



## Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 06:43 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

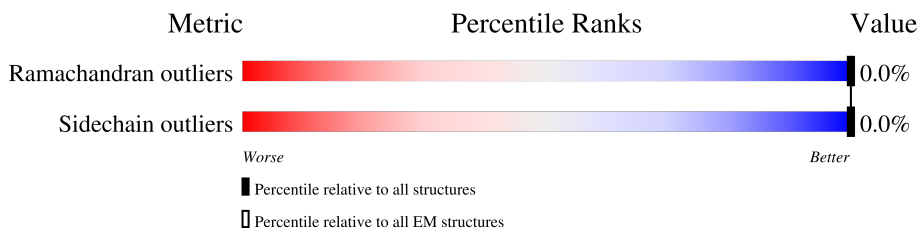
# 1 Overall quality at a glance i

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.







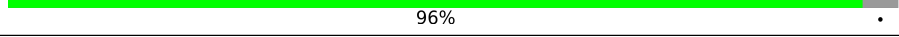
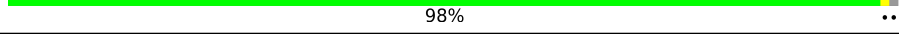

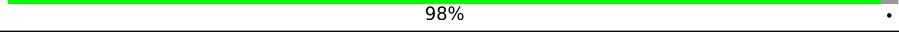
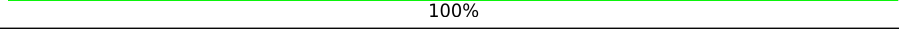

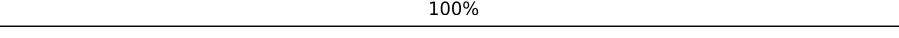
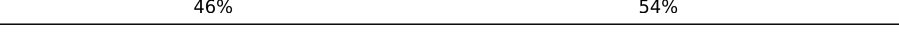
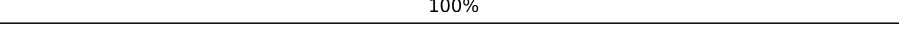
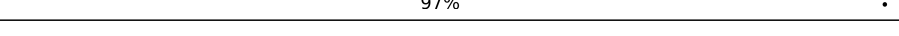


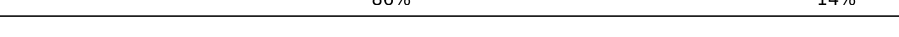

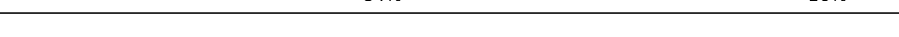






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	 69% 31%
11	K	138	 86% 14%
12	L	187	 88% 12%
13	M	154	 79% 21%
14	N	156	 96% .
15	O	101	 98% ..
16	P	397	 91% 9%
17	Q	292	 98% .
18	R	387	 100%
19	S	279	 48% 52%
20	T	443	 100%
21	U	227	 46% 54%
22	V	546	 100%
23	W	162	 97% .
24	X	149	 84% 16%
25	Y	64	 84% 16%
26	Z	124	 86% 14%
27	a	129	 63% . 36%
28	b	172	 84% 16%
29	c	67	 88% 12%
30	d	86	 99% .
31	e	219	 99% .
32	f	65	 98% .
33	g	55	 91% 9%
34	h	142	 76% 24%

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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
			Total	C	N	O	S		
1	A	239	1839	1165	311	352	11	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called Acyl carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called ASHI.

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

- Molecule 25 is a protein called P9.

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

- Molecule 26 is a protein called KFYI.

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

- Molecule 27 is a protein called AGGG.



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

- Molecule 28 is a protein called ESSS.

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

- Molecule 29 is a protein called B9.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

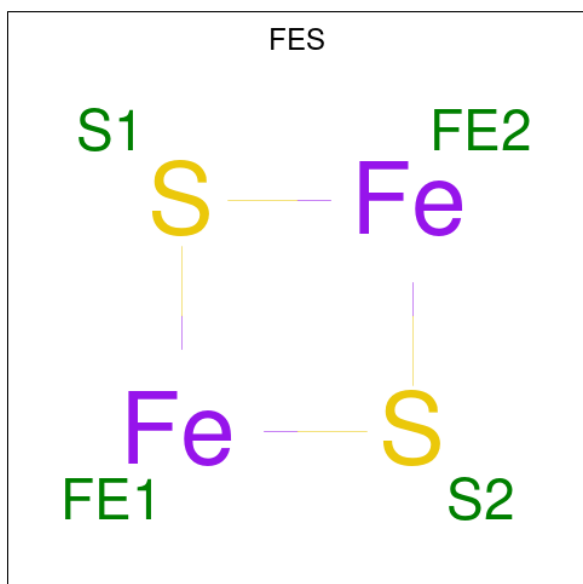
- Molecule 49 is a protein called NUOP8.

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: Fe<sub>2</sub>S<sub>2</sub>).



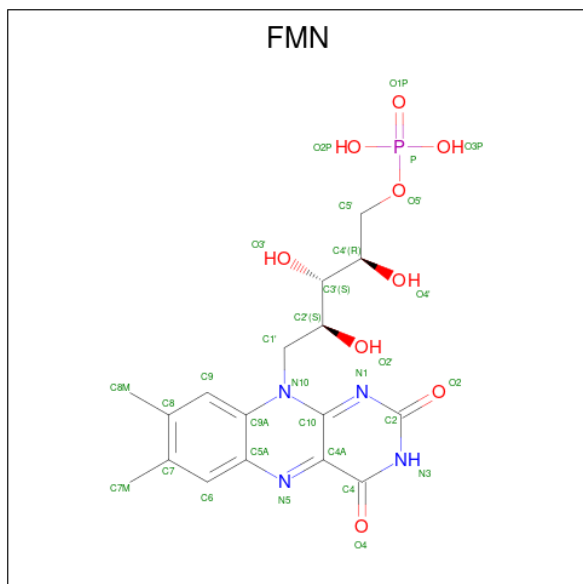
Mol	Chain	Residues	Atoms			AltConf
51	A	1	Total	Fe	S	0
			4	2	2	

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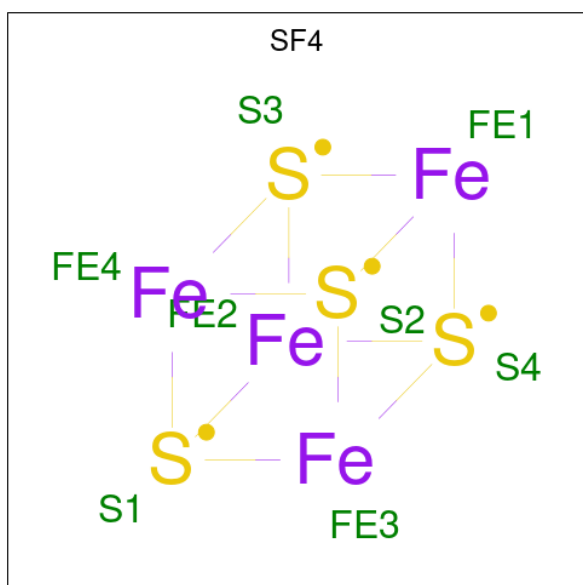
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
51	C	1	4	2	2	0

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



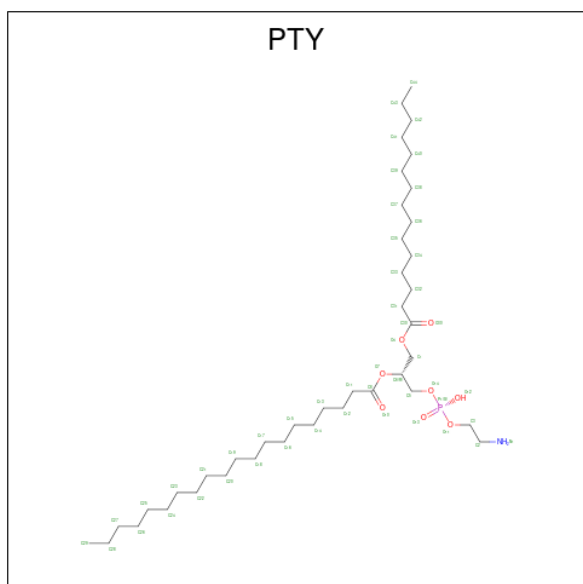
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	B	1	31	17	4	9	1	0

- 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:  $C_{40}H_{80}NO_8P$ ).



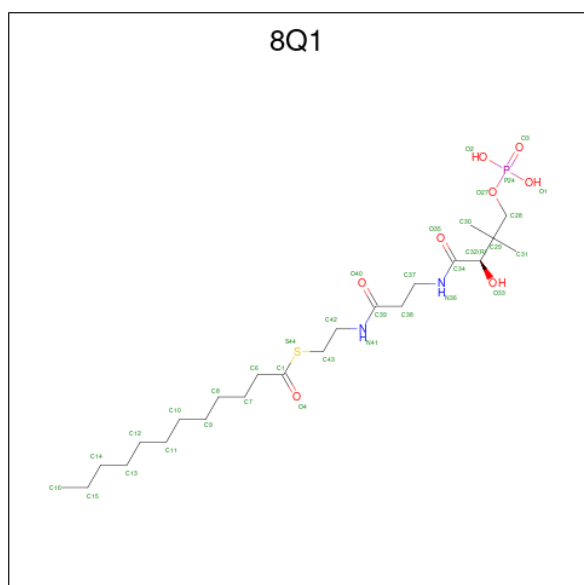
Mol	Chain	Residues	Atoms					AltConf
54	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
54	R	1	Total	C	N	O	P	0
			34	24	1	8	1	
54	R	1	Total	C	N	O	P	0
			44	34	1	8	1	
54	R	1	Total	C	N	O	P	0
			40	30	1	8	1	
54	S	1	Total	C	N	O	P	0
			46	36	1	8	1	

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

- Molecule 55 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS).



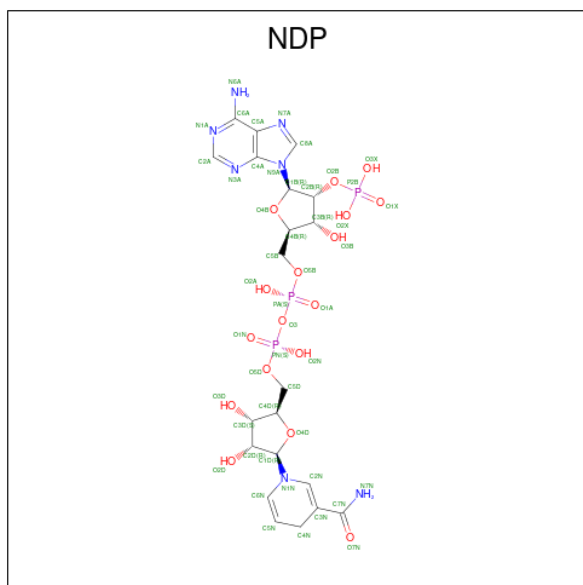
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
55	J	1	Total 35	C 23	N 2	O 8	P 1	S 1	0

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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

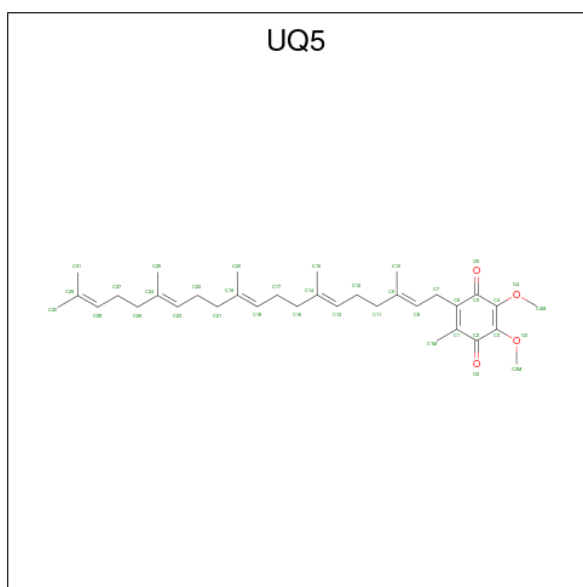
- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



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

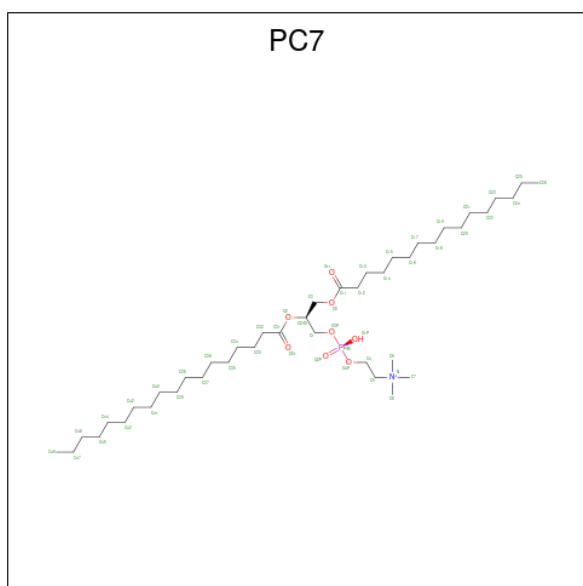
- Molecule 57 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula:  $C_{34}H_{50}O_4$ ).





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

- 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: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P).



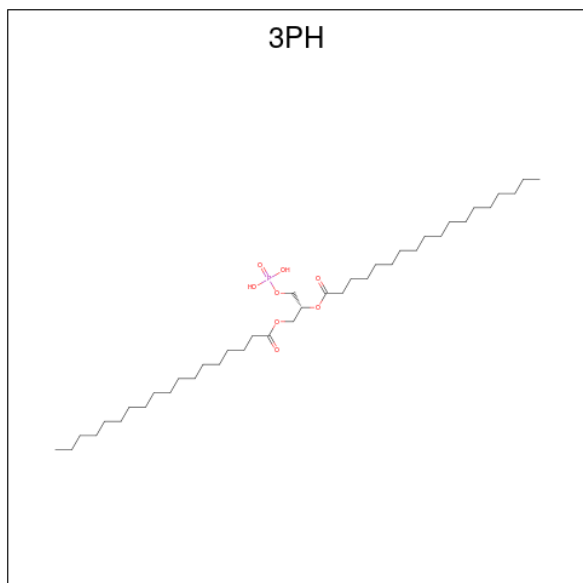
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	Q	1	33	23	1	8	1	0
58	R	1	44	34	1	8	1	0

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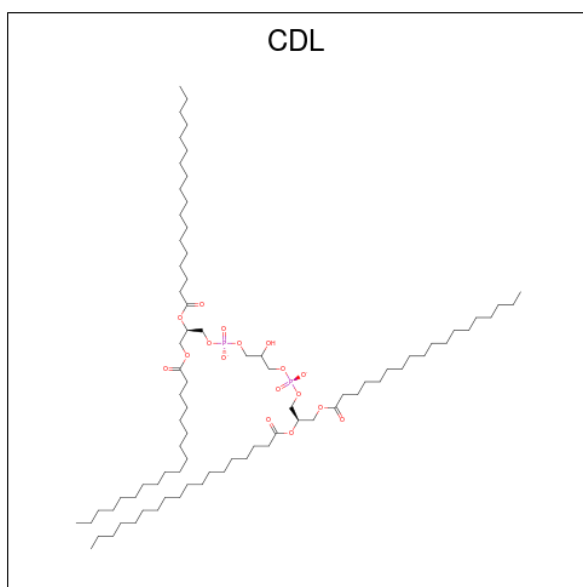
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
58	T	1	Total	C	N	O	P	0
			52	42	1	8	1	
58	u	1	Total	C	N	O	P	0
			42	32	1	8	1	

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



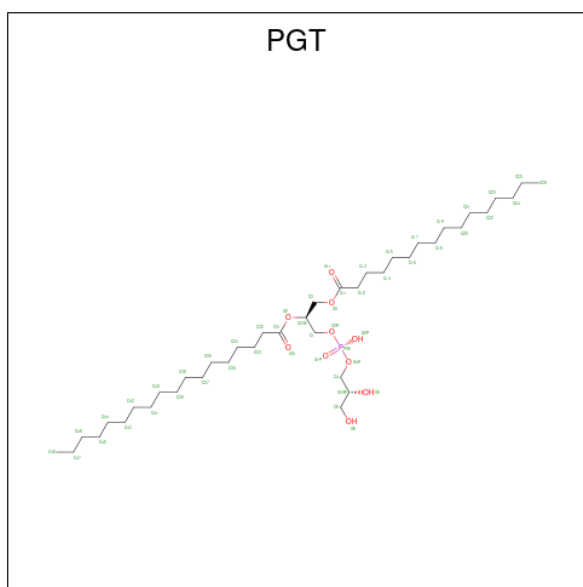
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
59	R	1	Total	C	O	P	0
			32	23	8	1	
59	S	1	Total	C	O	P	0
			37	28	8	1	
59	V	1	Total	C	O	P	0
			42	33	8	1	
59	V	1	Total	C	O	P	0
			41	32	8	1	
59	c	1	Total	C	O	P	0
			48	39	8	1	
59	g	1	Total	C	O	P	0
			37	28	8	1	
59	h	1	Total	C	O	P	0
			45	36	8	1	
59	w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

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



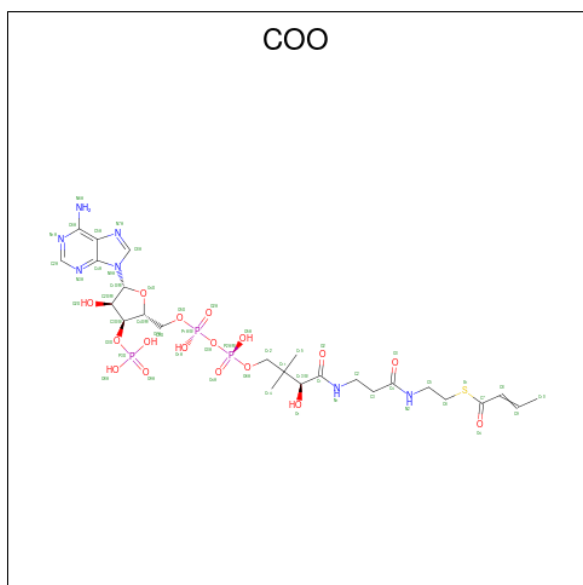
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
60	R	1	63	44	17	2	0
60	V	1	64	45	17	2	0
60	W	1	95	76	17	2	0
60	h	1	77	58	17	2	0
60	u	1	83	64	17	2	0
60	u	1	71	52	17	2	0
60	x	1	92	73	17	2	0
60	y	1	55	36	17	2	0

- Molecule 61 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



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

- Molecule 62 is CROTONYL COENZYME A (three-letter code: COO) (formula:  $C_{25}H_{40}N_7O_{17}P_3S$ ).



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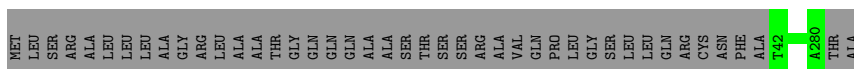
Mol	Chain	Residues	Atoms		AltConf
64	m	32	Total 32	O 32	0
64	n	7	Total 7	O 7	0
64	o	51	Total 51	O 51	0
64	p	21	Total 21	O 21	0
64	q	24	Total 24	O 24	0
64	r	12	Total 12	O 12	0
64	s	39	Total 39	O 39	0
64	t	55	Total 55	O 55	0
64	u	41	Total 41	O 41	0
64	v	2	Total 2	O 2	0
64	w	16	Total 16	O 16	0
64	x	22	Total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

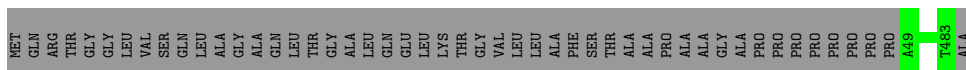
- Molecule 1: NADH:ubiquinone oxidoreductase 24 kD subunit

Chain A:  85% 15%



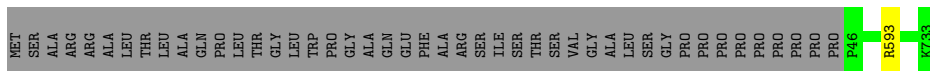
- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:  90% 10%




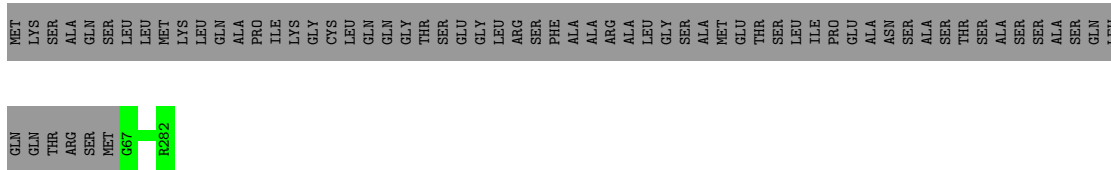
- Molecule 3: NADH:ubiquinone oxidoreductase 78 kDa subunit

Chain C:  94% 6%




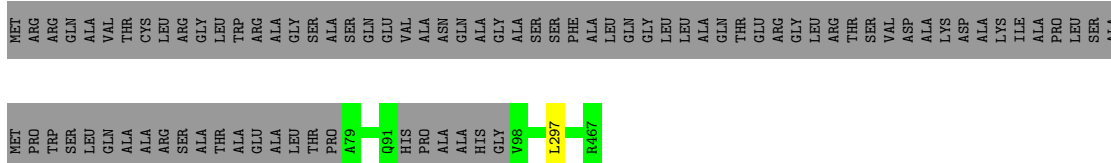
- Molecule 4: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

Chain D:  77% 23%



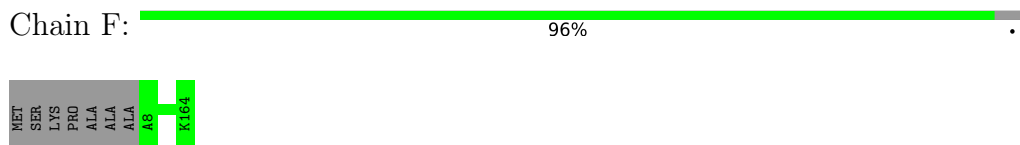
- Molecule 5: NADH:ubiquinone oxidoreductase 49 kD subunit

Chain E:  82% 18%

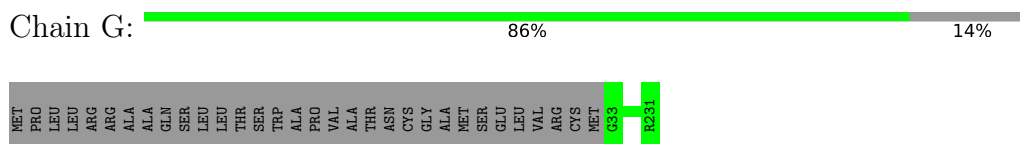




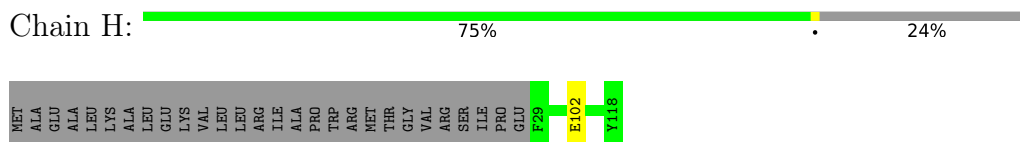
- Molecule 6: NADH:ubiquinone oxidoreductase subunit 10



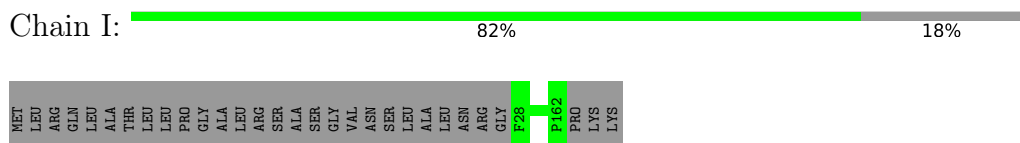
- Molecule 7: NADH:ubiquinone oxidoreductase subunit 8



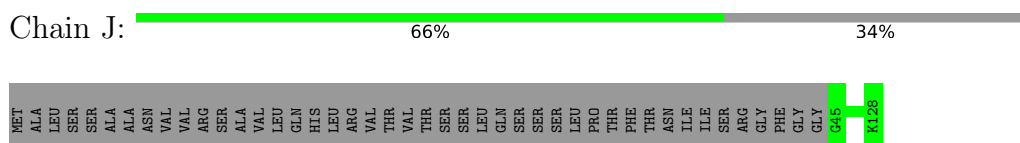
- Molecule 8: B14.5a



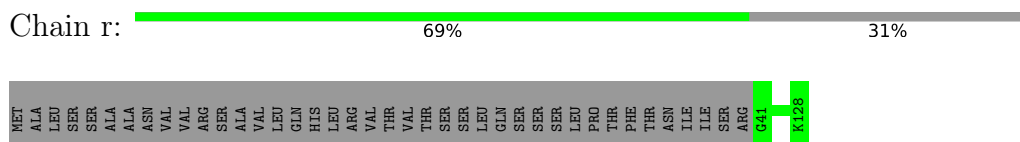
- Molecule 9: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit



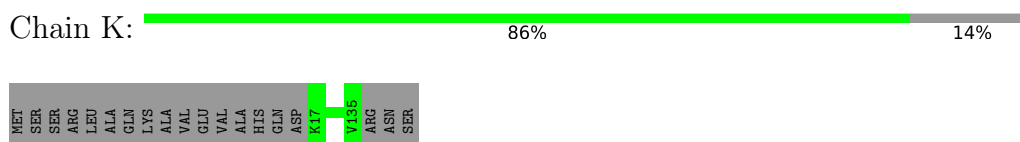
- Molecule 10: Acyl carrier protein




- Molecule 10: Acyl carrier protein



- Molecule 11: NADH:ubiquinone oxidoreductase B14 subunit




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

Chain L:  88% 12%

MET  
GLN  
ARG  
SER  
ILE  
LEU  
SER  
SER  
ALA  
LEU  
LEU  
PRO  
PRO  
ARG  
LEU  
LEU  
GLY  
VAL  
ARG  
E19  
R182  
ARG  
ALA  
ALA  
ALA  
LYS

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

Chain M:  79% 21%

MET  
ALA  
LEU  
GLN  
ALA  
THR  
SER  
SER  
GLN  
LEU  
ALA  
ARG  
HIS  
VAL  
ILE  
SER  
LYS  
THR  
LEU  
GLY  
GLY  
ALA  
PHE  
ALA  
THR  
LYS  
ALA  
ALA  
ASP  
V29  
G149  
GLY  
ALA  
HIS  
HIS

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

Chain N:  96% .

MET  
S2  
P151  
ALA  
ASN  
LYS  
SER  
ALA

- Molecule 15: NADH:ubiquinone oxidoreductase B8 subunit

Chain O:  98% ..

MET  
A2  
L7  
E101

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

Chain P:  91% 9%

MET  
LEU  
PRO  
ILE  
LEU  
GLY  
ARG  
ASN  
ALA  
ALA  
GLY  
SER  
ALA  
LEU  
ALA  
ARG  
LEU  
ALA  
GLY  
LEU  
ARG  
TRP  
ALA  
ALA  
ALA  
SER  
GLN  
SER  
SER  
ASP  
T33  
K314  
I395  
LYS  
GLN

- Molecule 17: NADH-ubiquinone oxidoreductase chain 1

Chain Q:  98% .

H1  
P198  
GLU  
ALA  
GLU  
LEU  
VAL  
ALA  
G205  
I292

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

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

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

- Molecule 20: NADH-ubiquinone oxidoreductase chain 4



H1 Y195 A443

- Molecule 21: NADH dehydrogenase subunit 4L



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

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

ARG SER Y123 K227

- Molecule 22: NADH-ubiquinone oxidoreductase chain 5



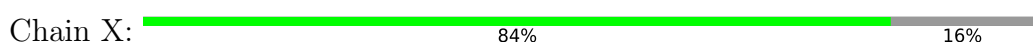
H1 F8 P519 A546

- Molecule 23: NADH-ubiquinone oxidoreductase chain 6




H1 Y157 ARG THR THR GLY ARG

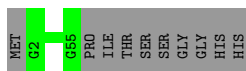
- Molecule 24: ASH1




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

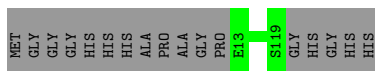
- Molecule 25: P9

Chain Y:  84% 16%



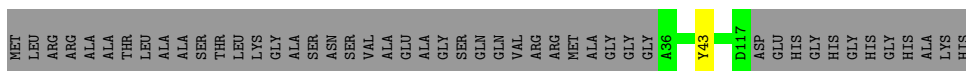
- Molecule 26: KFYI

Chain Z:  86% 14%




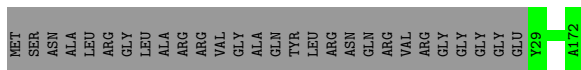
- Molecule 27: AGGG

Chain a:  63% 36%




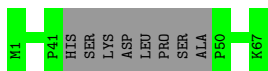
- Molecule 28: ESSS

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%



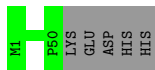
- Molecule 32: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit

Chain f:  98%



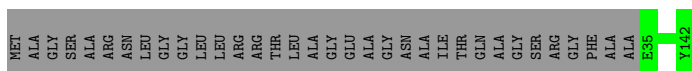
- Molecule 33: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit

Chain g: 91% 9%



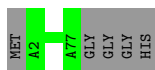
- Molecule 34: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

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% .



