



Full wwPDB EM Validation Report ⓘ

Jan 26, 2023 – 05:33 am GMT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

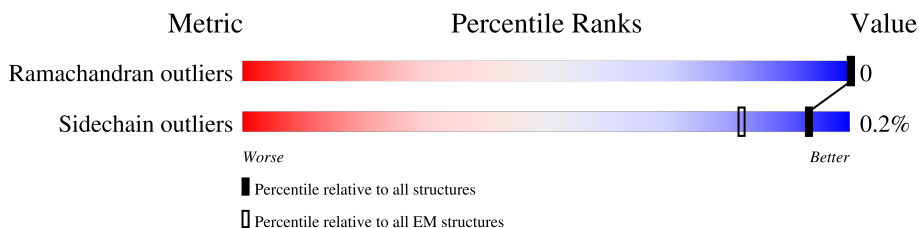
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.09 Å.

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




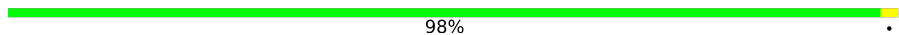
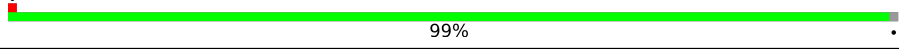
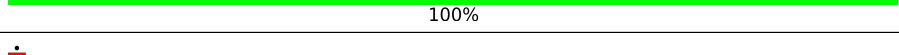
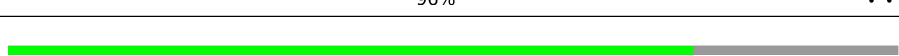



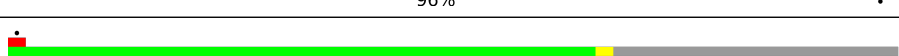

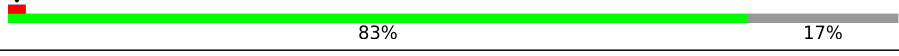

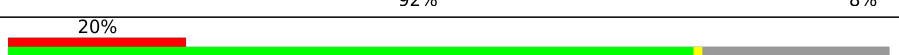

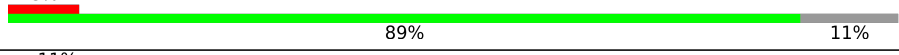


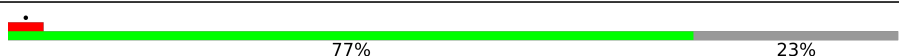
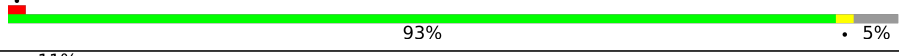

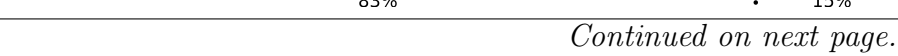


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	119	77% 21%
2	B	218	71% 28%
3	C	190	94% 5%
4	D	394	98%
5	E	255	6% 75% 25%
6	F	486	89% 11%
7	G	748	91% 8%
8	H	325	100%
9	I	222	74% 26%

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Mol	Chain	Length	Quality of chain
10	J	205	 84% 15%
11	K	100	 98%
12	L	669	 99%
13	M	495	 100%
14	N	499	 96%
15	O	159	 77% 23%
16	P	402	 79% 21%
17	Q	154	 68% 32%
18	R	110	 66% 34%
19	S	97	 96%
20	T	122	 66% 32%
21	U	126	 69% 31%
22	V	169	 83% 17%
23	W	133	 83% 16%
24	X	106	 92% 8%
25	Y	159	 77% 21%
26	Z	143	 87% 13%
27	a	65	 89% 11%
28	b	65	 66% 34%
29	c	88	 86% 14%
30	d	81	 91% 7%
31	e	83	 77% 23%
32	f	106	 93% 5%
33	g	114	68% 31%
34	i	98	83% 15%

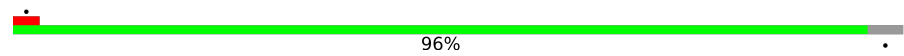
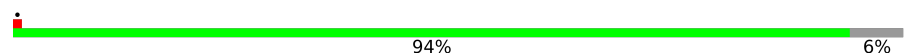
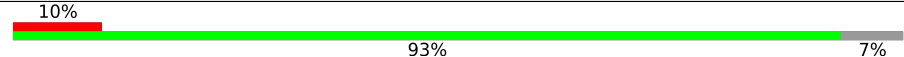
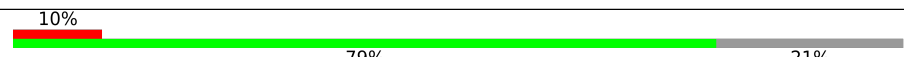
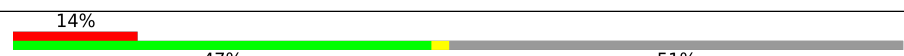
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Mol	Chain	Length	Quality of chain
35	j	69	74% 26%
36	k	72	65% 33%
37	l	125	58% 41%
38	m	71	99%
39	n	117	91% 7%
40	o	103	9% 77% 22%
41	p	106	84% 15%
42	q	159	50% 50%
43	u	63	25% 87% 13%
44	v	113	26% 74%
45	x	256	82% 18%
46	y	278	95% 5%
47	z	275	84% 15%
48	AA	503	17% 89% 11%
48	BA	503	17% 89% 10%
49	AB	531	92% 8%
49	BB	531	91% 8%
50	AC	393	97%
50	BC	393	97%
51	AD	272	31% 72% 28%
51	BD	272	27% 71% 28%
52	AE	307	79% 21%
52	BE	307	79% 21%
53	AF	122	95% 5%
53	BF	122	95% 5%

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Mol	Chain	Length	Quality of chain
54	AG	72	 96%
54	BG	72	 94%
55	AH	69	 93%
55	BH	69	 90%
56	AI	72	 76%
56	BI	72	 79%
57	AJ	57	 47%
57	BJ	57	 49%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
73	COO	y	302	X	-	-	-

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 29 is a protein called Transmembrane protein.

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

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

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

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

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

- Molecule 32 is a protein called At4g16450.

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

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

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

- Molecule 34 is a protein called At1g67350.

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

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

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

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

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

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

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

- Molecule 38 is a protein called AT2G31490 protein.

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

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

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

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

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

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

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

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

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

- Molecule 43 is a protein called Uncharacterized protein At1g67785.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 50 is a protein called Cytochrome b.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

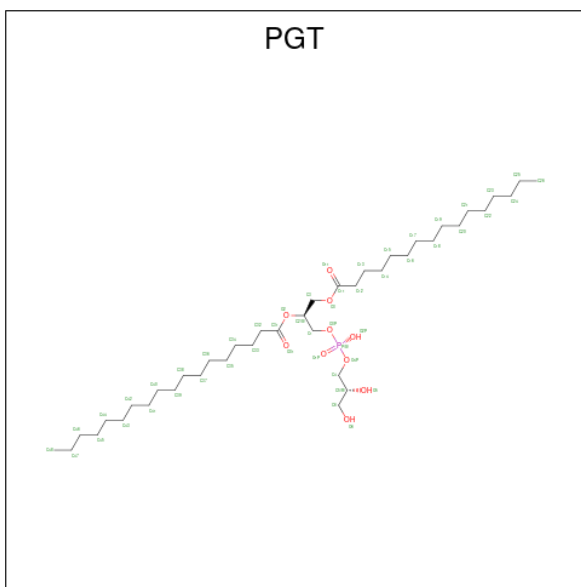
Mol	Chain	Residues	Atoms				AltConf	Trace
57	AJ	28	Total	C	N	O	0	0
			203	137	33	33		

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

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



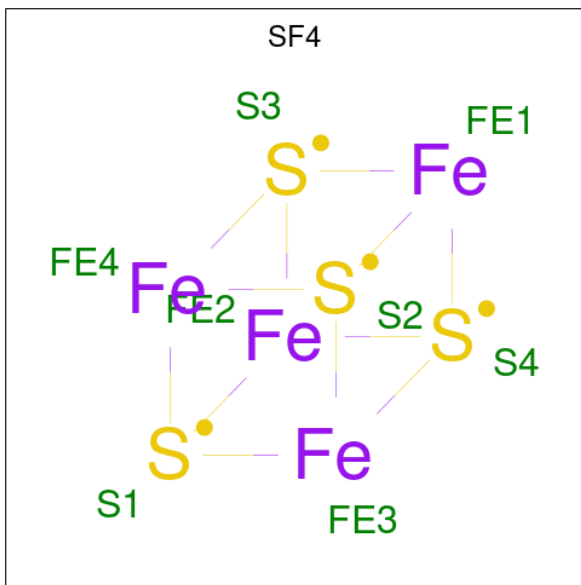
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
58	A	1	51	40	10	1	0
58	L	1	132	99	30	3	0
58	L	1	132	99	30	3	0
58	L	1	132	99	30	3	0
58	M	1	29	18	10	1	0
58	y	1	41	30	10	1	0
58	AC	1	92	70	20	2	0
58	AC	1	92	70	20	2	0
58	AF	1	51	40	10	1	0

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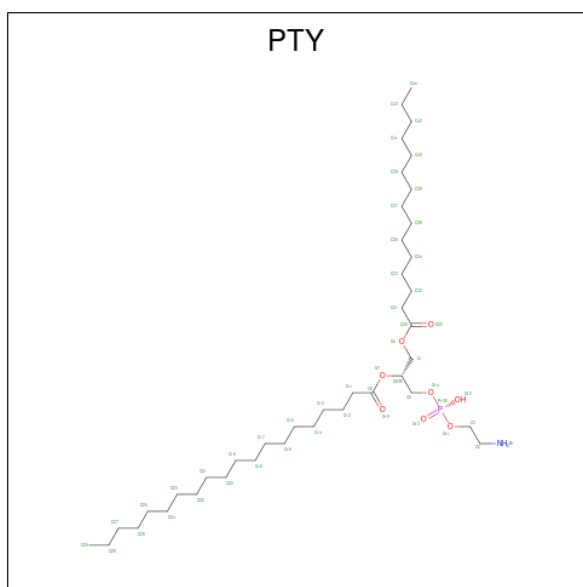
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
58	BC	1	37	26	10	1	0

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



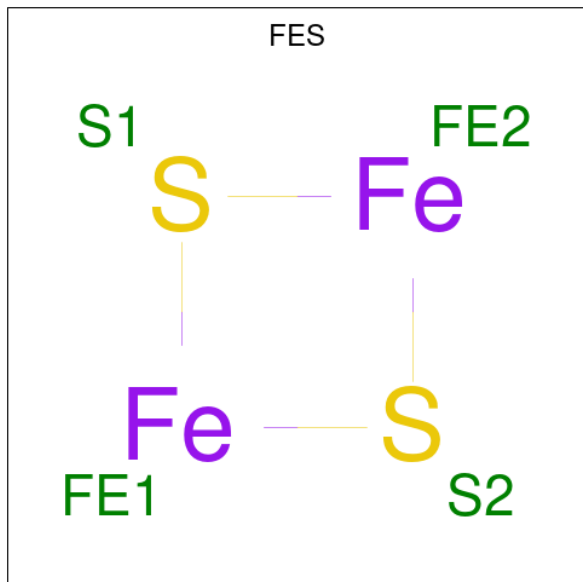
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	B	1	8	4	4	0
59	F	1	8	4	4	0
59	G	1	16	8	8	0
59	G	1	16	8	8	0
59	I	1	16	8	8	0
59	I	1	16	8	8	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	D	1	Total 50	40	1	8	1	0
60	L	1	Total 42	32	1	8	1	0
60	M	1	Total 87	67	2	16	2	0
60	M	1	Total 87	67	2	16	2	0
60	N	1	Total 135	105	3	24	3	0
60	N	1	Total 135	105	3	24	3	0
60	N	1	Total 135	105	3	24	3	0
60	Y	1	Total 31	21	1	8	1	0
60	d	1	Total 39	29	1	8	1	0
60	m	1	Total 50	40	1	8	1	0
60	z	1	Total 50	40	1	8	1	0
60	AB	1	Total 41	31	1	8	1	0
60	BB	1	Total 29	19	1	8	1	0
60	BF	1	Total 40	30	1	8	1	0

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



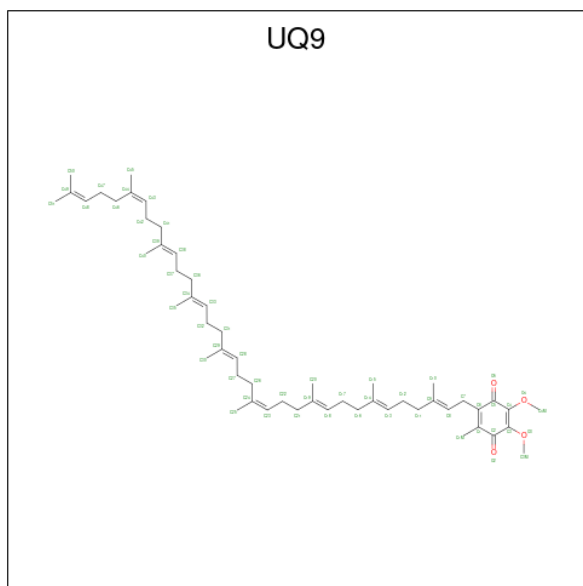
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
61	E	1	4	2	2	0
61	G	1	4	2	2	0
61	AD	1	4	2	2	0
61	BD	1	4	2	2	0

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



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

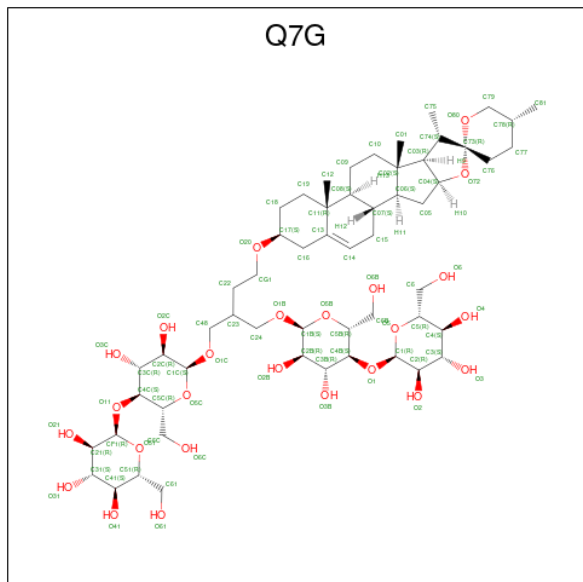
- Molecule 63 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



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

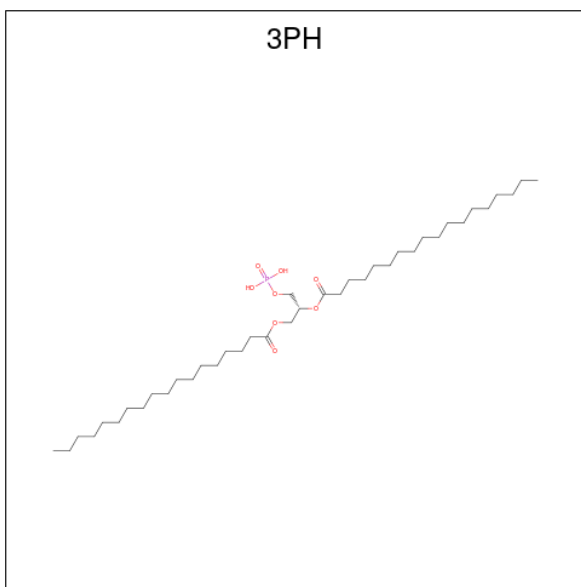
- Molecule 64 is 2-[[[4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl]oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-al

pha-D-glucopyranoside (three-letter code: Q7G) (formula: $C_{56}H_{92}O_{25}$) (labeled as "Ligand of Interest" by depositor).



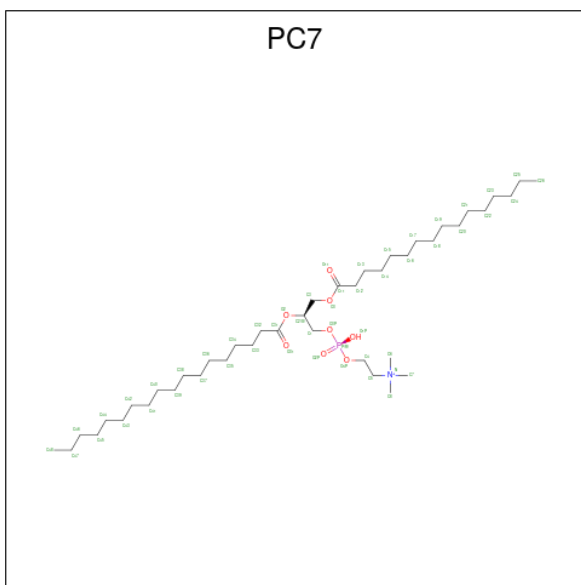
Mol	Chain	Residues	Atoms			AltConf
64	H	1	Total	C	O	0
			81	56	25	
64	K	1	Total	C	O	0
			81	56	25	
64	M	1	Total	C	O	0
			39	34	5	
64	a	1	Total	C	O	0
			39	34	5	
64	BC	1	Total	C	O	0
			78	68	10	
64	BC	1	Total	C	O	0
			78	68	10	

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



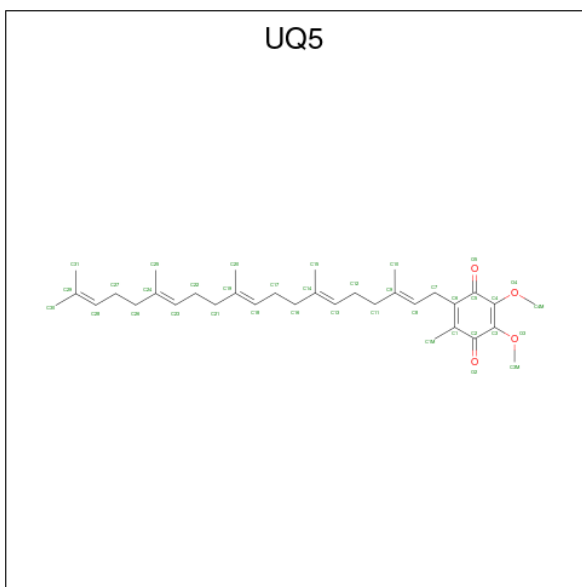
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
65	L	1	37	28	8	1	0
65	M	1	41	32	8	1	0
65	Y	1	33	24	8	1	0
65	f	1	84	66	16	2	0
65	f	1	84	66	16	2	0
65	l	1	37	28	8	1	0
65	AC	1	33	24	8	1	0
65	AI	1	32	23	8	1	0
65	BC	1	44	35	8	1	0
65	BJ	1	89	71	16	2	0
65	BJ	1	89	71	16	2	0

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



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

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

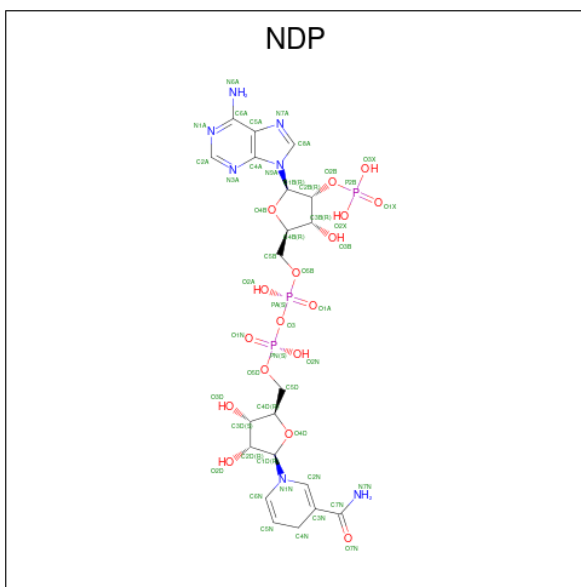


Mol	Chain	Residues	Atoms			AltConf
67	L	1	Total	C	O	0
			38	34	4	
67	AC	1	Total	C	O	0
			76	68	8	
67	AC	1	Total	C	O	0
			76	68	8	
67	BC	1	Total	C	O	0
			38	34	4	

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

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

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

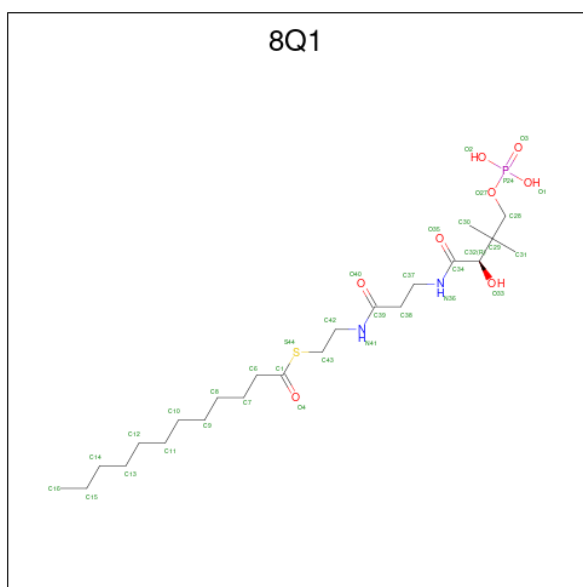


Mol	Chain	Residues	Atoms					AltConf
69	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

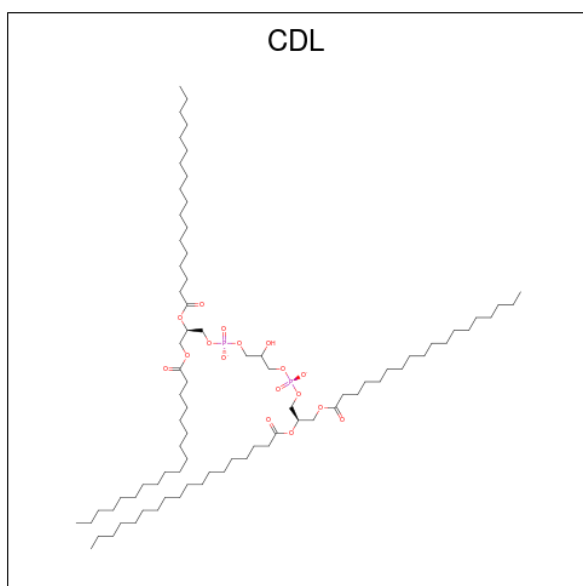
Mol	Chain	Residues	Atoms		AltConf
70	R	1	Total	Zn	0
			1	1	
70	y	1	Total	Zn	0
			1	1	
70	AB	1	Total	Zn	0
			1	1	
70	BB	1	Total	Zn	0
			1	1	

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



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

- Molecule 72 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



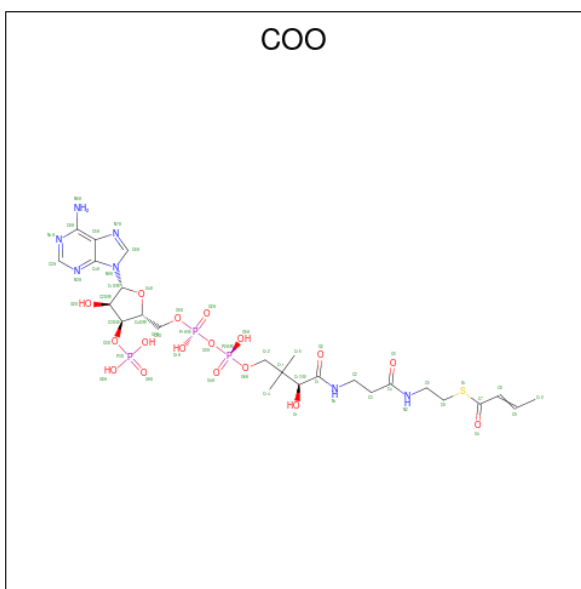
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
72	u	1	Total	C	O	P	0
			200	162	34	4	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
72	u	1	Total 200	C 162	O 34	P 4	0
72	AC	1	Total 166	C 128	O 34	P 4	0
72	AC	1	Total 166	C 128	O 34	P 4	0
72	AE	1	Total 85	C 66	O 17	P 2	0
72	BC	1	Total 158	C 120	O 34	P 4	0
72	BC	1	Total 158	C 120	O 34	P 4	0
72	BE	1	Total 88	C 69	O 17	P 2	0
72	BG	1	Total 70	C 51	O 17	P 2	0

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



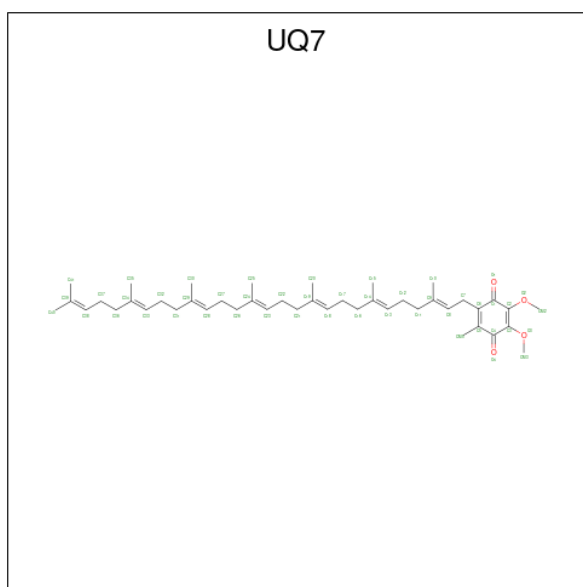
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
73	y	1	Total 53	C 25	N 7	O 17	P 3	S 1	0

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
74	AC	1	Total 86	C 68	Fe 2	N 8	O 8	0
74	AC	1	Total 86	C 68	Fe 2	N 8	O 8	0
74	AE	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	BC	1	Total 86	C 68	Fe 2	N 8	O 8	0
74	BC	1	Total 86	C 68	Fe 2	N 8	O 8	0
74	BE	1	Total 43	C 34	Fe 1	N 4	O 4	0

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



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

- Molecule 76 is water.

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

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

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

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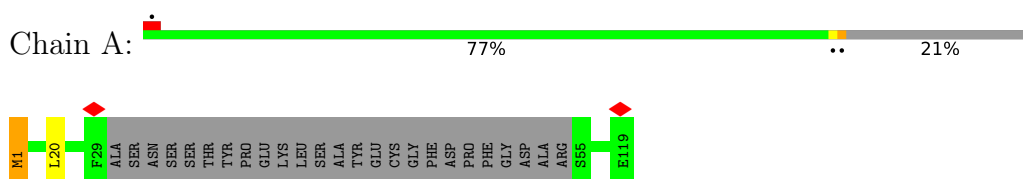
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Mol	Chain	Residues	Atoms		AltConf
76	AG	25	Total 25	O 25	0
76	AH	13	Total 13	O 13	0
76	AI	20	Total 20	O 20	0
76	BA	77	Total 77	O 77	0
76	BB	260	Total 260	O 260	0
76	BC	148	Total 148	O 148	0
76	BD	43	Total 43	O 43	0
76	BE	118	Total 118	O 118	0
76	BF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

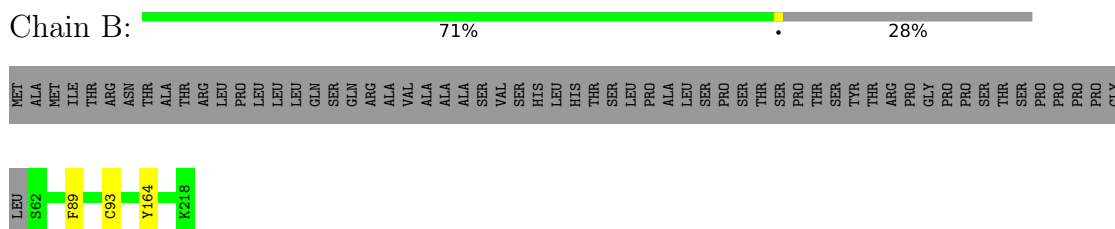
3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

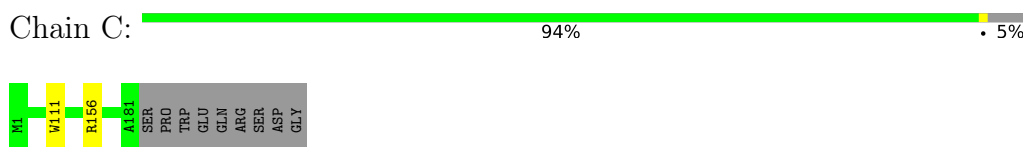
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



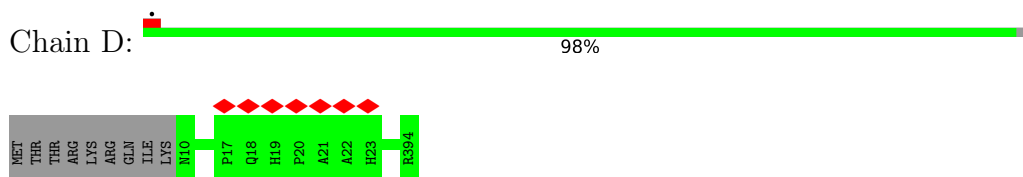
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



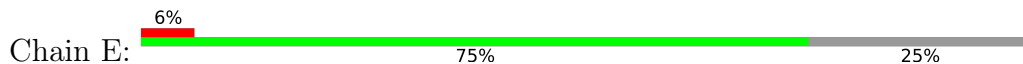
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

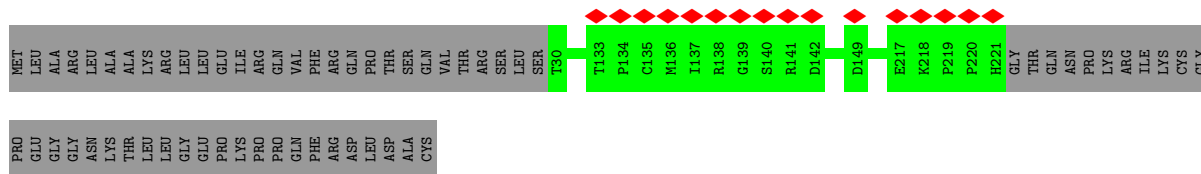


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2



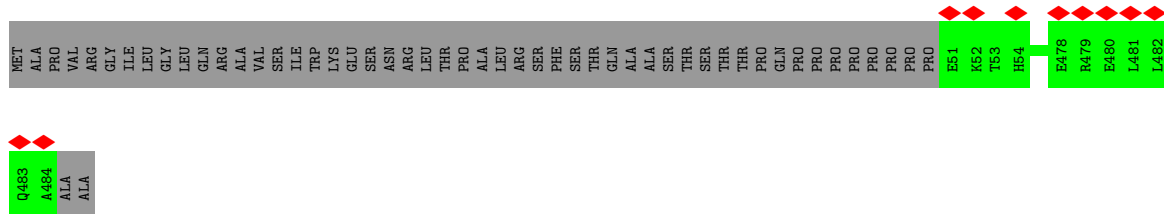
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





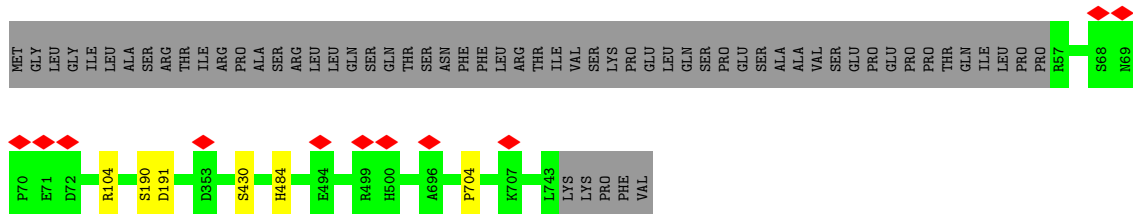
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 89% 11%



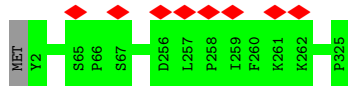
• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial

Chain G: 91% 8%



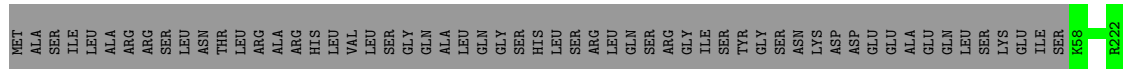
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 100%



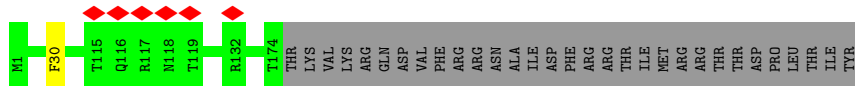
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I: 74% 26%

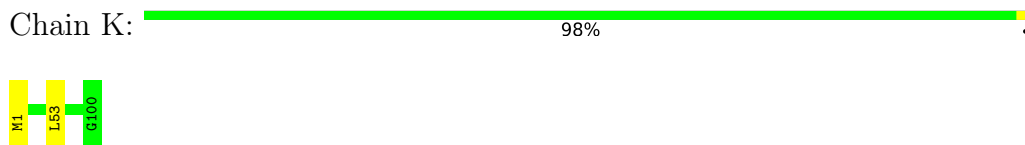


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

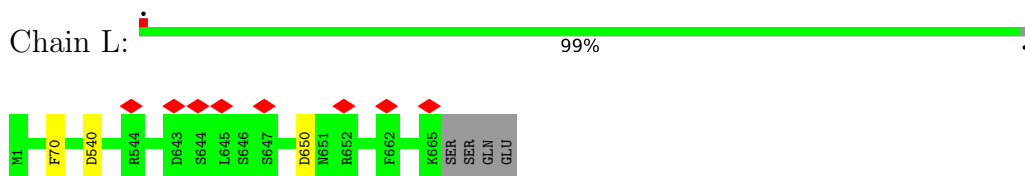
Chain J: 84% 15%



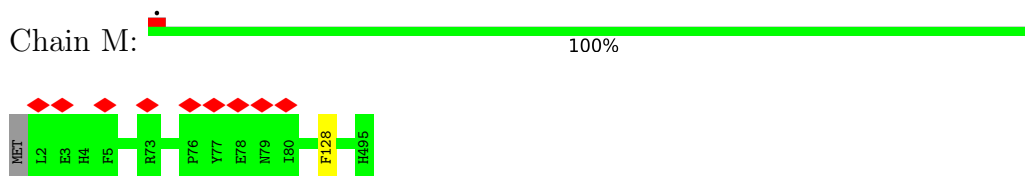
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



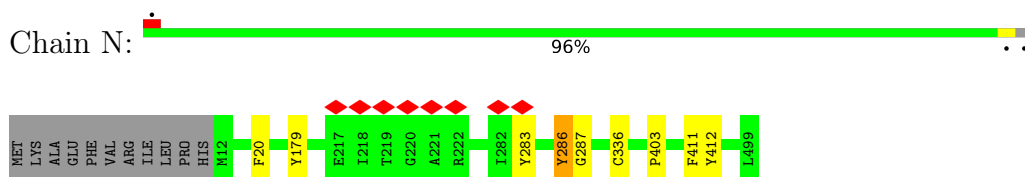
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



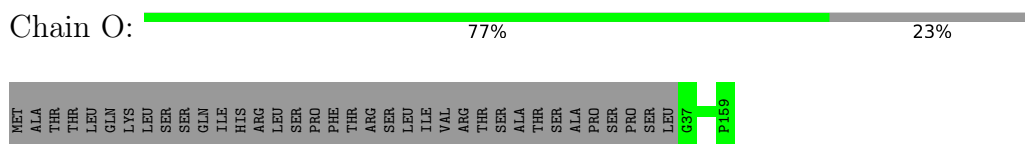
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



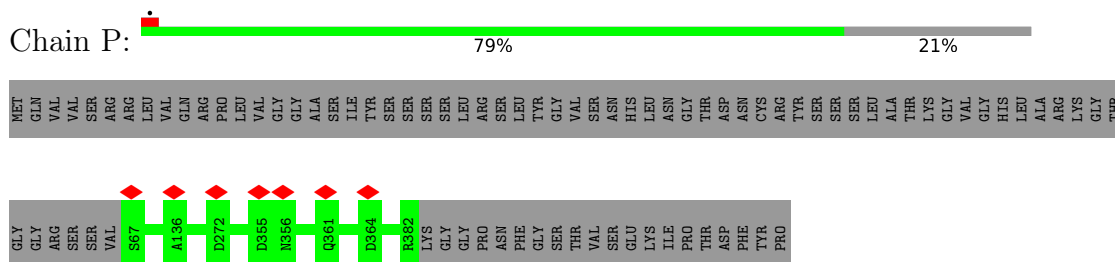
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



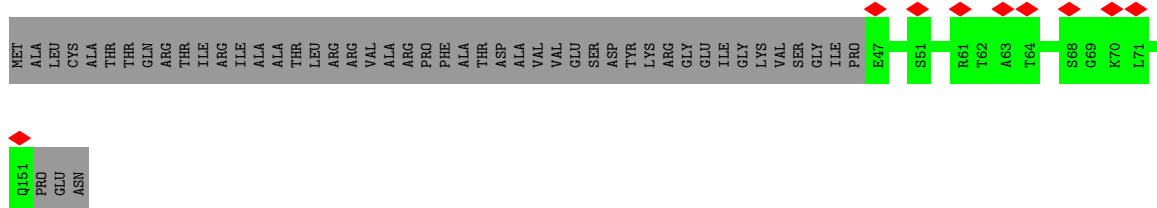
- Molecule 15: 2Fe-2S ferredoxin-like superfamily protein



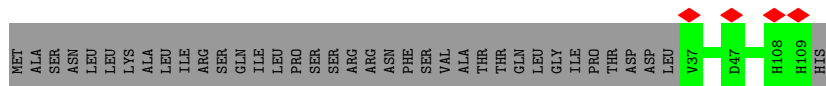
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



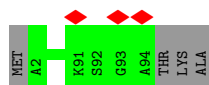
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



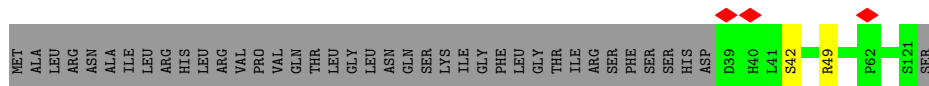
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



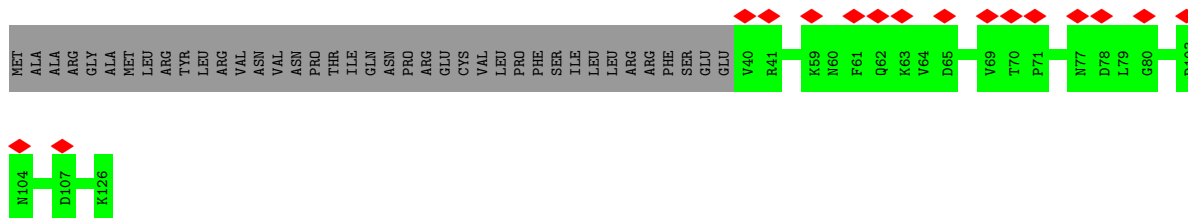
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



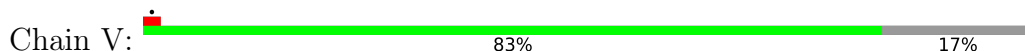
- Molecule 20: Acyl carrier protein 1, mitochondrial

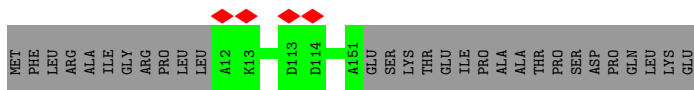


- Molecule 21: Acyl carrier protein 2, mitochondrial

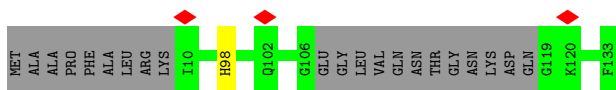
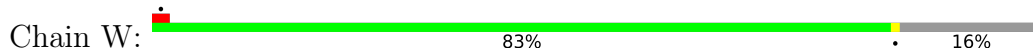


- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

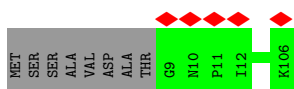




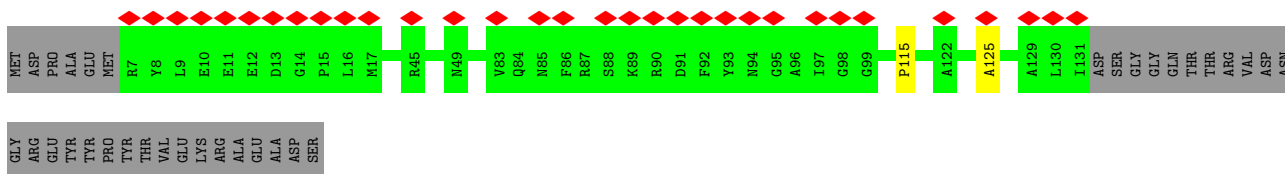
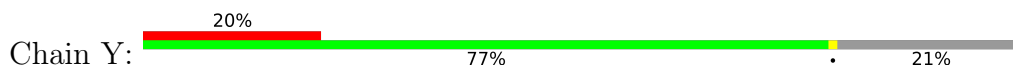
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



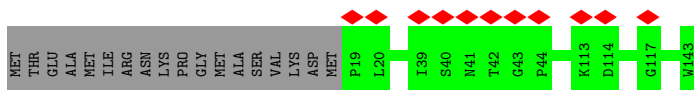
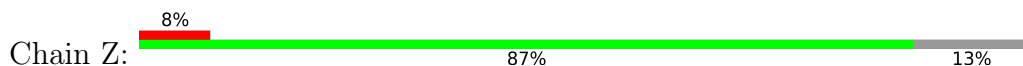
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



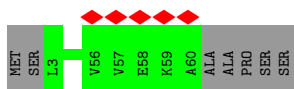
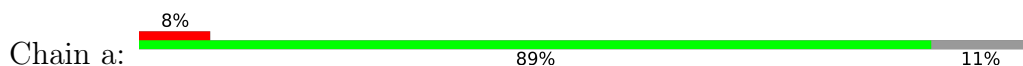
- Molecule 25: Outer envelope pore protein 16-3, chloroplastic/mitochondrial



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A

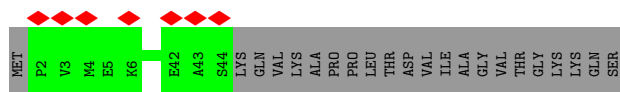


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

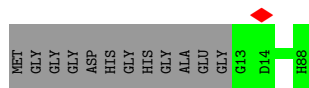
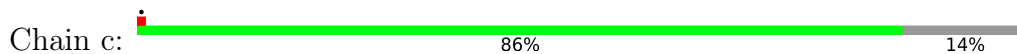


- Molecule 28: At2g46540/F11C10.23

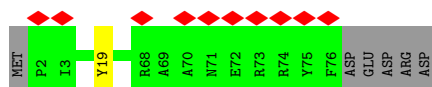




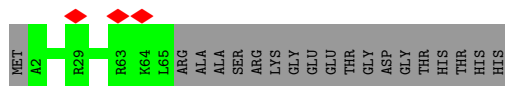
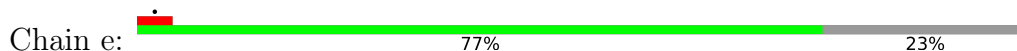
- Molecule 29: Transmembrane protein



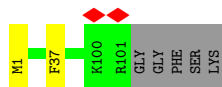
- Molecule 30: Excitatory amino acid transporter



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



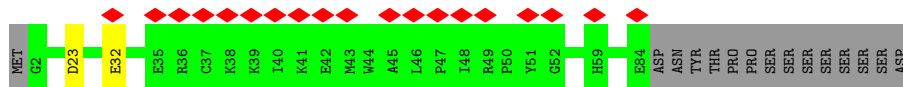
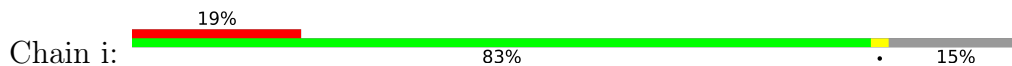
- Molecule 32: At4g16450



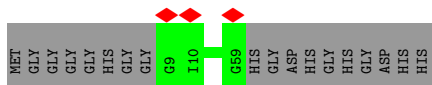
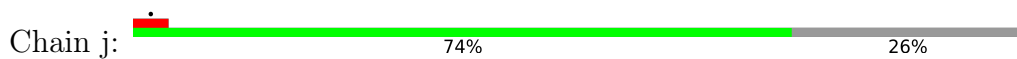
- Molecule 33: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



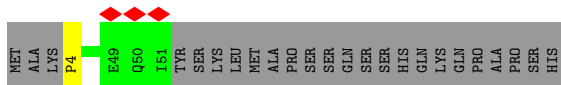
- Molecule 34: At1g67350



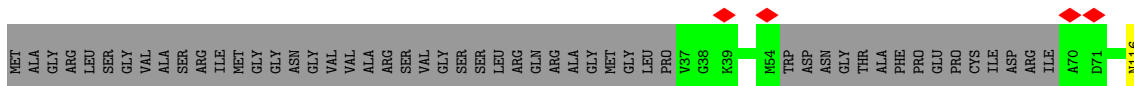
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2



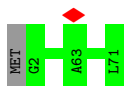
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



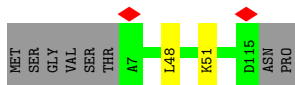
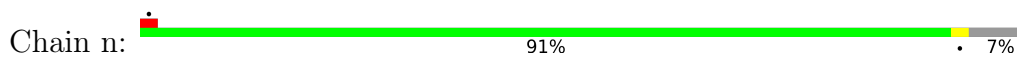
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



