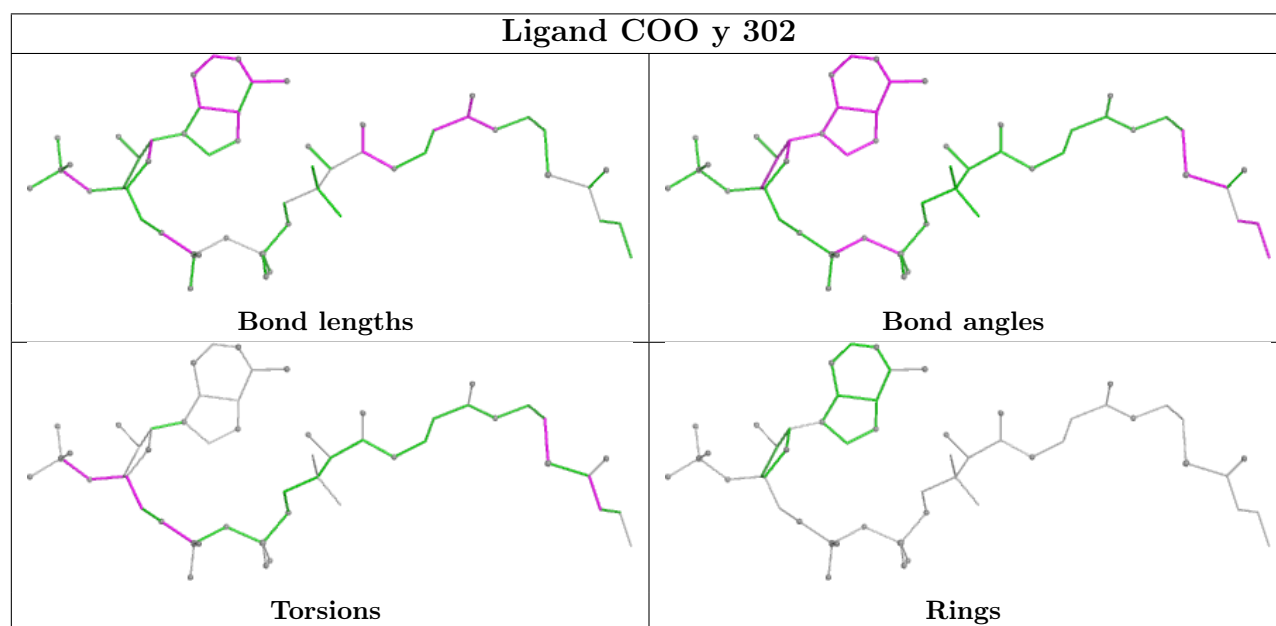
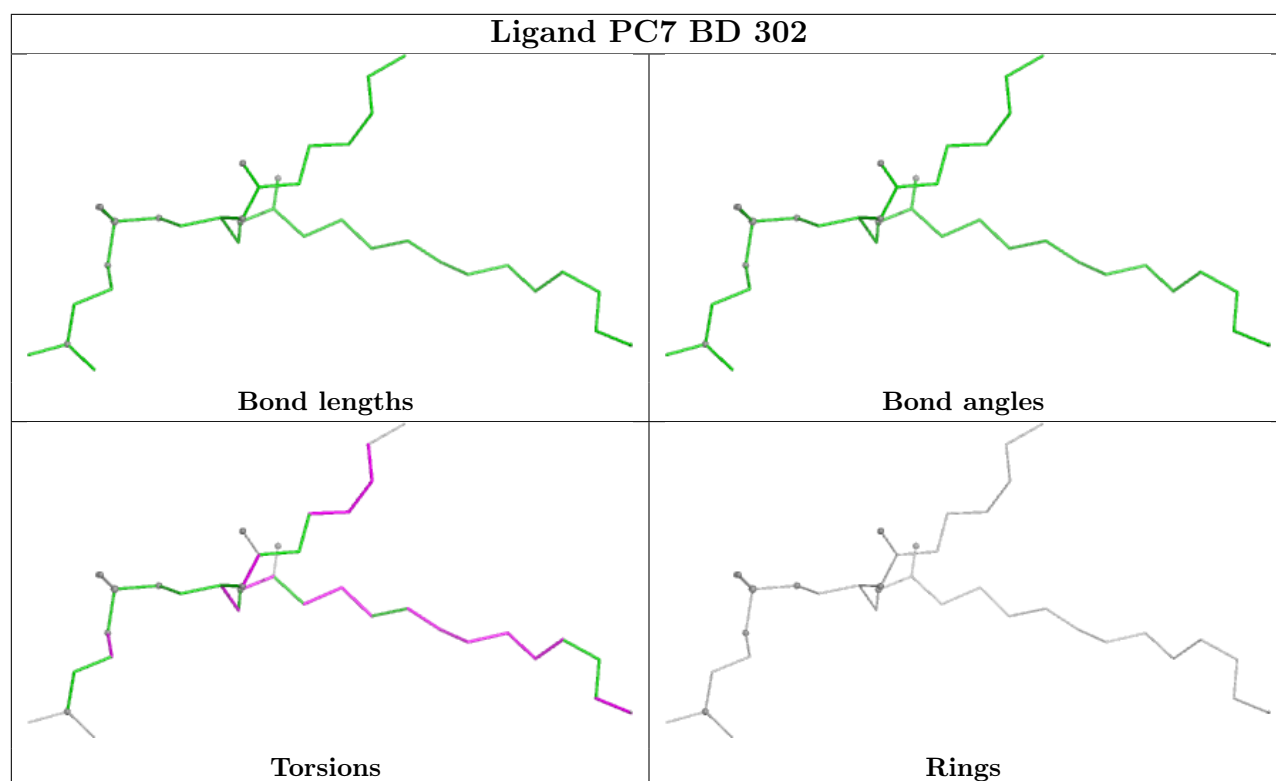
Rings

