



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2025 – 06:40 am GMT

PDB ID : 9F5Y
EMDB ID : EMD-50203
Title : Structure of the Chlamydomonas reinhardtii respiratory complex I from respiratory supercomplex
Authors : Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on : 2024-04-30
Resolution : 2.51 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.5

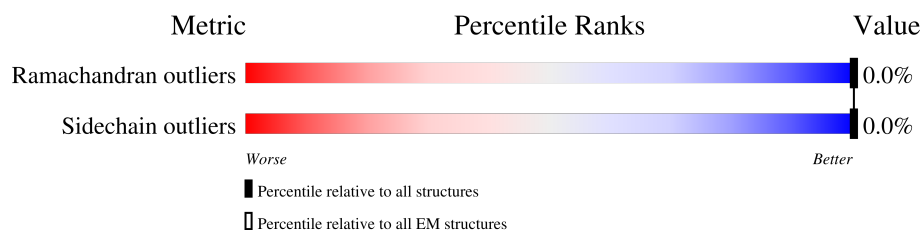
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 2.51 Å.

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







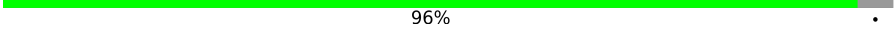
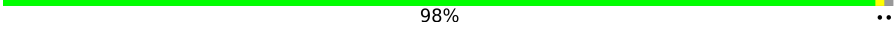

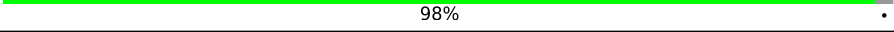
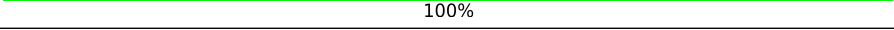

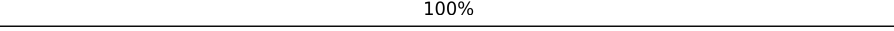
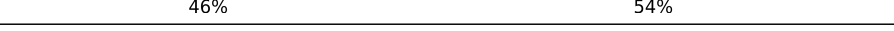
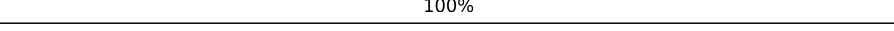
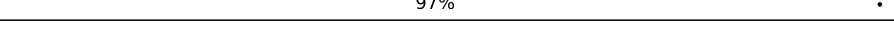





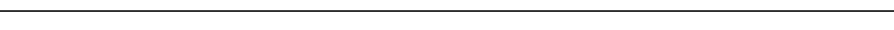

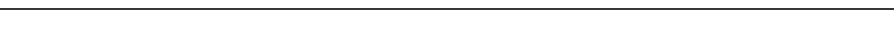
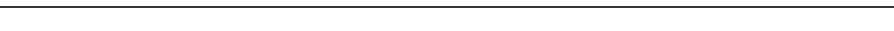


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	282	 85% 15%
2	B	484	 90% 10%
3	C	733	 94% 6%
4	D	282	 77% 23%
5	E	467	 82% 18%
6	F	164	 96% .
7	G	231	 86% 14%
8	H	118	 75% . 24%
9	I	165	 82% 18%
10	J	128	 66% 34%

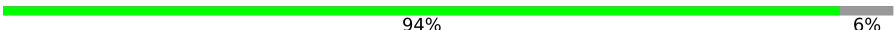
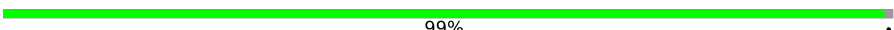
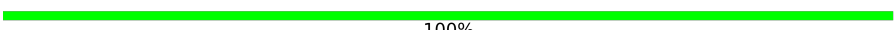
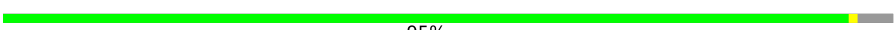








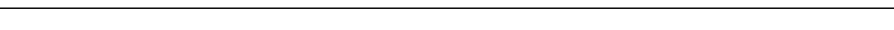
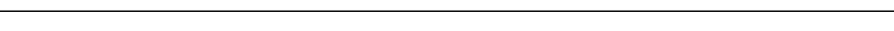
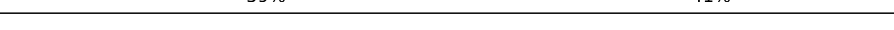

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Mol	Chain	Length	Quality of chain
10	r	128	
11	K	138	
12	L	187	
13	M	154	
14	N	156	
15	O	101	
16	P	397	
17	Q	292	
18	R	387	
19	S	279	
20	T	443	
21	U	227	
22	V	546	
23	W	162	
24	X	149	
25	Y	64	
26	Z	124	
27	a	129	
28	b	172	
29	c	67	
30	d	86	
31	e	219	
32	f	65	
33	g	55	
34	h	142	

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Mol	Chain	Length	Quality of chain
35	i	81	 94% 6%
36	j	86	 99% .
37	k	117	 100%
38	l	121	 95% . .
39	m	142	 97% .
40	n	106	 98% .
41	o	155	 98% .
42	p	130	 99% .
43	q	197	 80% 20%
44	s	312	 100%
45	t	279	 90% 9%
46	u	229	 100%
47	v	45	 100%
48	w	109	 59% 41%
49	x	157	 53% 47%
50	y	118	 97% .

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 75117 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 24 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase 78 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		

- Molecule 4 is a protein called NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase 49 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	383	Total	C	N	O	S	0	0
			3085	1971	537	554	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		

- Molecule 7 is a protein called NADH:ubiquinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		

- Molecule 8 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		

- Molecule 9 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
10	r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase 13 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		

- Molecule 16 is a protein called Putative NADH:ubiquinone oxidoreductase 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		

- Molecule 21 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		

- Molecule 24 is a protein called ASH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		

- Molecule 25 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		

- Molecule 26 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		

- Molecule 27 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		

- Molecule 28 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		

- Molecule 29 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		

- Molecule 30 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		

- Molecule 31 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		

- Molecule 32 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		

- Molecule 33 is a protein called Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		

- Molecule 34 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase 15 kDa subunit-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase 20,9 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		

- Molecule 40 is a protein called Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		

- Molecule 41 is a protein called Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		

- Molecule 42 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		

- Molecule 43 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		

- Molecule 44 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		

- Molecule 45 is a protein called CAG2 - CA-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		

- Molecule 46 is a protein called CAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		

- Molecule 47 is a protein called P10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		

- Molecule 48 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		

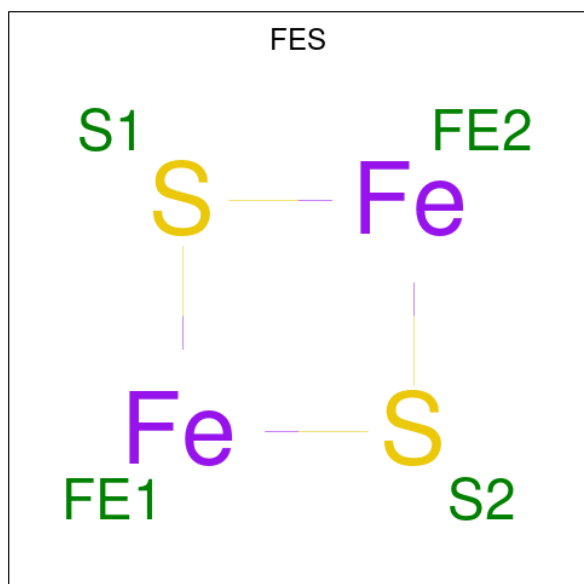
- Molecule 49 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		

- Molecule 50 is a protein called NUOP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



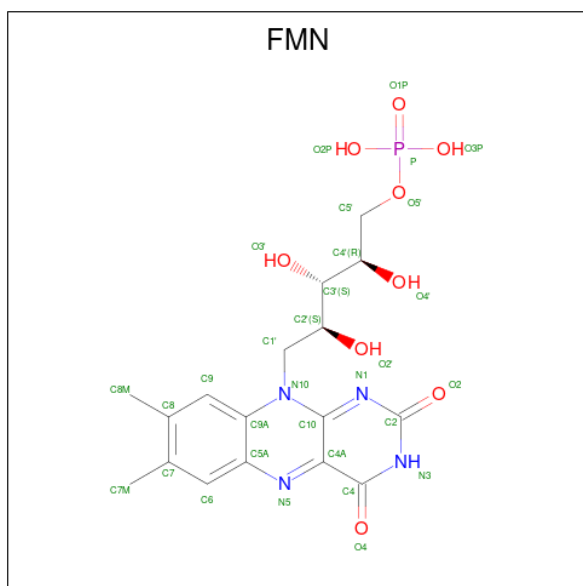
Mol	Chain	Residues	Atoms			AltConf
51	A	1	Total	Fe	S	0
			4	2	2	

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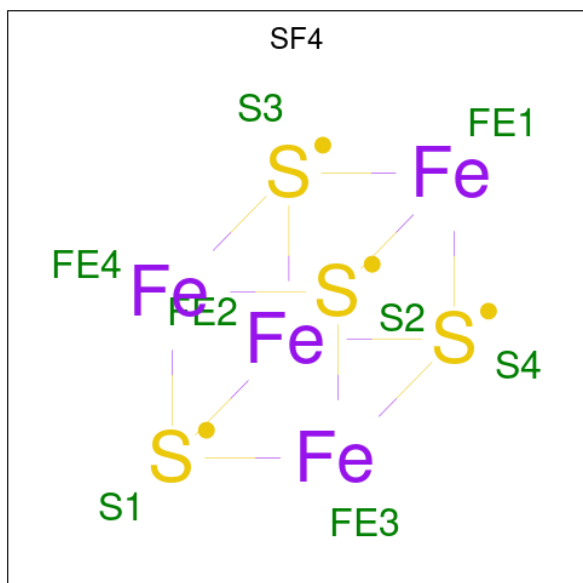
Mol	Chain	Residues	Atoms			AltConf
51	C	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



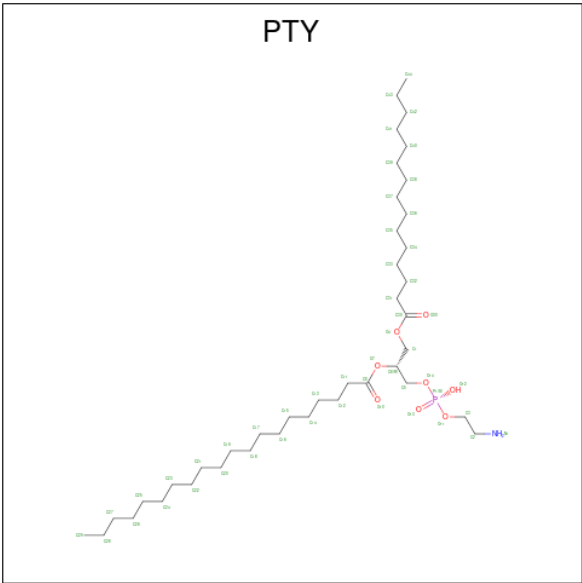
Mol	Chain	Residues	Atoms					AltConf
52	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 53 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
53	B	1	Total	Fe	S	0
			8	4	4	
53	C	1	Total	Fe	S	0
			8	4	4	
53	C	1	Total	Fe	S	0
			8	4	4	
53	F	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 54 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).



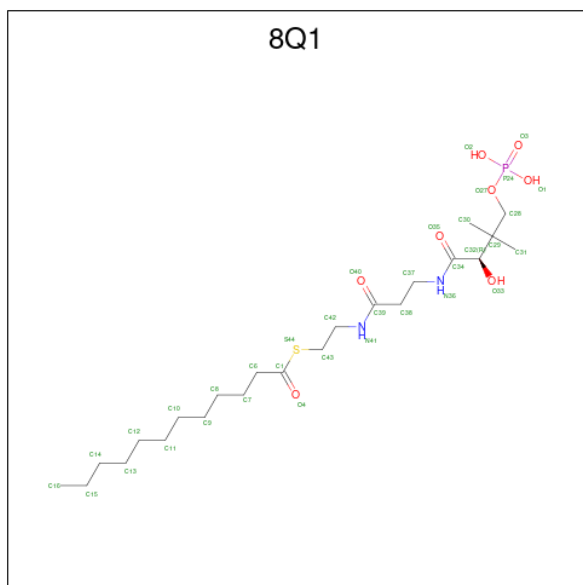
Mol	Chain	Residues	Atoms					AltConf
54	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
54	R	1	Total	C	N	O	P	0
			34	24	1	8	1	
54	R	1	Total	C	N	O	P	0
			44	34	1	8	1	
54	R	1	Total	C	N	O	P	0
			40	30	1	8	1	
54	S	1	Total	C	N	O	P	0
			46	36	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
54	T	1	Total	C	N	O	P	0
			50	40	1	8	1	
54	T	1	Total	C	N	O	P	0
			28	18	1	8	1	
54	T	1	Total	C	N	O	P	0
			26	16	1	8	1	
54	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
54	V	1	Total	C	N	O	P	0
			50	40	1	8	1	
54	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
54	e	1	Total	C	N	O	P	0
			25	15	1	8	1	
54	e	1	Total	C	N	O	P	0
			43	33	1	8	1	
54	h	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	x	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 55 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



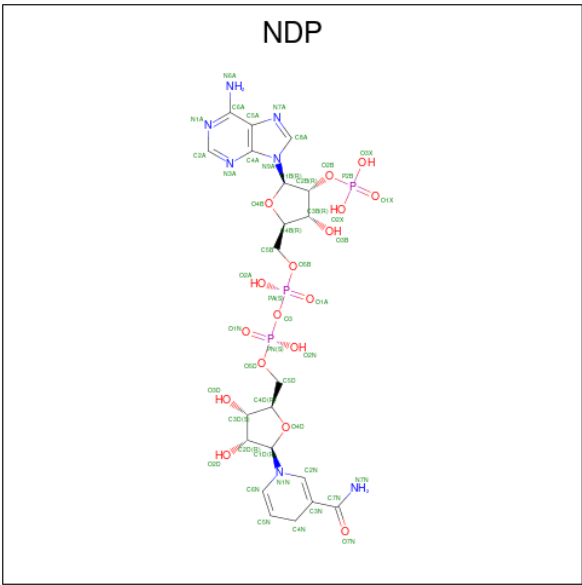
Mol	Chain	Residues	Atoms						AltConf
55	J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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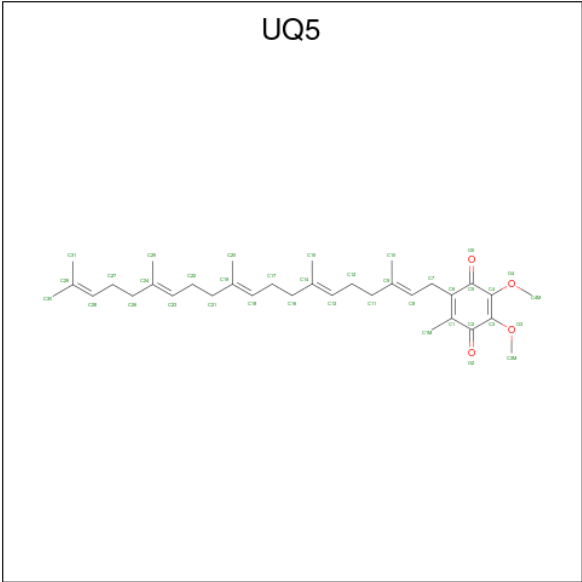
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
55	r	1	35	23	2	8	1	1	0

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



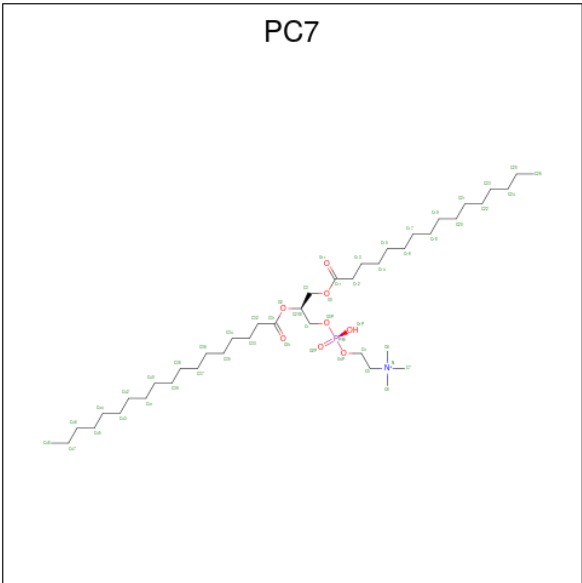
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	P	1	48	21	7	17	3	0

- Molecule 57 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: C₃₄H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
57	Q	1	Total	C	O	0
			38	34	4	

- Molecule 58 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C₄₂H₈₅NO₈P).



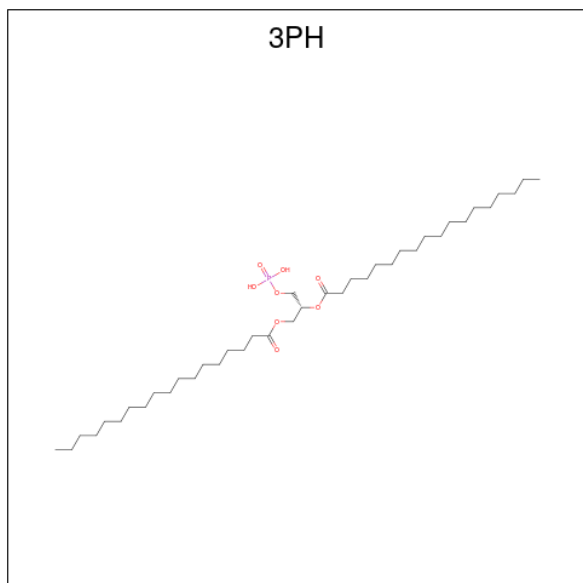
Mol	Chain	Residues	Atoms					AltConf
58	Q	1	Total	C	N	O	P	0
			33	23	1	8	1	
58	R	1	Total	C	N	O	P	0
			44	34	1	8	1	

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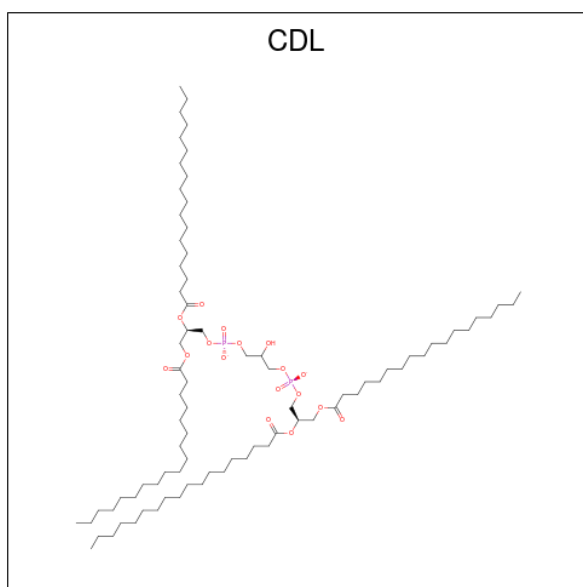
Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	P	0
			52	42	1	8	1	
58	u	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 59 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



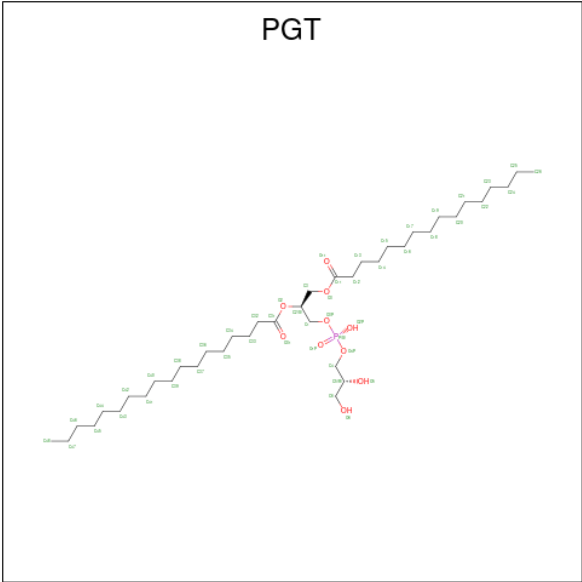
Mol	Chain	Residues	Atoms				AltConf
59	R	1	Total 32	C 23	O 8	P 1	0
59	S	1	Total 37	C 28	O 8	P 1	0
59	V	1	Total 42	C 33	O 8	P 1	0
59	V	1	Total 41	C 32	O 8	P 1	0
59	c	1	Total 48	C 39	O 8	P 1	0
59	g	1	Total 37	C 28	O 8	P 1	0
59	h	1	Total 45	C 36	O 8	P 1	0
59	w	1	Total 45	C 36	O 8	P 1	0

- Molecule 60 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



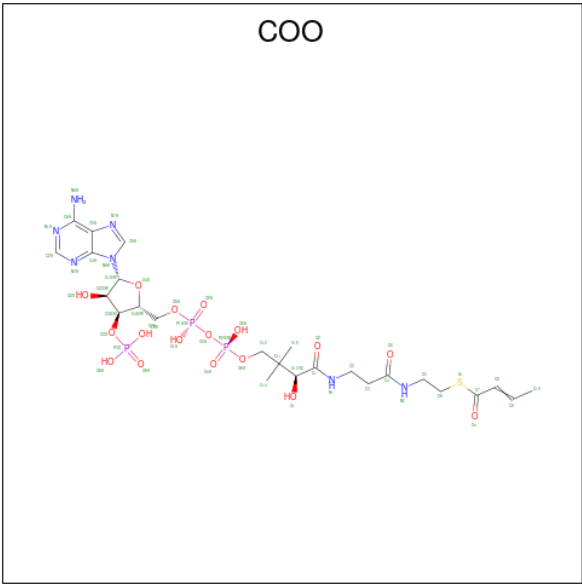
Mol	Chain	Residues	Atoms				AltConf
60	R	1	Total	C	O	P	0
			63	44	17	2	
60	V	1	Total	C	O	P	0
			64	45	17	2	
60	W	1	Total	C	O	P	0
			95	76	17	2	
60	h	1	Total	C	O	P	0
			77	58	17	2	
60	u	1	Total	C	O	P	0
			83	64	17	2	
60	u	1	Total	C	O	P	0
			71	52	17	2	
60	x	1	Total	C	O	P	0
			92	73	17	2	
60	y	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 61 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
61	T	1	Total	C	O	P	0
			48	37	10	1	
61	T	1	Total	C	O	P	0
			40	29	10	1	
61	b	1	Total	C	O	P	0
			44	33	10	1	
61	l	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 62 is CROTONYL COENZYME A (three-letter code: COO) (formula: C₂₅H₄₀N₇O₁₇P₃S).