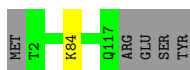
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain k: 100%

There are no outlier residues recorded for this chain.

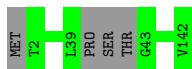
- Molecule 38: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

Chain l: 95% . .



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

Chain m: 97% .



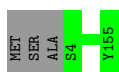
- Molecule 40: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

Chain n: 98%



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

Chain o: 98%



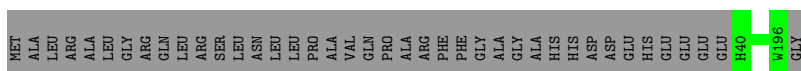
- Molecule 42: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

Chain p: 99%



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

Chain q: 80%



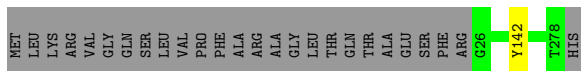
- Molecule 44: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

Chain s: 100%



- Molecule 45: CAG2 - CA-like

Chain t: 90%



- Molecule 46: CAG1

Chain u: 100%

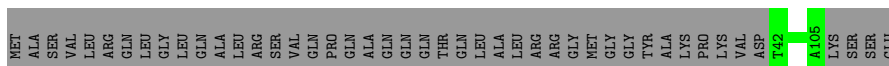


- Molecule 47: P10

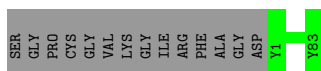
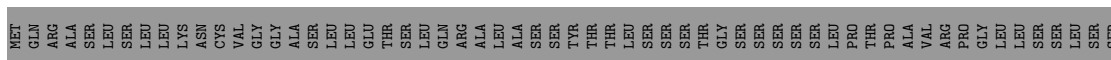


There are no outlier residues recorded for this chain.

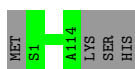
- Molecule 48: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit



- 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 i

### 5.1 Standard geometry i

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	314	MET	CA-CB-CG	5.76	123.09	113.30
8	H	102	GLU	C-N-CA	5.64	135.79	121.70
22	V	8	PHE	CB-CG-CD2	5.12	124.38	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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 [i](#)

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%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

All (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
59	V	602	3PH	P-O11	3.38	1.71	1.60
59	h	201	3PH	P-O11	3.30	1.70	1.60
59	c	101	3PH	P-O11	3.29	1.70	1.60
59	V	601	3PH	P-O11	3.27	1.70	1.60
59	w	201	3PH	P-O11	3.25	1.70	1.60
59	R	401	3PH	P-O11	3.25	1.70	1.60
59	S	301	3PH	P-O11	3.24	1.70	1.60
56	P	401	NDP	C6N-C5N	3.23	1.39	1.33
59	g	101	3PH	P-O11	3.19	1.70	1.60
55	r	200	8Q1	C1-S44	2.55	1.82	1.76
62	s	401	COO	C5A-C4A	2.43	1.47	1.40
55	r	200	8Q1	C6-C1	2.42	1.53	1.50
55	r	200	8Q1	O40-C39	-2.39	1.18	1.23
55	J	200	8Q1	O40-C39	-2.36	1.18	1.23
55	J	200	8Q1	C1-S44	2.31	1.81	1.76
56	P	401	NDP	C5A-C4A	2.29	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	J	200	8Q1	C6-C1	2.25	1.53	1.50
60	x	101	CDL	PB2-OB4	-2.19	1.45	1.55
52	B	501	FMN	C10-N1	2.13	1.37	1.33
60	y	201	CDL	PB2-OB4	-2.01	1.45	1.55

All (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
59	h	201	3PH	O32-C31-C32	-11.56	78.63	123.73
55	J	200	8Q1	C6-C1-S44	6.65	121.19	113.46
55	r	200	8Q1	C6-C1-S44	5.50	119.86	113.46
55	r	200	8Q1	C32-C34-N36	5.00	126.53	116.58
62	s	401	COO	C14-C11-C12	4.96	116.33	108.23
62	s	401	COO	C14-C11-C13	4.05	115.84	108.82
55	J	200	8Q1	O4-C1-C6	-3.86	119.43	123.99
56	P	401	NDP	PN-O3-PA	-3.77	119.91	132.83
59	V	602	3PH	C2-O21-C21	3.35	126.03	117.79
55	r	200	8Q1	C37-C38-C39	-3.32	106.83	112.36
55	r	200	8Q1	O4-C1-C6	-3.24	120.16	123.99
56	P	401	NDP	N3A-C2A-N1A	-3.18	123.71	128.68
62	s	401	COO	N3A-C2A-N1A	-3.17	123.72	128.68
62	s	401	COO	P1A-O3A-P2A	-3.14	122.05	132.83
52	B	501	FMN	C4-N3-C2	-3.12	119.88	125.64
55	r	200	8Q1	O35-C34-N36	-3.06	116.42	122.99
54	T	501	PTY	C6-O7-C8	3.06	125.32	117.79
62	s	401	COO	C4A-C5A-N7A	-2.94	106.33	109.40
62	s	401	COO	C3X-C2X-C1X	2.93	106.37	99.89
62	s	401	COO	C10-C9-C8	-2.88	119.65	125.34
52	B	501	FMN	C4A-C10-N10	2.75	120.51	116.48
52	B	501	FMN	C4A-C4-N3	2.71	120.06	113.19
56	P	401	NDP	C4A-C5A-N7A	-2.65	106.64	109.40
55	r	200	8Q1	C38-C39-N41	2.64	120.87	116.42
55	r	200	8Q1	C43-S44-C1	2.64	110.08	101.87
55	J	200	8Q1	O4-C1-S44	-2.49	119.38	122.61
52	B	501	FMN	O4-C4-C4A	-2.46	120.07	126.60
55	J	200	8Q1	C38-C39-N41	2.44	120.53	116.42
59	w	201	3PH	C2-O21-C21	2.42	123.74	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	Q	301	UQ5	C12-C13-C14	2.41	133.47	127.66
59	w	201	3PH	O13-P-O11	-2.40	100.35	106.73
58	u	601	PC7	O3-C3-C2	2.36	115.29	108.43
57	Q	301	UQ5	C8-C7-C6	2.35	118.39	112.05
55	J	200	8Q1	C43-S44-C1	2.34	109.15	101.87
57	Q	301	UQ5	C12-C11-C9	2.29	120.50	112.98
55	r	200	8Q1	C37-N36-C34	2.27	126.64	122.59
52	B	501	FMN	C4A-C10-N1	-2.27	119.47	124.73
61	T	502	PGT	C3-C2-C1	2.25	117.11	111.79
52	B	501	FMN	C10-C4A-N5	-2.22	120.14	124.86
61	l	701	PGT	C2-O2-C31	2.17	123.14	117.79
55	r	200	8Q1	C31-C29-C32	2.15	112.55	108.82
59	c	101	3PH	O13-P-O11	-2.14	101.03	106.73
59	h	201	3PH	O14-P-O13	2.13	115.77	107.64
59	g	101	3PH	O13-P-O11	-2.10	101.14	106.73
59	R	401	3PH	O13-P-O11	-2.09	101.17	106.73
59	S	301	3PH	O13-P-O11	-2.09	101.17	106.73
52	B	501	FMN	C9A-C5A-N5	-2.06	120.19	122.43
59	h	201	3PH	O13-P-O11	-2.06	101.24	106.73
59	V	601	3PH	O13-P-O11	-2.04	101.31	106.73
58	u	601	PC7	C3-C2-C1	2.03	116.59	111.79
55	r	200	8Q1	O4-C1-S44	-2.03	119.98	122.61
52	B	501	FMN	C5A-C9A-N10	2.02	120.04	117.95
59	R	401	3PH	O14-P-O13	2.02	115.35	107.64
59	w	201	3PH	O14-P-O13	2.02	115.35	107.64

There are no chirality outliers.

All (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
54	R	402	PTY	C6-C5-O14-P1
54	R	402	PTY	C3-O11-P1-O12
54	R	404	PTY	C11-C8-O7-C6
54	R	404	PTY	C5-O14-P1-O12
54	R	406	PTY	O14-C5-C6-O7
54	R	406	PTY	C11-C8-O7-C6
54	R	406	PTY	C5-O14-P1-O11