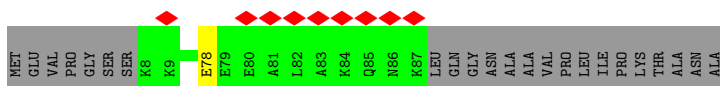
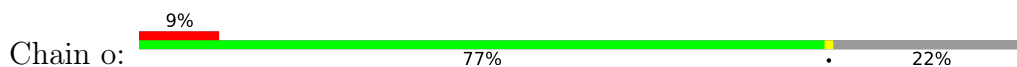
- Molecule 38: AT2G31490 protein



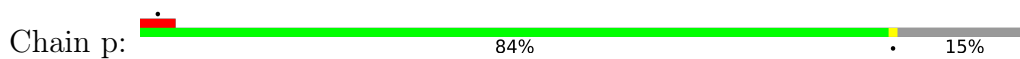
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



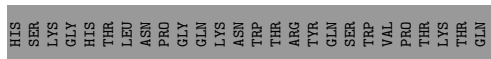
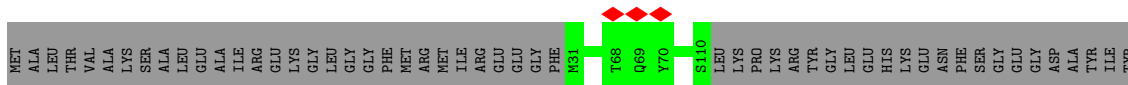
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



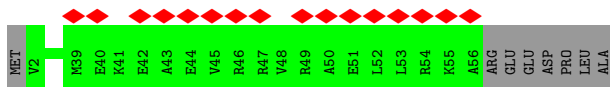
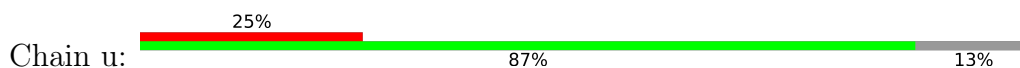
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B



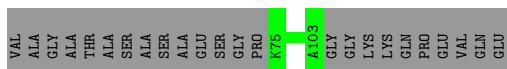
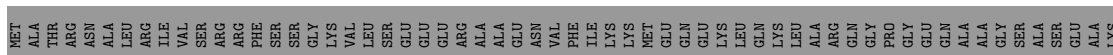
- Molecule 42: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



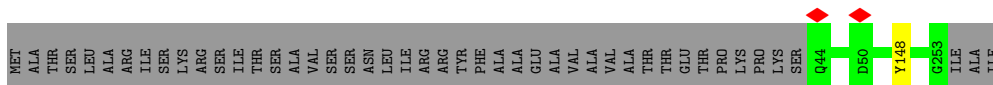
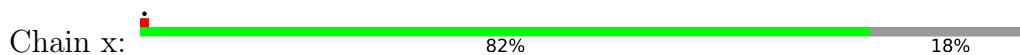
- Molecule 43: Uncharacterized protein At1g67785



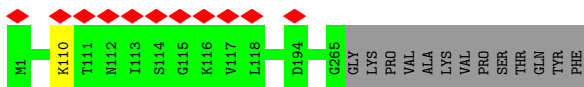
- Molecule 44: Uncharacterized protein At2g27730, mitochondrial



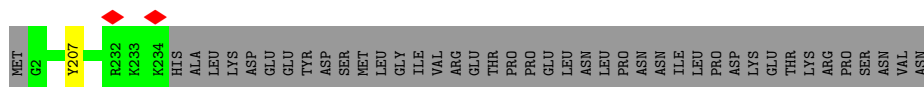
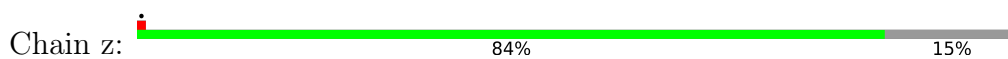
- Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial



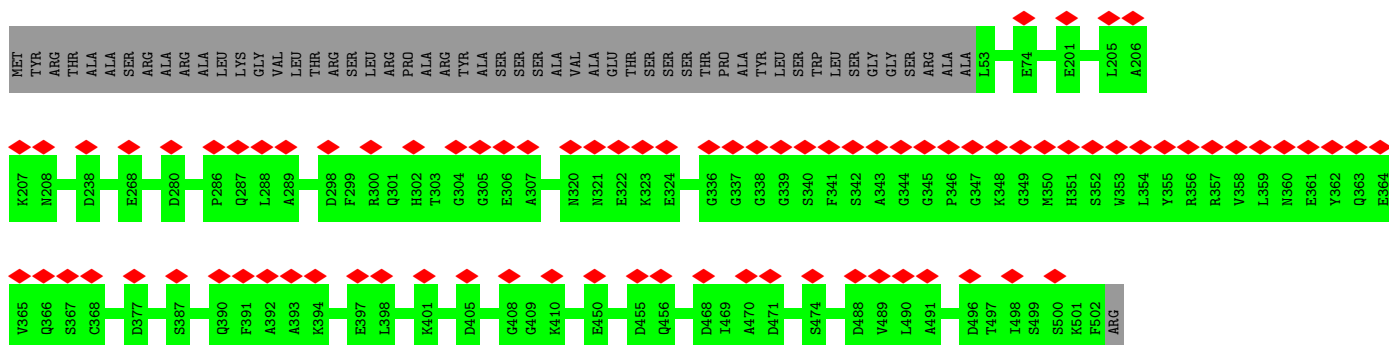
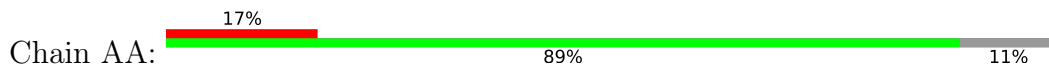
- Molecule 46: Gamma carbonic anhydrase 2, mitochondrial



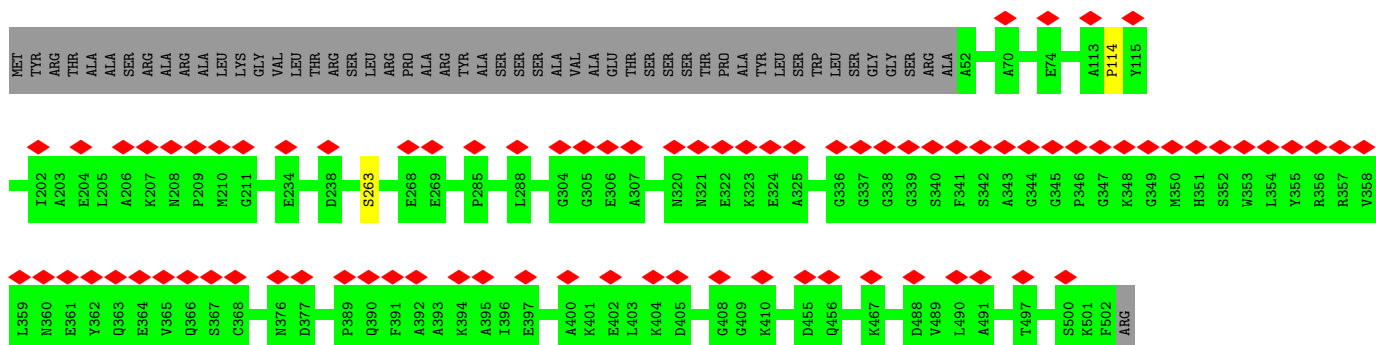
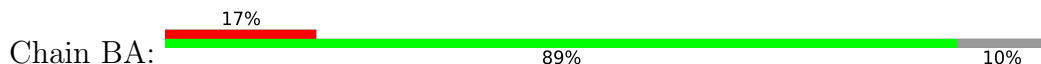
- Molecule 47: Gamma carbonic anhydrase 1, mitochondrial



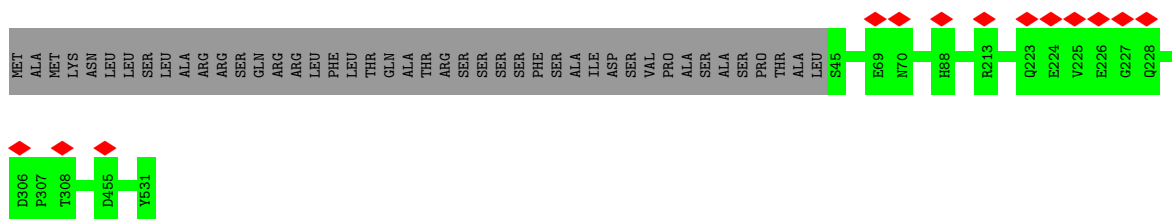
- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial



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

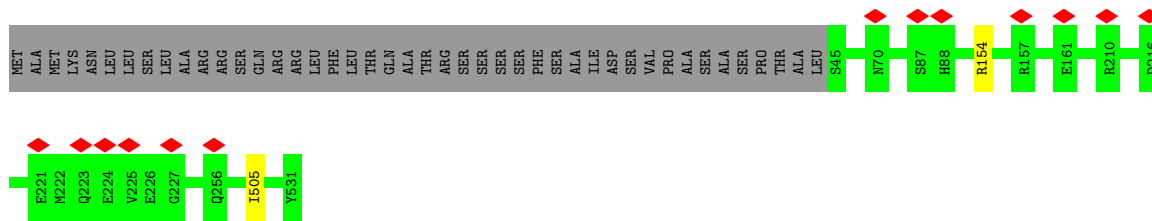


- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

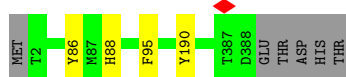


- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

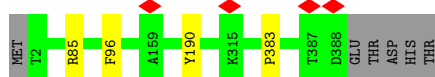




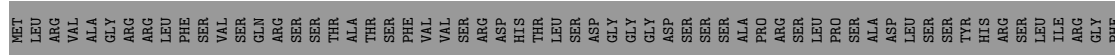
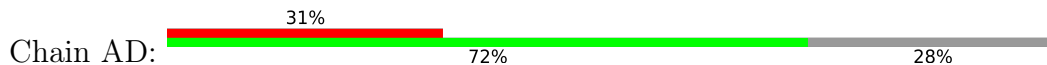
• Molecule 50: Cytochrome b



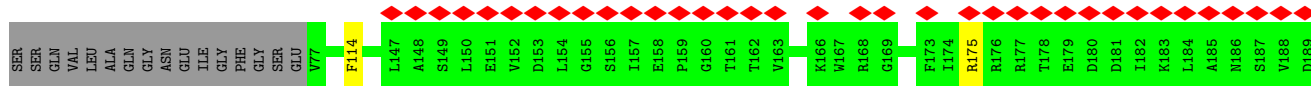
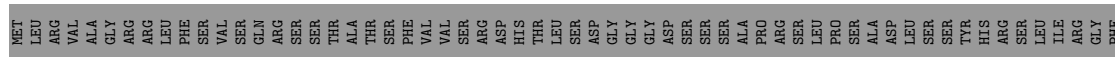
• Molecule 50: Cytochrome b



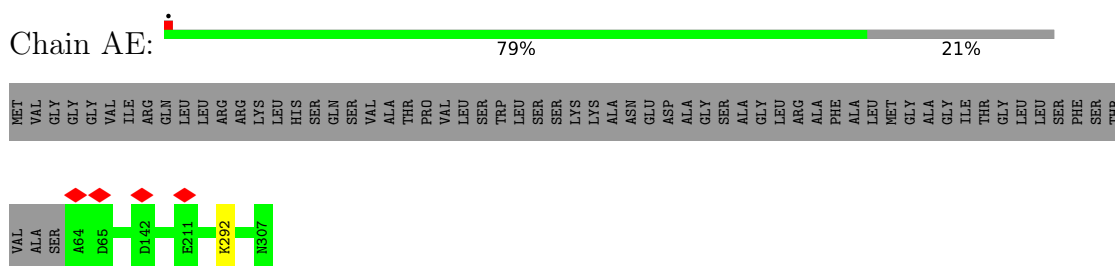
• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial



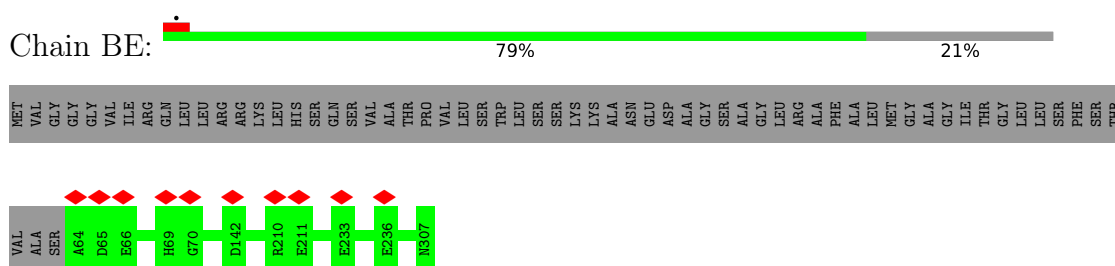
• Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial



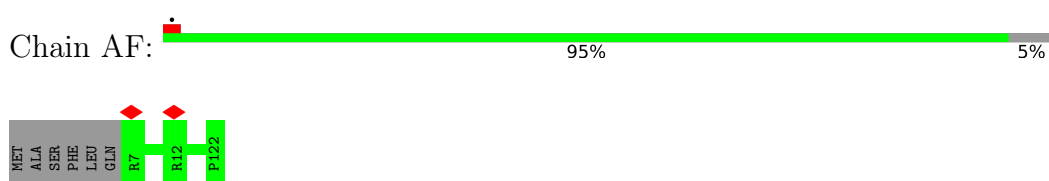
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial



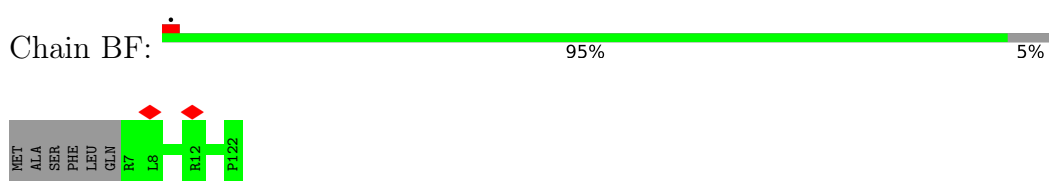
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial



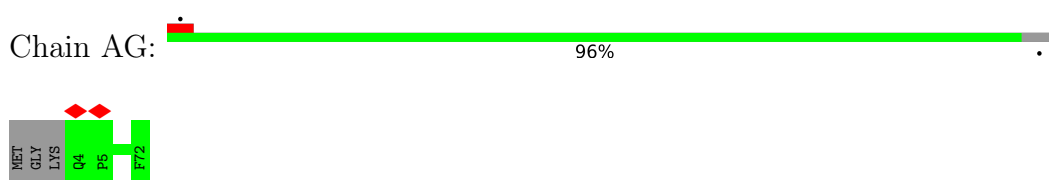
- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial



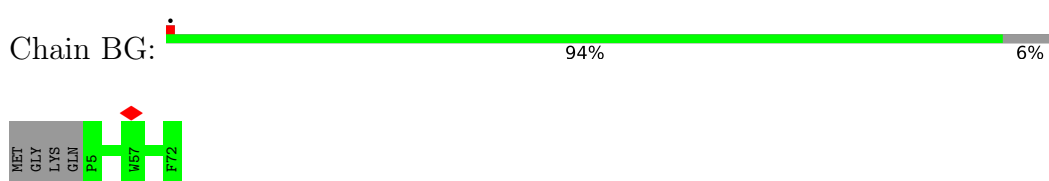
- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial



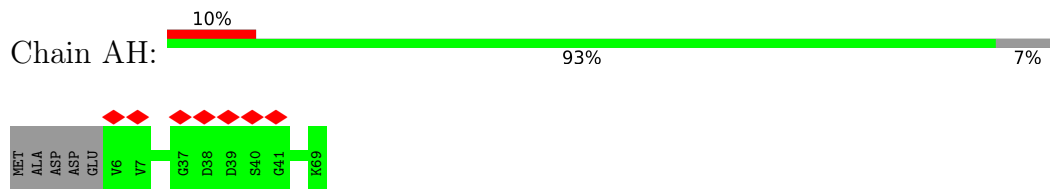
- Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial



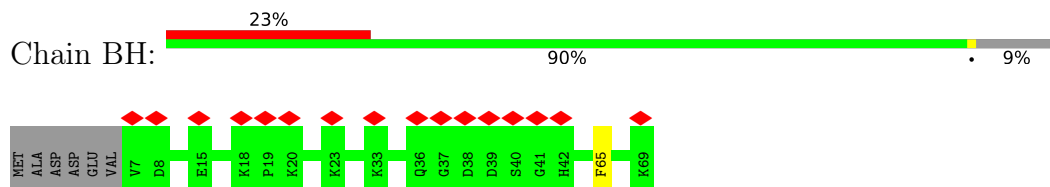
- Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial



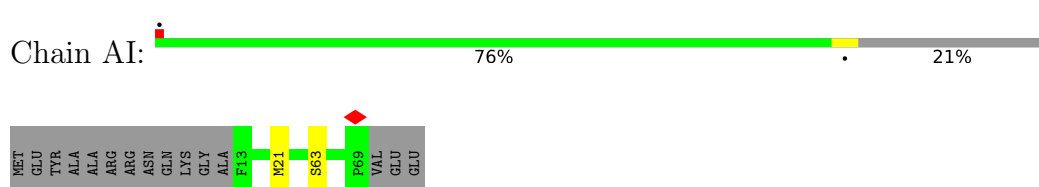
- Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial



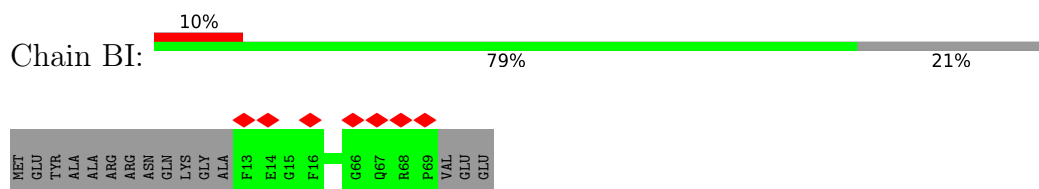
- Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial



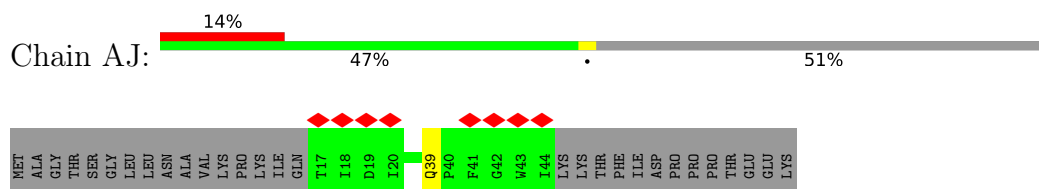
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



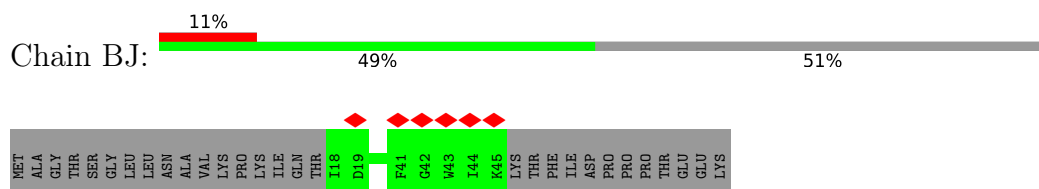
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



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



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



4 Experimental information

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

5 Model quality i

5.1 Standard geometry i

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

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	0.30	0/820	0.50	1/1113 (0.1%)
2	B	0.58	0/1279	0.68	0/1734
3	C	0.49	0/1590	0.66	1/2152 (0.0%)
4	D	0.51	0/3149	0.65	0/4259
5	E	0.53	0/1535	0.65	0/2084
6	F	0.26	0/3441	0.50	0/4641
7	G	0.33	0/5338	0.57	5/7231 (0.1%)
8	H	0.29	0/2609	0.49	0/3553
9	I	0.48	0/1378	0.62	0/1862
10	J	0.43	0/1435	0.60	0/1957
11	K	0.70	1/785 (0.1%)	0.74	0/1062
12	L	0.53	1/5368 (0.0%)	0.71	3/7291 (0.0%)
13	M	0.42	0/4066	0.60	0/5525
14	N	0.50	1/3948 (0.0%)	0.65	2/5360 (0.0%)
15	O	0.41	0/979	0.59	0/1326
16	P	0.44	0/2509	0.65	0/3401
17	Q	0.24	0/862	0.44	0/1166
18	R	0.33	0/585	0.52	0/793
19	S	0.38	0/739	0.58	0/996
20	T	0.57	1/671 (0.1%)	0.74	1/911 (0.1%)
21	U	0.29	0/687	0.46	0/929
22	V	0.46	0/1146	0.65	0/1555
23	W	0.36	0/923	0.62	1/1249 (0.1%)
24	X	0.28	0/790	0.51	0/1060
25	Y	0.47	2/944 (0.2%)	0.59	0/1277
26	Z	0.35	0/1027	0.57	0/1392
27	a	0.28	0/481	0.54	0/646
28	b	0.26	0/320	0.54	0/434
29	c	0.40	0/637	0.58	0/860
30	d	0.46	0/605	0.60	0/815
31	e	0.50	0/559	0.65	0/745

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.27	0/771	0.48	0/1042
33	g	0.36	0/661	0.68	2/899 (0.2%)
34	i	0.51	0/741	0.81	2/997 (0.2%)
35	j	0.42	0/433	0.63	0/592
36	k	0.46	0/392	0.81	2/526 (0.4%)
37	l	0.41	0/575	0.63	1/781 (0.1%)
38	m	0.48	0/592	0.73	0/793
39	n	0.67	2/938 (0.2%)	0.83	0/1273
40	o	0.56	0/666	0.82	1/886 (0.1%)
41	p	0.64	1/777 (0.1%)	0.84	0/1043
42	q	0.28	0/690	0.50	0/936
43	u	0.25	0/472	0.45	0/632
44	v	0.25	0/222	0.42	0/300
45	x	0.51	0/1669	0.61	0/2279
46	y	0.41	0/2046	0.59	0/2772
47	z	0.44	0/1804	0.64	0/2441
48	AA	0.38	0/3503	0.62	0/4752
48	BA	0.44	1/3508 (0.0%)	0.62	1/4759 (0.0%)
49	AB	0.36	0/3908	0.58	0/5305
49	BB	0.33	0/3908	0.56	1/5305 (0.0%)
50	AC	0.46	1/3208 (0.0%)	0.60	1/4395 (0.0%)
50	BC	0.47	0/3208	0.66	2/4395 (0.0%)
51	AD	0.34	0/1567	0.55	0/2135
51	BD	0.38	0/1558	0.62	2/2123 (0.1%)
52	AE	0.36	0/1968	0.56	0/2672
52	BE	0.37	0/1968	0.55	0/2672
53	AF	0.54	0/993	0.72	0/1336
53	BF	0.45	0/993	0.67	0/1336
54	AG	0.46	0/600	0.59	0/815
54	BG	0.38	0/591	0.65	0/802
55	AH	0.29	0/531	0.47	0/713
55	BH	0.43	0/524	0.69	1/703 (0.1%)
56	AI	0.69	1/488 (0.2%)	0.78	0/655
56	BI	0.40	0/488	0.71	0/655
57	AJ	0.43	0/210	0.76	1/290 (0.3%)
57	BJ	0.27	0/212	0.40	0/291
All	All	0.43	12/98588 (0.0%)	0.62	31/133680 (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
1	A	0	1
14	N	0	2
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	51	LYS	C-O	10.06	1.42	1.23
14	N	403	PRO	N-CD	-7.51	1.37	1.47
56	AI	63	SER	CA-CB	-6.47	1.43	1.52
48	BA	263	SER	CA-CB	-6.20	1.43	1.52
12	L	650	ASP	C-O	5.74	1.34	1.23
20	T	42	SER	CA-CB	-5.53	1.44	1.52
25	Y	115	PRO	N-CD	-5.51	1.40	1.47
50	AC	88	HIS	C-O	-5.40	1.13	1.23
11	K	53	LEU	C-O	-5.40	1.13	1.23
41	p	13	SER	CA-CB	-5.36	1.45	1.52
39	n	48	LEU	C-O	5.22	1.33	1.23
25	Y	125	ALA	C-O	-5.19	1.13	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	191	ASP	CB-CA-C	-10.44	89.52	110.40
12	L	650	ASP	CB-CA-C	-9.74	90.92	110.40
34	i	32	GLU	C-N-CA	-7.91	101.92	121.70
12	L	70	PHE	CB-CA-C	7.75	125.90	110.40
33	g	50	PRO	N-CD-CG	-7.53	91.90	103.20
33	g	50	PRO	CA-CB-CG	-6.47	91.71	104.00
50	BC	96	PHE	CB-CA-C	6.30	123.01	110.40
7	G	190	SER	N-CA-CB	6.03	119.54	110.50
12	L	540	ASP	CB-CA-C	5.75	121.89	110.40
51	BD	175	ARG	CB-CA-C	-5.74	98.92	110.40
55	BH	65	PHE	CB-CA-C	5.74	121.88	110.40
48	BA	114	PRO	CA-N-CD	-5.68	103.54	111.50
37	l	116	ASN	CB-CA-C	5.65	121.70	110.40
14	N	286	TYR	CB-CA-C	5.61	121.62	110.40
3	C	156	ARG	CG-CD-NE	-5.52	100.21	111.80
40	o	78	GLU	CB-CA-C	-5.52	99.37	110.40
7	G	430	SER	N-CA-CB	5.44	118.67	110.50
1	A	20	LEU	CA-CB-CG	5.43	127.79	115.30
51	BD	114	PHE	CB-CA-C	5.37	121.14	110.40
50	AC	86	TYR	CB-CA-C	5.36	121.13	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	23	ASP	O-C-N	-5.35	114.14	122.70
7	G	484	HIS	CB-CA-C	5.23	120.85	110.40
14	N	287	GLY	N-CA-C	5.20	126.09	113.10
7	G	704	PRO	N-CD-CG	-5.18	95.42	103.20
36	k	4	PRO	N-CA-CB	5.10	109.42	103.30
49	BB	154	ARG	CB-CA-C	-5.06	100.27	110.40
57	AJ	39	GLN	CB-CA-C	5.05	120.50	110.40
23	W	98	HIS	N-CA-CB	-5.05	101.51	110.60
20	T	49	ARG	CB-CG-CD	-5.03	98.52	111.60
36	k	4	PRO	N-CA-C	-5.02	99.04	112.10
50	BC	383	PRO	N-CD-CG	-5.01	95.69	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts [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	90/119 (76%)	89 (99%)	1 (1%)	0	100	100
2	B	155/218 (71%)	149 (96%)	6 (4%)	0	100	100
3	C	179/190 (94%)	176 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	383/394 (97%)	366 (96%)	17 (4%)	0	100	100
5	E	190/255 (74%)	178 (94%)	12 (6%)	0	100	100
6	F	432/486 (89%)	421 (98%)	11 (2%)	0	100	100
7	G	685/748 (92%)	668 (98%)	17 (2%)	0	100	100
8	H	322/325 (99%)	314 (98%)	8 (2%)	0	100	100
9	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
10	J	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
11	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
12	L	663/669 (99%)	637 (96%)	26 (4%)	0	100	100
13	M	493/495 (100%)	487 (99%)	6 (1%)	0	100	100
14	N	488/499 (98%)	474 (97%)	14 (3%)	0	100	100
15	O	121/159 (76%)	117 (97%)	4 (3%)	0	100	100
16	P	314/402 (78%)	301 (96%)	13 (4%)	0	100	100
17	Q	103/154 (67%)	100 (97%)	3 (3%)	0	100	100
18	R	71/110 (64%)	70 (99%)	1 (1%)	0	100	100
19	S	91/97 (94%)	89 (98%)	2 (2%)	0	100	100
20	T	81/122 (66%)	78 (96%)	3 (4%)	0	100	100
21	U	85/126 (68%)	77 (91%)	8 (9%)	0	100	100
22	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
23	W	108/133 (81%)	99 (92%)	9 (8%)	0	100	100
24	X	96/106 (91%)	95 (99%)	1 (1%)	0	100	100
25	Y	123/159 (77%)	117 (95%)	6 (5%)	0	100	100
26	Z	123/143 (86%)	122 (99%)	1 (1%)	0	100	100
27	a	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
28	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
29	c	74/88 (84%)	73 (99%)	1 (1%)	0	100	100
30	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
31	e	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
32	f	99/106 (93%)	98 (99%)	1 (1%)	0	100	100
33	g	77/114 (68%)	77 (100%)	0	0	100	100
34	i	81/98 (83%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	j	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
36	k	46/72 (64%)	45 (98%)	1 (2%)	0	100	100
37	l	70/125 (56%)	69 (99%)	1 (1%)	0	100	100
38	m	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
39	n	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
40	o	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
41	p	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
42	q	79/159 (50%)	75 (95%)	4 (5%)	0	100	100
43	u	53/63 (84%)	53 (100%)	0	0	100	100
44	v	27/113 (24%)	27 (100%)	0	0	100	100
45	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
46	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
47	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100
48	AA	448/503 (89%)	431 (96%)	17 (4%)	0	100	100
48	BA	449/503 (89%)	431 (96%)	18 (4%)	0	100	100
49	AB	485/531 (91%)	475 (98%)	10 (2%)	0	100	100
49	BB	485/531 (91%)	476 (98%)	9 (2%)	0	100	100
50	AC	385/393 (98%)	375 (97%)	10 (3%)	0	100	100
50	BC	385/393 (98%)	374 (97%)	11 (3%)	0	100	100
51	AD	194/272 (71%)	182 (94%)	12 (6%)	0	100	100
51	BD	193/272 (71%)	181 (94%)	12 (6%)	0	100	100
52	AE	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
52	BE	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
53	AF	114/122 (93%)	114 (100%)	0	0	100	100
53	BF	114/122 (93%)	114 (100%)	0	0	100	100
54	AG	67/72 (93%)	67 (100%)	0	0	100	100
54	BG	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
55	AH	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
55	BH	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
56	AI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
56	BI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	AJ	26/57 (46%)	25 (96%)	1 (4%)	0	100	100
57	BJ	26/57 (46%)	23 (88%)	3 (12%)	0	100	100
All	All	12051/14108 (85%)	11717 (97%)	334 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [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	85/105 (81%)	85 (100%)	0	100	100
2	B	132/184 (72%)	129 (98%)	3 (2%)	50	55
3	C	171/179 (96%)	170 (99%)	1 (1%)	86	90
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	166 (100%)	0	100	100
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	570/625 (91%)	569 (100%)	1 (0%)	93	96
8	H	271/272 (100%)	271 (100%)	0	100	100
9	I	147/195 (75%)	147 (100%)	0	100	100
10	J	156/186 (84%)	155 (99%)	1 (1%)	86	90
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	564/568 (99%)	564 (100%)	0	100	100
13	M	434/434 (100%)	433 (100%)	1 (0%)	93	96
14	N	408/416 (98%)	403 (99%)	5 (1%)	71	77
15	O	108/141 (77%)	108 (100%)	0	100	100
16	P	263/334 (79%)	263 (100%)	0	100	100
17	Q	89/128 (70%)	89 (100%)	0	100	100
18	R	64/97 (66%)	64 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	78/112 (70%)	78 (100%)	0	100	100
21	U	78/113 (69%)	78 (100%)	0	100	100
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	98/114 (86%)	98 (100%)	0	100	100
24	X	88/94 (94%)	88 (100%)	0	100	100
25	Y	92/120 (77%)	92 (100%)	0	100	100
26	Z	100/115 (87%)	100 (100%)	0	100	100
27	a	48/53 (91%)	48 (100%)	0	100	100
28	b	35/53 (66%)	35 (100%)	0	100	100
29	c	66/71 (93%)	66 (100%)	0	100	100
30	d	60/66 (91%)	59 (98%)	1 (2%)	60	67
31	e	59/73 (81%)	59 (100%)	0	100	100
32	f	80/83 (96%)	79 (99%)	1 (1%)	69	75
33	g	68/96 (71%)	68 (100%)	0	100	100
34	i	75/90 (83%)	75 (100%)	0	100	100
35	j	42/51 (82%)	42 (100%)	0	100	100
36	k	39/60 (65%)	39 (100%)	0	100	100
37	l	60/97 (62%)	60 (100%)	0	100	100
38	m	58/59 (98%)	58 (100%)	0	100	100
39	n	92/99 (93%)	92 (100%)	0	100	100
40	o	70/87 (80%)	70 (100%)	0	100	100
41	p	80/93 (86%)	80 (100%)	0	100	100
42	q	69/133 (52%)	69 (100%)	0	100	100
43	u	47/54 (87%)	47 (100%)	0	100	100
44	v	22/84 (26%)	22 (100%)	0	100	100
45	x	179/216 (83%)	178 (99%)	1 (1%)	86	90
46	y	221/232 (95%)	220 (100%)	1 (0%)	88	92
47	z	188/228 (82%)	187 (100%)	1 (0%)	88	92
48	AA	369/408 (90%)	369 (100%)	0	100	100
48	BA	369/408 (90%)	369 (100%)	0	100	100
49	AB	415/452 (92%)	415 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BB	415/452 (92%)	414 (100%)	1 (0%)	93	96
50	AC	330/336 (98%)	328 (99%)	2 (1%)	86	90
50	BC	330/336 (98%)	328 (99%)	2 (1%)	86	90
51	AD	170/232 (73%)	169 (99%)	1 (1%)	86	90
51	BD	169/232 (73%)	169 (100%)	0	100	100
52	AE	200/247 (81%)	199 (100%)	1 (0%)	88	92
52	BE	200/247 (81%)	200 (100%)	0	100	100
53	AF	105/110 (96%)	105 (100%)	0	100	100
53	BF	105/110 (96%)	105 (100%)	0	100	100
54	AG	63/65 (97%)	63 (100%)	0	100	100
54	BG	62/65 (95%)	62 (100%)	0	100	100
55	AH	58/62 (94%)	58 (100%)	0	100	100
55	BH	57/62 (92%)	57 (100%)	0	100	100
56	AI	48/59 (81%)	47 (98%)	1 (2%)	53	59
56	BI	48/59 (81%)	48 (100%)	0	100	100
57	AJ	16/41 (39%)	16 (100%)	0	100	100
57	BJ	16/41 (39%)	16 (100%)	0	100	100
All	All	10339/11908 (87%)	10314 (100%)	25 (0%)	93	96

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	89	PHE
2	B	93	CYS
2	B	164	TYR
3	C	111	TRP
7	G	104	ARG
10	J	30	PHE
13	M	128	PHE
14	N	20	PHE
14	N	179	TYR
14	N	283	TYR
14	N	286	TYR
14	N	336	CYS
30	d	19	TYR
32	f	37	PHE

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Mol	Chain	Res	Type
45	x	148	TYR
46	y	110	LYS
47	z	207	TYR
50	AC	95	PHE
50	AC	190	TYR
51	AD	194	ARG
52	AE	292	LYS
56	AI	21	MET
49	BB	505	ILE
50	BC	85	ARG
50	BC	190	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	23	HIS
4	D	311	HIS
4	D	372	HIS
6	F	304	HIS
12	L	318	GLN
13	M	341	HIS
20	T	118	HIS
38	m	25	HIS
39	n	39	HIS
42	q	85	ASN
48	AA	133	ASN
49	AB	192	GLN
49	AB	316	ASN
50	AC	6	GLN
50	AC	13	GLN
50	AC	209	GLN
53	AF	20	HIS
54	AG	36	HIS
48	BA	293	GLN
50	BC	13	GLN
50	BC	219	HIS
50	BC	274	HIS
50	BC	329	GLN
51	BD	96	HIS
52	BE	307	ASN
53	BF	64	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

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

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
1	FME	A	1	1	-	0/7/9/11	-
11	FME	K	1	11	-	5/7/9/11	-
32	FME	f	1	32	-	5/7/9/11	-

All (2) bond length outliers are listed below:

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

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-3.69	115.10	124.78
11	K	1	FME	C-CA-N	3.58	116.19	109.73

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

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 5 are monoatomic - leaving 86 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
66	PC7	L	706	-	39,39,51	1.08	3 (7%)	45,47,59	1.10	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	3PH	l	201	-	36,36,47	0.71	1 (2%)	40,41,52	0.70	1 (2%)
60	PTY	Y	202	-	30,30,49	0.35	0	33,35,54	0.37	0
60	PTY	N	503	-	49,49,49	0.27	0	52,54,54	0.36	0
59	SF4	B	500	2	0,12,12	-	-	-	-	-
61	FES	E	500	5	0,4,4	-	-	-	-	-
59	SF4	G	803	7	0,12,12	-	-	-	-	-
67	UQ5	AC	404	-	38,38,38	0.45	0	46,49,49	0.82	1 (2%)
72	CDL	BC	407	-	80,80,99	0.30	0	86,92,111	0.38	0
72	CDL	BE	402	-	87,87,99	0.93	8 (9%)	93,99,111	1.11	4 (4%)
60	PTY	M	504	-	49,49,49	0.29	0	52,54,54	0.40	0
59	SF4	I	501	9	0,12,12	-	-	-	-	-
72	CDL	AC	408	-	80,80,99	0.30	0	86,92,111	0.35	0
73	COO	y	302	-	45,55,55	3.88	16 (35%)	55,81,81	2.59	10 (18%)
66	PC7	AG	101	-	51,51,51	0.97	4 (7%)	57,59,59	1.01	2 (3%)
63	UQ9	H	401	-	35,35,58	2.48	11 (31%)	42,45,73	2.16	13 (30%)
58	PGT	BC	406	-	36,36,50	0.33	0	39,42,56	0.45	0
62	FMN	F	500	-	33,33,33	0.61	0	48,50,50	0.67	1 (2%)
65	3PH	AI	101	-	31,31,47	0.76	1 (3%)	35,36,52	0.76	2 (5%)
60	PTY	M	503	-	36,36,49	0.31	0	39,41,54	0.46	0
58	PGT	AC	406	-	40,40,50	0.32	0	43,46,56	0.33	0
60	PTY	m	101	-	49,49,49	0.26	0	52,54,54	0.35	0
64	Q7G	M	505	-	44,44,90	0.85	1 (2%)	66,68,138	1.75	17 (25%)
66	PC7	f	203	-	47,47,51	0.28	0	53,55,59	0.31	0
58	PGT	L	703	-	50,50,50	0.29	0	53,56,56	0.31	0
61	FES	BD	301	51	0,4,4	-	-	-	-	-
64	Q7G	BC	410	-	44,44,90	0.75	1 (2%)	66,68,138	1.44	10 (15%)
66	PC7	BC	409	-	40,40,51	0.34	0	46,48,59	0.51	0
66	PC7	v	201	-	51,51,51	0.97	4 (7%)	57,59,59	1.13	3 (5%)
58	PGT	y	303	-	40,40,50	1.17	4 (10%)	43,46,56	1.11	2 (4%)
60	PTY	BB	602	-	28,28,49	0.36	0	31,33,54	0.52	0
66	PC7	d	102	-	51,51,51	0.41	0	57,59,59	0.52	0
60	PTY	D	401	-	49,49,49	0.88	4 (8%)	52,54,54	1.03	2 (3%)
60	PTY	N	502	-	44,44,49	0.29	0	47,49,54	0.41	0
75	UQ7	BC	404	-	48,48,48	0.66	2 (4%)	58,61,61	0.77	3 (5%)
72	CDL	AE	402	-	84,84,99	0.29	0	90,96,111	0.36	0
65	3PH	BJ	102	-	47,47,47	0.63	1 (2%)	51,52,52	0.59	1 (1%)
66	PC7	AC	410	-	50,50,51	0.35	0	56,58,59	0.47	0
72	CDL	BG	101	-	69,69,99	1.04	8 (11%)	75,81,111	1.16	5 (6%)
74	HEM	BC	402	50	41,50,50	1.78	8 (19%)	45,82,82	2.04	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	3PH	f	202	-	42,42,47	0.67	1 (2%)	46,47,52	0.64	2 (4%)
65	3PH	L	701	-	36,36,47	0.54	0	40,41,52	0.73	2 (5%)
60	PTY	N	501	-	39,39,49	0.30	0	42,44,54	0.35	0
61	FES	G	801	7	0,4,4	-	-	-	-	-
72	CDL	BC	408	-	76,76,99	0.31	0	82,88,111	0.33	0
58	PGT	AF	201	-	50,50,50	1.07	3 (6%)	53,56,56	1.06	2 (3%)
71	8Q1	W	200	-	31,34,34	0.32	0	40,43,43	0.46	0
60	PTY	AB	602	-	40,40,49	0.30	0	43,45,54	0.32	0
60	PTY	z	301	-	49,49,49	0.86	3 (6%)	52,54,54	1.17	3 (5%)
64	Q7G	K	201	-	90,90,90	0.78	2 (2%)	136,138,138	1.33	19 (13%)
64	Q7G	H	402	-	90,90,90	0.70	3 (3%)	136,138,138	1.17	10 (7%)
64	Q7G	BC	411	-	44,44,90	0.76	1 (2%)	66,68,138	1.37	13 (19%)
58	PGT	L	702	-	35,35,50	0.31	0	38,41,56	0.40	0
58	PGT	A	201	-	50,50,50	1.08	4 (8%)	53,56,56	1.08	3 (5%)
69	NDP	P	500	-	45,52,52	0.73	0	53,80,80	0.84	1 (1%)
74	HEM	BC	401	50	41,50,50	1.65	9 (21%)	45,82,82	1.92	14 (31%)
60	PTY	d	101	-	38,38,49	0.31	0	41,43,54	0.40	0
58	PGT	M	502	-	28,28,50	0.34	0	31,34,56	0.38	0
72	CDL	AC	409	-	84,84,99	0.31	0	90,96,111	0.36	0
72	CDL	u	101	-	99,99,99	0.88	7 (7%)	105,111,111	1.07	5 (4%)
59	SF4	I	500	9	0,12,12	-	-	-	-	-
65	3PH	M	501	-	40,40,47	0.70	1 (2%)	44,45,52	0.66	1 (2%)
72	CDL	u	102	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
64	Q7G	a	101	-	44,44,90	0.66	0	66,68,138	1.32	9 (13%)
66	PC7	BD	302	-	38,38,51	0.34	0	44,46,59	0.46	0
65	3PH	BC	405	-	43,43,47	0.65	1 (2%)	47,48,52	0.62	1 (2%)
66	PC7	AB	603	-	33,33,51	0.38	0	39,41,59	0.43	0
74	HEM	AC	402	50	41,50,50	1.59	8 (19%)	45,82,82	1.88	9 (20%)
61	FES	AD	301	51	0,4,4	-	-	-	-	-
74	HEM	BE	401	52	41,50,50	1.79	10 (24%)	45,82,82	2.40	14 (31%)
60	PTY	L	705	-	41,41,49	0.96	4 (9%)	44,46,54	1.07	2 (4%)
74	HEM	AE	401	52	41,50,50	1.44	3 (7%)	45,82,82	1.43	10 (22%)
65	3PH	f	201	-	40,40,47	0.67	1 (2%)	44,45,52	0.73	2 (4%)
67	UQ5	BC	403	-	38,38,38	0.48	0	46,49,49	0.62	1 (2%)
59	SF4	G	802	7	0,12,12	-	-	-	-	-
60	PTY	BF	201	-	39,39,49	0.97	4 (10%)	42,44,54	1.06	2 (4%)
65	3PH	Y	201	-	32,32,47	0.35	0	36,37,52	0.34	0
74	HEM	AC	401	50	41,50,50	1.49	6 (14%)	45,82,82	1.45	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PGT	L	704	-	44,44,50	1.13	4 (9%)	47,50,56	1.06	2 (4%)
58	PGT	AC	407	-	50,50,50	1.09	3 (6%)	53,56,56	1.04	2 (3%)
67	UQ5	AC	403	-	38,38,38	0.77	2 (5%)	46,49,49	0.51	0
71	8Q1	T	200	-	31,34,34	0.38	0	40,43,43	1.14	3 (7%)
59	SF4	F	501	6	0,12,12	-	-	-	-	-
65	3PH	AC	405	-	32,32,47	0.33	0	36,37,52	0.41	0
67	UQ5	L	707	-	38,38,38	0.76	2 (5%)	46,49,49	0.84	3 (6%)
65	3PH	BJ	101	-	40,40,47	0.68	1 (2%)	44,45,52	0.65	1 (2%)