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

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	s	1	Total	Zn	0
			1	1	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	24	Total	O	0
			24	24	
64	B	66	Total	O	0
			66	66	
64	C	168	Total	O	0
			168	168	
64	D	66	Total	O	0
			66	66	
64	E	87	Total	O	0
			87	87	
64	F	39	Total	O	0
			39	39	
64	G	62	Total	O	0
			62	62	
64	H	16	Total	O	0
			16	16	
64	I	19	Total	O	0
			19	19	
64	K	16	Total	O	0
			16	16	
64	L	68	Total	O	0
			68	68	
64	M	30	Total	O	0
			30	30	
64	N	53	Total	O	0
			53	53	
64	O	6	Total	O	0
			6	6	
64	P	69	Total	O	0
			69	69	
64	Q	24	Total	O	0
			24	24	

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Mol	Chain	Residues	Atoms		AltConf
64	R	64	Total 64	O 64	0
64	S	22	Total 22	O 22	0
64	T	85	Total 85	O 85	0
64	U	14	Total 14	O 14	0
64	V	99	Total 99	O 99	0
64	W	25	Total 25	O 25	0
64	X	50	Total 50	O 50	0
64	Y	4	Total 4	O 4	0
64	Z	20	Total 20	O 20	0
64	a	6	Total 6	O 6	0
64	b	24	Total 24	O 24	0
64	c	1	Total 1	O 1	0
64	d	12	Total 12	O 12	0
64	e	55	Total 55	O 55	0
64	f	10	Total 10	O 10	0
64	g	7	Total 7	O 7	0
64	h	38	Total 38	O 38	0
64	i	30	Total 30	O 30	0
64	j	29	Total 29	O 29	0
64	k	51	Total 51	O 51	0
64	l	17	Total 17	O 17	0

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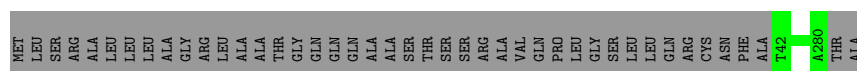
Mol	Chain	Residues	Atoms		AltConf
64	m	32	Total 32	O 32	0
64	n	7	Total 7	O 7	0
64	o	51	Total 51	O 51	0
64	p	21	Total 21	O 21	0
64	q	24	Total 24	O 24	0
64	r	12	Total 12	O 12	0
64	s	39	Total 39	O 39	0
64	t	55	Total 55	O 55	0
64	u	41	Total 41	O 41	0
64	v	2	Total 2	O 2	0
64	w	16	Total 16	O 16	0
64	x	22	Total 22	O 22	0
64	y	29	Total 29	O 29	0

3 Residue-property plots [i](#)


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

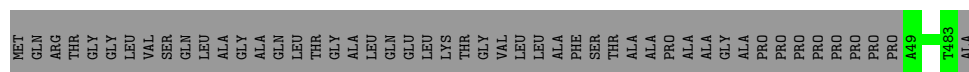
- Molecule 1: NADH:ubiquinone oxidoreductase 24 kD subunit

Chain A: 



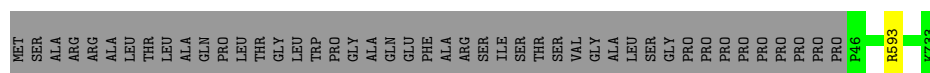
- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B: 




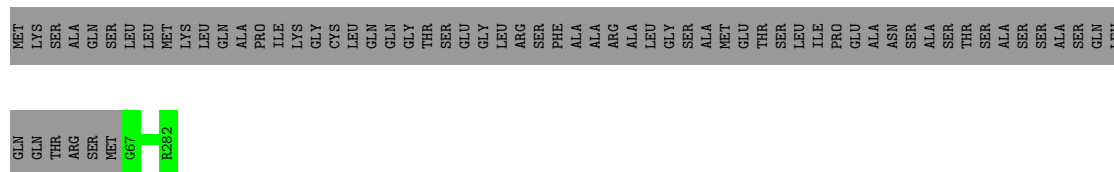
- Molecule 3: NADH:ubiquinone oxidoreductase 78 kDa subunit

Chain C: 




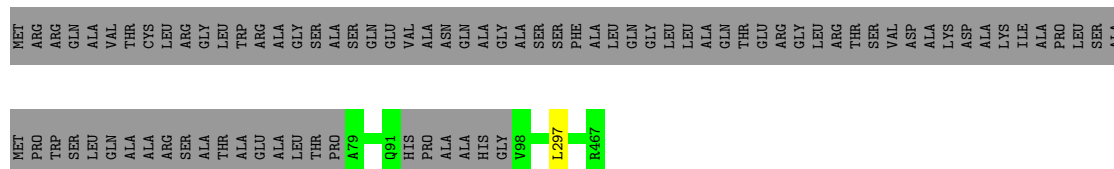
- Molecule 4: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

Chain D: 



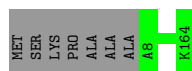
- Molecule 5: NADH:ubiquinone oxidoreductase 49 kD subunit

Chain E: 



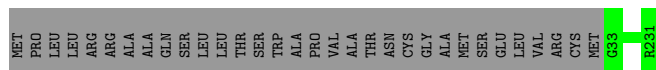
- Molecule 6: NADH:ubiquinone oxidoreductase subunit 10

Chain F:  96%




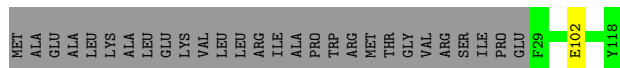
- Molecule 7: NADH:ubiquinone oxidoreductase subunit 8

Chain G:  86%




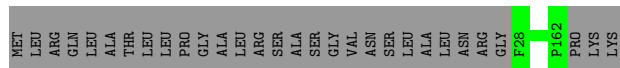
- Molecule 8: B14.5a

Chain H:  75%



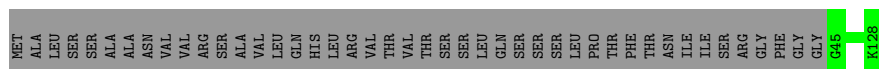
- Molecule 9: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit

Chain I:  82%



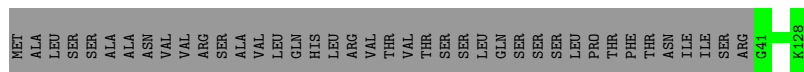
- Molecule 10: Acyl carrier protein

Chain J:  66%




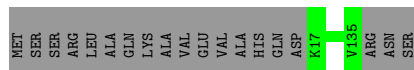
- Molecule 10: Acyl carrier protein

Chain r:  69%




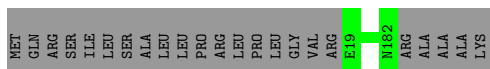
- Molecule 11: NADH:ubiquinone oxidoreductase B14 subunit

Chain K:  86%




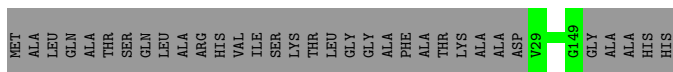
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:  88% 12%



- Molecule 13: NADH:ubiquinone oxidoreductase 13 kD-like subunit

Chain M:  79% 21%



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:  96% .



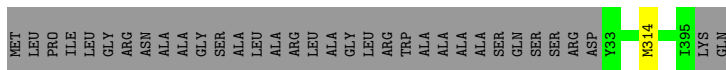
- Molecule 15: NADH:ubiquinone oxidoreductase B8 subunit

Chain O:  98% ..



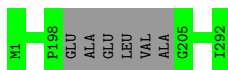
- Molecule 16: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

Chain P:  91% 9%



- Molecule 17: NADH-ubiquinone oxidoreductase chain 1

Chain Q:  98% .



- Molecule 18: NADH-ubiquinone oxidoreductase chain 2

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: NADH-ubiquinone oxidoreductase chain 3

Chain S:  48% 52%

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

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

PHE ALA LEU PRO MET GLN GLN SER VAL PHE GLY Y132 Y204 GLU CYS PHE ASP ALA PHE PHE GLY GLU ALA ARG GLN PHE S219 L224 E279

- Molecule 20: NADH-ubiquinone oxidoreductase chain 4

Chain T:  100%

H1 Y195 A443

- Molecule 21: NADH dehydrogenase subunit 4L

Chain U:  46%  54%

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

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

ARG SER Y123 K227

- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain V:  100%



H1 F8 P519 A546

- Molecule 23: NADH-ubiquinone oxidoreductase chain 6

Chain W:  97%


H1 Y157 ARG THR THR GLY ARG

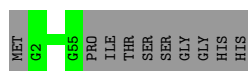
- Molecule 24: ASH1

Chain X:  84%  16%


MET SER LEU ASN SER LEU ARG GLY LEU LEU ARG ALA SER LEU GLN ALA LYS ASN ALA LEU PRO ALA LYS ALA G25 Y149

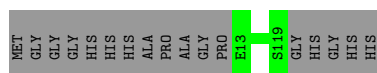
- Molecule 25: P9

Chain Y:  84% 16%



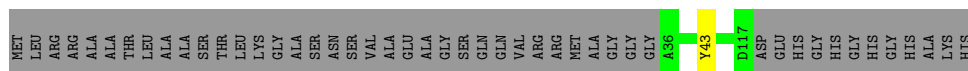
- Molecule 26: KFYI

Chain Z:  86% 14%




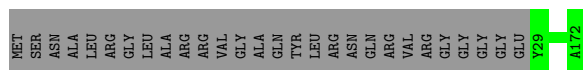
- Molecule 27: AGGG

Chain a:  63% 36%




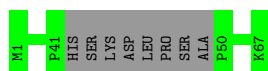
- Molecule 28: ESSS

Chain b:  84% 16%



- Molecule 29: B9

Chain c:  88% 12%



- Molecule 30: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit

Chain d:  99%



- Molecule 31: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit

Chain e:  99%



- Molecule 32: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit

Chain f:  98%



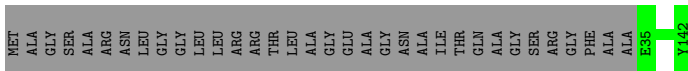
- Molecule 33: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit

Chain g: 91% 9%



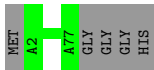
- Molecule 34: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

Chain h: 76% 24%



- Molecule 35: NADH:ubiquinone oxidoreductase 15 kDa subunit-like

Chain i: 94% 6%



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain j: 99% .



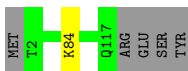
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain k: 100%

There are no outlier residues recorded for this chain.

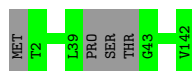
- Molecule 38: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

Chain l: 95% . .



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain m: 97% .



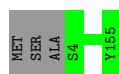
- Molecule 40: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

Chain n: 98% .



- Molecule 41: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit

Chain o: 98% .



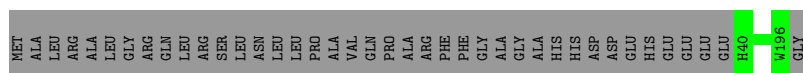
- Molecule 42: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

Chain p: 99% .



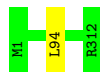
- Molecule 43: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

Chain q: 80% 20%



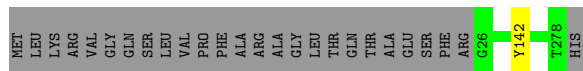
- Molecule 44: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

Chain s: 100%



- Molecule 45: CAG2 - CA-like

Chain t: 90% 9%



- Molecule 46: CAG1

Chain u: 100%

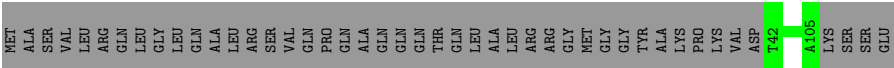


- Molecule 47: P10

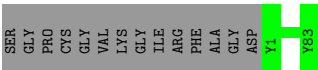
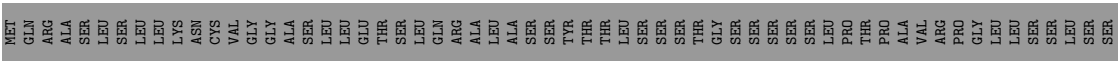


There are no outlier residues recorded for this chain.

- Molecule 48: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit



- Molecule 49: NUOP8



- Molecule 50: NUOP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.31	0/1878	0.54	0/2549
2	B	0.33	0/3400	0.56	0/4573
3	C	0.31	0/5272	0.56	0/7143
4	D	0.36	0/1843	0.58	0/2506
5	E	0.38	0/3158	0.61	1/4270 (0.0%)
6	F	0.41	0/1258	0.57	0/1706
7	G	0.32	0/1648	0.60	0/2222
8	H	0.35	0/773	0.60	1/1046 (0.1%)
9	I	0.31	0/1061	0.49	0/1441
10	J	0.29	0/649	0.49	0/875
10	r	0.32	0/673	0.47	0/906
11	K	0.34	0/1007	0.59	0/1348
12	L	0.33	0/1306	0.59	0/1769
13	M	0.31	0/936	0.52	0/1276
14	N	0.32	0/1277	0.52	0/1735
15	O	0.28	0/772	0.60	1/1037 (0.1%)
16	P	0.30	0/2879	0.55	1/3905 (0.0%)
17	Q	0.36	0/2234	0.58	0/3034
18	R	0.36	0/3100	0.55	0/4226
19	S	0.37	0/1106	0.57	1/1512 (0.1%)
20	T	0.37	1/3533 (0.0%)	0.56	0/4825
21	U	0.34	0/819	0.53	0/1112
22	V	0.36	0/4258	0.57	2/5792 (0.0%)
23	W	0.34	0/1239	0.52	0/1686
24	X	0.36	0/1081	0.55	0/1479
25	Y	0.32	0/411	0.49	0/557
26	Z	0.33	0/894	0.53	0/1218
27	a	0.33	0/698	0.47	0/949
28	b	0.35	0/1201	0.56	0/1623
29	c	0.31	0/463	0.53	0/623
30	d	0.37	0/721	0.53	0/968
31	e	0.34	0/1688	0.54	0/2301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.32	0/547	0.53	0/740
33	g	0.30	0/433	0.55	0/587
34	h	0.34	0/948	0.55	0/1285
35	i	0.32	0/644	0.60	0/860
36	j	0.34	0/732	0.54	0/983
37	k	0.32	0/1011	0.55	0/1361
38	l	0.33	0/936	0.49	0/1278
39	m	0.36	0/1155	0.56	0/1558
40	n	0.32	0/886	0.50	0/1188
41	o	0.33	0/1265	0.59	0/1705
42	p	0.32	0/1095	0.55	0/1480
43	q	0.32	0/1308	0.51	0/1779
44	s	0.32	0/2353	0.53	1/3202 (0.0%)
45	t	0.32	0/2043	0.56	0/2778
46	u	0.32	0/1730	0.54	0/2341
47	v	0.33	0/369	0.48	0/498
48	w	0.34	0/521	0.49	0/702
49	x	0.34	0/727	0.49	0/994
50	y	0.34	0/963	0.52	0/1313
All	All	0.34	1/72902 (0.0%)	0.55	8/98844 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	e	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	195	VAL	CB-CG1	-5.47	1.41	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	7	LEU	CA-CB-CG	7.19	131.83	115.30
5	E	297	LEU	CA-CB-CG	6.98	131.35	115.30
19	S	224	LEU	CA-CB-CG	6.21	129.59	115.30
44	s	94	LEU	CA-CB-CG	5.91	128.90	115.30
22	V	8	PHE	CB-CG-CD1	-5.81	116.73	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	e	147	MET	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/282 (84%)	228 (96%)	9 (4%)	0	100	100
2	B	433/484 (90%)	417 (96%)	16 (4%)	0	100	100
3	C	686/733 (94%)	667 (97%)	19 (3%)	0	100	100
4	D	214/282 (76%)	204 (95%)	10 (5%)	0	100	100
5	E	379/467 (81%)	368 (97%)	11 (3%)	0	100	100
6	F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
7	G	197/231 (85%)	189 (96%)	8 (4%)	0	100	100
8	H	88/118 (75%)	81 (92%)	7 (8%)	0	100	100
9	I	133/165 (81%)	130 (98%)	3 (2%)	0	100	100
10	J	82/128 (64%)	76 (93%)	6 (7%)	0	100	100
10	r	86/128 (67%)	84 (98%)	2 (2%)	0	100	100
11	K	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
12	L	162/187 (87%)	155 (96%)	7 (4%)	0	100	100
13	M	119/154 (77%)	111 (93%)	8 (7%)	0	100	100
14	N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
15	O	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	361/397 (91%)	350 (97%)	11 (3%)	0	100	100
17	Q	282/292 (97%)	274 (97%)	8 (3%)	0	100	100
18	R	385/387 (100%)	369 (96%)	16 (4%)	0	100	100
19	S	130/279 (47%)	128 (98%)	2 (2%)	0	100	100
20	T	441/443 (100%)	431 (98%)	10 (2%)	0	100	100
21	U	103/227 (45%)	102 (99%)	1 (1%)	0	100	100
22	V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	44	64
23	W	155/162 (96%)	151 (97%)	4 (3%)	0	100	100
24	X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
25	Y	52/64 (81%)	52 (100%)	0	0	100	100
26	Z	105/124 (85%)	100 (95%)	5 (5%)	0	100	100
27	a	80/129 (62%)	78 (98%)	1 (1%)	1 (1%)	10	19
28	b	142/172 (83%)	139 (98%)	3 (2%)	0	100	100
29	c	55/67 (82%)	52 (94%)	3 (6%)	0	100	100
30	d	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
31	e	216/219 (99%)	214 (99%)	1 (0%)	1 (0%)	25	44
32	f	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
33	g	48/55 (87%)	42 (88%)	6 (12%)	0	100	100
34	h	106/142 (75%)	97 (92%)	9 (8%)	0	100	100
35	i	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
36	j	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
37	k	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
38	l	114/121 (94%)	110 (96%)	4 (4%)	0	100	100
39	m	134/142 (94%)	133 (99%)	1 (1%)	0	100	100
40	n	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
41	o	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
42	p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
43	q	155/197 (79%)	149 (96%)	6 (4%)	0	100	100
44	s	310/312 (99%)	303 (98%)	7 (2%)	0	100	100
45	t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
46	u	226/229 (99%)	220 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	v	43/45 (96%)	43 (100%)	0	0	100	100
48	w	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
49	x	81/157 (52%)	81 (100%)	0	0	100	100
50	y	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
All	All	8946/10307 (87%)	8662 (97%)	281 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	a	43	TYR
22	V	519	PRO
31	e	148	PRO

5.3.2 Protein sidechains [i](#)

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	197/228 (86%)	197 (100%)	0	100	100
2	B	344/377 (91%)	344 (100%)	0	100	100
3	C	537/572 (94%)	536 (100%)	1 (0%)	92	97
4	D	196/248 (79%)	196 (100%)	0	100	100
5	E	329/388 (85%)	329 (100%)	0	100	100
6	F	129/133 (97%)	129 (100%)	0	100	100
7	G	172/198 (87%)	172 (100%)	0	100	100
8	H	82/105 (78%)	82 (100%)	0	100	100
9	I	111/134 (83%)	111 (100%)	0	100	100
10	J	71/108 (66%)	71 (100%)	0	100	100
10	r	72/108 (67%)	72 (100%)	0	100	100
11	K	106/122 (87%)	106 (100%)	0	100	100
12	L	130/148 (88%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	100/121 (83%)	100 (100%)	0	100	100
14	N	128/132 (97%)	128 (100%)	0	100	100
15	O	80/81 (99%)	80 (100%)	0	100	100
16	P	305/327 (93%)	305 (100%)	0	100	100
17	Q	230/234 (98%)	230 (100%)	0	100	100
18	R	321/321 (100%)	321 (100%)	0	100	100
19	S	111/217 (51%)	111 (100%)	0	100	100
20	T	374/374 (100%)	374 (100%)	0	100	100
21	U	84/180 (47%)	84 (100%)	0	100	100
22	V	439/439 (100%)	439 (100%)	0	100	100
23	W	131/135 (97%)	131 (100%)	0	100	100
24	X	105/122 (86%)	105 (100%)	0	100	100
25	Y	38/46 (83%)	38 (100%)	0	100	100
26	Z	93/102 (91%)	93 (100%)	0	100	100
27	a	68/98 (69%)	68 (100%)	0	100	100
28	b	119/138 (86%)	119 (100%)	0	100	100
29	c	49/56 (88%)	49 (100%)	0	100	100
30	d	63/64 (98%)	63 (100%)	0	100	100
31	e	163/164 (99%)	163 (100%)	0	100	100
32	f	52/53 (98%)	52 (100%)	0	100	100
33	g	40/45 (89%)	40 (100%)	0	100	100
34	h	91/110 (83%)	91 (100%)	0	100	100
35	i	65/67 (97%)	65 (100%)	0	100	100
36	j	72/73 (99%)	72 (100%)	0	100	100
37	k	102/102 (100%)	102 (100%)	0	100	100
38	l	94/99 (95%)	93 (99%)	1 (1%)	70	87
39	m	118/122 (97%)	118 (100%)	0	100	100
40	n	92/94 (98%)	92 (100%)	0	100	100
41	o	130/132 (98%)	130 (100%)	0	100	100
42	p	109/110 (99%)	109 (100%)	0	100	100
43	q	135/165 (82%)	135 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	s	243/243 (100%)	243 (100%)	0	100	100
45	t	212/233 (91%)	211 (100%)	1 (0%)	86	95
46	u	180/181 (99%)	180 (100%)	0	100	100
47	v	38/38 (100%)	38 (100%)	0	100	100
48	w	55/91 (60%)	55 (100%)	0	100	100
49	x	70/130 (54%)	70 (100%)	0	100	100
50	y	102/106 (96%)	102 (100%)	0	100	100
All	All	7477/8414 (89%)	7474 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	593	ARG
38	l	84	LYS
45	t	142	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	279	ASN
3	C	297	ASN
3	C	618	GLN
38	l	41	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 54 ligands modelled in this entry, 1 is monoatomic - leaving 53 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$
58	PC7	u	601	-	41,41,51	0.55	0	47,49,59	0.68	2 (4%)
51	FES	C	801	3	0,4,4	-	-	-		
60	CDL	W	701	-	94,94,99	0.35	0	100,106,111	0.28	0
60	CDL	x	101	-	91,91,99	0.40	1 (1%)	97,103,111	0.24	0
53	SF4	G	301	7	0,12,12	-	-	-		
54	PTY	V	605	-	49,49,49	0.46	0	52,54,54	0.38	0
53	SF4	C	802	3	0,12,12	-	-	-		
54	PTY	R	406	-	39,39,49	0.53	0	42,44,54	0.51	0
51	FES	A	301	1	0,4,4	-	-	-		
59	3PH	R	401	-	31,31,47	0.75	1 (3%)	35,36,52	0.73	2 (5%)
53	SF4	F	201	6	0,12,12	-	-	-		
59	3PH	V	601	-	41,41,47	0.66	1 (2%)	45,46,52	0.63	1 (2%)
60	CDL	y	201	-	54,54,99	0.53	1 (1%)	60,66,111	0.32	0
54	PTY	e	302	-	42,42,49	0.52	0	45,47,54	0.42	0
60	CDL	u	603	-	70,70,99	0.43	0	76,82,111	0.28	0
54	PTY	e	301	-	24,24,49	0.64	0	27,29,54	0.52	0
53	SF4	C	803	3	0,12,12	-	-	-		
53	SF4	B	502	2	0,12,12	-	-	-		
60	CDL	V	603	-	63,63,99	0.41	0	69,75,111	0.25	0
54	PTY	T	506	-	25,25,49	0.64	0	28,30,54	0.47	0
54	PTY	R	402	-	33,33,49	0.53	0	36,38,54	0.43	0
55	8Q1	r	200	-	31,34,34	1.76	5 (16%)	40,43,43	1.88	10 (25%)
61	PGT	l	701	-	50,50,50	0.48	0	53,56,56	0.59	1 (1%)
60	CDL	u	602	-	82,82,99	0.38	0	88,94,111	0.30	0
52	FMN	B	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.25	8 (16%)
55	8Q1	J	200	-	31,34,34	1.69	5 (16%)	40,43,43	1.71	5 (12%)
54	PTY	T	501	-	49,49,49	0.46	0	52,54,54	0.62	1 (1%)
60	CDL	R	405	-	62,62,99	0.40	0	68,74,111	0.28	0
59	3PH	c	101	-	47,47,47	0.62	1 (2%)	51,52,52	0.63	1 (1%)
54	PTY	T	504	-	27,27,49	0.65	0	30,32,54	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PTY	h	202	-	45,45,49	0.47	0	48,50,54	0.46	0
54	PTY	R	404	-	43,43,49	0.51	0	46,48,54	0.46	0
57	UQ5	Q	301	-	38,38,38	0.51	0	46,49,49	0.83	3 (6%)
59	3PH	g	101	-	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
59	3PH	w	201	-	44,44,47	0.64	1 (2%)	48,49,52	0.75	3 (6%)
59	3PH	h	201	-	44,44,47	0.65	1 (2%)	48,49,52	3.77	5 (10%)
58	PC7	R	403	-	43,43,51	0.53	0	49,51,59	0.61	0
54	PTY	S	302	-	45,45,49	0.49	0	48,50,54	0.41	0
61	PGT	b	601	-	43,43,50	0.53	0	46,49,56	0.51	0
62	COO	s	401	-	45,55,55	0.82	1 (2%)	55,81,81	4.26	10 (18%)
54	PTY	x	102	-	49,49,49	0.46	0	52,54,54	0.40	0
58	PC7	T	503	-	51,51,51	0.50	0	57,59,59	0.59	0
53	SF4	G	302	7	0,12,12	-	-	-	-	-
54	PTY	V	606	-	34,34,49	0.56	0	37,39,54	0.44	0
61	PGT	T	502	-	47,47,50	0.53	0	50,53,56	0.56	1 (2%)
61	PGT	T	505	-	39,39,50	0.54	0	42,45,56	0.50	0
59	3PH	S	301	-	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
54	PTY	G	303	-	42,42,49	0.49	0	45,47,54	0.44	0
60	CDL	h	203	-	76,76,99	0.37	0	82,88,111	0.25	0
56	NDP	P	401	-	45,52,52	0.97	2 (4%)	53,80,80	1.19	3 (5%)
59	3PH	V	602	-	40,40,47	0.67	1 (2%)	44,45,52	0.82	1 (2%)
54	PTY	V	604	-	39,39,49	0.54	0	42,44,54	0.50	0
58	PC7	Q	302	-	32,32,51	0.59	0	38,40,59	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC7	u	601	-	-	15/45/45/55	-
51	FES	C	801	3	-	-	0/1/1/1
60	CDL	W	701	-	-	62/105/105/110	-
60	CDL	x	101	-	-	65/102/102/110	-
53	SF4	G	301	7	-	-	0/6/5/5
54	PTY	V	605	-	-	25/53/53/53	-
53	SF4	C	802	3	-	-	0/6/5/5
54	PTY	R	406	-	-	15/43/43/53	-
51	FES	A	301	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	3PH	R	401	-	-	13/33/33/49	-
53	SF4	F	201	6	-	-	0/6/5/5
59	3PH	V	601	-	-	18/43/43/49	-
60	CDL	y	201	-	-	30/65/65/110	-
54	PTY	e	302	-	-	22/46/46/53	-
60	CDL	u	603	-	-	57/81/81/110	-
54	PTY	e	301	-	-	9/28/28/53	-
53	SF4	C	803	3	-	-	0/6/5/5
53	SF4	B	502	2	-	-	0/6/5/5
60	CDL	V	603	-	-	42/74/74/110	-
54	PTY	T	506	-	-	15/29/29/53	-
54	PTY	R	402	-	-	11/37/37/53	-
55	8Q1	r	200	-	-	19/41/41/41	-
61	PGT	l	701	-	-	27/55/55/55	-
60	CDL	u	602	-	-	51/93/93/110	-
52	FMN	B	501	-	-	4/18/18/18	0/3/3/3
55	8Q1	J	200	-	-	11/41/41/41	-
54	PTY	T	501	-	-	19/53/53/53	-
60	CDL	R	405	-	-	43/73/73/110	-
59	3PH	c	101	-	-	13/49/49/49	-
54	PTY	T	504	-	-	11/31/31/53	-
54	PTY	h	202	-	-	20/49/49/53	-
54	PTY	R	404	-	-	21/47/47/53	-
57	UQ5	Q	301	-	-	4/33/57/57	0/1/1/1
59	3PH	g	101	-	-	10/38/38/49	-
59	3PH	w	201	-	-	21/46/46/49	-
59	3PH	h	201	-	-	19/46/46/49	-
58	PC7	R	403	-	-	15/47/47/55	-
54	PTY	S	302	-	-	21/49/49/53	-
61	PGT	b	601	-	-	27/48/48/55	-
62	COO	s	401	-	-	22/50/70/70	0/3/3/3
54	PTY	x	102	-	-	18/53/53/53	-
58	PC7	T	503	-	-	22/55/55/55	-
54	PTY	V	606	-	-	18/38/38/53	-
53	SF4	G	302	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PGT	T	502	-	-	20/52/52/55	-
61	PGT	T	505	-	-	18/44/44/55	-
59	3PH	S	301	-	-	13/38/38/49	-
54	PTY	G	303	-	-	6/46/46/53	-
60	CDL	h	203	-	-	58/87/87/110	-
56	NDP	P	401	-	-	9/30/77/77	0/5/5/5
59	3PH	V	602	-	-	17/42/42/49	-
54	PTY	V	604	-	-	15/43/43/53	-
58	PC7	Q	302	-	-	14/36/36/55	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	200	8Q1	C34-N36	5.99	1.46	1.33
55	J	200	8Q1	C34-N36	5.48	1.45	1.33
55	r	200	8Q1	C39-N41	5.24	1.45	1.33
55	J	200	8Q1	C39-N41	5.13	1.45	1.33
52	B	501	FMN	C4A-N5	3.60	1.37	1.30