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Mol	Chain	Res	Type	Atoms
54	S	302	PTY	C3-O11-P1-O12
54	S	302	PTY	C5-O14-P1-O13
54	T	501	PTY	N1-C2-C3-O11
54	T	501	PTY	C3-O11-P1-O12
54	T	501	PTY	C5-O14-P1-O11
54	T	504	PTY	N1-C2-C3-O11
54	T	504	PTY	C5-O14-P1-O12
54	V	604	PTY	N1-C2-C3-O11
54	V	604	PTY	C3-O11-P1-O12
54	V	604	PTY	C3-O11-P1-O13
54	V	605	PTY	N1-C2-C3-O11
54	V	605	PTY	C3-O11-P1-O13
54	V	605	PTY	C5-O14-P1-O12
54	e	301	PTY	N1-C2-C3-O11
54	e	301	PTY	C3-O11-P1-O13
54	e	301	PTY	C3-O11-P1-O14
54	e	302	PTY	O14-C5-C6-O7
54	e	302	PTY	O10-C8-O7-C6
54	e	302	PTY	C11-C8-O7-C6
54	e	302	PTY	C5-O14-P1-O12
54	h	202	PTY	O10-C8-O7-C6
54	h	202	PTY	C3-O11-P1-O14
54	h	202	PTY	C5-O14-P1-O12
54	x	102	PTY	O10-C8-O7-C6
54	x	102	PTY	C3-O11-P1-O13
55	J	200	8Q1	C1-C6-C7-C8
55	J	200	8Q1	O27-C28-C29-C32
55	r	200	8Q1	C1-C6-C7-C8
55	r	200	8Q1	O4-C1-S44-C43
55	r	200	8Q1	C6-C1-S44-C43
55	r	200	8Q1	C28-C29-C32-C34
55	r	200	8Q1	C28-C29-C32-O33
55	r	200	8Q1	C30-C29-C32-C34
55	r	200	8Q1	C30-C29-C32-O33
55	r	200	8Q1	C31-C29-C32-C34
55	r	200	8Q1	C31-C29-C32-O33
55	r	200	8Q1	O33-C32-C34-N36
55	r	200	8Q1	C32-C34-N36-C37
55	r	200	8Q1	C28-O27-P24-O1
56	P	401	NDP	C5B-O5B-PA-O1A
56	P	401	NDP	C5D-O5D-PN-O1N
56	P	401	NDP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
57	Q	301	UQ5	C19-C21-C22-C23
58	Q	302	PC7	C4-O4P-P-O3P
58	Q	302	PC7	C4-O4P-P-O1P
58	Q	302	PC7	C4-O4P-P-O2P
58	R	403	PC7	C1-O3P-P-O1P
58	R	403	PC7	C1-O3P-P-O2P
58	R	403	PC7	C1-O3P-P-O4P
58	R	403	PC7	O4P-C4-C5-N
58	T	503	PC7	C32-C31-O2-C2
58	T	503	PC7	C4-O4P-P-O2P
58	T	503	PC7	O4P-C4-C5-N
58	u	601	PC7	C32-C31-O2-C2
58	u	601	PC7	C4-O4P-P-O1P
59	R	401	3PH	C1-O11-P-O13
59	R	401	3PH	C1-O11-P-O14
59	S	301	3PH	C1-O11-P-O13
59	S	301	3PH	C1-O11-P-O14
59	S	301	3PH	C1-O11-P-O12
59	V	601	3PH	C1-O11-P-O13
59	V	601	3PH	C1-O11-P-O14
59	V	601	3PH	O22-C21-O21-C2
59	V	601	3PH	C22-C21-O21-C2
59	V	602	3PH	C1-O11-P-O13
59	V	602	3PH	C1-O11-P-O14
59	V	602	3PH	C1-O11-P-O12
59	V	602	3PH	C22-C21-O21-C2
59	c	101	3PH	C1-O11-P-O13
59	c	101	3PH	C1-O11-P-O14
59	c	101	3PH	C1-O11-P-O12
59	h	201	3PH	C1-O11-P-O13
59	h	201	3PH	C1-O11-P-O14
59	h	201	3PH	O11-C1-C2-O21
59	h	201	3PH	C22-C21-O21-C2
60	R	405	CDL	CA2-OA2-PA1-OA3
60	R	405	CDL	CA2-OA2-PA1-OA4
60	R	405	CDL	CA3-OA5-PA1-OA2
60	R	405	CDL	CA3-OA5-PA1-OA3
60	R	405	CDL	CA3-OA5-PA1-OA4
60	R	405	CDL	CB2-OB2-PB2-OB3
60	R	405	CDL	CB2-OB2-PB2-OB4
60	R	405	CDL	CB2-OB2-PB2-OB5
60	R	405	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
60	R	405	CDL	OB5-CB3-CB4-OB6
60	R	405	CDL	C51-CB5-OB6-CB4
60	V	603	CDL	CA2-OA2-PA1-OA3
60	V	603	CDL	C11-CA5-OA6-CA4
60	V	603	CDL	CB2-OB2-PB2-OB4
60	V	603	CDL	CB3-OB5-PB2-OB3
60	V	603	CDL	CB3-OB5-PB2-OB4
60	W	701	CDL	CA2-OA2-PA1-OA3
60	W	701	CDL	CA3-OA5-PA1-OA2
60	W	701	CDL	CA3-OA5-PA1-OA3
60	W	701	CDL	CA3-OA5-PA1-OA4
60	W	701	CDL	OA7-CA5-OA6-CA4
60	W	701	CDL	C11-CA5-OA6-CA4
60	h	203	CDL	CA2-C1-CB2-OB2
60	h	203	CDL	CA2-OA2-PA1-OA3
60	h	203	CDL	CA2-OA2-PA1-OA4
60	h	203	CDL	CA2-OA2-PA1-OA5
60	h	203	CDL	CA3-OA5-PA1-OA3
60	h	203	CDL	CA3-OA5-PA1-OA4
60	h	203	CDL	CB2-OB2-PB2-OB3
60	h	203	CDL	CB2-OB2-PB2-OB5
60	h	203	CDL	CB3-OB5-PB2-OB3
60	u	602	CDL	CA2-C1-CB2-OB2
60	u	602	CDL	CA2-OA2-PA1-OA3
60	u	602	CDL	CA2-OA2-PA1-OA4
60	u	602	CDL	CA2-OA2-PA1-OA5
60	u	602	CDL	CA3-OA5-PA1-OA2
60	u	602	CDL	CA3-OA5-PA1-OA3
60	u	602	CDL	CA3-OA5-PA1-OA4
60	u	602	CDL	C51-CB5-OB6-CB4
60	u	603	CDL	O1-C1-CB2-OB2
60	u	603	CDL	CA2-OA2-PA1-OA4
60	u	603	CDL	CA3-OA5-PA1-OA3
60	u	603	CDL	CB2-OB2-PB2-OB4
60	u	603	CDL	CB3-OB5-PB2-OB3
60	x	101	CDL	CA3-OA5-PA1-OA4
60	x	101	CDL	CB2-OB2-PB2-OB3
60	y	201	CDL	O1-C1-CB2-OB2
60	y	201	CDL	CA2-C1-CB2-OB2
60	y	201	CDL	CA3-OA5-PA1-OA3
60	y	201	CDL	CA3-OA5-PA1-OA4
61	T	502	PGT	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
61	T	505	PGT	C1-O3P-P-O4P
61	b	601	PGT	C2-C1-O3P-P
61	b	601	PGT	C1-O3P-P-O2P
61	b	601	PGT	C4-O4P-P-O1P
61	l	701	PGT	O3P-C1-C2-O2
61	l	701	PGT	C4-O4P-P-O1P
62	s	401	COO	C14-C11-C13-O1
62	s	401	COO	C12-C11-C13-O1
62	s	401	COO	C14-C11-C13-C1
62	s	401	COO	C12-C11-C13-C1
62	s	401	COO	C13-C11-C12-O6A
62	s	401	COO	C13-C1-N1-C2
62	s	401	COO	O2-C1-N1-C2
62	s	401	COO	C3-C4-N2-C5
62	s	401	COO	O3-C4-N2-C5
62	s	401	COO	O4-C7-S1-C6
62	s	401	COO	C8-C7-S1-C6
62	s	401	COO	S1-C7-C8-C9
54	R	404	PTY	O30-C30-O4-C1
54	V	606	PTY	O30-C30-O4-C1
59	g	101	3PH	O32-C31-O31-C3
60	V	603	CDL	OB9-CB7-OB8-CB6
60	W	701	CDL	OB9-CB7-OB8-CB6
60	u	602	CDL	OA9-CA7-OA8-CA6
61	l	701	PGT	O11-C11-O3-C3
54	R	404	PTY	C31-C30-O4-C1
54	V	606	PTY	C31-C30-O4-C1
60	V	603	CDL	C71-CB7-OB8-CB6
60	u	602	CDL	C31-CA7-OA8-CA6
61	b	601	PGT	C12-C11-O3-C3
54	h	202	PTY	O30-C30-O4-C1
59	h	201	3PH	O32-C31-O31-C3
61	b	601	PGT	O11-C11-O3-C3
54	R	404	PTY	O10-C8-O7-C6
54	R	406	PTY	O10-C8-O7-C6
58	T	503	PC7	O31-C31-O2-C2
58	u	601	PC7	O31-C31-O2-C2
59	V	602	3PH	O22-C21-O21-C2
60	R	405	CDL	OB7-CB5-OB6-CB4
60	V	603	CDL	OA7-CA5-OA6-CA4
60	W	701	CDL	OB7-CB5-OB6-CB4
60	u	602	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
59	g	101	3PH	C32-C31-O31-C3
60	W	701	CDL	C71-CB7-OB8-CB6
61	T	505	PGT	C12-C11-O3-C3
61	l	701	PGT	C12-C11-O3-C3
54	h	202	PTY	C11-C8-O7-C6
54	x	102	PTY	C11-C8-O7-C6
54	h	202	PTY	C31-C30-O4-C1
59	h	201	3PH	C32-C31-O31-C3
59	h	201	3PH	O22-C21-O21-C2
54	e	302	PTY	O30-C30-O4-C1
58	R	403	PC7	O11-C11-O3-C3
61	T	505	PGT	O11-C11-O3-C3
60	R	405	CDL	O1-C1-CA2-OA2
60	h	203	CDL	O1-C1-CB2-OB2
60	u	602	CDL	O1-C1-CB2-OB2
60	x	101	CDL	O1-C1-CB2-OB2
60	y	201	CDL	O1-C1-CA2-OA2
61	b	601	PGT	O4P-C4-C5-O5
54	e	301	PTY	C31-C30-O4-C1
54	e	302	PTY	C31-C30-O4-C1
60	u	603	CDL	C31-CA7-OA8-CA6
61	T	502	PGT	C12-C11-O3-C3
60	h	203	CDL	C71-C72-C73-C74
55	r	200	8Q1	O35-C34-N36-C37
54	T	501	PTY	C11-C8-O7-C6
60	W	701	CDL	C51-CB5-OB6-CB4
60	h	203	CDL	C75-C76-C77-C78
61	T	502	PGT	O11-C11-O3-C3
60	x	101	CDL	C72-C73-C74-C75
60	u	603	CDL	C13-C14-C15-C16
58	R	403	PC7	C12-C11-O3-C3
54	T	501	PTY	O10-C8-O7-C6
60	u	603	CDL	OA9-CA7-OA8-CA6
54	e	301	PTY	O30-C30-O4-C1
59	h	201	3PH	C3B-C3C-C3D-C3E
61	T	502	PGT	C17-C18-C19-C20
60	R	405	CDL	C71-CB7-OB8-CB6
60	W	701	CDL	C63-C64-C65-C66
59	S	301	3PH	C22-C21-O21-C2
60	W	701	CDL	CA2-C1-CB2-OB2
60	u	603	CDL	CA2-C1-CB2-OB2
60	y	201	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
60	R	405	CDL	OB9-CB7-OB8-CB6
58	Q	302	PC7	C4-C5-N-C7
59	R	401	3PH	C32-C31-O31-C3
60	x	101	CDL	C31-CA7-OA8-CA6
60	h	203	CDL	CB7-C71-C72-C73
60	h	203	CDL	C12-C13-C14-C15
58	T	503	PC7	O2-C2-C3-O3
60	u	603	CDL	OB6-CB4-CB6-OB8
60	y	201	CDL	OA6-CA4-CA6-OA8
59	R	401	3PH	O32-C31-O31-C3
60	h	203	CDL	C15-C16-C17-C18
60	u	603	CDL	C39-C40-C41-C42
58	T	503	PC7	C11-C12-C13-C14
59	S	301	3PH	C21-C22-C23-C24
60	R	405	CDL	CA7-C31-C32-C33
54	S	302	PTY	C30-C31-C32-C33
59	c	101	3PH	C31-C32-C33-C34
60	V	603	CDL	CB7-C71-C72-C73
60	h	203	CDL	CA7-C31-C32-C33
61	l	701	PGT	C31-C32-C33-C34
54	V	605	PTY	C13-C14-C15-C16
61	b	601	PGT	O5-C5-C6-O6
54	R	404	PTY	C30-C31-C32-C33
54	x	102	PTY	C8-C11-C12-C13
58	u	601	PC7	C31-C32-C33-C34
60	R	405	CDL	CB7-C71-C72-C73
60	V	603	CDL	CA7-C31-C32-C33
60	W	701	CDL	CB5-C51-C52-C53
60	u	602	CDL	CB7-C71-C72-C73
60	x	101	CDL	CB5-C51-C52-C53
60	y	201	CDL	CB7-C71-C72-C73
60	W	701	CDL	C74-C75-C76-C77
60	x	101	CDL	C13-C14-C15-C16
58	Q	302	PC7	C4-C5-N-C8
54	V	605	PTY	C30-C31-C32-C33
60	u	603	CDL	CB7-C71-C72-C73
59	R	401	3PH	C22-C21-O21-C2
60	x	101	CDL	OA9-CA7-OA8-CA6
54	V	605	PTY	C19-C20-C21-C22
60	W	701	CDL	O1-C1-CB2-OB2
61	T	505	PGT	O4P-C4-C5-O5
59	S	301	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
60	u	603	CDL	CA7-C31-C32-C33
60	u	603	CDL	C11-CA5-OA6-CA4
54	R	402	PTY	C3-O11-P1-O14
54	R	402	PTY	C5-O14-P1-O11
54	R	404	PTY	C5-O14-P1-O11
54	S	302	PTY	C3-O11-P1-O14
54	T	501	PTY	C3-O11-P1-O14
54	T	504	PTY	C5-O14-P1-O11
54	T	506	PTY	C3-O11-P1-O14
54	V	604	PTY	C3-O11-P1-O14
54	V	604	PTY	C5-O14-P1-O11
54	V	605	PTY	C5-O14-P1-O11
54	e	302	PTY	C5-O14-P1-O11
54	h	202	PTY	C5-O14-P1-O11
58	u	601	PC7	C4-O4P-P-O3P
60	R	405	CDL	CA2-OA2-PA1-OA5
60	V	603	CDL	CB2-OB2-PB2-OB5
60	V	603	CDL	CB3-OB5-PB2-OB2
60	W	701	CDL	CA2-OA2-PA1-OA5
60	W	701	CDL	CB3-OB5-PB2-OB2
60	h	203	CDL	CA3-OA5-PA1-OA2
60	h	203	CDL	CB3-OB5-PB2-OB2
60	u	602	CDL	CB2-OB2-PB2-OB5
60	u	603	CDL	CA2-OA2-PA1-OA5
60	u	603	CDL	CB2-OB2-PB2-OB5
60	u	603	CDL	CB3-OB5-PB2-OB2
60	x	101	CDL	CA3-OA5-PA1-OA2
60	y	201	CDL	CA3-OA5-PA1-OA2
60	y	201	CDL	CB2-OB2-PB2-OB5
61	T	502	PGT	C4-O4P-P-O3P
61	b	601	PGT	C1-O3P-P-O4P
61	l	701	PGT	C4-O4P-P-O3P
60	W	701	CDL	C18-C19-C20-C21
59	w	201	3PH	C21-C22-C23-C24
60	x	101	CDL	CA2-C1-CB2-OB2
61	T	505	PGT	O4P-C4-C5-C6
59	R	401	3PH	O22-C21-O21-C2
60	u	603	CDL	OA7-CA5-OA6-CA4
59	w	201	3PH	C32-C31-O31-C3
59	V	602	3PH	C26-C27-C28-C29
60	u	603	CDL	C20-C21-C22-C23
60	u	603	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
60	u	603	CDL	C36-C37-C38-C39
60	x	101	CDL	C77-C78-C79-C80
61	T	502	PGT	C14-C15-C16-C17
54	V	605	PTY	C11-C8-O7-C6
61	T	505	PGT	C32-C31-O2-C2
54	S	302	PTY	C11-C12-C13-C14
54	e	302	PTY	C34-C35-C36-C37
60	W	701	CDL	C83-C84-C85-C86
60	h	203	CDL	C19-C20-C21-C22
60	u	602	CDL	C36-C37-C38-C39
60	u	603	CDL	C14-C15-C16-C17
60	u	603	CDL	C33-C34-C35-C36
55	J	200	8Q1	O27-C28-C29-C30
55	J	200	8Q1	O27-C28-C29-C31
62	s	401	COO	C15-C11-C12-O6A
54	T	501	PTY	C37-C38-C39-C40
58	T	503	PC7	C32-C33-C34-C35
60	R	405	CDL	C72-C73-C74-C75
60	W	701	CDL	C77-C78-C79-C80
60	x	101	CDL	C23-C24-C25-C26
59	V	601	3PH	C2C-C2D-C2E-C2F
60	W	701	CDL	C61-C62-C63-C64
54	V	605	PTY	C32-C33-C34-C35
54	V	606	PTY	C13-C14-C15-C16
59	g	101	3PH	C3E-C3F-C3G-C3H
60	W	701	CDL	C34-C35-C36-C37
60	h	203	CDL	C11-C12-C13-C14
60	h	203	CDL	C72-C73-C74-C75
60	u	603	CDL	C12-C13-C14-C15
60	y	201	CDL	C72-C73-C74-C75
61	b	601	PGT	C37-C38-C39-C40
61	l	701	PGT	C39-C40-C41-C42
54	S	302	PTY	C33-C34-C35-C36
55	r	200	8Q1	C12-C13-C14-C15
59	h	201	3PH	C2A-C2B-C2C-C2D
60	R	405	CDL	C11-C12-C13-C14
60	u	603	CDL	C40-C41-C42-C43
61	b	601	PGT	C36-C37-C38-C39
54	R	402	PTY	C8-C11-C12-C13
54	e	302	PTY	C30-C31-C32-C33
58	T	503	PC7	C13-C14-C15-C16
60	W	701	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
60	u	602	CDL	C57-C58-C59-C60
54	x	102	PTY	C16-C17-C18-C19
58	T	503	PC7	C33-C34-C35-C36
59	S	301	3PH	C37-C38-C39-C3A
60	W	701	CDL	C51-C52-C53-C54
60	W	701	CDL	C59-C60-C61-C62
60	u	602	CDL	C62-C63-C64-C65
60	u	603	CDL	CA5-C11-C12-C13
60	R	405	CDL	C75-C76-C77-C78
60	W	701	CDL	C35-C36-C37-C38
54	T	504	PTY	C32-C33-C34-C35
60	h	203	CDL	C20-C21-C22-C23
60	u	602	CDL	C63-C64-C65-C66
60	u	603	CDL	C16-C17-C18-C19
60	u	603	CDL	C38-C39-C40-C41
60	u	603	CDL	C42-C43-C44-C45
60	x	101	CDL	C79-C80-C81-C82
61	T	502	PGT	C4-C5-C6-O6
61	b	601	PGT	C4-C5-C6-O6
61	l	701	PGT	C4-C5-C6-O6
54	V	605	PTY	O10-C8-O7-C6
61	T	505	PGT	O31-C31-O2-C2
61	l	701	PGT	O31-C31-O2-C2
61	l	701	PGT	C32-C31-O2-C2
59	V	602	3PH	C2B-C2C-C2D-C2E
60	V	603	CDL	C71-C72-C73-C74
60	W	701	CDL	C32-C33-C34-C35
60	h	203	CDL	C73-C74-C75-C76
60	x	101	CDL	C16-C17-C18-C19
59	g	101	3PH	C21-C22-C23-C24
54	V	605	PTY	C33-C34-C35-C36
54	x	102	PTY	C22-C23-C24-C25
55	r	200	8Q1	C11-C10-C9-C8
58	Q	302	PC7	C12-C13-C14-C15
58	T	503	PC7	C40-C41-C42-C43
59	c	101	3PH	C33-C34-C35-C36
60	h	203	CDL	C57-C58-C59-C60
60	x	101	CDL	C21-C22-C23-C24
61	T	505	PGT	C32-C33-C34-C35
61	T	505	PGT	C19-C20-C21-C22
60	x	101	CDL	C15-C16-C17-C18
61	b	601	PGT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
59	c	101	3PH	C35-C36-C37-C38
60	W	701	CDL	C11-C12-C13-C14
60	h	203	CDL	C32-C33-C34-C35
61	b	601	PGT	C32-C33-C34-C35
59	w	201	3PH	O32-C31-O31-C3
54	R	404	PTY	C25-C26-C27-C28
54	S	302	PTY	C37-C38-C39-C40
58	T	503	PC7	C39-C40-C41-C42
60	h	203	CDL	C31-C32-C33-C34
60	h	203	CDL	C80-C81-C82-C83
61	T	502	PGT	C16-C17-C18-C19
60	V	603	CDL	C11-C12-C13-C14
60	x	101	CDL	C11-C12-C13-C14
62	s	401	COO	N2-C5-C6-S1
54	T	506	PTY	C12-C13-C14-C15
54	e	302	PTY	C13-C14-C15-C16
58	T	503	PC7	C38-C39-C40-C41
60	V	603	CDL	C13-C14-C15-C16
60	x	101	CDL	C62-C63-C64-C65
60	x	101	CDL	C63-C64-C65-C66
59	g	101	3PH	C37-C38-C39-C3A
60	V	603	CDL	C34-C35-C36-C37
60	u	602	CDL	C16-C17-C18-C19
60	x	101	CDL	C57-C58-C59-C60
61	b	601	PGT	C17-C18-C19-C20
58	Q	302	PC7	C11-C12-C13-C14
58	T	503	PC7	C17-C18-C19-C20
60	x	101	CDL	C54-C55-C56-C57
60	h	203	CDL	C11-CA5-OA6-CA4
60	h	203	CDL	C51-CB5-OB6-CB4
54	R	406	PTY	C14-C15-C16-C17
60	W	701	CDL	C17-C18-C19-C20
61	T	505	PGT	C18-C19-C20-C21
60	u	603	CDL	C34-C35-C36-C37
59	w	201	3PH	O22-C21-O21-C2
60	h	203	CDL	OA7-CA5-OA6-CA4
60	h	203	CDL	OB7-CB5-OB6-CB4
59	R	401	3PH	C36-C37-C38-C39
60	x	101	CDL	C80-C81-C82-C83
59	h	201	3PH	C33-C34-C35-C36
60	W	701	CDL	C62-C63-C64-C65
60	W	701	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
60	W	701	CDL	C81-C82-C83-C84
54	T	504	PTY	C11-C8-O7-C6
54	R	404	PTY	C24-C25-C26-C27
59	w	201	3PH	C38-C39-C3A-C3B
60	W	701	CDL	C14-C15-C16-C17
61	T	505	PGT	C15-C16-C17-C18
61	l	701	PGT	C11-C12-C13-C14
54	T	501	PTY	C19-C20-C21-C22
58	T	503	PC7	C44-C45-C46-C47
60	y	201	CDL	OB7-CB5-OB6-CB4
60	u	603	CDL	C71-CB7-OB8-CB6
60	u	603	CDL	C71-C72-C73-C74
62	s	401	COO	O4-C7-C8-C9
54	V	604	PTY	C34-C35-C36-C37
58	T	503	PC7	C15-C16-C17-C18
55	J	200	8Q1	C10-C11-C12-C13
60	W	701	CDL	C80-C81-C82-C83
60	u	602	CDL	C13-C14-C15-C16
60	u	602	CDL	C33-C34-C35-C36
61	l	701	PGT	C40-C41-C42-C43
54	T	501	PTY	C6-C1-O4-C30
58	u	601	PC7	C39-C40-C41-C42
60	u	602	CDL	C54-C55-C56-C57
58	Q	302	PC7	C32-C31-O2-C2
59	w	201	3PH	C22-C21-O21-C2
60	R	405	CDL	C11-CA5-OA6-CA4
60	u	602	CDL	C11-CA5-OA6-CA4
60	y	201	CDL	C51-CB5-OB6-CB4
59	V	602	3PH	C2A-C2B-C2C-C2D
60	x	101	CDL	C55-C56-C57-C58
54	T	504	PTY	O10-C8-O7-C6
58	Q	302	PC7	O31-C31-O2-C2
54	R	402	PTY	O4-C1-C6-O7
54	T	506	PTY	O4-C1-C6-O7
54	R	404	PTY	C16-C17-C18-C19
60	R	405	CDL	C32-C33-C34-C35
58	Q	302	PC7	C4-C5-N-C6
60	V	603	CDL	C33-C34-C35-C36
60	x	101	CDL	C51-C52-C53-C54
54	x	102	PTY	C20-C21-C22-C23
60	V	603	CDL	C51-CB5-OB6-CB4
60	x	101	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
60	x	101	CDL	C83-C84-C85-C86
54	T	506	PTY	C5-O14-P1-O11
54	V	605	PTY	C3-O11-P1-O14
60	u	603	CDL	CA3-OA5-PA1-OA2
59	h	201	3PH	C36-C37-C38-C39
60	u	603	CDL	C15-C16-C17-C18
54	T	504	PTY	C30-C31-C32-C33
54	V	605	PTY	C6-C5-O14-P1
60	h	203	CDL	CB4-CB3-OB5-PB2
60	h	203	CDL	C16-C17-C18-C19
61	T	502	PGT	C36-C37-C38-C39
60	x	101	CDL	C71-CB7-OB8-CB6
59	V	601	3PH	O11-C1-C2-C3
59	c	101	3PH	O11-C1-C2-C3
59	h	201	3PH	O11-C1-C2-C3
61	l	701	PGT	O3P-C1-C2-C3
60	u	602	CDL	C11-C12-C13-C14
60	x	101	CDL	C19-C20-C21-C22
60	u	602	CDL	C18-C19-C20-C21
54	T	501	PTY	C21-C22-C23-C24
59	V	602	3PH	C34-C35-C36-C37
60	x	101	CDL	C12-C13-C14-C15
54	e	302	PTY	C31-C32-C33-C34
58	T	503	PC7	C42-C43-C44-C45
59	w	201	3PH	C2A-C2B-C2C-C2D
60	W	701	CDL	CB2-C1-CA2-OA2
60	u	602	CDL	OA7-CA5-OA6-CA4
60	x	101	CDL	C74-C75-C76-C77
60	V	603	CDL	C21-C22-C23-C24
54	e	302	PTY	C8-C11-C12-C13
60	u	603	CDL	OB9-CB7-OB8-CB6
54	R	404	PTY	C33-C34-C35-C36
54	R	404	PTY	O4-C1-C6-C5
60	R	405	CDL	C77-C78-C79-C80
60	V	603	CDL	C32-C33-C34-C35
60	h	203	CDL	CB3-CB4-CB6-OB8
60	h	203	CDL	C76-C77-C78-C79
60	u	603	CDL	CB3-CB4-CB6-OB8
60	x	101	CDL	CA3-CA4-CA6-OA8
60	y	201	CDL	CA3-CA4-CA6-OA8
61	l	701	PGT	C41-C42-C43-C44
54	R	402	PTY	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
60	u	603	CDL	C37-C38-C39-C40
60	V	603	CDL	C23-C24-C25-C26
60	u	603	CDL	C44-C45-C46-C47
60	x	101	CDL	CB7-C71-C72-C73
55	r	200	8Q1	O33-C32-C34-O35
54	V	605	PTY	C35-C36-C37-C38
60	u	602	CDL	C37-C38-C39-C40
60	u	602	CDL	C61-C62-C63-C64
59	V	601	3PH	C37-C38-C39-C3A
54	T	501	PTY	C32-C33-C34-C35
58	T	503	PC7	C45-C46-C47-C48
54	G	303	PTY	C8-C11-C12-C13
54	T	506	PTY	C31-C30-O4-C1
54	e	302	PTY	C17-C18-C19-C20
61	T	502	PGT	C20-C21-C22-C23
58	T	503	PC7	C23-C24-C25-C26
60	W	701	CDL	C19-C20-C21-C22
60	x	101	CDL	C36-C37-C38-C39
60	W	701	CDL	CB6-CB4-OB6-CB5
60	R	405	CDL	OA7-CA5-OA6-CA4
60	u	602	CDL	C74-C75-C76-C77
58	R	403	PC7	C2-C1-O3P-P
59	h	201	3PH	C1-O11-P-O12
60	W	701	CDL	C54-C55-C56-C57
60	W	701	CDL	C75-C76-C77-C78
54	T	501	PTY	C31-C30-O4-C1
54	S	302	PTY	O14-C5-C6-O7
54	V	605	PTY	C12-C11-C8-O7
61	b	601	PGT	C11-C12-C13-C14
61	b	601	PGT	C18-C19-C20-C21
54	V	605	PTY	C39-C40-C41-C42
59	g	101	3PH	C38-C39-C3A-C3B
60	u	603	CDL	C51-C52-C53-C54
54	S	302	PTY	O4-C1-C6-O7
60	x	101	CDL	OB9-CB7-OB8-CB6
54	S	302	PTY	C8-C11-C12-C13
59	h	201	3PH	C3D-C3E-C3F-C3G
60	x	101	CDL	C32-C33-C34-C35
60	x	101	CDL	C61-C62-C63-C64
60	y	201	CDL	C12-C13-C14-C15
62	s	401	COO	P1A-O3A-P2A-O4A
60	y	201	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
59	S	301	3PH	C32-C33-C34-C35
59	S	301	3PH	C38-C39-C3A-C3B
59	S	301	3PH	C39-C3A-C3B-C3C
60	R	405	CDL	C12-C13-C14-C15
60	V	603	CDL	C19-C20-C21-C22
60	W	701	CDL	C31-CA7-OA8-CA6
58	Q	302	PC7	C14-C15-C16-C17
60	h	203	CDL	C56-C57-C58-C59
54	R	404	PTY	O14-C5-C6-C1
54	R	406	PTY	O14-C5-C6-C1
54	e	302	PTY	O14-C5-C6-C1
60	R	405	CDL	OB5-CB3-CB4-CB6
60	V	603	CDL	OA5-CA3-CA4-CA6
60	y	201	CDL	OB5-CB3-CB4-CB6
60	W	701	CDL	C40-C41-C42-C43
60	u	602	CDL	C71-CB7-OB8-CB6
59	h	201	3PH	C26-C27-C28-C29
60	x	101	CDL	C18-C19-C20-C21
60	x	101	CDL	C56-C57-C58-C59
61	T	502	PGT	C18-C19-C20-C21
60	V	603	CDL	OB7-CB5-OB6-CB4
60	W	701	CDL	C52-C53-C54-C55
60	W	701	CDL	C82-C83-C84-C85
59	V	601	3PH	C2B-C2C-C2D-C2E
54	e	302	PTY	C39-C40-C41-C42
61	l	701	PGT	C34-C35-C36-C37
60	u	603	CDL	CA4-CA3-OA5-PA1
54	h	202	PTY	C31-C32-C33-C34
60	h	203	CDL	C33-C34-C35-C36
54	V	604	PTY	C37-C38-C39-C40
60	h	203	CDL	C77-C78-C79-C80
54	R	402	PTY	O4-C1-C6-C5
54	S	302	PTY	O4-C1-C6-C5
54	T	506	PTY	O4-C1-C6-C5
54	V	604	PTY	O4-C1-C6-C5
58	T	503	PC7	C1-C2-C3-O3
60	V	603	CDL	CA3-CA4-CA6-OA8
60	h	203	CDL	CA3-CA4-CA6-OA8
60	y	201	CDL	CB3-CB4-CB6-OB8
61	T	505	PGT	C1-C2-C3-O3
54	S	302	PTY	C12-C13-C14-C15
60	V	603	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
54	T	501	PTY	O30-C30-O4-C1
54	T	506	PTY	O30-C30-O4-C1
59	w	201	3PH	C3C-C3D-C3E-C3F
54	V	606	PTY	C14-C15-C16-C17
60	W	701	CDL	C60-C61-C62-C63
61	T	505	PGT	C14-C15-C16-C17
58	T	503	PC7	C16-C17-C18-C19
54	S	302	PTY	C5-O14-P1-O11
60	x	101	CDL	CB3-OB5-PB2-OB2
54	T	504	PTY	O14-C5-C6-O7
58	u	601	PC7	C16-C17-C18-C19
60	V	603	CDL	O1-C1-CA2-OA2
54	R	404	PTY	C23-C24-C25-C26
60	u	602	CDL	C22-C23-C24-C25
54	S	302	PTY	C13-C14-C15-C16
54	S	302	PTY	C38-C39-C40-C41
59	c	101	3PH	C22-C23-C24-C25
54	V	604	PTY	O4-C1-C6-O7
58	R	403	PC7	O2-C2-C3-O3
58	u	601	PC7	O2-C2-C3-O3
59	h	201	3PH	O21-C2-C3-O31
60	y	201	CDL	OB6-CB4-CB6-OB8
61	T	505	PGT	O2-C2-C3-O3
61	b	601	PGT	O2-C2-C3-O3
61	T	502	PGT	O2-C31-C32-C33
58	u	601	PC7	C32-C33-C34-C35
60	h	203	CDL	CA5-C11-C12-C13
60	R	405	CDL	CB2-C1-CA2-OA2
60	u	603	CDL	CB2-C1-CA2-OA2
54	x	102	PTY	C26-C27-C28-C29
61	l	701	PGT	C20-C21-C22-C23
60	u	602	CDL	C24-C25-C26-C27
60	u	602	CDL	CA5-C11-C12-C13
54	V	606	PTY	C11-C12-C13-C14
60	h	203	CDL	C55-C56-C57-C58
60	u	602	CDL	C51-C52-C53-C54
60	u	603	CDL	C21-C22-C23-C24
60	y	201	CDL	C51-C52-C53-C54
54	V	604	PTY	C6-C5-O14-P1
59	R	401	3PH	C2-C1-O11-P
54	T	501	PTY	C11-C12-C13-C14
60	R	405	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
54	G	303	PTY	C37-C38-C39-C40
54	R	406	PTY	C39-C40-C41-C42
54	e	301	PTY	C30-C31-C32-C33
54	V	606	PTY	C11-C8-O7-C6
54	S	302	PTY	O14-C5-C6-C1
54	T	506	PTY	O14-C5-C6-C1
58	u	601	PC7	O3P-C1-C2-C3
60	u	602	CDL	OB5-CB3-CB4-CB6
61	T	502	PGT	O3P-C1-C2-C3
61	T	505	PGT	O3P-C1-C2-C3
60	u	602	CDL	C15-C16-C17-C18
60	x	101	CDL	C75-C76-C77-C78
54	T	501	PTY	C33-C34-C35-C36
55	J	200	8Q1	C7-C8-C9-C10
60	u	602	CDL	C59-C60-C61-C62
58	Q	302	PC7	C12-C11-O3-C3
54	T	501	PTY	C40-C41-C42-C43
55	r	200	8Q1	C28-O27-P24-O2
56	P	401	NDP	C2B-O2B-P2B-O1X
60	u	602	CDL	C20-C21-C22-C23
60	V	603	CDL	C72-C73-C74-C75
54	x	102	PTY	C31-C30-O4-C1
54	G	303	PTY	C32-C33-C34-C35
59	R	401	3PH	C3-C2-O21-C21
59	w	201	3PH	C3-C2-O21-C21
61	l	701	PGT	C3-C2-O2-C31
59	c	101	3PH	C29-C2A-C2B-C2C
60	W	701	CDL	C64-C65-C66-C67
59	g	101	3PH	C32-C33-C34-C35
59	R	401	3PH	C26-C27-C28-C29
60	h	203	CDL	C17-C18-C19-C20
60	u	602	CDL	C58-C59-C60-C61
58	u	601	PC7	C1-C2-C3-O3
59	h	201	3PH	C1-C2-C3-O31
60	R	405	CDL	CB3-CB4-CB6-OB8
61	b	601	PGT	C1-C2-C3-O3
54	R	404	PTY	O14-C5-C6-O7
54	T	506	PTY	O14-C5-C6-O7
58	u	601	PC7	O3P-C1-C2-O2
59	c	101	3PH	O11-C1-C2-O21
59	w	201	3PH	O11-C1-C2-O21
60	V	603	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
60	h	203	CDL	OB5-CB3-CB4-OB6
59	w	201	3PH	C29-C2A-C2B-C2C
60	y	201	CDL	C11-C12-C13-C14
54	V	606	PTY	O10-C8-O7-C6
60	V	603	CDL	C12-C13-C14-C15
60	W	701	CDL	OA9-CA7-OA8-CA6
54	R	404	PTY	O4-C1-C6-O7
54	R	406	PTY	O4-C1-C6-O7
54	V	605	PTY	O4-C1-C6-O7
54	V	606	PTY	O4-C1-C6-O7
59	w	201	3PH	O21-C2-C3-O31
60	R	405	CDL	OB6-CB4-CB6-OB8
60	V	603	CDL	OA6-CA4-CA6-OA8
60	W	701	CDL	OB6-CB4-CB6-OB8
60	h	203	CDL	OA6-CA4-CA6-OA8
61	l	701	PGT	O2-C2-C3-O3
60	u	602	CDL	OB9-CB7-OB8-CB6
60	V	603	CDL	C32-C31-CA7-OA8
60	W	701	CDL	C44-C45-C46-C47
60	h	203	CDL	C51-C52-C53-C54
60	h	203	CDL	C78-C79-C80-C81
56	P	401	NDP	C5B-O5B-PA-O3
61	T	502	PGT	O5-C5-C6-O6
54	V	604	PTY	C11-C8-O7-C6
54	x	102	PTY	C32-C33-C34-C35
60	W	701	CDL	C71-C72-C73-C74
54	V	604	PTY	O10-C8-O7-C6
54	x	102	PTY	O30-C30-O4-C1
58	Q	302	PC7	O11-C11-O3-C3
60	R	405	CDL	C31-CA7-OA8-CA6
59	R	401	3PH	C25-C26-C27-C28
60	h	203	CDL	C74-C75-C76-C77
60	x	101	CDL	C84-C85-C86-C87
54	R	404	PTY	C13-C14-C15-C16
54	R	404	PTY	C3-O11-P1-O14
54	V	606	PTY	C5-O14-P1-O11
54	e	301	PTY	C5-O14-P1-O11
56	P	401	NDP	O4D-C1D-N1N-C6N
58	R	403	PC7	C4-O4P-P-O3P
60	V	603	CDL	C35-C36-C37-C38
60	W	701	CDL	C43-C44-C45-C46
60	V	603	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
60	W	701	CDL	CB4-CB3-OB5-PB2
54	R	402	PTY	C5-O14-P1-O13
54	R	406	PTY	C5-O14-P1-O12
54	T	501	PTY	C3-O11-P1-O13
54	T	501	PTY	C5-O14-P1-O12
54	T	506	PTY	C3-O11-P1-O13
54	T	506	PTY	C5-O14-P1-O12
54	T	506	PTY	C5-O14-P1-O13
54	V	604	PTY	C5-O14-P1-O13
54	V	605	PTY	C3-O11-P1-O12
54	h	202	PTY	C3-O11-P1-O12
60	R	405	CDL	CB3-OB5-PB2-OB4
60	V	603	CDL	CA2-OA2-PA1-OA4
60	V	603	CDL	CA3-OA5-PA1-OA3
60	W	701	CDL	CA2-OA2-PA1-OA4
60	W	701	CDL	CB3-OB5-PB2-OB3
60	h	203	CDL	CB3-OB5-PB2-OB4
60	u	602	CDL	CB2-OB2-PB2-OB3
60	u	602	CDL	CB2-OB2-PB2-OB4
60	u	603	CDL	CA3-OA5-PA1-OA4
60	u	603	CDL	CB2-OB2-PB2-OB3
60	u	603	CDL	CB3-OB5-PB2-OB4
60	x	101	CDL	CA3-OA5-PA1-OA3
60	y	201	CDL	CB2-OB2-PB2-OB3
60	y	201	CDL	CB2-OB2-PB2-OB4
61	T	502	PGT	C4-O4P-P-O2P
61	T	505	PGT	C1-O3P-P-O2P
54	V	605	PTY	O14-C5-C6-C1
60	V	603	CDL	OB5-CB3-CB4-CB6
60	h	203	CDL	OA5-CA3-CA4-CA6
60	h	203	CDL	OB5-CB3-CB4-CB6
60	y	201	CDL	OA5-CA3-CA4-CA6
61	T	502	PGT	C35-C36-C37-C38
54	e	302	PTY	C18-C19-C20-C21
59	w	201	3PH	C3A-C3B-C3C-C3D
60	W	701	CDL	C36-C37-C38-C39
61	T	502	PGT	C41-C42-C43-C44
54	S	302	PTY	C2-C3-O11-P1
54	V	606	PTY	C2-C3-O11-P1
60	W	701	CDL	C31-C32-C33-C34
61	l	701	PGT	C38-C39-C40-C41
60	x	101	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
61	b	601	PGT	O4P-C4-C5-C6
59	S	301	3PH	C22-C23-C24-C25
52	B	501	FMN	N10-C1'-C2'-O2'
59	V	601	3PH	O11-C1-C2-O21
60	V	603	CDL	OB5-CB3-CB4-OB6
60	u	602	CDL	OB5-CB3-CB4-OB6
60	u	603	CDL	OB5-CB3-CB4-OB6
60	x	101	CDL	CA7-C31-C32-C33
60	y	201	CDL	OB5-CB3-CB4-OB6
61	T	502	PGT	O3P-C1-C2-O2
58	R	403	PC7	C12-C13-C14-C15
61	b	601	PGT	C40-C41-C42-C43
60	x	101	CDL	C78-C79-C80-C81
54	V	606	PTY	C32-C33-C34-C35
60	W	701	CDL	O1-C1-CA2-OA2
60	x	101	CDL	C82-C83-C84-C85
54	R	406	PTY	O4-C1-C6-C5
54	V	605	PTY	O4-C1-C6-C5
60	h	203	CDL	OB6-CB4-CB6-OB8
60	u	603	CDL	OA6-CA4-CA6-OA8
54	S	302	PTY	C15-C16-C17-C18
54	V	604	PTY	C11-C12-C13-C14
60	R	405	CDL	OA9-CA7-OA8-CA6
60	u	602	CDL	C17-C18-C19-C20
60	x	101	CDL	C52-C53-C54-C55
54	h	202	PTY	C36-C37-C38-C39
54	h	202	PTY	C33-C34-C35-C36
59	g	101	3PH	C39-C3A-C3B-C3C
61	b	601	PGT	C38-C39-C40-C41
54	V	605	PTY	C34-C35-C36-C37
54	e	302	PTY	C33-C34-C35-C36
59	V	601	3PH	C29-C2A-C2B-C2C
60	y	201	CDL	C15-C16-C17-C18
54	e	302	PTY	C40-C41-C42-C43
54	V	606	PTY	C15-C16-C17-C18
54	S	302	PTY	C17-C18-C19-C20
61	b	601	PGT	C32-C31-O2-C2
62	s	401	COO	C2X-C3X-O3X-P3X
54	V	606	PTY	C36-C37-C38-C39
60	u	603	CDL	C32-C33-C34-C35
60	x	101	CDL	C17-C18-C19-C20
54	R	404	PTY	C1-C6-O7-C8

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Mol	Chain	Res	Type	Atoms
54	T	501	PTY	C1-C6-O7-C8
59	V	602	3PH	C1-C2-O21-C21
60	R	405	CDL	CB6-CB4-OB6-CB5
60	u	602	CDL	CB6-CB4-OB6-CB5
61	l	701	PGT	C21-C22-C23-C24
55	r	200	8Q1	C28-O27-P24-O3
58	u	601	PC7	C38-C39-C40-C41
61	T	505	PGT	O3P-C1-C2-O2
61	b	601	PGT	O31-C31-O2-C2
59	h	201	3PH	C3A-C3B-C3C-C3D
60	W	701	CDL	C84-C85-C86-C87
60	x	101	CDL	OA6-CA4-CA6-OA8
54	V	604	PTY	C32-C33-C34-C35
54	G	303	PTY	C3-O11-P1-O14
54	R	406	PTY	C3-O11-P1-O14
54	T	504	PTY	C3-O11-P1-O14
54	V	606	PTY	C3-O11-P1-O14
54	e	302	PTY	C3-O11-P1-O14
54	x	102	PTY	C3-O11-P1-O14
58	Q	302	PC7	C1-O3P-P-O4P
58	T	503	PC7	C4-O4P-P-O3P
60	u	602	CDL	CB3-OB5-PB2-OB2
60	y	201	CDL	CB3-OB5-PB2-OB2
61	b	601	PGT	C4-O4P-P-O3P
59	V	601	3PH	C2D-C2E-C2F-C2G
60	R	405	CDL	C52-C53-C54-C55
58	R	403	PC7	C1-C2-C3-O3
60	W	701	CDL	CB3-CB4-CB6-OB8
59	V	601	3PH	C23-C24-C25-C26
60	x	101	CDL	CA5-C11-C12-C13
59	V	601	3PH	C33-C34-C35-C36
62	s	401	COO	P1A-O3A-P2A-O5A
54	R	406	PTY	C35-C36-C37-C38
55	J	200	8Q1	C11-C12-C13-C14
60	u	603	CDL	C17-C18-C19-C20
59	S	301	3PH	C2-C1-O11-P
60	u	602	CDL	CA4-CA3-OA5-PA1
60	x	101	CDL	C14-C15-C16-C17
59	V	602	3PH	C33-C34-C35-C36
61	l	701	PGT	C37-C38-C39-C40
60	u	602	CDL	CA7-C31-C32-C33
54	G	303	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
54	x	102	PTY	C31-C32-C33-C34
54	R	404	PTY	C22-C23-C24-C25
54	x	102	PTY	C40-C41-C42-C43
60	W	701	CDL	C42-C43-C44-C45
54	h	202	PTY	C8-C11-C12-C13
59	V	601	3PH	C34-C35-C36-C37
54	V	605	PTY	C17-C18-C19-C20
62	s	401	COO	O2-C1-C13-C11
59	R	401	3PH	C37-C38-C39-C3A
54	x	102	PTY	C38-C39-C40-C41
60	y	201	CDL	C32-C33-C34-C35
54	h	202	PTY	C41-C42-C43-C44
54	e	301	PTY	O4-C1-C6-O7
60	R	405	CDL	C1-CB2-OB2-PB2
54	V	605	PTY	C12-C11-C8-O10
54	e	302	PTY	C14-C15-C16-C17
60	x	101	CDL	C71-C72-C73-C74
54	R	402	PTY	C11-C12-C13-C14
54	x	102	PTY	O4-C1-C6-C5
59	V	602	3PH	C1-C2-C3-O31
59	w	201	3PH	C1-C2-C3-O31
58	u	601	PC7	C35-C36-C37-C38
60	V	603	CDL	C17-C18-C19-C20
54	V	606	PTY	C16-C17-C18-C19
54	h	202	PTY	C38-C39-C40-C41
60	W	701	CDL	CA7-C31-C32-C33
61	b	601	PGT	C34-C35-C36-C37
62	s	401	COO	N1-C1-C13-C11
60	h	203	CDL	C72-C71-CB7-OB8
54	R	406	PTY	C32-C33-C34-C35
61	l	701	PGT	O5-C5-C6-O6
60	y	201	CDL	CA5-C11-C12-C13
55	J	200	8Q1	C13-C14-C15-C16
59	w	201	3PH	C22-C23-C24-C25
58	u	601	PC7	C37-C38-C39-C40
60	h	203	CDL	C13-C14-C15-C16
58	R	403	PC7	C36-C37-C38-C39
59	c	101	3PH	C34-C35-C36-C37
60	h	203	CDL	C54-C55-C56-C57
57	Q	301	UQ5	C14-C16-C17-C18
54	T	506	PTY	C14-C15-C16-C17
60	u	602	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
55	r	200	8Q1	C6-C7-C8-C9
54	V	606	PTY	C31-C32-C33-C34
60	W	701	CDL	C55-C56-C57-C58
54	V	606	PTY	O4-C1-C6-C5
54	T	504	PTY	C33-C34-C35-C36
55	J	200	8Q1	O4-C1-S44-C43
59	g	101	3PH	C24-C25-C26-C27
59	V	602	3PH	C3A-C3B-C3C-C3D
54	V	605	PTY	O14-C5-C6-O7
60	h	203	CDL	OA5-CA3-CA4-OA6
59	V	602	3PH	C23-C24-C25-C26
59	w	201	3PH	C35-C36-C37-C38
60	u	603	CDL	C43-C44-C45-C46
60	R	405	CDL	C33-C34-C35-C36
54	T	504	PTY	O14-C5-C6-C1
60	x	101	CDL	C35-C36-C37-C38
61	l	701	PGT	C33-C34-C35-C36
54	h	202	PTY	O4-C1-C6-O7
62	s	401	COO	C3X-O3X-P3X-O9A
54	e	302	PTY	C12-C11-C8-O7
59	w	201	3PH	C34-C35-C36-C37
58	R	403	PC7	C44-C45-C46-C47
59	h	201	3PH	C24-C25-C26-C27
59	w	201	3PH	C2B-C2C-C2D-C2E
60	x	101	CDL	C33-C34-C35-C36
60	u	603	CDL	C12-C11-CA5-OA6
57	Q	301	UQ5	C11-C12-C13-C14
55	J	200	8Q1	C9-C10-C11-C12
54	T	506	PTY	O10-C8-O7-C6
58	T	503	PC7	C37-C38-C39-C40
59	S	301	3PH	C27-C28-C29-C2A
60	x	101	CDL	C52-C51-CB5-OB6
60	x	101	CDL	C72-C71-CB7-OB8
59	w	201	3PH	C32-C33-C34-C35
54	S	302	PTY	C12-C11-C8-O7
57	Q	301	UQ5	C5-C4-O4-C4M
59	R	401	3PH	C1-O11-P-O12
59	V	601	3PH	C1-O11-P-O12
61	l	701	PGT	C1-C2-C3-O3
54	R	406	PTY	C16-C17-C18-C19
54	h	202	PTY	O4-C30-C31-C32
59	V	601	3PH	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
61	l	701	PGT	C35-C36-C37-C38
60	x	101	CDL	C76-C77-C78-C79
60	u	603	CDL	OB5-CB3-CB4-CB6
60	R	405	CDL	C72-C71-CB7-OB8
56	P	401	NDP	C5D-O5D-PN-O3
62	s	401	COO	C3X-O3X-P3X-O8A
59	w	201	3PH	C39-C3A-C3B-C3C
54	R	404	PTY	C17-C18-C19-C20
61	T	502	PGT	C31-C32-C33-C34
54	h	202	PTY	C14-C15-C16-C17
54	x	102	PTY	C21-C22-C23-C24
60	u	603	CDL	C52-C51-CB5-OB6
60	x	101	CDL	C81-C82-C83-C84
54	e	302	PTY	C12-C11-C8-O10
59	V	601	3PH	C27-C28-C29-C2A
61	T	502	PGT	O31-C31-C32-C33
56	P	401	NDP	PA-O3-PN-O2N
54	T	506	PTY	C11-C8-O7-C6
54	S	302	PTY	C12-C11-C8-O10
59	g	101	3PH	C23-C24-C25-C26
60	u	602	CDL	C32-C33-C34-C35
60	V	603	CDL	CA2-C1-CB2-OB2
59	V	602	3PH	C35-C36-C37-C38
55	J	200	8Q1	C6-C7-C8-C9
54	h	202	PTY	O30-C30-C31-C32
60	x	101	CDL	C52-C51-CB5-OB7
54	e	301	PTY	O4-C1-C6-C5
60	u	603	CDL	CA3-CA4-CA6-OA8
58	R	403	PC7	C16-C17-C18-C19
60	R	405	CDL	CB3-OB5-PB2-OB2
60	V	603	CDL	CA2-OA2-PA1-OA5
60	x	101	CDL	CB2-OB2-PB2-OB5
61	l	701	PGT	O4P-C4-C5-O5
59	V	602	3PH	C32-C33-C34-C35
60	R	405	CDL	C34-C35-C36-C37
60	W	701	CDL	C41-C42-C43-C44
54	R	406	PTY	C3-O11-P1-O13
60	V	603	CDL	CA3-OA5-PA1-OA4
60	u	602	CDL	CB3-OB5-PB2-OB3
60	x	101	CDL	CB2-OB2-PB2-OB4
60	x	101	CDL	CB3-OB5-PB2-OB3
60	y	201	CDL	CB3-OB5-PB2-OB3