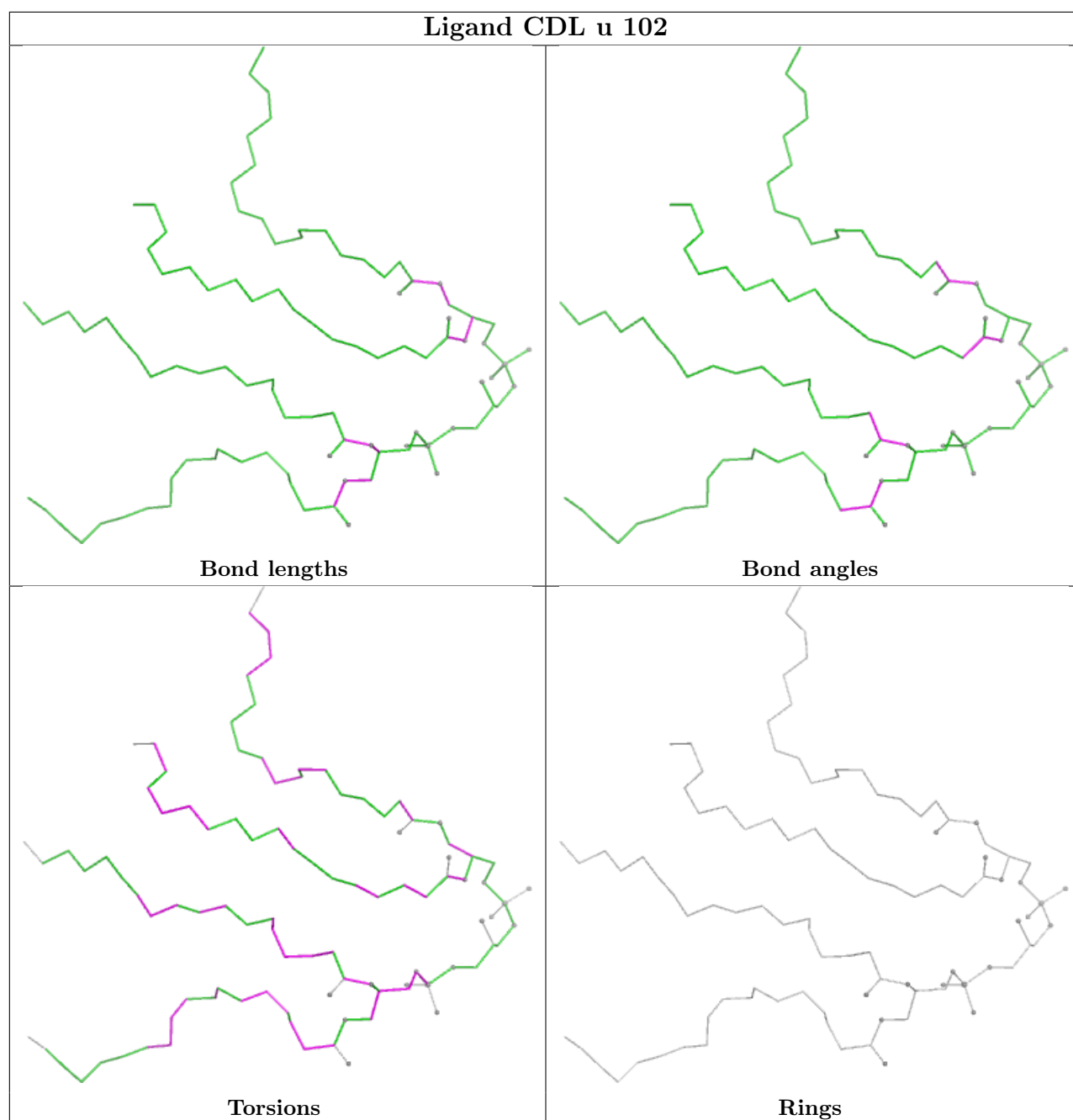


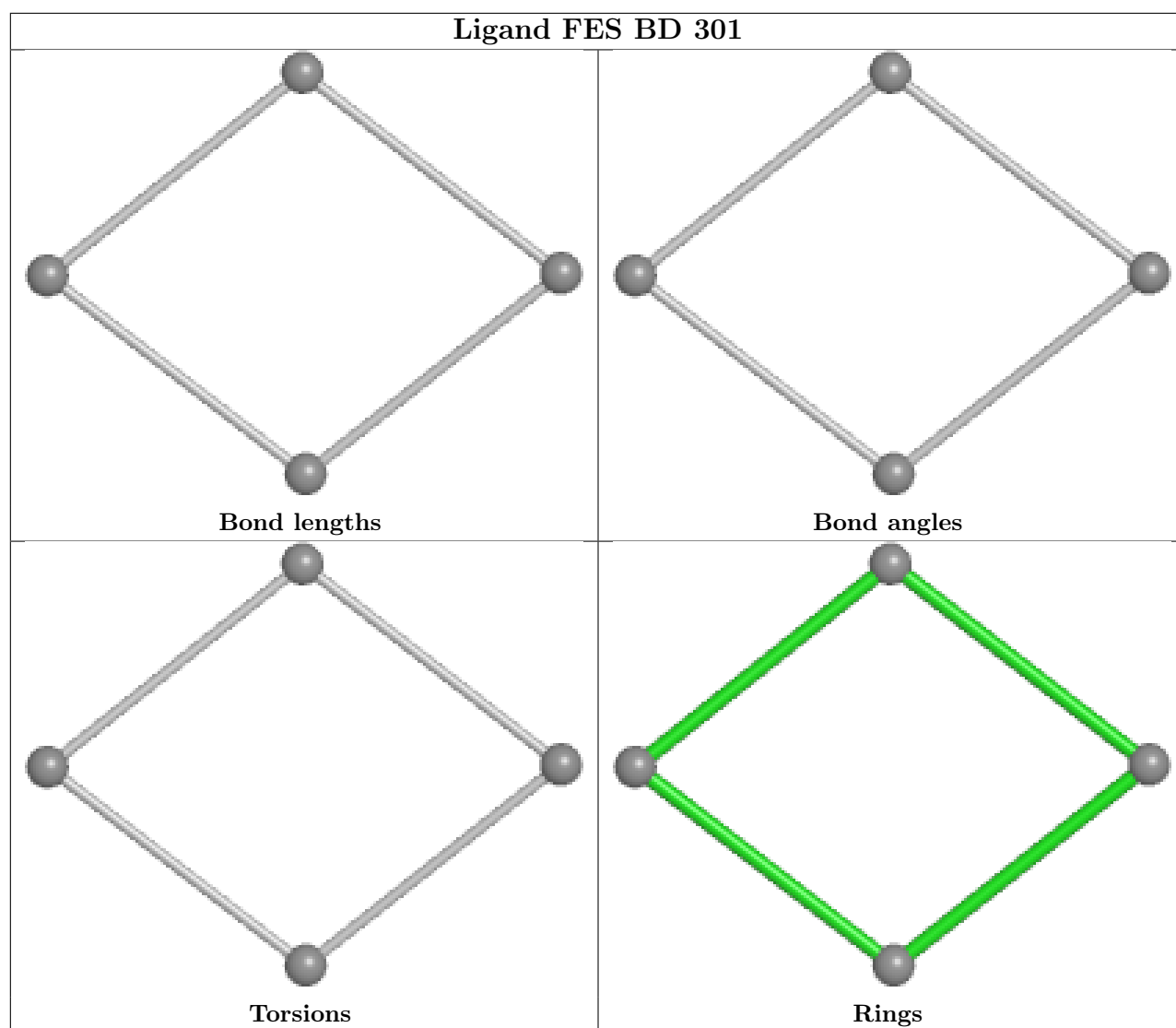












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

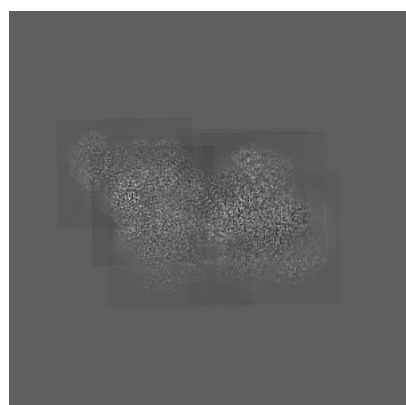
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16168. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

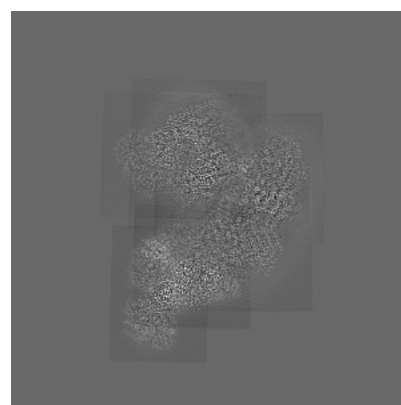
6.1.1 Primary map



X



Y

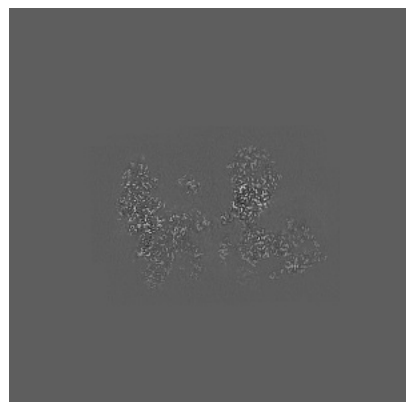


Z

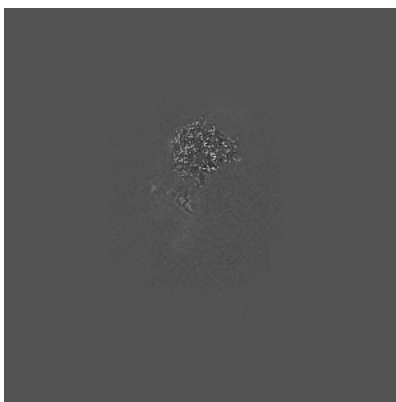
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