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	s	401	COO	C15-C11-C12	-19.13	77.03	108.23
59	h	201	3PH	O31-C31-O32	-17.93	78.33	123.59
62	s	401	COO	C15-C11-C13	-16.74	79.80	108.82
62	s	401	COO	C15-C11-C14	-15.18	78.23	109.17
59	h	201	3PH	O31-C31-C32	14.35	156.94	111.91

There are no chirality outliers.

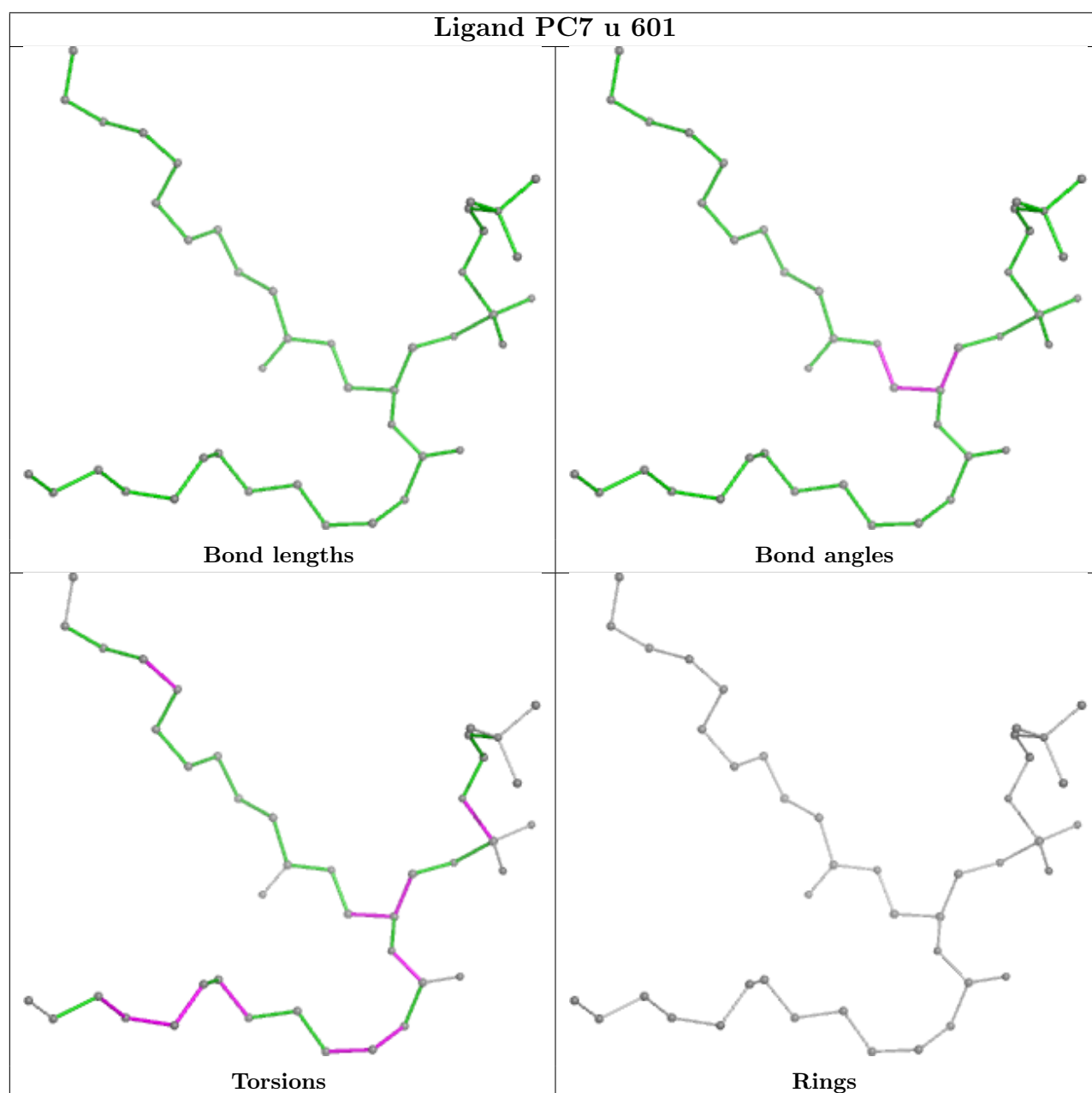
5 of 1005 torsion outliers are listed below:

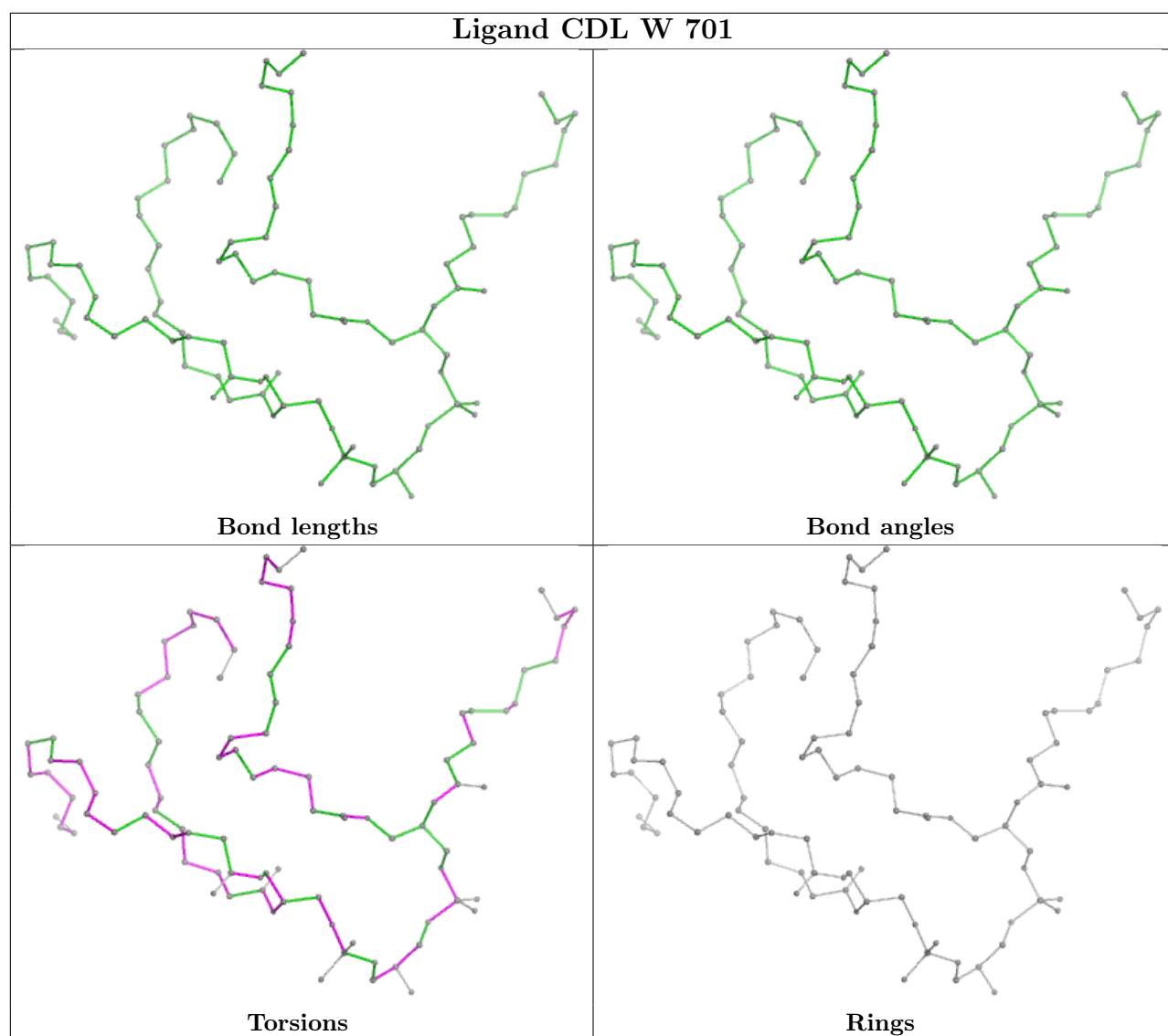
Mol	Chain	Res	Type	Atoms
52	B	501	FMN	C5'-O5'-P-O1P
52	B	501	FMN	C5'-O5'-P-O2P
52	B	501	FMN	C5'-O5'-P-O3P
54	G	303	PTY	C3-O11-P1-O13
54	R	402	PTY	C2-C3-O11-P1

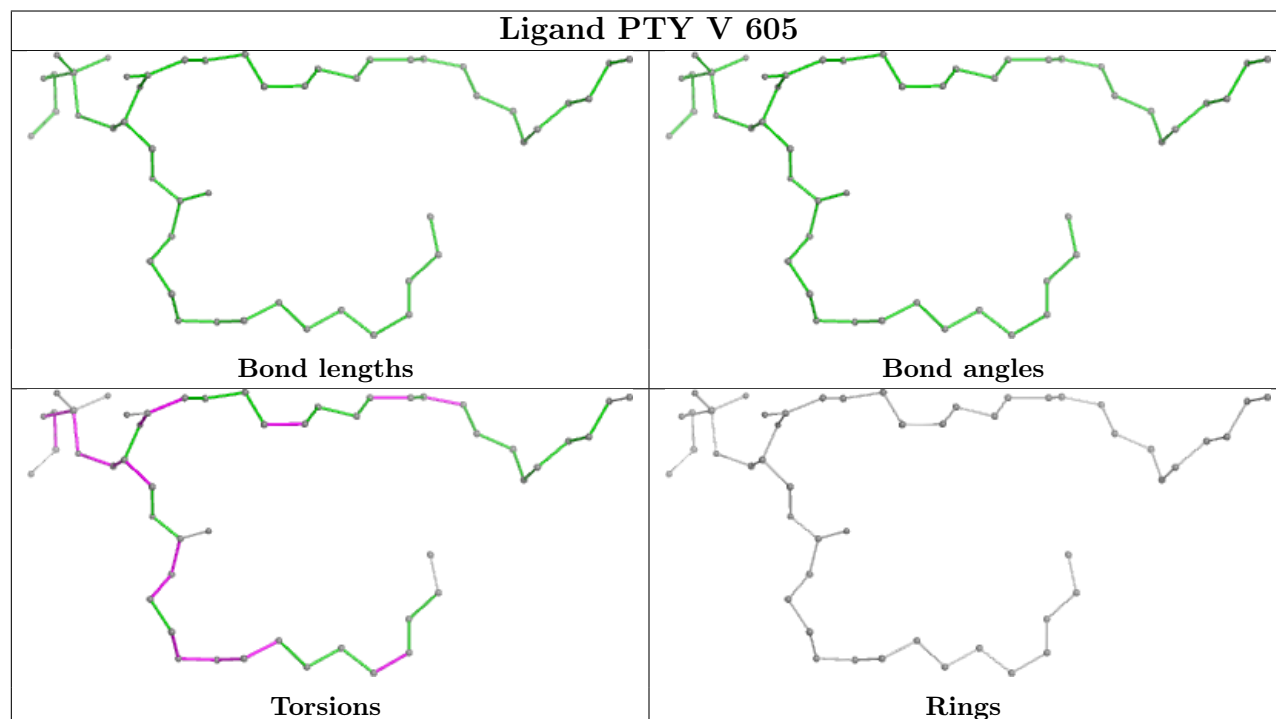
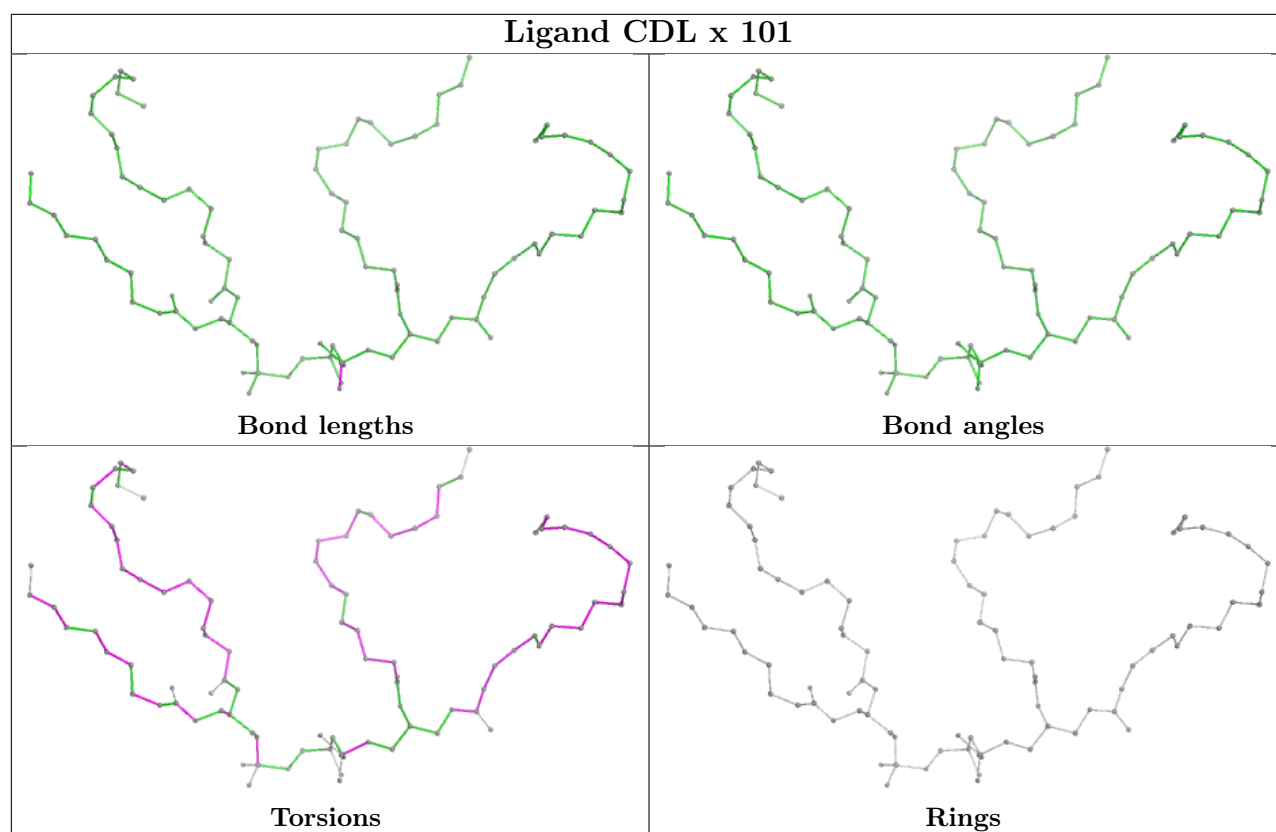
There are no ring outliers.

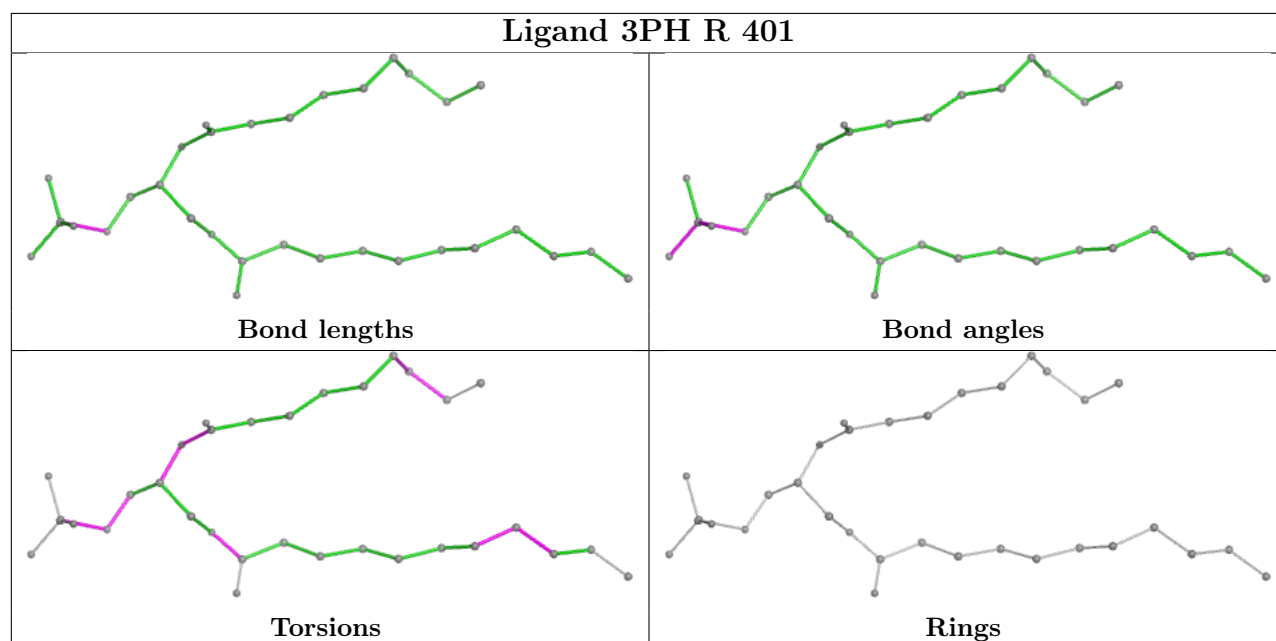
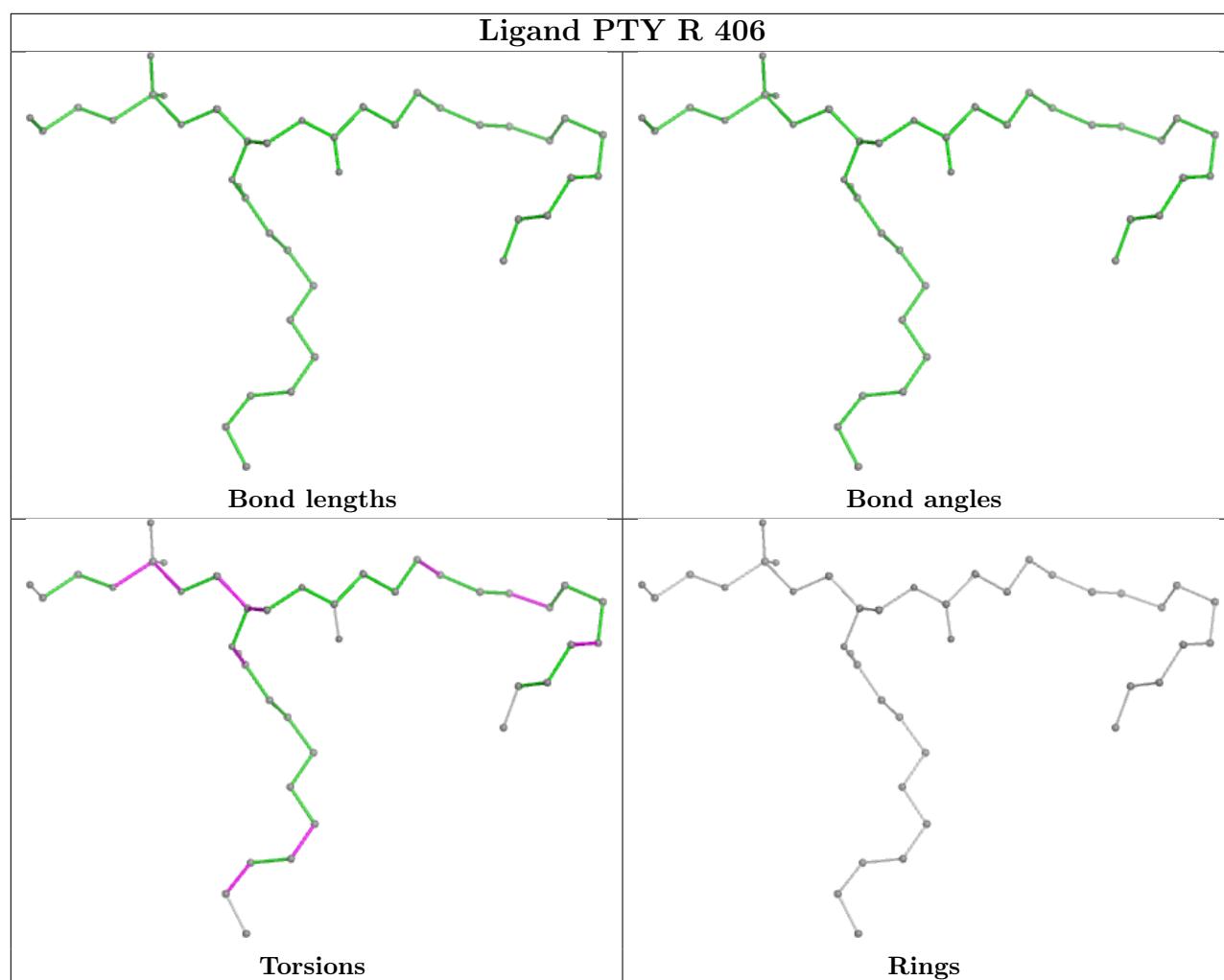
No monomer is involved in short contacts.