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
66	PC7	L	706	-	-	17/43/43/55	-
65	3PH	l	201	-	-	11/38/38/49	-
60	PTY	Y	202	-	-	6/34/34/53	-
60	PTY	N	503	-	-	17/53/53/53	-
59	SF4	B	500	2	-	-	0/6/5/5
61	FES	E	500	5	-	-	0/1/1/1
59	SF4	G	803	7	-	-	0/6/5/5
67	UQ5	AC	404	-	-	13/33/57/57	0/1/1/1
72	CDL	BC	407	-	-	47/91/91/110	-
72	CDL	BE	402	-	-	35/98/98/110	-
60	PTY	M	504	-	-	34/53/53/53	-
72	CDL	AC	408	-	-	50/91/91/110	-
59	SF4	I	501	9	-	-	0/6/5/5
73	COO	y	302	-	1/1/12/16	11/50/70/70	0/3/3/3
66	PC7	AG	101	-	-	20/55/55/55	-
63	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
58	PGT	BC	406	-	-	26/41/41/55	-
62	FMN	F	500	-	-	2/18/18/18	0/3/3/3
65	3PH	AI	101	-	-	15/33/33/49	-
60	PTY	M	503	-	-	22/40/40/53	-
58	PGT	AC	406	-	-	20/45/45/55	-
60	PTY	m	101	-	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	Q7G	M	505	-	-	6/12/100/200	0/6/6/10
66	PC7	f	203	-	-	25/51/51/55	-
58	PGT	L	703	-	-	13/55/55/55	-
61	FES	BD	301	51	-	-	0/1/1/1
64	Q7G	BC	410	-	-	6/12/100/200	0/6/6/10
66	PC7	BC	409	-	-	25/44/44/55	-
66	PC7	v	201	-	-	25/55/55/55	-
58	PGT	y	303	-	-	28/45/45/55	-
60	PTY	BB	602	-	-	16/32/32/53	-
66	PC7	d	102	-	-	27/55/55/55	-
60	PTY	D	401	-	-	19/53/53/53	-
60	PTY	N	502	-	-	29/48/48/53	-
75	UQ7	BC	404	-	-	19/45/69/69	0/1/1/1
72	CDL	AE	402	-	-	41/95/95/110	-
65	3PH	BJ	102	-	-	13/49/49/49	-
66	PC7	AC	410	-	-	20/54/54/55	-
72	CDL	BG	101	-	-	38/80/80/110	-
74	HEM	BC	402	50	-	2/12/54/54	-
65	3PH	f	202	-	-	18/44/44/49	-
65	3PH	L	701	-	-	14/38/38/49	-
60	PTY	N	501	-	-	13/43/43/53	-
61	FES	G	801	7	-	-	0/1/1/1
72	CDL	BC	408	-	-	36/87/87/110	-
58	PGT	AF	201	-	-	37/55/55/55	-
71	8Q1	W	200	-	-	11/41/41/41	-
60	PTY	AB	602	-	-	24/44/44/53	-
60	PTY	z	301	-	-	27/53/53/53	-
64	Q7G	K	201	-	-	6/32/200/200	0/10/10/10
64	Q7G	H	402	-	-	12/32/200/200	0/10/10/10
64	Q7G	BC	411	-	-	4/12/100/200	0/6/6/10
58	PGT	L	702	-	-	20/40/40/55	-
58	PGT	A	201	-	-	26/55/55/55	-
69	NDP	P	500	-	-	7/30/77/77	0/5/5/5
74	HEM	BC	401	50	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PTY	d	101	-	-	25/42/42/53	-
58	PGT	M	502	-	-	18/33/33/55	-
72	CDL	AC	409	-	-	52/95/95/110	-
72	CDL	u	101	-	-	49/110/110/110	-
59	SF4	I	500	9	-	-	0/6/5/5
65	3PH	M	501	-	-	19/42/42/49	-
72	CDL	u	102	-	-	44/110/110/110	-
64	Q7G	a	101	-	-	4/12/100/200	0/6/6/10
66	PC7	BD	302	-	-	18/42/42/55	-
65	3PH	BC	405	-	-	20/45/45/49	-
66	PC7	AB	603	-	-	18/37/37/55	-
74	HEM	AC	402	50	-	6/12/54/54	-
61	FES	AD	301	51	-	-	0/1/1/1
74	HEM	BE	401	52	-	4/12/54/54	-
60	PTY	L	705	-	-	20/45/45/53	-
74	HEM	AE	401	52	-	2/12/54/54	-
65	3PH	f	201	-	-	14/42/42/49	-
67	UQ5	BC	403	-	-	9/33/57/57	0/1/1/1
65	3PH	Y	201	-	-	18/34/34/49	-
60	PTY	BF	201	-	-	18/43/43/53	-
74	HEM	AC	401	50	-	2/12/54/54	-
59	SF4	G	802	7	-	-	0/6/5/5
58	PGT	L	704	-	-	29/49/49/55	-
58	PGT	AC	407	-	-	22/55/55/55	-
67	UQ5	AC	403	-	-	16/33/57/57	0/1/1/1
71	8Q1	T	200	-	-	24/41/41/41	-
59	SF4	F	501	6	-	-	0/6/5/5
65	3PH	AC	405	-	-	23/34/34/49	-
67	UQ5	L	707	-	-	16/33/57/57	0/1/1/1
65	3PH	BJ	101	-	-	14/42/42/49	-

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	y	302	COO	C2A-N1A	-15.18	1.05	1.33
63	H	401	UQ9	C6-C1	9.79	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	y	302	COO	C2A-N3A	-8.71	1.18	1.32
73	y	302	COO	C5A-C4A	8.18	1.62	1.40
73	y	302	COO	C1-N1	7.47	1.49	1.33
73	y	302	COO	C4-N2	6.79	1.48	1.33
74	BC	402	HEM	C1B-NB	-6.36	1.29	1.40
73	y	302	COO	O4X-C1X	5.84	1.49	1.41
73	y	302	COO	C4A-N3A	5.80	1.43	1.35
74	BE	401	HEM	C1B-NB	-5.62	1.30	1.40
73	y	302	COO	C6A-N1A	-5.46	1.13	1.37
74	BC	401	HEM	C1B-NB	-4.85	1.31	1.40
63	H	401	UQ9	C4-C3	4.39	1.54	1.36
63	H	401	UQ9	C7-C8	4.14	1.56	1.50
74	BC	402	HEM	FE-NB	4.07	2.17	1.96
74	AC	402	HEM	C1B-NB	-4.07	1.33	1.40
73	y	302	COO	C5A-N7A	-4.06	1.25	1.39
74	BC	401	HEM	C4D-ND	-4.00	1.33	1.40
74	BC	402	HEM	C4D-ND	-3.96	1.33	1.40
74	AE	401	HEM	C3C-C2C	-3.93	1.34	1.40
74	AC	402	HEM	C4D-ND	-3.88	1.33	1.40
74	AE	401	HEM	C3C-CAC	3.82	1.55	1.47
74	AC	401	HEM	C3C-CAC	3.80	1.55	1.47
74	AC	401	HEM	C3C-C2C	-3.77	1.35	1.40
74	BE	401	HEM	C4D-ND	-3.66	1.34	1.40
74	BE	401	HEM	C4B-NB	-3.66	1.31	1.38
74	BC	402	HEM	C4B-NB	-3.60	1.31	1.38
73	y	302	COO	C2X-C1X	-3.46	1.48	1.53
74	AC	402	HEM	C4B-NB	-3.42	1.31	1.38
74	AC	402	HEM	FE-NB	3.41	2.13	1.96
73	y	302	COO	P3X-O3X	3.36	1.65	1.59
74	BC	401	HEM	O2A-CGA	-3.35	1.19	1.30
65	M	501	3PH	P-O11	3.31	1.70	1.60
65	f	202	3PH	P-O11	3.29	1.70	1.60
65	BJ	102	3PH	P-O11	3.29	1.70	1.60
65	AI	101	3PH	P-O11	3.26	1.70	1.60
65	BC	405	3PH	P-O11	3.26	1.70	1.60
65	BJ	101	3PH	P-O11	3.25	1.70	1.60
65	l	201	3PH	P-O11	3.23	1.70	1.60
65	f	201	3PH	P-O11	3.23	1.70	1.60
58	A	201	PGT	O3-C11	3.17	1.42	1.33
58	AF	201	PGT	O3-C11	3.16	1.42	1.33
74	BC	402	HEM	C1D-ND	-3.15	1.32	1.38
73	y	302	COO	C6A-N6A	3.14	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AC	407	PGT	O3-C11	3.10	1.42	1.33
58	L	704	PGT	O3-C11	3.10	1.42	1.33
58	AC	407	PGT	O2-C31	3.07	1.43	1.34
74	BE	401	HEM	O2A-CGA	-2.99	1.20	1.30
74	AC	401	HEM	CAB-C3B	2.98	1.55	1.47
74	AC	402	HEM	O2D-CGD	-2.95	1.20	1.30
58	AF	201	PGT	O2-C31	2.90	1.42	1.34
64	K	201	Q7G	O1B-C1B	2.89	1.45	1.40
58	A	201	PGT	O2-C31	2.86	1.42	1.34
58	y	303	PGT	O2-C31	2.86	1.42	1.34
74	BC	402	HEM	O2A-CGA	-2.85	1.21	1.30
74	AE	401	HEM	CAB-C3B	2.85	1.55	1.47
67	L	707	UQ5	C4-C5	-2.85	1.40	1.48
74	BE	401	HEM	FE-NB	2.84	2.10	1.96
74	BE	401	HEM	C1D-ND	-2.84	1.33	1.38
72	u	101	CDL	OA6-CA4	-2.79	1.39	1.46
58	y	303	PGT	O3-C11	2.79	1.41	1.33
74	BC	401	HEM	FE-NB	2.75	2.10	1.96
67	AC	403	UQ5	C3-C2	-2.74	1.41	1.48
58	L	704	PGT	O2-C31	2.72	1.42	1.34
72	BG	101	CDL	OA6-CA4	-2.70	1.39	1.46
72	u	102	CDL	OA6-CA4	-2.70	1.39	1.46
74	AC	402	HEM	C1D-ND	-2.68	1.33	1.38
74	BC	401	HEM	C1D-ND	-2.68	1.33	1.38
74	AC	402	HEM	O2A-CGA	-2.65	1.21	1.30
66	L	706	PC7	O2-C2	-2.64	1.40	1.46
60	z	301	PTY	O7-C6	-2.63	1.40	1.46
73	y	302	COO	C3-C4	2.60	1.56	1.51
66	AG	101	PC7	O2-C2	-2.60	1.40	1.46
72	BG	101	CDL	OB6-CB4	-2.59	1.40	1.46
64	BC	410	Q7G	C11-C08	-2.58	1.51	1.56
64	H	402	Q7G	C11-C08	-2.57	1.51	1.56
63	H	401	UQ9	C11-C9	2.57	1.56	1.51
60	L	705	PTY	O7-C6	-2.56	1.40	1.46
72	BE	402	CDL	OB6-CB4	-2.55	1.40	1.46
74	BE	401	HEM	C3C-C2C	-2.54	1.36	1.40
60	z	301	PTY	O4-C1	-2.54	1.39	1.45
72	u	101	CDL	OA8-CA7	2.53	1.40	1.33
60	D	401	PTY	O7-C6	-2.52	1.40	1.46
64	M	505	Q7G	C11-C08	-2.51	1.51	1.56
60	BF	201	PTY	O7-C6	-2.51	1.40	1.46
72	u	101	CDL	OB6-CB5	2.50	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	BE	401	HEM	O2D-CGD	-2.50	1.22	1.30
72	u	101	CDL	OB8-CB7	2.50	1.40	1.33
72	u	102	CDL	OB6-CB4	-2.49	1.40	1.46
74	BC	401	HEM	O2D-CGD	-2.48	1.22	1.30
60	L	705	PTY	O4-C30	2.47	1.40	1.33
72	u	102	CDL	OB8-CB7	2.47	1.40	1.33
72	BG	101	CDL	OB8-CB7	2.47	1.40	1.33
72	BG	101	CDL	OA8-CA7	2.47	1.40	1.33
63	H	401	UQ9	C16-C14	2.46	1.56	1.51
66	v	201	PC7	O3-C11	2.46	1.40	1.33
72	BE	402	CDL	OA8-CA7	2.44	1.40	1.33
75	BC	404	UQ7	C3-C4	-2.43	1.41	1.48
72	BE	402	CDL	OB8-CB7	2.42	1.40	1.33
60	D	401	PTY	O4-C30	2.41	1.40	1.33
66	L	706	PC7	O3-C11	2.41	1.40	1.33
72	u	102	CDL	OA8-CA7	2.40	1.40	1.33
74	BC	401	HEM	C3D-C2D	-2.39	1.31	1.36
66	AG	101	PC7	O3-C11	2.39	1.40	1.33
64	BC	411	Q7G	C11-C08	-2.39	1.52	1.56
74	BC	401	HEM	C4B-NB	-2.38	1.33	1.38
63	H	401	UQ9	C21-C19	2.38	1.56	1.51
66	v	201	PC7	O2-C2	-2.37	1.40	1.46
74	BC	402	HEM	O2D-CGD	-2.37	1.22	1.30
67	AC	403	UQ5	C4-C5	-2.36	1.42	1.48
66	v	201	PC7	O3-C3	-2.35	1.39	1.45
60	BF	201	PTY	O4-C30	2.35	1.40	1.33
63	H	401	UQ9	C26-C24	2.33	1.56	1.51
73	y	302	COO	P1A-O5X	2.31	1.68	1.59
72	BE	402	CDL	OA6-CA5	2.30	1.40	1.34
58	AC	407	PGT	P-O3P	2.28	1.68	1.59
74	BC	401	HEM	C1B-C2B	-2.28	1.40	1.44
72	u	101	CDL	OA8-CA6	-2.28	1.40	1.45
73	y	302	COO	O3-C4	-2.28	1.18	1.23
63	H	401	UQ9	C7-C6	2.27	1.55	1.51
60	L	705	PTY	O4-C1	-2.26	1.40	1.45
63	H	401	UQ9	O4-C4M	-2.25	1.40	1.45
58	L	704	PGT	P-O3P	2.23	1.68	1.59
74	BE	401	HEM	C1B-C2B	-2.23	1.40	1.44
64	K	201	Q7G	O1C-C1C	2.21	1.44	1.40
58	y	303	PGT	P-O3P	2.20	1.68	1.59
58	AF	201	PGT	P-O3P	2.19	1.68	1.59
58	A	201	PGT	P-O3P	2.19	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	u	102	CDL	OB6-CB5	2.17	1.40	1.34
60	BF	201	PTY	O7-C8	2.17	1.40	1.34
60	L	705	PTY	O7-C8	2.16	1.40	1.34
66	AG	101	PC7	O3-C3	-2.16	1.40	1.45
58	L	704	PGT	O2-C2	-2.16	1.41	1.46
72	BE	402	CDL	OA6-CA4	-2.16	1.41	1.46
72	BE	402	CDL	OA8-CA6	-2.16	1.40	1.45
75	BC	404	UQ7	C2-C1	-2.15	1.42	1.48
72	BG	101	CDL	OA8-CA6	-2.14	1.40	1.45
60	D	401	PTY	O7-C8	2.14	1.40	1.34
60	D	401	PTY	O4-C1	-2.14	1.40	1.45
72	BE	402	CDL	OB8-CB6	-2.14	1.40	1.45
58	A	201	PGT	O2-C2	-2.14	1.41	1.46
72	BG	101	CDL	OA6-CA5	2.12	1.40	1.34
72	BE	402	CDL	OB6-CB5	2.12	1.40	1.34
74	AC	401	HEM	CMB-C2B	2.12	1.55	1.50
74	AC	401	HEM	FE-ND	2.11	2.07	1.96
72	BG	101	CDL	OB6-CB5	2.11	1.40	1.34
60	BF	201	PTY	O4-C1	-2.11	1.40	1.45
66	L	706	PC7	O3-C3	-2.11	1.40	1.45
63	H	401	UQ9	O5-C5	-2.10	1.18	1.23
72	BG	101	CDL	OB8-CB6	-2.10	1.40	1.45
66	AG	101	PC7	O2-C31	2.09	1.40	1.34
66	v	201	PC7	O2-C31	2.08	1.40	1.34
58	y	303	PGT	O3-C3	-2.08	1.40	1.45
64	H	402	Q7G	O1B-C1B	2.08	1.43	1.40
64	H	402	Q7G	O1C-C1C	2.08	1.43	1.40
72	u	101	CDL	OB6-CB4	-2.07	1.41	1.46
60	z	301	PTY	O4-C30	2.06	1.39	1.33
63	H	401	UQ9	C6-C5	2.05	1.52	1.46
74	AC	401	HEM	FE-NB	2.05	2.07	1.96
72	u	102	CDL	OA8-CA6	-2.05	1.40	1.45
72	u	101	CDL	OB8-CB6	-2.04	1.40	1.45
72	u	102	CDL	OA6-CA5	2.03	1.40	1.34
72	u	102	CDL	OB8-CB6	-2.03	1.40	1.45
73	y	302	COO	O2-C1	-2.02	1.19	1.23
74	BE	401	HEM	FE-ND	-2.02	1.86	1.96
67	L	707	UQ5	C3-C2	-2.01	1.43	1.48
74	AC	402	HEM	C1B-C2B	-2.01	1.40	1.44
74	BC	402	HEM	C3B-C4B	2.01	1.48	1.44

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	y	302	COO	C4A-C5A-N7A	-13.98	94.83	109.40
63	H	401	UQ9	C7-C8-C9	-7.98	113.50	126.79
74	BE	401	HEM	CHC-C4B-NB	7.95	133.06	124.43
73	y	302	COO	C6-S1-C7	7.70	109.48	99.80
74	AC	402	HEM	C1B-NB-C4B	6.12	111.40	105.07
74	BC	402	HEM	C1B-NB-C4B	6.11	111.38	105.07
74	BE	401	HEM	C1B-NB-C4B	5.66	110.92	105.07
74	BE	401	HEM	CHD-C1D-ND	5.11	129.98	124.43
64	M	505	Q7G	C05-C06-C02	-4.82	97.49	103.91
74	BE	401	HEM	O2A-CGA-O1A	-4.75	111.45	123.30
74	BC	402	HEM	CHC-C4B-NB	4.65	129.48	124.43
74	AC	402	HEM	CHC-C4B-NB	4.63	129.46	124.43
63	H	401	UQ9	C7-C6-C5	4.63	124.05	118.48
73	y	302	COO	C2A-N1A-C6A	4.59	126.60	118.75
74	BC	401	HEM	C1B-NB-C4B	4.56	109.78	105.07
64	K	201	Q7G	C15-C07-C06	-4.37	104.58	110.91
66	v	201	PC7	O2-C31-C32	4.34	120.86	111.50
72	BE	402	CDL	OA6-CA5-C11	4.29	120.76	111.50
71	T	200	8Q1	C37-C38-C39	-4.20	105.37	112.36
74	BC	401	HEM	CHC-C4B-NB	4.17	128.96	124.43
58	A	201	PGT	O2-C31-C32	4.07	120.28	111.50
64	K	201	Q7G	C76-C73-C74	-4.05	107.36	115.69
72	u	102	CDL	OB6-CB5-C51	4.04	120.22	111.50
60	z	301	PTY	O7-C8-C11	3.97	120.05	111.50
72	BG	101	CDL	OA6-CA5-C11	3.94	120.00	111.50
58	L	704	PGT	O2-C31-C32	3.92	119.96	111.50
58	AC	407	PGT	O2-C31-C32	3.92	119.96	111.50
58	y	303	PGT	O2-C31-C32	3.92	119.95	111.50
64	M	505	Q7G	CG1-C22-C23	-3.91	108.93	113.88
72	BE	402	CDL	OB6-CB5-C51	3.89	119.89	111.50
72	BG	101	CDL	OB6-CB5-C51	3.88	119.86	111.50
58	AF	201	PGT	O2-C31-C32	3.86	119.83	111.50
74	AC	402	HEM	C4C-CHD-C1D	3.86	127.65	122.56
64	BC	410	Q7G	C02-C06-C07	-3.86	108.66	114.38
60	L	705	PTY	O7-C8-C11	3.85	119.80	111.50
74	BC	402	HEM	C4B-CHC-C1C	3.84	127.62	122.56
64	M	505	Q7G	C16-C13-C11	3.82	121.50	116.42
64	K	201	Q7G	O80-C73-C76	-3.82	107.22	110.77
60	BF	201	PTY	O7-C8-C11	3.81	119.72	111.50
66	AG	101	PC7	O2-C31-C32	3.80	119.69	111.50
64	M	505	Q7G	C09-C08-C11	-3.74	108.16	113.08
72	u	101	CDL	OA6-CA5-C11	3.73	119.54	111.50
74	BC	402	HEM	CHA-C4D-ND	3.69	128.94	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	M	505	Q7G	C09-C10-C02	-3.65	106.53	112.78
64	M	505	Q7G	C76-C73-C74	-3.61	108.26	115.69
74	BC	402	HEM	C4D-ND-C1D	3.60	108.79	105.07
74	BC	401	HEM	O2A-CGA-O1A	-3.59	114.34	123.30
60	D	401	PTY	O7-C8-C11	3.59	119.23	111.50
72	u	102	CDL	OA6-CA5-C11	3.55	119.16	111.50
67	AC	404	UQ5	C7-C6-C5	-3.55	114.21	118.48
66	L	706	PC7	O2-C31-C32	3.53	119.11	111.50
73	y	302	COO	C3X-C2X-C1X	3.50	107.65	99.89
74	BC	401	HEM	CMD-C2D-C1D	3.45	130.29	125.04
64	K	201	Q7G	C16-C13-C14	-3.44	115.65	120.61
74	BC	401	HEM	CHD-C1D-ND	3.39	128.12	124.43
63	H	401	UQ9	C1M-C1-C6	-3.39	118.87	124.40
74	AC	401	HEM	C4D-ND-C1D	3.34	108.52	105.07
74	BE	401	HEM	CBA-CAA-C2A	3.33	118.30	112.62
64	BC	410	Q7G	C12-C11-C08	-3.30	107.75	111.68
74	AC	402	HEM	O2D-CGD-O1D	-3.29	115.10	123.30
74	AC	401	HEM	C1B-NB-C4B	3.27	108.45	105.07
72	u	101	CDL	OB6-CB5-C51	3.27	118.54	111.50
73	y	302	COO	C5A-C6A-N6A	-3.25	115.41	120.35
74	AC	401	HEM	C4B-CHC-C1C	3.24	126.83	122.56
74	BC	402	HEM	O2D-CGD-O1D	-3.20	115.32	123.30
64	a	101	Q7G	C02-C06-C07	-3.19	109.65	114.38
74	BE	401	HEM	CHD-C1D-C2D	-3.19	120.00	124.98
63	H	401	UQ9	C27-C26-C24	-3.18	109.42	114.62
64	BC	410	Q7G	C07-C15-C14	-3.17	108.17	112.73
64	BC	410	Q7G	CG1-C22-C23	-3.14	109.90	113.88
64	H	402	Q7G	C3B-C4B-C5B	-3.11	103.79	110.93
64	BC	411	Q7G	C19-C11-C08	3.11	113.07	108.73
64	H	402	Q7G	C09-C10-C02	-3.11	107.45	112.78
64	BC	410	Q7G	C02-C03-C74	-3.10	110.00	120.56
74	BE	401	HEM	O2A-CGA-CBA	3.10	124.00	114.03
72	u	101	CDL	OA8-CA7-C31	3.10	121.64	111.91
64	a	101	Q7G	C76-C73-C74	-3.09	109.33	115.69
63	H	401	UQ9	C22-C23-C24	-3.07	120.26	127.66
63	H	401	UQ9	C17-C18-C19	-3.06	120.30	127.66
64	BC	411	Q7G	C02-C06-C07	-3.05	109.86	114.38
64	M	505	Q7G	O80-C79-C78	-3.01	107.85	112.18
64	M	505	Q7G	C02-C03-C74	-3.00	110.35	120.56
74	BC	402	HEM	CHD-C1D-ND	2.99	127.68	124.43
63	H	401	UQ9	C12-C13-C14	-2.96	120.53	127.66
74	BE	401	HEM	CHA-C4D-ND	2.95	128.03	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	BC	410	Q7G	C76-C73-C74	-2.94	109.64	115.69
66	L	706	PC7	O3-C11-C12	2.93	121.10	111.91
74	BE	401	HEM	CHC-C4B-C3B	-2.92	120.10	124.57
74	BC	401	HEM	CHA-C4D-ND	2.91	127.97	124.38
64	BC	411	Q7G	C12-C11-C08	-2.89	108.23	111.68
74	AC	402	HEM	CHA-C4D-ND	2.89	127.95	124.38
73	y	302	COO	C5A-C6A-N1A	2.89	126.90	120.35
63	H	401	UQ9	C8-C7-C6	2.88	119.81	112.05
74	AE	401	HEM	C1B-NB-C4B	2.88	108.04	105.07
67	L	707	UQ5	C1-C6-C5	-2.87	116.88	119.58
63	H	401	UQ9	C20-C19-C21	2.87	120.10	115.27
58	AF	201	PGT	O3-C11-C12	2.87	120.90	111.91
74	BE	401	HEM	O2D-CGD-O1D	-2.86	116.16	123.30
66	v	201	PC7	O3-C11-C12	2.81	120.74	111.91
64	K	201	Q7G	O1B-C1B-C2B	2.78	112.65	108.30
64	M	505	Q7G	C02-C06-C07	-2.77	110.28	114.38
74	BC	402	HEM	C4B-C3B-C2B	-2.77	104.92	107.11
74	AE	401	HEM	C4D-ND-C1D	2.76	107.92	105.07
64	M	505	Q7G	C19-C11-C13	2.75	113.79	108.75
64	H	402	Q7G	C76-C73-C74	-2.73	110.07	115.69
64	K	201	Q7G	C81-C78-C79	-2.72	106.39	111.18
64	BC	411	Q7G	CG1-C22-C23	-2.72	110.44	113.88
64	BC	410	Q7G	C11-C08-C07	-2.72	108.66	112.73
64	H	402	Q7G	C02-C03-C74	-2.71	111.35	120.56
64	H	402	Q7G	C09-C08-C11	-2.70	109.52	113.08
72	u	102	CDL	OB8-CB7-C71	2.68	120.33	111.91
74	AC	402	HEM	CHD-C1D-ND	2.68	127.34	124.43
73	y	302	COO	C10-C9-C8	-2.68	120.06	125.34
64	M	505	Q7G	C12-C11-C08	-2.67	108.50	111.68
74	BC	402	HEM	O2D-CGD-CBD	2.66	122.56	114.03
64	a	101	Q7G	C02-C03-C74	-2.65	111.56	120.56
60	D	401	PTY	O4-C30-C31	2.64	120.18	111.91
74	BC	402	HEM	O2A-CGA-O1A	-2.63	116.74	123.30
63	H	401	UQ9	C25-C24-C26	2.63	119.69	115.27
72	u	101	CDL	OB8-CB7-C71	2.62	120.14	111.91
74	BC	401	HEM	O2D-CGD-CBD	2.62	122.45	114.03
64	BC	411	Q7G	C09-C10-C02	-2.62	108.29	112.78
64	H	402	Q7G	C12-C11-C08	-2.61	108.57	111.68
67	L	707	UQ5	C7-C6-C5	2.61	121.62	118.48
74	BC	401	HEM	CHB-C1B-NB	2.60	127.59	124.38
74	BC	401	HEM	CBD-CAD-C3D	-2.59	105.44	112.63
64	BC	411	Q7G	C02-C03-C74	-2.58	111.78	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	303	PGT	O3-C11-C12	2.58	119.99	111.91
64	K	201	Q7G	CG1-C22-C23	-2.57	110.62	113.88
74	AC	401	HEM	C4C-CHD-C1D	2.57	125.95	122.56
64	K	201	Q7G	C02-C03-C74	-2.56	111.84	120.56
72	BE	402	CDL	OA8-CA7-C31	2.56	119.94	111.91
73	y	302	COO	P1A-O3A-P2A	-2.55	124.09	132.83
74	AE	401	HEM	C4B-CHC-C1C	2.54	125.91	122.56
72	BG	101	CDL	OB8-CB7-C71	2.53	119.86	111.91
74	BE	401	HEM	C4D-ND-C1D	2.53	107.69	105.07
60	BF	201	PTY	O4-C30-C31	2.53	119.85	111.91
58	AC	407	PGT	O3-C11-C12	2.53	119.85	111.91
63	H	401	UQ9	C15-C14-C16	2.53	119.52	115.27
72	u	102	CDL	OA8-CA7-C31	2.53	119.83	111.91
64	a	101	Q7G	C12-C11-C08	-2.51	108.68	111.68
72	BG	101	CDL	OA8-CA7-C31	2.51	119.77	111.91
66	AG	101	PC7	O3-C11-C12	2.50	119.77	111.91
64	H	402	Q7G	C05-C06-C02	-2.50	100.58	103.91
64	BC	411	Q7G	C11-C08-C07	-2.50	108.99	112.73
74	BC	402	HEM	CBD-CAD-C3D	-2.49	105.72	112.63
64	M	505	Q7G	C75-C74-C03	-2.48	109.00	114.50
73	y	302	COO	C1X-N9A-C4A	-2.47	122.30	126.64
66	v	201	PC7	C2-O2-C31	-2.47	111.70	117.79
74	BC	401	HEM	CHD-C1D-C2D	-2.46	121.14	124.98
74	AE	401	HEM	CAA-CBA-CGA	-2.46	106.87	113.76
64	a	101	Q7G	O80-C79-C78	-2.45	108.65	112.18
72	BE	402	CDL	OB8-CB7-C71	2.45	119.60	111.91
74	AC	402	HEM	CBD-CAD-C3D	-2.45	105.82	112.63
74	BC	401	HEM	O2D-CGD-O1D	-2.45	117.20	123.30
64	K	201	Q7G	C76-C77-C78	-2.45	106.65	111.81
64	BC	411	Q7G	C76-C73-C74	-2.44	110.67	115.69
58	A	201	PGT	O3-C11-C12	2.44	119.56	111.91
58	L	704	PGT	O3-C11-C12	2.44	119.56	111.91
67	L	707	UQ5	C3-C4-C5	-2.43	115.90	120.68
65	f	202	3PH	O13-P-O11	-2.42	100.28	106.73
64	K	201	Q7G	C61-C51-C41	-2.42	107.33	113.00
64	M	505	Q7G	C01-C02-C06	-2.42	107.21	111.71
64	a	101	Q7G	C08-C11-C13	2.40	113.42	109.65
64	M	505	Q7G	C15-C07-C08	-2.39	106.81	109.71
69	P	500	NDP	C5A-C6A-N6A	2.38	123.97	120.35
64	H	402	Q7G	CF1-O11-C4C	-2.38	112.08	117.96
75	BC	404	UQ7	C17-C16-C14	2.38	120.79	112.98
64	a	101	Q7G	CG1-C22-C23	-2.37	110.89	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	BC	401	HEM	O2A-CGA-CBA	2.36	121.62	114.03
65	f	201	3PH	C3-C2-C1	2.35	117.36	111.79
64	BC	411	Q7G	C17-C16-C13	-2.34	107.88	111.52
60	z	301	PTY	O4-C30-C31	2.34	119.24	111.91
64	BC	410	Q7G	C09-C08-C11	-2.33	110.00	113.08
64	a	101	Q7G	C75-C74-C73	-2.33	110.67	114.92
64	K	201	Q7G	C1C-O5C-C5C	2.32	118.25	113.69
65	l	201	3PH	O13-P-O11	-2.32	100.56	106.73
65	BC	405	3PH	O13-P-O11	-2.31	100.58	106.73
64	H	402	Q7G	C75-C74-C73	-2.31	110.70	114.92
65	L	701	3PH	O21-C21-C22	-2.30	106.54	111.50
72	BG	101	CDL	CA4-OA6-CA5	-2.30	112.14	117.79
64	M	505	Q7G	C16-C13-C14	-2.29	117.30	120.61
65	M	501	3PH	O13-P-O11	-2.29	100.63	106.73
64	BC	411	Q7G	C15-C07-C06	-2.29	107.59	110.91
60	L	705	PTY	O4-C30-C31	2.29	119.08	111.91
66	L	706	PC7	C2-O2-C31	-2.28	112.17	117.79
74	BC	401	HEM	C4B-C3B-C2B	-2.28	105.30	107.11
74	AE	401	HEM	C3B-C2B-C1B	2.27	108.17	106.49
74	AE	401	HEM	CMC-C2C-C3C	2.26	128.91	124.68
74	AE	401	HEM	C3D-C4D-ND	-2.26	107.65	110.17
64	K	201	Q7G	C05-C06-C02	-2.26	100.90	103.91
75	BC	404	UQ7	C16-C17-C18	2.26	119.31	111.88
64	K	201	Q7G	O80-C73-C74	2.24	115.24	107.38
74	BE	401	HEM	CHB-C1B-NB	2.24	127.14	124.38
64	M	505	Q7G	C10-C02-C03	-2.23	111.89	115.46
64	BC	411	Q7G	C16-C13-C14	-2.22	117.41	120.61
63	H	401	UQ9	C6-C1-C2	2.22	120.94	119.18
64	BC	410	Q7G	C09-C10-C02	-2.21	108.99	112.78
64	K	201	Q7G	C77-C76-C73	-2.21	108.12	111.93
74	AC	401	HEM	CMC-C2C-C3C	2.20	128.80	124.68
65	L	701	3PH	C3-C2-C1	2.19	116.96	111.79
65	f	201	3PH	O13-P-O11	-2.19	100.92	106.73
74	AC	402	HEM	CHB-C1B-NB	2.18	127.08	124.38
64	K	201	Q7G	O72-C73-C76	2.18	113.64	108.60
65	BJ	101	3PH	O13-P-O11	-2.18	100.94	106.73
65	AI	101	3PH	O13-P-O11	-2.17	100.97	106.73
64	K	201	Q7G	C48-O1C-C1C	2.17	117.97	113.74
64	a	101	Q7G	C07-C15-C14	-2.16	109.63	112.73
74	AC	401	HEM	C3D-C4D-ND	-2.16	107.76	110.17
64	M	505	Q7G	C10-C02-C06	2.16	110.62	107.27
74	BE	401	HEM	CBD-CAD-C3D	-2.14	106.69	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	y	302	COO	C2X-C3X-C4X	2.14	107.01	103.22
74	BC	402	HEM	C4A-C3A-C2A	2.13	108.48	107.00
63	H	401	UQ9	C10-C9-C8	-2.12	118.23	123.68
65	BJ	102	3PH	O13-P-O11	-2.12	101.09	106.73
74	AE	401	HEM	CBD-CAD-C3D	-2.12	106.75	112.63
75	BC	404	UQ7	C11-C12-C13	2.12	118.84	111.88
74	BC	402	HEM	O2A-CGA-CBA	2.11	120.80	114.03
64	BC	411	Q7G	C75-C74-C03	-2.10	109.83	114.50
74	BC	401	HEM	CAD-C3D-C4D	2.10	128.33	124.66
64	K	201	Q7G	C08-C07-C06	-2.10	106.28	109.09
64	BC	410	Q7G	C75-C74-C03	-2.10	109.84	114.50
60	z	301	PTY	C6-O7-C8	-2.09	112.66	117.79
64	BC	411	Q7G	C16-C13-C11	2.08	119.19	116.42
64	K	201	Q7G	C03-C02-C06	-2.08	97.17	100.23
65	f	202	3PH	O14-P-O13	2.08	115.57	107.64
74	BC	402	HEM	CHA-C4D-C3D	-2.07	121.44	125.33
62	F	500	FMN	C4-N3-C2	-2.07	121.81	125.64
74	AC	402	HEM	CAD-CBD-CGD	2.06	118.04	113.60
67	BC	403	UQ5	C6-C1-C2	2.06	120.81	119.18
74	AE	401	HEM	CHC-C4B-NB	2.04	126.65	124.43
64	K	201	Q7G	C19-C11-C08	2.04	111.57	108.73
71	T	200	8Q1	C42-N41-C39	2.04	126.62	122.84
74	BE	401	HEM	CMC-C2C-C3C	2.03	128.48	124.68
65	AI	101	3PH	C3-C2-C1	2.03	116.58	111.79
64	H	402	Q7G	C08-C07-C06	-2.02	106.39	109.09
71	T	200	8Q1	C37-N36-C34	2.01	126.18	122.59
72	u	101	CDL	OA8-CA7-OA9	-2.01	118.51	123.59
74	AE	401	HEM	C4C-CHD-C1D	2.01	125.21	122.56
58	A	201	PGT	C2-O2-C31	-2.00	112.86	117.79
74	BC	402	HEM	C4C-CHD-C1D	2.00	125.20	122.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
73	y	302	COO	C13