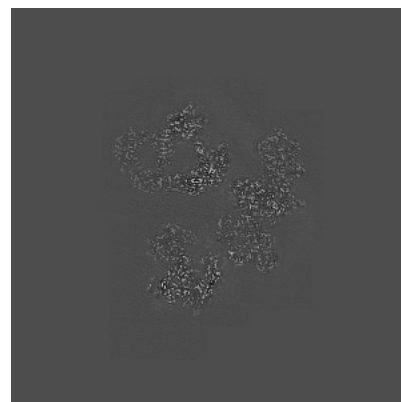
6.2.1 Primary map



X Index: 375



Y Index: 375



Z Index: 375

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

6.3 Largest variance slices [i](#)

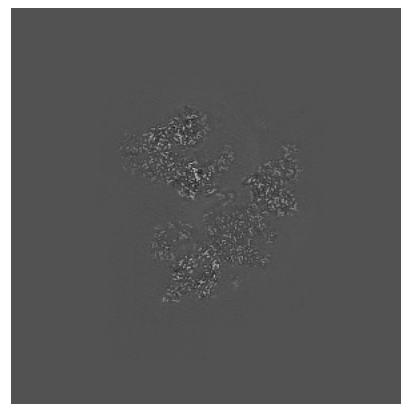
6.3.1 Primary map



X Index: 289



Y Index: 236

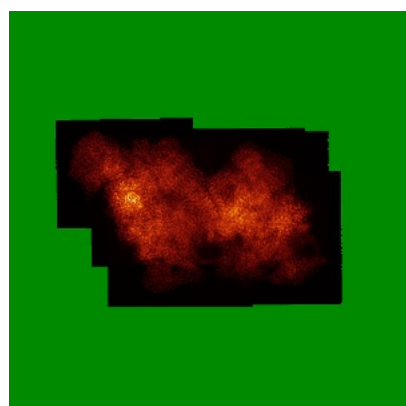


Z Index: 355

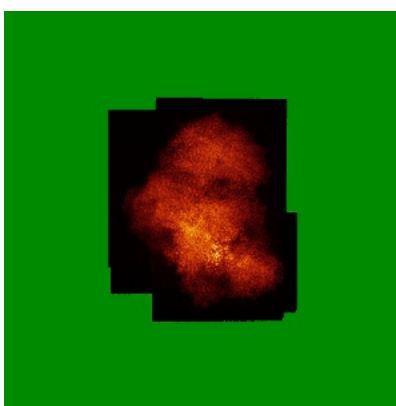
The images above show the largest variance slices of the map in three orthogonal directions.