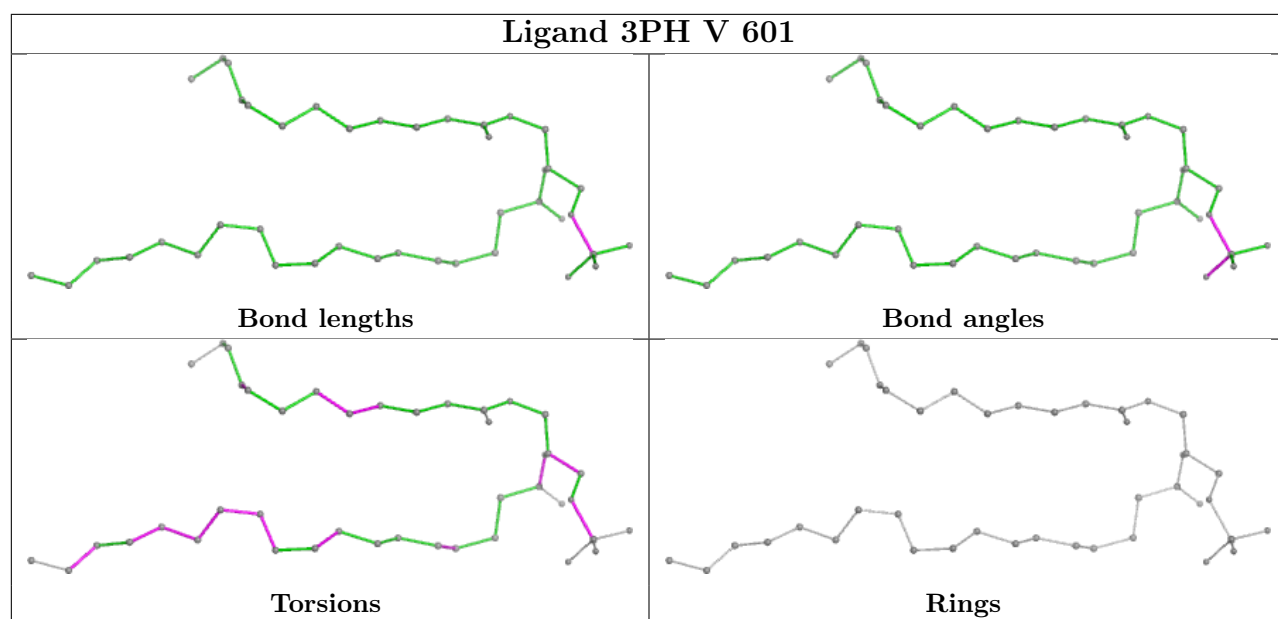
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

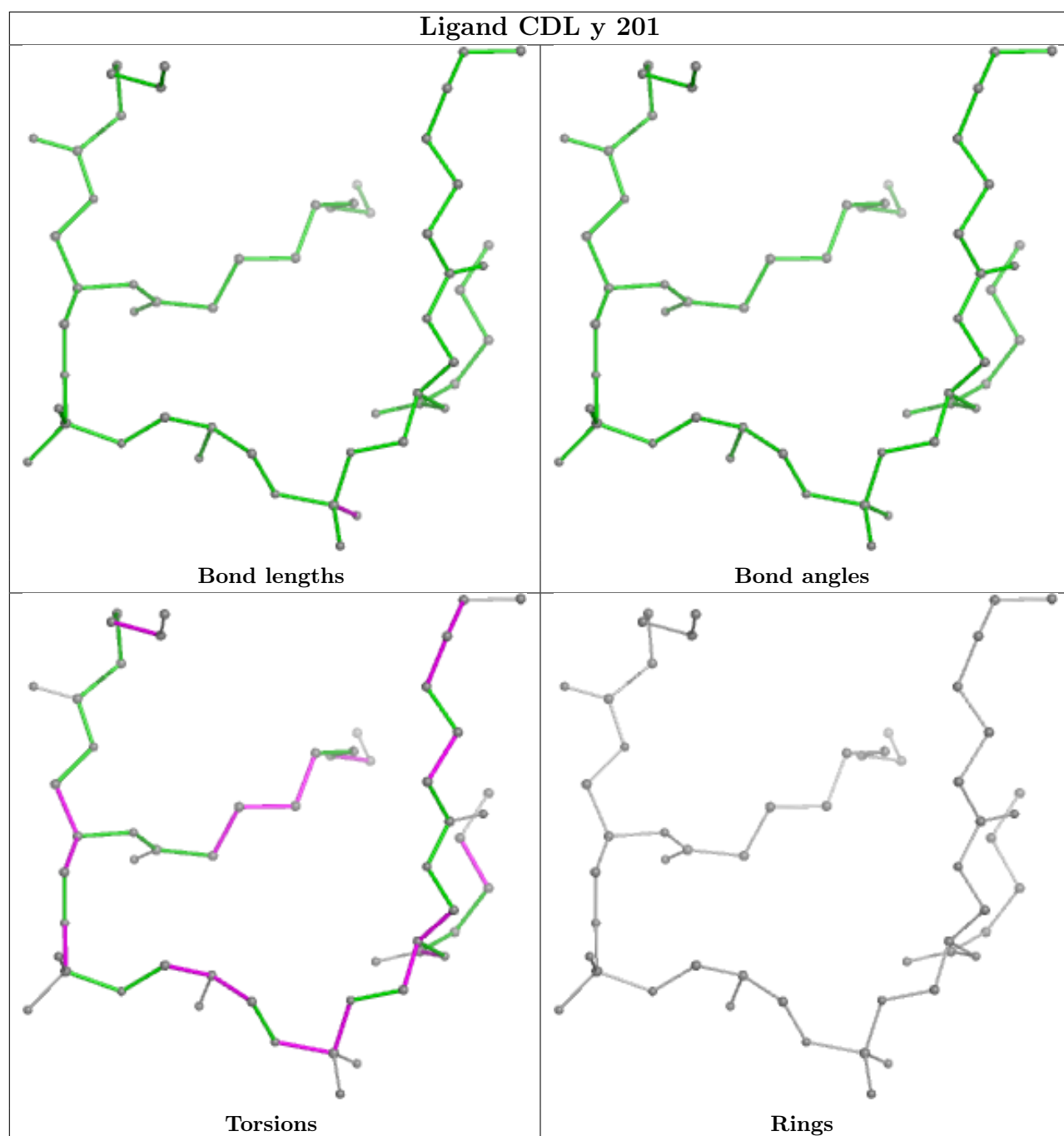


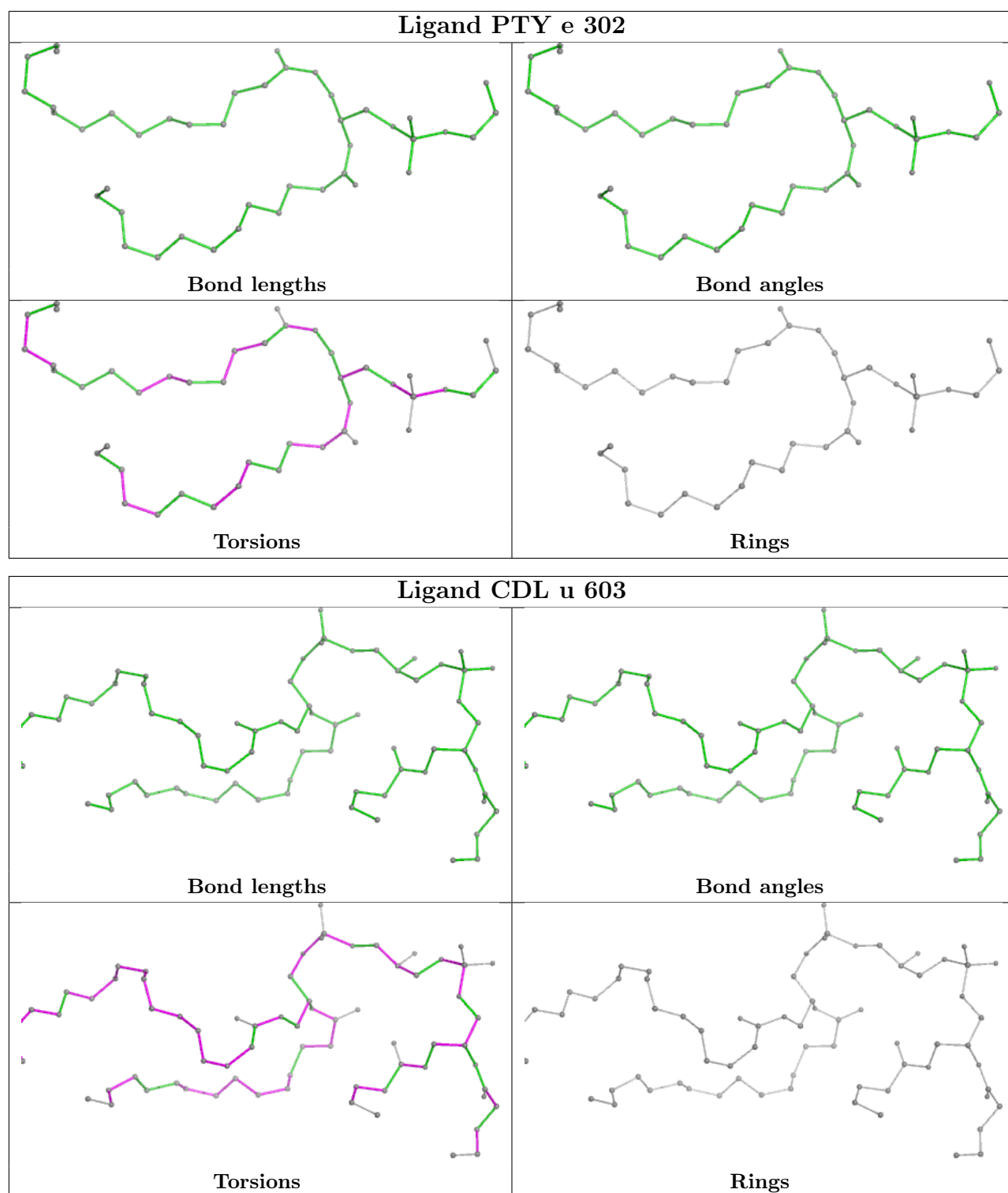


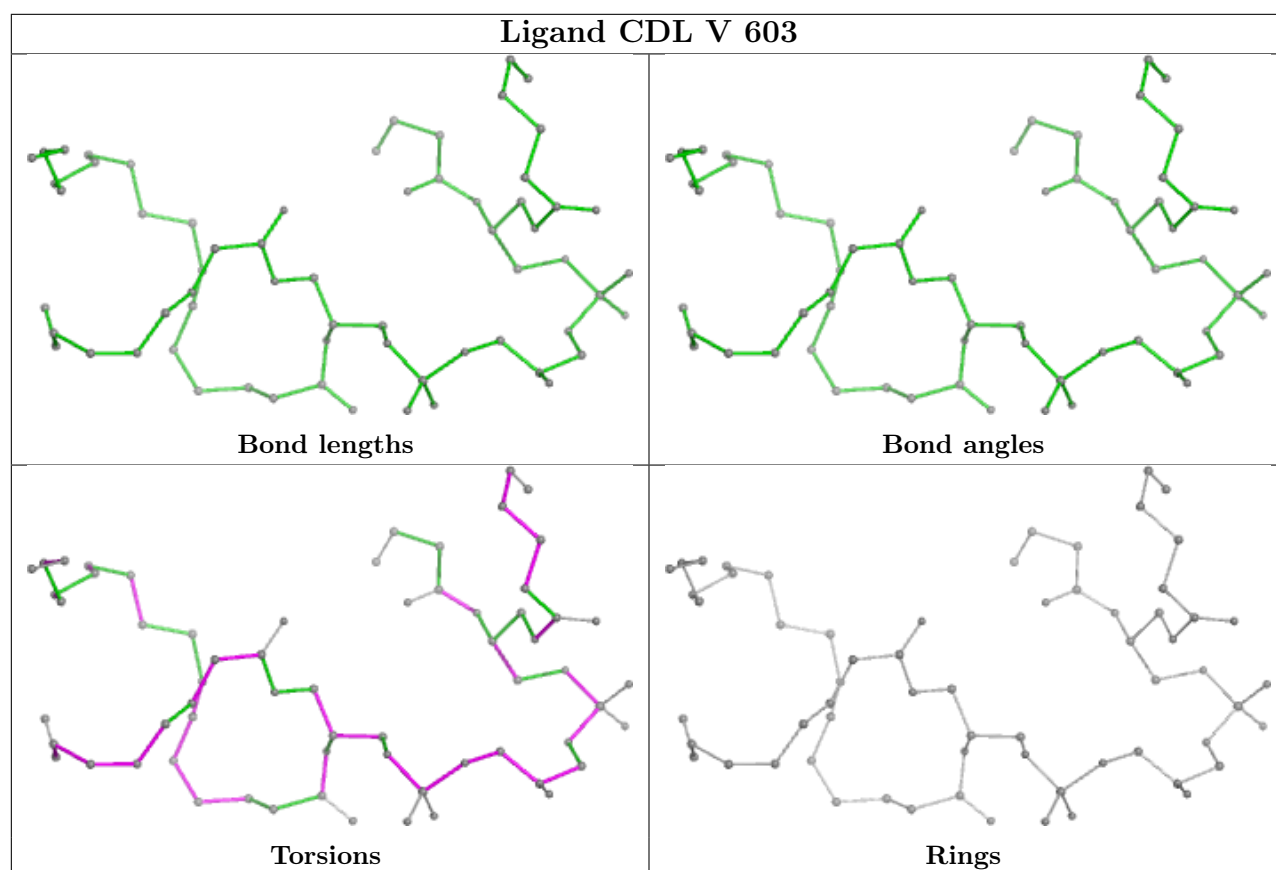
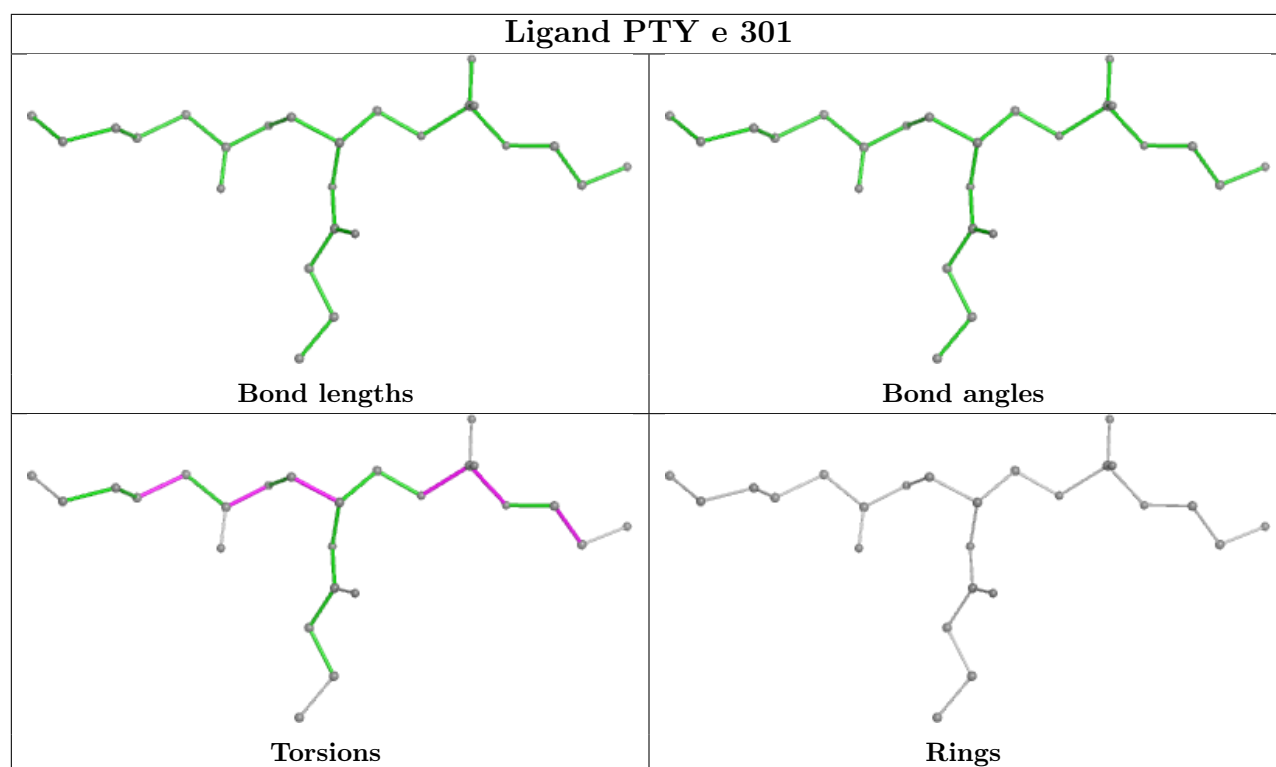


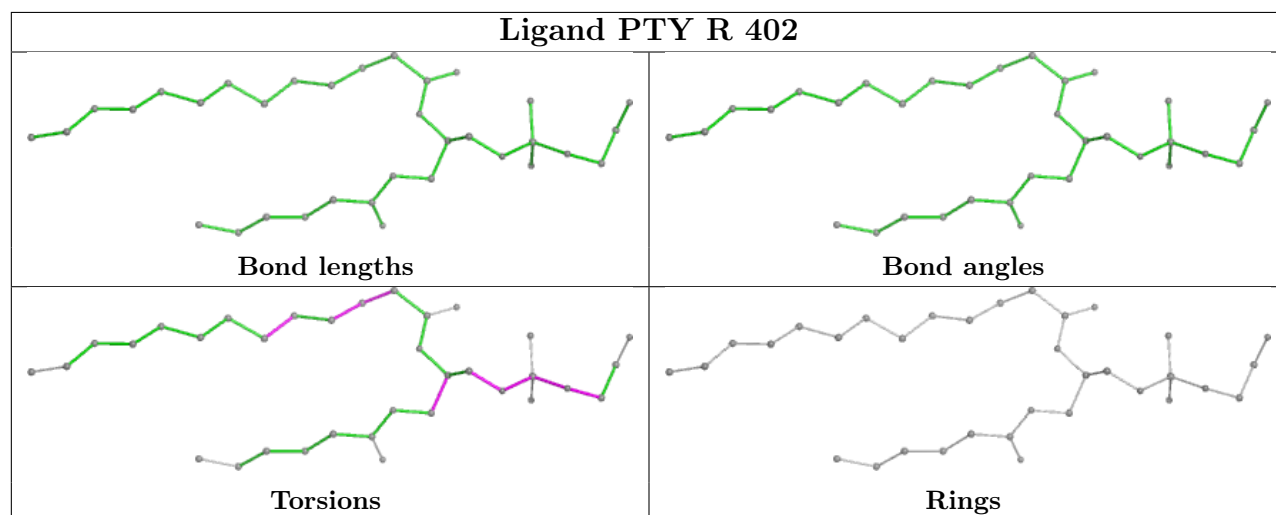
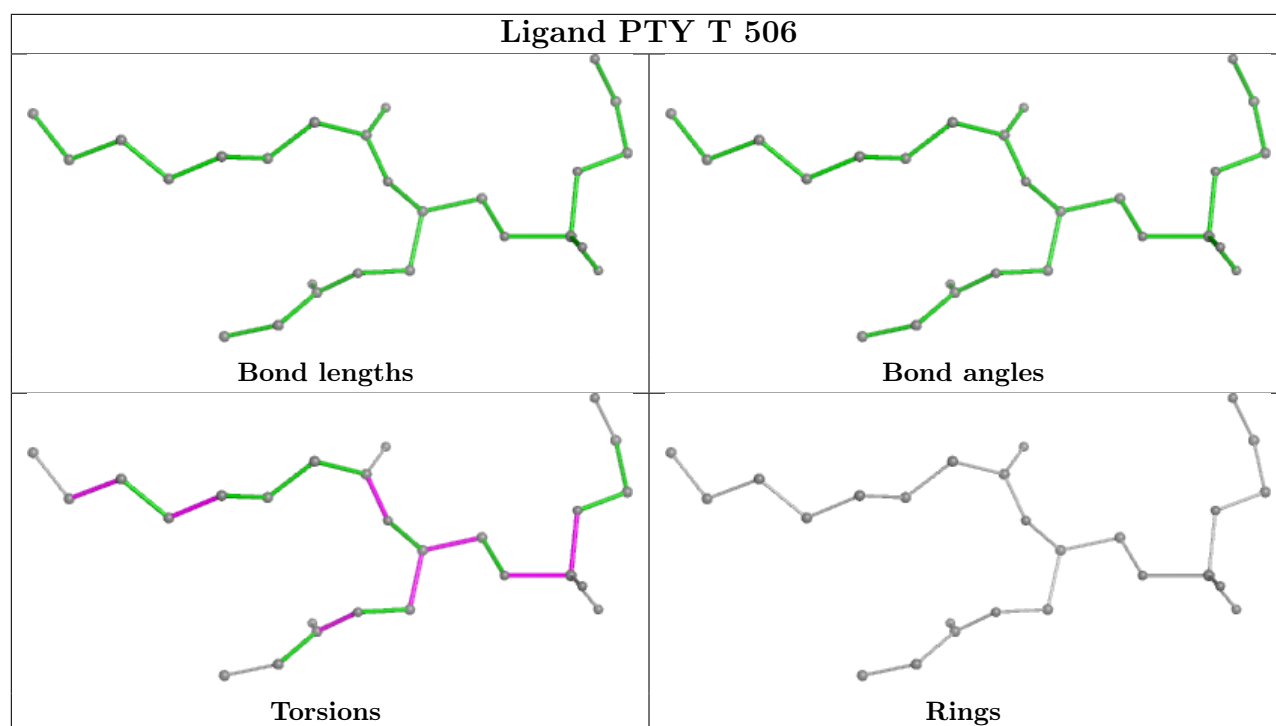