All (1485) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
58	L	702	PGT	O31-C31-O2-C2
58	L	704	PGT	C32-C31-O2-C2
58	L	704	PGT	O2-C2-C3-O3
58	L	704	PGT	C1-O3P-P-O1P
58	M	502	PGT	C1-O3P-P-O1P
58	M	502	PGT	C4-O4P-P-O1P
58	M	502	PGT	C4-O4P-P-O2P
58	M	502	PGT	C4-C5-C6-O6
58	y	303	PGT	O2-C2-C3-O3
58	AC	406	PGT	C1-O3P-P-O1P
58	AC	406	PGT	C4-O4P-P-O1P
58	AC	406	PGT	C4-O4P-P-O2P
58	AC	406	PGT	C4-C5-C6-O6
58	AC	407	PGT	C32-C31-O2-C2
58	AC	407	PGT	C4-C5-C6-O6
58	AF	201	PGT	C1-O3P-P-O2P
58	AF	201	PGT	C1-O3P-P-O4P
58	AF	201	PGT	C4-O4P-P-O2P
58	BC	406	PGT	C32-C31-O2-C2
58	BC	406	PGT	O31-C31-O2-C2
58	BC	406	PGT	C1-O3P-P-O1P
58	BC	406	PGT	C1-O3P-P-O2P
58	BC	406	PGT	C1-O3P-P-O4P
58	BC	406	PGT	C4-O4P-P-O2P
58	BC	406	PGT	O4P-C4-C5-C6
58	BC	406	PGT	C4-C5-C6-O6
60	D	401	PTY	C3-O11-P1-O12
60	L	705	PTY	N1-C2-C3-O11
60	L	705	PTY	C2-C3-O11-P1
60	M	503	PTY	C11-C8-O7-C6
60	M	504	PTY	N1-C2-C3-O11
60	M	504	PTY	O10-C8-O7-C6
60	M	504	PTY	C11-C8-O7-C6
60	N	501	PTY	C3-O11-P1-O13
60	N	501	PTY	C5-O14-P1-O12
60	N	502	PTY	C2-C3-O11-P1
60	N	502	PTY	C3-O11-P1-O14
60	N	503	PTY	N1-C2-C3-O11
60	Y	202	PTY	O10-C8-O7-C6
60	Y	202	PTY	C11-C8-O7-C6
60	d	101	PTY	C3-O11-P1-O12
60	m	101	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
60	z	301	PTY	O10-C8-O7-C6
60	z	301	PTY	C11-C8-O7-C6
60	AB	602	PTY	N1-C2-C3-O11
60	BB	602	PTY	N1-C2-C3-O11
60	BB	602	PTY	O10-C8-O7-C6
60	BB	602	PTY	C11-C8-O7-C6
60	BF	201	PTY	N1-C2-C3-O11
60	BF	201	PTY	C3-O11-P1-O12
63	H	401	UQ9	C12-C11-C9-C10
63	H	401	UQ9	C12-C11-C9-C8
63	H	401	UQ9	C1-C6-C7-C8
63	H	401	UQ9	C5-C6-C7-C8
64	H	402	Q7G	CG1-C22-C23-C48
64	H	402	Q7G	C48-C23-C24-O1B
64	K	201	Q7G	C2B-C1B-O1B-C24
64	K	201	Q7G	O5B-C1B-O1B-C24
64	M	505	Q7G	C22-CG1-O20-C17
64	a	101	Q7G	C18-C17-O20-CG1
65	L	701	3PH	C22-C21-O21-C2
65	Y	201	3PH	C1-O11-P-O13
65	Y	201	3PH	C1-O11-P-O14
65	f	201	3PH	C1-O11-P-O13
65	f	201	3PH	C1-O11-P-O12
65	f	202	3PH	C22-C21-O21-C2
65	l	201	3PH	O22-C21-O21-C2
65	l	201	3PH	C22-C21-O21-C2
65	AC	405	3PH	C1-O11-P-O13
65	AC	405	3PH	C1-O11-P-O14
65	AC	405	3PH	O22-C21-O21-C2
65	AC	405	3PH	C22-C21-O21-C2
65	AI	101	3PH	C1-O11-P-O13
65	AI	101	3PH	C1-O11-P-O14
65	AI	101	3PH	C32-C31-O31-C3
65	BJ	101	3PH	C1-O11-P-O13
66	L	706	PC7	C32-C31-O2-C2
66	L	706	PC7	O31-C31-O2-C2
66	L	706	PC7	C4-O4P-P-O2P
66	L	706	PC7	O4P-C4-C5-N
66	f	203	PC7	C32-C31-O2-C2
66	f	203	PC7	O31-C31-O2-C2
66	f	203	PC7	C4-O4P-P-O1P
66	AB	603	PC7	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
66	AB	603	PC7	O31-C31-O2-C2
66	AB	603	PC7	C1-O3P-P-O2P
66	AC	410	PC7	C32-C31-O2-C2
66	AC	410	PC7	O31-C31-O2-C2
66	AG	101	PC7	C32-C31-O2-C2
66	BC	409	PC7	C32-C31-O2-C2
66	BC	409	PC7	O2-C2-C3-O3
66	BC	409	PC7	C4-O4P-P-O2P
66	BD	302	PC7	C32-C31-O2-C2
67	L	707	UQ5	C7-C8-C9-C10
67	L	707	UQ5	C7-C8-C9-C11
67	L	707	UQ5	C9-C11-C12-C13
67	L	707	UQ5	C14-C16-C17-C18
67	L	707	UQ5	C19-C21-C22-C23
67	L	707	UQ5	C27-C28-C29-C31
67	AC	403	UQ5	C7-C8-C9-C10
67	AC	403	UQ5	C7-C8-C9-C11
67	AC	403	UQ5	C12-C13-C14-C15
67	AC	403	UQ5	C17-C18-C19-C20
67	BC	403	UQ5	C9-C11-C12-C13
71	T	200	8Q1	C28-C29-C32-C34
71	T	200	8Q1	C30-C29-C32-C34
71	T	200	8Q1	C30-C29-C32-O33
71	T	200	8Q1	C31-C29-C32-C34
71	T	200	8Q1	C32-C34-N36-C37
71	T	200	8Q1	O35-C34-N36-C37
71	T	200	8Q1	C38-C39-N41-C42
71	T	200	8Q1	O40-C39-N41-C42
71	T	200	8Q1	N41-C42-C43-S44
71	T	200	8Q1	C28-O27-P24-O2
71	T	200	8Q1	C28-O27-P24-O1
71	W	200	8Q1	O27-C28-C29-C32
71	W	200	8Q1	C29-C28-O27-P24
71	W	200	8Q1	C28-C29-C32-C34
71	W	200	8Q1	C28-C29-C32-O33
71	W	200	8Q1	C30-C29-C32-O33
71	W	200	8Q1	C31-C29-C32-C34
71	W	200	8Q1	C31-C29-C32-O33
71	W	200	8Q1	C28-O27-P24-O1
72	u	101	CDL	O1-C1-CB2-OB2
72	u	101	CDL	OA9-CA7-OA8-CA6
72	u	101	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
72	u	102	CDL	CB3-OB5-PB2-OB4
72	u	102	CDL	OB7-CB5-OB6-CB4
72	u	102	CDL	C51-CB5-OB6-CB4
72	AC	408	CDL	C11-CA5-OA6-CA4
72	AC	408	CDL	CB2-OB2-PB2-OB4
72	AC	408	CDL	OB5-CB3-CB4-OB6
72	AC	408	CDL	C51-CB5-OB6-CB4
72	AC	409	CDL	CA2-C1-CB2-OB2
72	AC	409	CDL	CB2-OB2-PB2-OB3
72	AE	402	CDL	C11-CA5-OA6-CA4
72	AE	402	CDL	CB3-OB5-PB2-OB4
72	BC	407	CDL	CA2-OA2-PA1-OA3
72	BC	407	CDL	OA7-CA5-OA6-CA4
72	BC	407	CDL	C11-CA5-OA6-CA4
72	BC	407	CDL	CB2-OB2-PB2-OB3
72	BC	407	CDL	CB2-OB2-PB2-OB4
72	BC	408	CDL	CB2-OB2-PB2-OB4
72	BC	408	CDL	CB3-OB5-PB2-OB2
72	BC	408	CDL	CB3-OB5-PB2-OB3
72	BC	408	CDL	CB3-OB5-PB2-OB4
72	BE	402	CDL	CA6-CA4-OA6-CA5
72	BE	402	CDL	C11-CA5-OA6-CA4
72	BE	402	CDL	CB3-OB5-PB2-OB2
72	BE	402	CDL	CB3-OB5-PB2-OB3
72	BE	402	CDL	CB3-OB5-PB2-OB4
72	BG	101	CDL	CA3-OA5-PA1-OA3
72	BG	101	CDL	CA3-OA5-PA1-OA4
72	BG	101	CDL	C11-CA5-OA6-CA4
72	BG	101	CDL	CB4-CB3-OB5-PB2
73	y	302	COO	C5X-O5X-P1A-O2A
73	y	302	COO	C5X-O5X-P1A-O1A
73	y	302	COO	C5-C6-S1-C7
73	y	302	COO	S1-C7-C8-C9
75	BC	404	UQ7	C17-C18-C19-C20
75	BC	404	UQ7	C17-C18-C19-C21
75	BC	404	UQ7	C18-C19-C21-C22
75	BC	404	UQ7	C20-C19-C21-C22
58	M	502	PGT	O11-C11-O3-C3
60	N	501	PTY	O30-C30-O4-C1
60	BB	602	PTY	O30-C30-O4-C1
65	AI	101	3PH	O32-C31-O31-C3
66	BD	302	PC7	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
72	AC	409	CDL	OB9-CB7-OB8-CB6
58	M	502	PGT	C12-C11-O3-C3
60	N	501	PTY	C31-C30-O4-C1
60	BB	602	PTY	C31-C30-O4-C1
66	BD	302	PC7	C12-C11-O3-C3
72	AC	409	CDL	C71-CB7-OB8-CB6
67	L	707	UQ5	C27-C28-C29-C30
58	AF	201	PGT	O11-C11-O3-C3
60	M	503	PTY	O30-C30-O4-C1
65	BC	405	3PH	O32-C31-O31-C3
65	BJ	101	3PH	O32-C31-O31-C3
72	AE	402	CDL	OB9-CB7-OB8-CB6
72	BG	101	CDL	OB9-CB7-OB8-CB6
58	A	201	PGT	O31-C31-O2-C2
58	L	704	PGT	O31-C31-O2-C2
58	AC	407	PGT	O31-C31-O2-C2
60	M	503	PTY	O10-C8-O7-C6
60	N	502	PTY	O10-C8-O7-C6
65	L	701	3PH	O22-C21-O21-C2
66	AG	101	PC7	O31-C31-O2-C2
66	BC	409	PC7	O31-C31-O2-C2
72	AC	408	CDL	OA7-CA5-OA6-CA4
72	AC	408	CDL	OB7-CB5-OB6-CB4
72	AE	402	CDL	OA7-CA5-OA6-CA4
72	BG	101	CDL	OA7-CA5-OA6-CA4
65	BJ	101	3PH	C32-C31-O31-C3
72	BG	101	CDL	C71-CB7-OB8-CB6
60	N	502	PTY	C11-C8-O7-C6
72	AE	402	CDL	OA9-CA7-OA8-CA6
58	AF	201	PGT	C12-C11-O3-C3
60	M	503	PTY	C31-C30-O4-C1
60	M	504	PTY	C31-C30-O4-C1
65	BC	405	3PH	C32-C31-O31-C3
66	d	102	PC7	C12-C11-O3-C3
72	AE	402	CDL	C71-CB7-OB8-CB6
67	L	707	UQ5	C17-C18-C19-C20
65	f	202	3PH	O22-C21-O21-C2
66	BD	302	PC7	O31-C31-O2-C2
72	BE	402	CDL	OA7-CA5-OA6-CA4
67	L	707	UQ5	C17-C18-C19-C21
67	AC	403	UQ5	C17-C18-C19-C21
66	d	102	PC7	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
58	BC	406	PGT	O4P-C4-C5-O5
72	BE	402	CDL	O1-C1-CA2-OA2
72	BG	101	CDL	O1-C1-CA2-OA2
58	L	702	PGT	C12-C11-O3-C3
60	d	101	PTY	C31-C30-O4-C1
72	AE	402	CDL	C31-CA7-OA8-CA6
72	AC	409	CDL	C51-CB5-OB6-CB4
72	AC	409	CDL	C19-C20-C21-C22
60	N	502	PTY	C12-C13-C14-C15
60	d	101	PTY	C17-C18-C19-C20
66	f	203	PC7	C41-C42-C43-C44
72	AC	409	CDL	C40-C41-C42-C43
66	v	201	PC7	C2-C1-O3P-P
60	M	504	PTY	O30-C30-O4-C1
67	L	707	UQ5	C12-C11-C9-C10
67	AC	403	UQ5	C15-C14-C16-C17
67	BC	403	UQ5	C25-C24-C26-C27
75	BC	404	UQ7	C15-C14-C16-C17
75	BC	404	UQ7	C25-C24-C26-C27
67	L	707	UQ5	C12-C11-C9-C8
67	AC	403	UQ5	C13-C14-C16-C17
67	BC	403	UQ5	C23-C24-C26-C27
75	BC	404	UQ7	C13-C14-C16-C17
75	BC	404	UQ7	C23-C24-C26-C27
60	AB	602	PTY	C15-C16-C17-C18
72	AC	408	CDL	C55-C56-C57-C58
67	AC	404	UQ5	C14-C16-C17-C18
67	AC	404	UQ5	C19-C21-C22-C23
67	AC	404	UQ5	C24-C26-C27-C28
67	BC	403	UQ5	C19-C21-C22-C23
73	y	302	COO	C4X-C3X-O3X-P3X
72	BC	407	CDL	C56-C57-C58-C59
65	L	701	3PH	C22-C23-C24-C25
58	L	702	PGT	O11-C11-O3-C3
60	d	101	PTY	O30-C30-O4-C1
58	L	702	PGT	O4P-C4-C5-C6
58	y	303	PGT	O4P-C4-C5-C6
72	BG	101	CDL	CB2-C1-CA2-OA2
66	v	201	PC7	C4-C5-N-C6
66	AC	410	PC7	C4-C5-N-C8
66	AC	410	PC7	C4-C5-N-C6
58	y	303	PGT	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
65	L	701	3PH	C32-C31-O31-C3
72	u	101	CDL	C71-CB7-OB8-CB6
58	y	303	PGT	C14-C15-C16-C17
60	M	504	PTY	C8-C11-C12-C13
60	D	401	PTY	C35-C36-C37-C38
58	L	702	PGT	O4P-C4-C5-O5
58	BC	406	PGT	O2-C2-C3-O3
58	AC	406	PGT	C44-C45-C46-C47
72	BG	101	CDL	C40-C41-C42-C43
72	AC	409	CDL	OB7-CB5-OB6-CB4
60	z	301	PTY	C31-C32-C33-C34
60	z	301	PTY	C38-C39-C40-C41
65	AC	405	3PH	C31-C32-C33-C34
65	BC	405	3PH	C21-C22-C23-C24
72	u	101	CDL	CB5-C51-C52-C53
69	P	500	NDP	C2D-C1D-N1N-C6N
65	L	701	3PH	O32-C31-O31-C3
66	d	102	PC7	C17-C18-C19-C20
60	AB	602	PTY	C31-C30-O4-C1
72	BC	407	CDL	C71-CB7-OB8-CB6
58	y	303	PGT	C12-C13-C14-C15
72	u	101	CDL	C32-C33-C34-C35
58	A	201	PGT	O5-C5-C6-O6
58	AC	407	PGT	O5-C5-C6-O6
58	BC	406	PGT	O5-C5-C6-O6
58	L	704	PGT	C31-C32-C33-C34
60	m	101	PTY	C30-C31-C32-C33
65	L	701	3PH	C21-C22-C23-C24
65	Y	201	3PH	C21-C22-C23-C24
65	BJ	101	3PH	C21-C22-C23-C24
65	BJ	102	3PH	C31-C32-C33-C34
72	u	101	CDL	CA5-C11-C12-C13
72	AC	409	CDL	CB5-C51-C52-C53
72	AE	402	CDL	CA5-C11-C12-C13
72	BC	408	CDL	CA7-C31-C32-C33
58	A	201	PGT	C17-C18-C19-C20
72	BC	408	CDL	C71-CB7-OB8-CB6
67	AC	403	UQ5	C12-C13-C14-C16
58	L	702	PGT	C31-C32-C33-C34
58	L	702	PGT	C11-C12-C13-C14
60	z	301	PTY	C8-C11-C12-C13
60	AB	602	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
72	AC	408	CDL	CA5-C11-C12-C13
58	L	703	PGT	C32-C31-O2-C2
64	H	402	Q7G	C22-C23-C24-O1B
60	AB	602	PTY	O30-C30-O4-C1
60	N	501	PTY	C8-C11-C12-C13
72	AE	402	CDL	C14-C15-C16-C17
72	BC	407	CDL	OB9-CB7-OB8-CB6
67	AC	403	UQ5	C9-C11-C12-C13
67	BC	403	UQ5	C24-C26-C27-C28
75	BC	404	UQ7	C29-C31-C32-C33
72	AE	402	CDL	CB5-C51-C52-C53
58	L	704	PGT	O4P-C4-C5-O5
58	M	502	PGT	O4P-C4-C5-O5
58	y	303	PGT	O4P-C4-C5-O5
72	AC	408	CDL	C31-CA7-OA8-CA6
72	BG	101	CDL	C31-CA7-OA8-CA6
58	A	201	PGT	C36-C37-C38-C39
58	y	303	PGT	O11-C11-O3-C3
72	u	101	CDL	OB9-CB7-OB8-CB6
60	d	101	PTY	C8-C11-C12-C13
72	AC	409	CDL	CA7-C31-C32-C33
72	BC	408	CDL	OB9-CB7-OB8-CB6
60	d	101	PTY	C11-C8-O7-C6
60	L	705	PTY	C16-C17-C18-C19
58	M	502	PGT	C4-O4P-P-O3P
58	y	303	PGT	C4-O4P-P-O3P
58	AC	406	PGT	C4-O4P-P-O3P
58	AF	201	PGT	C4-O4P-P-O3P
58	BC	406	PGT	C4-O4P-P-O3P
60	D	401	PTY	C3-O11-P1-O14
60	M	503	PTY	C3-O11-P1-O14
60	M	504	PTY	C3-O11-P1-O14
60	N	501	PTY	C5-O14-P1-O11
60	N	502	PTY	C5-O14-P1-O11
60	d	101	PTY	C3-O11-P1-O14
60	z	301	PTY	C3-O11-P1-O14
60	AB	602	PTY	C3-O11-P1-O14
60	BF	201	PTY	C3-O11-P1-O14
66	L	706	PC7	C4-O4P-P-O3P
66	f	203	PC7	C1-O3P-P-O4P
66	f	203	PC7	C4-O4P-P-O3P
66	AB	603	PC7	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
66	BC	409	PC7	C4-O4P-P-O3P
72	u	101	CDL	CB3-OB5-PB2-OB2
72	u	102	CDL	CB3-OB5-PB2-OB2
72	AC	408	CDL	CA2-OA2-PA1-OA5
72	AC	409	CDL	CB2-OB2-PB2-OB5
72	AC	409	CDL	CB3-OB5-PB2-OB2
72	AE	402	CDL	CB3-OB5-PB2-OB2
72	BC	407	CDL	CB2-OB2-PB2-OB5
72	BC	408	CDL	CB2-OB2-PB2-OB5
72	BG	101	CDL	CA3-OA5-PA1-OA2
72	BG	101	CDL	CB2-OB2-PB2-OB5
65	M	501	3PH	C31-C32-C33-C34
58	A	201	PGT	O4P-C4-C5-C6
58	L	704	PGT	O4P-C4-C5-C6
58	M	502	PGT	O4P-C4-C5-C6
58	AF	201	PGT	O4P-C4-C5-C6
72	u	101	CDL	CA2-C1-CB2-OB2
72	BE	402	CDL	CB2-C1-CA2-OA2
58	L	703	PGT	O31-C31-O2-C2
60	d	101	PTY	O10-C8-O7-C6
67	BC	403	UQ5	C12-C11-C9-C10
66	v	201	PC7	C4-C5-N-C8
66	BC	409	PC7	C4-C5-N-C7
66	BC	409	PC7	C4-C5-N-C8
66	BC	409	PC7	C4-C5-N-C6
65	M	501	3PH	C21-C22-C23-C24
72	BC	408	CDL	CB5-C51-C52-C53
58	BC	406	PGT	C13-C14-C15-C16
65	M	501	3PH	C36-C37-C38-C39
65	Y	201	3PH	C33-C34-C35-C36
72	BC	408	CDL	C35-C36-C37-C38
66	v	201	PC7	C32-C31-O2-C2
72	BC	408	CDL	C11-CA5-OA6-CA4
58	L	704	PGT	C15-C16-C17-C18
58	y	303	PGT	C33-C34-C35-C36
58	AC	407	PGT	C15-C16-C17-C18
58	AF	201	PGT	C42-C43-C44-C45
58	BC	406	PGT	C15-C16-C17-C18
60	L	705	PTY	C35-C36-C37-C38
60	N	503	PTY	C11-C12-C13-C14
60	BF	201	PTY	C34-C35-C36-C37
65	f	202	3PH	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
66	d	102	PC7	C39-C40-C41-C42
66	d	102	PC7	C32-C33-C34-C35
66	f	203	PC7	C39-C40-C41-C42
66	AC	410	PC7	C36-C37-C38-C39
66	BC	409	PC7	C33-C34-C35-C36
72	AC	409	CDL	C73-C74-C75-C76
72	AE	402	CDL	C22-C23-C24-C25
72	AE	402	CDL	C35-C36-C37-C38
72	BC	408	CDL	C13-C14-C15-C16
72	BC	408	CDL	C52-C53-C54-C55
72	BE	402	CDL	C15-C16-C17-C18
71	W	200	8Q1	O27-C28-C29-C30
71	W	200	8Q1	O27-C28-C29-C31
72	BC	407	CDL	C31-CA7-OA8-CA6
58	A	201	PGT	C15-C16-C17-C18
58	AC	407	PGT	C40-C41-C42-C43
60	d	101	PTY	C14-C15-C16-C17
65	AC	405	3PH	C34-C35-C36-C37
66	f	203	PC7	C33-C34-C35-C36
66	AC	410	PC7	C17-C18-C19-C20
72	AC	409	CDL	C16-C17-C18-C19
72	BC	407	CDL	C16-C17-C18-C19
72	BC	407	CDL	C78-C79-C80-C81
72	BC	408	CDL	OA7-CA5-OA6-CA4
66	L	706	PC7	C31-C32-C33-C34
58	AC	407	PGT	C18-C19-C20-C21
60	L	705	PTY	C33-C34-C35-C36
60	d	101	PTY	C11-C12-C13-C14
65	AI	101	3PH	C33-C34-C35-C36
66	AG	101	PC7	C21-C22-C23-C24
72	AC	408	CDL	C18-C19-C20-C21
72	BE	402	CDL	C12-C13-C14-C15
58	A	201	PGT	C20-C21-C22-C23
58	y	303	PGT	C13-C14-C15-C16
60	M	504	PTY	C32-C33-C34-C35
60	N	502	PTY	C20-C21-C22-C23
60	d	101	PTY	C16-C17-C18-C19
60	d	101	PTY	C18-C19-C20-C21
60	z	301	PTY	C33-C34-C35-C36
66	AC	410	PC7	C15-C16-C17-C18
66	AG	101	PC7	C39-C40-C41-C42
66	BC	409	PC7	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
72	u	101	CDL	C76-C77-C78-C79
72	u	102	CDL	C37-C38-C39-C40
72	AE	402	CDL	C37-C38-C39-C40
72	BC	407	CDL	C80-C81-C82-C83
58	AC	407	PGT	O4P-C4-C5-O5
58	AF	201	PGT	O4P-C4-C5-O5
72	AC	408	CDL	O1-C1-CB2-OB2
72	AC	409	CDL	O1-C1-CA2-OA2
72	AC	409	CDL	O1-C1-CB2-OB2
60	N	502	PTY	C37-C38-C39-C40
60	d	101	PTY	C13-C14-C15-C16
60	AB	602	PTY	C36-C37-C38-C39
72	BC	407	CDL	C59-C60-C61-C62
58	AC	406	PGT	C11-C12-C13-C14
58	BC	406	PGT	C11-C12-C13-C14
60	AB	602	PTY	C30-C31-C32-C33
72	BG	101	CDL	CB7-C71-C72-C73
60	M	503	PTY	C31-C32-C33-C34
60	N	503	PTY	C13-C14-C15-C16
60	m	101	PTY	C13-C14-C15-C16
65	AI	101	3PH	C22-C23-C24-C25
66	d	102	PC7	C37-C38-C39-C40
66	AB	603	PC7	C13-C14-C15-C16
72	BC	408	CDL	C11-C12-C13-C14
72	BG	101	CDL	OA9-CA7-OA8-CA6
58	AF	201	PGT	C37-C38-C39-C40
65	AI	101	3PH	C38-C39-C3A-C3B
65	BJ	101	3PH	C22-C23-C24-C25
66	L	706	PC7	C39-C40-C41-C42
66	v	201	PC7	C12-C13-C14-C15
66	BD	302	PC7	C17-C18-C19-C20
72	u	101	CDL	C36-C37-C38-C39
72	AC	408	CDL	C83-C84-C85-C86
72	BC	407	CDL	C13-C14-C15-C16
58	AF	201	PGT	C2-C3-O3-C11
66	L	706	PC7	C11-C12-C13-C14
58	A	201	PGT	C22-C23-C24-C25
58	L	704	PGT	C18-C19-C20-C21
58	AF	201	PGT	C40-C41-C42-C43
60	M	503	PTY	C15-C16-C17-C18
60	M	504	PTY	C15-C16-C17-C18
60	M	504	PTY	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
60	N	502	PTY	C38-C39-C40-C41
60	N	503	PTY	C21-C22-C23-C24
65	AI	101	3PH	C36-C37-C38-C39
66	d	102	PC7	C43-C44-C45-C46
66	v	201	PC7	C18-C19-C20-C21
72	AE	402	CDL	C31-C32-C33-C34
64	BC	410	Q7G	C16-C17-O20-CG1
64	BC	410	Q7G	C18-C17-O20-CG1
60	D	401	PTY	C17-C18-C19-C20
72	AC	409	CDL	C36-C37-C38-C39
72	AC	409	CDL	C39-C40-C41-C42
58	A	201	PGT	C4-C5-C6-O6
58	L	704	PGT	C4-C5-C6-O6
58	AF	201	PGT	C4-C5-C6-O6
64	H	402	Q7G	O5-C1-O1-C4B
64	K	201	Q7G	C22-CG1-O20-C17
64	BC	410	Q7G	C22-CG1-O20-C17
60	AB	602	PTY	C11-C8-O7-C6
65	M	501	3PH	C22-C21-O21-C2
58	L	704	PGT	C33-C34-C35-C36
58	L	704	PGT	C20-C21-C22-C23
60	D	401	PTY	C33-C34-C35-C36
60	d	101	PTY	C19-C20-C21-C22
65	Y	201	3PH	C27-C28-C29-C2A
65	Y	201	3PH	C28-C29-C2A-C2B
65	AC	405	3PH	C36-C37-C38-C39
66	v	201	PC7	C38-C39-C40-C41
72	AE	402	CDL	C16-C17-C18-C19
75	BC	404	UQ7	C12-C13-C14-C16
60	BB	602	PTY	C30-C31-C32-C33
72	AE	402	CDL	CB7-C71-C72-C73
72	BE	402	CDL	CB7-C71-C72-C73
58	A	201	PGT	C13-C14-C15-C16
58	L	702	PGT	C13-C14-C15-C16
58	y	303	PGT	C15-C16-C17-C18
58	AC	407	PGT	C19-C20-C21-C22
58	BC	406	PGT	C17-C18-C19-C20
60	M	504	PTY	C35-C36-C37-C38
60	N	503	PTY	C24-C25-C26-C27
72	AC	408	CDL	C57-C58-C59-C60
72	AC	409	CDL	C18-C19-C20-C21
72	AC	409	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
72	BC	408	CDL	C56-C57-C58-C59
66	v	201	PC7	C4-C5-N-C7
66	AC	410	PC7	C4-C5-N-C7
67	BC	403	UQ5	C14-C16-C17-C18
58	L	703	PGT	C14-C15-C16-C17
58	L	704	PGT	C17-C18-C19-C20
58	AC	406	PGT	C42-C43-C44-C45
58	AC	406	PGT	C37-C38-C39-C40
60	z	301	PTY	C32-C33-C34-C35
65	f	202	3PH	C28-C29-C2A-C2B
72	AC	408	CDL	C75-C76-C77-C78
72	BE	402	CDL	C19-C20-C21-C22
58	L	702	PGT	C34-C35-C36-C37
71	T	200	8Q1	C11-C10-C9-C8
72	u	101	CDL	C61-C62-C63-C64
72	AC	409	CDL	C71-C72-C73-C74
65	AC	405	3PH	C21-C22-C23-C24
72	u	101	CDL	CB7-C71-C72-C73
58	AC	406	PGT	C39-C40-C41-C42
60	M	504	PTY	C33-C34-C35-C36
60	d	101	PTY	C15-C16-C17-C18
66	d	102	PC7	C18-C19-C20-C21
66	AC	410	PC7	C32-C33-C34-C35
72	AC	408	CDL	C71-CB7-OB8-CB6
58	L	703	PGT	C15-C16-C17-C18
65	AC	405	3PH	C33-C34-C35-C36
66	f	203	PC7	C43-C44-C45-C46
66	f	203	PC7	C16-C17-C18-C19
64	BC	411	Q7G	C23-C48-O1C-C1C
58	AF	201	PGT	C16-C17-C18-C19
60	L	705	PTY	C32-C33-C34-C35
60	L	705	PTY	C40-C41-C42-C43
66	BD	302	PC7	C32-C33-C34-C35
72	AE	402	CDL	CA7-C31-C32-C33
72	AC	408	CDL	OA9-CA7-OA8-CA6
72	AC	408	CDL	C80-C81-C82-C83
66	v	201	PC7	O31-C31-O2-C2
58	y	303	PGT	C38-C39-C40-C41
58	AC	407	PGT	C13-C14-C15-C16
65	BC	405	3PH	C33-C34-C35-C36
66	v	201	PC7	C13-C14-C15-C16
72	AC	409	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
72	u	102	CDL	CA5-C11-C12-C13
58	L	704	PGT	C36-C37-C38-C39
58	AC	407	PGT	C33-C34-C35-C36
75	BC	404	UQ7	C37-C38-C39-C40
58	AC	406	PGT	O5-C5-C6-O6
58	AF	201	PGT	O5-C5-C6-O6
64	H	402	Q7G	CG1-C22-C23-C24
58	A	201	PGT	C34-C35-C36-C37
58	AF	201	PGT	C36-C37-C38-C39
60	D	401	PTY	C14-C15-C16-C17
60	N	503	PTY	C32-C33-C34-C35
66	d	102	PC7	C36-C37-C38-C39
66	AC	410	PC7	C18-C19-C20-C21
72	u	101	CDL	C51-C52-C53-C54
72	AC	409	CDL	C35-C36-C37-C38
72	AC	409	CDL	C41-C42-C43-C44
72	AC	408	CDL	CA7-C31-C32-C33
58	y	303	PGT	C34-C35-C36-C37
60	d	101	PTY	C20-C21-C22-C23
64	H	402	Q7G	C2-C1-O1-C4B
65	M	501	3PH	C25-C26-C27-C28
65	M	501	3PH	C2C-C2D-C2E-C2F
65	AC	405	3PH	C37-C38-C39-C3A
58	L	704	PGT	C34-C35-C36-C37
60	M	504	PTY	C34-C35-C36-C37
72	BE	402	CDL	C79-C80-C81-C82
60	N	502	PTY	C8-C11-C12-C13
58	AC	407	PGT	O4P-C4-C5-C6
72	BC	408	CDL	CA2-C1-CB2-OB2
60	N	502	PTY	C15-C16-C17-C18
60	BF	201	PTY	C13-C14-C15-C16
65	Y	201	3PH	C23-C24-C25-C26
65	Y	201	3PH	C24-C25-C26-C27
65	f	202	3PH	C38-C39-C3A-C3B
66	BD	302	PC7	C15-C16-C17-C18
60	AB	602	PTY	O10-C8-O7-C6
65	M	501	3PH	O22-C21-O21-C2
60	BF	201	PTY	C40-C41-C42-C43
66	L	706	PC7	C32-C33-C34-C35
72	AE	402	CDL	C32-C33-C34-C35
72	BC	407	CDL	OA9-CA7-OA8-CA6
60	N	502	PTY	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
60	AB	602	PTY	C38-C39-C40-C41
65	l	201	3PH	C32-C33-C34-C35
66	d	102	PC7	C15-C16-C17-C18
71	T	200	8Q1	C12-C13-C14-C15
58	AC	406	PGT	C33-C34-C35-C36
58	AC	407	PGT	C43-C44-C45-C46
60	N	502	PTY	C19-C20-C21-C22
72	AC	408	CDL	C12-C13-C14-C15
65	M	501	3PH	C32-C31-O31-C3
72	u	102	CDL	C11-CA5-OA6-CA4
72	BC	408	CDL	C51-CB5-OB6-CB4
58	BC	406	PGT	C20-C21-C22-C23
60	D	401	PTY	C37-C38-C39-C40
60	N	502	PTY	C40-C41-C42-C43
65	L	701	3PH	C2D-C2E-C2F-C2G
72	BC	407	CDL	C77-C78-C79-C80
72	AC	408	CDL	OB9-CB7-OB8-CB6
60	N	503	PTY	C8-C11-C12-C13
69	P	500	NDP	C2D-C1D-N1N-C2N
60	D	401	PTY	C12-C13-C14-C15
60	M	504	PTY	C37-C38-C39-C40
60	AB	602	PTY	C13-C14-C15-C16
65	BJ	102	3PH	C32-C33-C34-C35
65	M	501	3PH	C27-C28-C29-C2A
65	f	201	3PH	C23-C24-C25-C26
72	BC	408	CDL	C41-C42-C43-C44
67	AC	404	UQ5	C18-C19-C21-C22
66	v	201	PC7	C33-C34-C35-C36
72	BC	407	CDL	OB7-CB5-OB6-CB4
60	N	503	PTY	C30-C31-C32-C33
65	BC	405	3PH	C31-C32-C33-C34
66	AB	603	PC7	C11-C12-C13-C14
72	BC	408	CDL	CB7-C71-C72-C73
66	BC	409	PC7	C35-C36-C37-C38
72	AC	408	CDL	C17-C18-C19-C20
73	y	302	COO	O4-C7-C8-C9
58	y	303	PGT	C36-C37-C38-C39
65	AC	405	3PH	C38-C39-C3A-C3B
66	v	201	PC7	C32-C33-C34-C35
72	AC	409	CDL	C58-C59-C60-C61
71	T	200	8Q1	C11-C12-C13-C14
60	N	503	PTY	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
65	L	701	3PH	C26-C27-C28-C29
65	AC	405	3PH	C32-C33-C34-C35
66	AC	410	PC7	C34-C35-C36-C37
66	AG	101	PC7	C20-C21-C22-C23
72	AC	409	CDL	C57-C58-C59-C60
60	L	705	PTY	C31-C32-C33-C34
65	BC	405	3PH	C34-C35-C36-C37
72	AE	402	CDL	C21-C22-C23-C24
75	BC	404	UQ7	C9-C11-C12-C13
72	AC	409	CDL	C20-C21-C22-C23
58	AC	406	PGT	C32-C31-O2-C2
65	AI	101	3PH	C22-C21-O21-C2
72	BC	407	CDL	C51-CB5-OB6-CB4
72	BC	407	CDL	OB5-CB3-CB4-OB6
58	A	201	PGT	C12-C13-C14-C15
72	BC	408	CDL	O1-C1-CB2-OB2
58	AC	406	PGT	O31-C31-O2-C2
65	AI	101	3PH	O22-C21-O21-C2
63	H	401	UQ9	C24-C26-C27-C28
60	N	503	PTY	C33-C34-C35-C36
72	AC	409	CDL	C53-C54-C55-C56
72	u	102	CDL	C16-C17-C18-C19
72	AE	402	CDL	C71-C72-C73-C74
72	u	102	CDL	CB5-C51-C52-C53
67	BC	403	UQ5	C12-C11-C9-C8
73	y	302	COO	O4X-C4X-C5X-O5X
72	AC	408	CDL	C14-C15-C16-C17
66	L	706	PC7	C33-C34-C35-C36
72	u	102	CDL	C51-C52-C53-C54
72	u	102	CDL	C53-C54-C55-C56
72	AC	408	CDL	C76-C77-C78-C79
72	AC	409	CDL	C23-C24-C25-C26
72	AE	402	CDL	C40-C41-C42-C43
60	z	301	PTY	C34-C35-C36-C37
66	d	102	PC7	C33-C34-C35-C36
66	AB	603	PC7	C35-C36-C37-C38
72	u	102	CDL	OA7-CA5-OA6-CA4
72	BC	408	CDL	OB7-CB5-OB6-CB4
58	M	502	PGT	C32-C31-O2-C2
65	Y	201	3PH	C29-C2A-C2B-C2C
71	T	200	8Q1	C7-C8-C9-C10
72	u	102	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
72	AE	402	CDL	C11-C12-C13-C14
72	BC	407	CDL	C73-C74-C75-C76
72	BG	101	CDL	C38-C39-C40-C41
60	m	101	PTY	C5-O14-P1-O11
66	BC	409	PC7	C1-O3P-P-O4P
72	AC	408	CDL	CB2-OB2-PB2-OB5
66	f	203	PC7	C15-C16-C17-C18
60	d	101	PTY	C30-C31-C32-C33
60	z	301	PTY	C36-C37-C38-C39
72	u	102	CDL	C12-C13-C14-C15
58	L	702	PGT	O3P-C1-C2-C3
60	z	301	PTY	O14-C5-C6-C1
65	Y	201	3PH	O11-C1-C2-C3
65	f	202	3PH	O11-C1-C2-C3
65	l	201	3PH	O11-C1-C2-C3
66	L	706	PC7	O3P-C1-C2-C3
72	u	102	CDL	OB5-CB3-CB4-CB6
60	N	502	PTY	C17-C18-C19-C20
65	f	201	3PH	C37-C38-C39-C3A
60	z	301	PTY	C20-C21-C22-C23
67	AC	403	UQ5	C27-C28-C29-C30
72	AC	409	CDL	CA5-C11-C12-C13
58	AC	407	PGT	C32-C33-C34-C35
58	AF	201	PGT	C38-C39-C40-C41
72	u	102	CDL	C58-C59-C60-C61
67	AC	404	UQ5	C20-C19-C21-C22
65	M	501	3PH	C22-C23-C24-C25
72	BC	408	CDL	C37-C38-C39-C40
58	y	303	PGT	C35-C36-C37-C38
60	M	504	PTY	C14-C15-C16-C17
60	N	503	PTY	C22-C23-C24-C25
66	v	201	PC7	C16-C17-C18-C19
72	u	101	CDL	C15-C16-C17-C18
72	AC	408	CDL	C54-C55-C56-C57
58	AC	407	PGT	C31-C32-C33-C34
65	M	501	3PH	O32-C31-O31-C3
66	AG	101	PC7	C14-C15-C16-C17
58	L	704	PGT	C1-C2-C3-O3
60	L	705	PTY	O4-C1-C6-C5
60	N	502	PTY	O4-C1-C6-C5
60	m	101	PTY	C37-C38-C39-C40
65	f	202	3PH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
65	AC	405	3PH	C1-C2-C3-O31
66	d	102	PC7	C1-C2-C3-O3
66	f	203	PC7	C1-C2-C3-O3
66	BC	409	PC7	C1-C2-C3-O3
72	AC	408	CDL	CA3-CA4-CA6-OA8
72	AE	402	CDL	CB3-CB4-CB6-OB8
72	BC	407	CDL	CA3-CA4-CA6-OA8
72	BE	402	CDL	CA3-CA4-CA6-OA8
72	BG	101	CDL	CB3-CB4-CB6-OB8
75	BC	404	UQ7	C37-C38-C39-C41
60	N	502	PTY	C21-C22-C23-C24
66	AC	410	PC7	C44-C45-C46-C47
71	T	200	8Q1	C13-C14-C15-C16
67	L	707	UQ5	C1-C6-C7-C8
58	AC	406	PGT	C45-C46-C47-C48
58	AC	406	PGT	C13-C14-C15-C16
60	D	401	PTY	C15-C16-C17-C18
66	AG	101	PC7	C15-C16-C17-C18
72	BC	407	CDL	C75-C76-C77-C78
60	M	503	PTY	C36-C37-C38-C39
72	u	101	CDL	C11-C12-C13-C14
72	u	101	CDL	C44-C45-C46-C47
72	AC	409	CDL	C52-C53-C54-C55
60	AB	602	PTY	C31-C32-C33-C34
72	AC	409	CDL	C22-C23-C24-C25
58	AC	407	PGT	C42-C43-C44-C45
65	AC	405	3PH	C39-C3A-C3B-C3C
65	BJ	102	3PH	C23-C24-C25-C26
72	u	101	CDL	C33-C34-C35-C36
65	f	202	3PH	C35-C36-C37-C38
65	AC	405	3PH	C25-C26-C27-C28
66	BC	409	PC7	C36-C37-C38-C39
58	BC	406	PGT	C31-C32-C33-C34
65	l	201	3PH	C21-C22-C23-C24
66	AG	101	PC7	C32-C33-C34-C35
60	N	503	PTY	C41-C42-C43-C44
71	T	200	8Q1	C6-C7-C8-C9
64	H	402	Q7G	O5C-C5C-C6C-O6C
67	AC	404	UQ5	C12-C11-C9-C10
67	AC	404	UQ5	C12-C11-C9-C8
65	f	201	3PH	C3F-C3G-C3H-C3I
66	f	203	PC7	C45-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
60	d	101	PTY	C22-C23-C24-C25
60	AB	602	PTY	C33-C34-C35-C36
66	BC	409	PC7	C41-C42-C43-C44
60	M	503	PTY	C1-C6-O7-C8
58	M	502	PGT	C13-C14-C15-C16
72	BC	407	CDL	C18-C19-C20-C21
60	d	101	PTY	C23-C24-C25-C26
65	Y	201	3PH	C1-O11-P-O12
65	AC	405	3PH	C1-O11-P-O12
65	AI	101	3PH	C1-O11-P-O12
72	AC	408	CDL	C1-CB2-OB2-PB2
65	M	501	3PH	C23-C24-C25-C26
72	AC	408	CDL	C15-C16-C17-C18
58	AF	201	PGT	O3P-C1-C2-O2
58	AF	201	PGT	C21-C22-C23-C24
65	BJ	101	3PH	C35-C36-C37-C38
72	u	102	CDL	C44-C45-C46-C47
66	v	201	PC7	C21-C22-C23-C24
72	AE	402	CDL	C74-C75-C76-C77
60	AB	602	PTY	C32-C33-C34-C35
60	BB	602	PTY	C11-C12-C13-C14
64	H	402	Q7G	C2C-C1C-O1C-C48
66	BD	302	PC7	C21-C22-C23-C24
58	L	702	PGT	O2-C2-C3-O3
60	BB	602	PTY	O4-C1-C6-O7
71	T	200	8Q1	C31-C29-C32-O33
58	A	201	PGT	C37-C38-C39-C40
72	u	102	CDL	C34-C35-C36-C37
72	u	102	CDL	C79-C80-C81-C82
72	AC	409	CDL	C11-C12-C13-C14
65	f	202	3PH	C21-C22-C23-C24
65	BJ	102	3PH	C32-C31-O31-C3
69	P	500	NDP	PN-O3-PA-O1A
60	d	101	PTY	C31-C32-C33-C34
72	BC	407	CDL	C19-C20-C21-C22
65	BJ	102	3PH	C35-C36-C37-C38
60	BB	602	PTY	C8-C11-C12-C13
64	H	402	Q7G	C3C-C4C-O11-CF1
66	v	201	PC7	C40-C41-C42-C43
64	BC	411	Q7G	C22-CG1-O20-C17
58	M	502	PGT	O31-C31-O2-C2
72	u	101	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
65	M	501	3PH	C2D-C2E-C2F-C2G
66	v	201	PC7	C45-C46-C47-C48
72	BC	407	CDL	C53-C54-C55-C56
60	Y	202	PTY	C31-C30-O4-C1
65	f	202	3PH	C32-C31-O31-C3
60	AB	602	PTY	C39-C40-C41-C42
72	BE	402	CDL	C11-C12-C13-C14
58	M	502	PGT	O3P-C1-C2-C3
60	d	101	PTY	O14-C5-C6-C1
65	L	701	3PH	O11-C1-C2-C3
66	d	102	PC7	O3P-C1-C2-C3
72	BC	407	CDL	OB5-CB3-CB4-CB6
60	L	705	PTY	C41-C42-C43-C44
60	BF	201	PTY	C11-C12-C13-C14
72	AC	408	CDL	C56-C57-C58-C59
60	m	101	PTY	N1-C2-C3-O11
60	M	504	PTY	C40-C41-C42-C43
65	l	201	3PH	C26-C27-C28-C29
72	u	102	CDL	C72-C71-CB7-OB8
60	M	504	PTY	C30-C31-C32-C33
58	L	704	PGT	C21-C22-C23-C24
72	AC	408	CDL	C82-C83-C84-C85
58	L	702	PGT	C35-C36-C37-C38
60	M	504	PTY	C21-C22-C23-C24
66	v	201	PC7	C41-C42-C43-C44
58	BC	406	PGT	C12-C11-O3-C3
75	BC	404	UQ7	C11-C12-C13-C14
65	M	501	3PH	C2A-C2B-C2C-C2D
65	f	202	3PH	C36-C37-C38-C39
58	AC	406	PGT	C5-C4-O4P-P
65	Y	201	3PH	C2-C1-O11-P
64	M	505	Q7G	C23-C48-O1C-C1C
60	D	401	PTY	C39-C40-C41-C42
65	AC	405	3PH	C24-C25-C26-C27
60	M	503	PTY	C16-C17-C18-C19
65	BC	405	3PH	C2B-C2C-C2D-C2E
58	y	303	PGT	C16-C17-C18-C19
60	AB	602	PTY	C16-C17-C18-C19
72	BC	407	CDL	C15-C16-C17-C18
72	BC	407	CDL	C79-C80-C81-C82
58	y	303	PGT	C1-C2-C3-O3
58	BC	406	PGT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
60	M	503	PTY	O4-C1-C6-C5
60	M	504	PTY	O4-C1-C6-C5
60	m	101	PTY	O4-C1-C6-C5
60	z	301	PTY	O4-C1-C6-C5
60	BB	602	PTY	O4-C1-C6-C5
65	l	201	3PH	C1-C2-C3-O31
66	BD	302	PC7	C1-C2-C3-O3
72	u	101	CDL	CA3-CA4-CA6-OA8
72	u	102	CDL	CA3-CA4-CA6-OA8
66	d	102	PC7	C38-C39-C40-C41
72	u	101	CDL	C31-C32-C33-C34
72	BE	402	CDL	C52-C53-C54-C55
58	A	201	PGT	C32-C33-C34-C35
60	M	503	PTY	C32-C33-C34-C35
60	M	504	PTY	C11-C12-C13-C14
58	AC	407	PGT	C34-C35-C36-C37
66	BD	302	PC7	C12-C13-C14-C15
58	AF	201	PGT	C32-C31-O2-C2
66	BD	302	PC7	C14-C15-C16-C17
65	BJ	101	3PH	C36-C37-C38-C39
72	AC	408	CDL	C52-C53-C54-C55
72	AE	402	CDL	C56-C57-C58-C59
72	AC	408	CDL	CA3-OA5-PA1-OA2
58	AF	201	PGT	C41-C42-C43-C44
72	BC	407	CDL	C64-C65-C66-C67
58	M	502	PGT	O5-C5-C6-O6
58	y	303	PGT	O5-C5-C6-O6
64	H	402	Q7G	C5C-C4C-O11-CF1
58	L	703	PGT	O3P-C1-C2-O2
65	l	201	3PH	O11-C1-C2-O21
66	d	102	PC7	O3P-C1-C2-O2
72	AE	402	CDL	C24-C25-C26-C27
60	N	501	PTY	C13-C14-C15-C16
60	M	504	PTY	C23-C24-C25-C26
72	u	102	CDL	C36-C37-C38-C39
58	AF	201	PGT	C34-C35-C36-C37
72	BC	408	CDL	C74-C75-C76-C77
60	N	503	PTY	C18-C19-C20-C21
60	L	705	PTY	O4-C1-C6-O7
60	M	503	PTY	O4-C1-C6-O7
60	N	502	PTY	O4-C1-C6-O7
65	l	201	3PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
66	BD	302	PC7	O2-C2-C3-O3
72	AC	408	CDL	OB6-CB4-CB6-OB8
72	AC	409	CDL	OA6-CA4-CA6-OA8
72	BG	101	CDL	OB6-CB4-CB6-OB8
72	AC	408	CDL	C84-C85-C86-C87
58	AC	406	PGT	O4P-C4-C5-C6
64	M	505	Q7G	C48-C23-C24-O1B
64	M	505	Q7G	C24-C23-C48-O1C
64	BC	410	Q7G	C24-C23-C48-O1C
60	L	705	PTY	C15-C16-C17-C18
66	L	706	PC7	C13-C14-C15-C16
72	u	101	CDL	OA7-CA5-OA6-CA4
58	L	704	PGT	C22-C23-C24-C25
66	AG	101	PC7	C17-C18-C19-C20
72	u	101	CDL	C12-C13-C14-C15
72	BE	402	CDL	C18-C19-C20-C21
66	AC	410	PC7	C35-C36-C37-C38
66	AG	101	PC7	C16-C17-C18-C19
58	L	704	PGT	C5-C4-O4P-P
58	AF	201	PGT	C5-C4-O4P-P
58	BC	406	PGT	C2-C1-O3P-P
65	AI	101	3PH	C2-C1-O11-P
72	u	102	CDL	CB4-CB3-OB5-PB2
60	Y	202	PTY	O30-C30-O4-C1
66	AB	603	PC7	C4-C5-N-C7
72	u	101	CDL	CA7-C31-C32-C33
60	M	503	PTY	C35-C36-C37-C38
72	u	102	CDL	C20-C21-C22-C23
72	AC	409	CDL	C74-C75-C76-C77
60	M	503	PTY	C34-C35-C36-C37
60	N	502	PTY	C13-C14-C15-C16
65	BJ	102	3PH	O32-C31-O31-C3
73	y	302	COO	C2X-C3X-O3X-P3X
58	AC	406	PGT	C38-C39-C40-C41
58	AF	201	PGT	O31-C31-O2-C2
72	AC	409	CDL	C11-CA5-OA6-CA4
58	L	704	PGT	C37-C38-C39-C40
60	z	301	PTY	C21-C22-C23-C24
64	BC	410	Q7G	C23-C22-CG1-O20
64	BC	411	Q7G	C23-C22-CG1-O20
58	L	702	PGT	C16-C17-C18-C19
60	M	503	PTY	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
60	D	401	PTY	C23-C24-C25-C26
64	M	505	Q7G	C22-C23-C24-O1B
72	AC	408	CDL	OB5-CB3-CB4-CB6
72	BG	101	CDL	OA5-CA3-CA4-CA6
58	A	201	PGT	C33-C34-C35-C36
72	BC	407	CDL	C83-C84-C85-C86
72	BG	101	CDL	C43-C44-C45-C46
66	d	102	PC7	C12-C13-C14-C15
72	AC	408	CDL	C58-C59-C60-C61
72	AC	408	CDL	C79-C80-C81-C82
72	BG	101	CDL	C41-C42-C43-C44
69	P	500	NDP	O4D-C1D-N1N-C6N
72	BG	101	CDL	C51-C52-C53-C54
65	f	201	3PH	C3A-C3B-C3C-C3D
58	AF	201	PGT	C17-C18-C19-C20
65	l	201	3PH	C32-C31-O31-C3
72	u	101	CDL	C14-C15-C16-C17
65	AC	405	3PH	C3-C2-O21-C21
72	u	101	CDL	CB6-CB4-OB6-CB5
72	AC	409	CDL	CB3-CB4-OB6-CB5
74	BE	401	HEM	C2B-C3B-CAB-CBB
75	BC	404	UQ7	C12-C13-C14-C15
65	f	202	3PH	C2D-C2E-C2F-C2G
60	L	705	PTY	C14-C15-C16-C17
72	BC	408	CDL	C55-C56-C57-C58
71	T	200	8Q1	N36-C37-C38-C39
58	L	702	PGT	C1-C2-C3-O3
58	M	502	PGT	C2-C1-O3P-P
58	AF	201	PGT	C1-C2-C3-O3
66	AB	603	PC7	C1-C2-C3-O3
72	AC	408	CDL	CB4-CB3-OB5-PB2
72	AC	409	CDL	CA3-CA4-CA6-OA8
60	d	101	PTY	O14-C5-C6-O7
65	L	701	3PH	O11-C1-C2-O21
65	BJ	102	3PH	O11-C1-C2-O21
66	f	203	PC7	O3P-C1-C2-O2
72	AC	409	CDL	C24-C25-C26-C27
72	BC	408	CDL	C31-C32-C33-C34
72	BC	408	CDL	C57-C58-C59-C60
72	AC	409	CDL	OA7-CA5-OA6-CA4
71	W	200	8Q1	C30-C29-C32-C34
65	f	202	3PH	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
60	z	301	PTY	C40-C41-C42-C43
58	AF	201	PGT	O2-C2-C3-O3
60	M	504	PTY	O4-C1-C6-O7
60	m	101	PTY	O4-C1-C6-O7
60	z	301	PTY	O4-C1-C6-O7
60	AB	602	PTY	O4-C1-C6-O7
66	f	203	PC7	O2-C2-C3-O3
66	v	201	PC7	O2-C2-C3-O3
66	AB	603	PC7	O2-C2-C3-O3
72	u	101	CDL	OA6-CA4-CA6-OA8
72	u	101	CDL	OB6-CB4-CB6-OB8
72	u	102	CDL	OA6-CA4-CA6-OA8
72	AE	402	CDL	OB6-CB4-CB6-OB8
72	BE	402	CDL	OB6-CB4-CB6-OB8
66	BD	302	PC7	C34-C35-C36-C37
60	L	705	PTY	C11-C12-C13-C14
66	BD	302	PC7	C33-C34-C35-C36
72	u	102	CDL	C75-C76-C77-C78
72	BC	408	CDL	C38-C39-C40-C41
58	L	704	PGT	C14-C15-C16-C17
72	AE	402	CDL	C20-C21-C22-C23
72	AE	402	CDL	C23-C24-C25-C26
58	BC	406	PGT	O11-C11-O3-C3
72	BG	101	CDL	CB4-CB6-OB8-CB7
58	L	702	PGT	C36-C37-C38-C39
73	y	302	COO	C3X-C4X-C5X-O5X
65	BC	405	3PH	C39-C3A-C3B-C3C
72	AC	409	CDL	C42-C43-C44-C45
60	D	401	PTY	C40-C41-C42-C43
72	BC	407	CDL	C12-C13-C14-C15
72	BG	101	CDL	C13-C14-C15-C16
66	BC	409	PC7	C31-C32-C33-C34
58	L	702	PGT	C4-O4P-P-O3P
58	L	704	PGT	C1-O3P-P-O4P
60	Y	202	PTY	C3-O11-P1-O14
60	Y	202	PTY	C5-O14-P1-O11
72	BC	407	CDL	CA2-OA2-PA1-OA5
72	BG	101	CDL	C31-C32-C33-C34
58	L	704	PGT	C2-C1-O3P-P
60	N	502	PTY	C6-C5-O14-P1
65	AC	405	3PH	C2-C1-O11-P
72	BE	402	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
65	l	201	3PH	O32-C31-O31-C3
58	y	303	PGT	C4-O4P-P-O1P
58	AF	201	PGT	C1-O3P-P-O1P
58	AF	201	PGT	C4-O4P-P-O1P
60	D	401	PTY	C3-O11-P1-O13
60	L	705	PTY	C3-O11-P1-O12
60	M	503	PTY	C3-O11-P1-O13
60	M	504	PTY	C3-O11-P1-O13
60	N	502	PTY	C3-O11-P1-O12
60	N	502	PTY	C5-O14-P1-O12
60	N	502	PTY	C5-O14-P1-O13
60	d	101	PTY	C3-O11-P1-O13
60	m	101	PTY	C5-O14-P1-O13
60	z	301	PTY	C3-O11-P1-O12
60	z	301	PTY	C3-O11-P1-O13
60	AB	602	PTY	C3-O11-P1-O13
60	BF	201	PTY	C3-O11-P1-O13
66	L	706	PC7	C4-O4P-P-O1P
66	f	203	PC7	C1-O3P-P-O1P
66	f	203	PC7	C1-O3P-P-O2P
66	f	203	PC7	C4-O4P-P-O2P
66	AB	603	PC7	C1-O3P-P-O1P
66	AG	101	PC7	C4-O4P-P-O2P
66	BC	409	PC7	C1-O3P-P-O1P
66	BC	409	PC7	C1-O3P-P-O2P
66	BC	409	PC7	C4-O4P-P-O1P
72	u	101	CDL	CB2-OB2-PB2-OB3
72	u	101	CDL	CB3-OB5-PB2-OB3
72	u	101	CDL	CB3-OB5-PB2-OB4
72	u	102	CDL	CB3-OB5-PB2-OB3
72	AC	408	CDL	CA2-OA2-PA1-OA4
72	AC	408	CDL	CB2-OB2-PB2-OB3
72	AC	409	CDL	CB2-OB2-PB2-OB4
72	AE	402	CDL	CB3-OB5-PB2-OB3
72	BG	101	CDL	CB2-OB2-PB2-OB3
58	y	303	PGT	C11-C12-C13-C14
64	H	402	Q7G	O5C-C1C-O1C-C48
58	A	201	PGT	C12-C11-O3-C3
66	v	201	PC7	C12-C11-O3-C3
58	L	703	PGT	O3P-C1-C2-C3
58	AF	201	PGT	O3P-C1-C2-C3
60	M	504	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
60	BB	602	PTY	O14-C5-C6-C1
65	M	501	3PH	O11-C1-C2-C3
65	BJ	102	3PH	O11-C1-C2-C3
66	f	203	PC7	O3P-C1-C2-C3
67	AC	403	UQ5	C14-C16-C17-C18
65	BJ	101	3PH	C33-C34-C35-C36
60	N	502	PTY	N1-C2-C3-O11
67	AC	403	UQ5	C27-C28-C29-C31
66	AB	603	PC7	C31-C32-C33-C34
63	H	401	UQ9	C5-C4-O4-C4M
67	AC	403	UQ5	C2-C3-O3-C3M
67	AC	404	UQ5	C2-C3-O3-C3M
60	z	301	PTY	C25-C26-C27-C28
66	d	102	PC7	C13-C14-C15-C16
66	BC	409	PC7	C34-C35-C36-C37
60	m	101	PTY	C2-C3-O11-P1
60	BF	201	PTY	C2-C3-O11-P1
60	M	504	PTY	C19-C20-C21-C22
66	BC	409	PC7	C40-C41-C42-C43
65	L	701	3PH	C32-C33-C34-C35
66	AC	410	PC7	C33-C34-C35-C36
72	BG	101	CDL	CA2-C1-CB2-OB2
72	u	101	CDL	OB7-CB5-OB6-CB4
67	AC	404	UQ5	C25-C24-C26-C27
58	L	702	PGT	O3P-C1-C2-O2
58	AF	201	PGT	C31-C32-C33-C34
60	M	504	PTY	O14-C5-C6-O7
60	z	301	PTY	O14-C5-C6-O7
60	BB	602	PTY	O14-C5-C6-O7
62	F	500	FMN	N10-C1'-C2'-O2'
62	F	500	FMN	N10-C1'-C2'-C3'
64	BC	411	Q7G	C23-C24-O1B-C1B
65	M	501	3PH	O11-C1-C2-O21
65	Y	201	3PH	O11-C1-C2-O21
65	f	202	3PH	O11-C1-C2-O21
66	L	706	PC7	O3P-C1-C2-O2
72	u	102	CDL	OB5-CB3-CB4-OB6
72	BG	101	CDL	OA5-CA3-CA4-OA6
65	BC	405	3PH	C36-C37-C38-C39
72	u	102	CDL	C22-C23-C24-C25
69	P	500	NDP	O4D-C1D-N1N-C2N
72	u	102	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
72	BC	408	CDL	C16-C17-C18-C19
66	d	102	PC7	C4-C5-N-C8
66	AC	410	PC7	C41-C42-C43-C44
66	AG	101	PC7	C13-C14-C15-C16
60	AB	602	PTY	O4-C1-C6-C5
66	f	203	PC7	C37-C38-C39-C40
71	T	200	8Q1	C28-C29-C32-O33
65	BC	405	3PH	O21-C2-C3-O31
72	AC	408	CDL	OA6-CA4-CA6-OA8
72	BC	407	CDL	OA6-CA4-CA6-OA8
72	BC	407	CDL	OB6-CB4-CB6-OB8
72	BE	402	CDL	OA6-CA4-CA6-OA8
60	N	503	PTY	C35-C36-C37-C38
65	f	202	3PH	C39-C3A-C3B-C3C
58	A	201	PGT	C41-C42-C43-C44
65	M	501	3PH	C32-C33-C34-C35
58	A	201	PGT	C19-C20-C21-C22
66	d	102	PC7	C19-C20-C21-C22
65	f	201	3PH	C22-C23-C24-C25
66	BC	409	PC7	C37-C38-C39-C40
72	u	101	CDL	C37-C38-C39-C40
72	AC	409	CDL	C33-C34-C35-C36
66	f	203	PC7	C44-C45-C46-C47
66	v	201	PC7	O11-C11-O3-C3
64	a	101	Q7G	CG1-C22-C23-C48
72	BC	407	CDL	C58-C59-C60-C61
60	m	101	PTY	C31-C32-C33-C34
58	AC	407	PGT	C35-C36-C37-C38
66	AB	603	PC7	C4-C5-N-C6
58	A	201	PGT	C21-C22-C23-C24
65	BJ	101	3PH	O22-C21-O21-C2
58	M	502	PGT	C33-C34-C35-C36
75	BC	404	UQ7	C4-C3-O3-CM3
72	AC	408	CDL	C32-C31-CA7-OA8
58	AF	201	PGT	C19-C20-C21-C22
60	BF	201	PTY	C41-C42-C43-C44
60	m	101	PTY	C24-C25-C26-C27
72	u	101	CDL	C41-C42-C43-C44
72	AC	408	CDL	C59-C60-C61-C62
58	BC	406	PGT	C1-C2-O2-C31
58	BC	406	PGT	C3-C2-O2-C31
72	BC	407	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
58	A	201	PGT	C42-C43-C44-C45
72	AE	402	CDL	C53-C54-C55-C56
58	A	201	PGT	O11-C11-O3-C3
66	f	203	PC7	C18-C19-C20-C21
60	D	401	PTY	C6-C5-O14-P1
65	BJ	101	3PH	C1-O11-P-O12
58	M	502	PGT	O3P-C1-C2-O2
72	BC	407	CDL	OA5-CA3-CA4-OA6
66	BC	409	PC7	C14-C15-C16-C17
72	BE	402	CDL	C38-C39-C40-C41
66	d	102	PC7	C4-C5-N-C7
67	AC	404	UQ5	C15-C14-C16-C17
72	u	102	CDL	C59-C60-C61-C62
72	AC	408	CDL	C64-C65-C66-C67
66	L	706	PC7	C37-C38-C39-C40
65	BJ	101	3PH	C22-C21-O21-C2
72	u	101	CDL	C51-CB5-OB6-CB4
58	AC	406	PGT	C35-C36-C37-C38
65	AC	405	3PH	O21-C2-C3-O31
66	d	102	PC7	O2-C2-C3-O3
58	A	201	PGT	C1-O3P-P-O4P
58	L	703	PGT	C4-O4P-P-O3P
58	y	303	PGT	C1-O3P-P-O4P
60	D	401	PTY	C5-O14-P1-O11
60	L	705	PTY	C5-O14-P1-O11
60	N	501	PTY	C3-O11-P1-O14
60	m	101	PTY	C3-O11-P1-O14
60	z	301	PTY	C5-O14-P1-O11
66	v	201	PC7	C4-O4P-P-O3P
72	BE	402	CDL	CB2-OB2-PB2-OB5
72	BG	101	CDL	CA2-OA2-PA1-OA5
58	AF	201	PGT	C11-C12-C13-C14
58	A	201	PGT	C39-C40-C41-C42
60	D	401	PTY	C22-C23-C24-C25
72	u	102	CDL	C78-C79-C80-C81
72	AC	408	CDL	CB3-CB4-CB6-OB8
72	u	102	CDL	C56-C57-C58-C59
60	N	501	PTY	O10-C8-O7-C6
72	u	102	CDL	C42-C43-C44-C45
72	AE	402	CDL	C19-C20-C21-C22
69	P	500	NDP	PN-O3-PA-O2A
60	M	504	PTY	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
60	AB	602	PTY	C17-C18-C19-C20
72	u	102	CDL	C73-C74-C75-C76
65	f	201	3PH	C2-C1-O11-P
60	M	504	PTY	C25-C26-C27-C28
58	L	704	PGT	O5-C5-C6-O6
72	u	102	CDL	C72-C73-C74-C75
60	AB	602	PTY	C34-C35-C36-C37
60	BB	602	PTY	C32-C33-C34-C35
66	AC	410	PC7	C22-C23-C24-C25
72	BC	408	CDL	C40-C41-C42-C43
58	AF	201	PGT	C15-C16-C17-C18
72	u	101	CDL	OA5-CA3-CA4-OA6
66	AB	603	PC7	C33-C34-C35-C36
72	BC	407	CDL	C63-C64-C65-C66
74	BE	401	HEM	C4B-C3B-CAB-CBB
65	BJ	102	3PH	C29-C2A-C2B-C2C
66	BC	409	PC7	C16-C17-C18-C19
66	d	102	PC7	C14-C15-C16-C17
66	AB	603	PC7	C4-C5-N-C8
72	BE	402	CDL	C78-C79-C80-C81
58	L	703	PGT	C16-C17-C18-C19
72	AC	409	CDL	C59-C60-C61-C62
72	u	102	CDL	C21-C22-C23-C24
72	AE	402	CDL	C54-C55-C56-C57
60	L	705	PTY	C37-C38-C39-C40
60	d	101	PTY	C24-C25-C26-C27
65	f	202	3PH	C2B-C2C-C2D-C2E
65	BJ	102	3PH	C26-C27-C28-C29
72	AE	402	CDL	C44-C45-C46-C47
67	AC	403	UQ5	C22-C23-C24-C25
64	BC	410	Q7G	C22-C23-C48-O1C
74	BE	401	HEM	CAA-CBA-CGA-O1A
74	BE	401	HEM	CAA-CBA-CGA-O2A
74	AE	401	HEM	CAA-CBA-CGA-O1A
74	BC	402	HEM	CAD-CBD-CGD-O1D
65	f	201	3PH	C1-C2-O21-C21
72	AC	408	CDL	C74-C75-C76-C77
66	d	102	PC7	C4-C5-N-C6
60	BF	201	PTY	O10-C8-O7-C6
65	BC	405	3PH	O22-C21-O21-C2
65	BJ	102	3PH	O22-C21-O21-C2
65	Y	201	3PH	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
72	AC	408	CDL	C78-C79-C80-C81
72	u	101	CDL	CB2-OB2-PB2-OB5
66	AG	101	PC7	C12-C11-O3-C3
74	BC	402	HEM	CAD-CBD-CGD-O2D
58	L	702	PGT	C37-C38-C39-C40
65	BC	405	3PH	C32-C33-C34-C35
72	BC	408	CDL	CB4-CB3-OB5-PB2
64	a	101	Q7G	CG1-C22-C23-C24
58	L	703	PGT	C32-C33-C34-C35
72	AC	408	CDL	C63-C64-C65-C66
72	BC	407	CDL	C74-C75-C76-C77
66	BC	409	PC7	O3P-C1-C2-C3
65	f	202	3PH	C24-C25-C26-C27
60	N	501	PTY	C11-C8-O7-C6
60	z	301	PTY	C26-C27-C28-C29
64	K	201	Q7G	C3C-C4C-O11-CF1
74	AC	402	HEM	CAD-CBD-CGD-O2D
65	f	201	3PH	C24-C25-C26-C27
65	BC	405	3PH	C37-C38-C39-C3A
65	BJ	102	3PH	C39-C3A-C3B-C3C
71	T	200	8Q1	C42-C43-S44-C1
74	AE	401	HEM	CAA-CBA-CGA-O2A
74	BC	401	HEM	CAA-CBA-CGA-O1A
60	M	503	PTY	C13-C14-C15-C16
60	N	502	PTY	C31-C30-O4-C1
66	v	201	PC7	C17-C18-C19-C20
72	u	101	CDL	C81-C82-C83-C84
75	BC	404	UQ7	C26-C27-C28-C29
72	BC	407	CDL	CA2-C1-CB2-OB2
74	AC	402	HEM	CAD-CBD-CGD-O1D
72	BE	402	CDL	C34-C35-C36-C37
74	BC	401	HEM	CAA-CBA-CGA-O2A
58	y	303	PGT	C37-C38-C39-C40
64	K	201	Q7G	C5C-C4C-O11-CF1
58	AC	407	PGT	C36-C37-C38-C39
60	N	502	PTY	O30-C30-O4-C1
60	BF	201	PTY	C39-C40-C41-C42
72	AC	409	CDL	C44-C45-C46-C47
72	BE	402	CDL	C37-C38-C39-C40
58	AC	407	PGT	C41-C42-C43-C44
66	v	201	PC7	C1-C2-C3-O3
72	u	102	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
74	AC	401	HEM	CAA-CBA-CGA-O2A
65	BC	405	3PH	C3F-C3G-C3H-C3I
72	AE	402	CDL	C72-C73-C74-C75
60	M	504	PTY	C26-C27-C28-C29
72	u	102	CDL	C72-C71-CB7-OB9
66	BD	302	PC7	C16-C17-C18-C19
72	u	101	CDL	C62-C63-C64-C65
65	BC	405	3PH	C22-C23-C24-C25
72	u	101	CDL	C21-C22-C23-C24
72	BG	101	CDL	C11-C12-C13-C14
58	y	303	PGT	O3P-C1-C2-O2
65	BC	405	3PH	O11-C1-C2-O21
72	AE	402	CDL	OB5-CB3-CB4-OB6
72	BG	101	CDL	OB5-CB3-CB4-OB6
60	M	503	PTY	C11-C12-C13-C14
72	AE	402	CDL	C59-C60-C61-C62
60	BF	201	PTY	C16-C17-C18-C19
72	BE	402	CDL	C77-C78-C79-C80
72	u	101	CDL	OA5-CA3-CA4-CA6
72	BG	101	CDL	OB5-CB3-CB4-CB6
66	AG	101	PC7	O11-C11-O3-C3
67	L	707	UQ5	C15-C14-C16-C17
67	L	707	UQ5	C20-C19-C21-C22
65	BJ	102	3PH	C22-C21-O21-C2
72	u	102	CDL	C24-C25-C26-C27
60	AB	602	PTY	C11-C12-C13-C14
66	L	706	PC7	O3-C11-C12-C13
66	v	201	PC7	O3-C11-C12-C13
60	d	101	PTY	C6-C5-O14-P1
60	BF	201	PTY	C12-C13-C14-C15
67	AC	404	UQ5	C4-C3-O3-C3M
72	AC	409	CDL	OB6-CB4-CB6-OB8
65	f	201	3PH	O31-C31-C32-C33
65	L	701	3PH	C1-O11-P-O14
65	f	201	3PH	C1-O11-P-O14
65	BJ	101	3PH	C1-O11-P-O14
63	H	401	UQ9	C15-C14-C16-C17
67	L	707	UQ5	C25-C24-C26-C27
58	L	703	PGT	C1-O3P-P-O4P
66	d	102	PC7	C4-O4P-P-O3P
67	AC	404	UQ5	C23-C24-C26-C27
66	AB	603	PC7	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
60	M	504	PTY	C12-C11-C8-O7
58	M	502	PGT	C32-C33-C34-C35
60	D	401	PTY	C21-C22-C23-C24
67	L	707	UQ5	C5-C6-C7-C8
66	d	102	PC7	C23-C24-C25-C26
64	a	101	Q7G	C23-C48-O1C-C1C
72	BE	402	CDL	C76-C77-C78-C79
72	BC	408	CDL	C12-C11-CA5-OA6
58	L	704	PGT	C35-C36-C37-C38
74	AC	402	HEM	C2B-C3B-CAB-CBB
60	L	705	PTY	O10-C8-O7-C6
65	f	201	3PH	O22-C21-O21-C2
65	f	202	3PH	C31-C32-C33-C34
72	BC	407	CDL	CB5-C51-C52-C53
72	BC	408	CDL	C12-C13-C14-C15
72	BG	101	CDL	C36-C37-C38-C39
72	BE	402	CDL	C32-C31-CA7-OA8
72	BG	101	CDL	C32-C31-CA7-OA8
60	N	502	PTY	C32-C33-C34-C35
75	BC	404	UQ7	C14-C16-C17-C18
71	T	200	8Q1	C28-O27-P24-O3
72	u	101	CDL	CB3-CB4-CB6-OB8
72	BC	407	CDL	CB3-CB4-CB6-OB8
74	AC	401	HEM	CAA-CBA-CGA-O1A
58	y	303	PGT	O3-C11-C12-C13
65	Y	201	3PH	O31-C31-C32-C33
72	BG	101	CDL	C72-C71-CB7-OB8
72	BC	408	CDL	C72-C73-C74-C75
66	f	203	PC7	C17-C18-C19-C20
74	AC	402	HEM	C4B-C3B-CAB-CBB
60	N	502	PTY	C36-C37-C38-C39
66	BD	302	PC7	C18-C19-C20-C21
66	AC	410	PC7	C23-C24-C25-C26
72	BG	101	CDL	O1-C1-CB2-OB2
67	AC	403	UQ5	C22-C23-C24-C26
63	H	401	UQ9	C13-C14-C16-C17
66	AC	410	PC7	C12-C13-C14-C15
72	u	101	CDL	C40-C41-C42-C43
65	BC	405	3PH	C22-C21-O21-C2
65	Y	201	3PH	C2A-C2B-C2C-C2D
58	y	303	PGT	O3P-C1-C2-C3
65	BC	405	3PH	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
72	AC	409	CDL	OA5-CA3-CA4-CA6
72	u	102	CDL	C43-C44-C45-C46
60	BF	201	PTY	O4-C30-C31-C32
65	AI	101	3PH	O31-C31-C32-C33
66	AG	101	PC7	O2-C31-C32-C33
60	M	503	PTY	C18-C19-C20-C21
73	y	302	COO	C5X-O5X-P1A-O3A
73	y	302	COO	C3X-O3X-P3X-O8A
58	L	703	PGT	C13-C14-C15-C16
72	BC	407	CDL	CA7-C31-C32-C33
60	BB	602	PTY	C31-C32-C33-C34
66	d	102	PC7	C45-C46-C47-C48
72	BC	407	CDL	C51-C52-C53-C54
60	M	503	PTY	O4-C30-C31-C32
60	N	501	PTY	O4-C30-C31-C32
66	AG	101	PC7	O3-C11-C12-C13
60	m	101	PTY	C16-C17-C18-C19
63	H	401	UQ9	C3-C4-O4-C4M
75	BC	404	UQ7	C2-C3-O3-CM3
69	P	500	NDP	O4B-C4B-C5B-O5B
60	N	503	PTY	C17-C18-C19-C20
64	K	201	Q7G	C23-C22-CG1-O20
64	M	505	Q7G	C23-C22-CG1-O20
60	BF	201	PTY	C11-C8-O7-C6
72	BC	408	CDL	C12-C11-CA5-OA7
66	AC	410	PC7	C16-C17-C18-C19
66	AB	603	PC7	O3-C11-C12-C13
60	L	705	PTY	C17-C18-C19-C20
58	y	303	PGT	O11-C11-C12-C13
58	y	303	PGT	C4-C5-C6-O6
65	L	701	3PH	C23-C24-C25-C26
72	BG	101	CDL	C32-C31-CA7-OA9
66	f	203	PC7	C14-C15-C16-C17
64	H	402	Q7G	C22-CG1-O20-C17
65	f	201	3PH	O32-C31-C32-C33
72	BG	101	CDL	C72-C71-CB7-OB9
67	BC	403	UQ5	C16-C17-C18-C19
65	Y	201	3PH	O32-C31-C32-C33
65	AI	101	3PH	C1-C2-C3-O31
65	BC	405	3PH	C1-C2-C3-O31
72	AC	409	CDL	CB3-CB4-CB6-OB8
72	BE	402	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
65	BJ	101	3PH	C37-C38-C39-C3A
66	BD	302	PC7	C11-C12-C13-C14
66	L	706	PC7	O11-C11-C12-C13
66	AG	101	PC7	O31-C31-C32-C33
66	AG	101	PC7	O11-C11-C12-C13
58	AF	201	PGT	C44-C45-C46-C47
60	AB	602	PTY	C35-C36-C37-C38
72	AE	402	CDL	C73-C74-C75-C76
72	AC	409	CDL	C52-C51-CB5-OB6
72	BE	402	CDL	C72-C71-CB7-OB8
65	M	501	3PH	C2E-C2F-C2G-C2H
72	u	101	CDL	C17-C18-C19-C20
67	AC	404	UQ5	C13-C14-C16-C17
58	AC	407	PGT	C39-C40-C41-C42
60	D	401	PTY	C41-C42-C43-C44
60	z	301	PTY	C15-C16-C17-C18
60	BF	201	PTY	C33-C34-C35-C36
58	L	703	PGT	C1-O3P-P-O1P
58	L	704	PGT	C4-O4P-P-O1P
60	m	101	PTY	C3-O11-P1-O13
60	z	301	PTY	C5-O14-P1-O13
66	d	102	PC7	C4-O4P-P-O2P
72	u	101	CDL	CA3-OA5-PA1-OA3
72	AC	408	CDL	CA3-OA5-PA1-OA3
72	AC	409	CDL	CB3-OB5-PB2-OB3
60	L	705	PTY	C11-C8-O7-C6
71	T	200	8Q1	C37-C38-C39-N41
65	AC	405	3PH	C3A-C3B-C3C-C3D
72	u	102	CDL	C52-C53-C54-C55
60	BB	602	PTY	C12-C11-C8-O7
65	L	701	3PH	C2E-C2F-C2G-C2H
58	L	703	PGT	C11-C12-C13-C14
60	z	301	PTY	N1-C2-C3-O11
60	M	503	PTY	O30-C30-C31-C32
60	M	504	PTY	C12-C11-C8-O10
66	AB	603	PC7	O11-C11-C12-C13
72	BE	402	CDL	C32-C31-CA7-OA9
72	u	101	CDL	C54-C55-C56-C57
66	AG	101	PC7	C22-C23-C24-C25
58	AC	407	PGT	C20-C21-C22-C23
58	L	704	PGT	C11-C12-C13-C14
60	N	501	PTY	O30-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
60	N	502	PTY	C18-C19-C20-C21
65	M	501	3PH	C28-C29-C2A-C2B
66	AG	101	PC7	C43-C44-C45-C46
60	D	401	PTY	C2-C3-O11-P1
60	M	504	PTY	C2-C3-O11-P1
60	BB	602	PTY	C2-C3-O11-P1
66	BD	302	PC7	C5-C4-O4P-P
66	f	203	PC7	C31-C32-C33-C34
60	BF	201	PTY	O30-C30-C31-C32
65	AI	101	3PH	O32-C31-C32-C33
60	N	503	PTY	O4-C30-C31-C32
60	m	101	PTY	C21-C22-C23-C24
72	BE	402	CDL	CB5-C51-C52-C53
72	BE	402	CDL	C13-C14-C15-C16
65	AC	405	3PH	O31-C31-C32-C33
72	AE	402	CDL	C12-C11-CA5-OA6
65	BJ	101	3PH	C39-C3A-C3B-C3C
66	AC	410	PC7	C19-C20-C21-C22
66	v	201	PC7	C11-C12-C13-C14
72	AE	402	CDL	C36-C37-C38-C39
72	BC	408	CDL	C34-C35-C36-C37
60	m	101	PTY	C19-C20-C21-C22
60	M	504	PTY	O4-C30-C31-C32
60	M	504	PTY	C39-C40-C41-C42
72	u	101	CDL	C43-C44-C45-C46
71	T	200	8Q1	C37-C38-C39-O40
72	AC	409	CDL	OA5-CA3-CA4-OA6
74	AC	402	HEM	C2A-CAA-CBA-CGA
60	N	503	PTY	O30-C30-C31-C32
72	BE	402	CDL	C59-C60-C61-C62
58	L	704	PGT	O2-C31-C32-C33
58	BC	406	PGT	O2-C31-C32-C33
72	u	102	CDL	C32-C31-CA7-OA8
72	BC	407	CDL	C32-C31-CA7-OA8
58	L	704	PGT	O31-C31-C32-C33
60	N	501	PTY	C12-C11-C8-O7
60	z	301	PTY	O4-C30-C31-C32
65	BC	405	3PH	O21-C21-C22-C23
67	AC	403	UQ5	C4-C3-O3-C3M
58	AF	201	PGT	C12-C13-C14-C15
72	u	101	CDL	C35-C36-C37-C38
58	BC	406	PGT	O31-C31-C32-C33