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

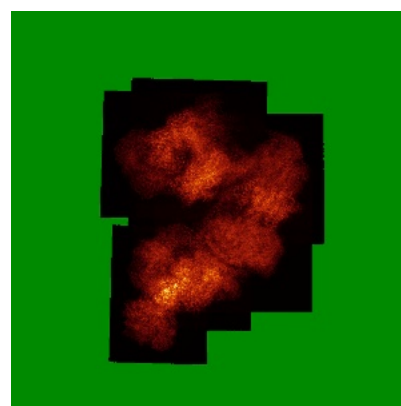
6.4.1 Primary map



X



Y

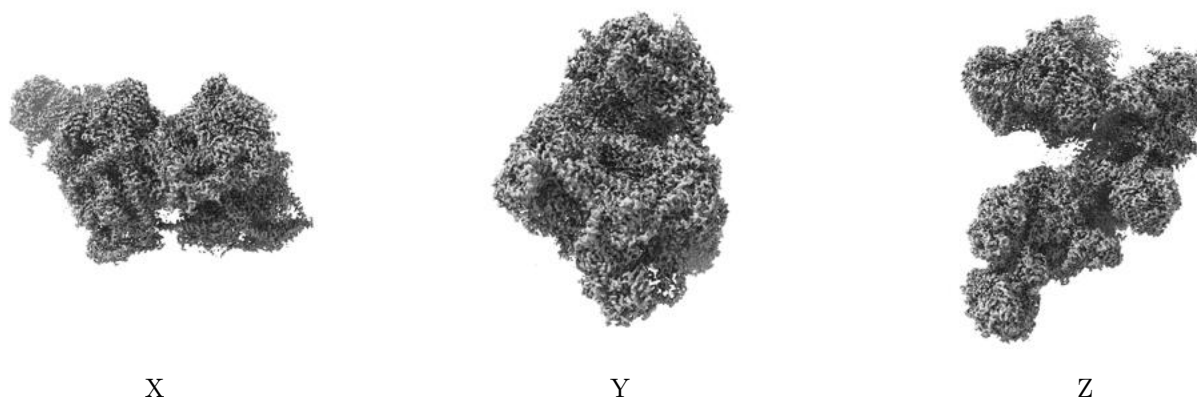


Z

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 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

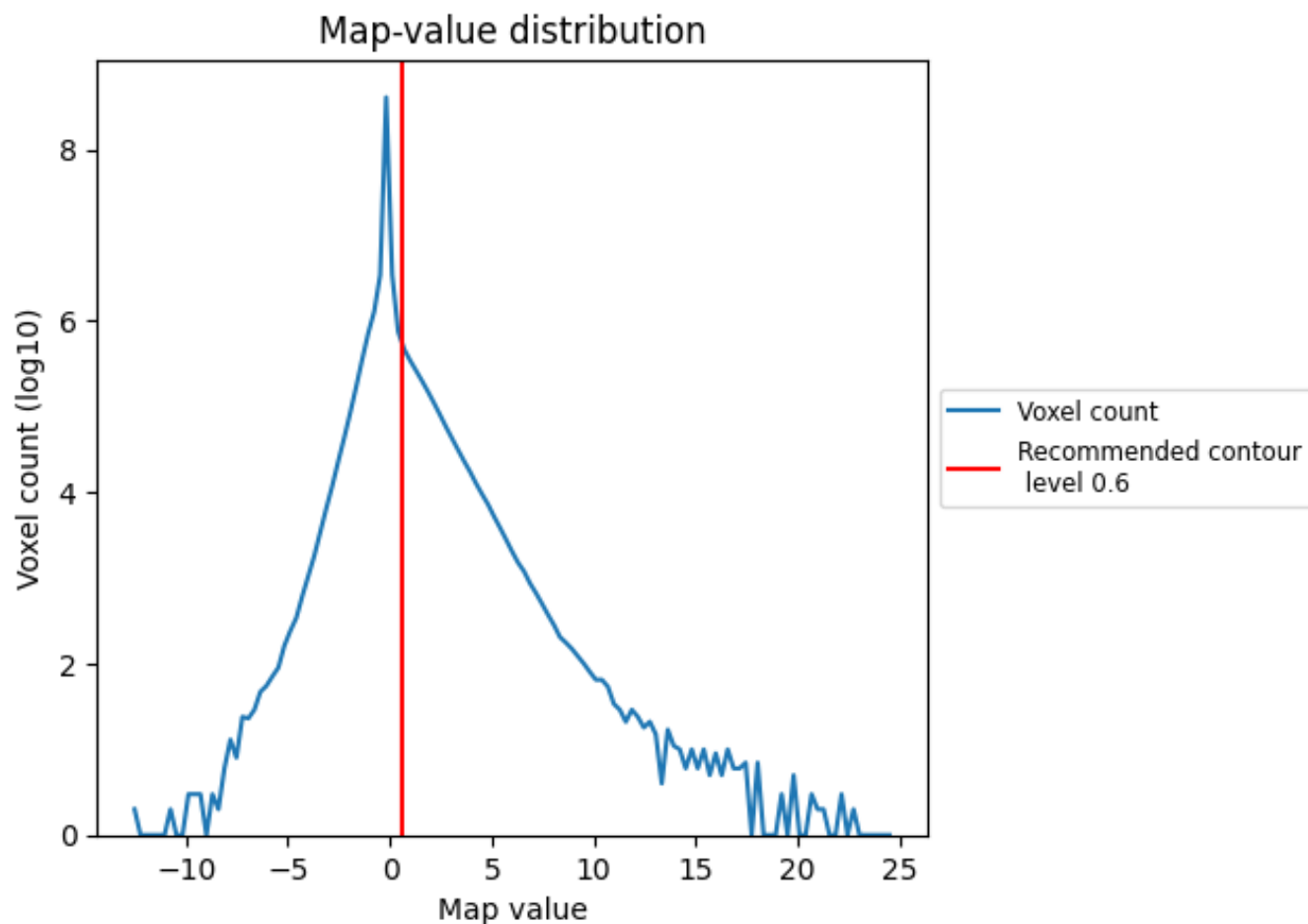
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