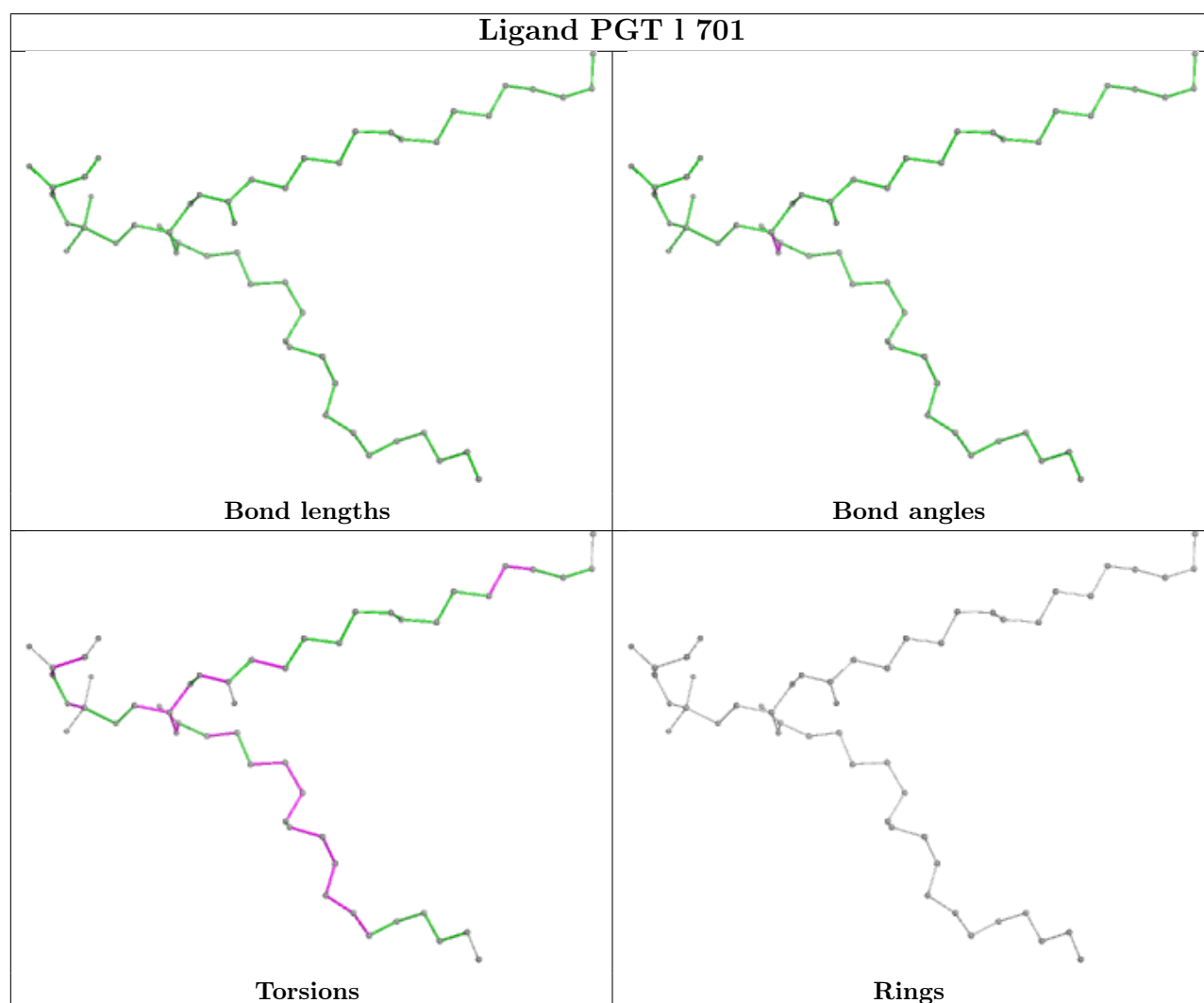
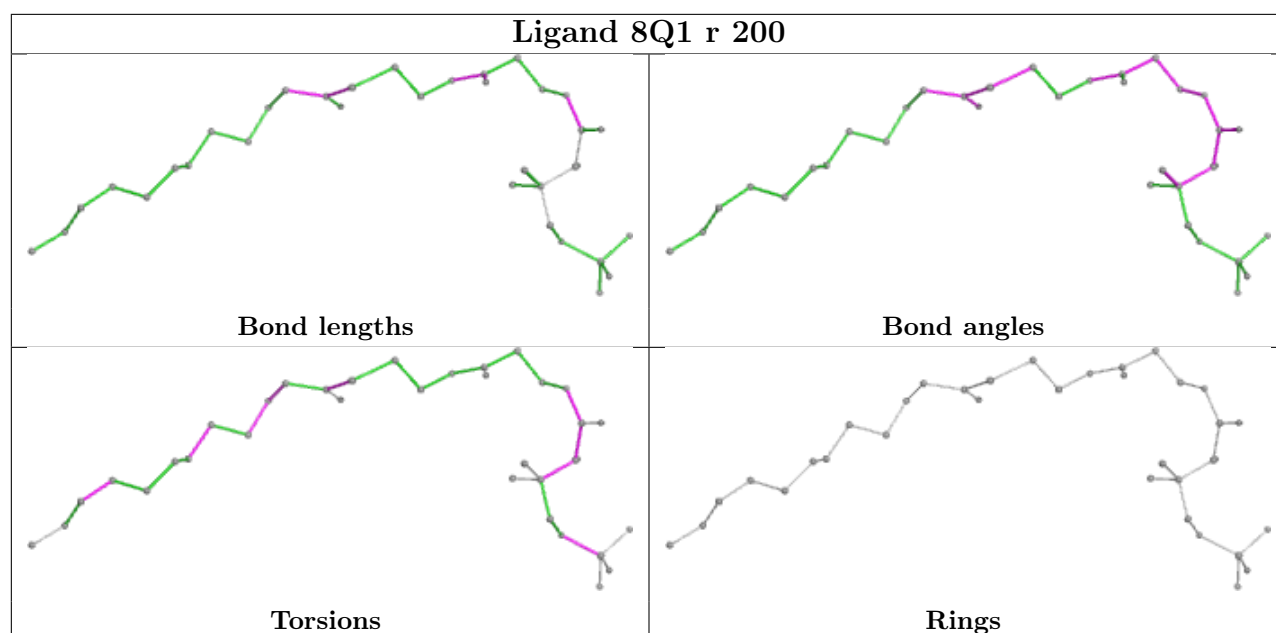


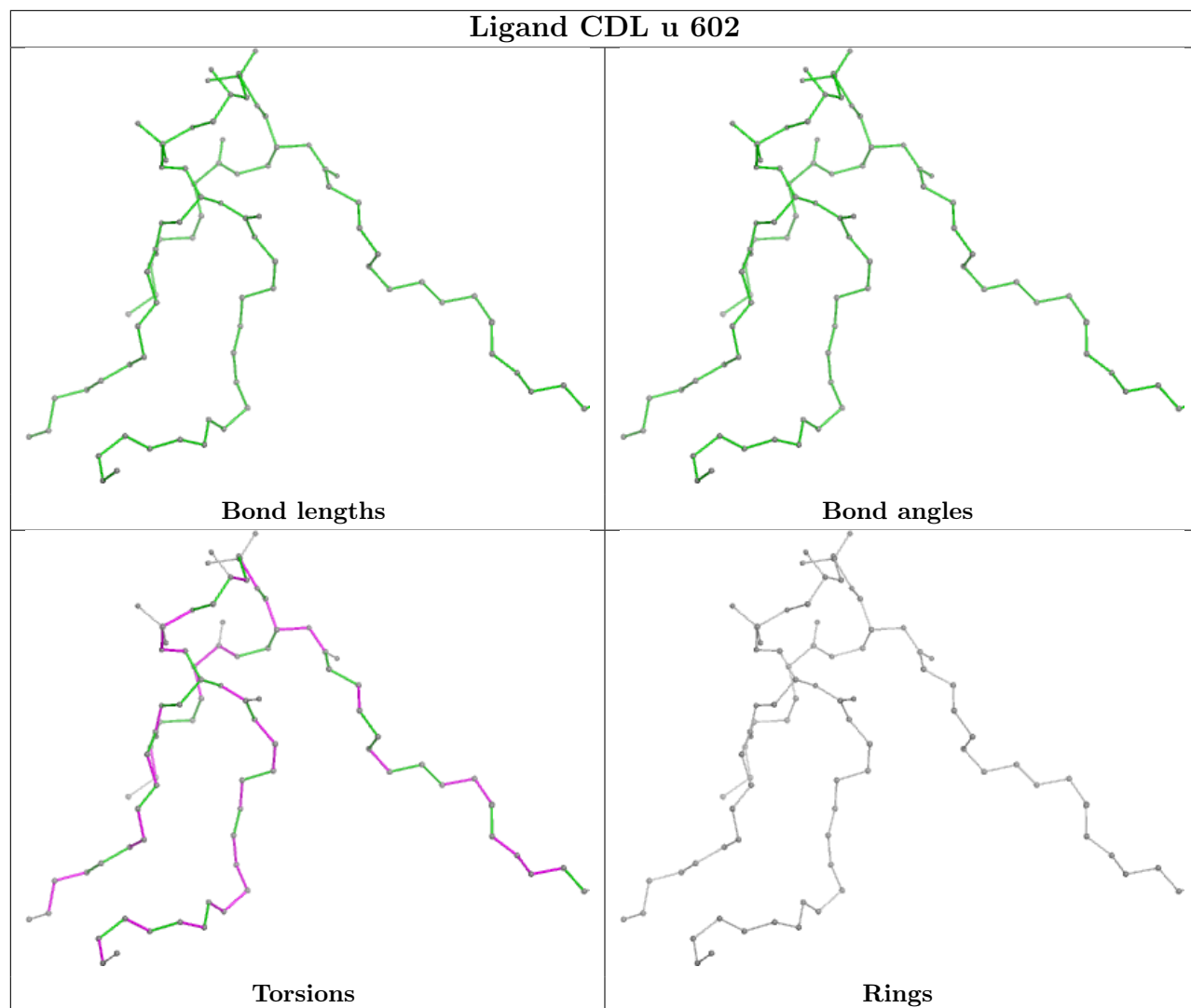


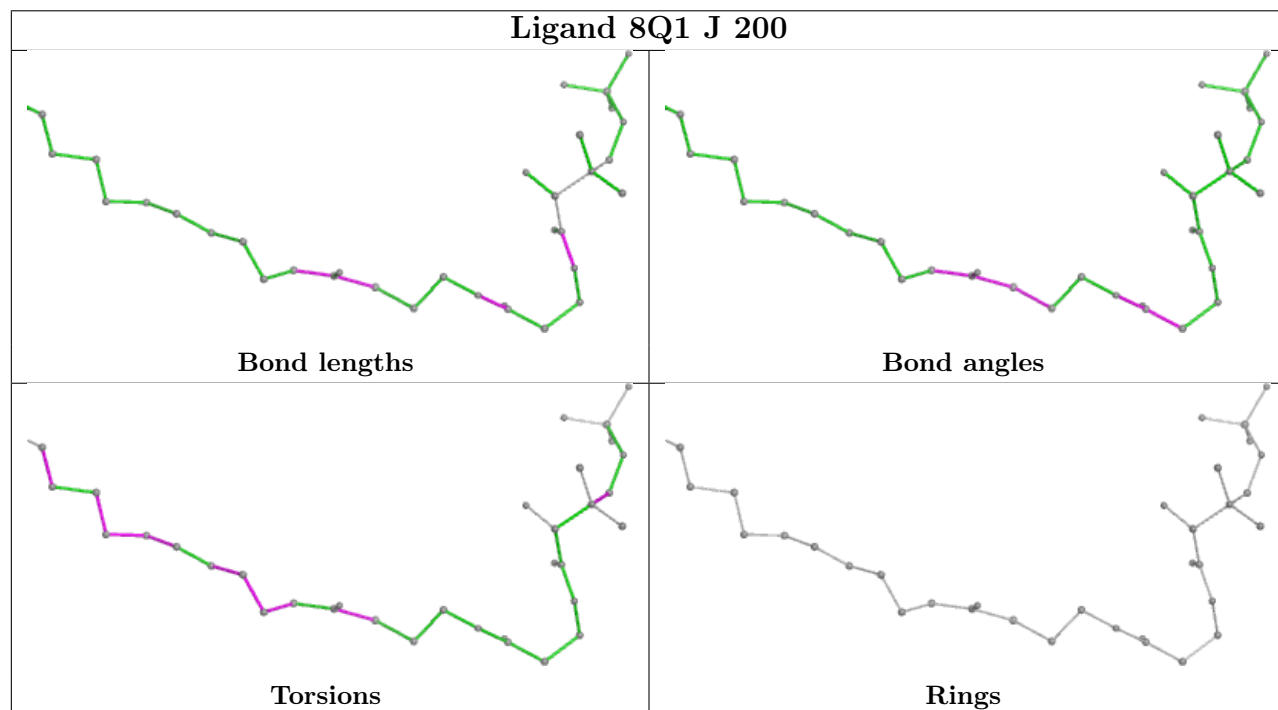
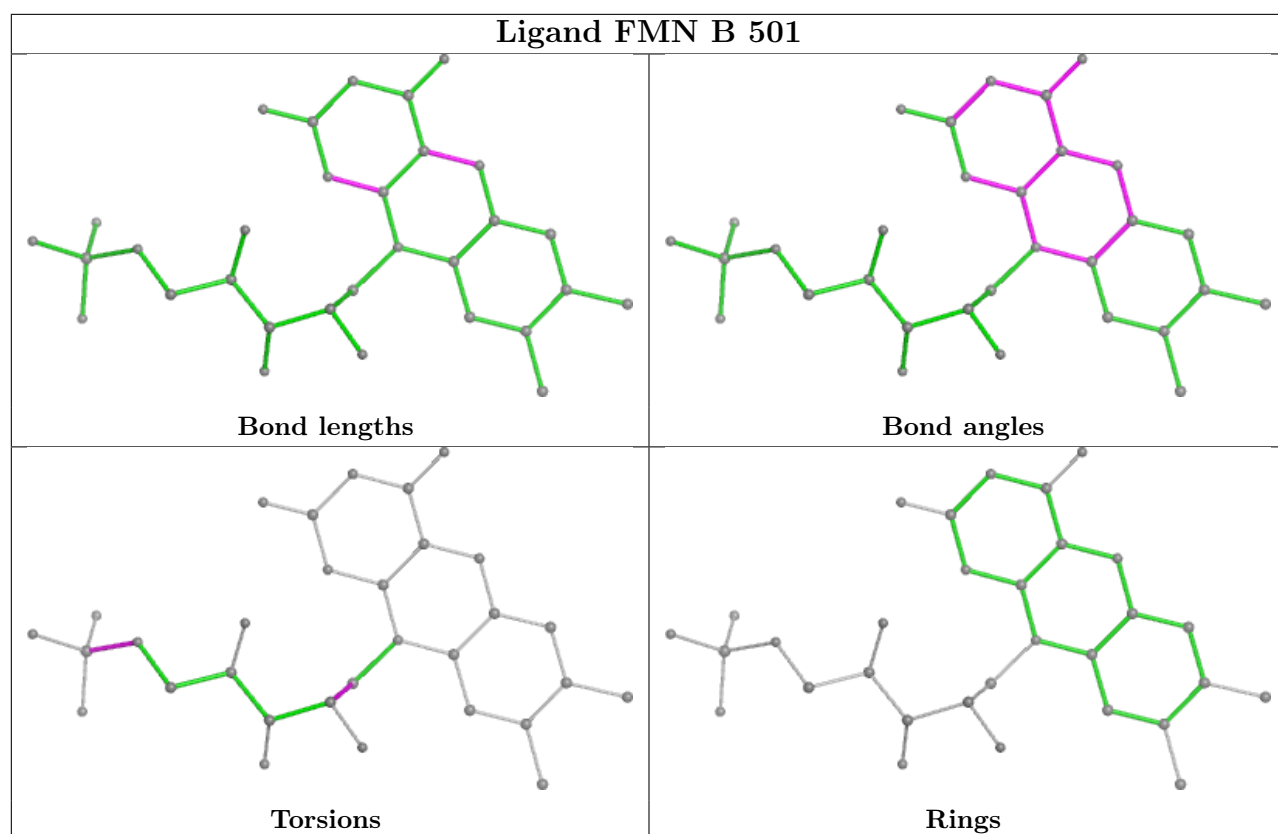


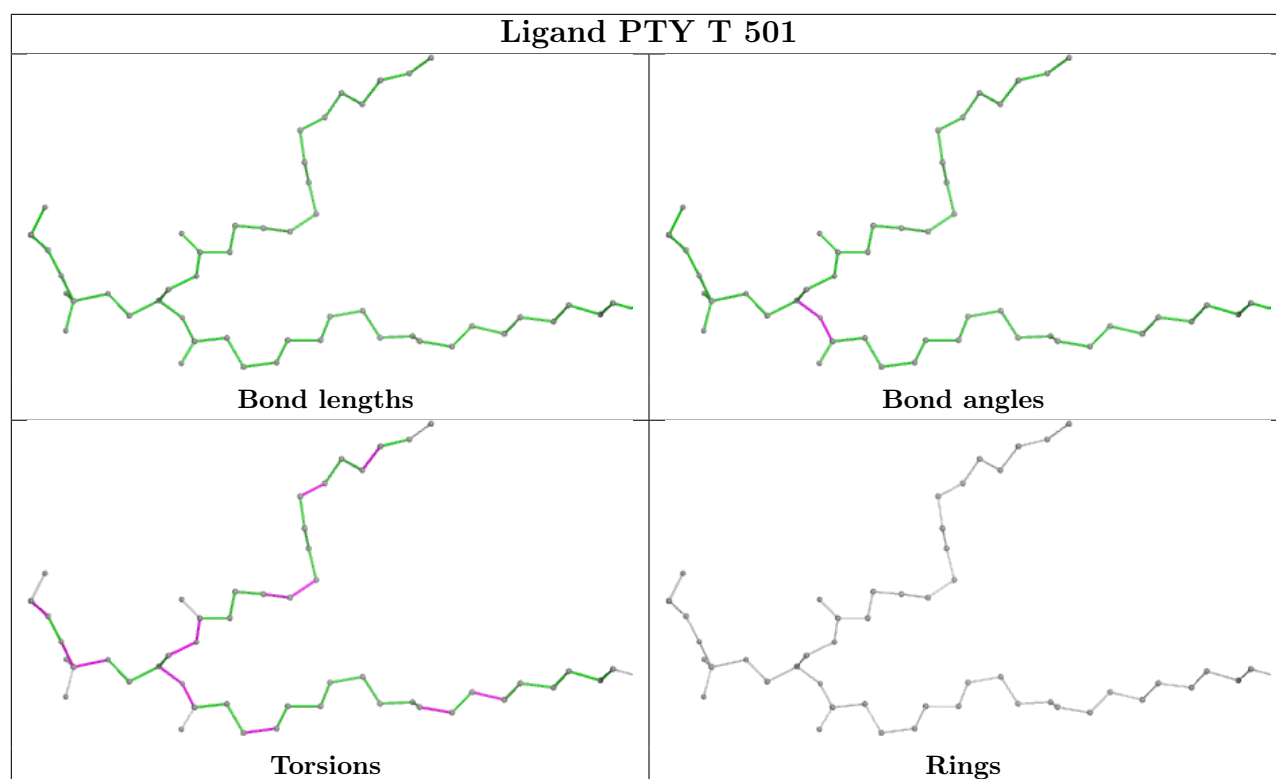


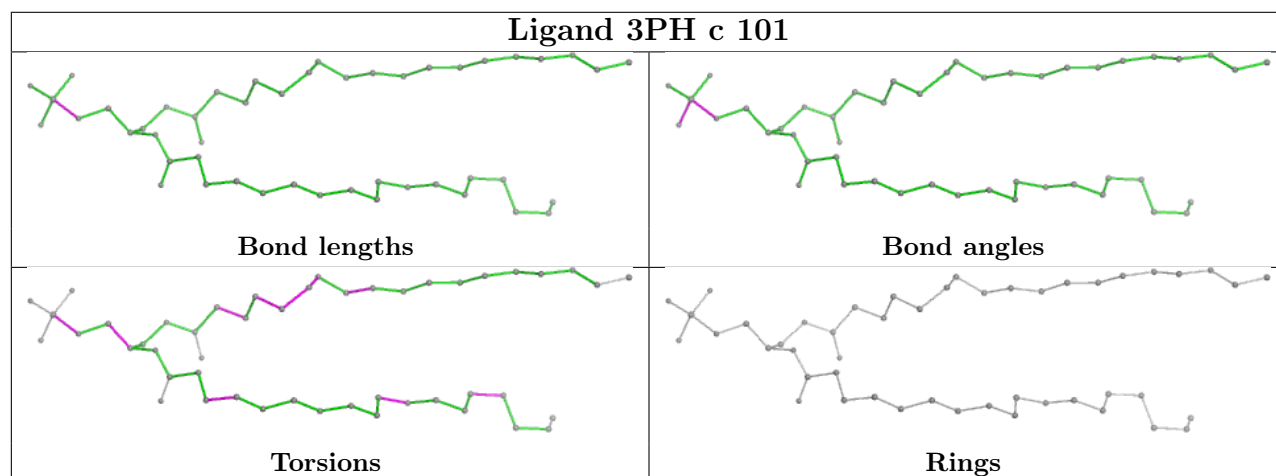
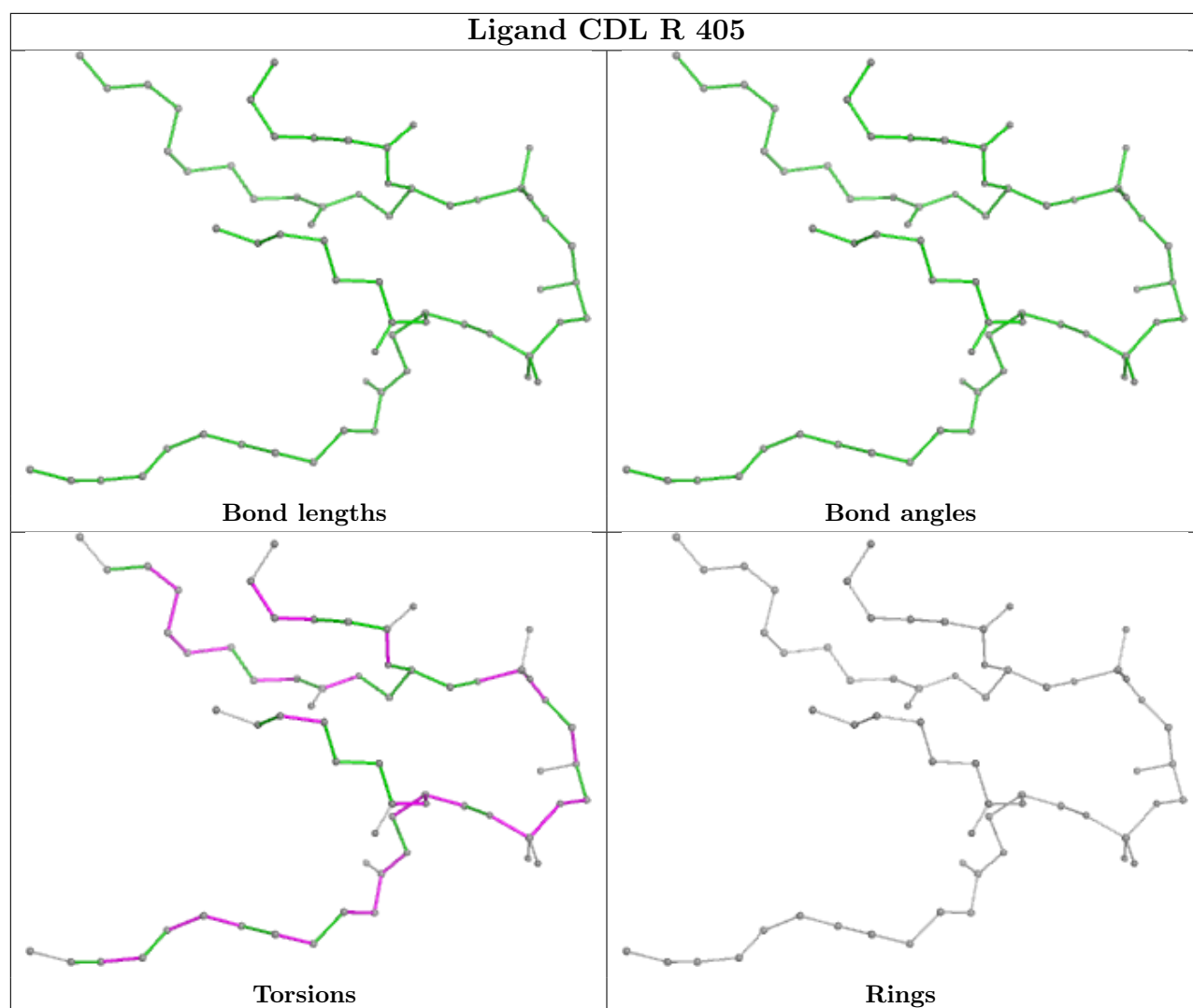