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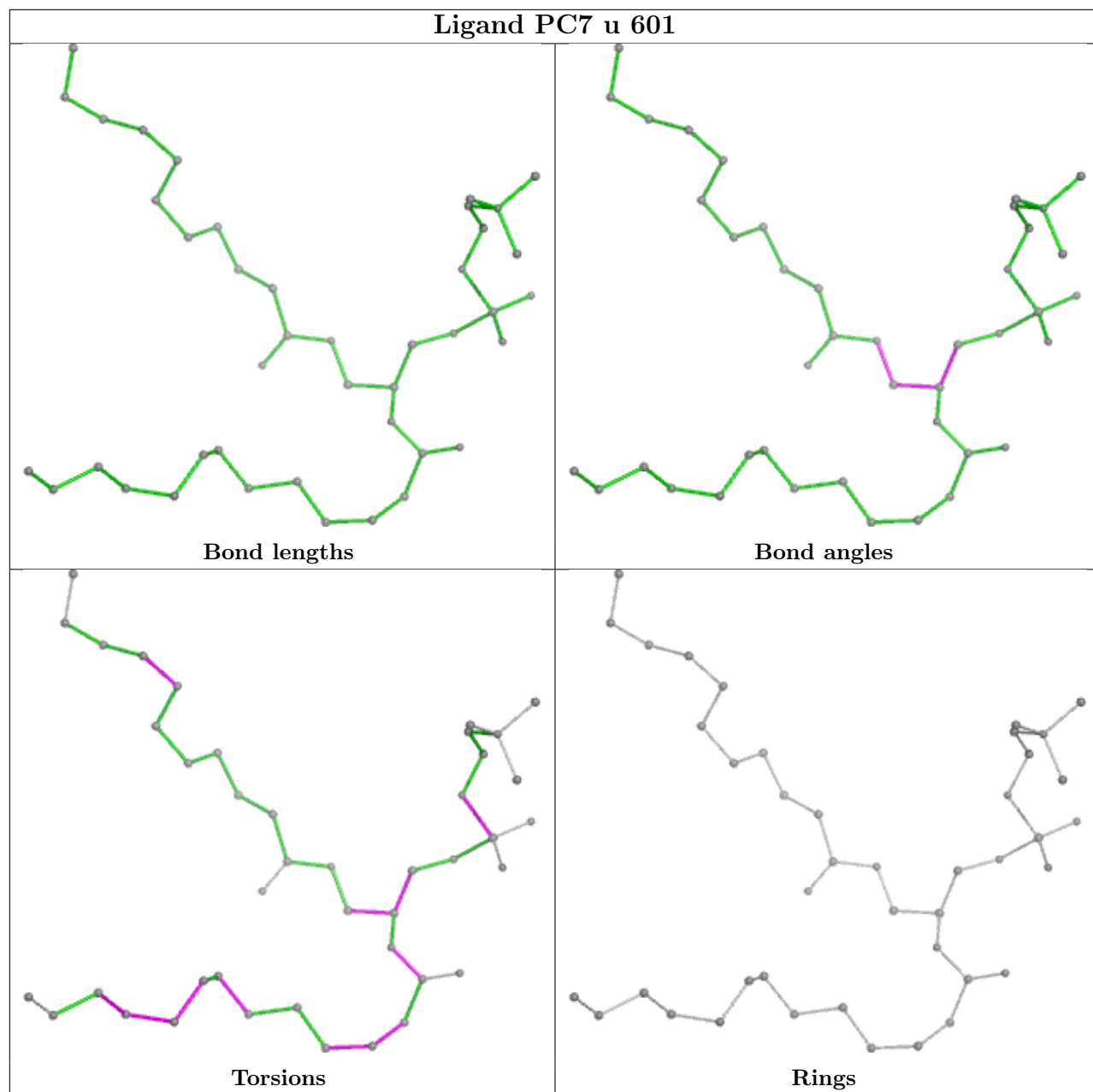
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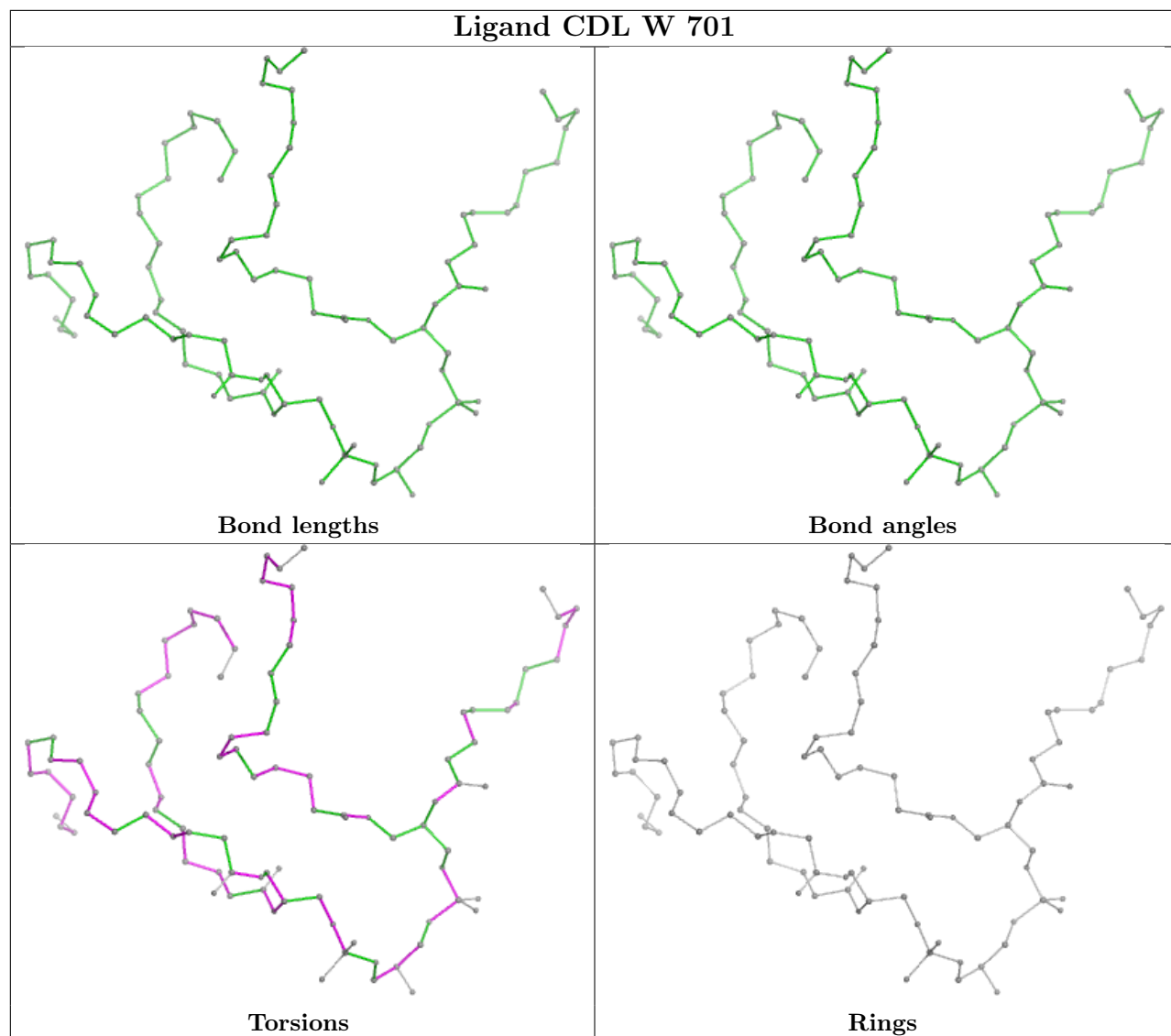
Mol	Chain	Res	Type	Atoms
61	T	505	PGT	C4-O4P-P-O1P
61	b	601	PGT	C4-O4P-P-O2P
61	l	701	PGT	C4-O4P-P-O2P
56	P	401	NDP	O4B-C4B-C5B-O5B
60	u	603	CDL	C52-C51-CB5-OB7
60	x	101	CDL	C72-C71-CB7-OB9
59	V	602	3PH	C25-C26-C27-C28
59	c	101	3PH	C37-C38-C39-C3A
58	R	403	PC7	C13-C14-C15-C16
59	c	101	3PH	C2D-C2E-C2F-C2G
61	b	601	PGT	C31-C32-C33-C34
59	w	201	3PH	C36-C37-C38-C39
54	h	202	PTY	C2-C3-O11-P1
60	u	603	CDL	C35-C36-C37-C38
54	V	606	PTY	C33-C34-C35-C36
60	h	203	CDL	C12-C11-CA5-OA6
60	R	405	CDL	C35-C36-C37-C38
54	V	605	PTY	O4-C30-C31-C32
60	h	203	CDL	C52-C51-CB5-OB6
54	x	102	PTY	C23-C24-C25-C26
60	x	101	CDL	C12-C11-CA5-OA7
60	x	101	CDL	C12-C11-CA5-OA6
60	h	203	CDL	C52-C51-CB5-OB7
60	u	603	CDL	O1-C1-CA2-OA2
59	V	601	3PH	C2F-C2G-C2H-C2I
60	R	405	CDL	C72-C71-CB7-OB9
54	h	202	PTY	C37-C38-C39-C40

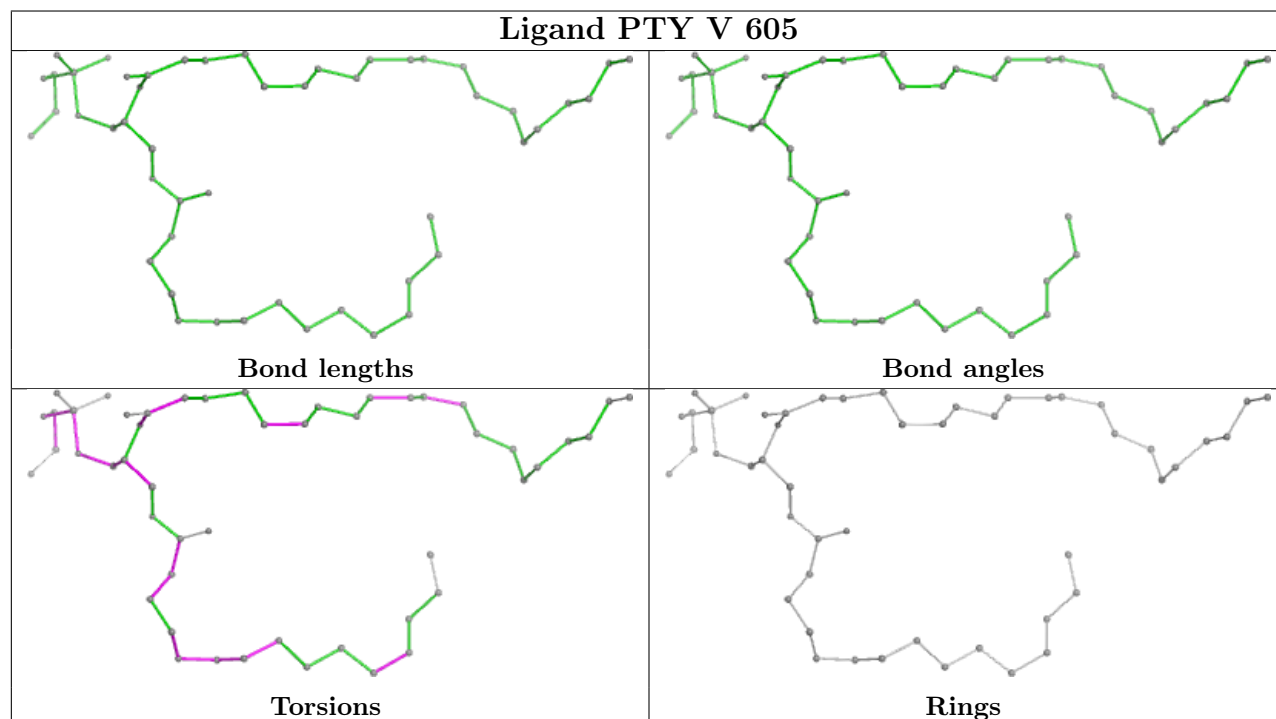
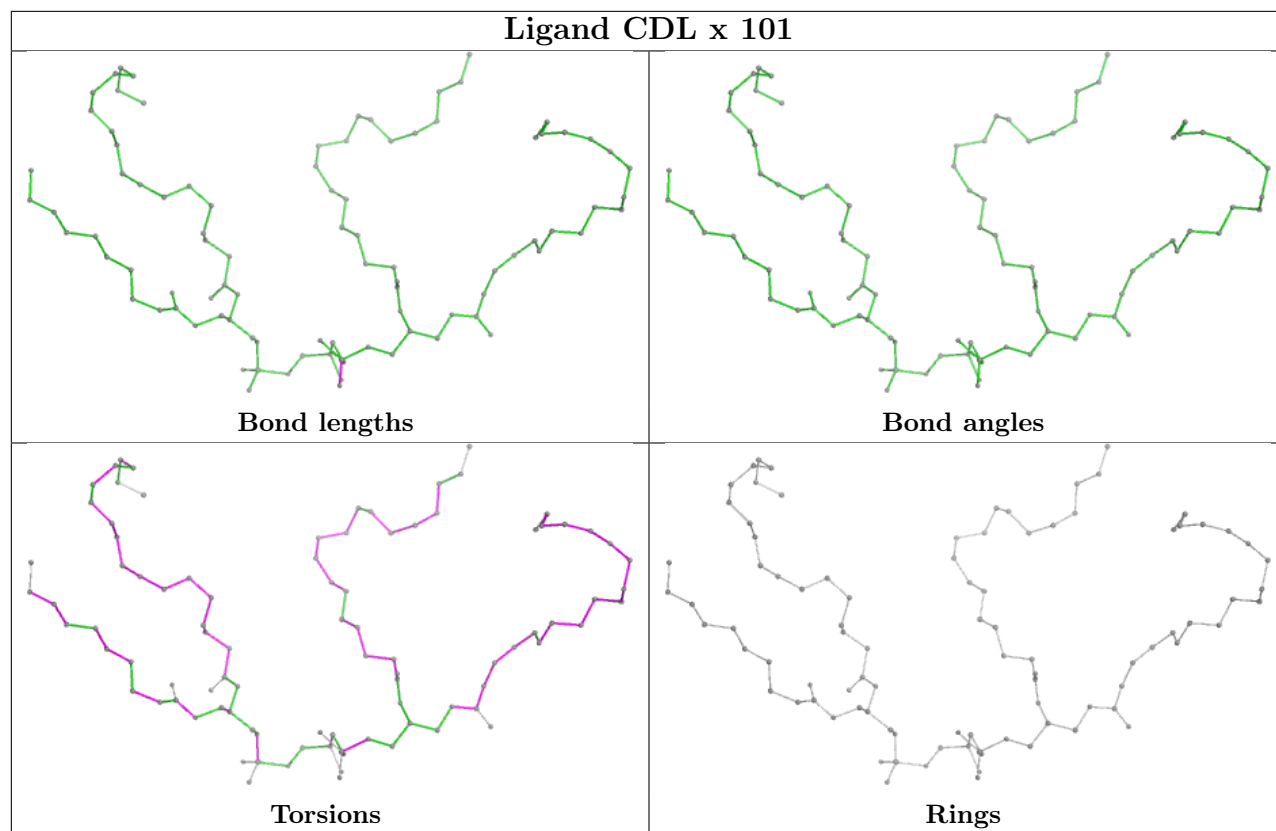
There are no ring outliers.

No monomer is involved in short contacts.

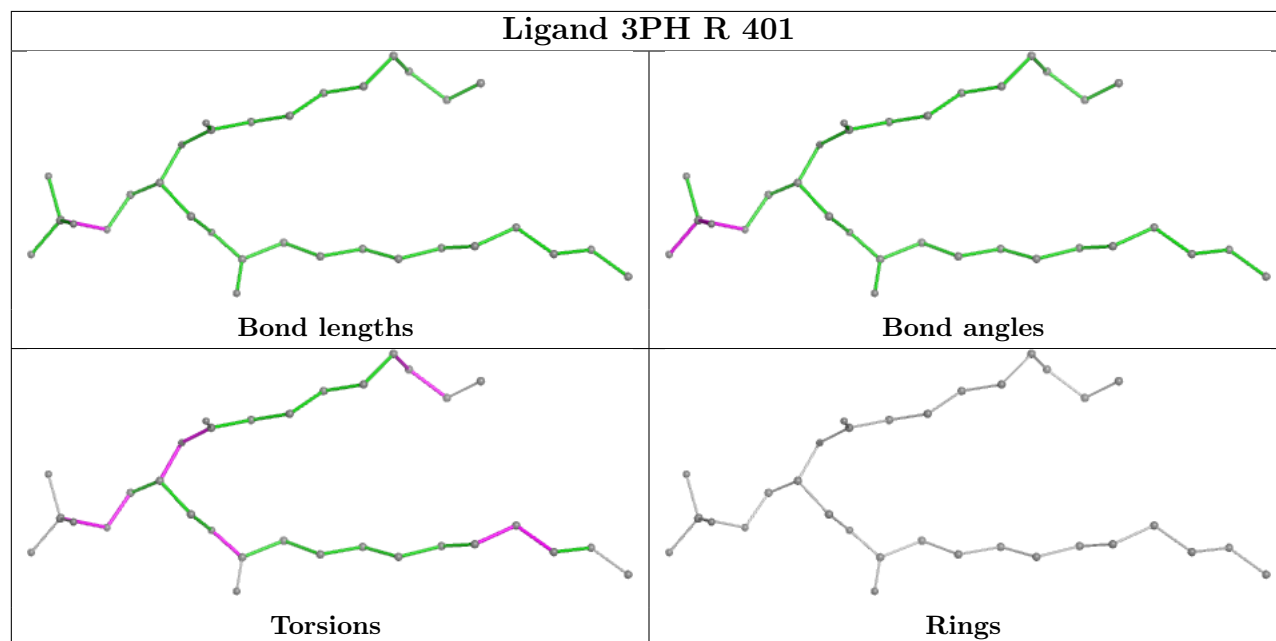
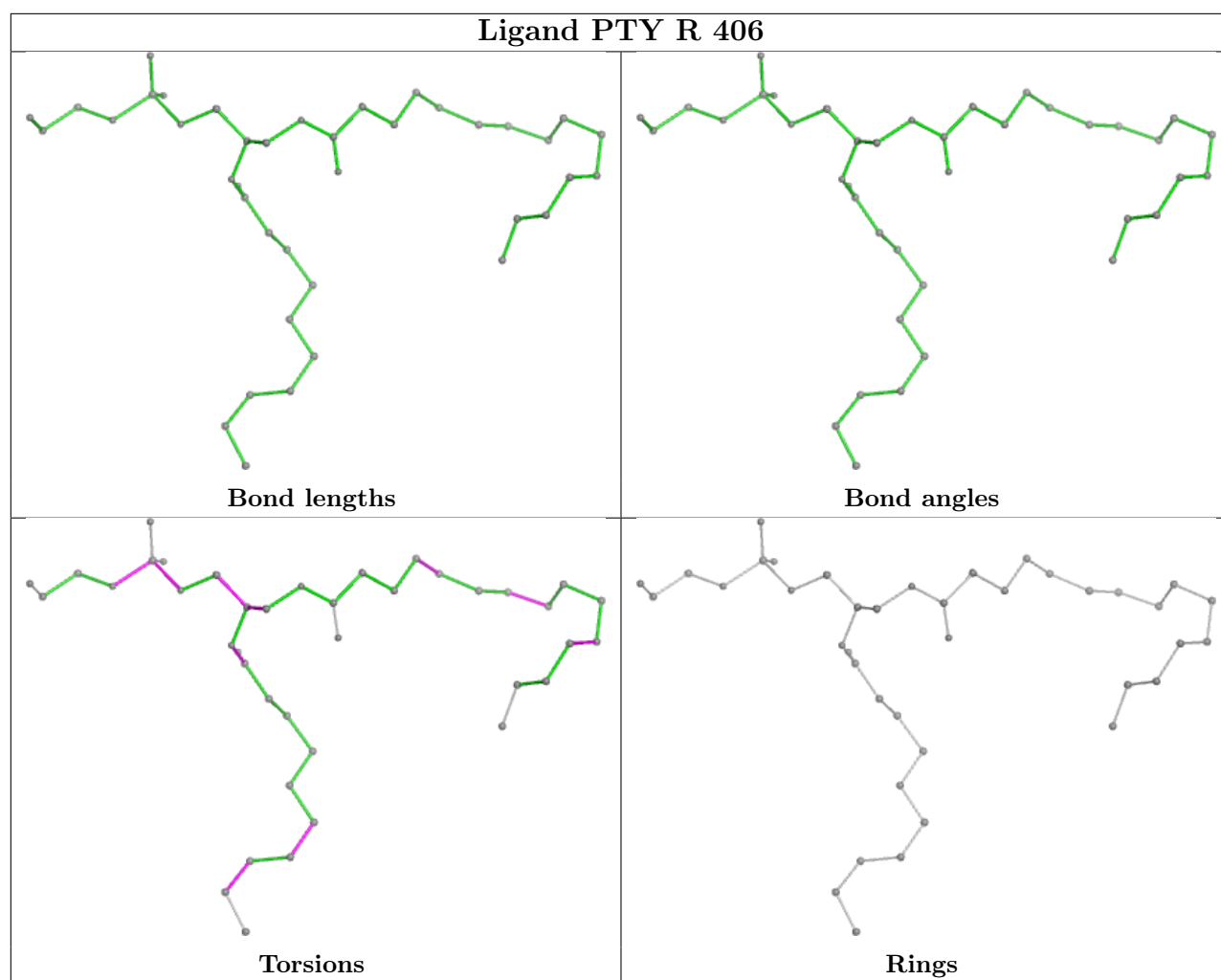
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