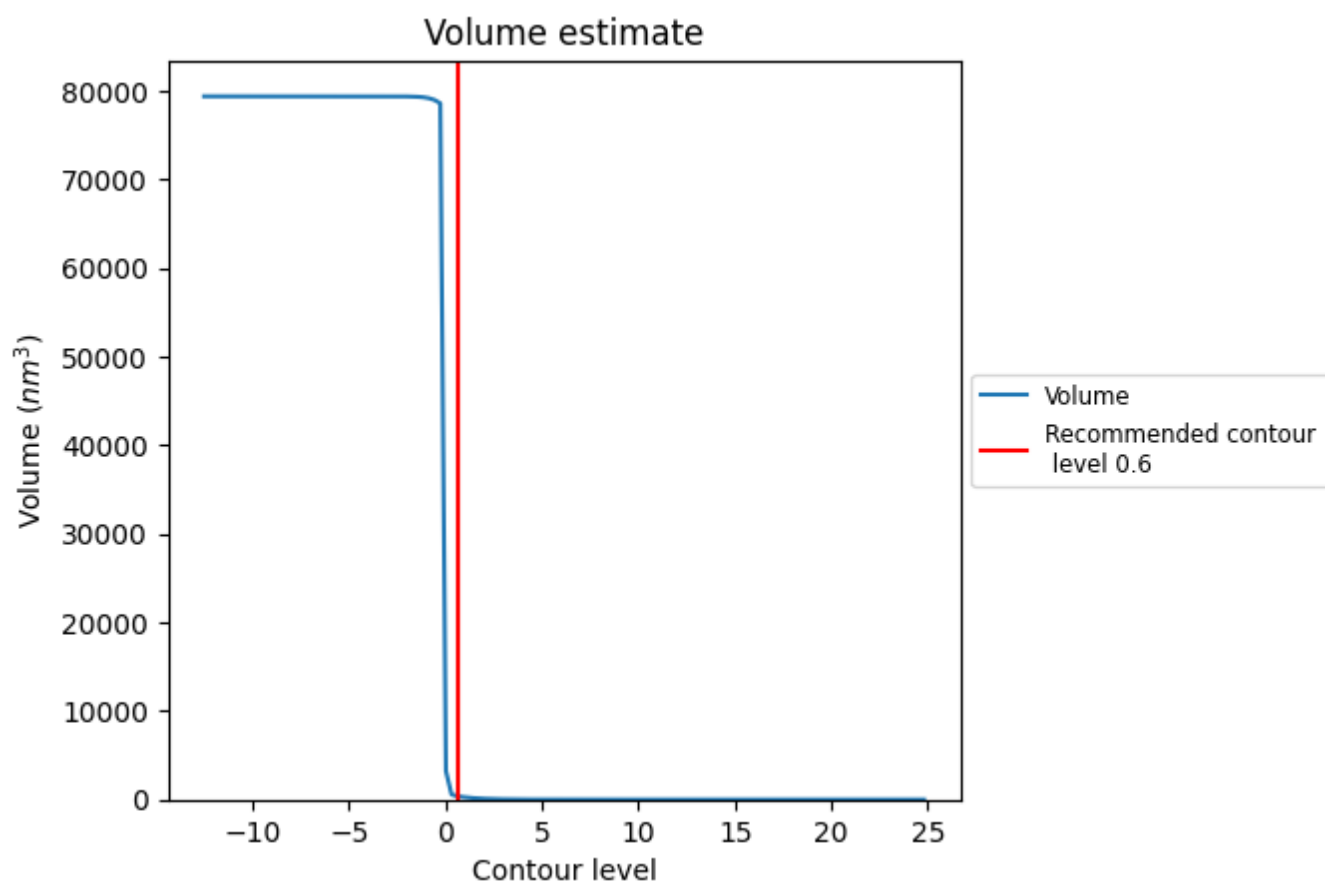
This section contains the results of statistical analysis of the map.

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.