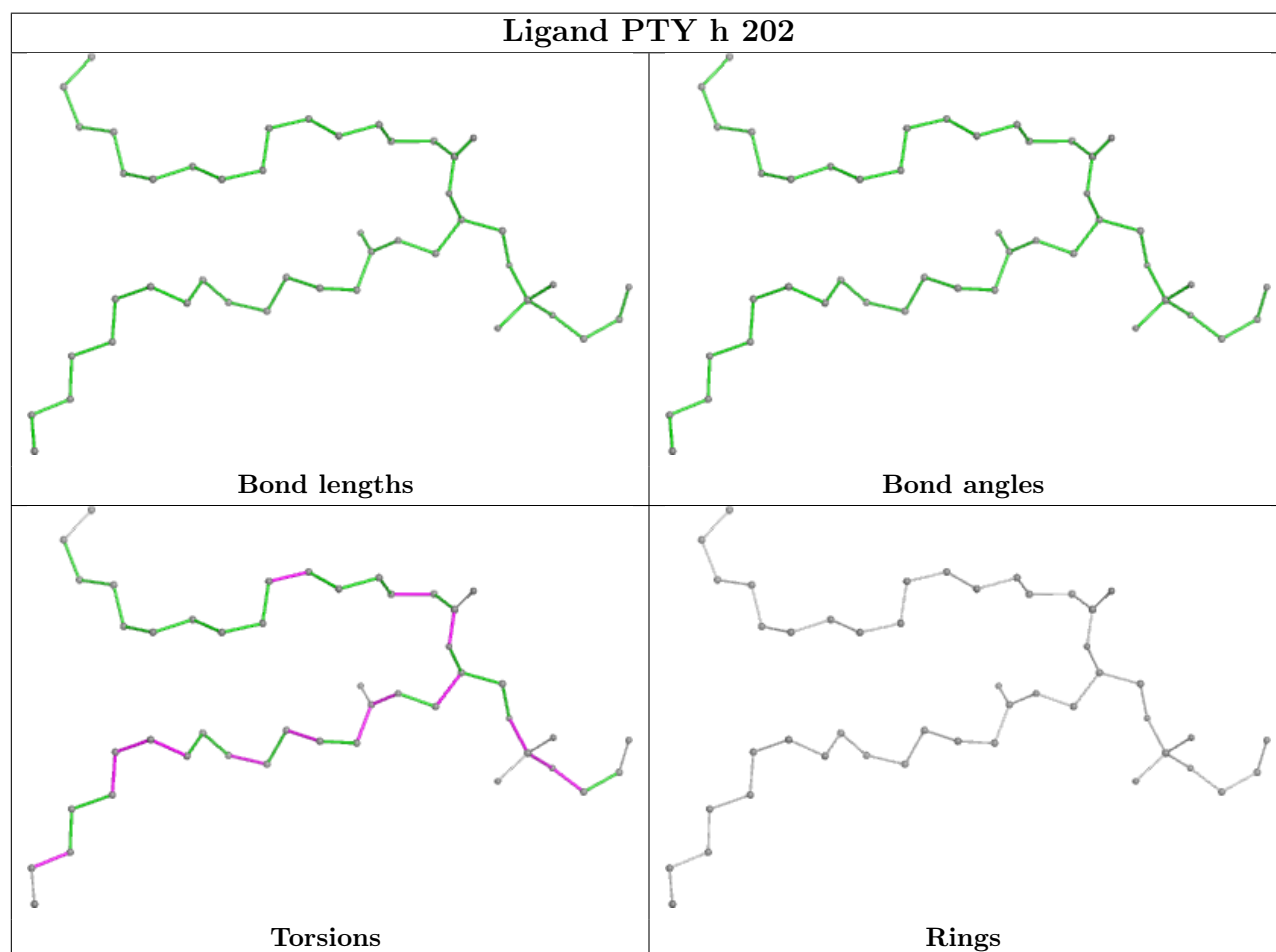
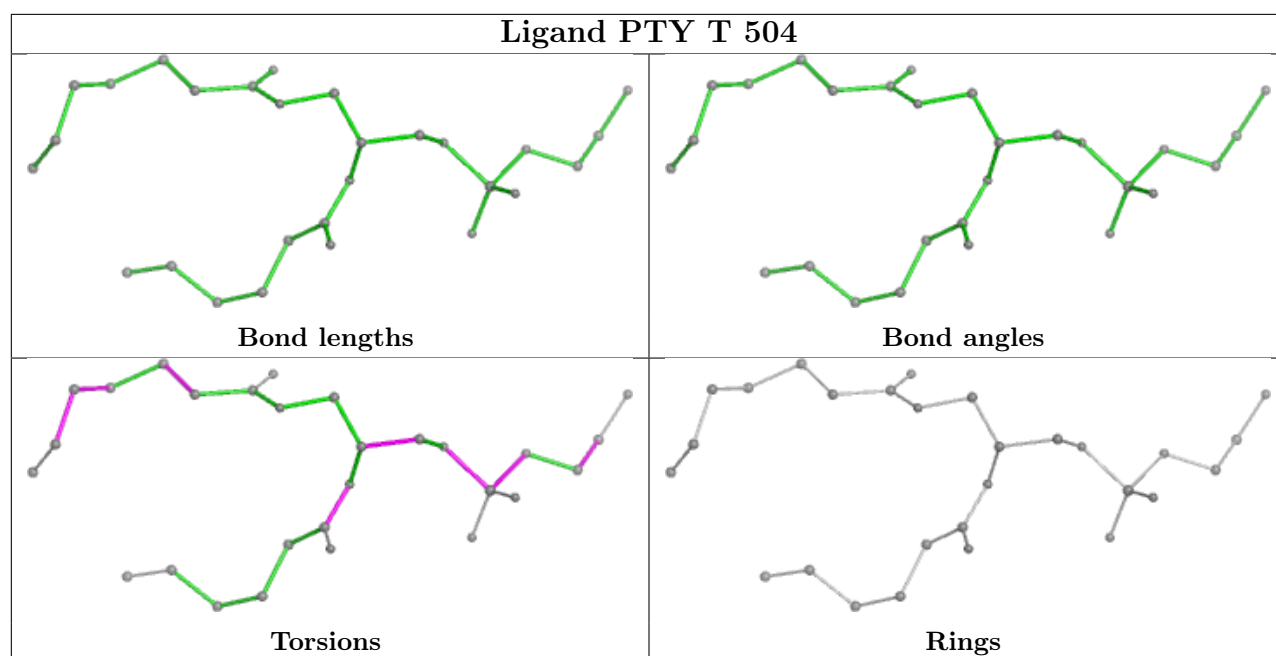


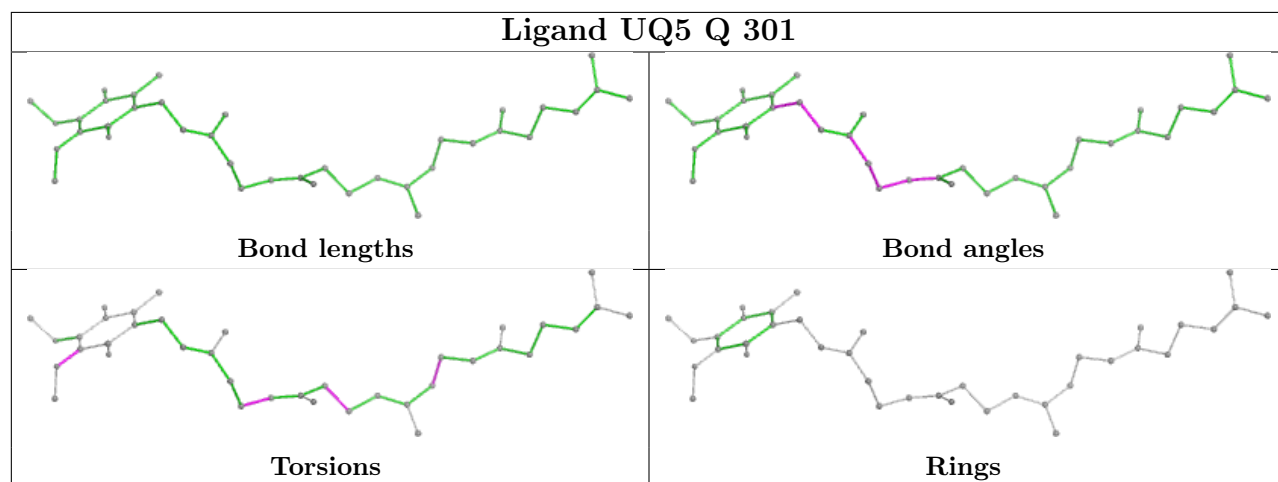
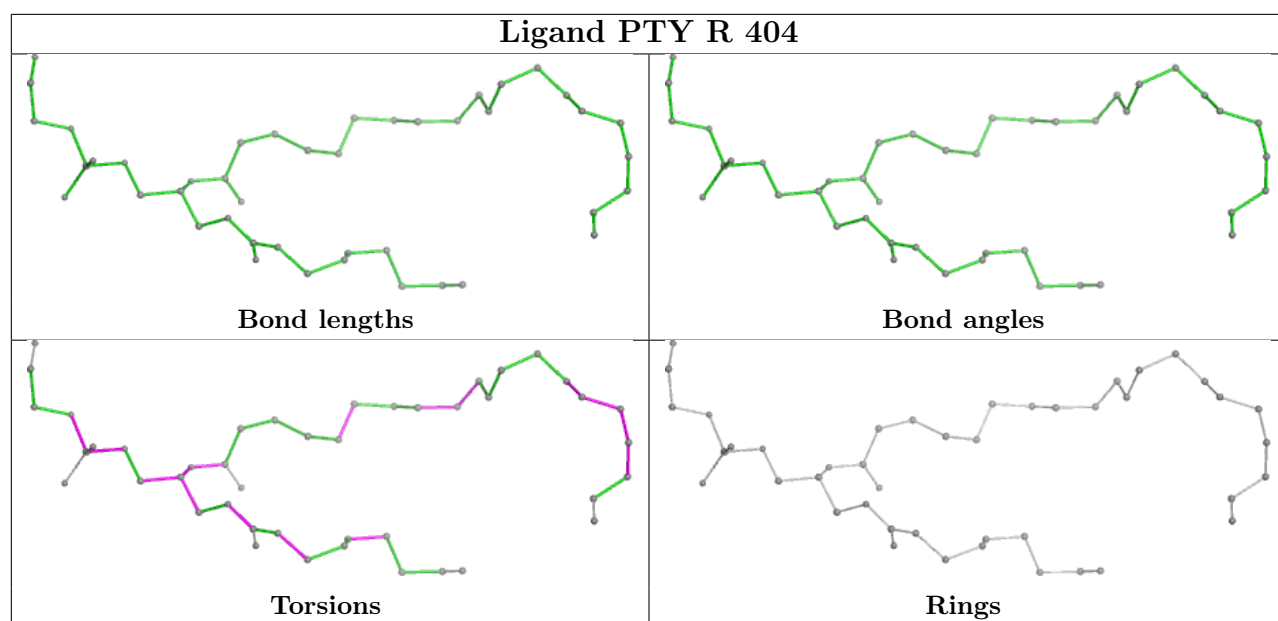


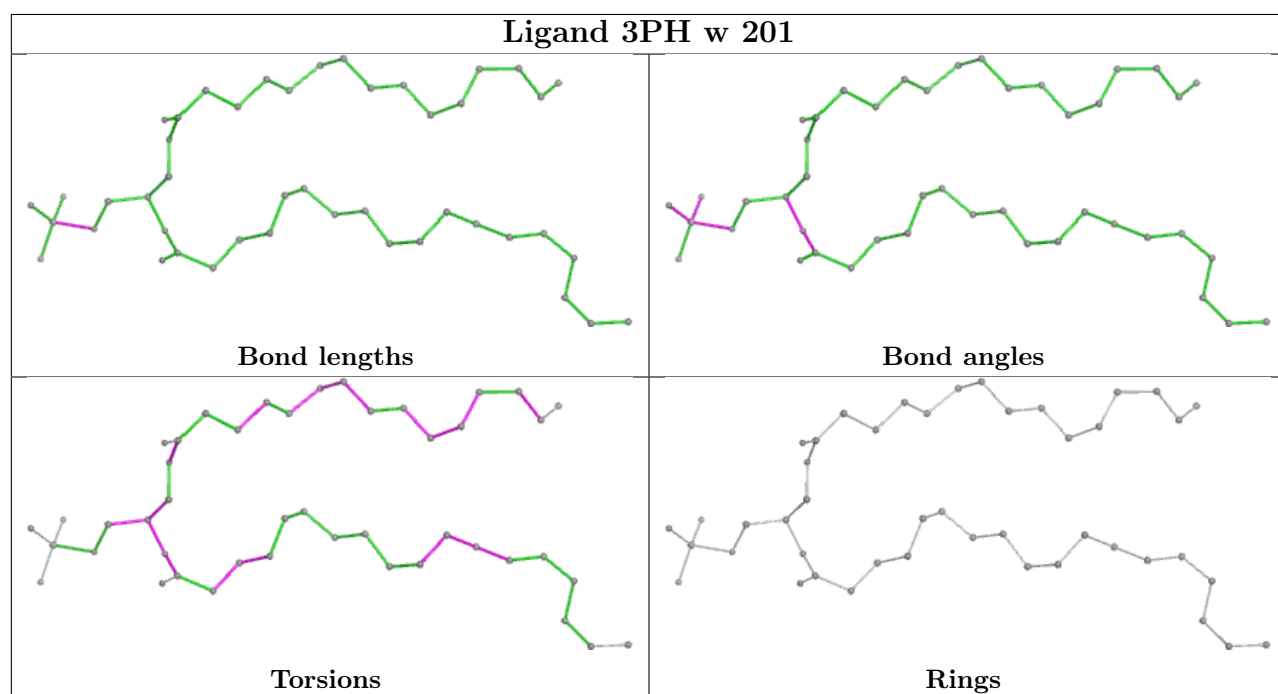
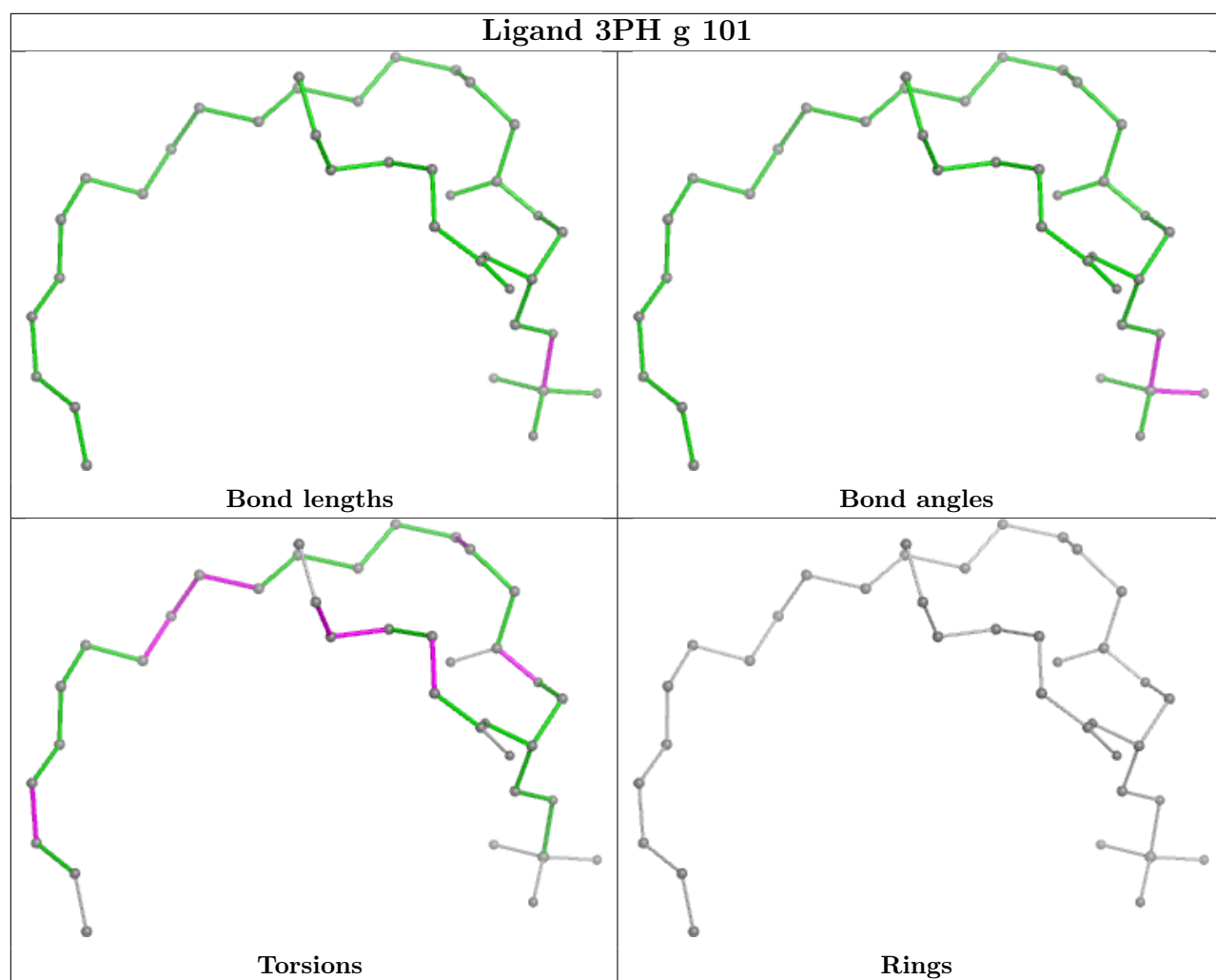


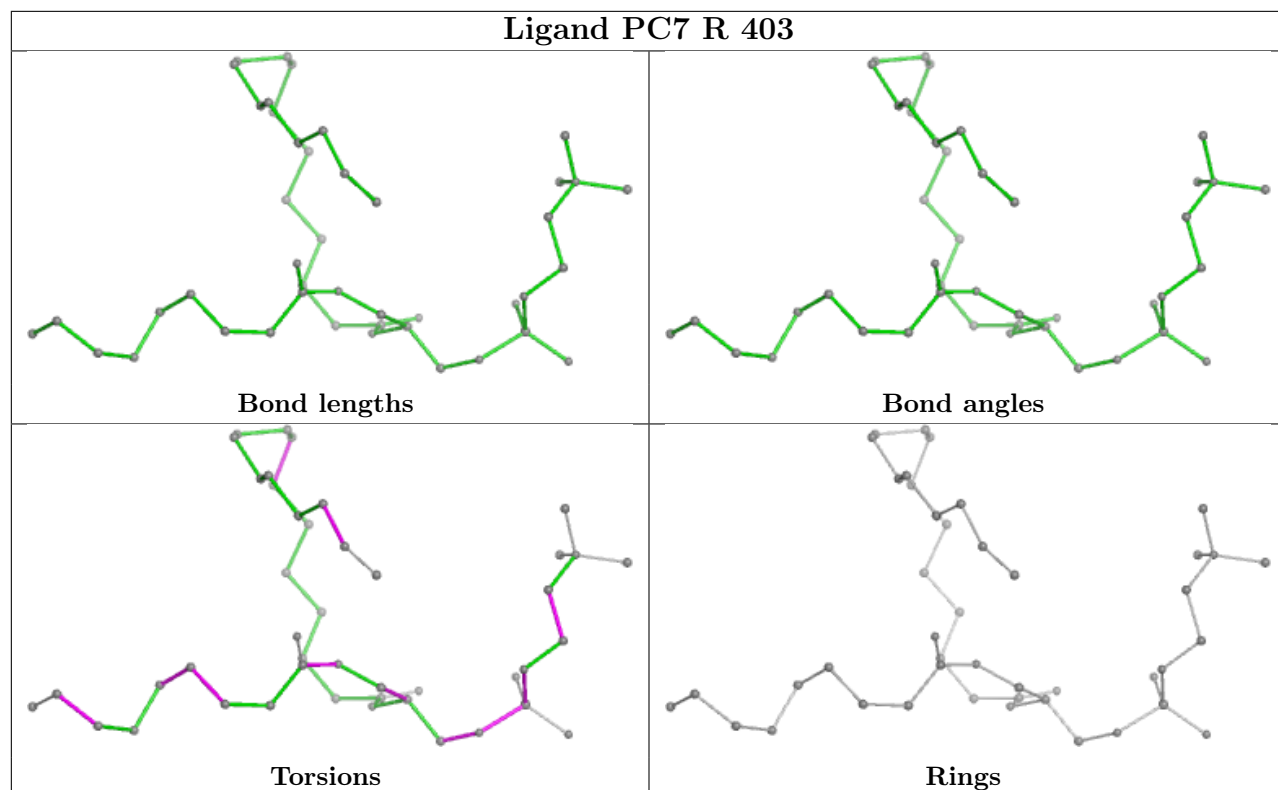
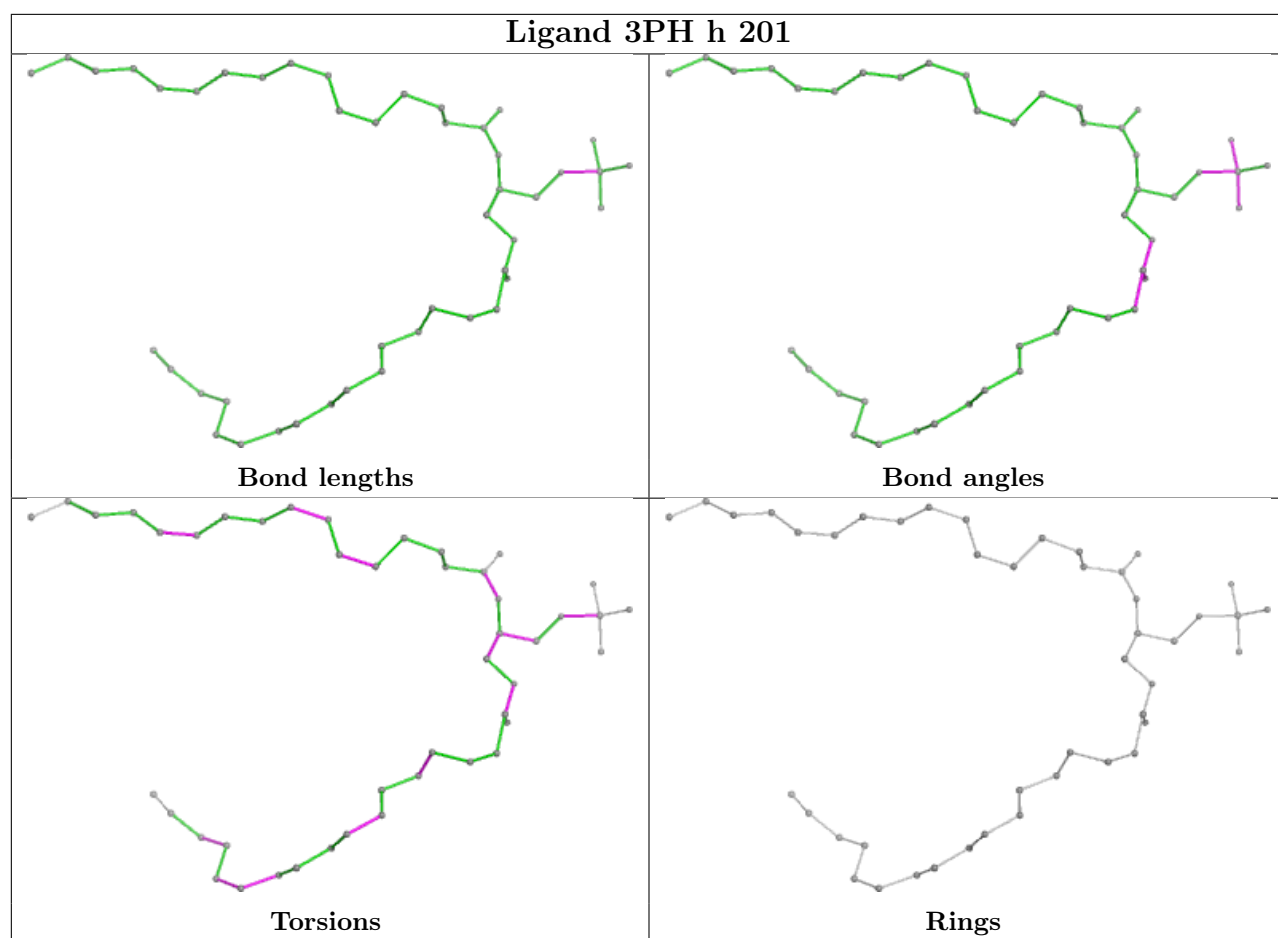