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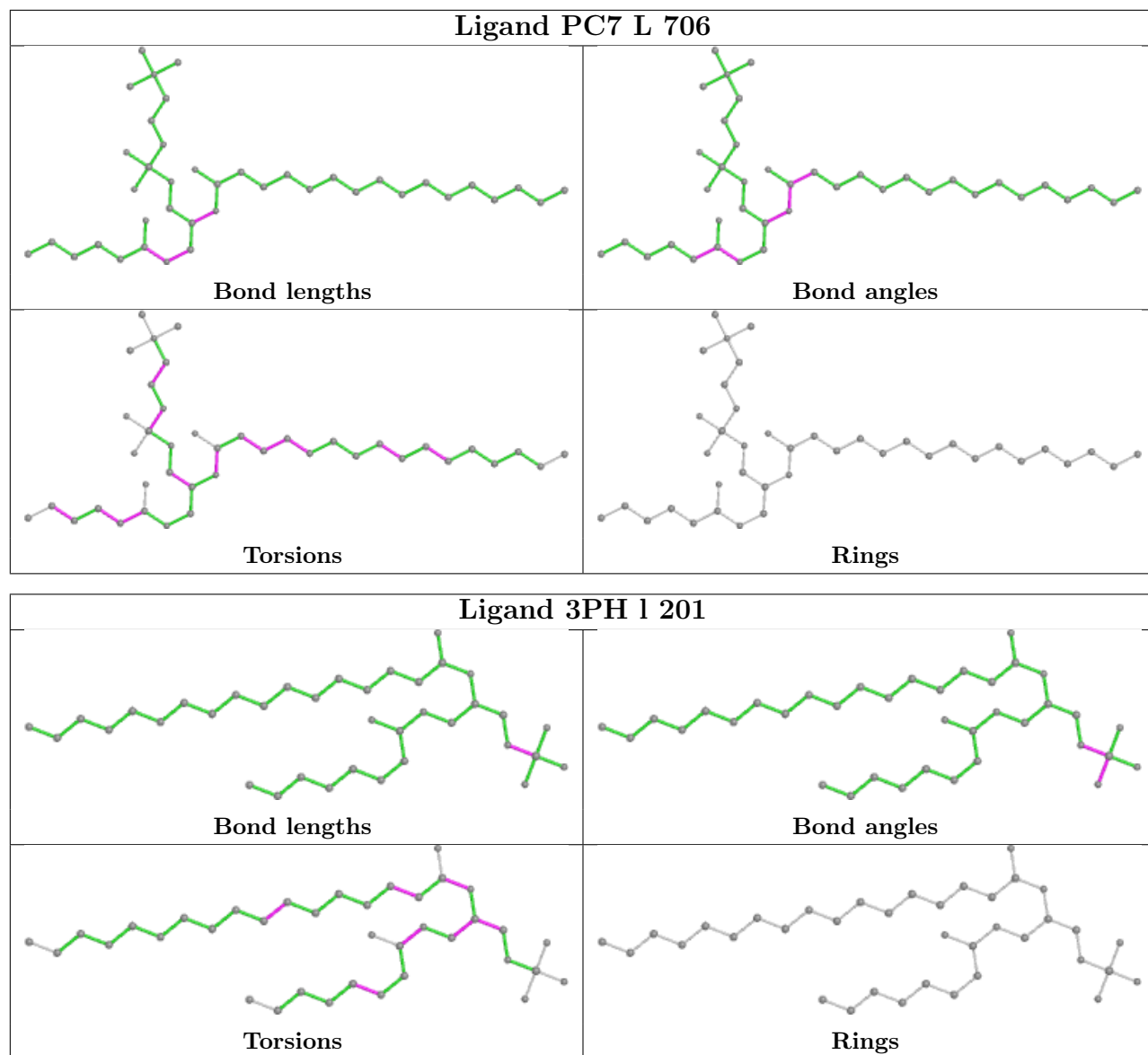
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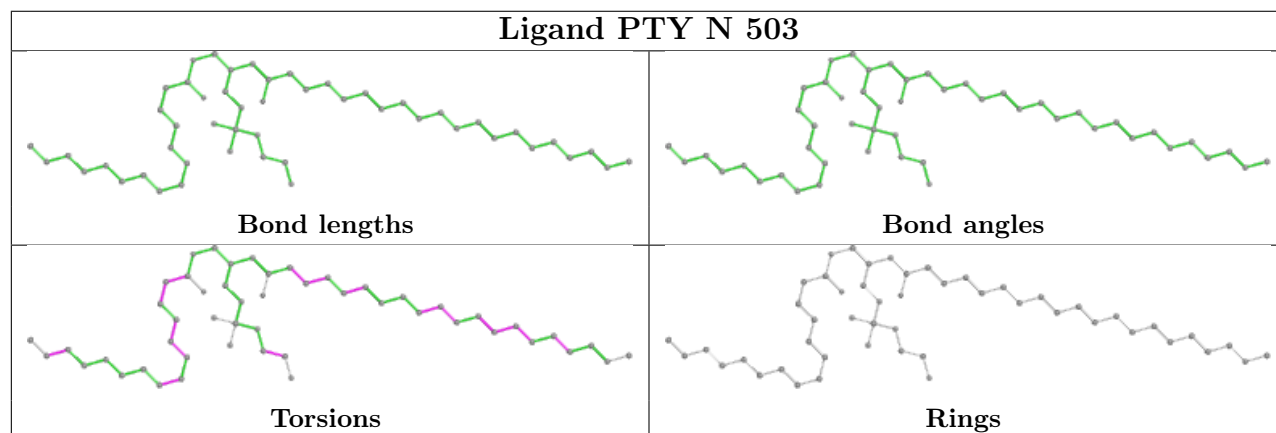
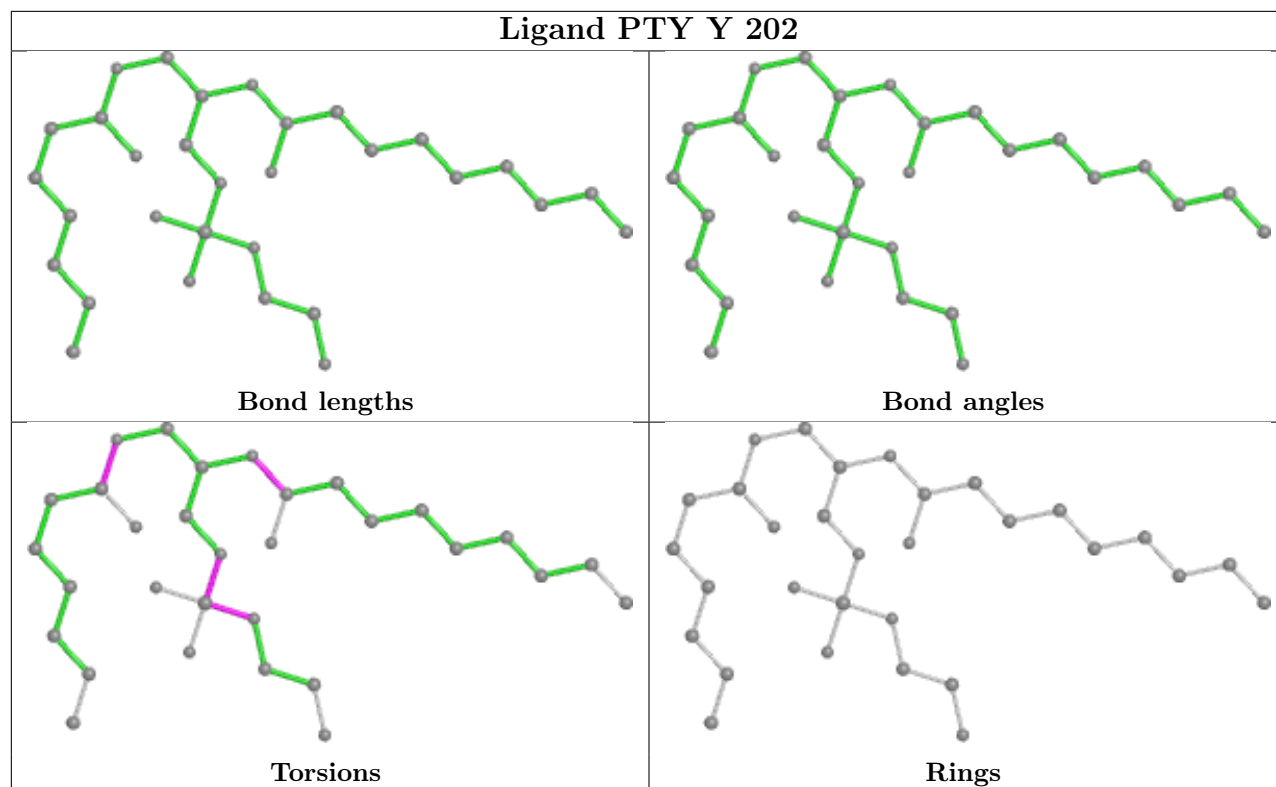
Mol	Chain	Res	Type	Atoms
72	BE	402	CDL	C72-C71-CB7-OB9
58	AF	201	PGT	C45-C46-C47-C48
58	y	303	PGT	C31-C32-C33-C34
60	z	301	PTY	O30-C30-C31-C32
72	u	102	CDL	C32-C31-CA7-OA9
65	AC	405	3PH	O32-C31-C32-C33
72	BC	407	CDL	C32-C31-CA7-OA9
65	Y	201	3PH	C34-C35-C36-C37
72	AC	409	CDL	C14-C15-C16-C17
58	A	201	PGT	O3-C11-C12-C13
58	L	702	PGT	O2-C31-C32-C33
74	AC	402	HEM	CAA-CBA-CGA-O1A

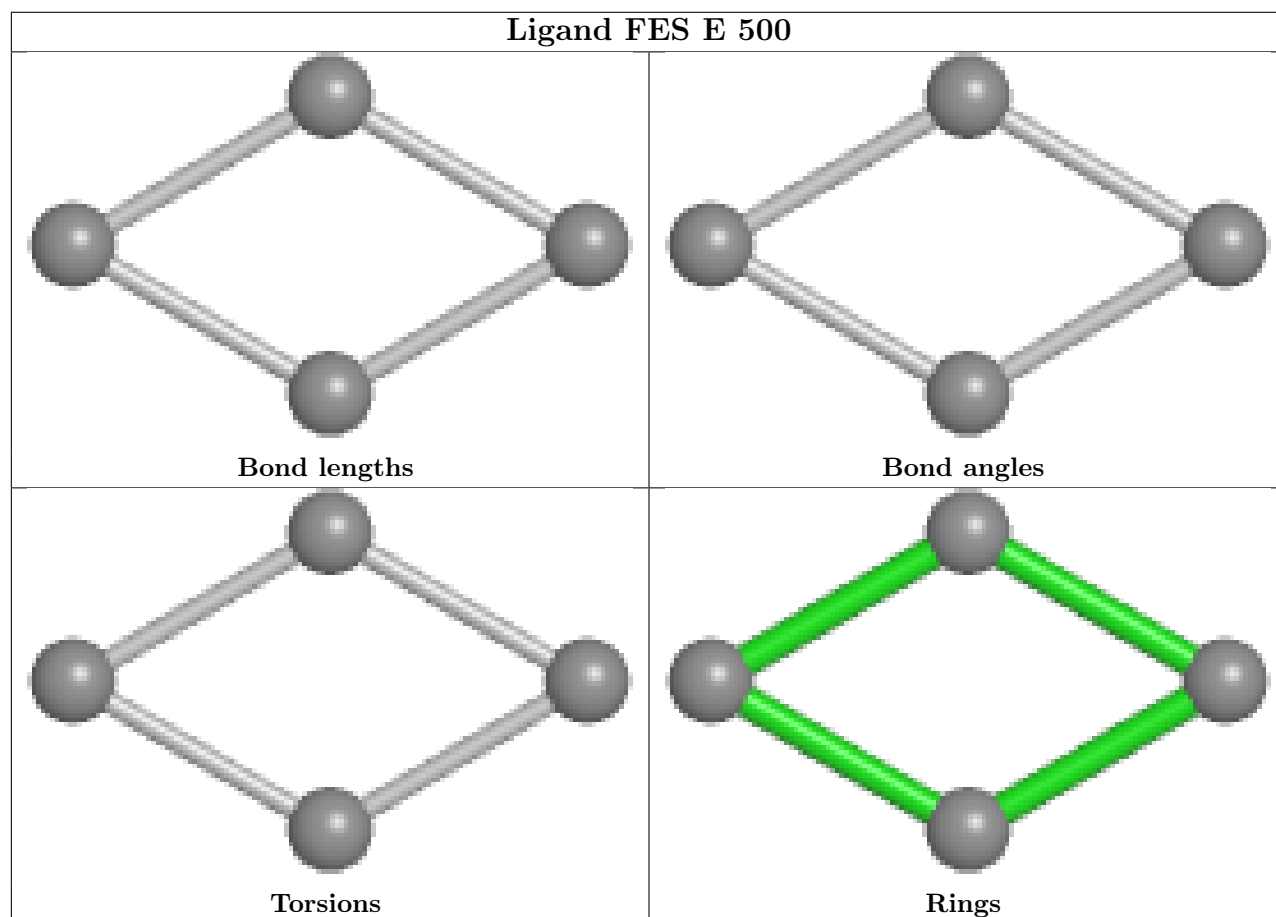
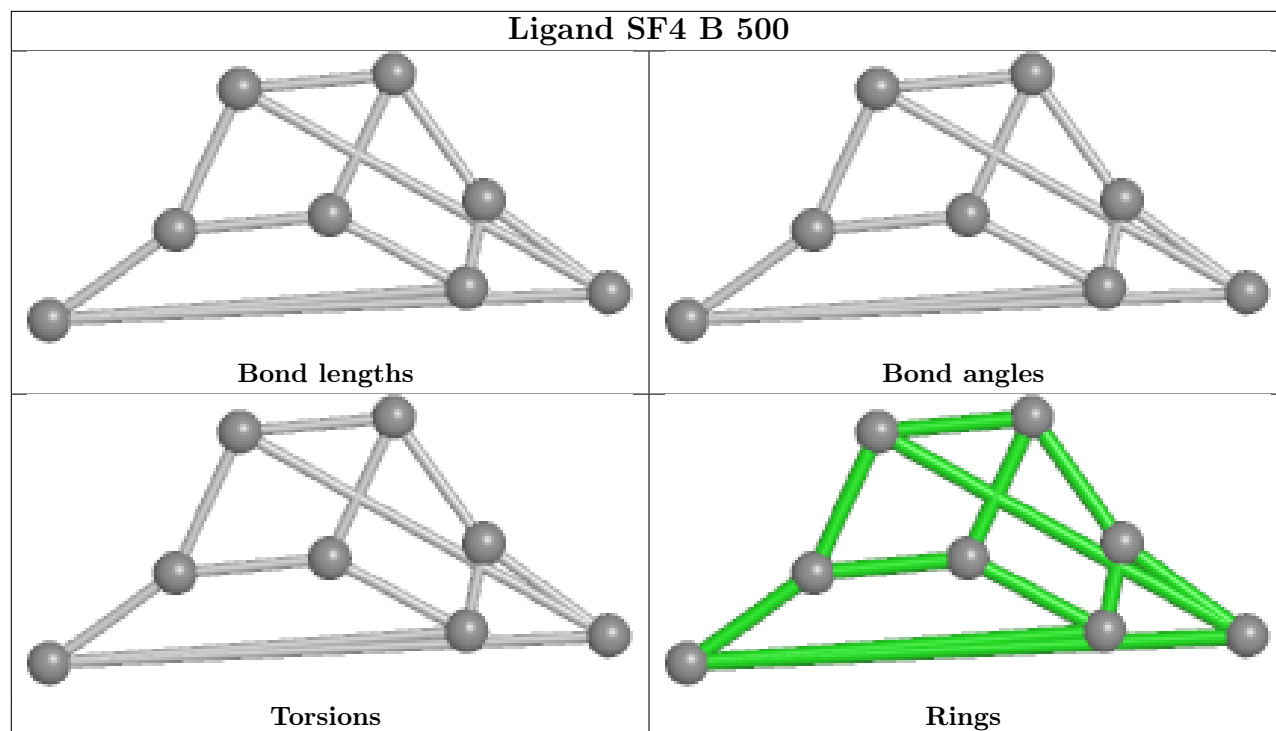
There are no ring outliers.

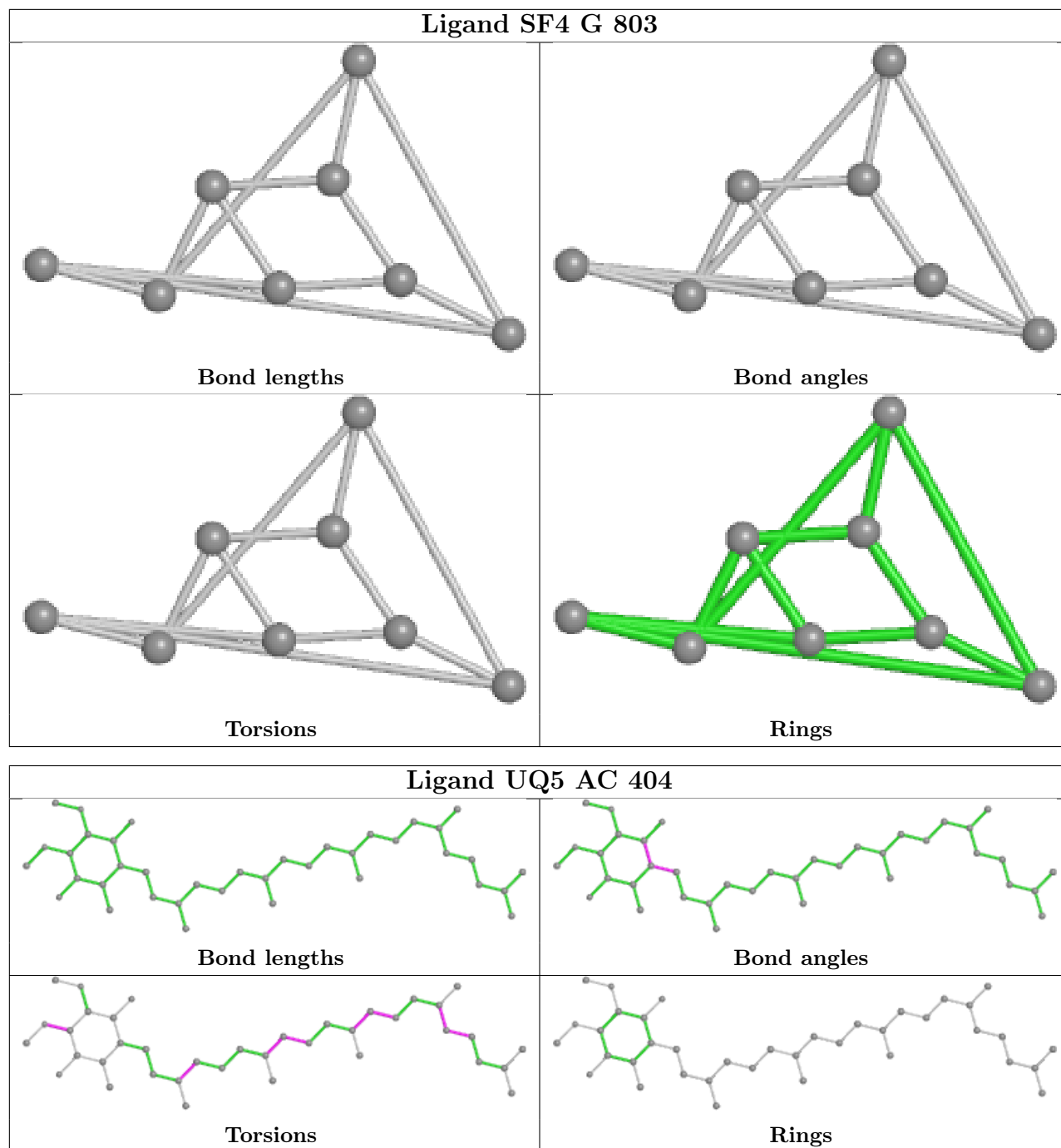
No monomer is involved in short contacts.