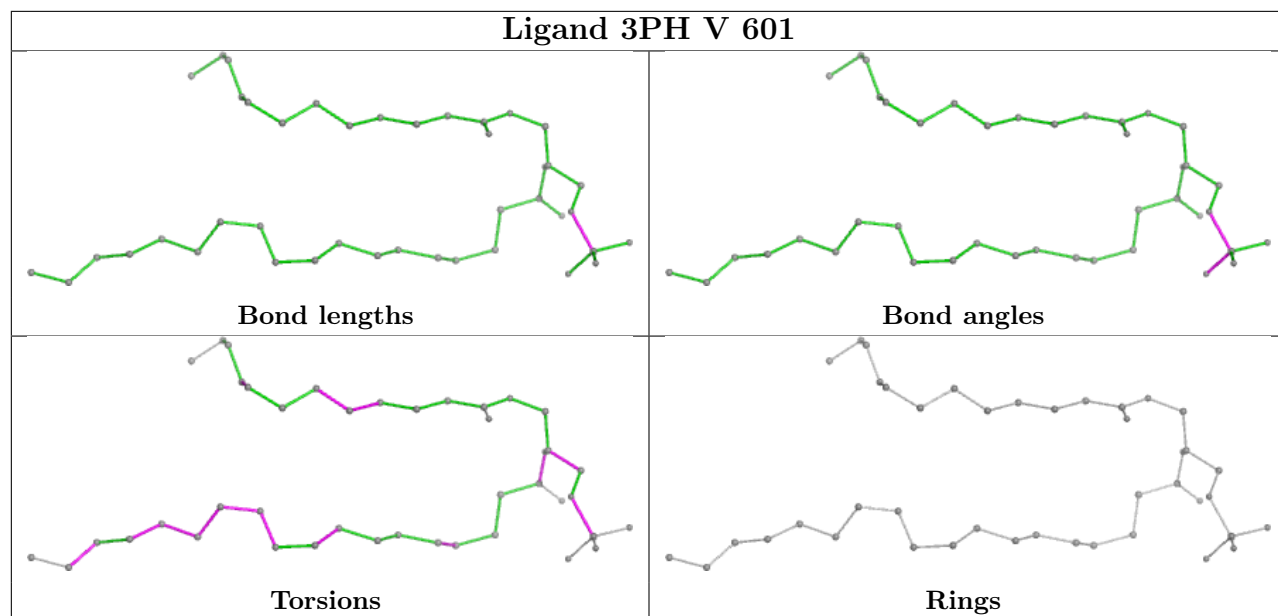


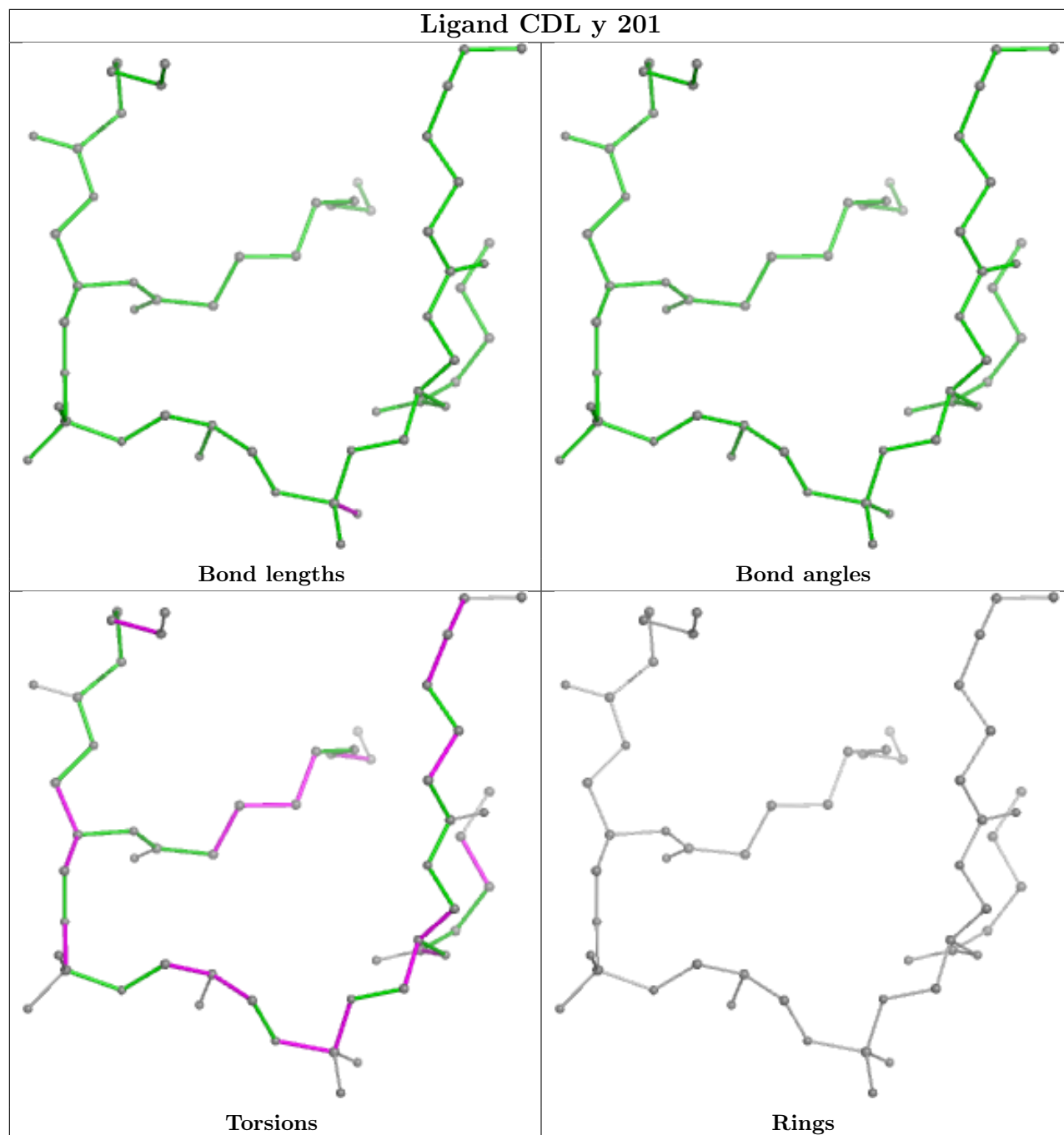


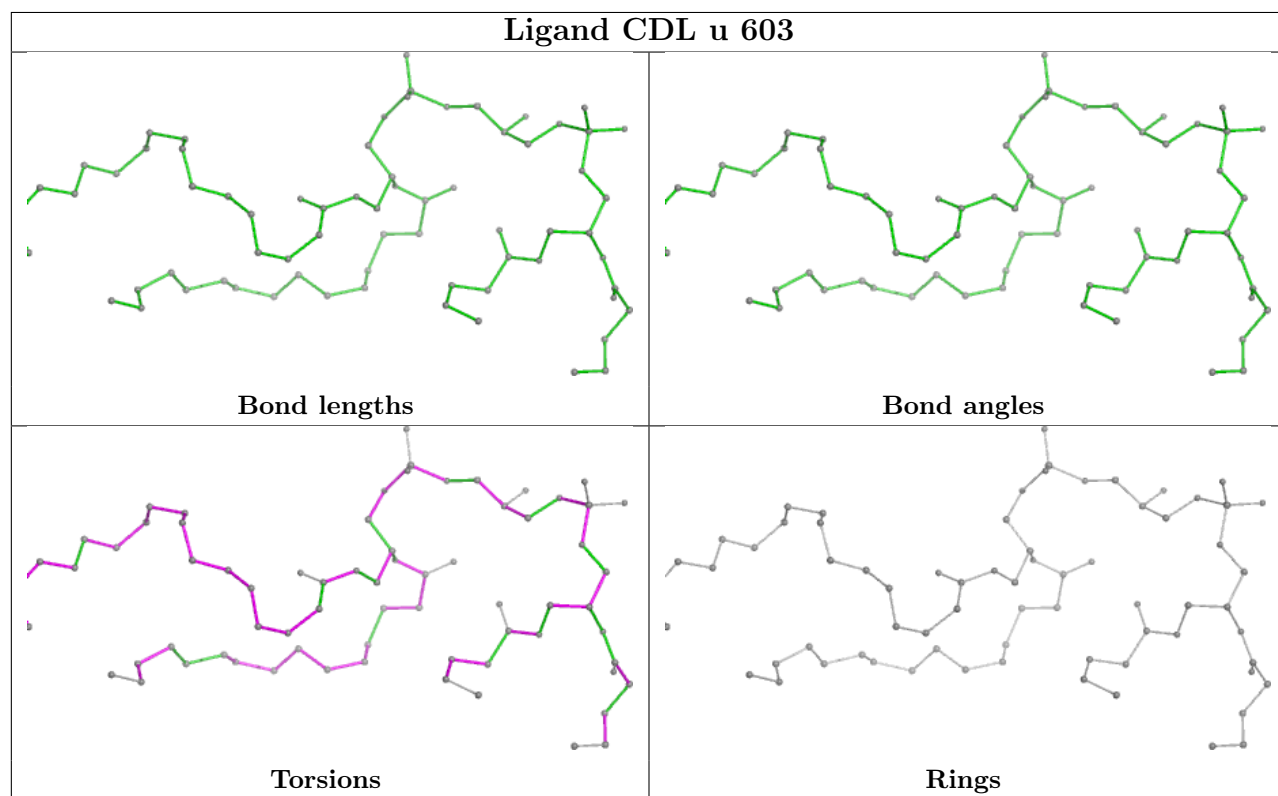
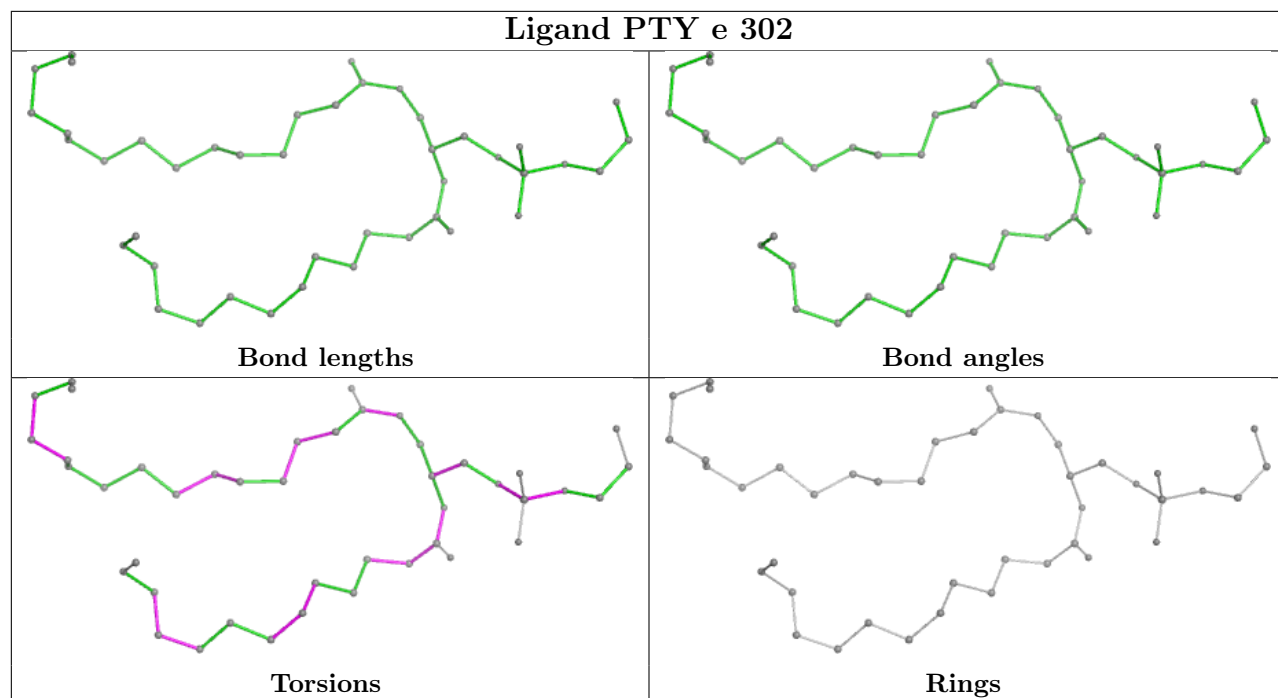


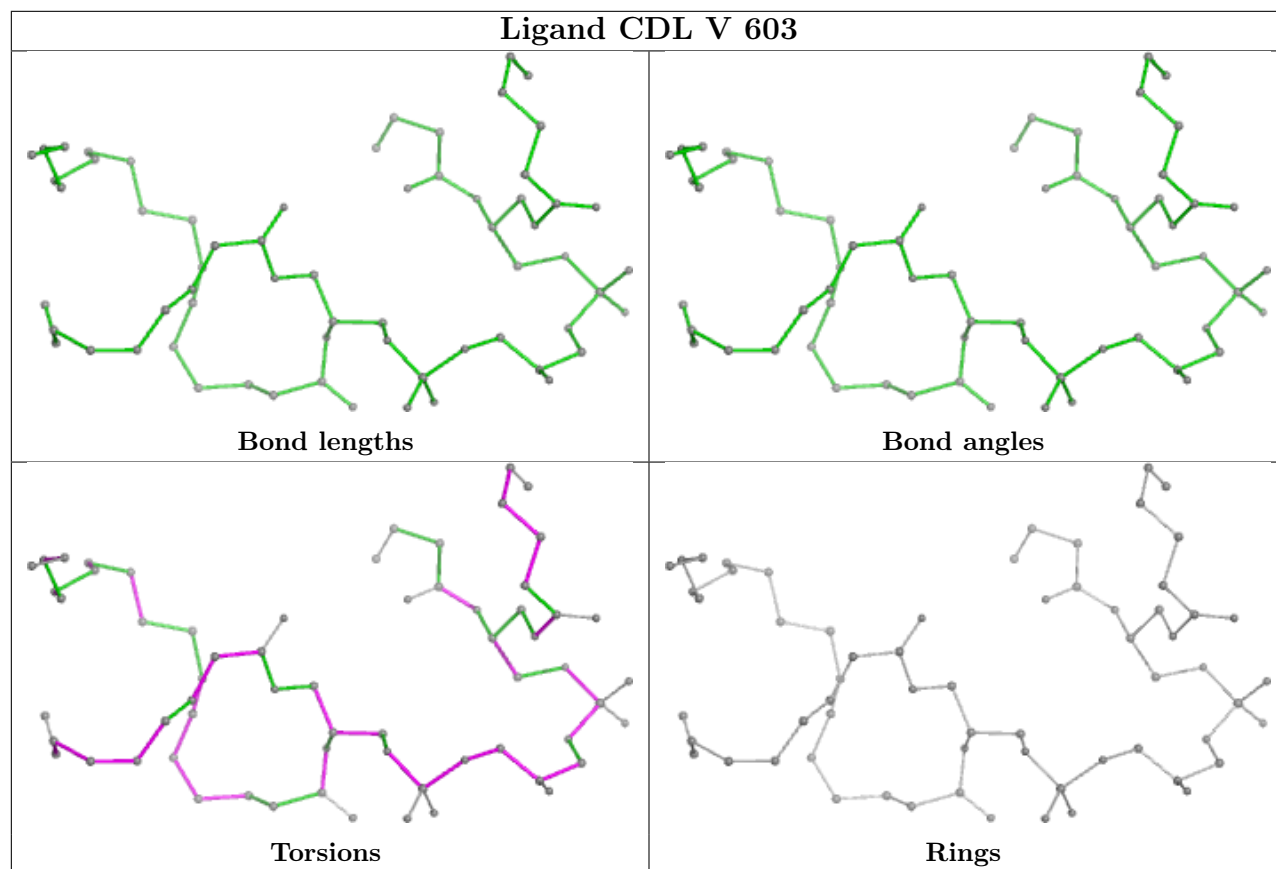
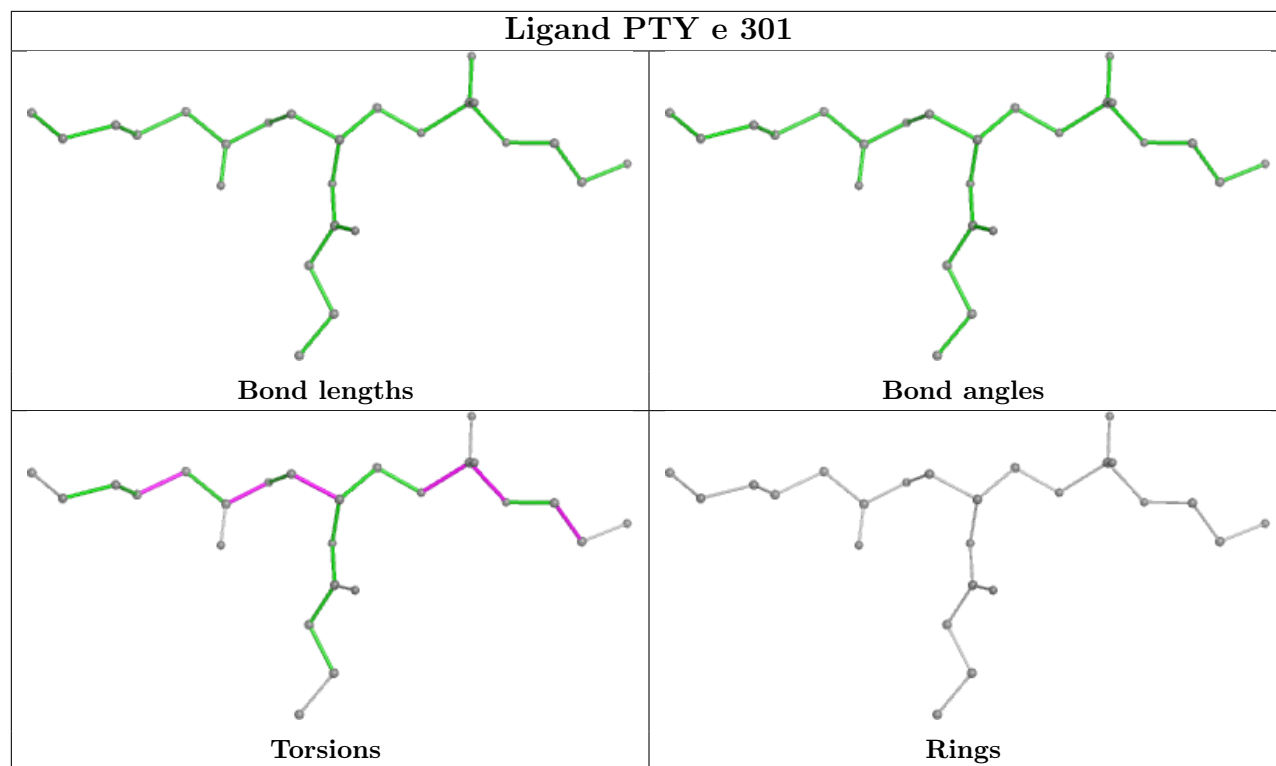


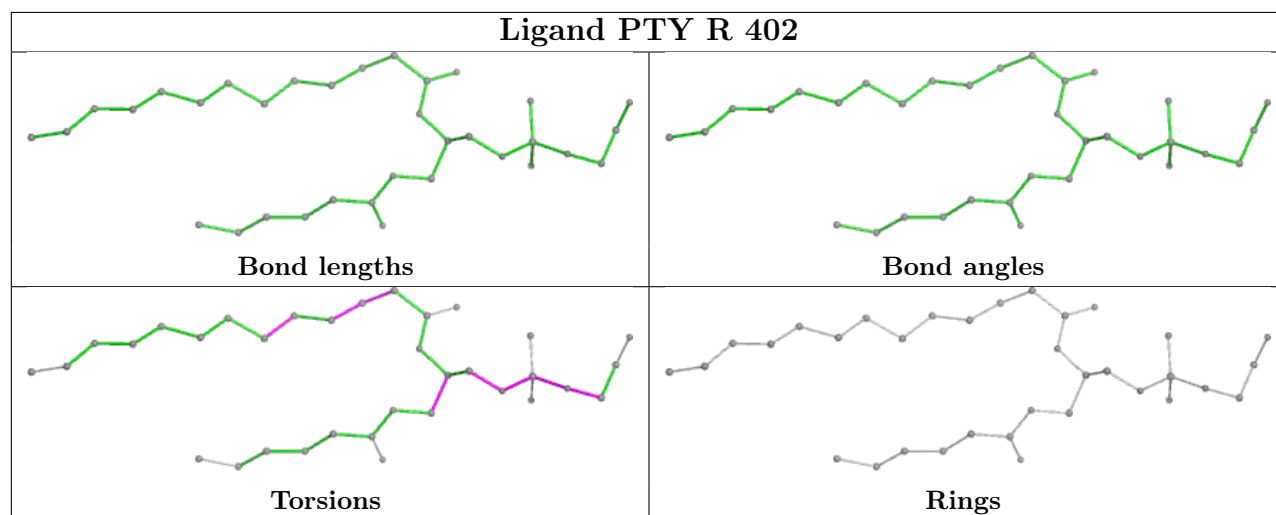
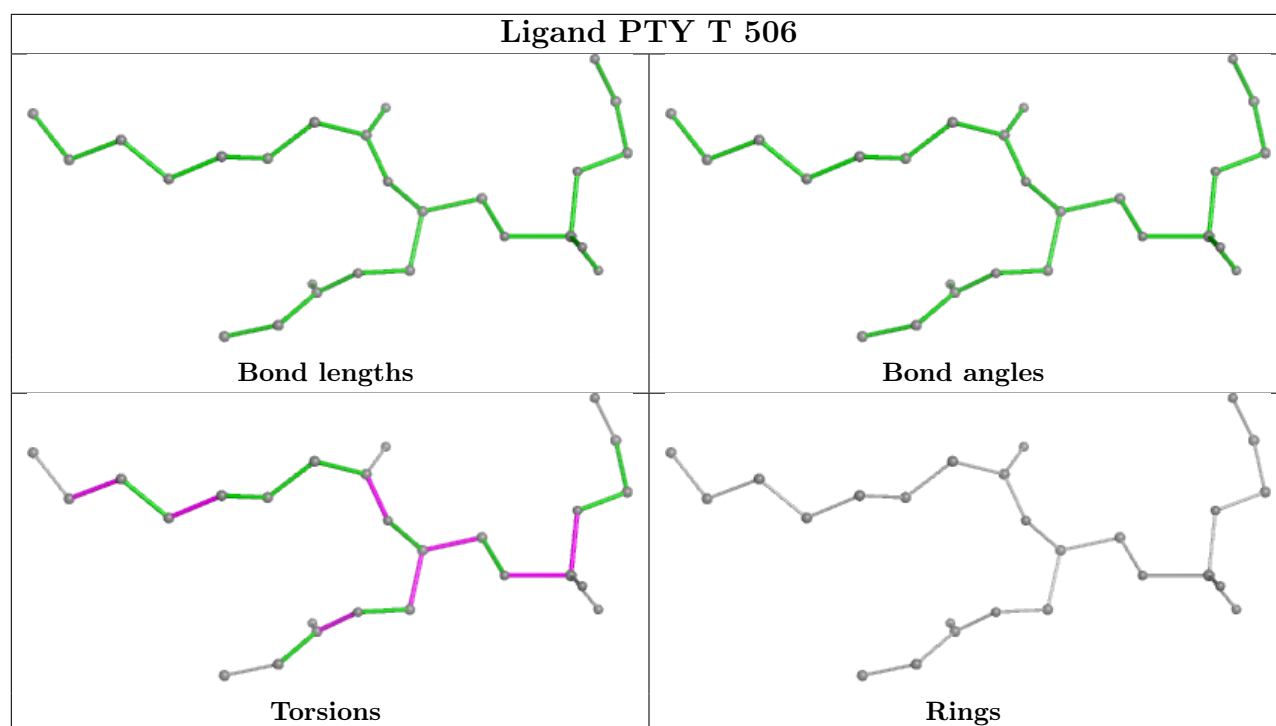


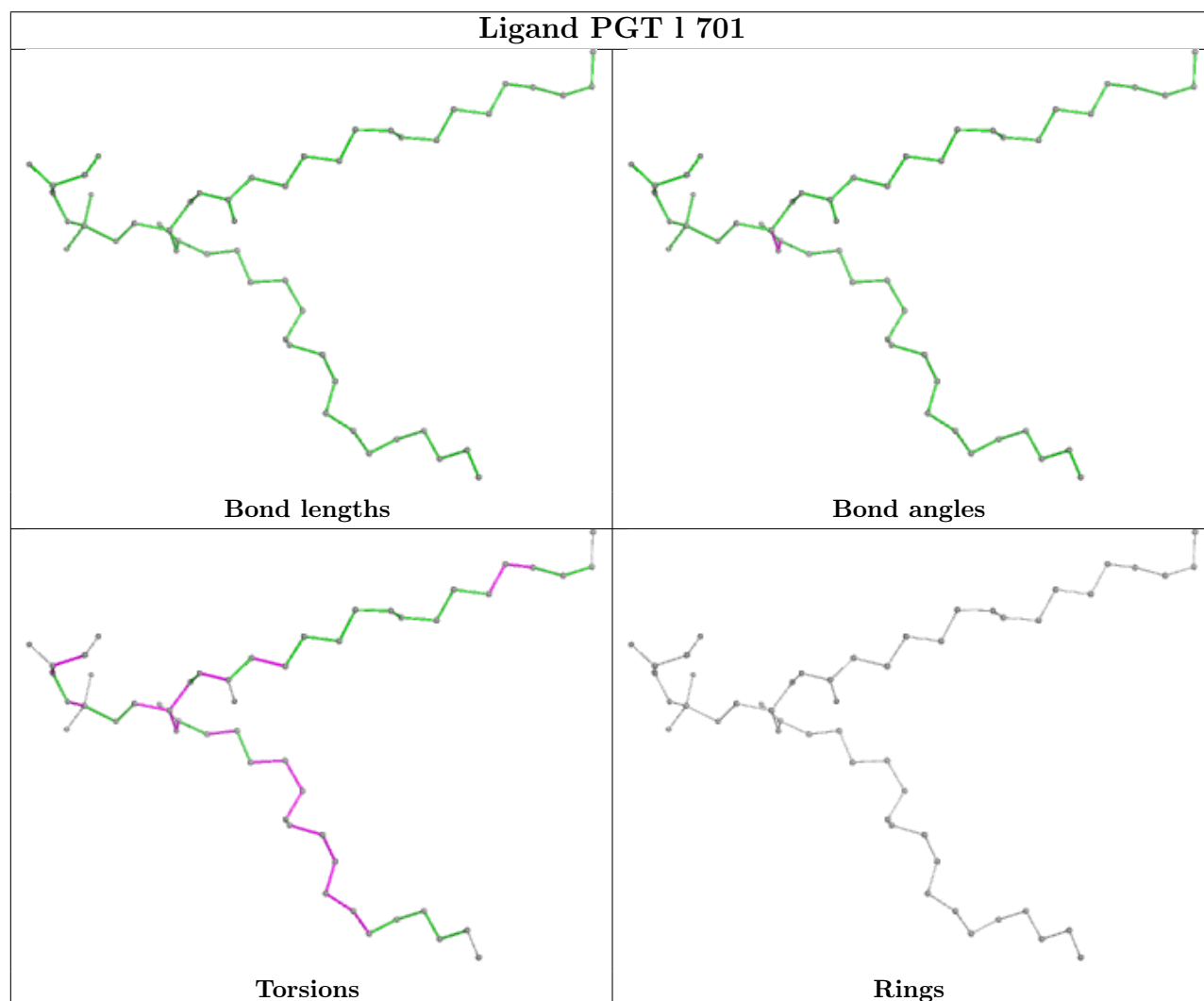
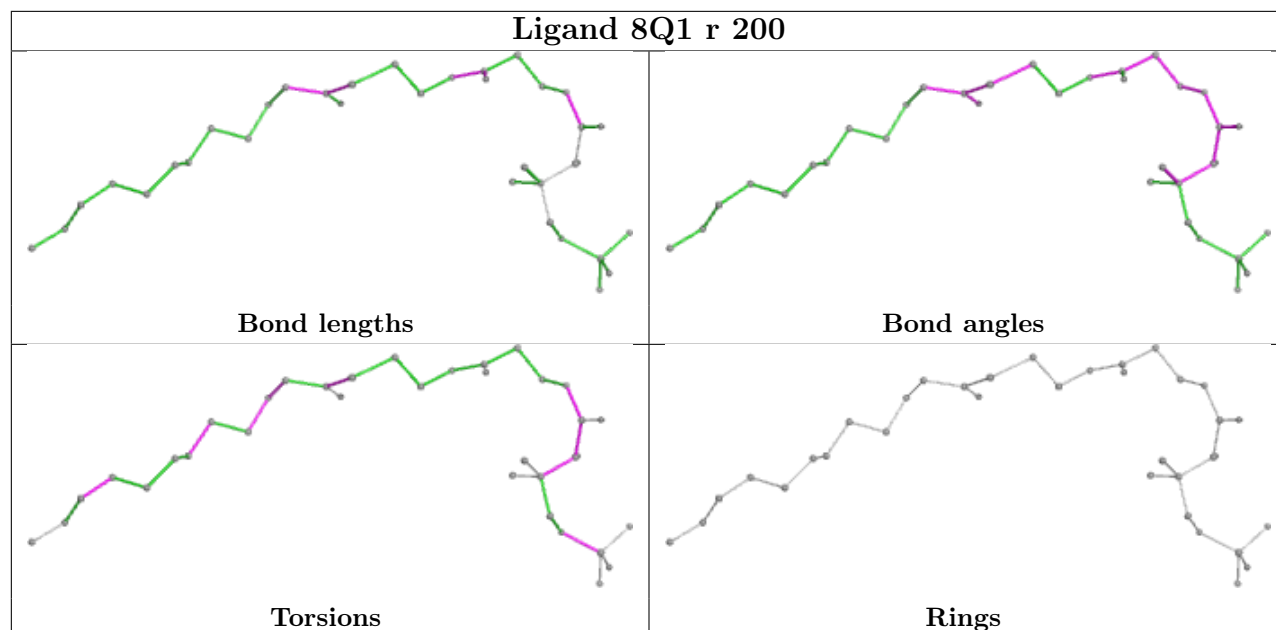