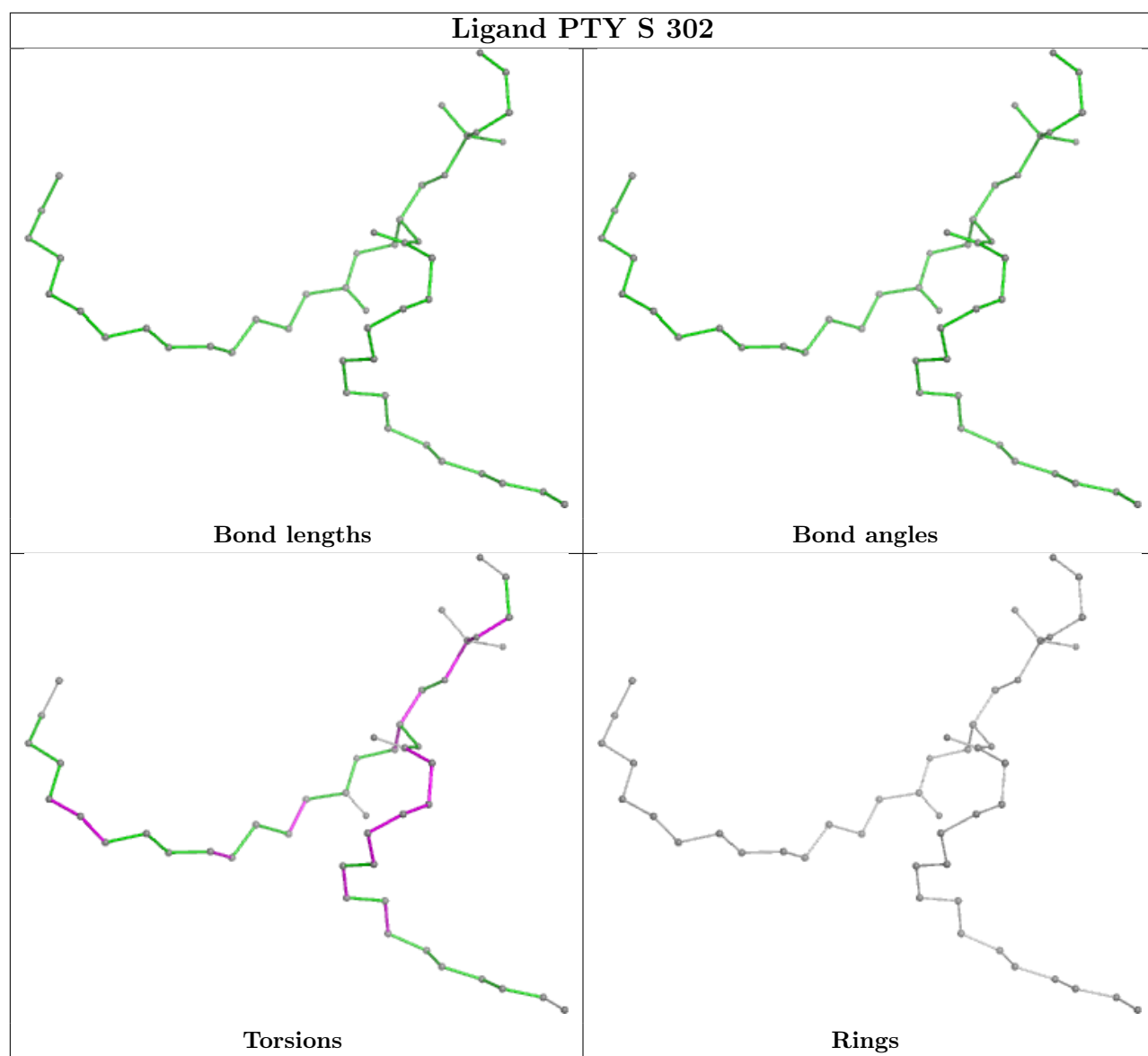


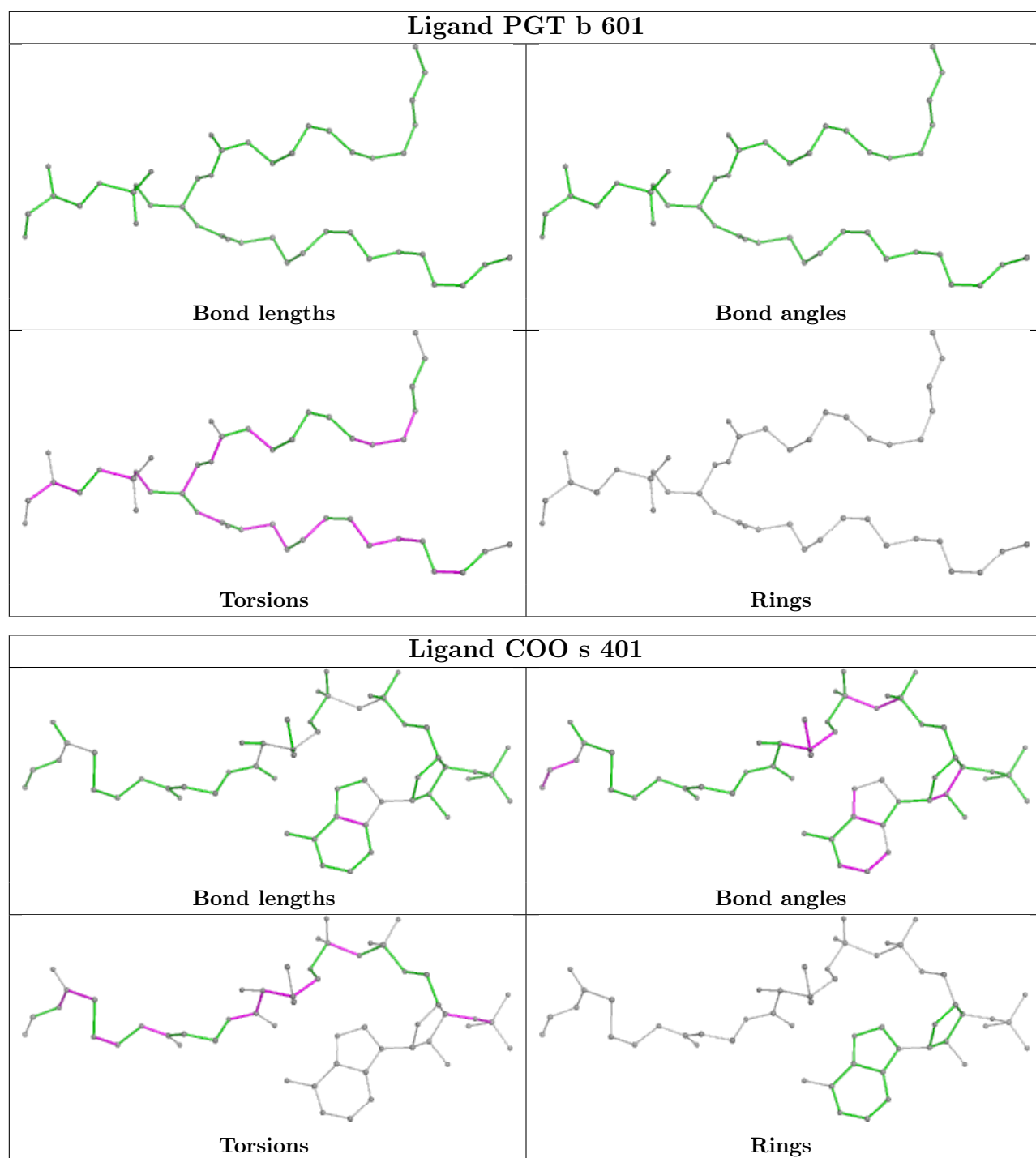


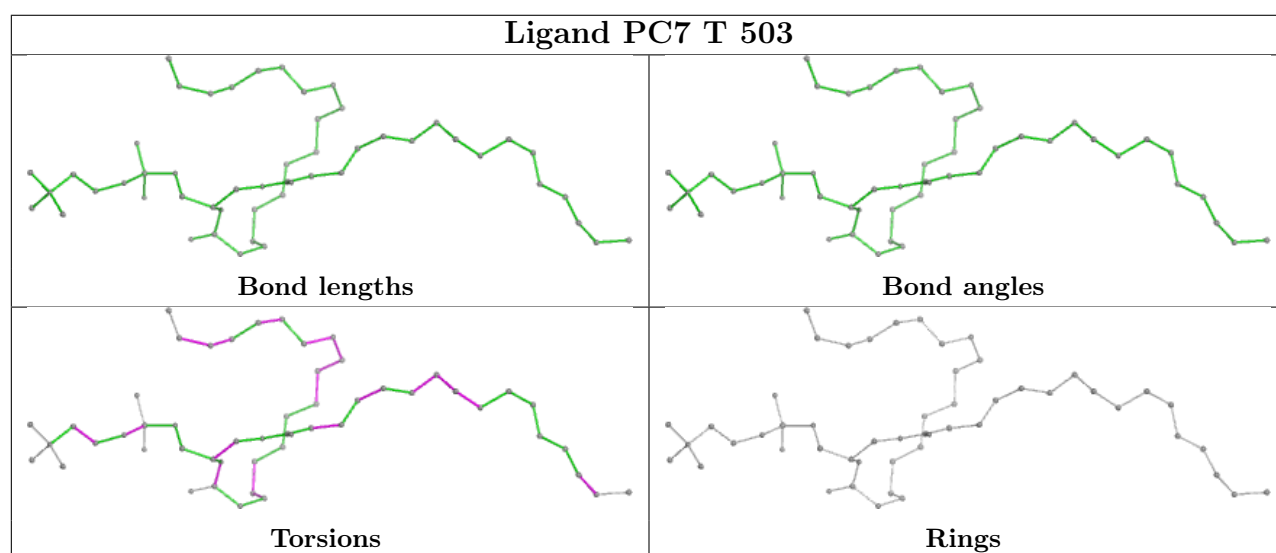
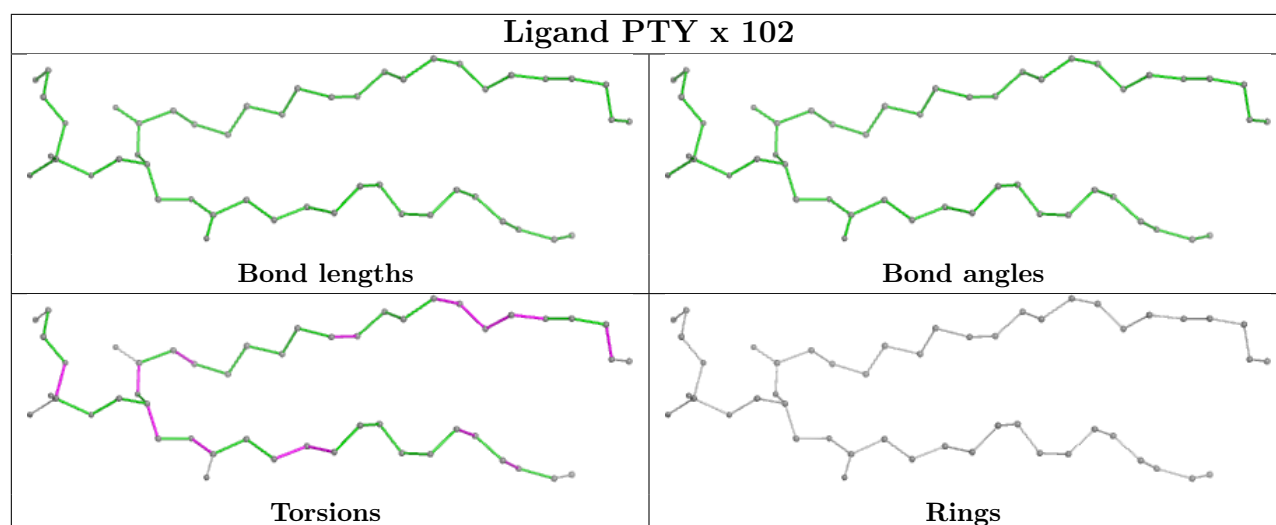


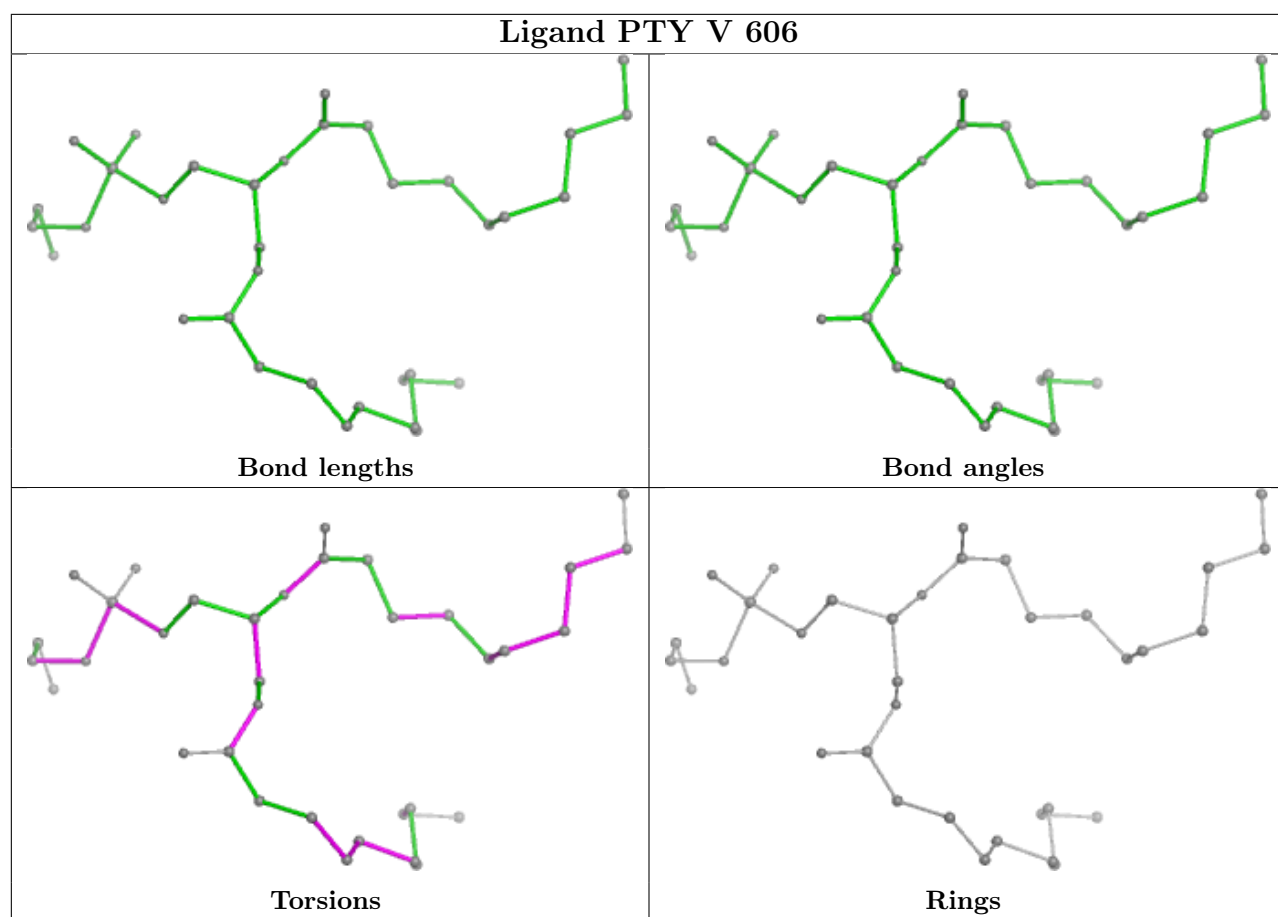


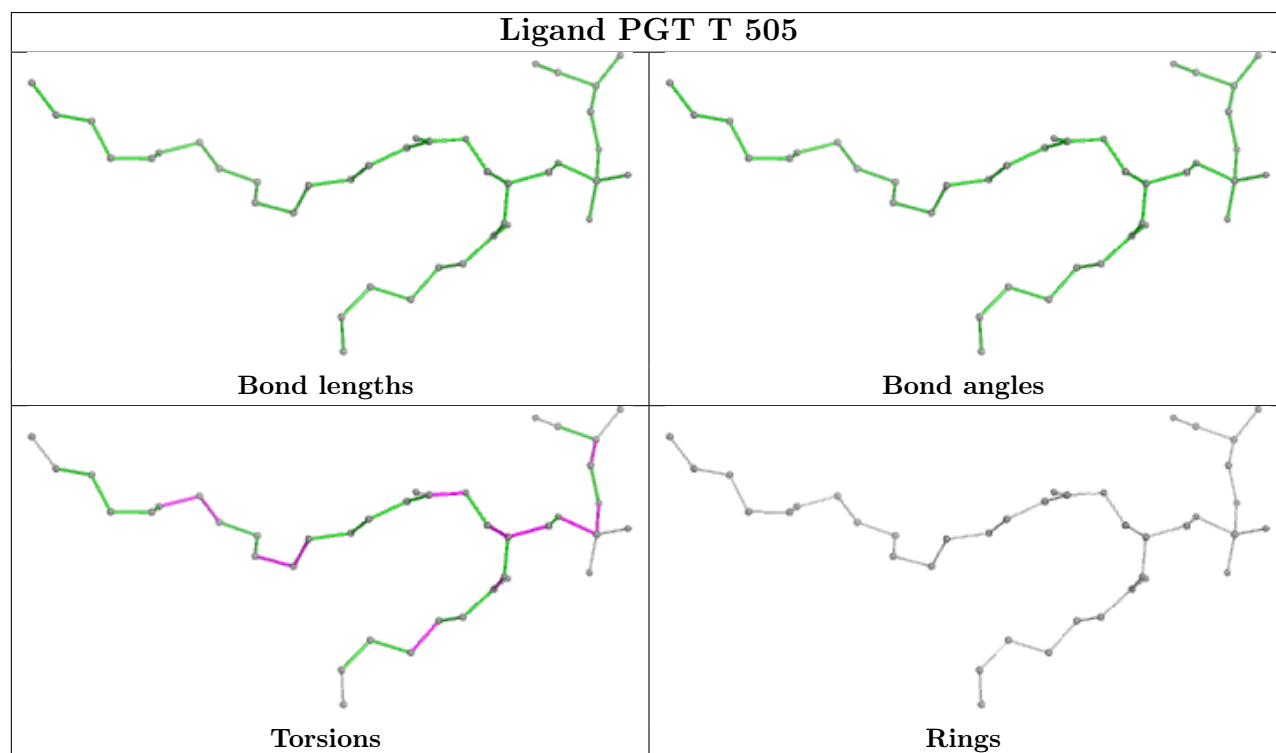
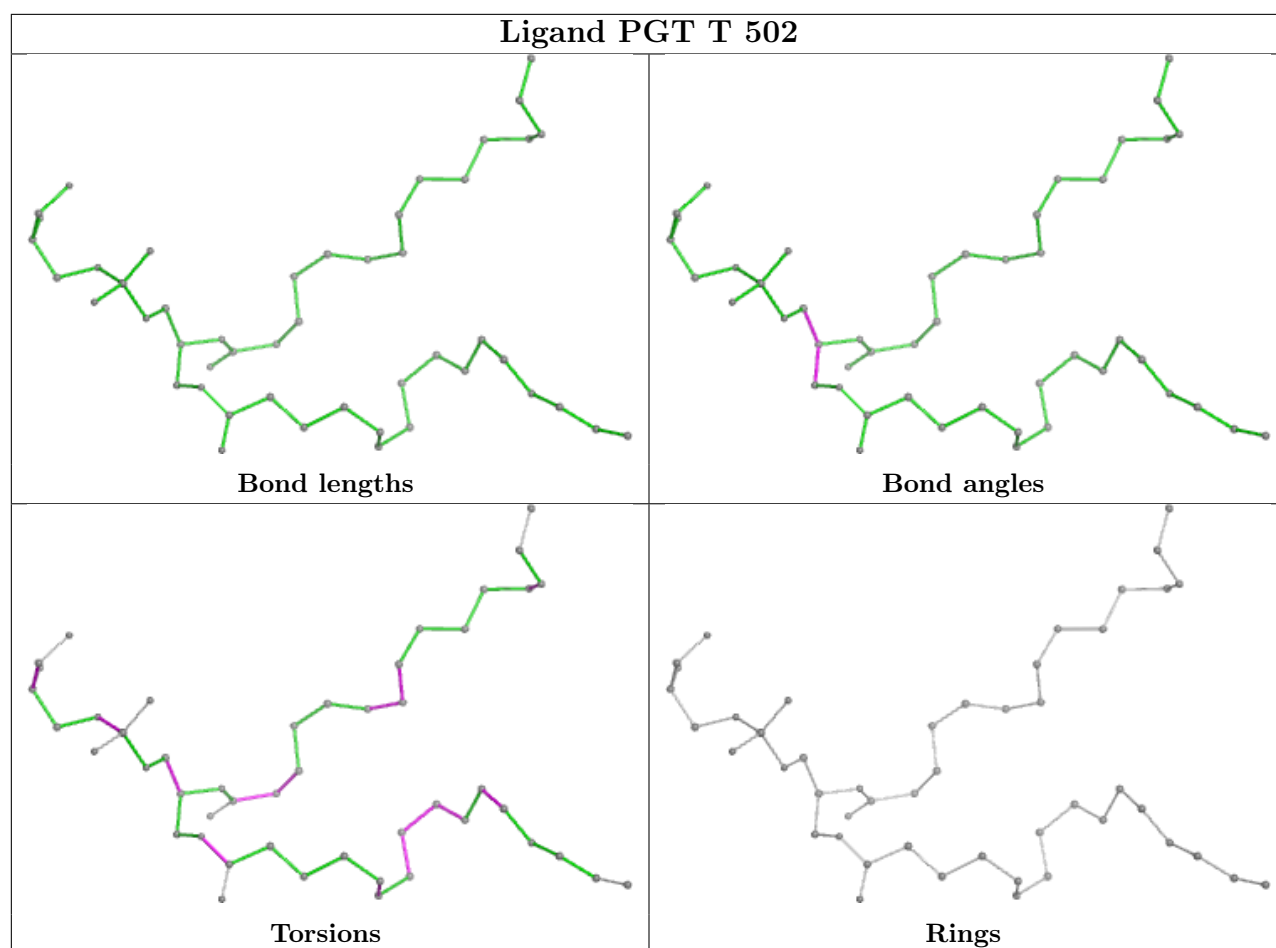