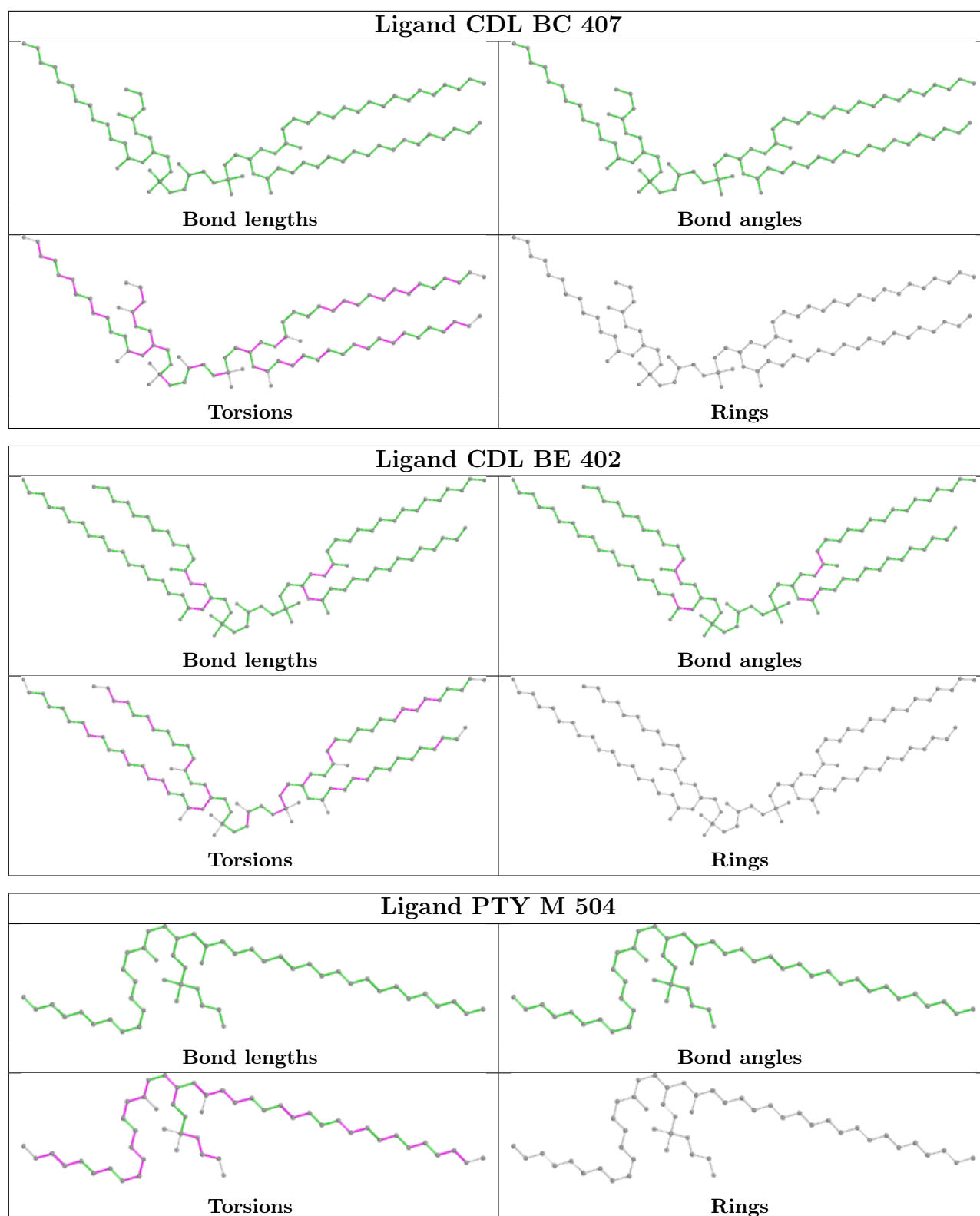
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

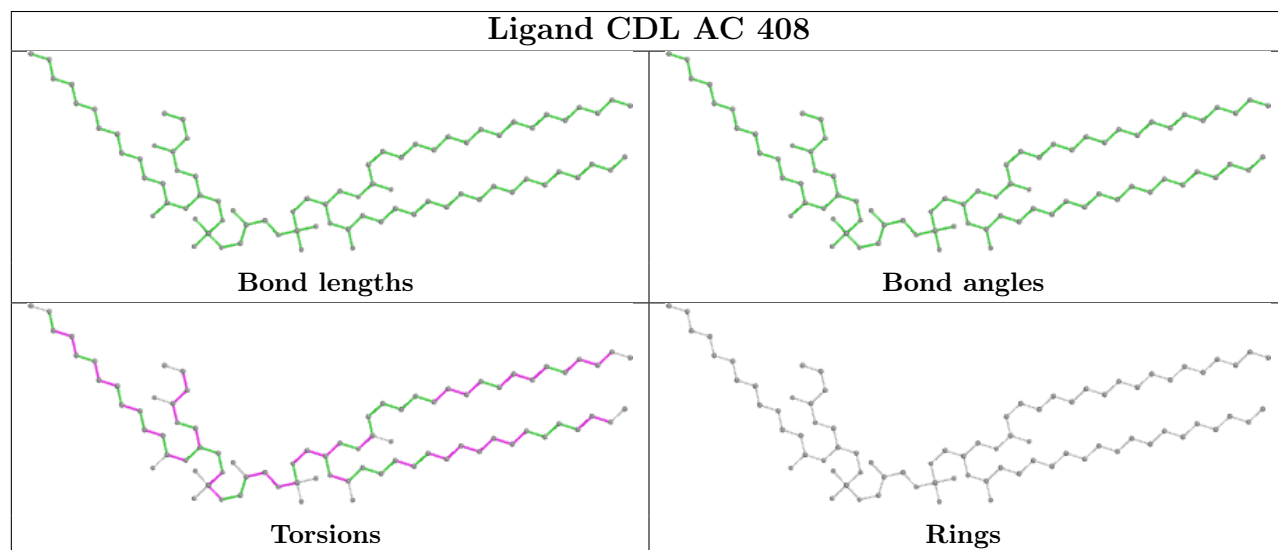
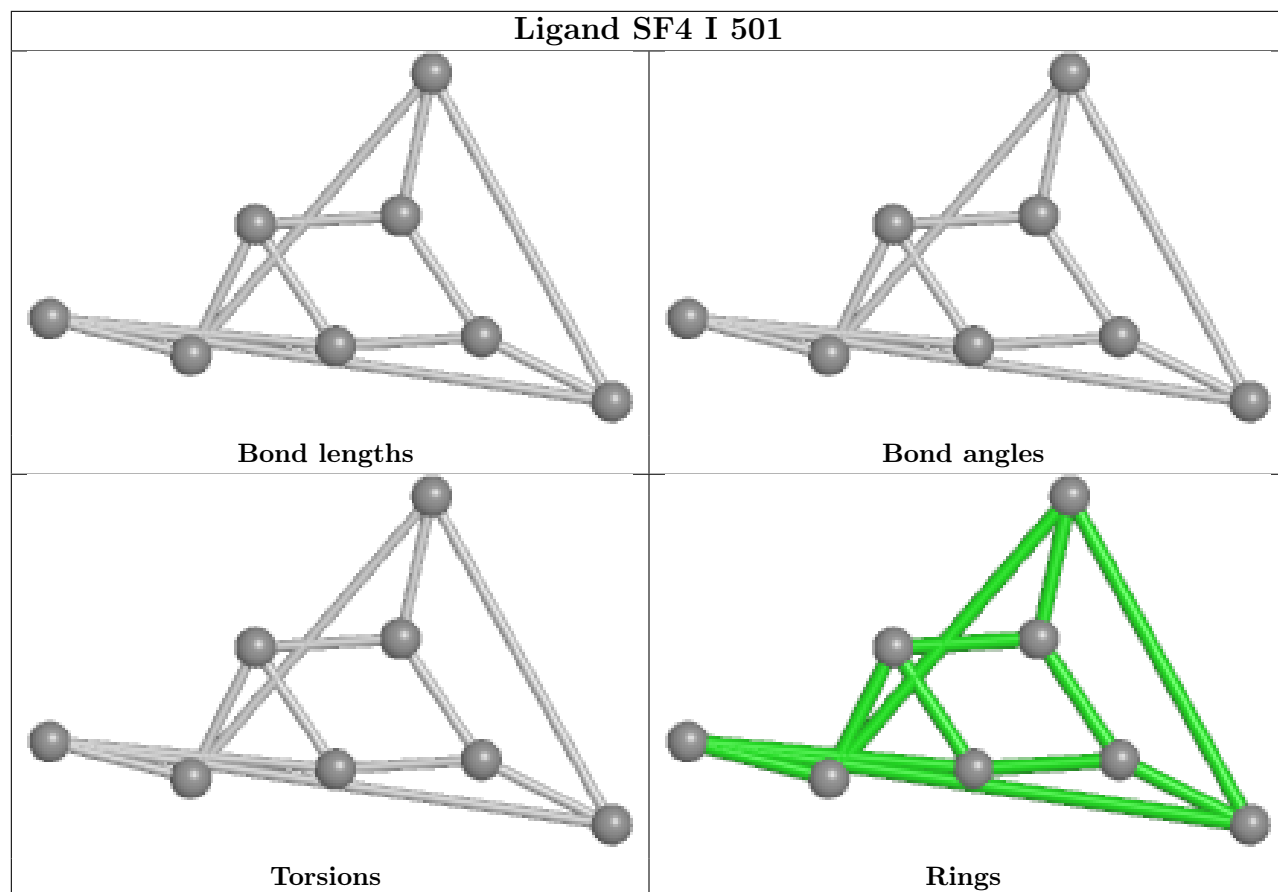


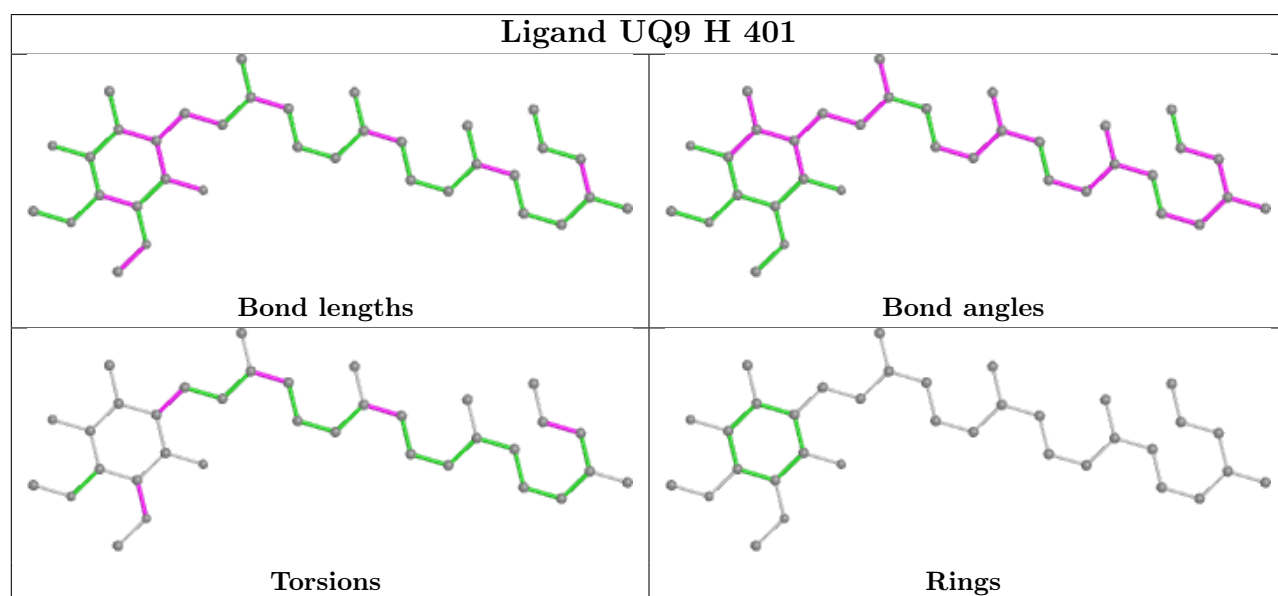
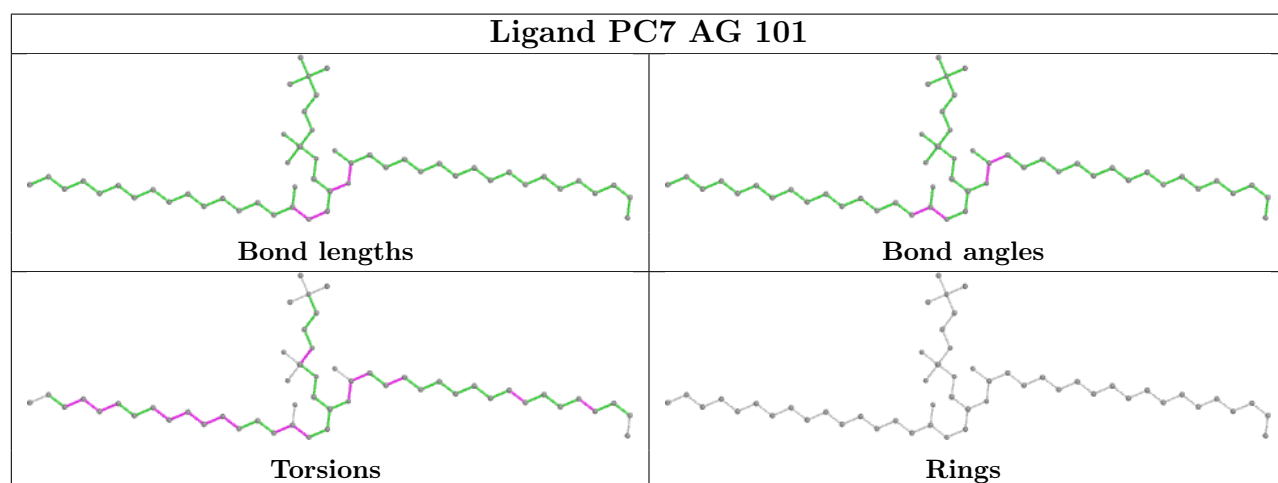
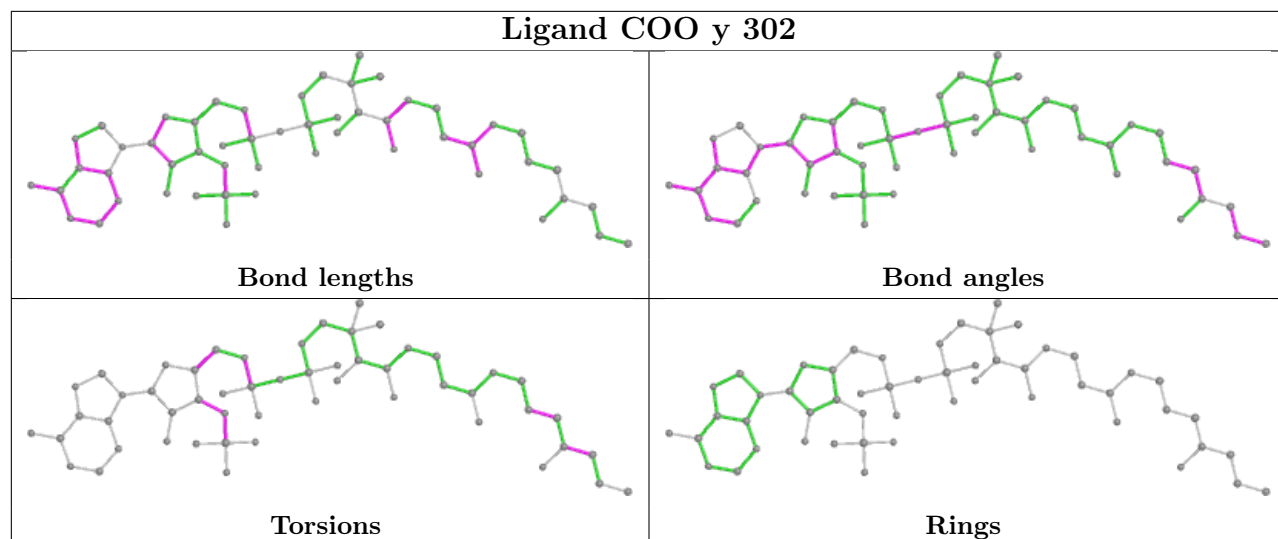


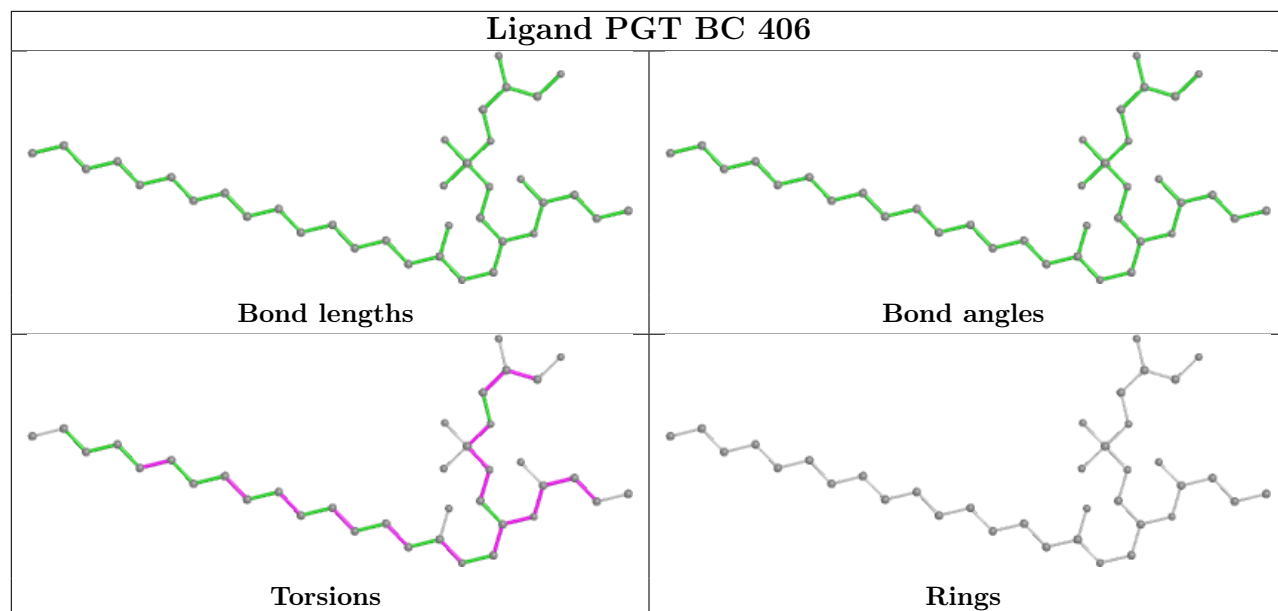


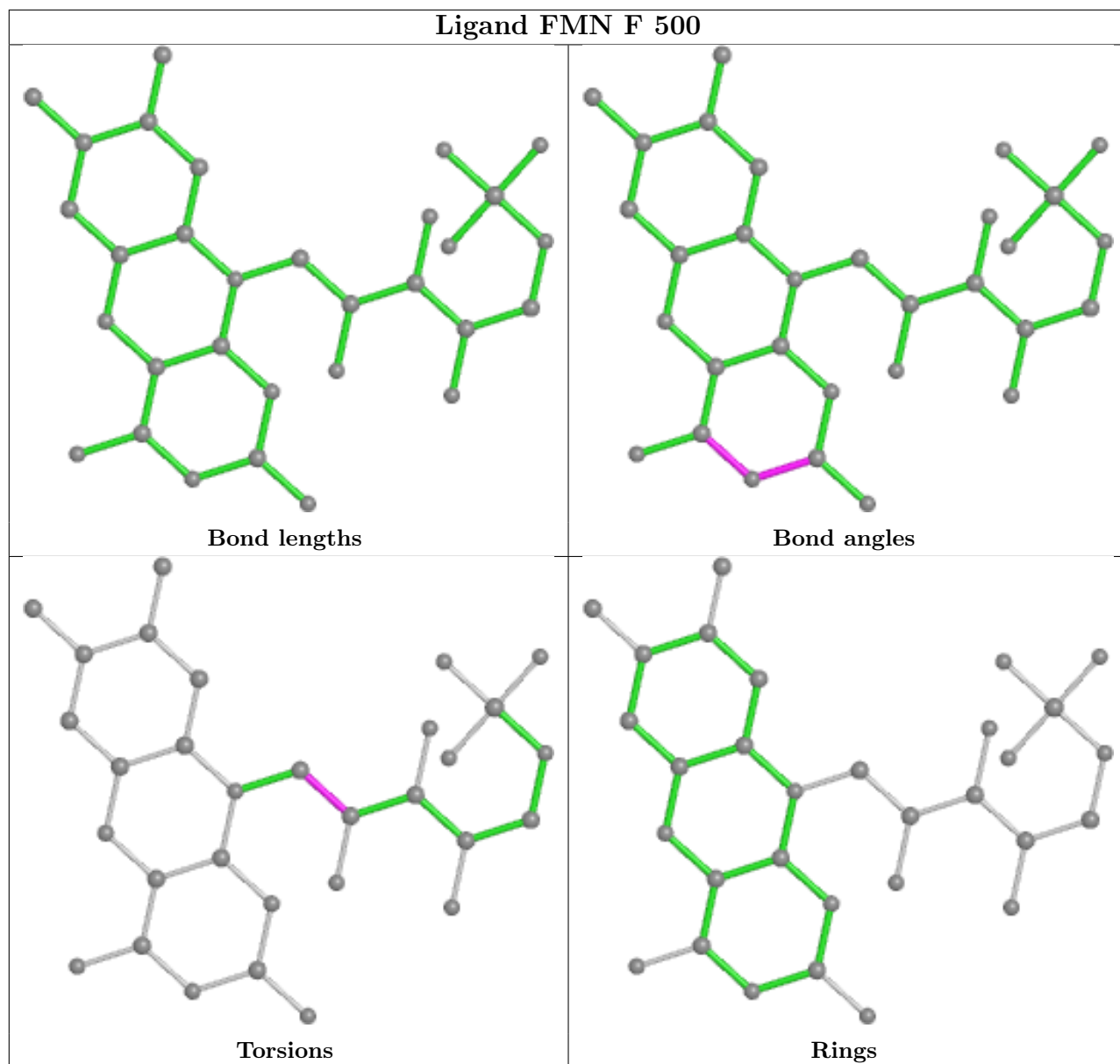


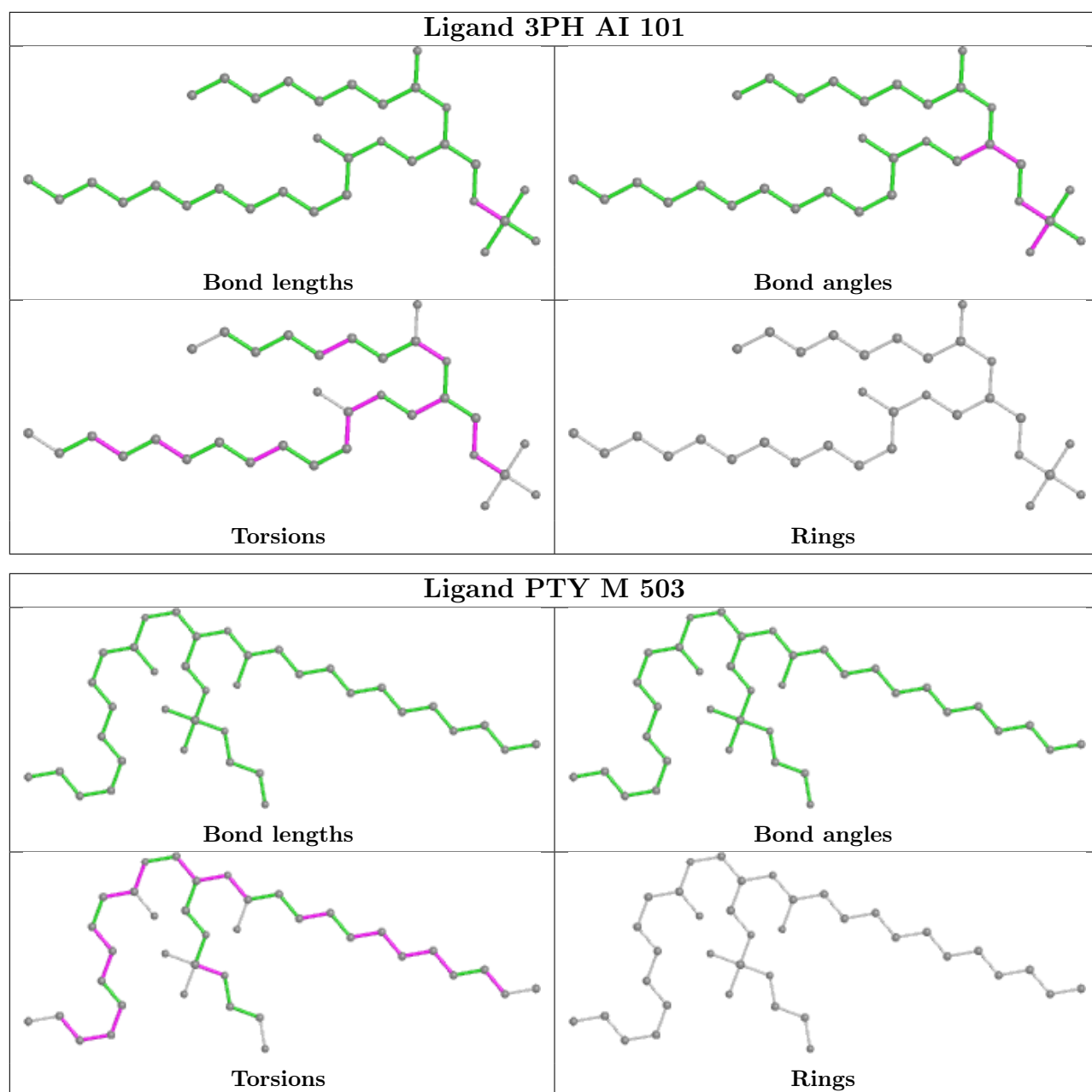


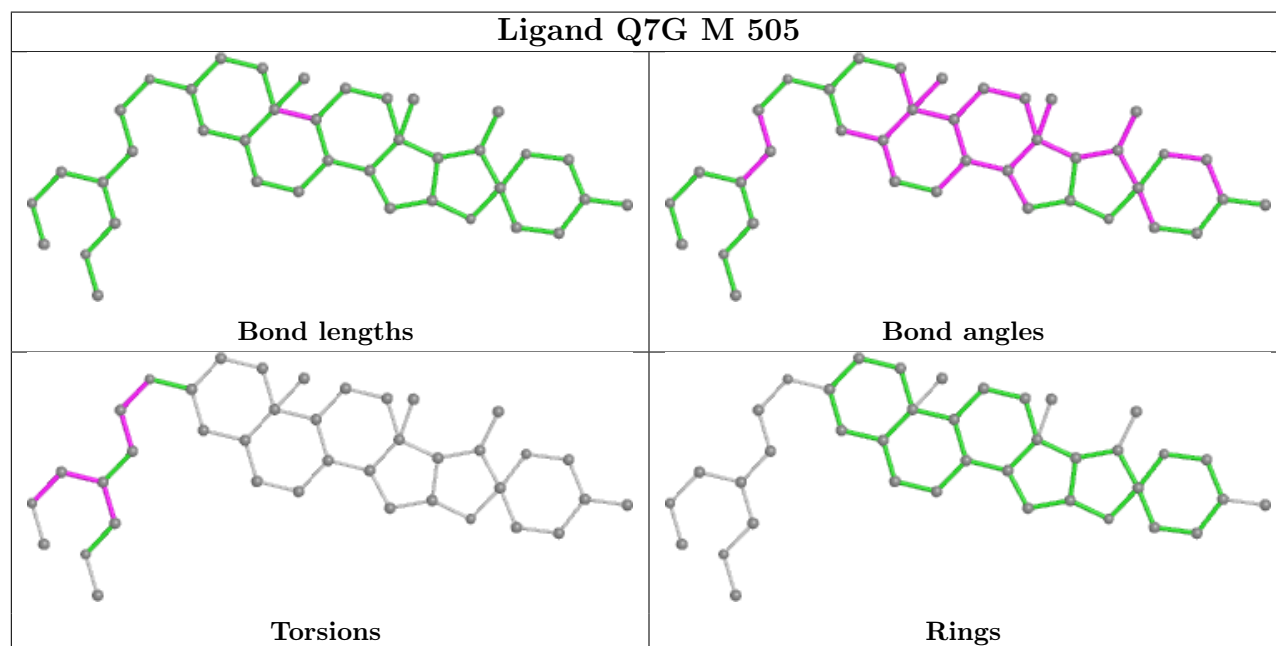
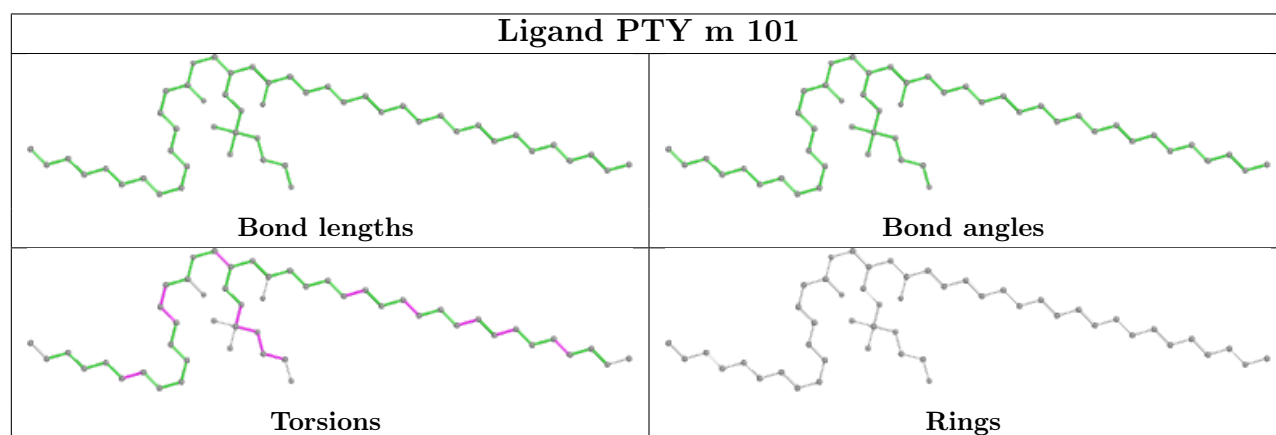
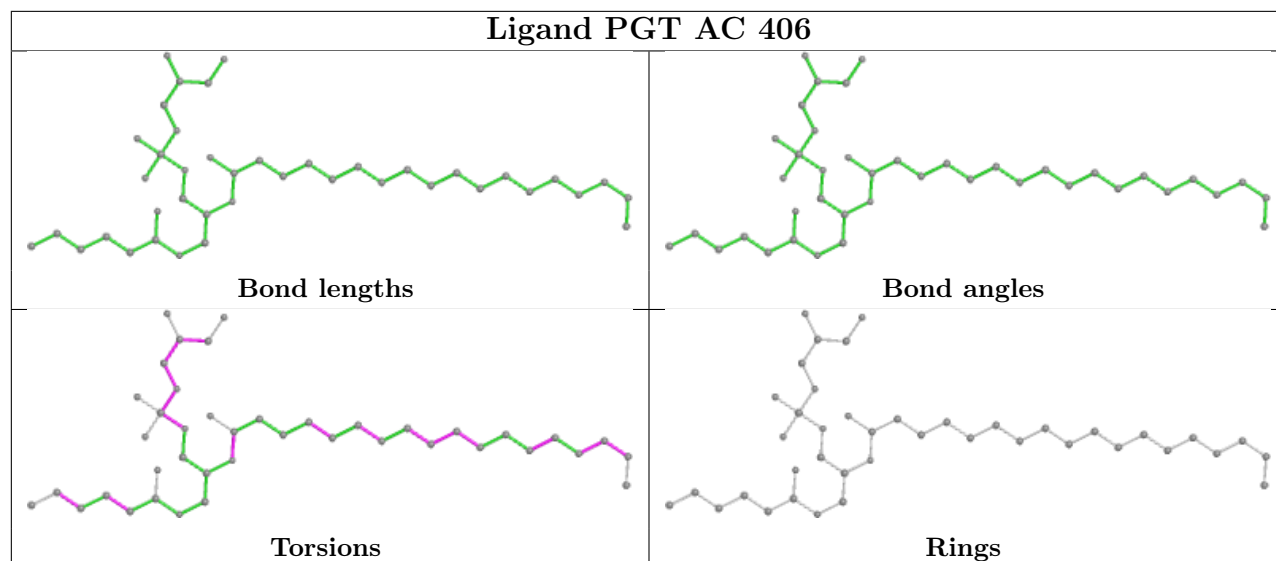


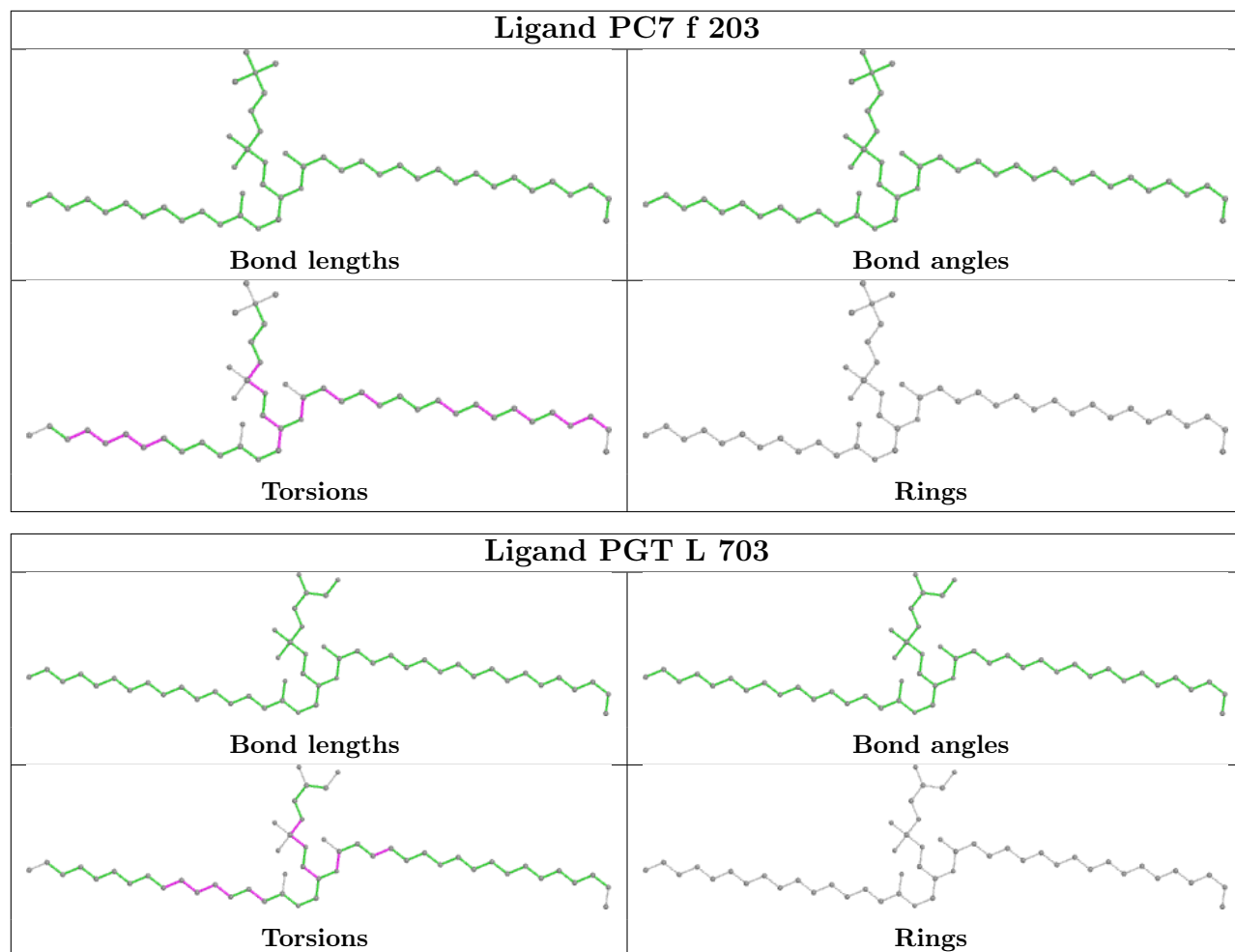


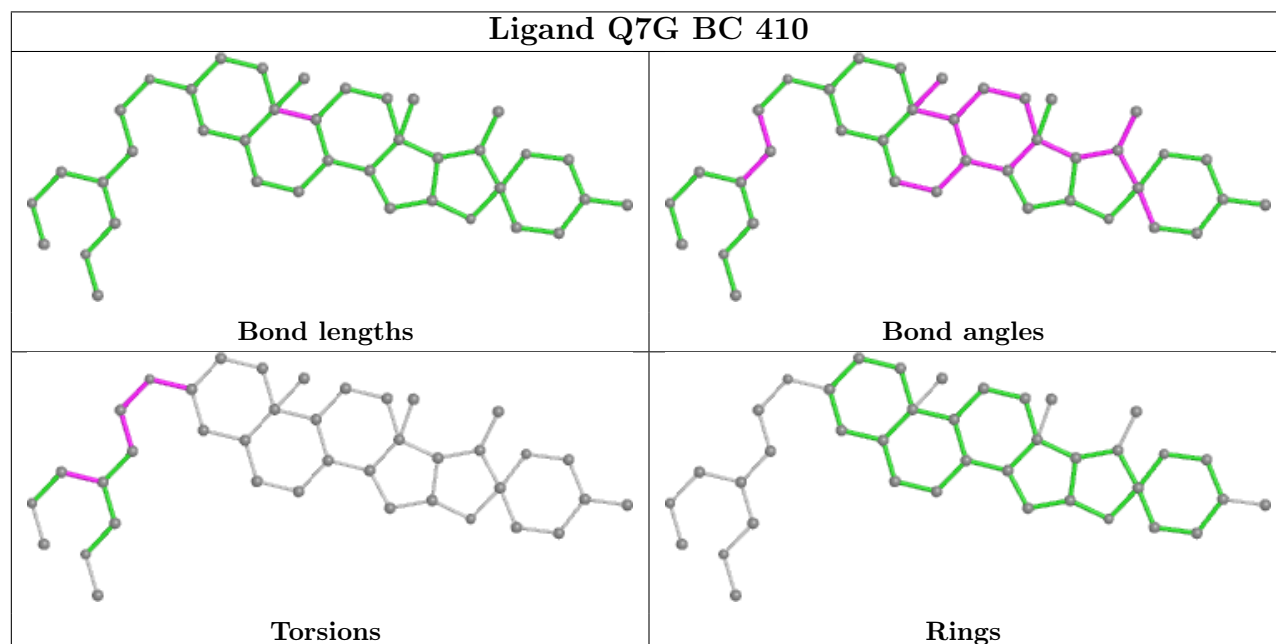
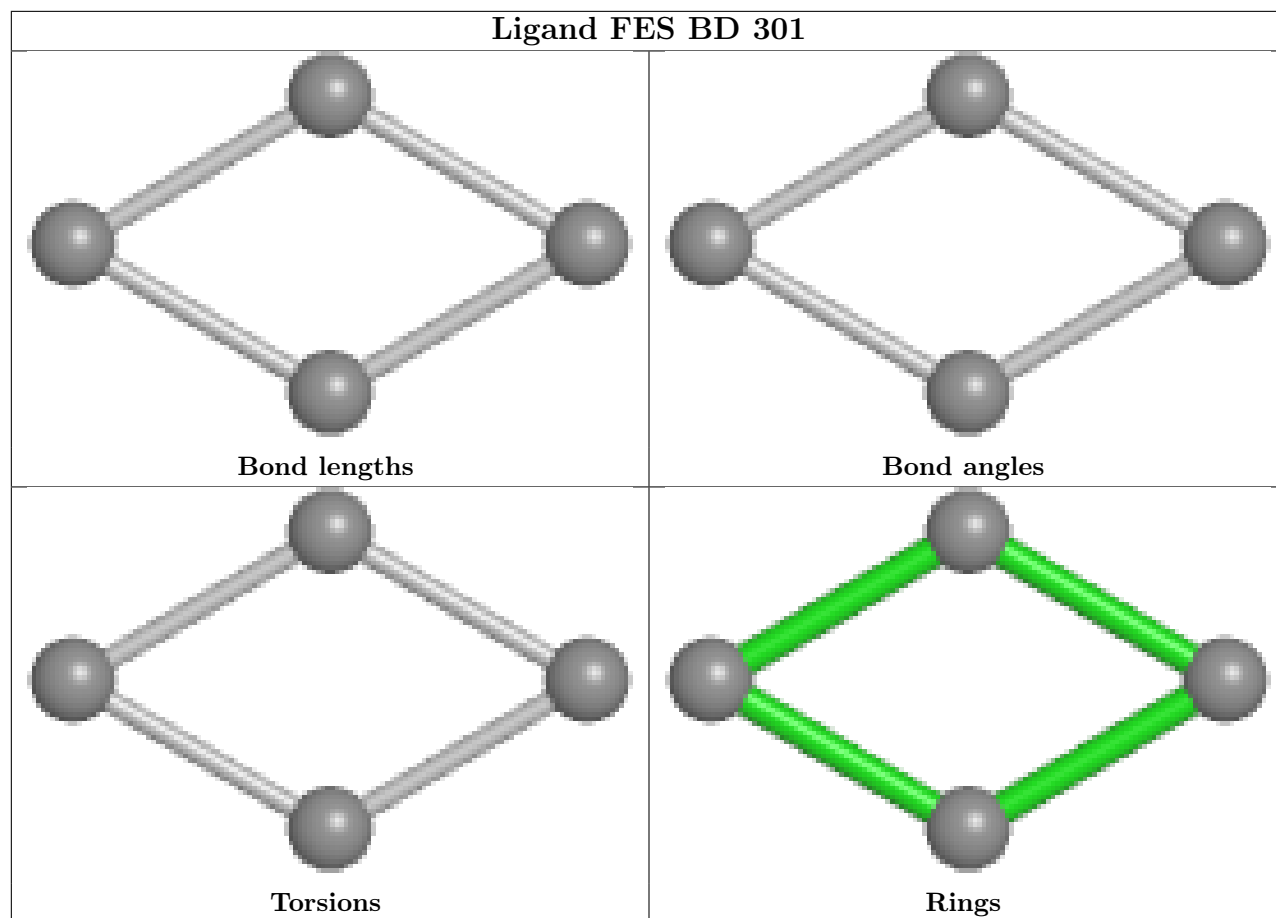