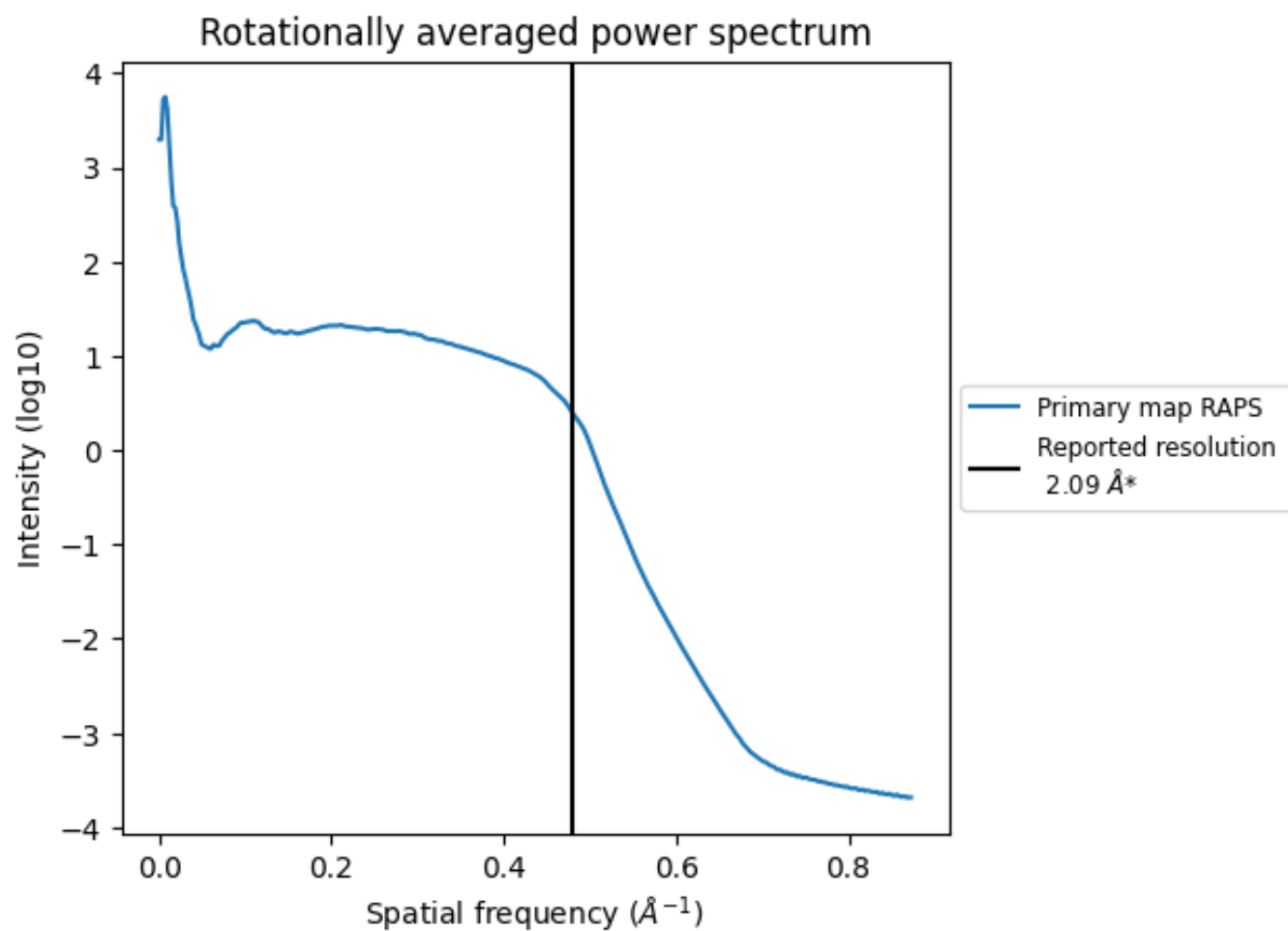
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390 nm^3 ; this corresponds to an approximate mass of 352 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 ⓘ

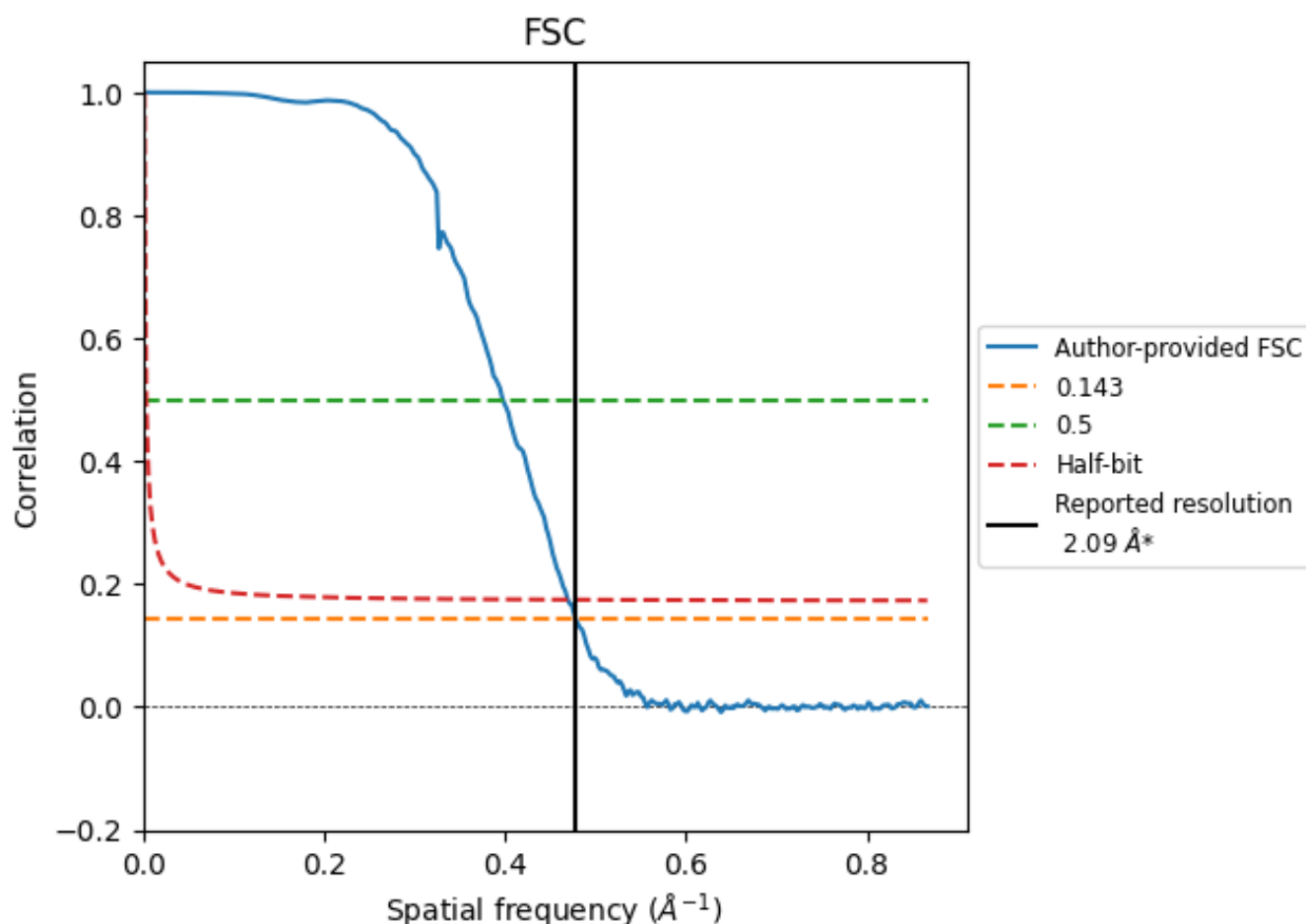


*Reported resolution corresponds to spatial frequency of 0.478 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.478 Å⁻¹