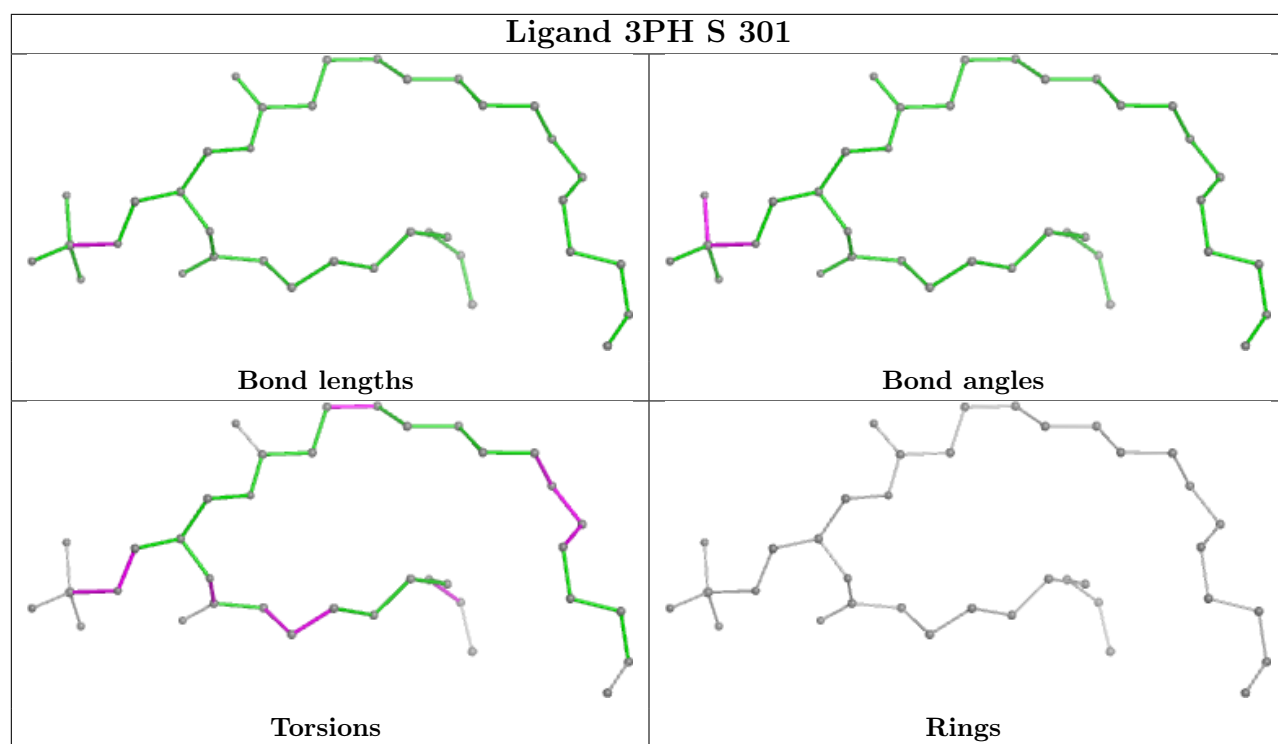


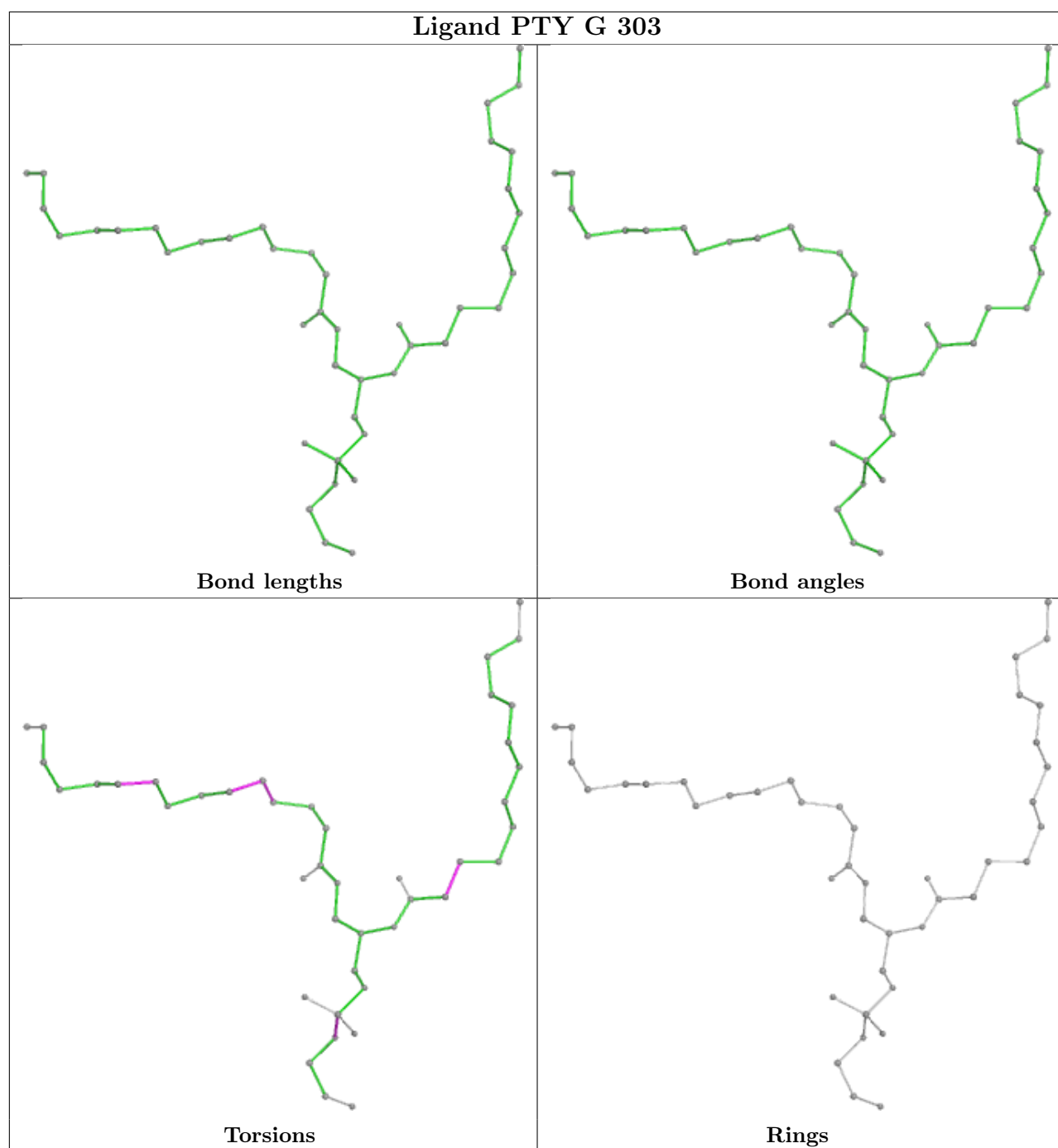


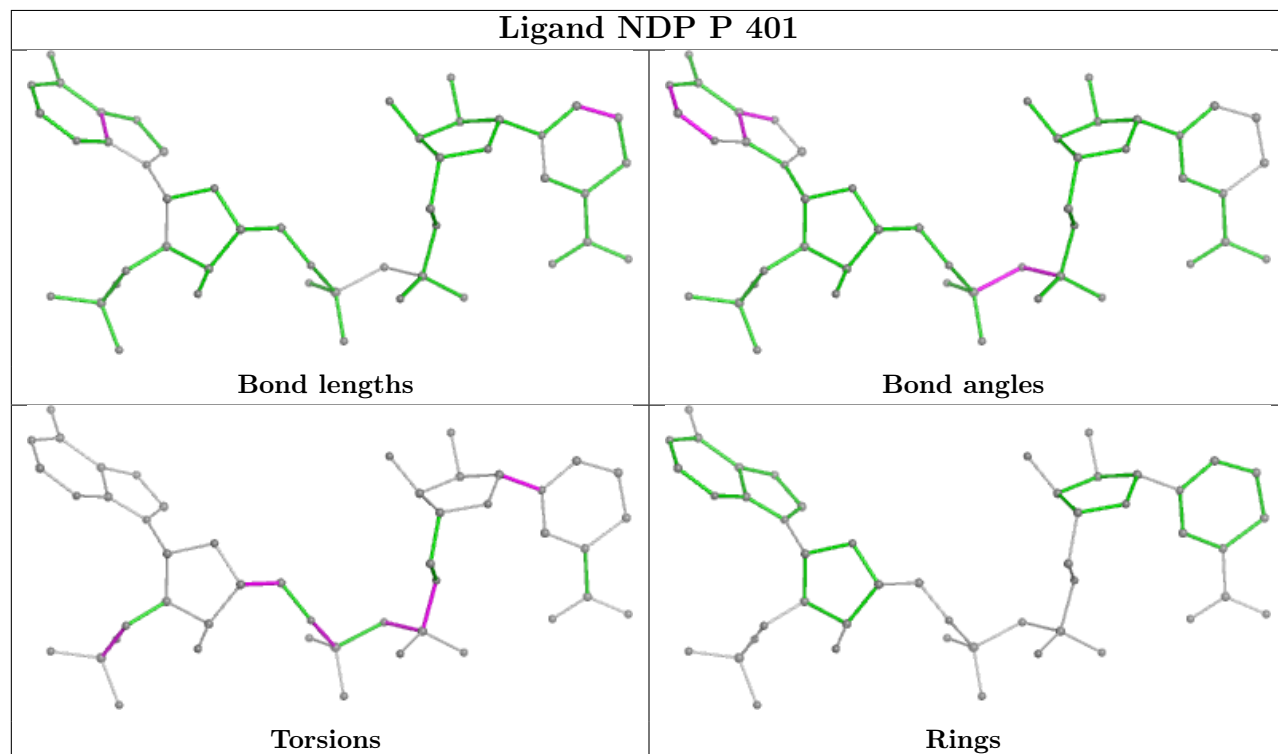
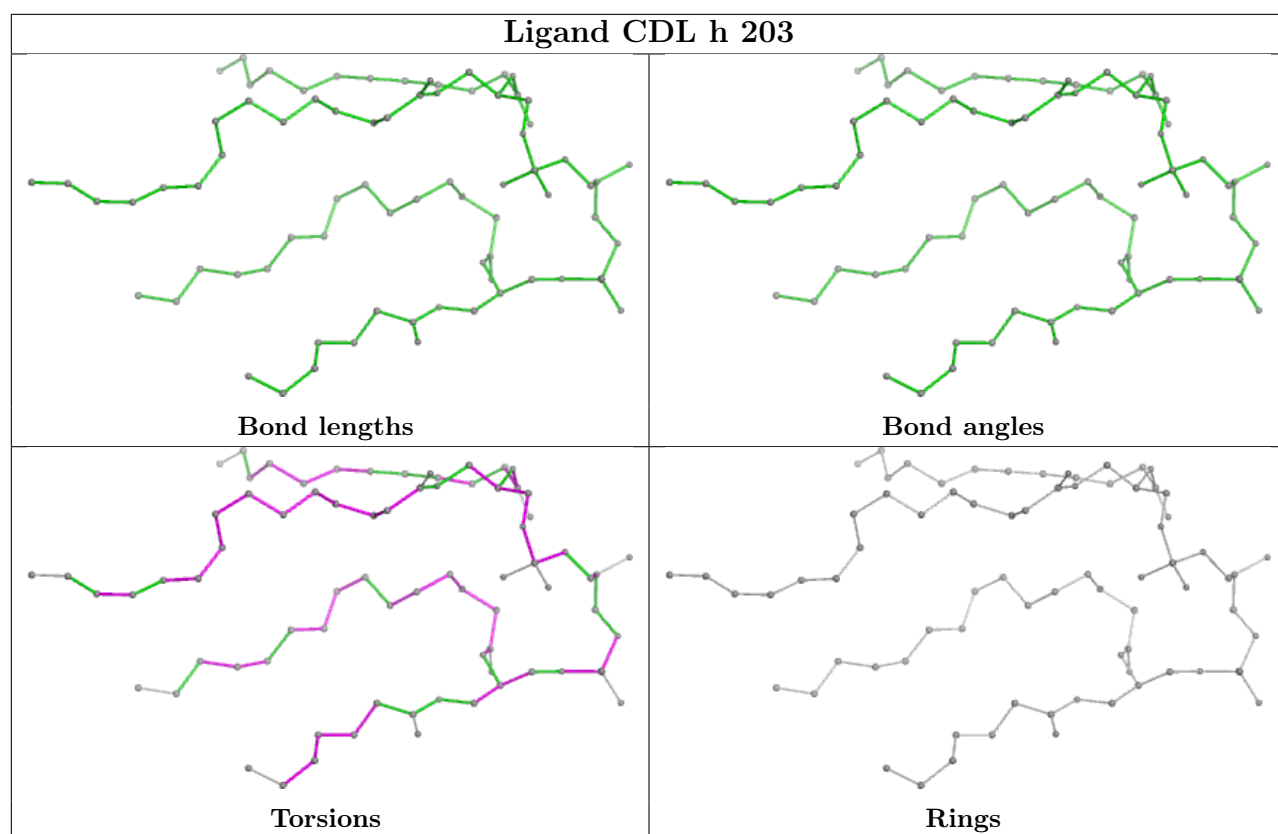


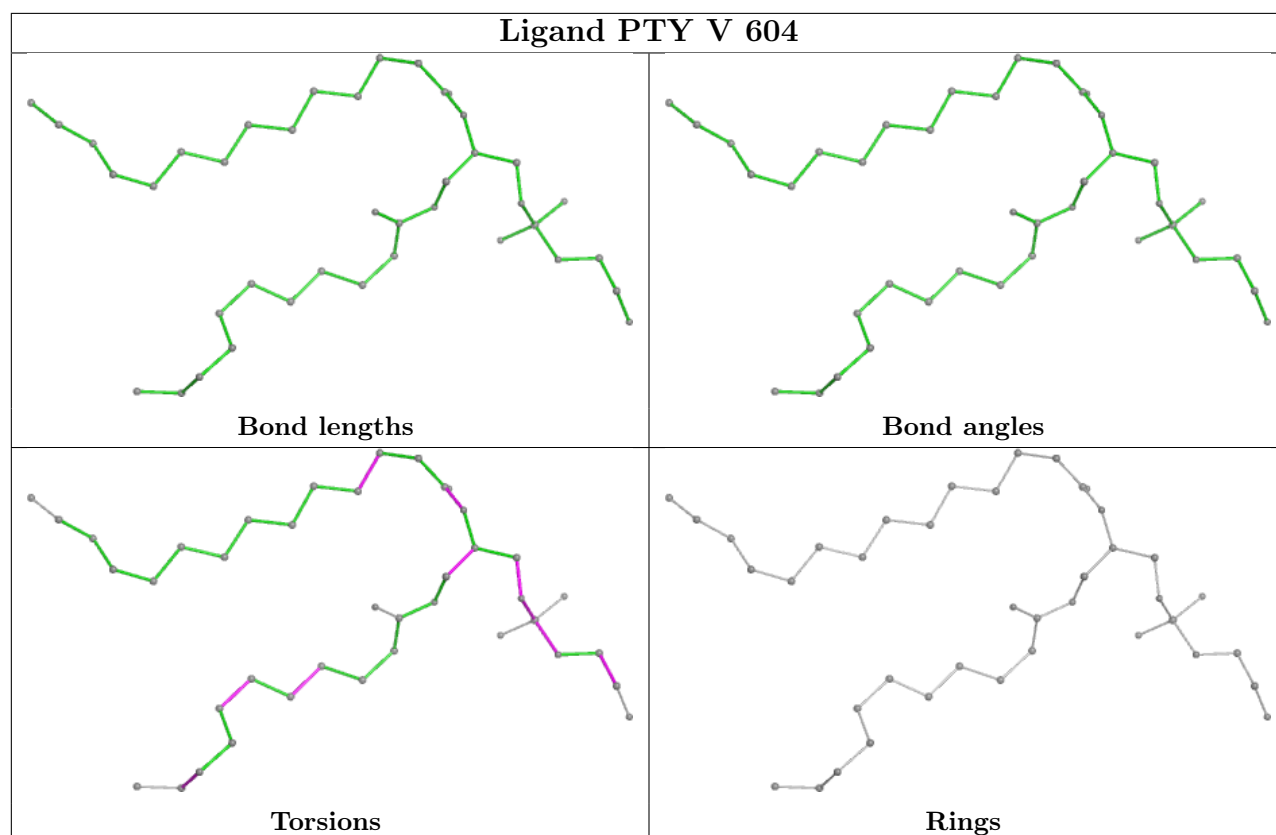
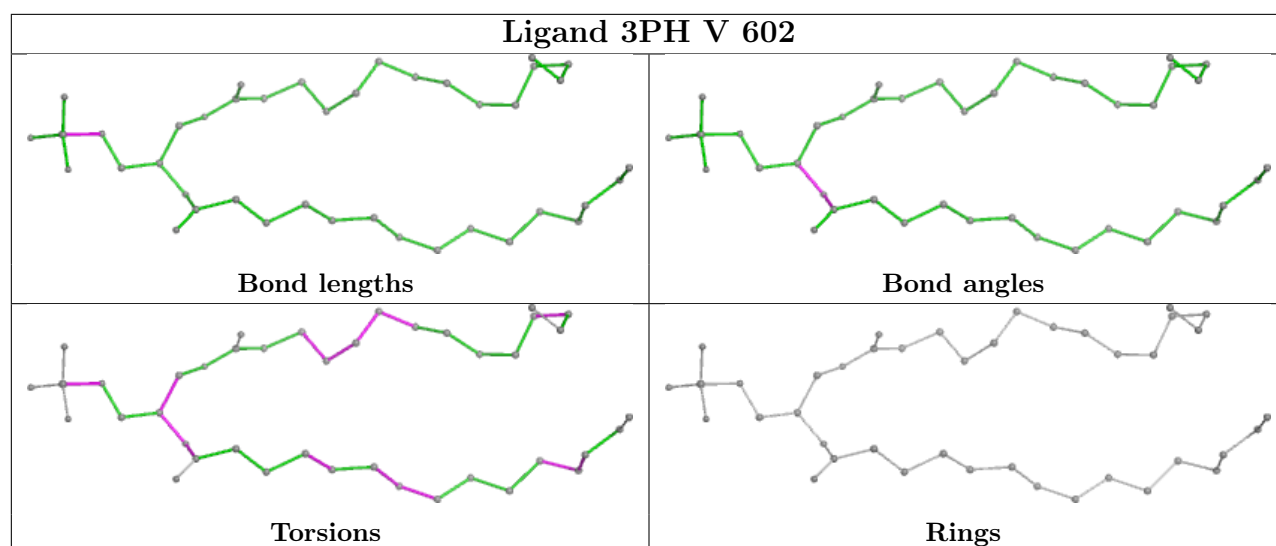


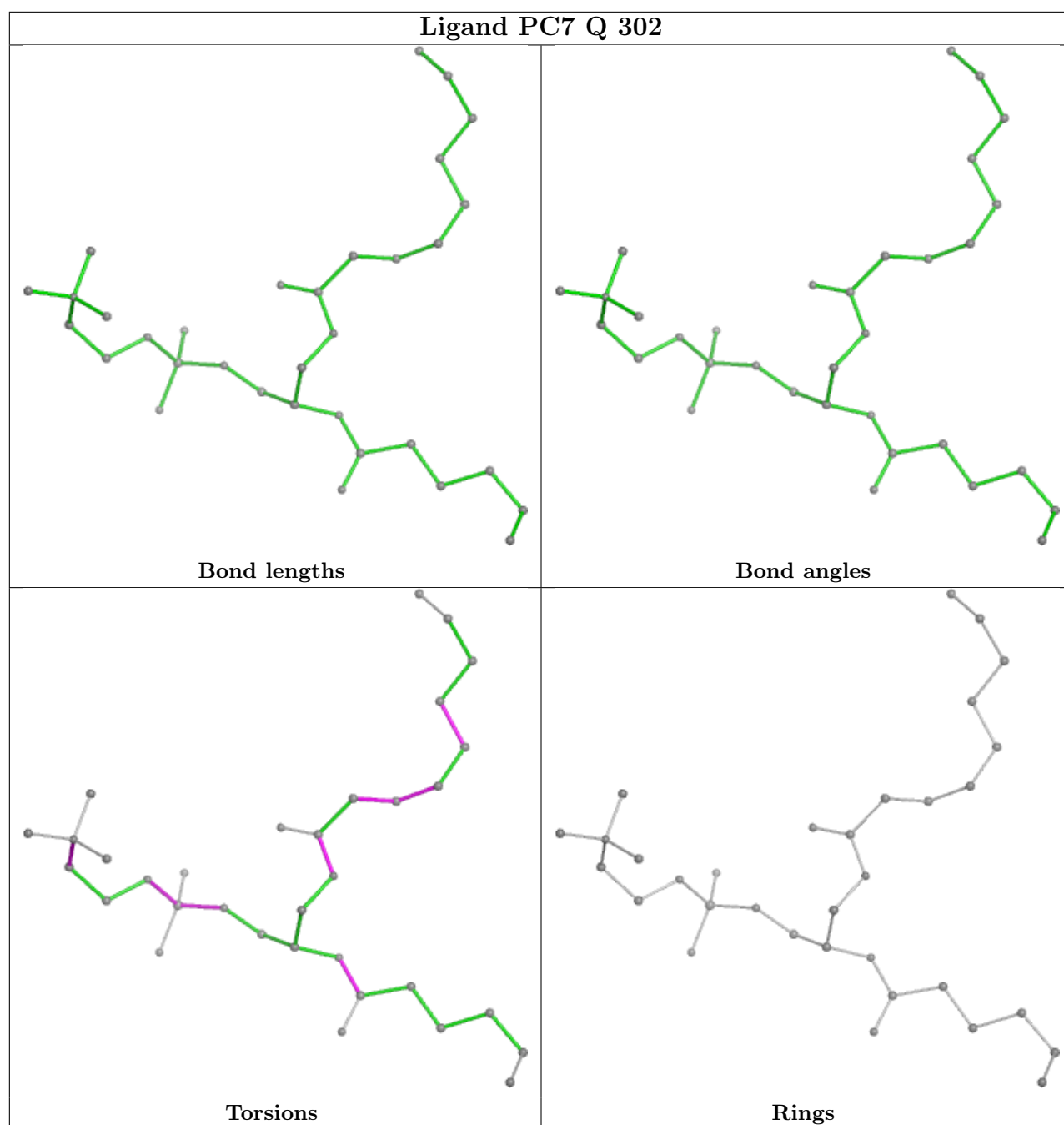












5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-50203. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.