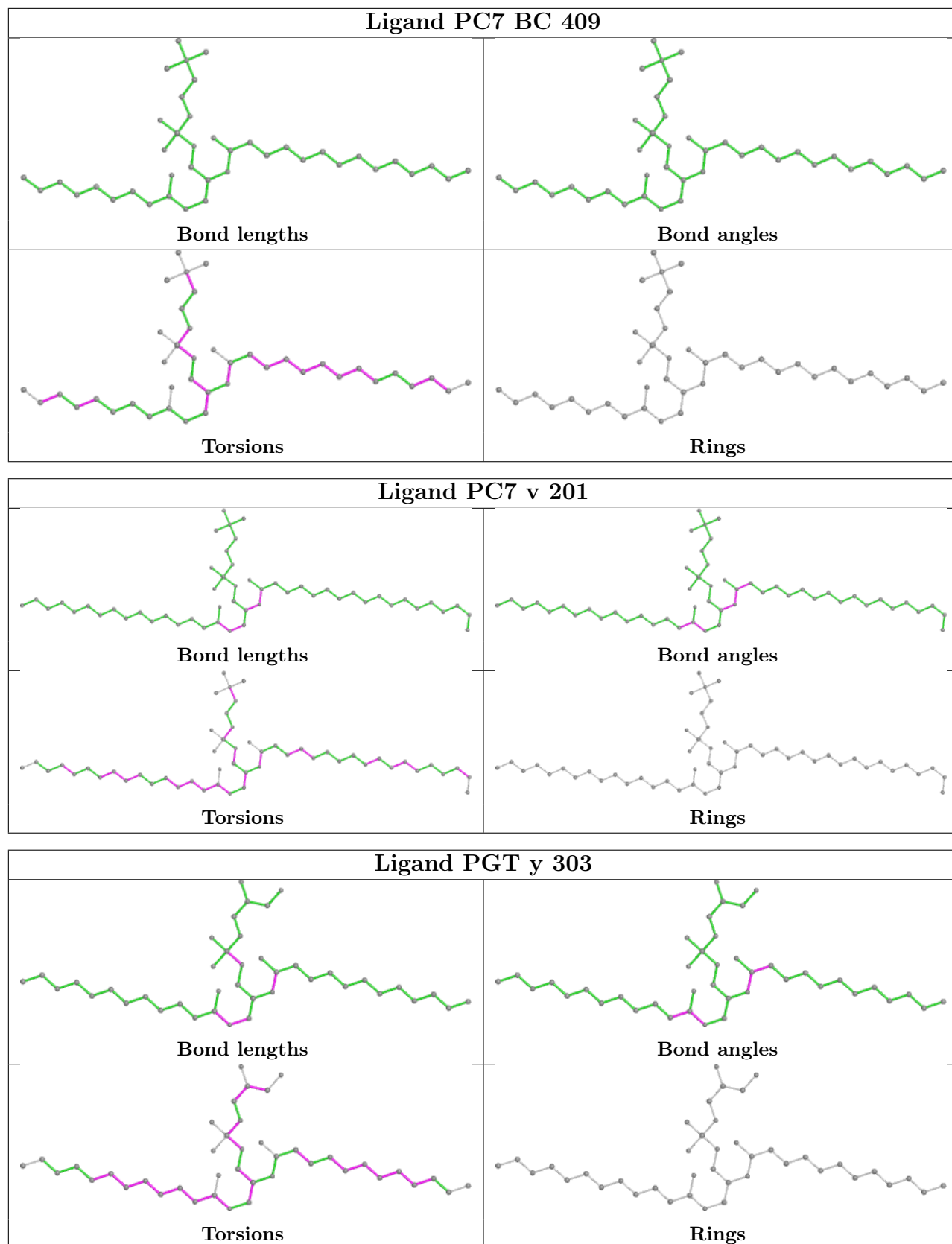


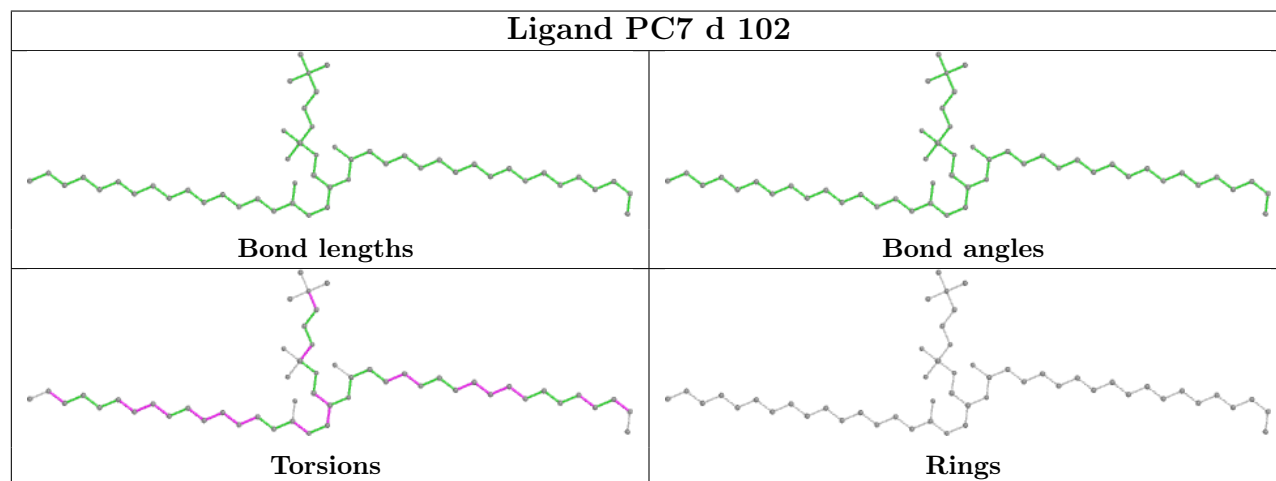
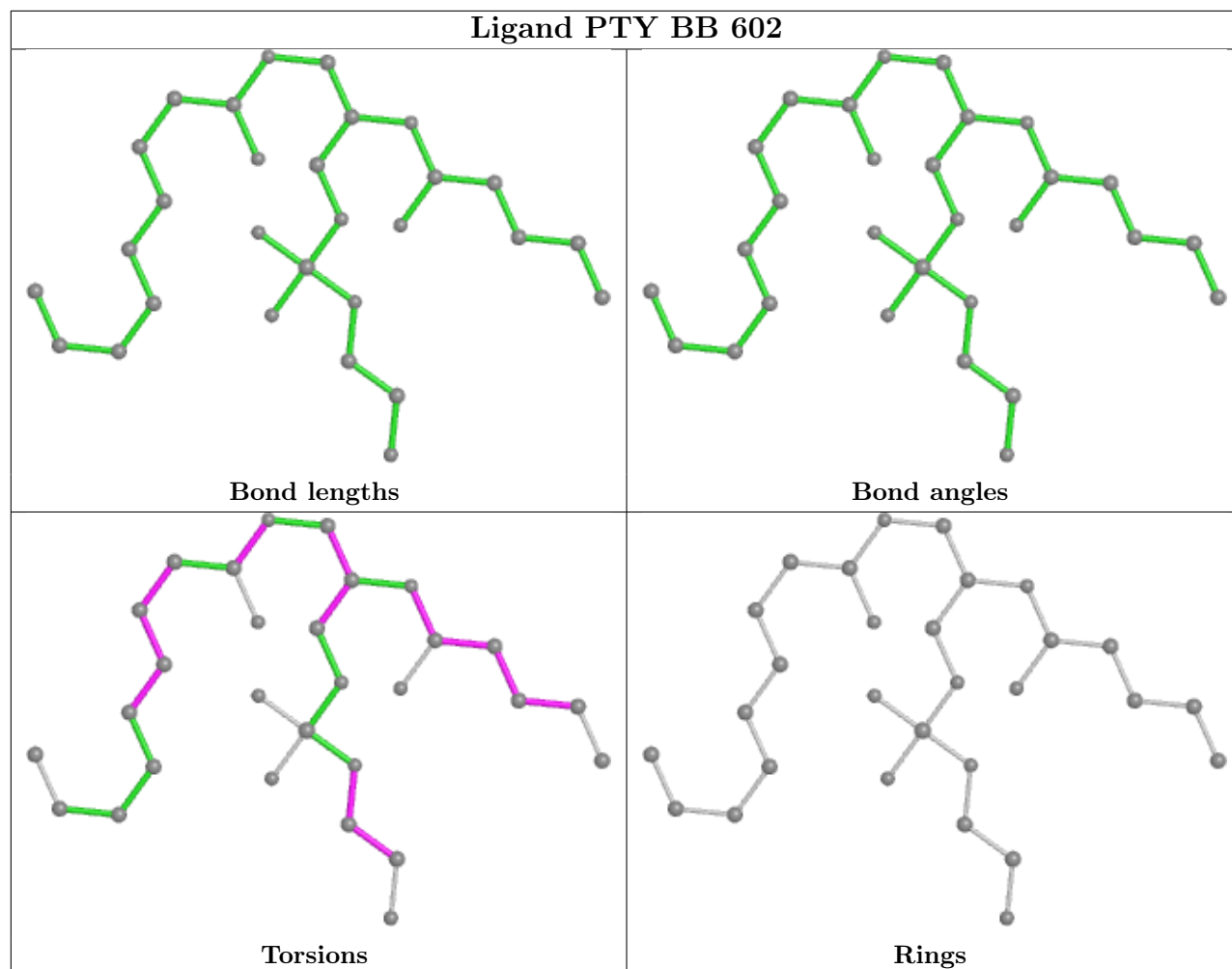


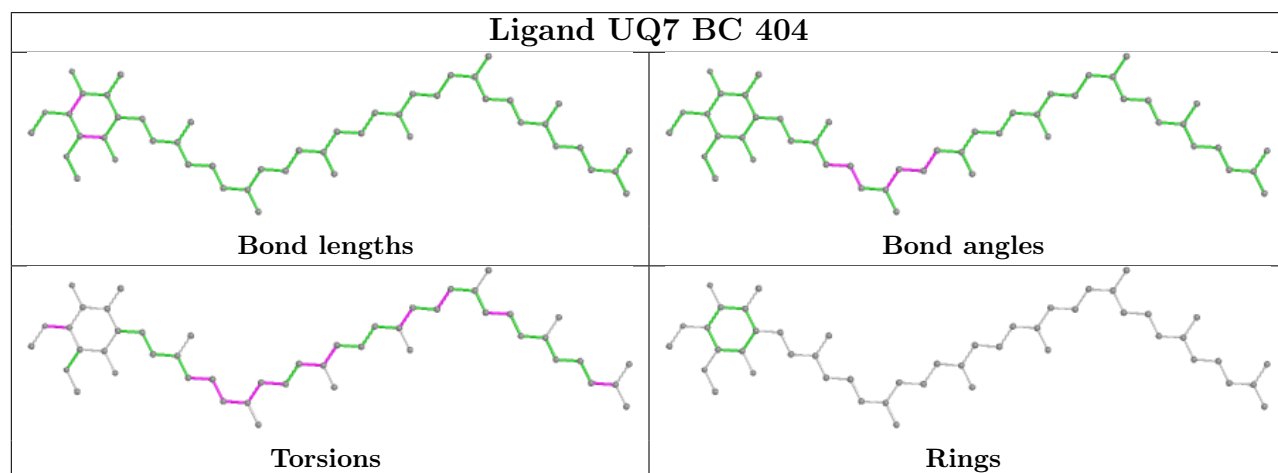
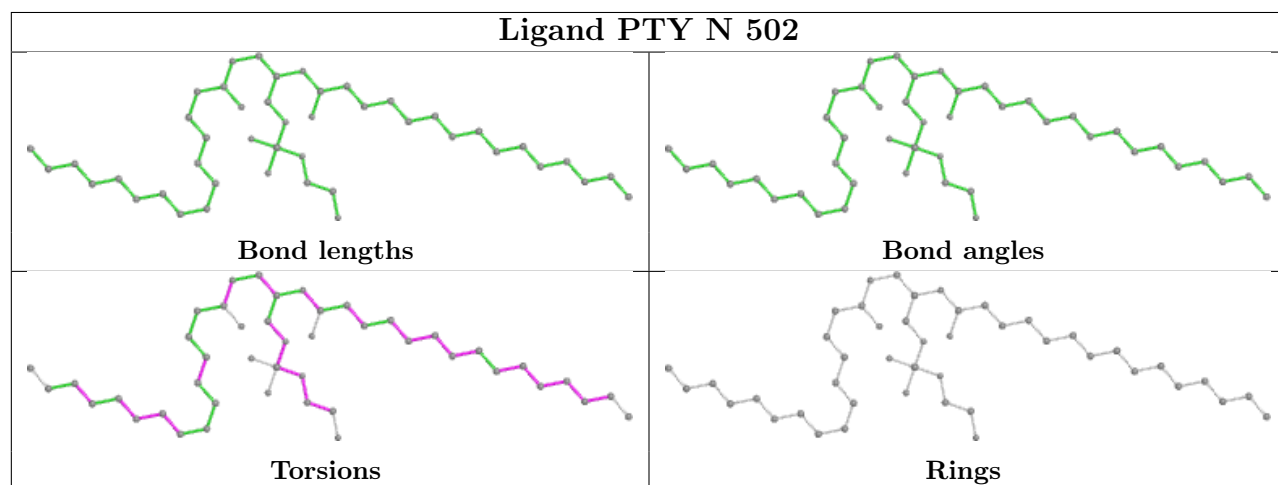
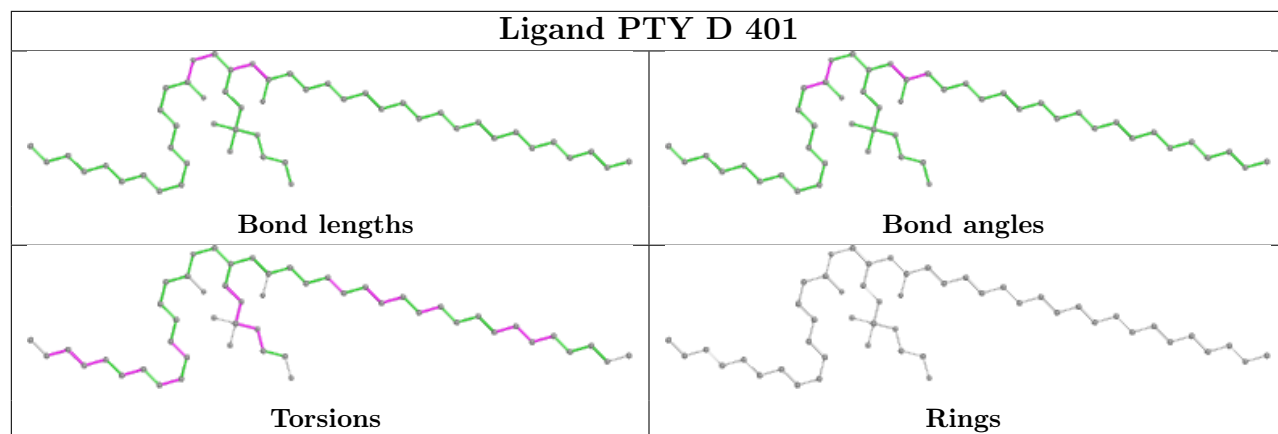


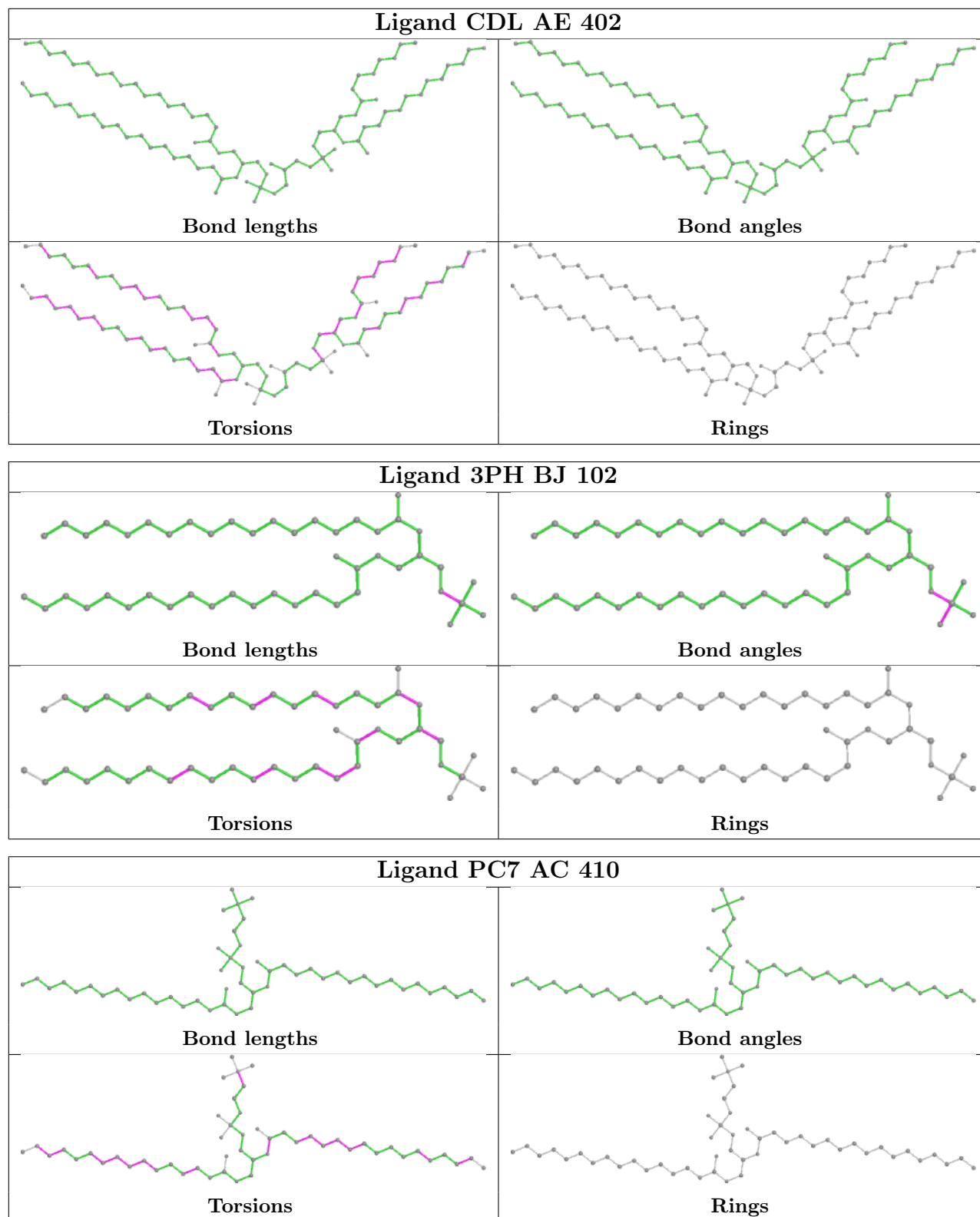


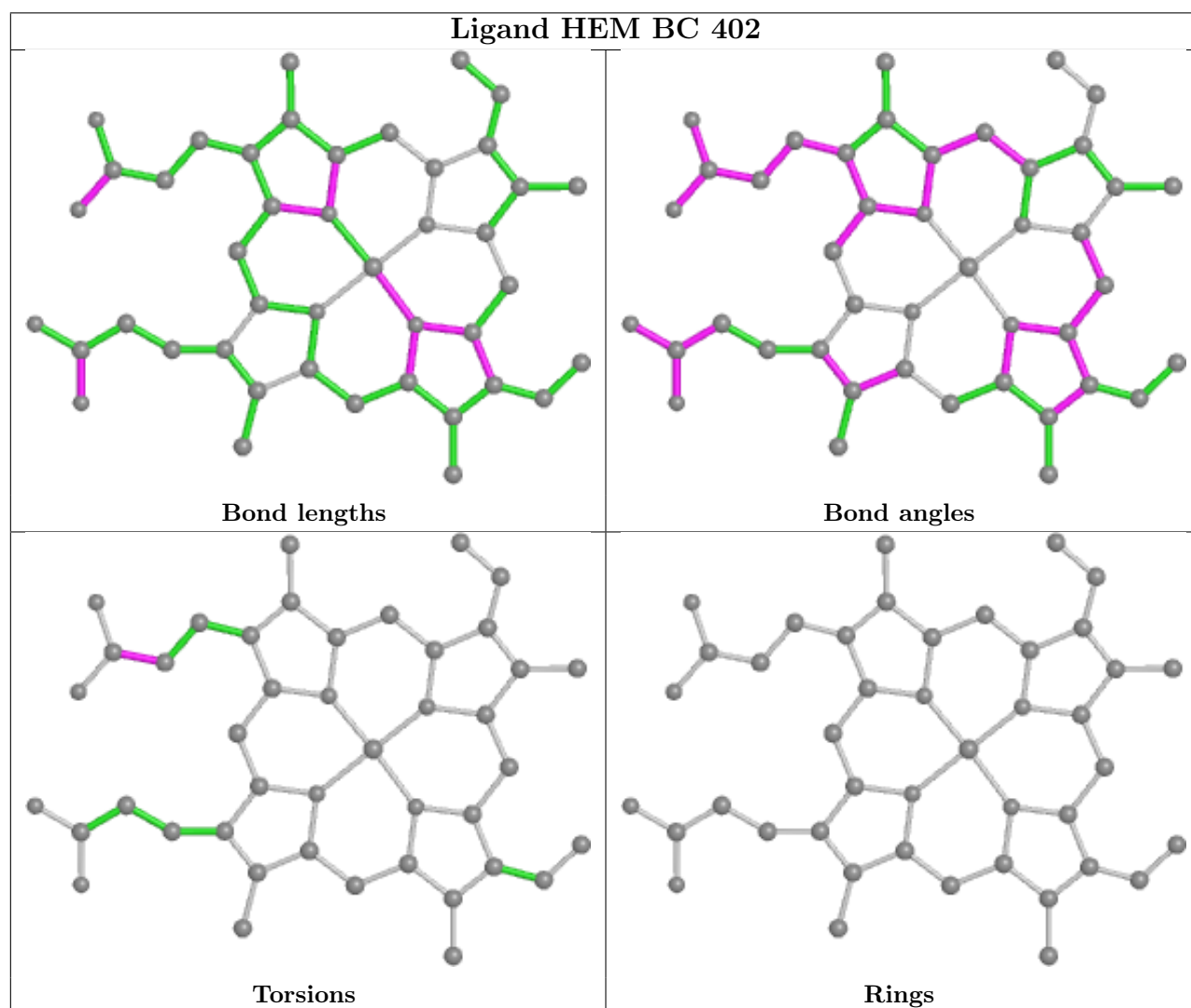
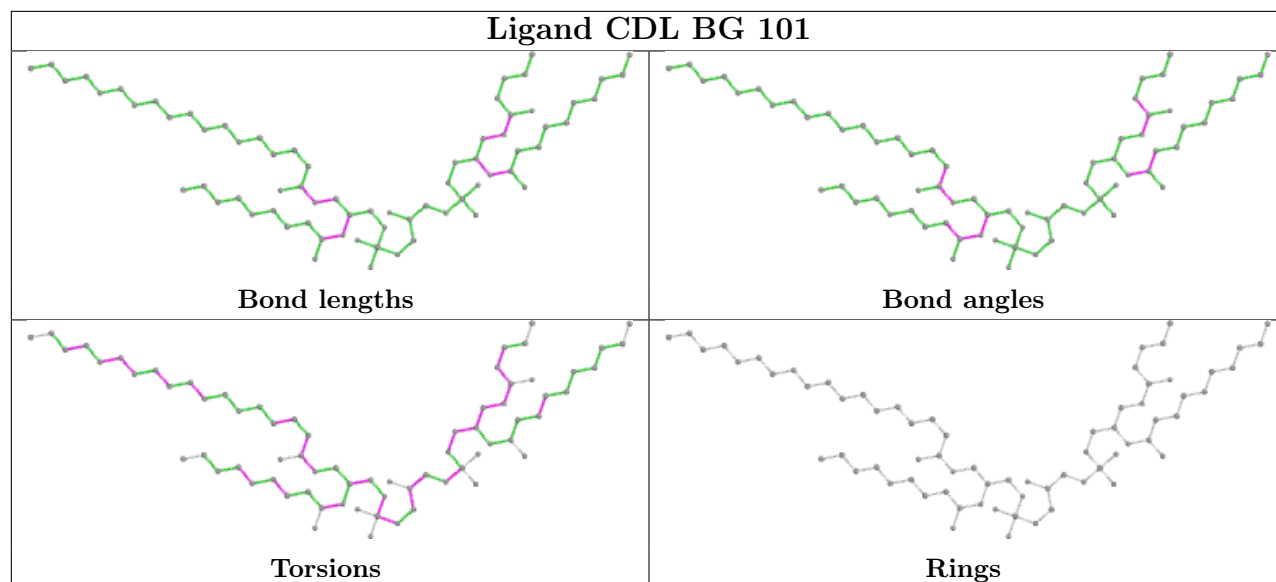


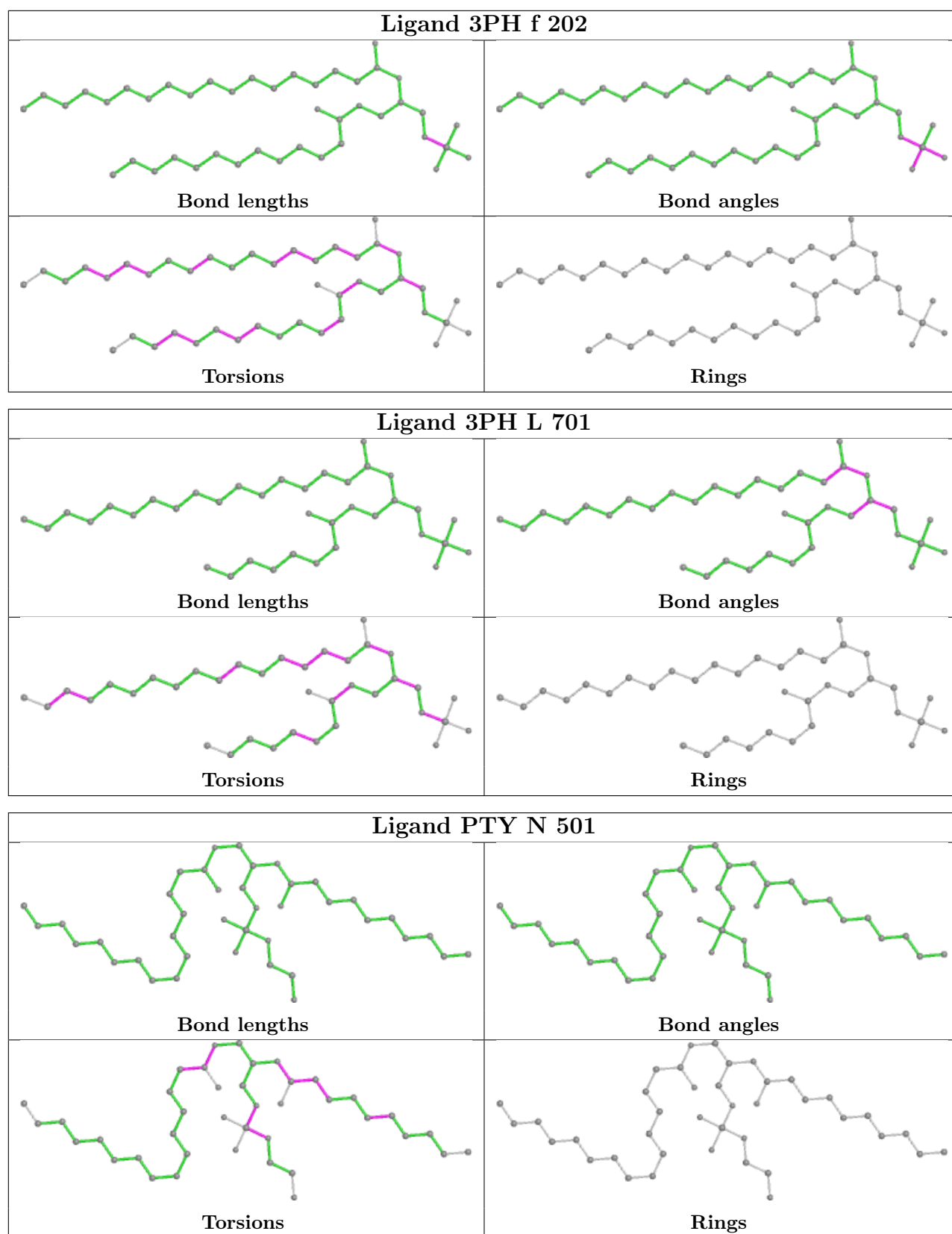


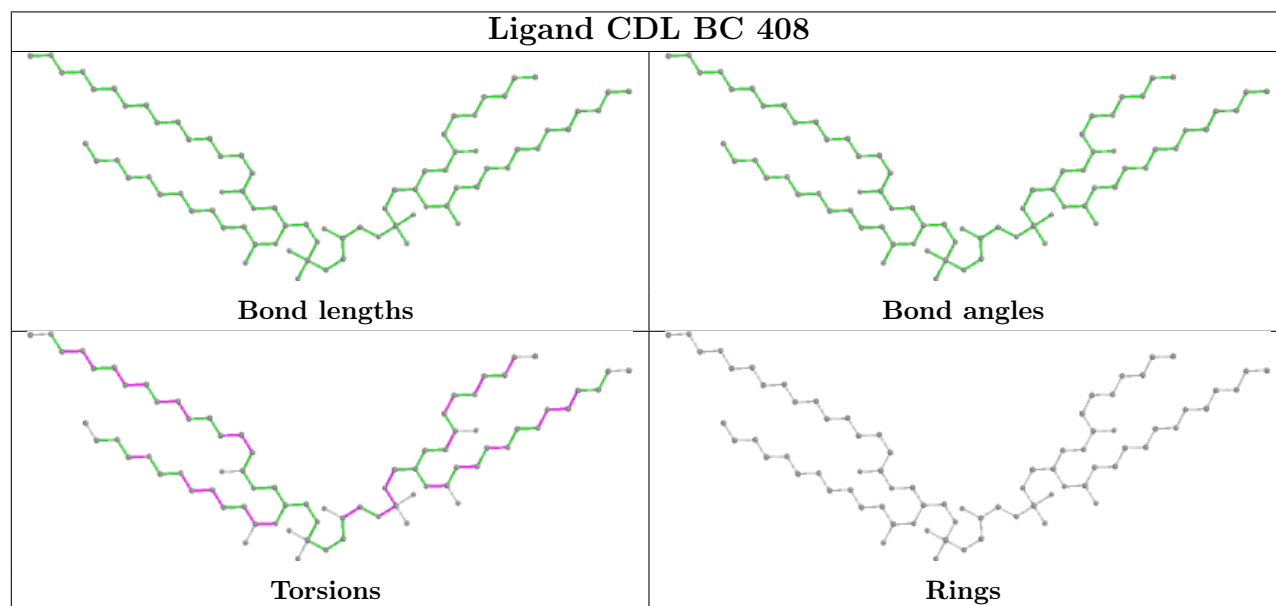
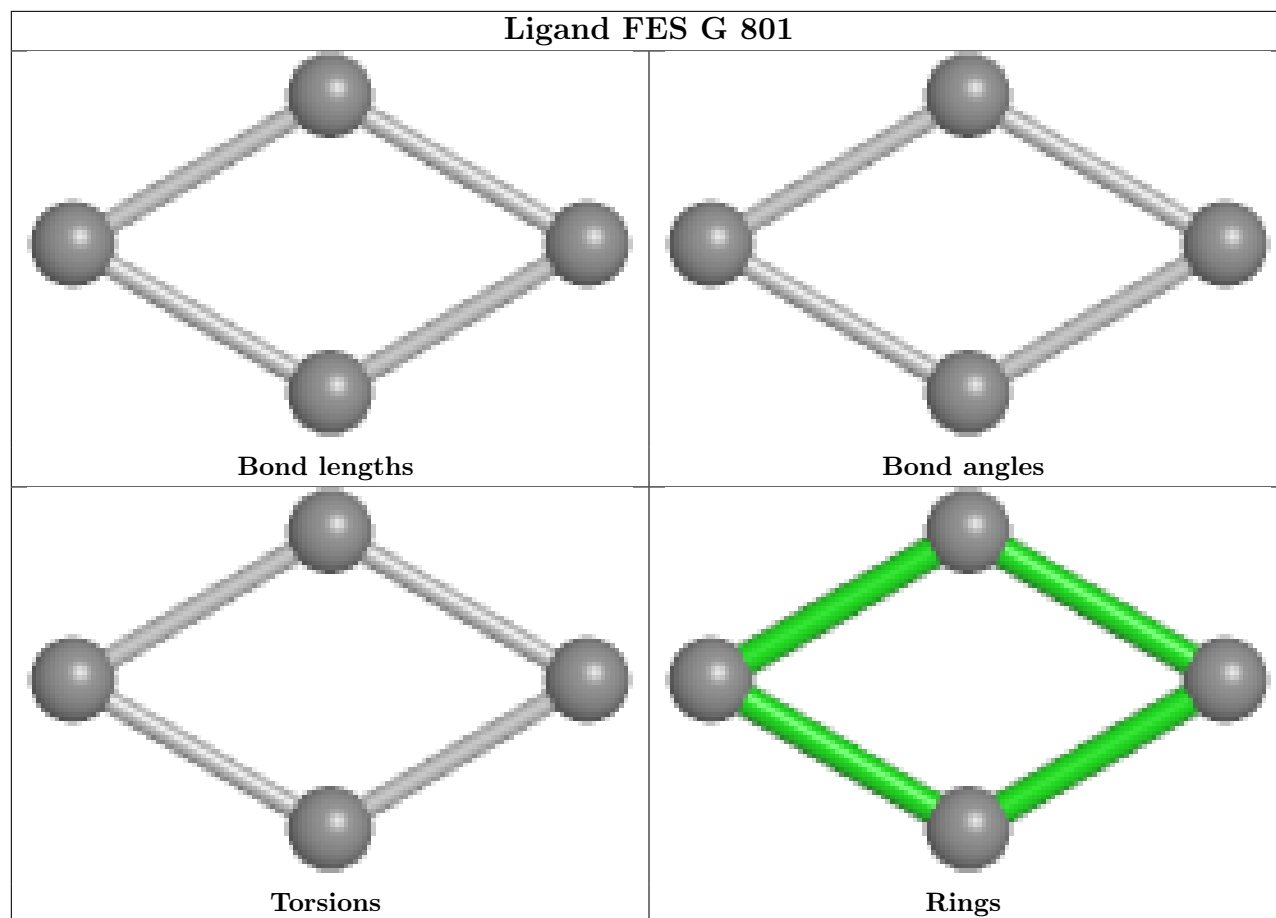


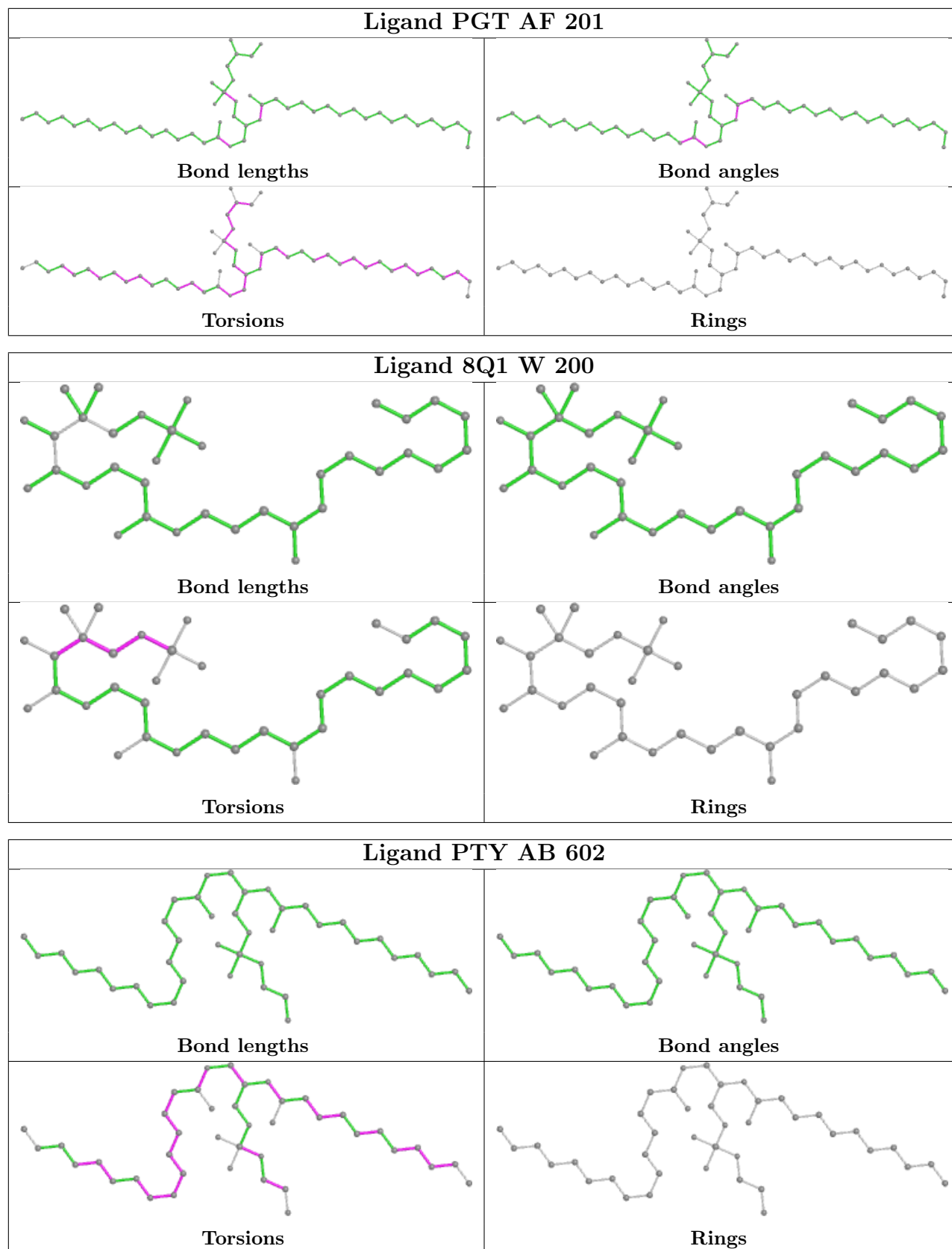


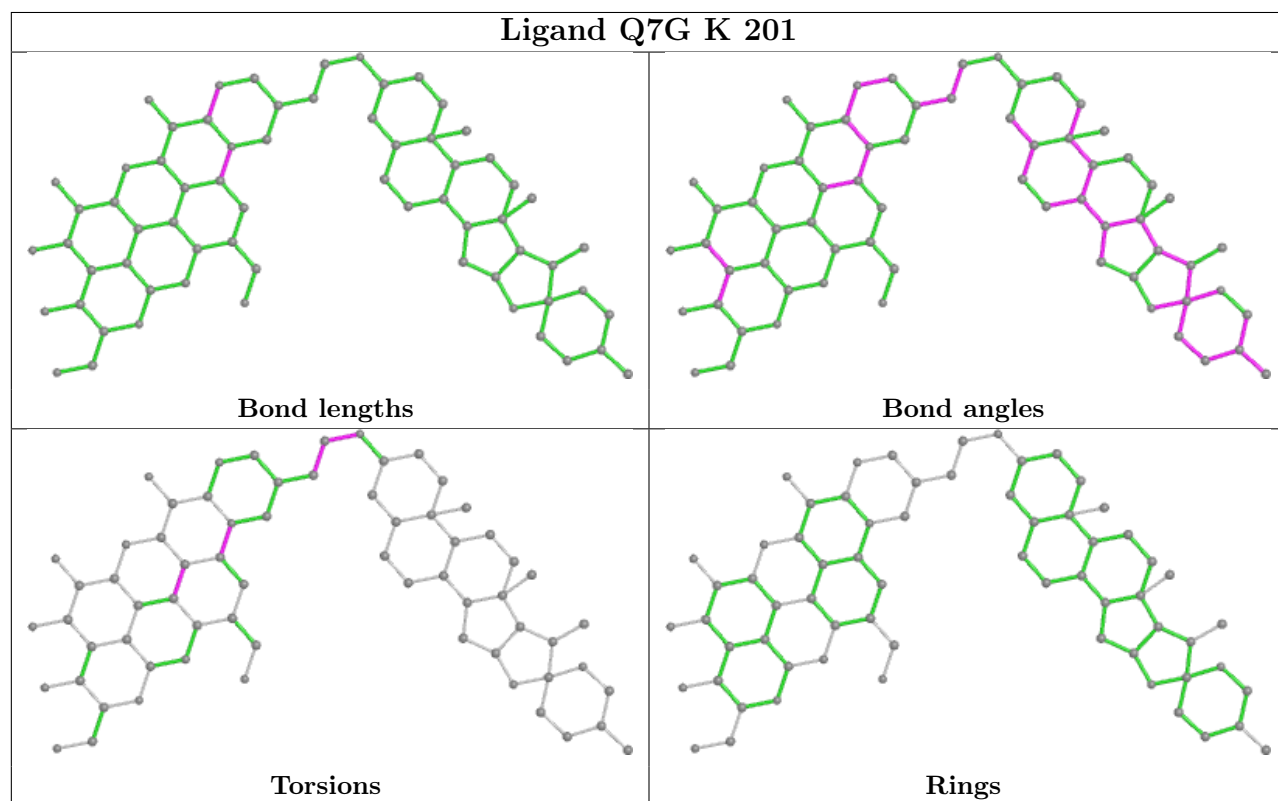
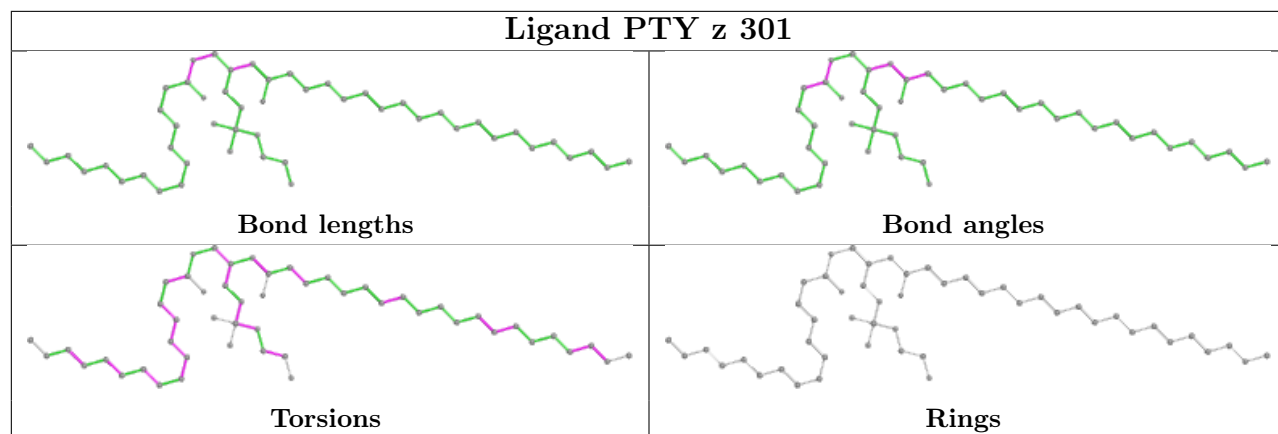


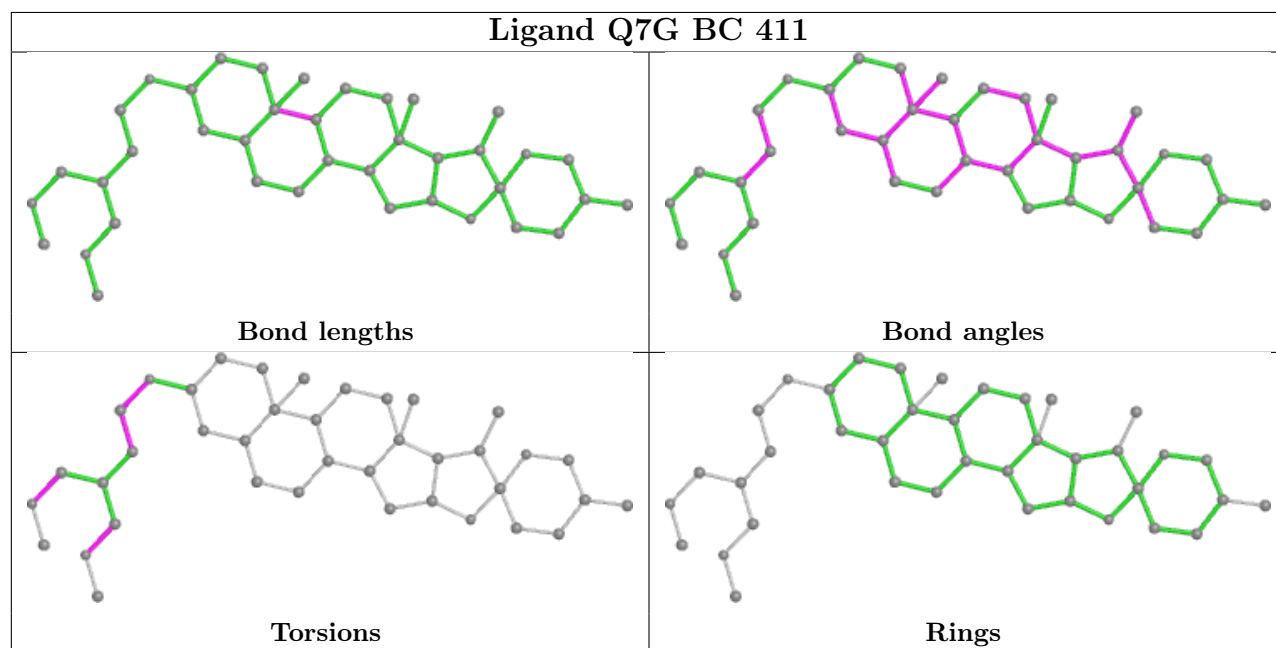
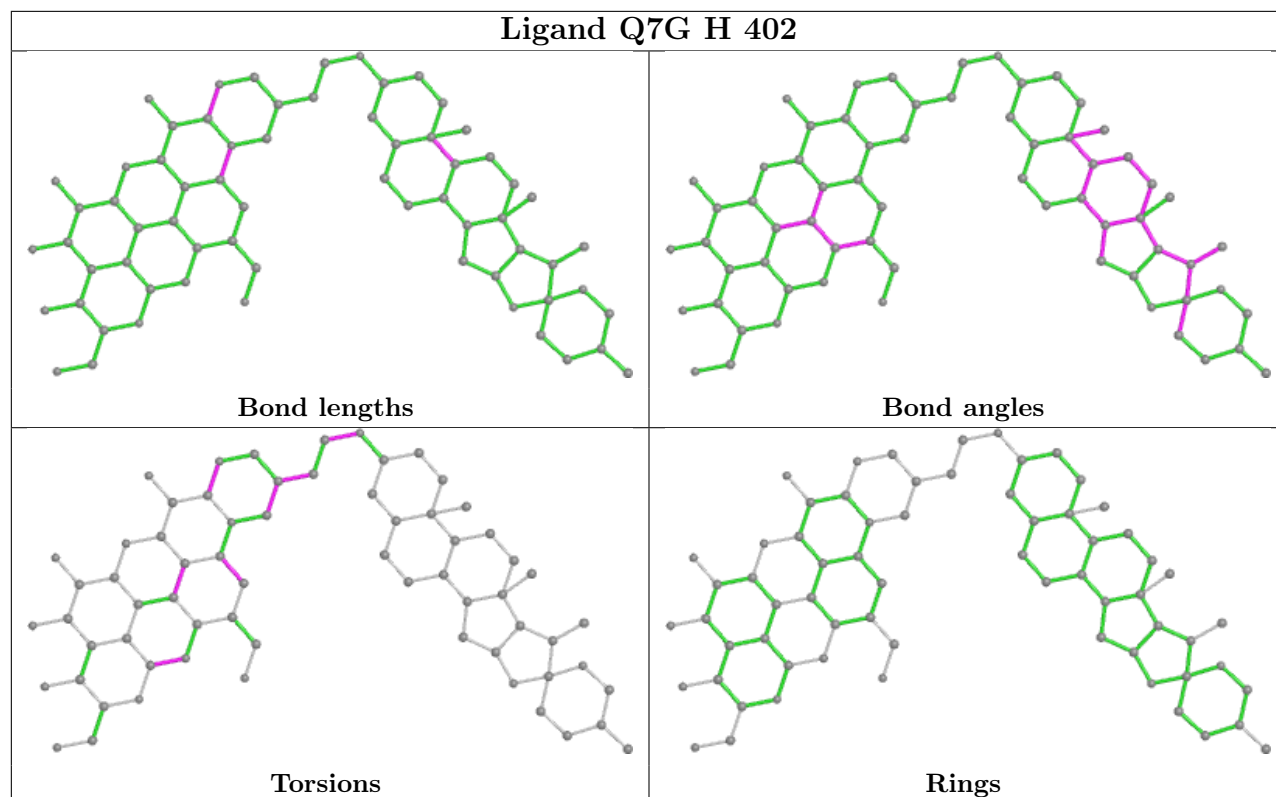