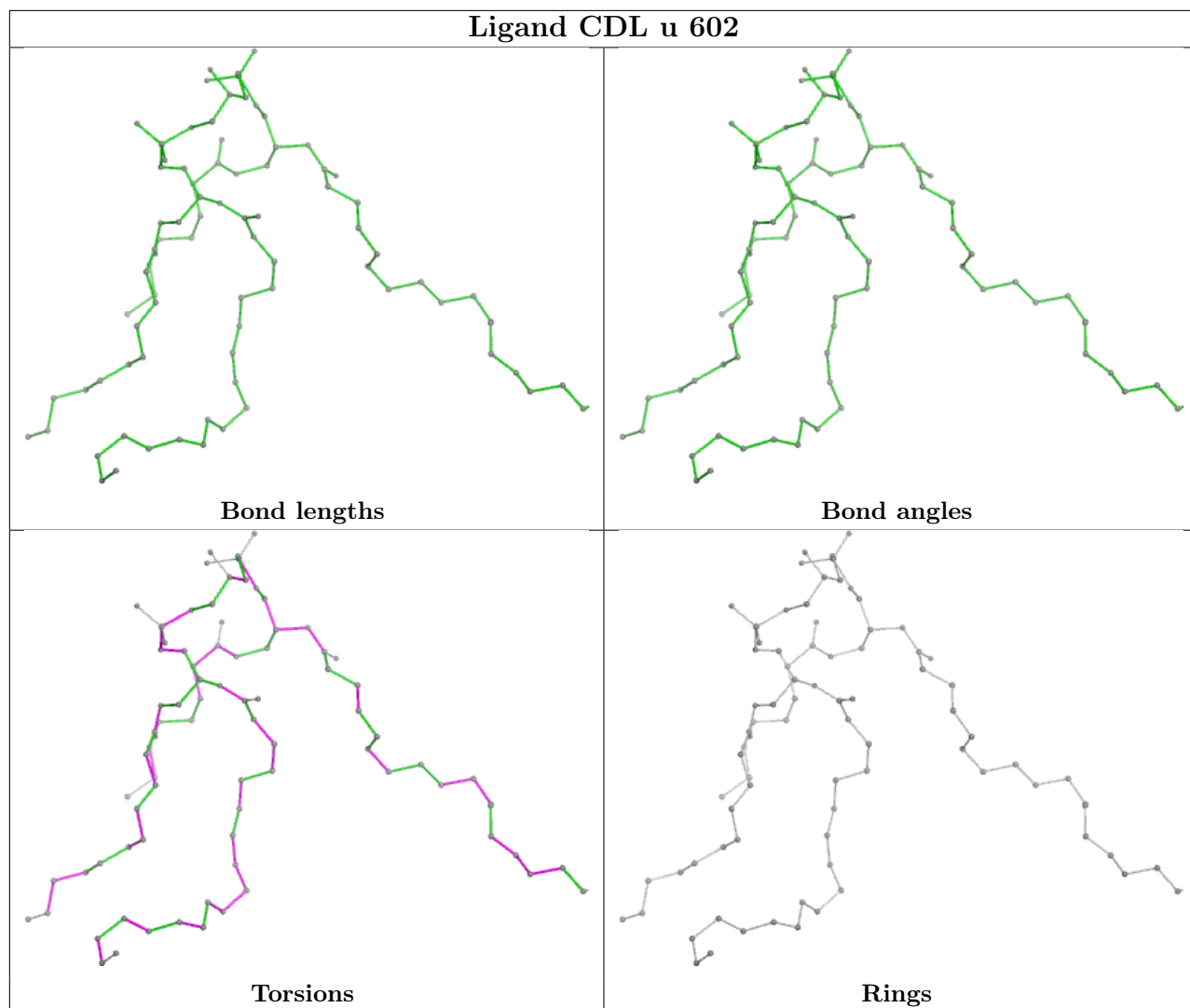




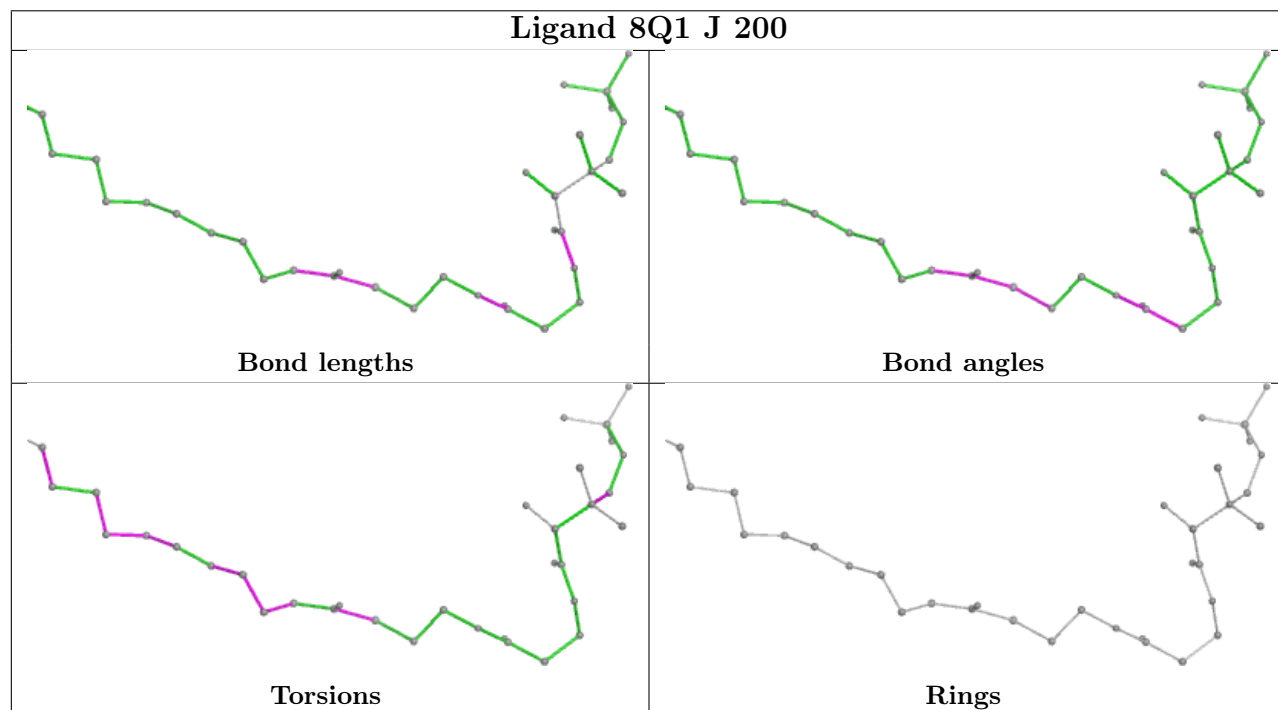
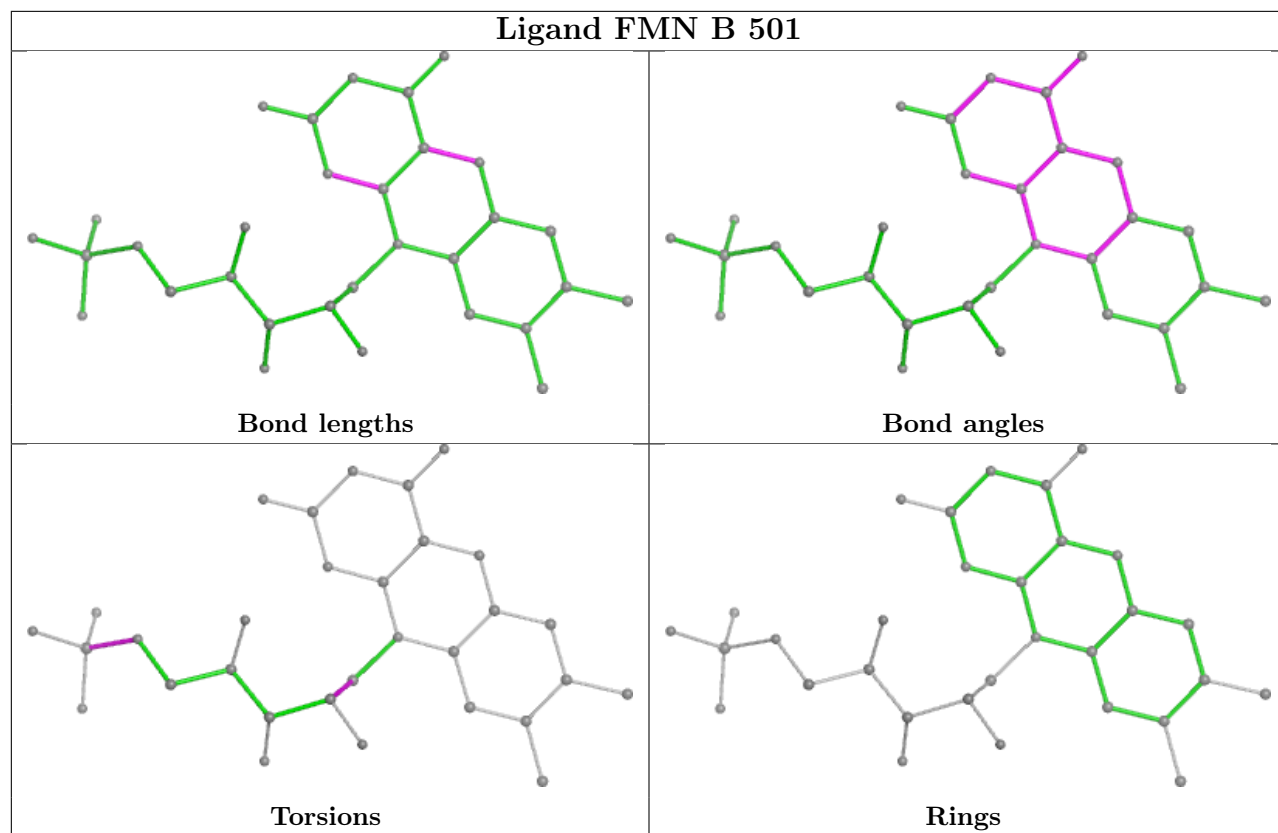


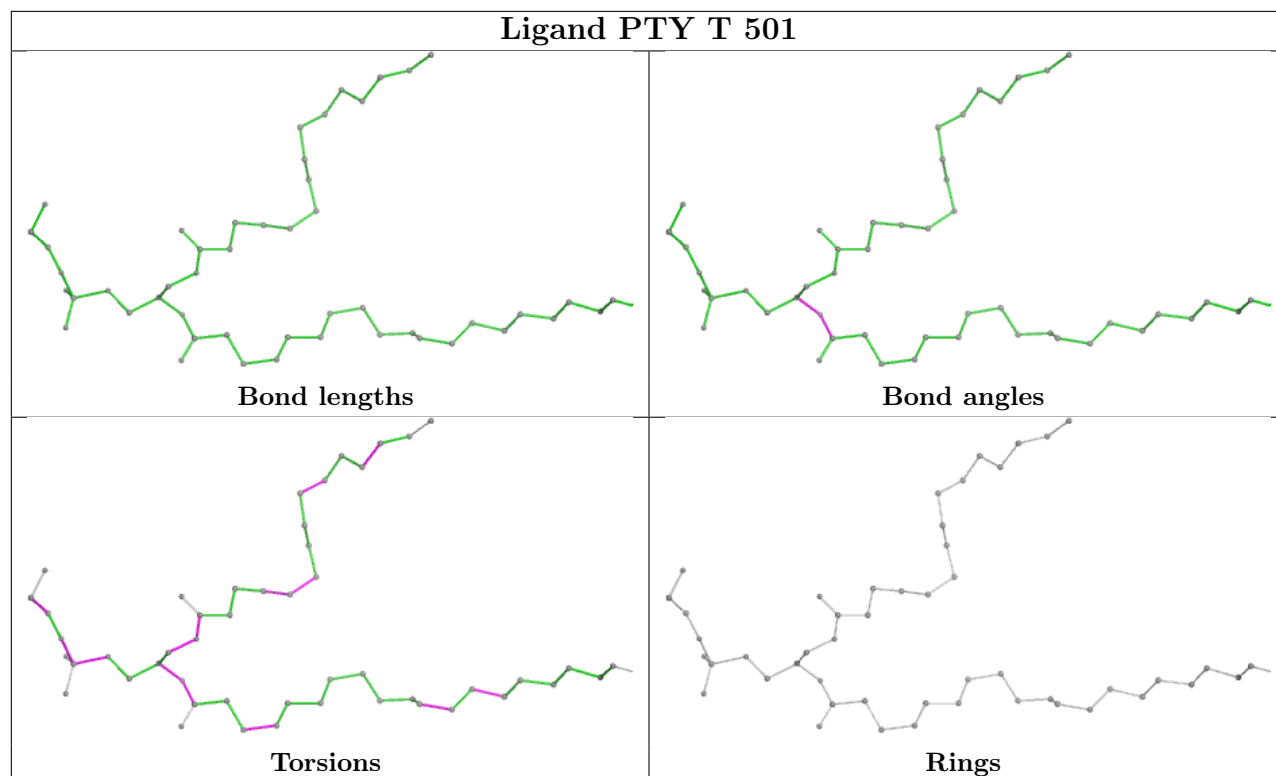


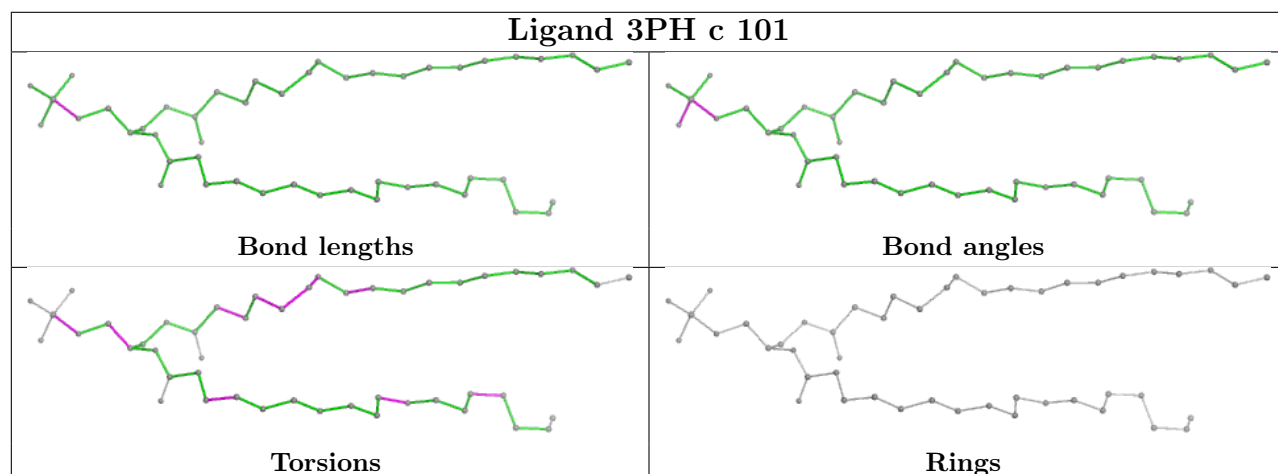
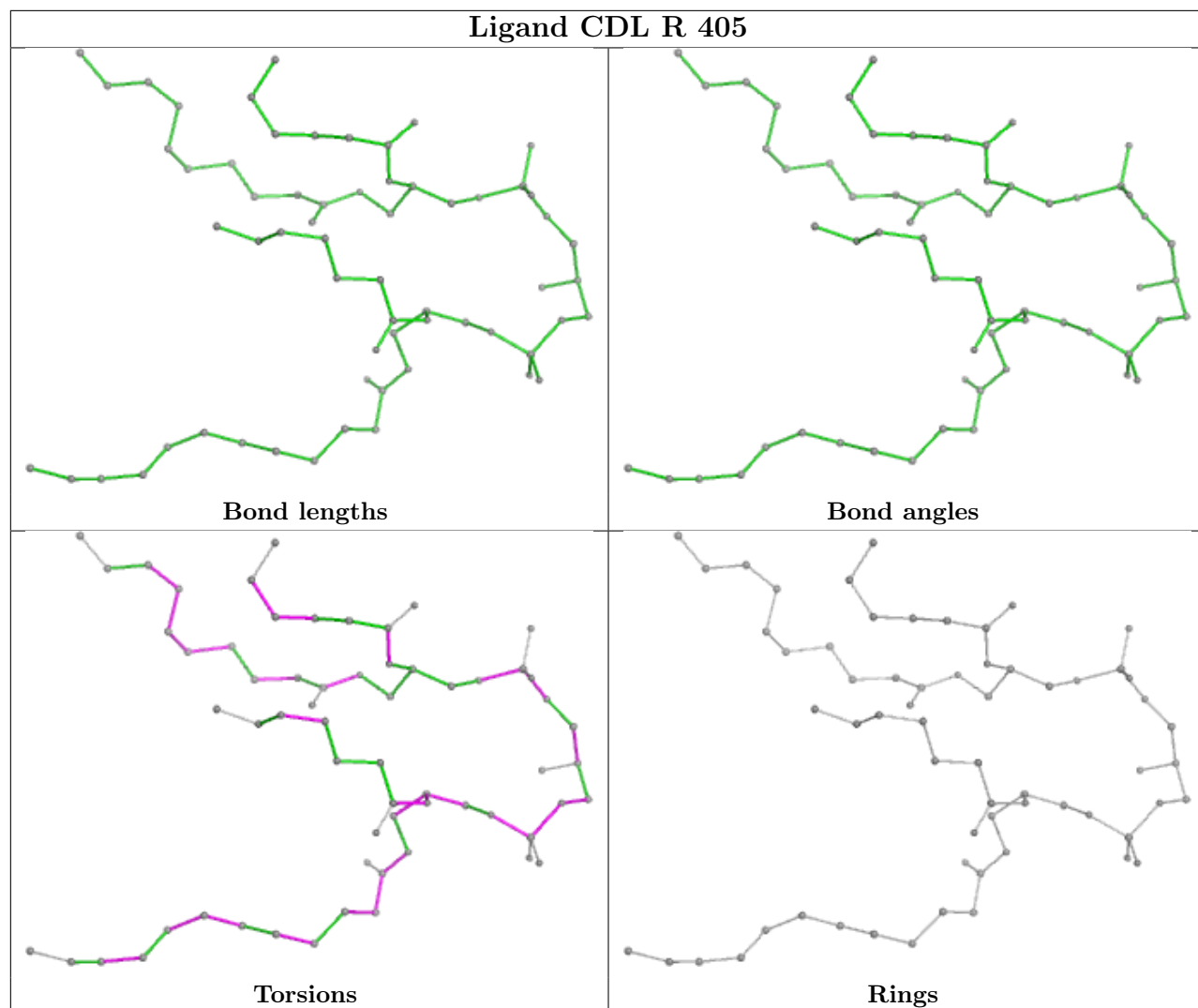


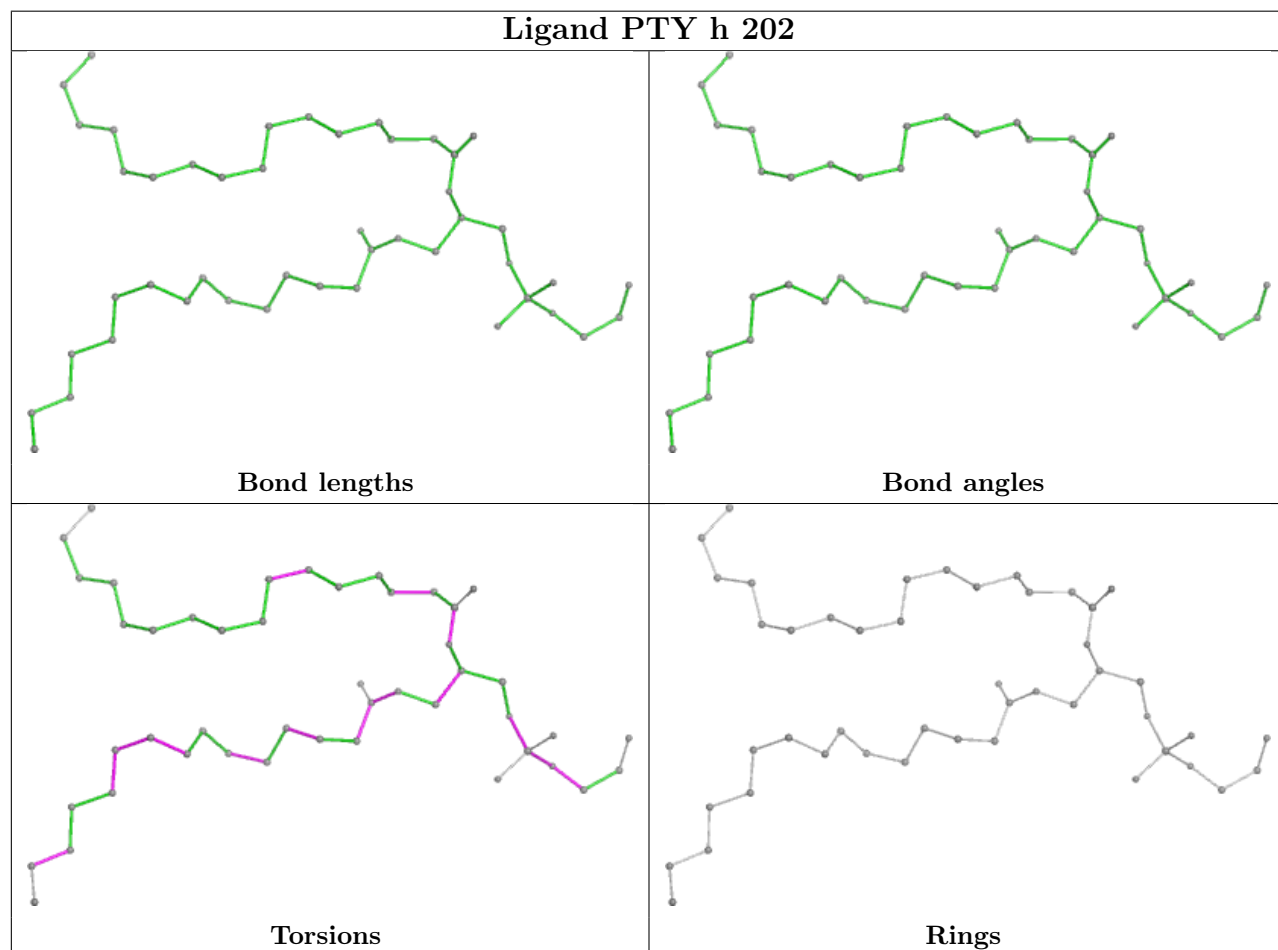
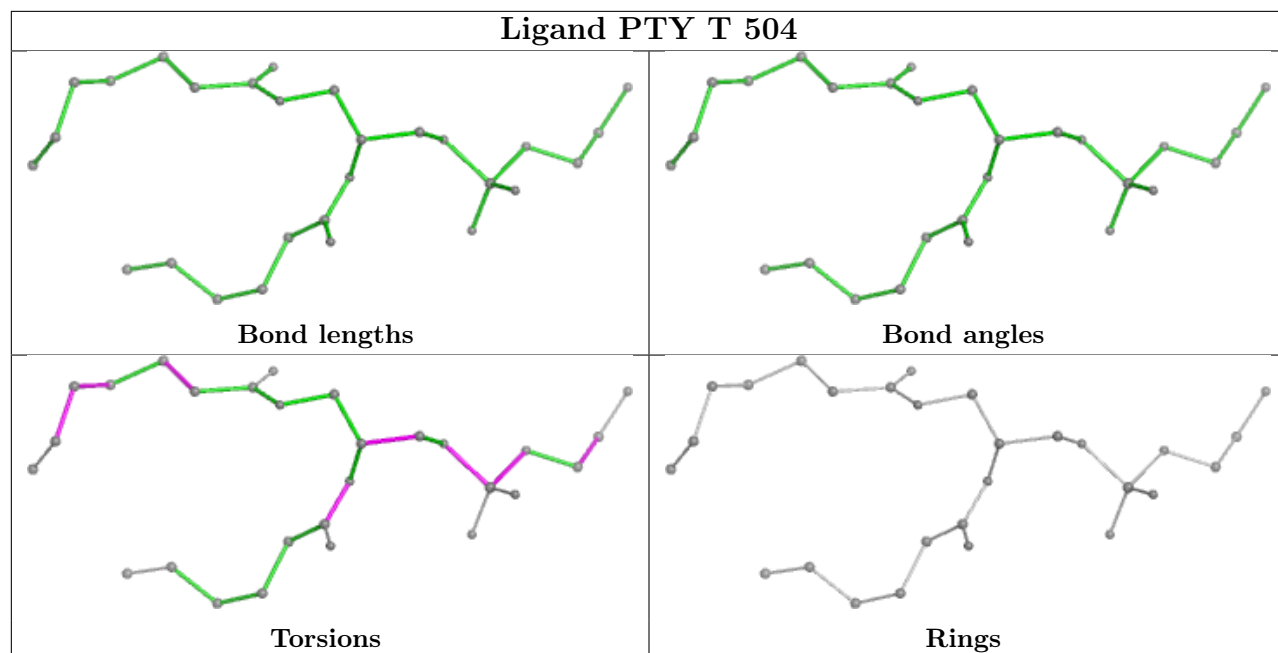


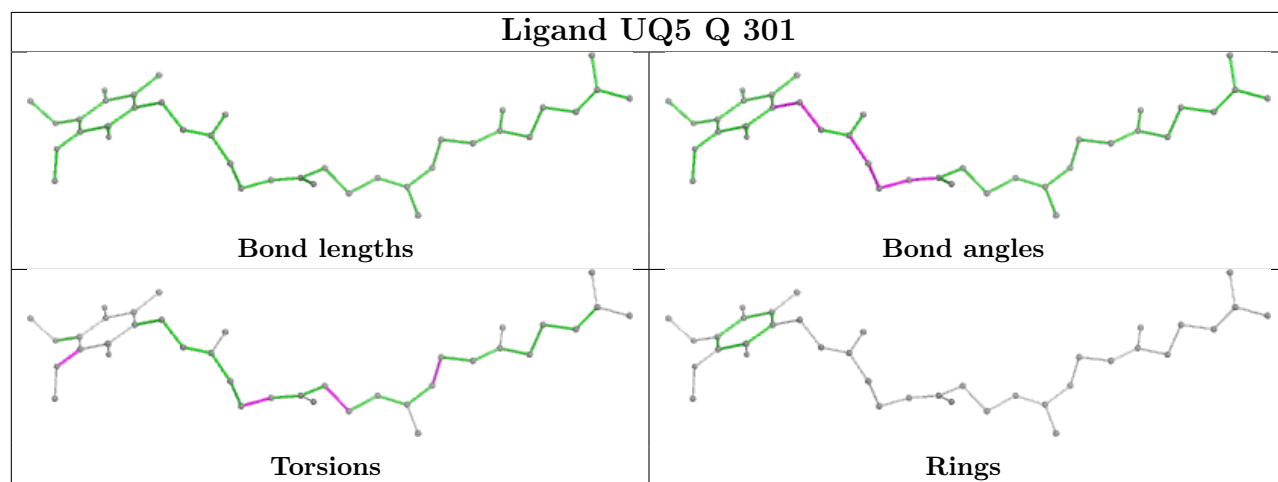
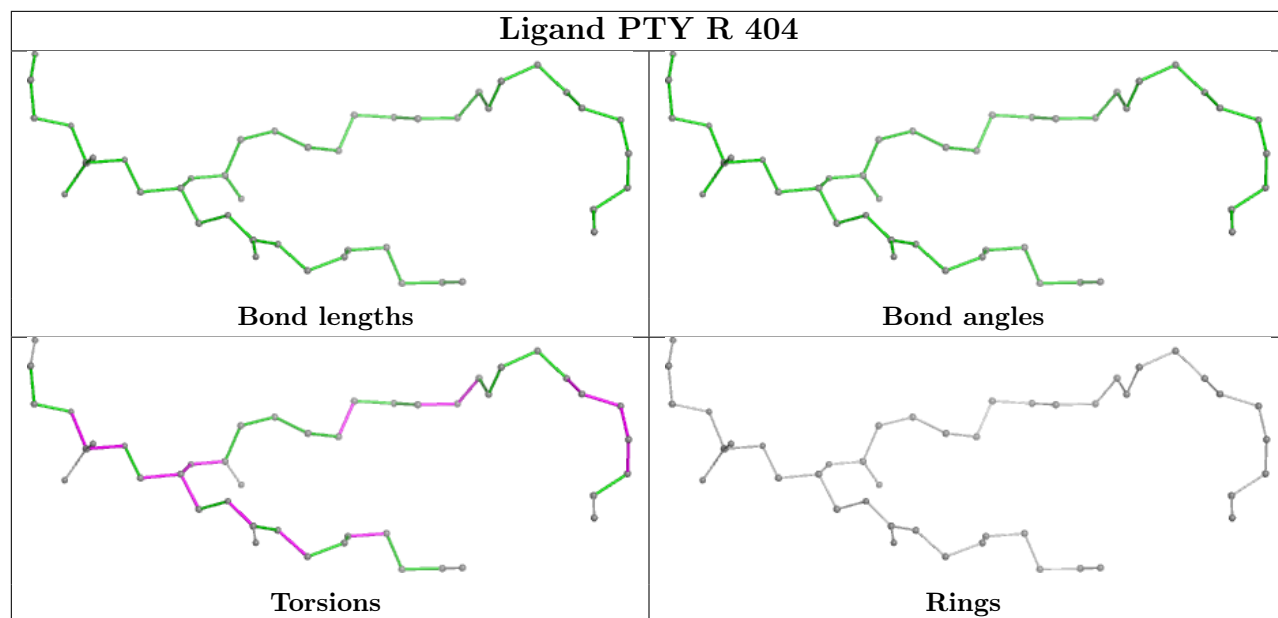