8.2 Resolution estimates [i](#)

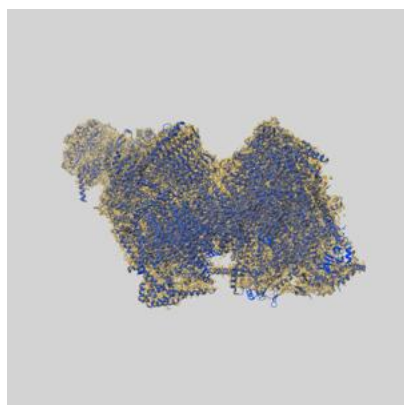
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.09	2.51	2.13
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

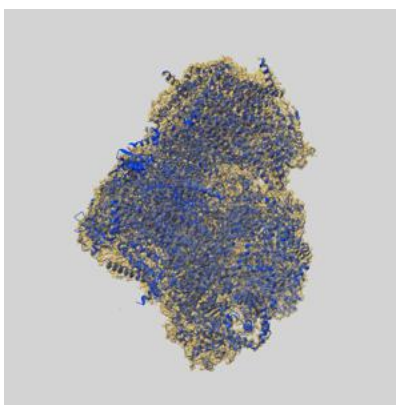
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16168 and PDB model 8BPX. Per-residue inclusion information can be found in section [3](#) on page [33](#).

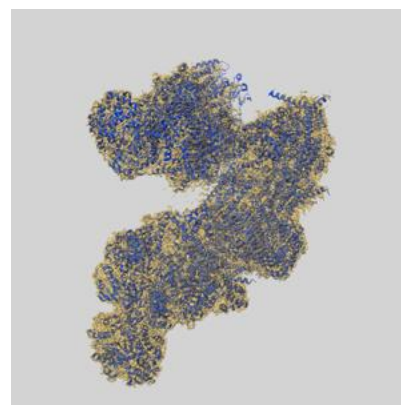
9.1 Map-model overlay [i](#)



X



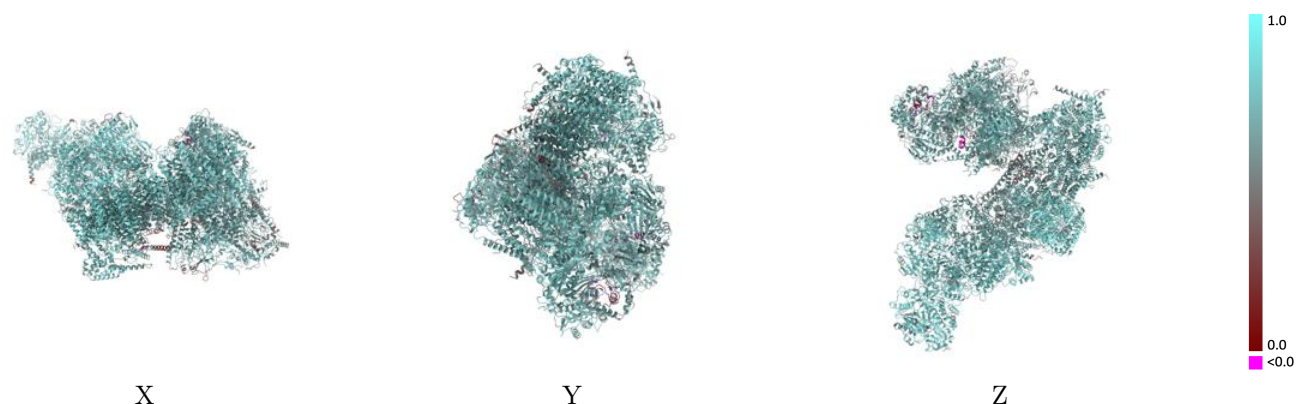
Y



Z

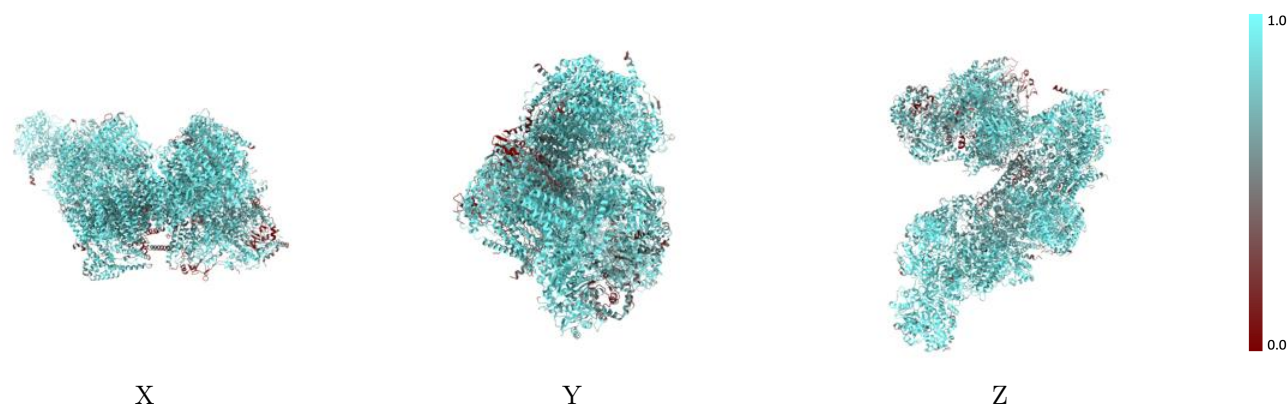
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



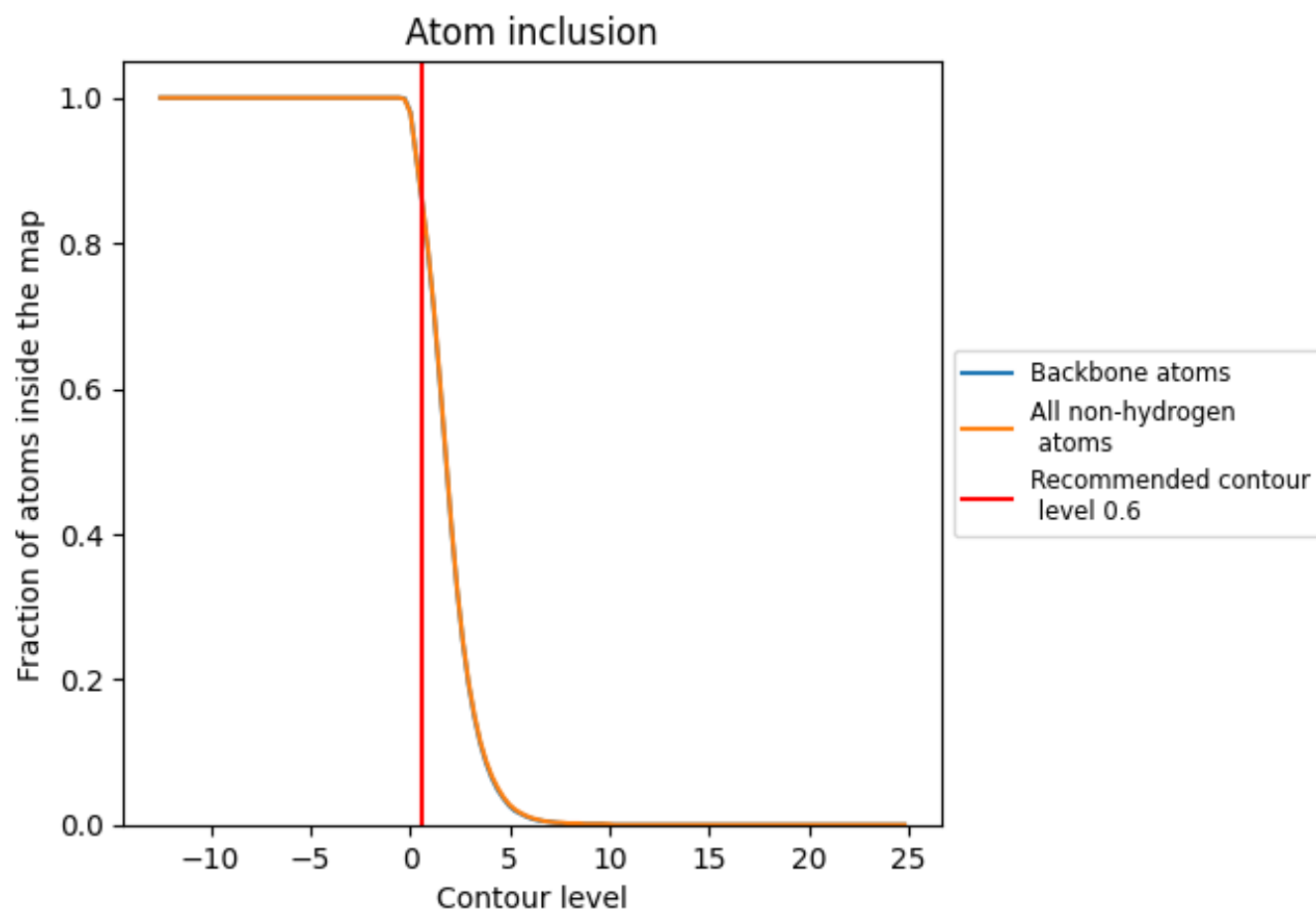
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.7070
A	 0.9390	 0.7560
AA	 0.6670	 0.5930
AB	 0.8810	 0.7020
AC	 0.9060	 0.7190
AD	 0.5260	 0.5880
AE	 0.9120	 0.7220
AF	 0.9330	 0.7300
AG	 0.8570	 0.6890
AH	 0.7710	 0.6450
AI	 0.8330	 0.6880
AJ	 0.5700	 0.5930
B	 0.9790	 0.8060
BA	 0.6820	 0.6050
BB	 0.8730	 0.7010
BC	 0.8880	 0.7010
BD	 0.5720	 0.5910
BE	 0.8800	 0.6940
BF	 0.9170	 0.6960
BG	 0.7870	 0.6430
BH	 0.6090	 0.5780
BI	 0.7820	 0.6380
BJ	 0.5730	 0.5980
C	 0.9580	 0.7940
D	 0.9530	 0.7910
E	 0.8470	 0.6810
F	 0.9330	 0.7460
G	 0.9220	 0.7420
H	 0.9250	 0.7710
I	 0.9650	 0.7850
J	 0.9060	 0.7450
K	 0.9170	 0.7600
L	 0.9240	 0.7200
M	 0.9270	 0.7270
N	 0.9420	 0.7730



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	 0.9360	 0.7570
P	 0.8670	 0.6930
Q	 0.8190	 0.6700
R	 0.8840	 0.7270
S	 0.9100	 0.7020
T	 0.8290	 0.6560
U	 0.6240	 0.5640
V	 0.8690	 0.7290
W	 0.8390	 0.6900
X	 0.8100	 0.7000
Y	 0.5890	 0.5500
Z	 0.8420	 0.7090
a	 0.8430	 0.7150
b	 0.7520	 0.6610
c	 0.9220	 0.7100
d	 0.7720	 0.6850
e	 0.8670	 0.7180
f	 0.8850	 0.7520
g	 0.7840	 0.6390
i	 0.6430	 0.5780
j	 0.8420	 0.6610
k	 0.8080	 0.6400
l	 0.8100	 0.6520
m	 0.8630	 0.6840
n	 0.9130	 0.6840
o	 0.8270	 0.6810
p	 0.8610	 0.6780
q	 0.9190	 0.7380
u	 0.5850	 0.5480
v	 0.8830	 0.7440
x	 0.9600	 0.7990
y	 0.9120	 0.7580
z	 0.9050	 0.7460