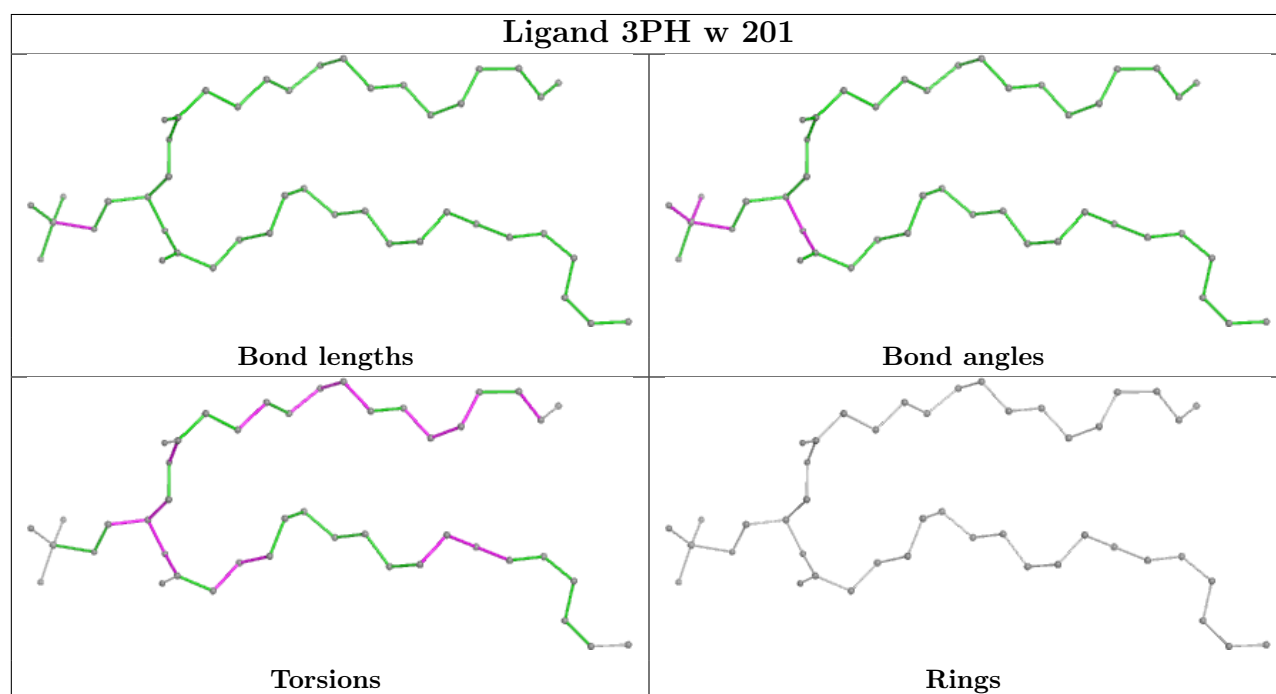
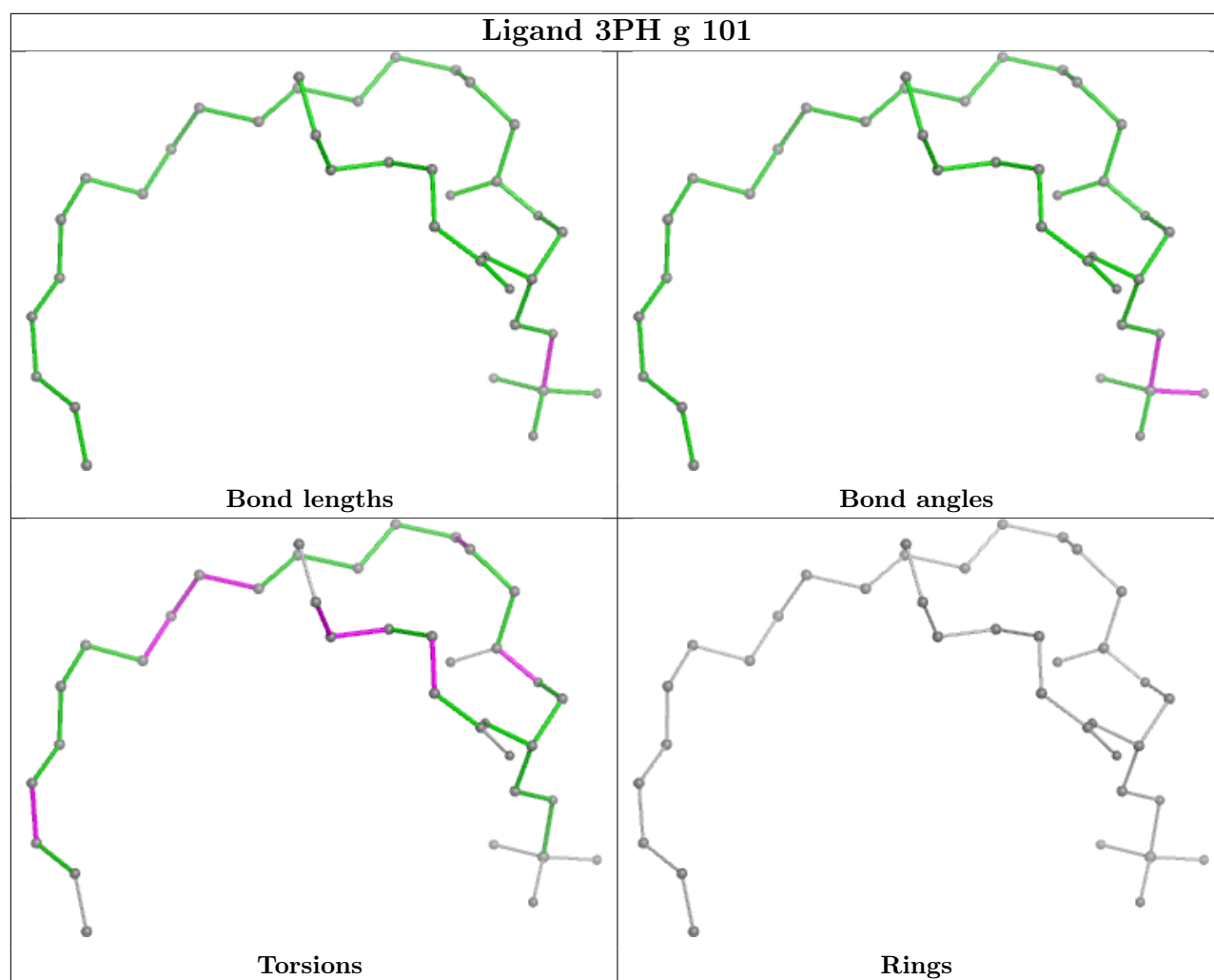


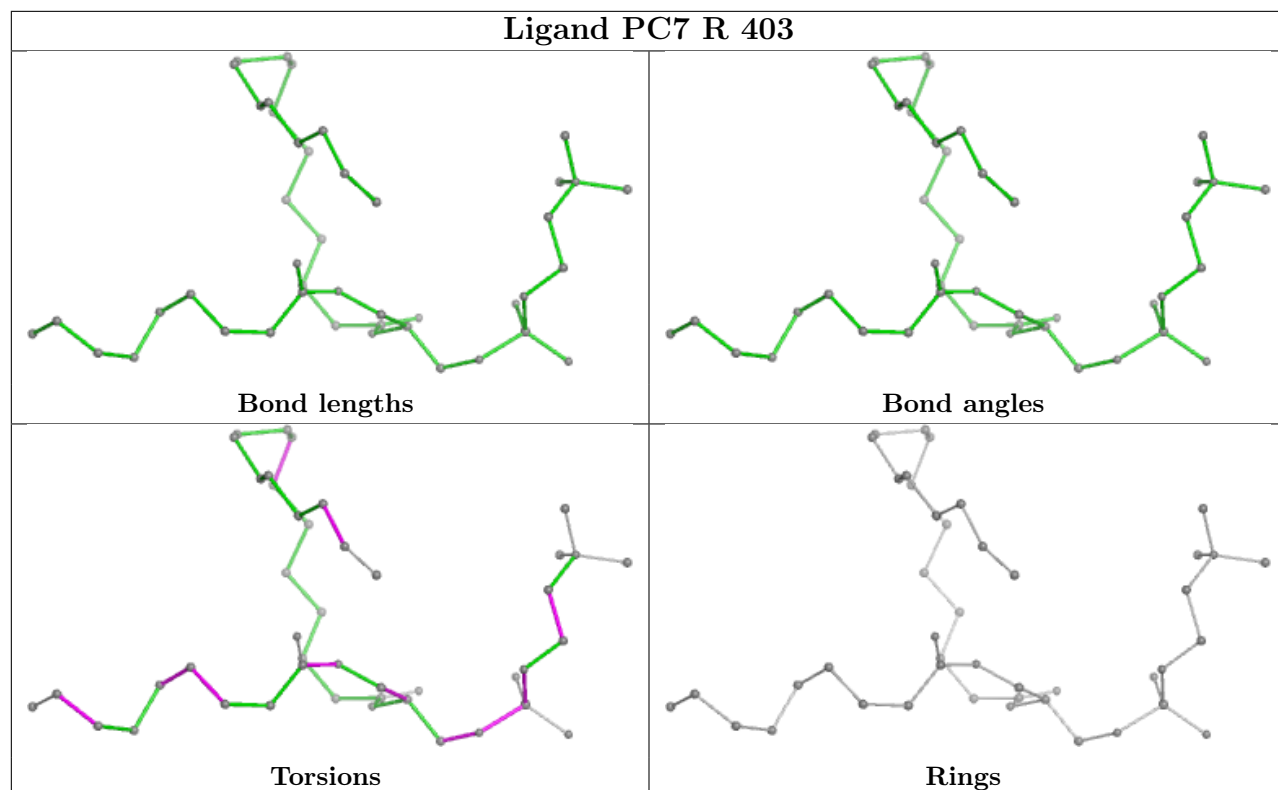
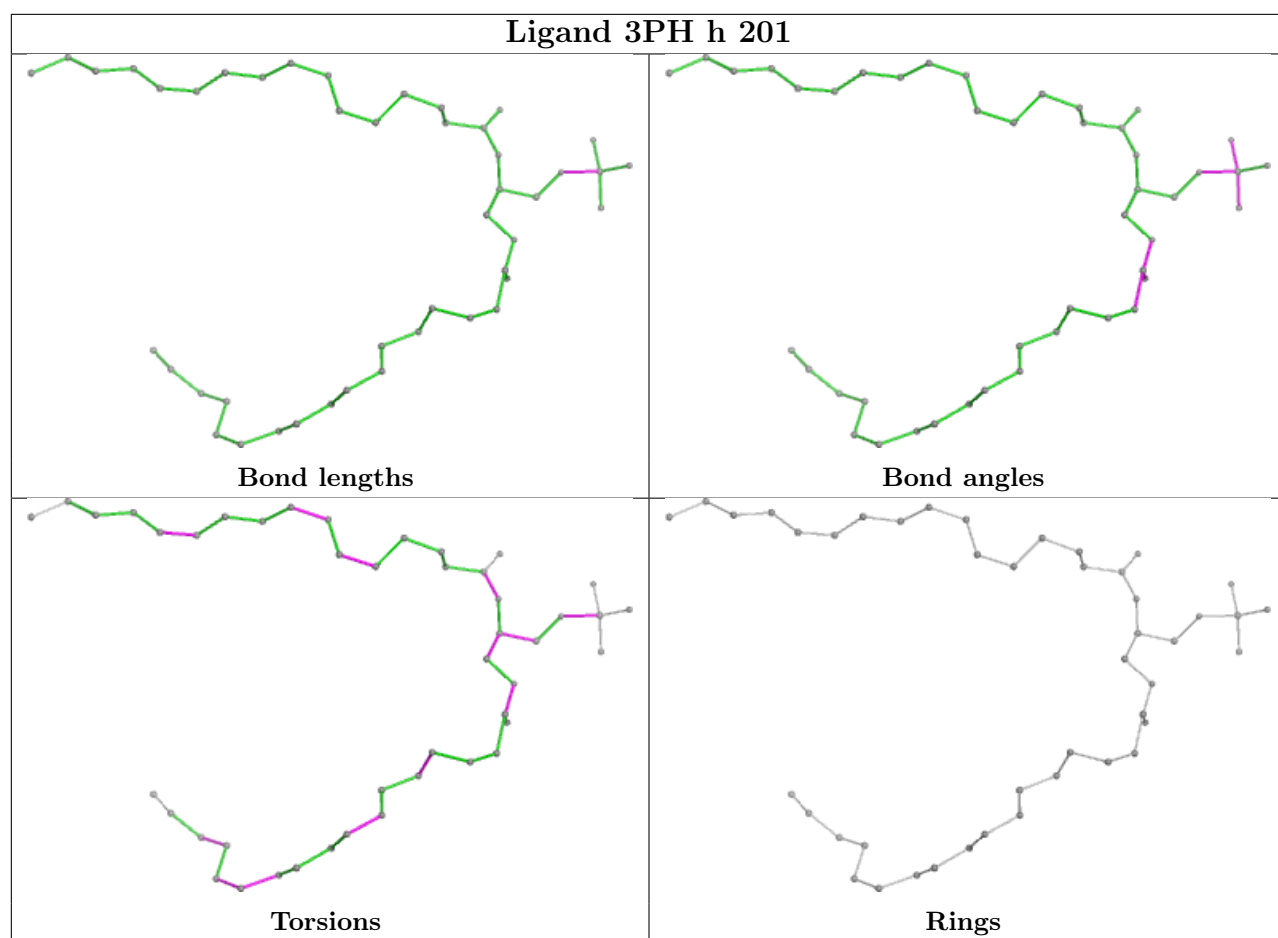


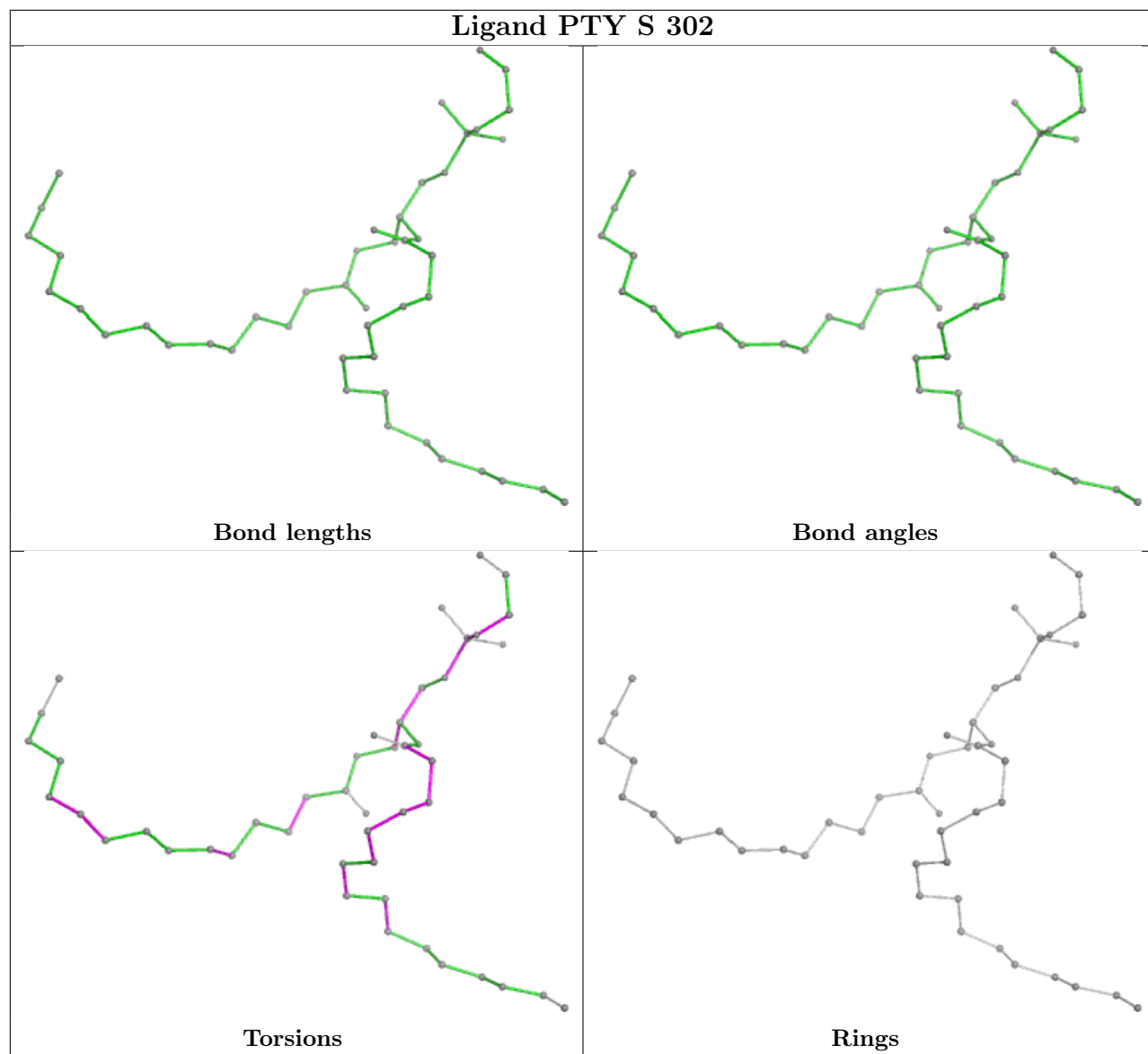




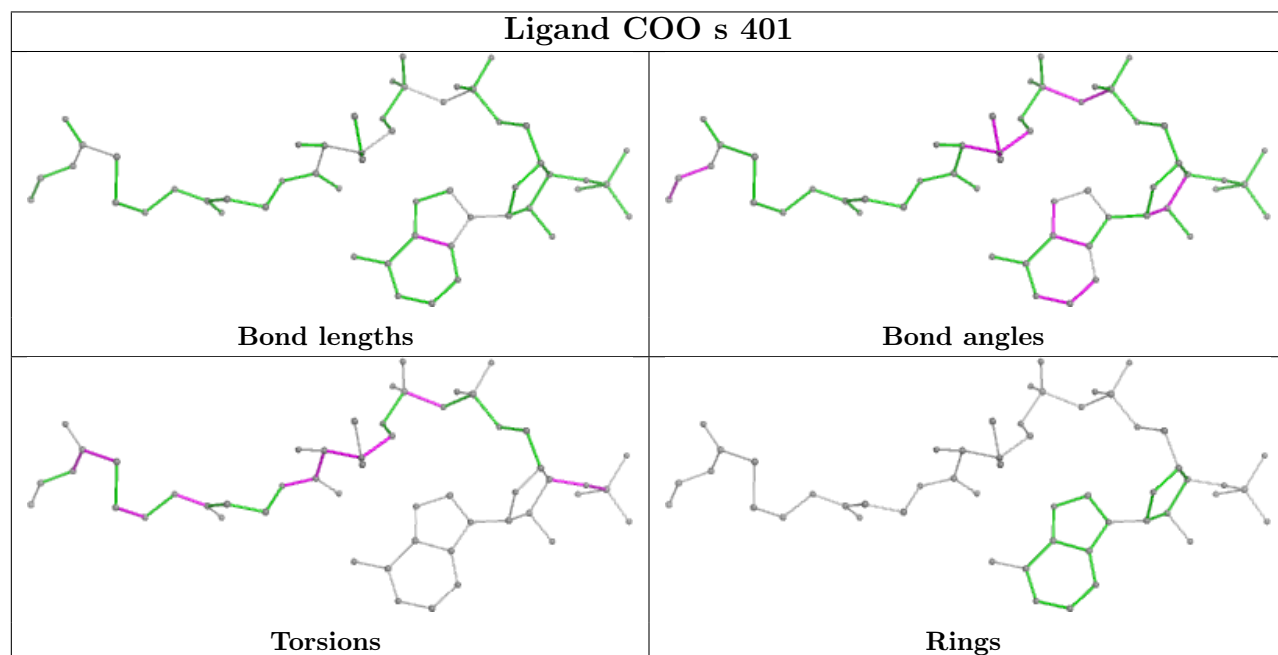
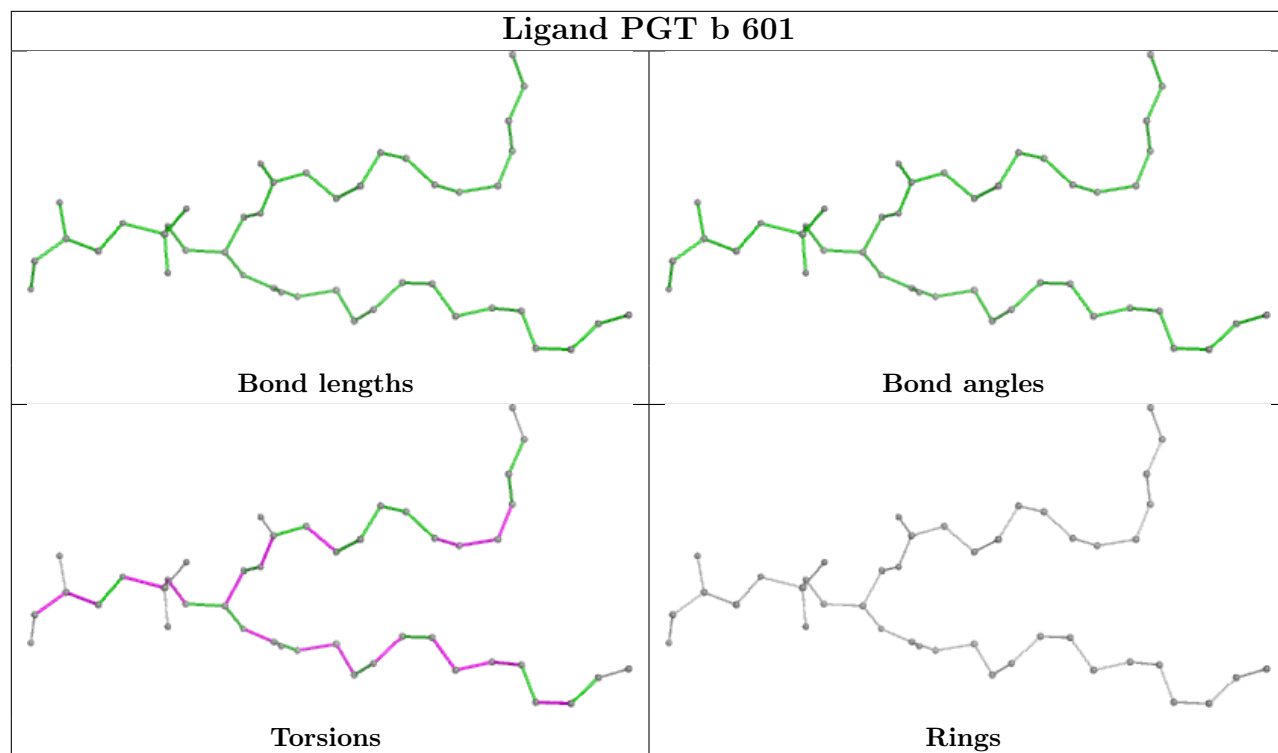


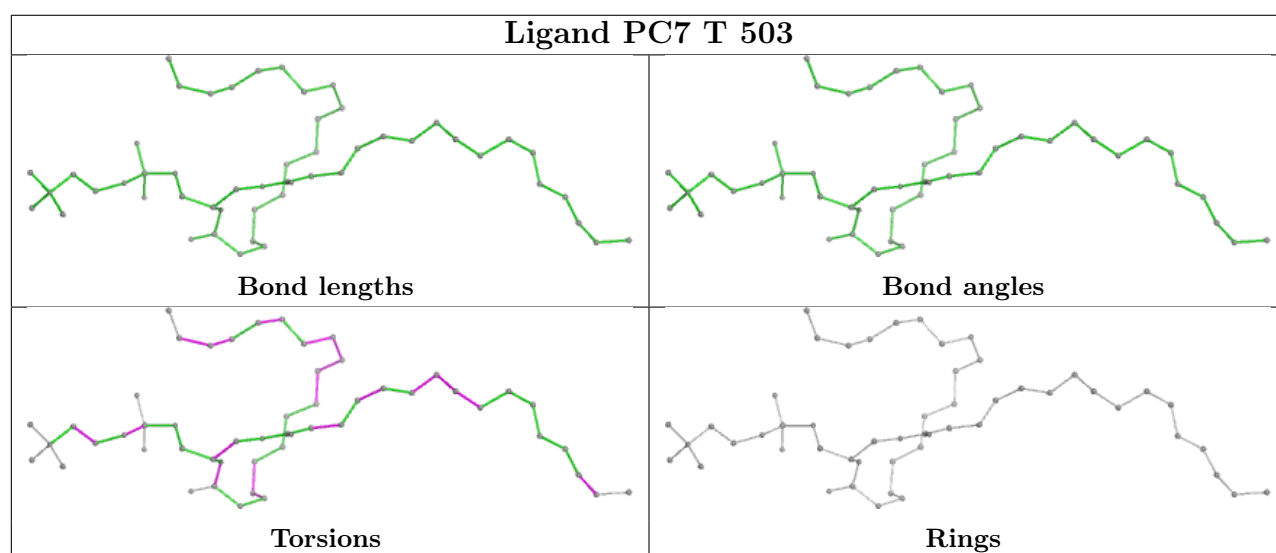
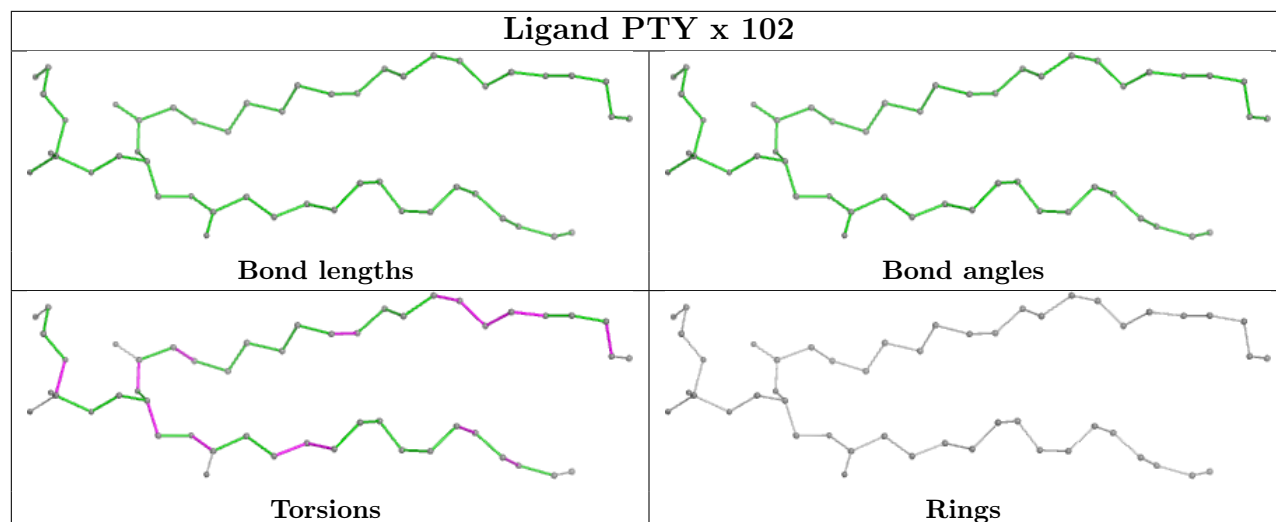


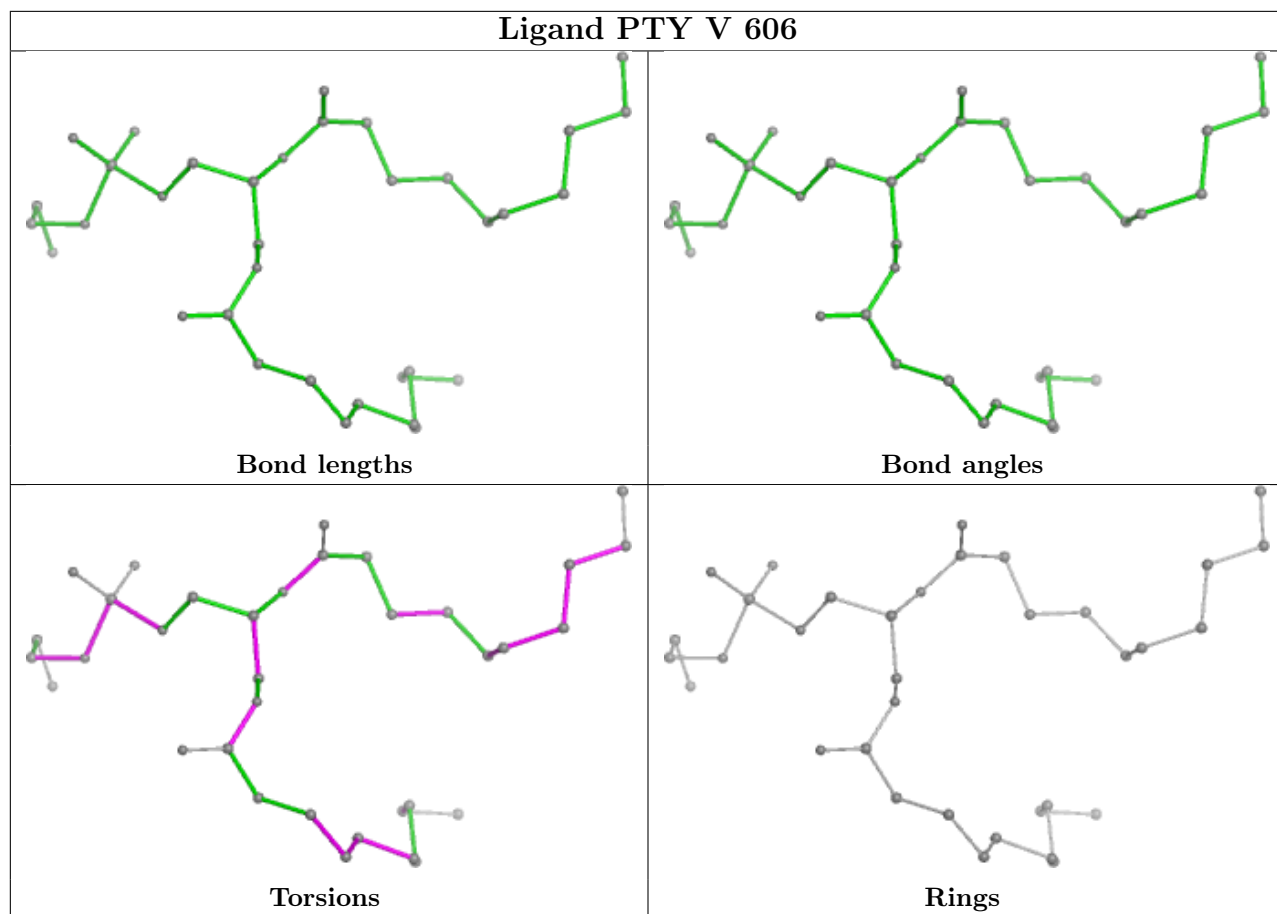


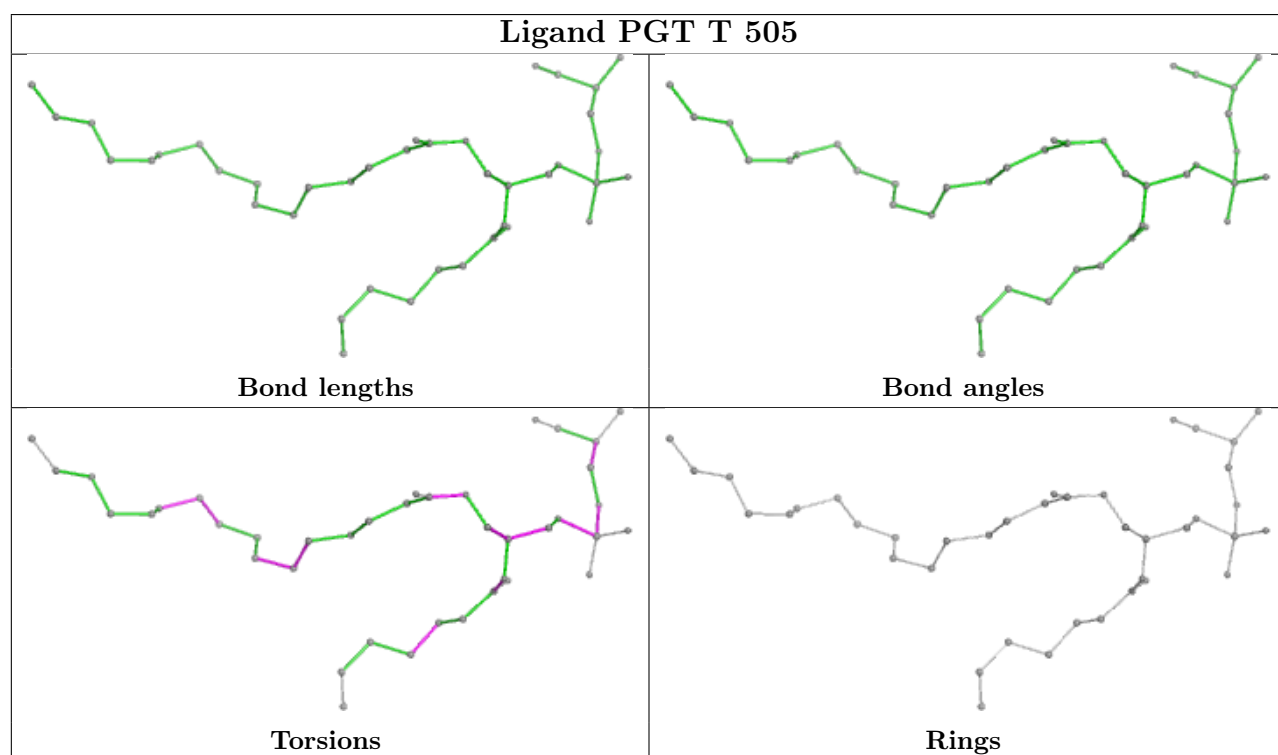
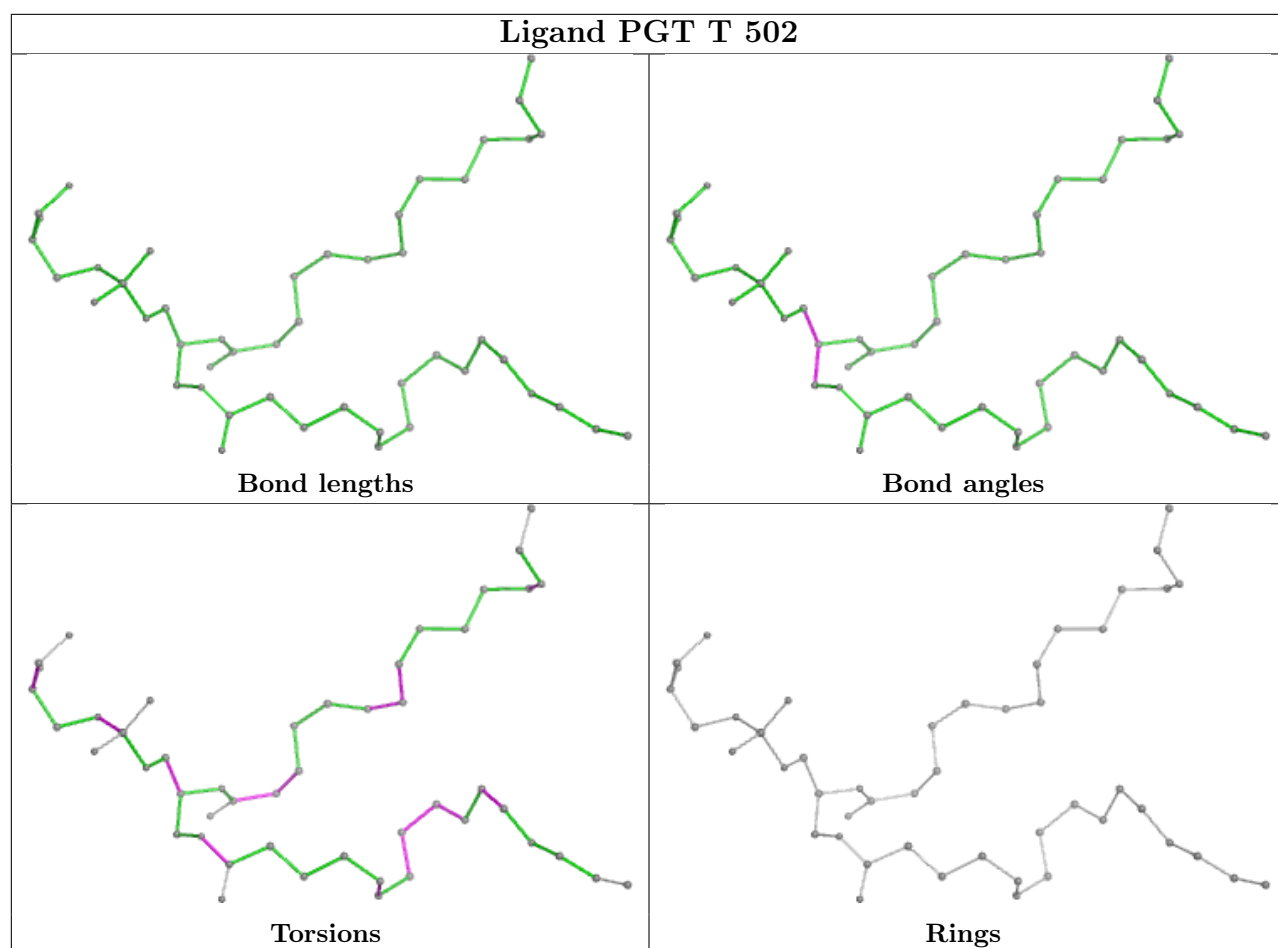


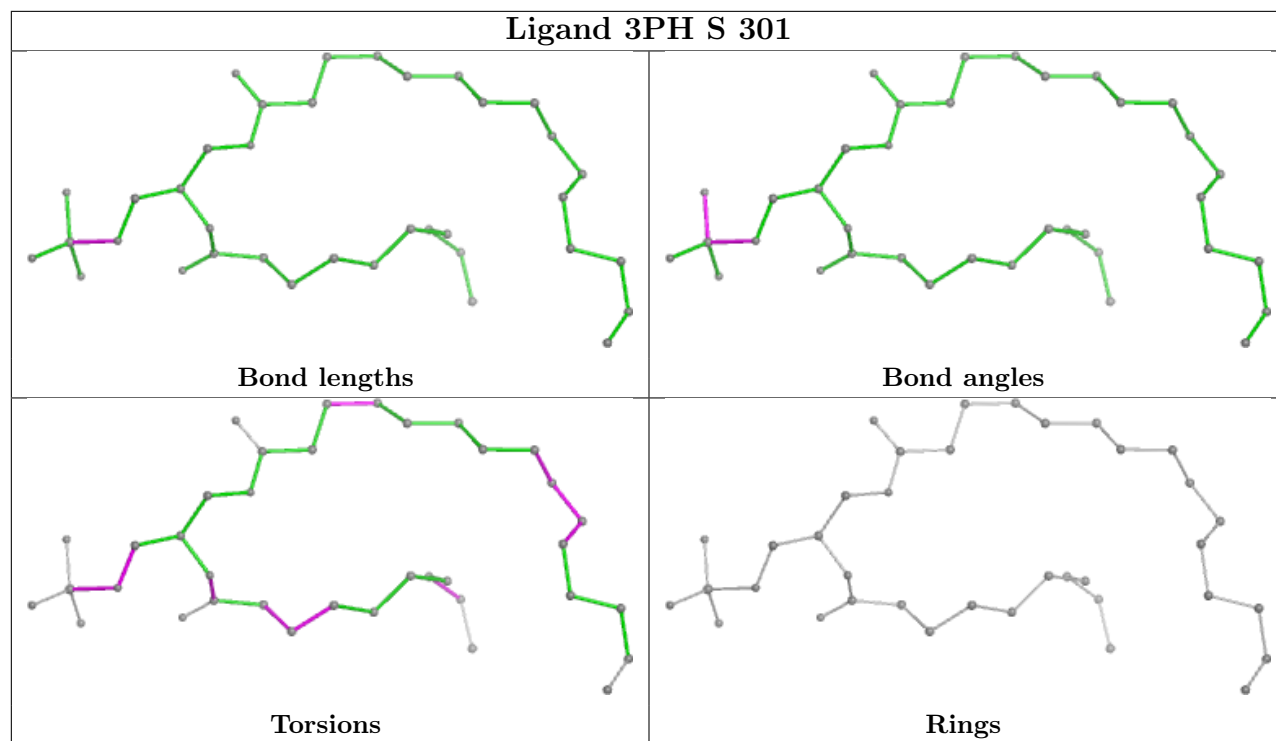


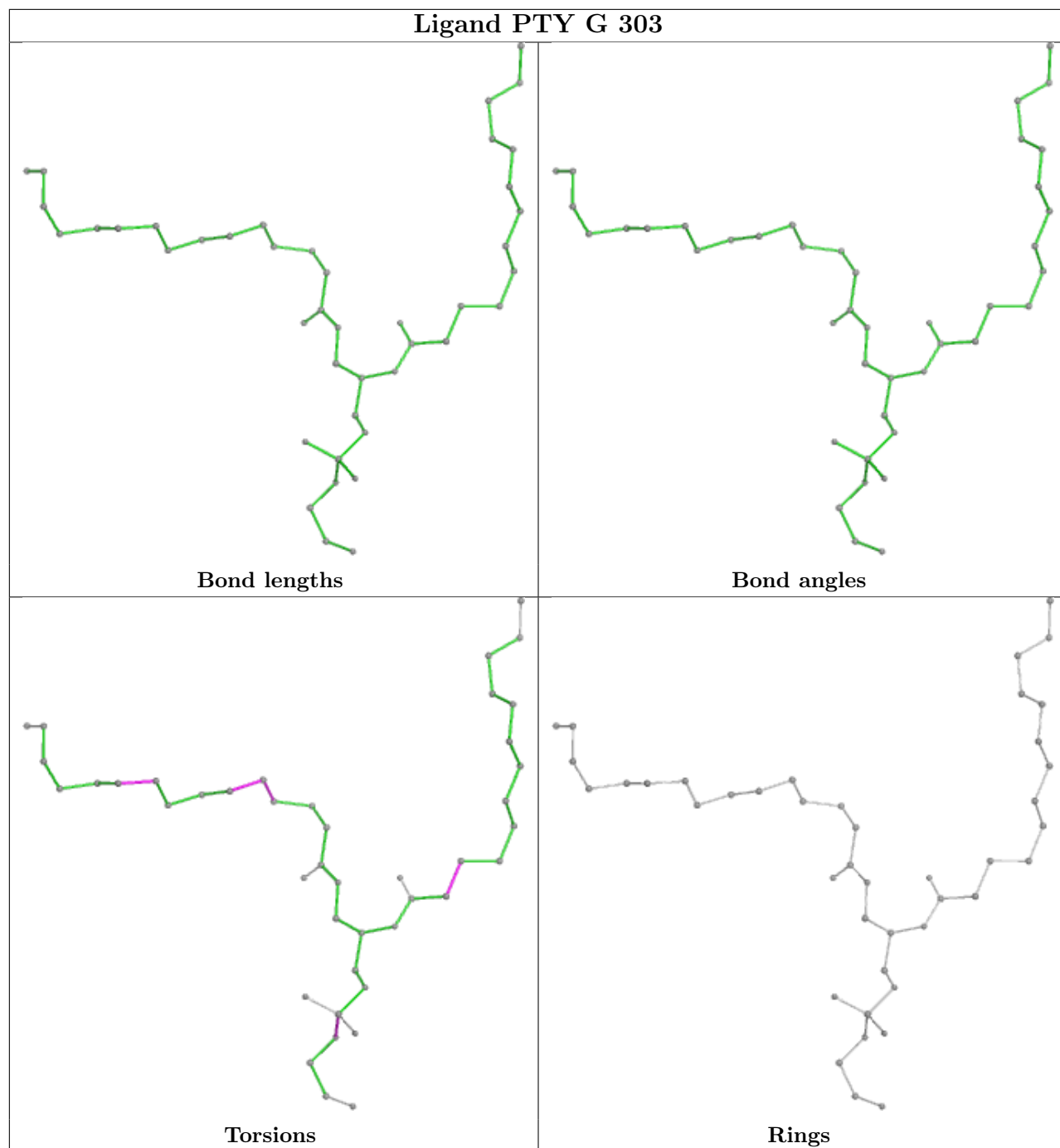


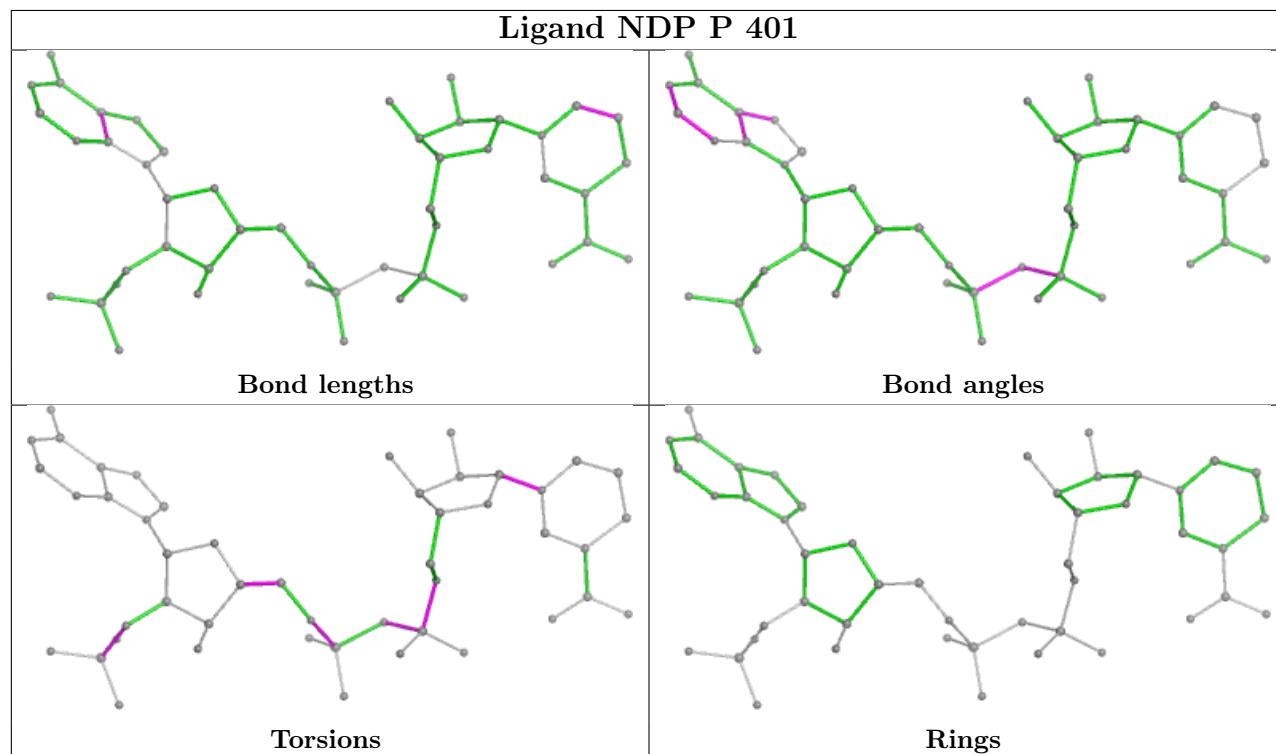
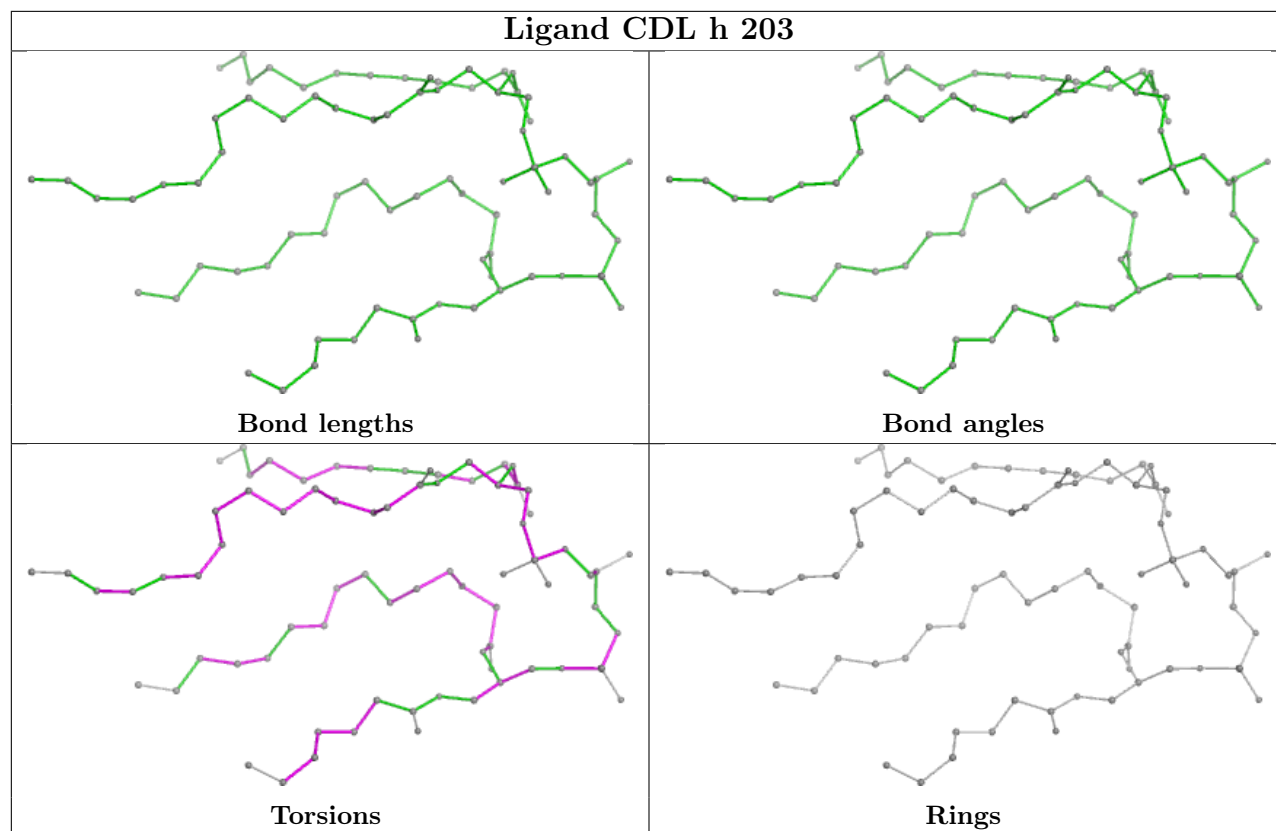


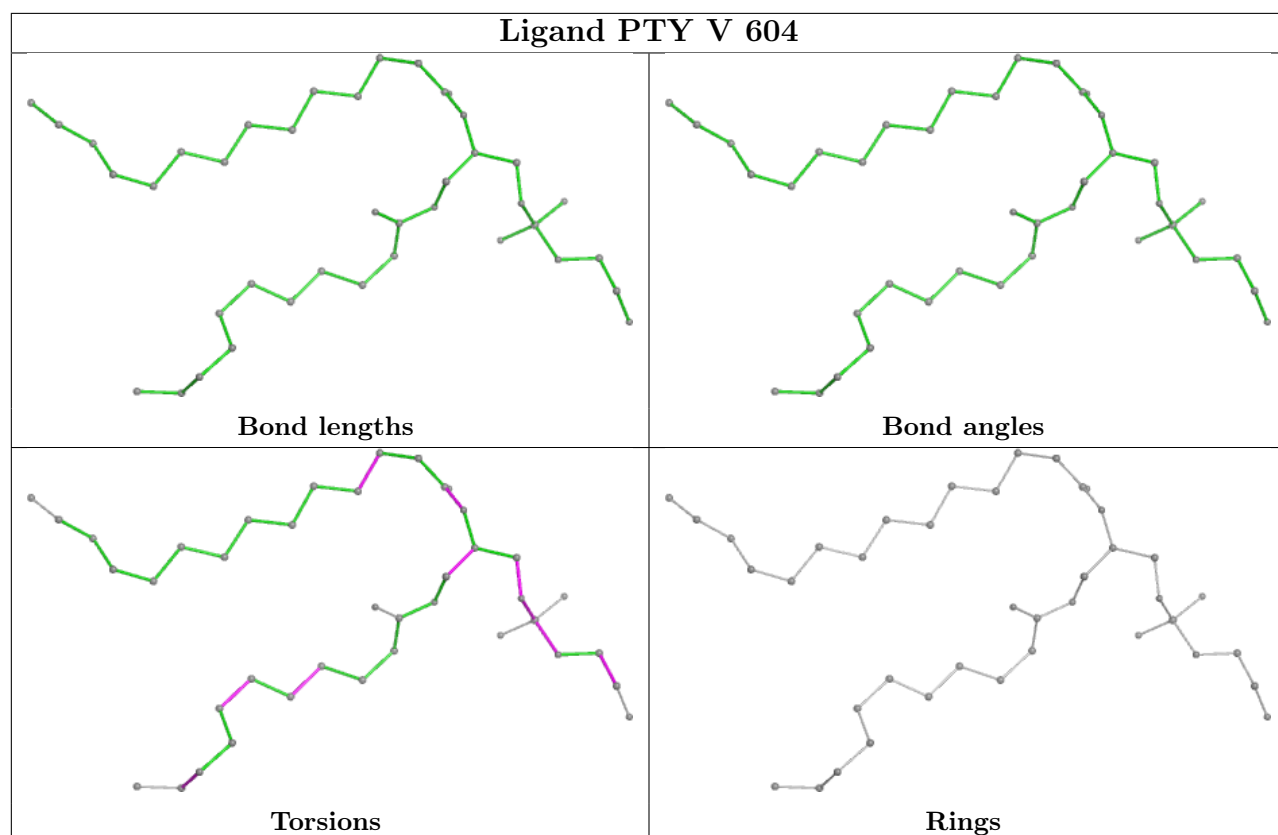
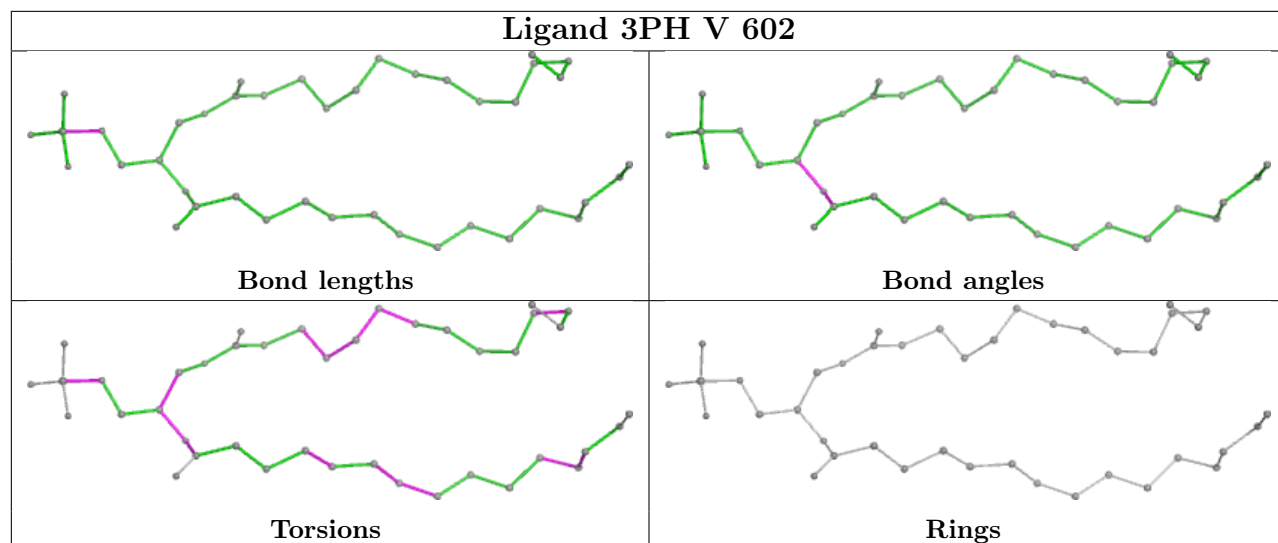




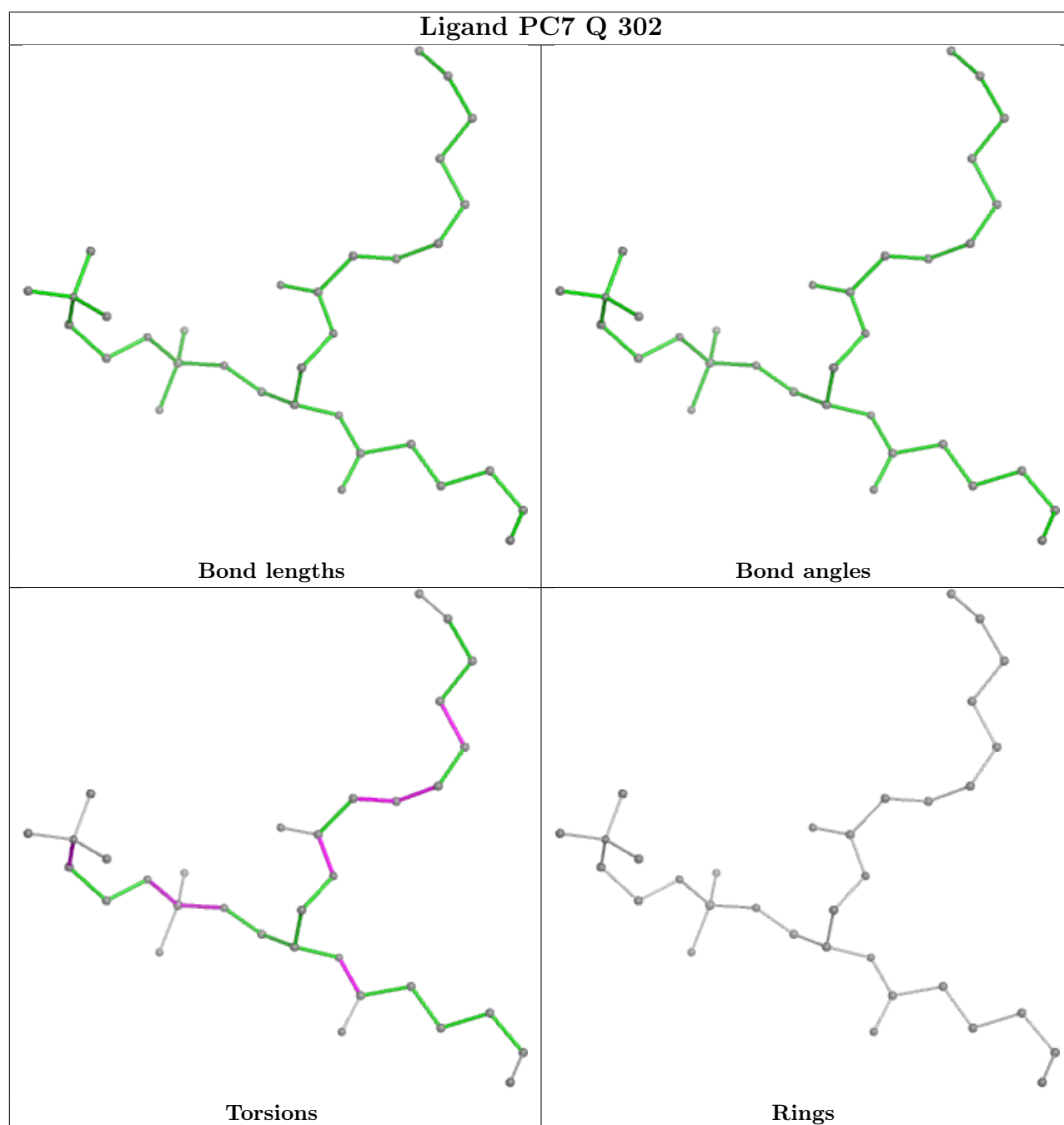












## 5.7 Other polymers [i](#)

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.