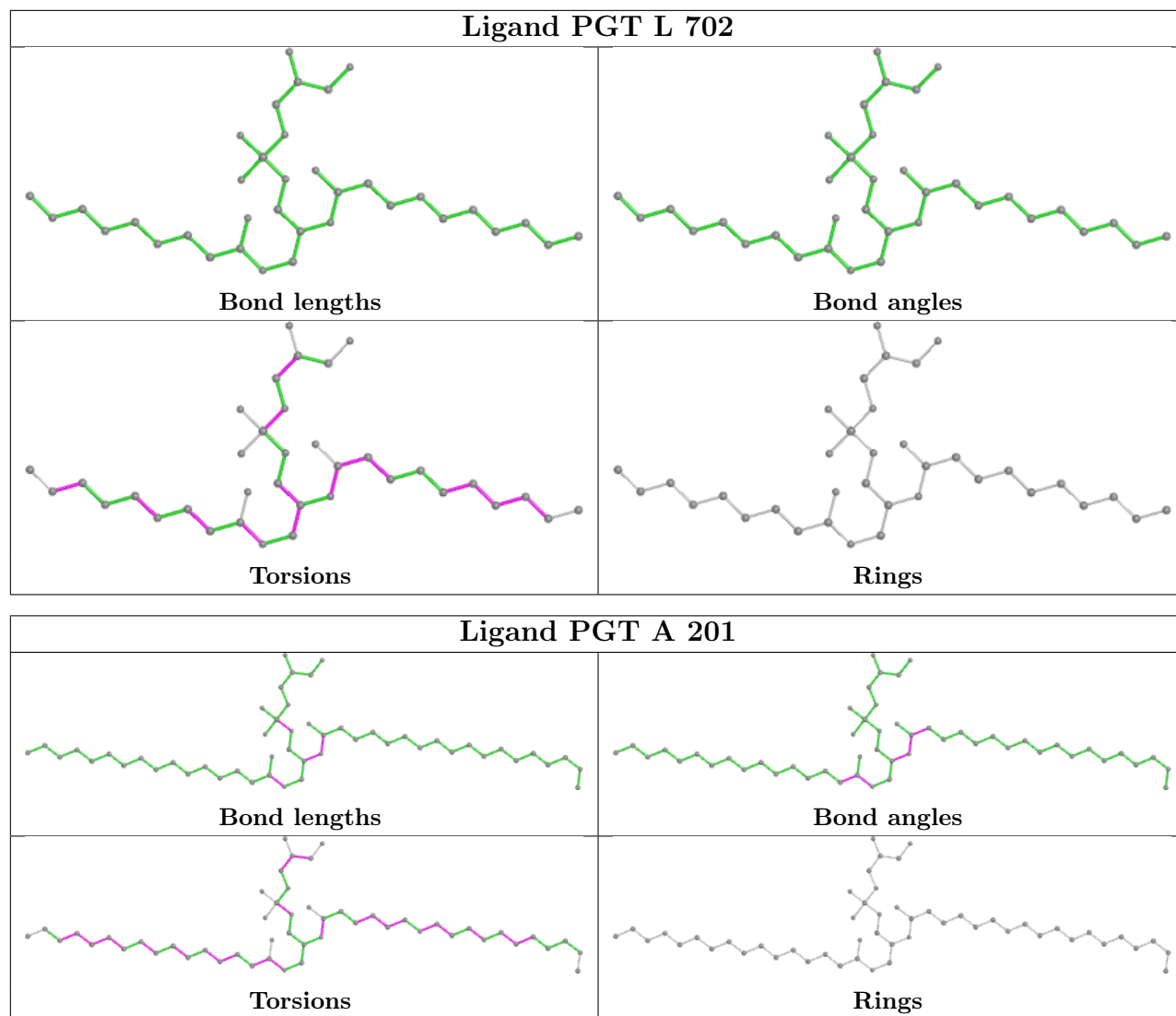


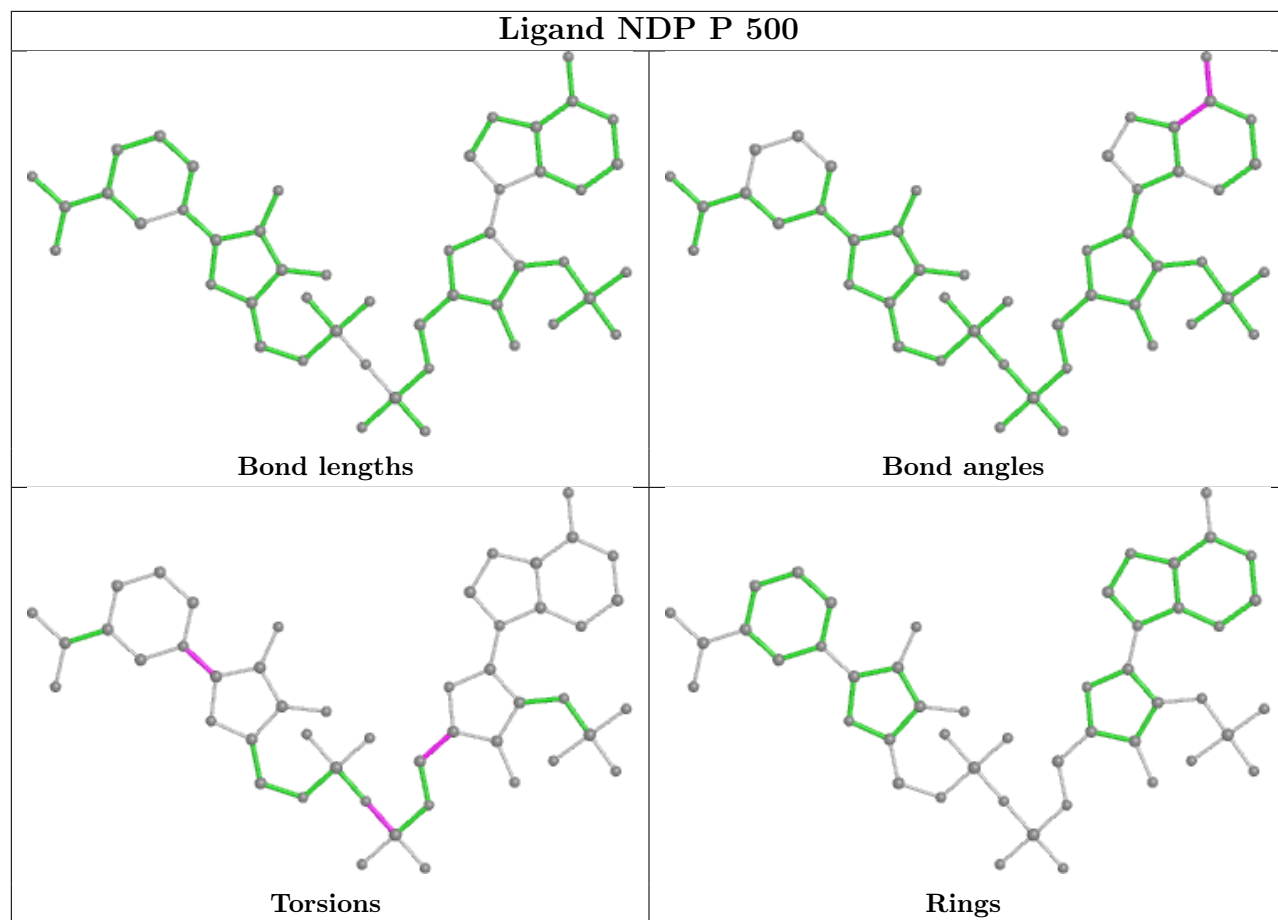


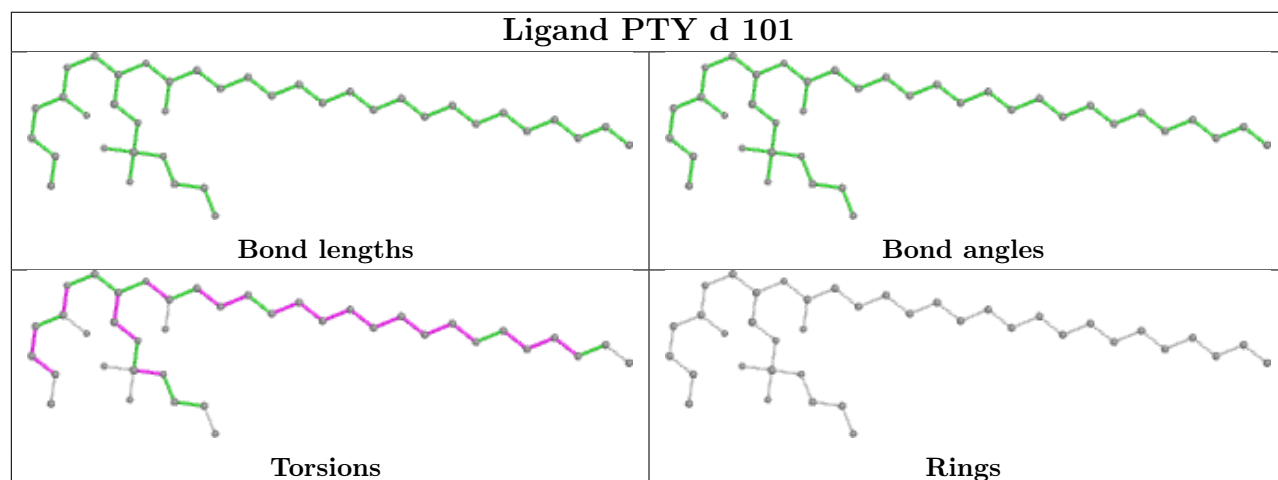
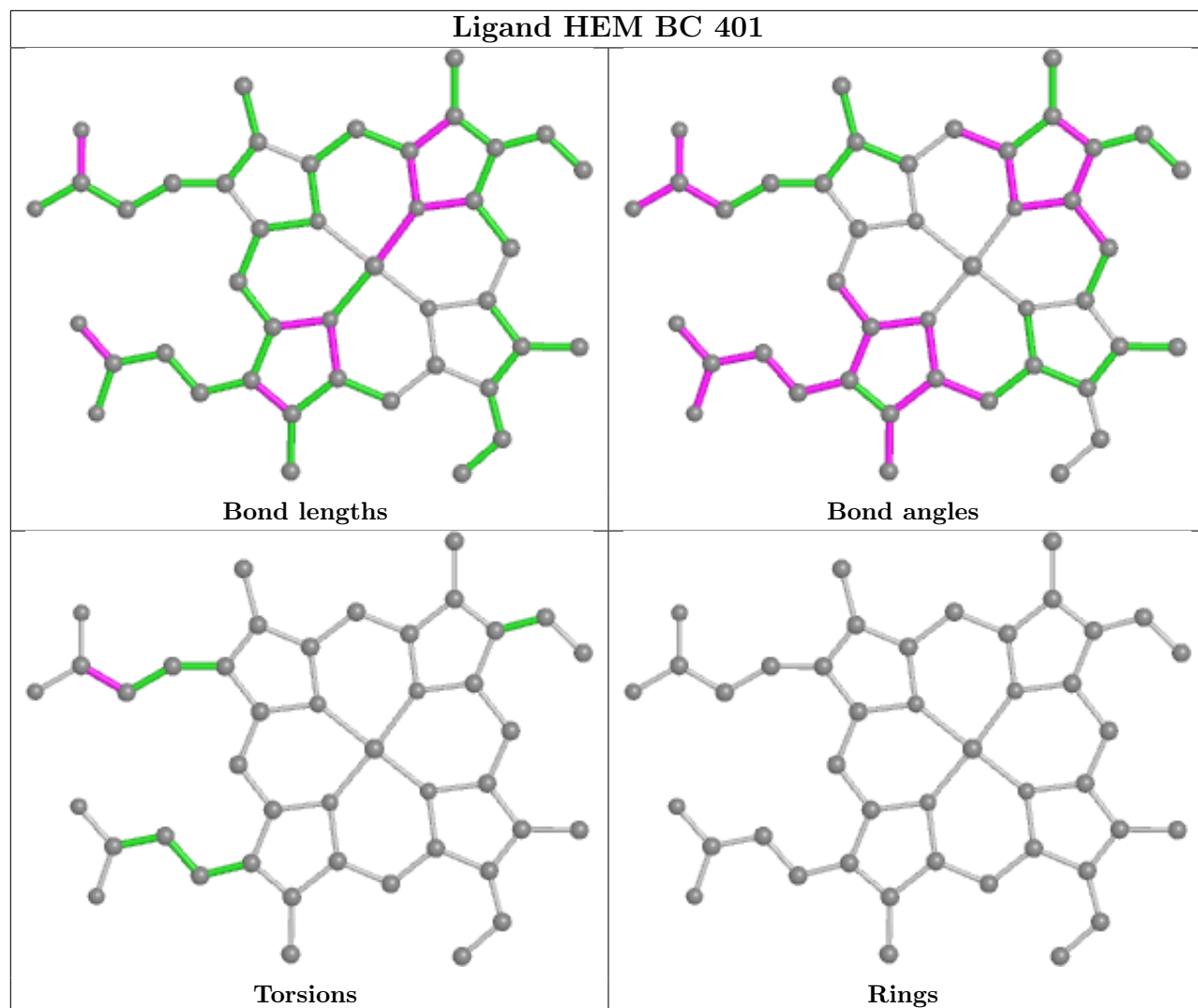


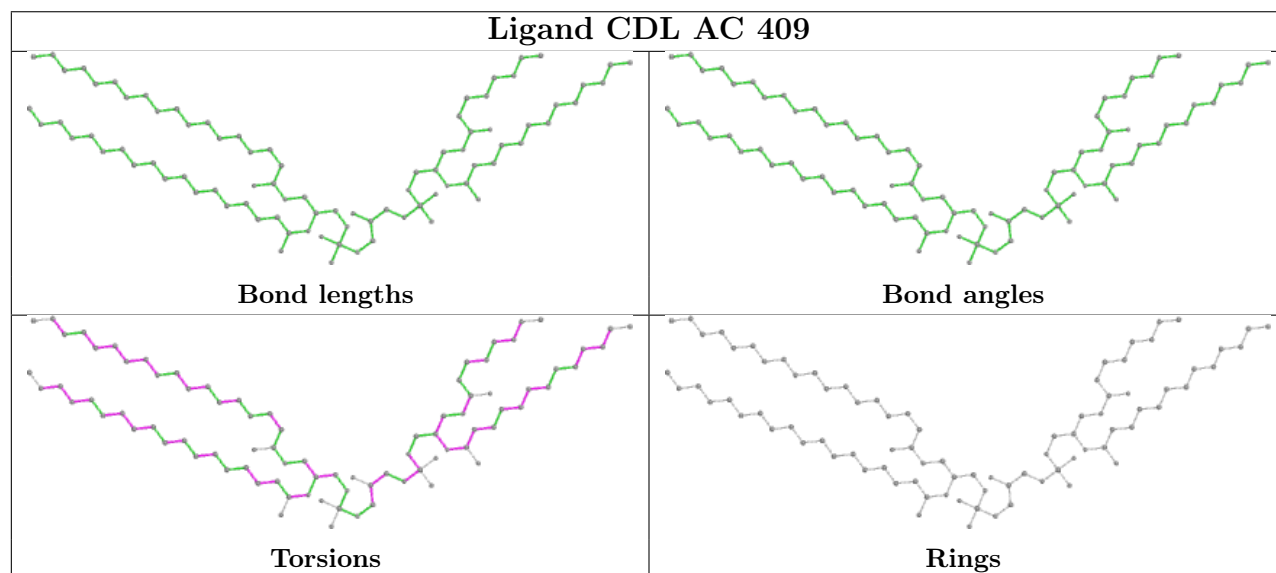
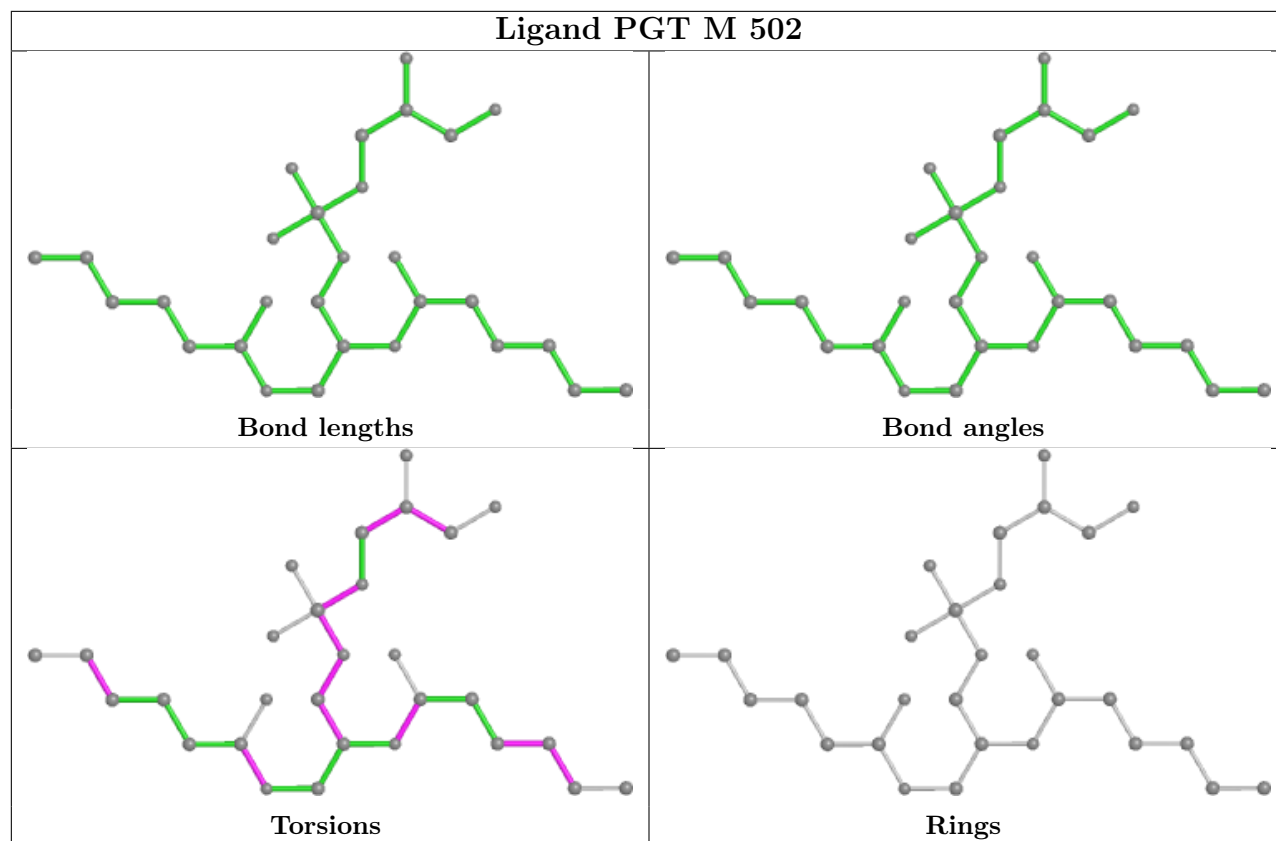


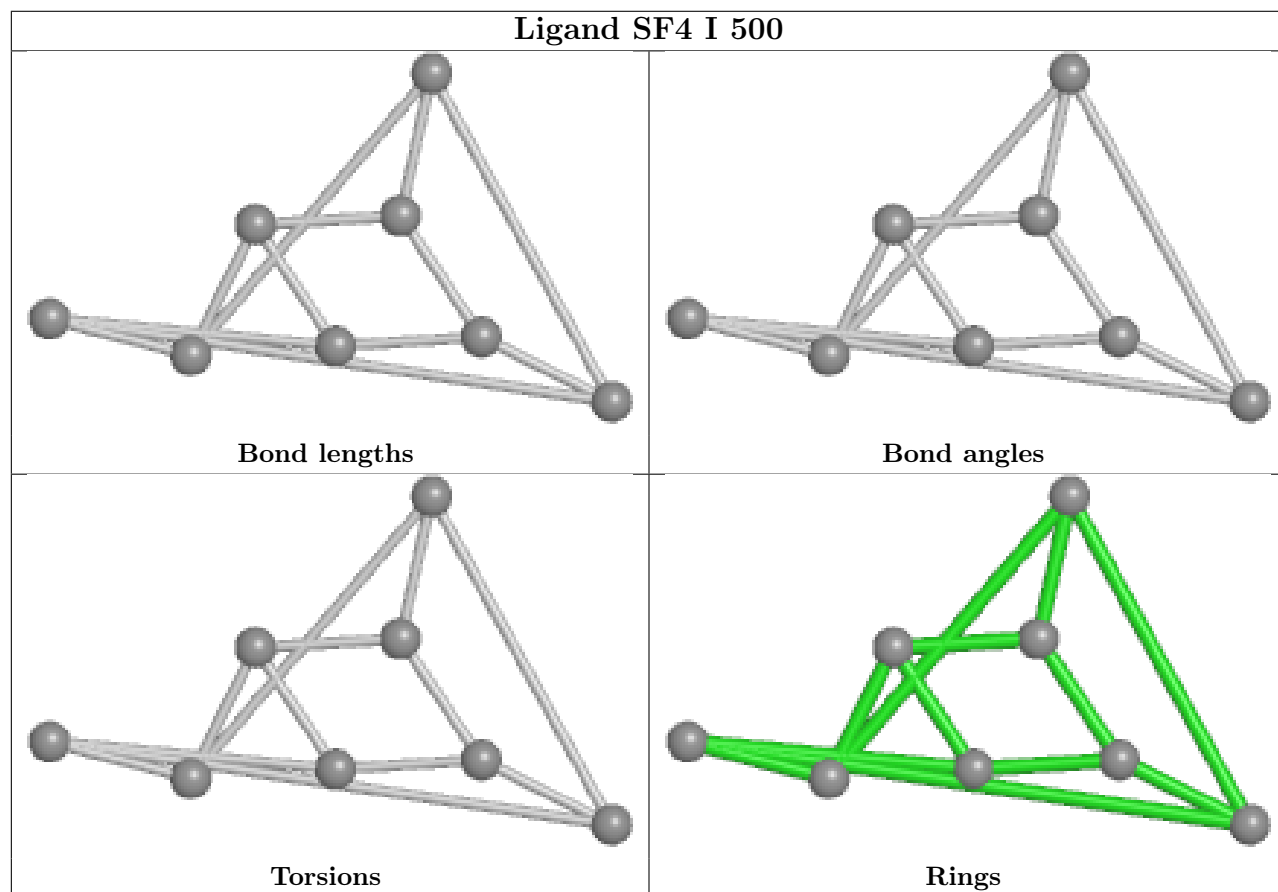
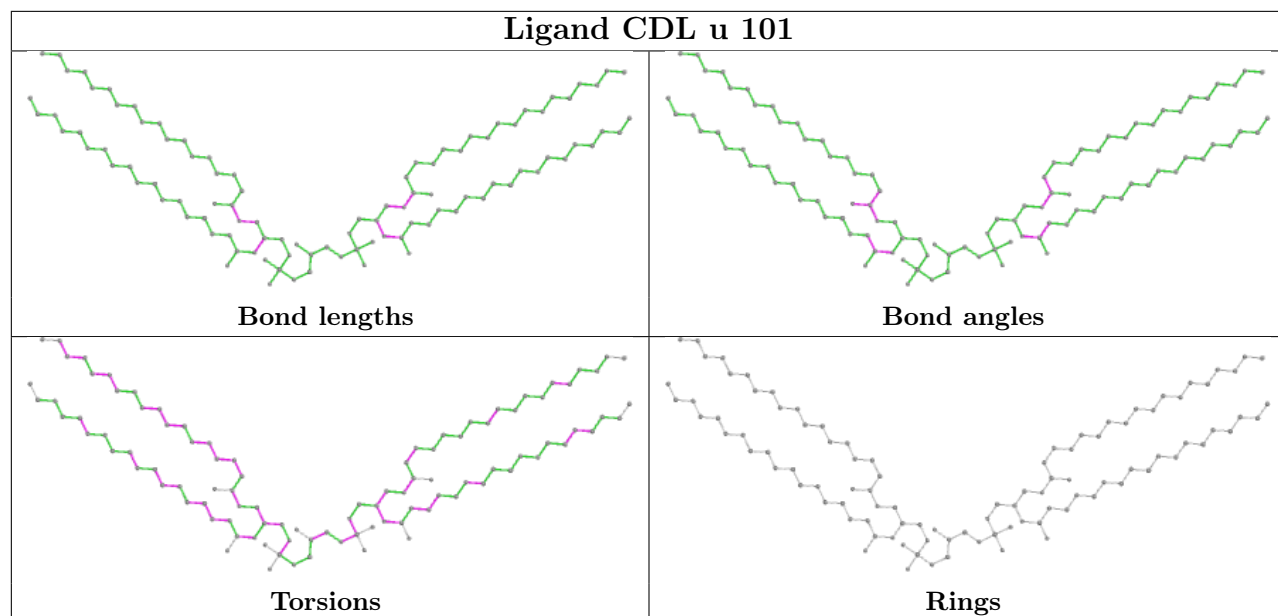


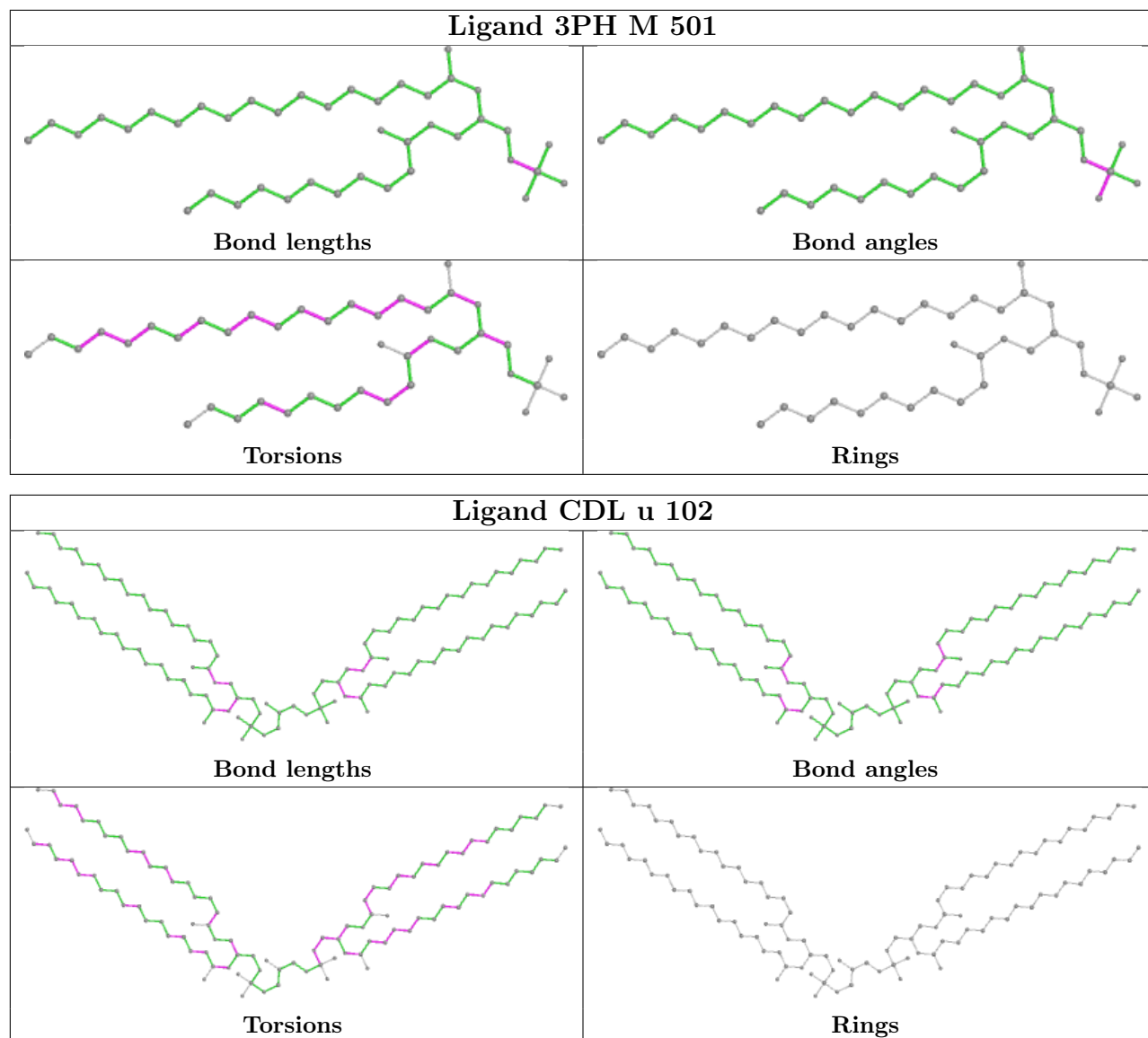


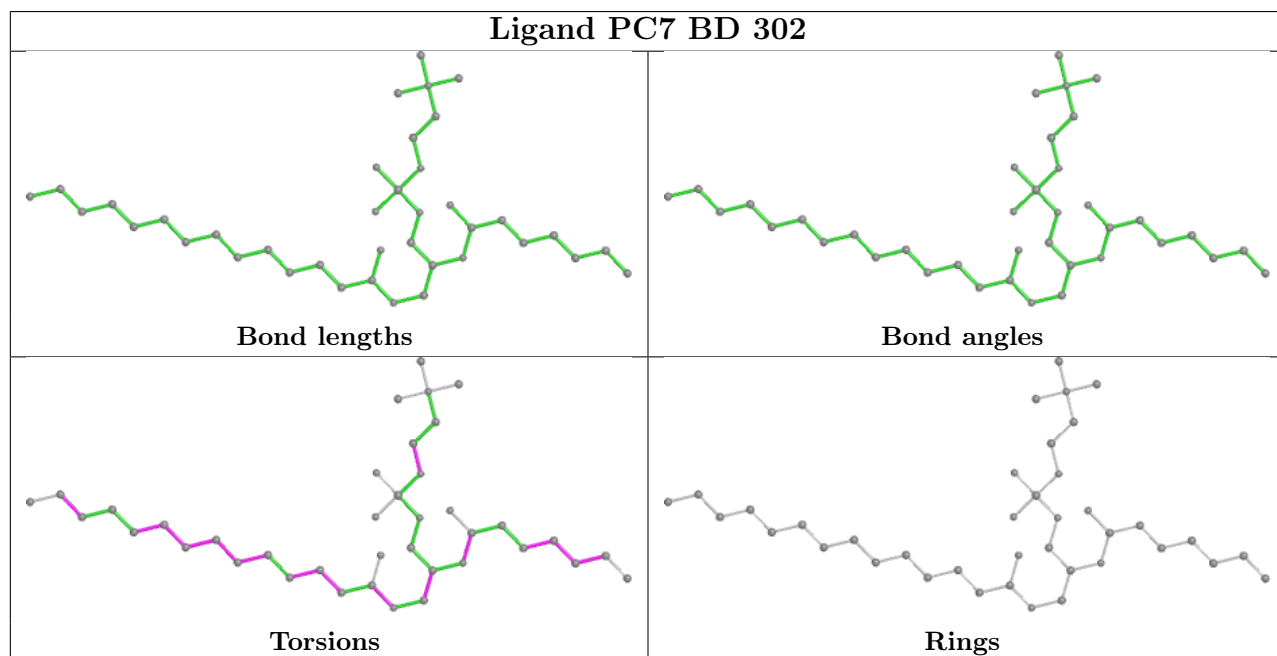
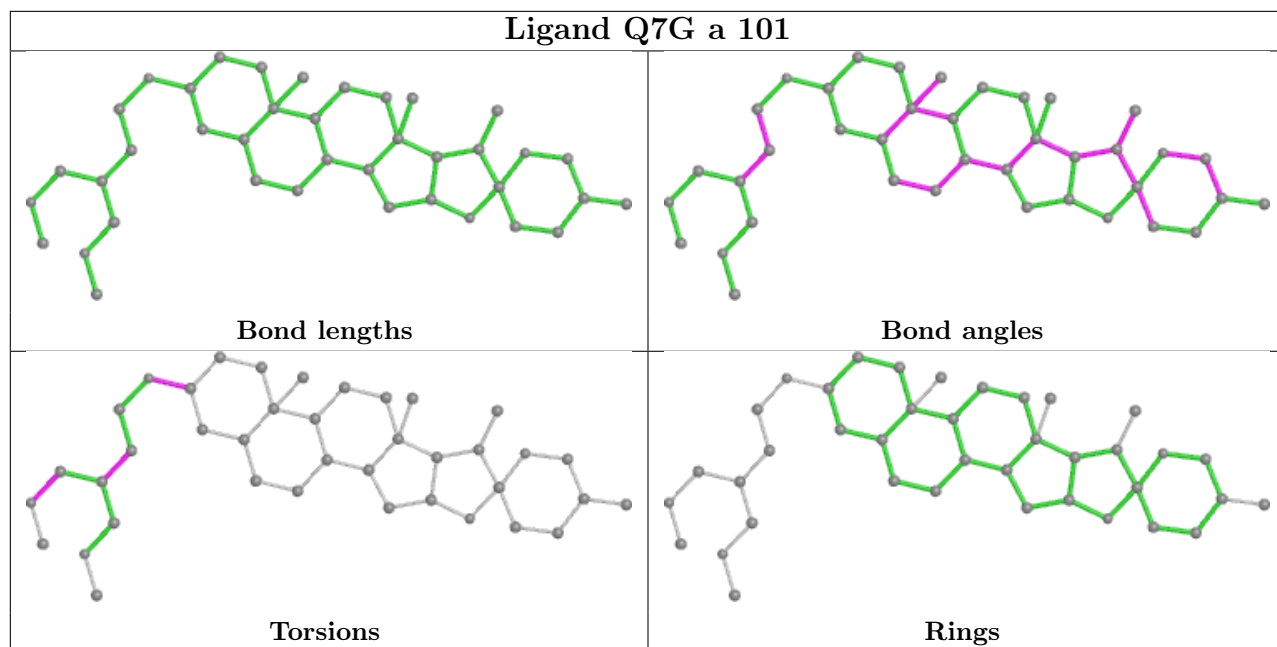


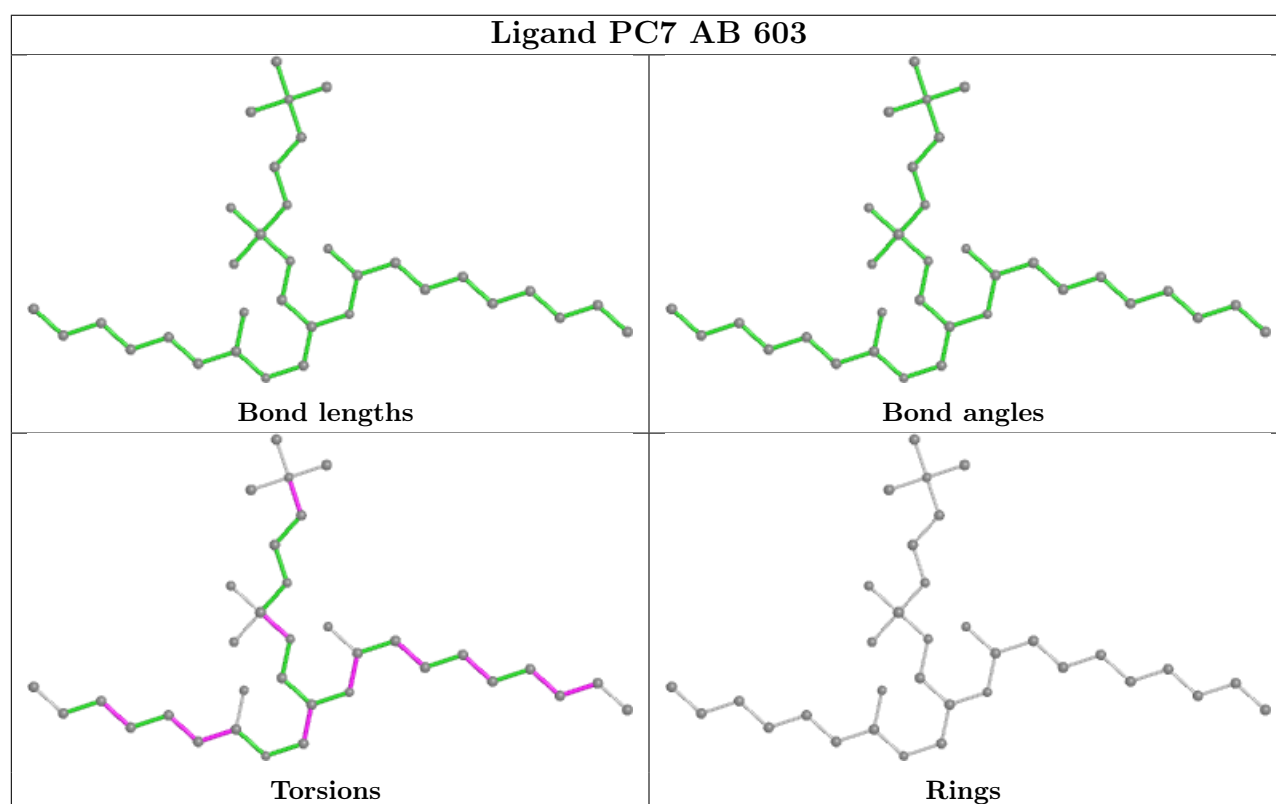
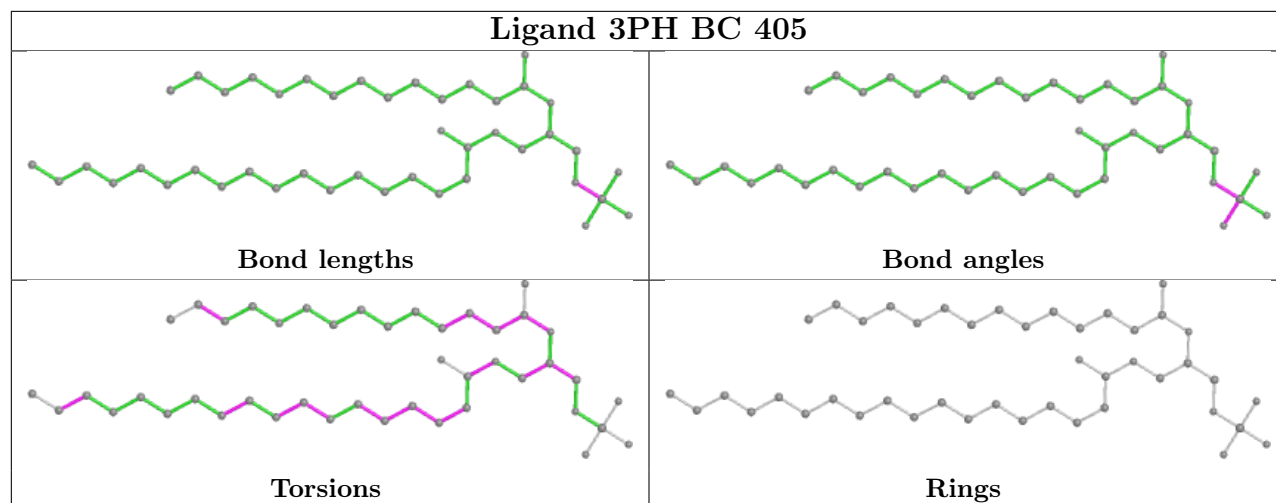


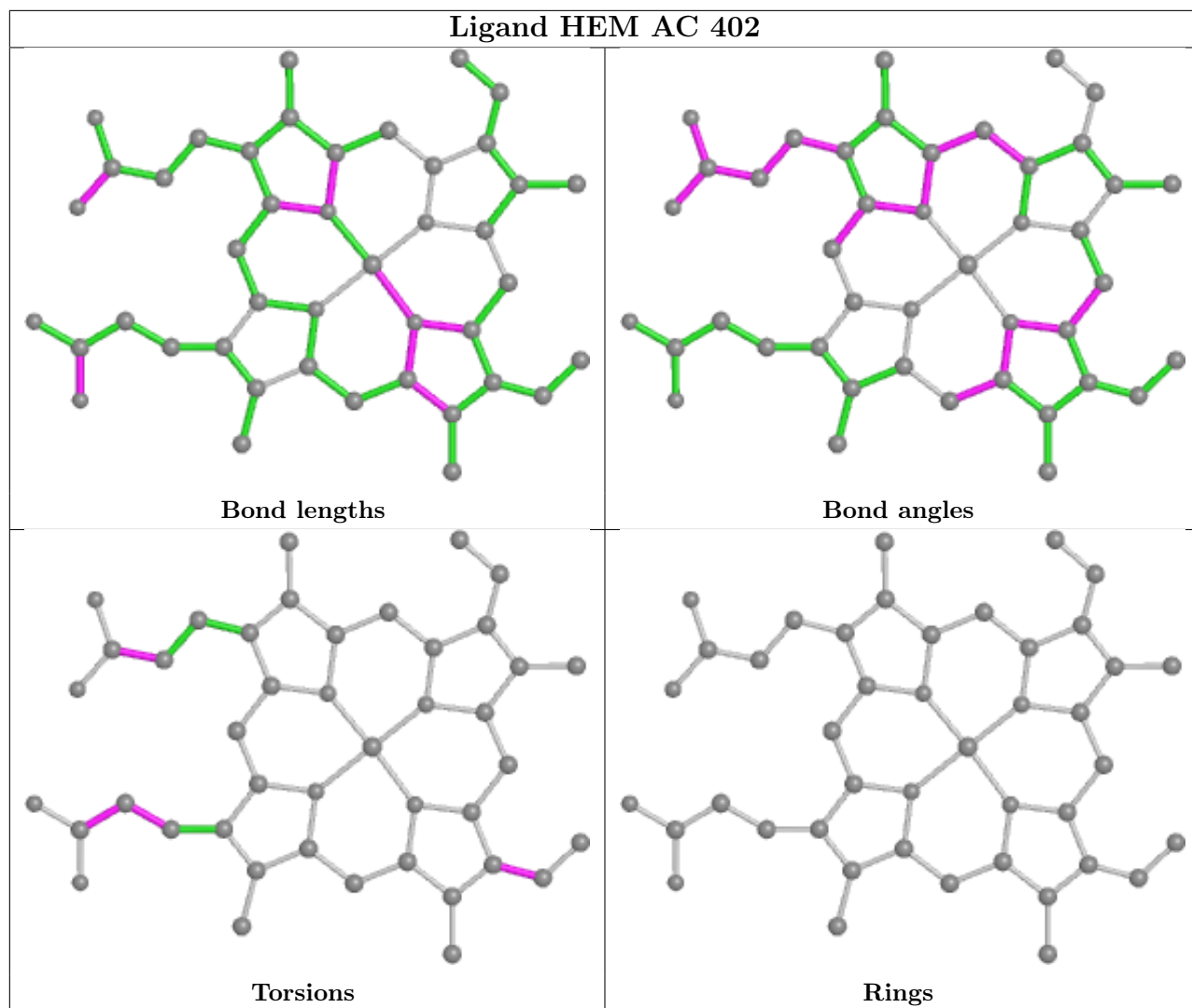


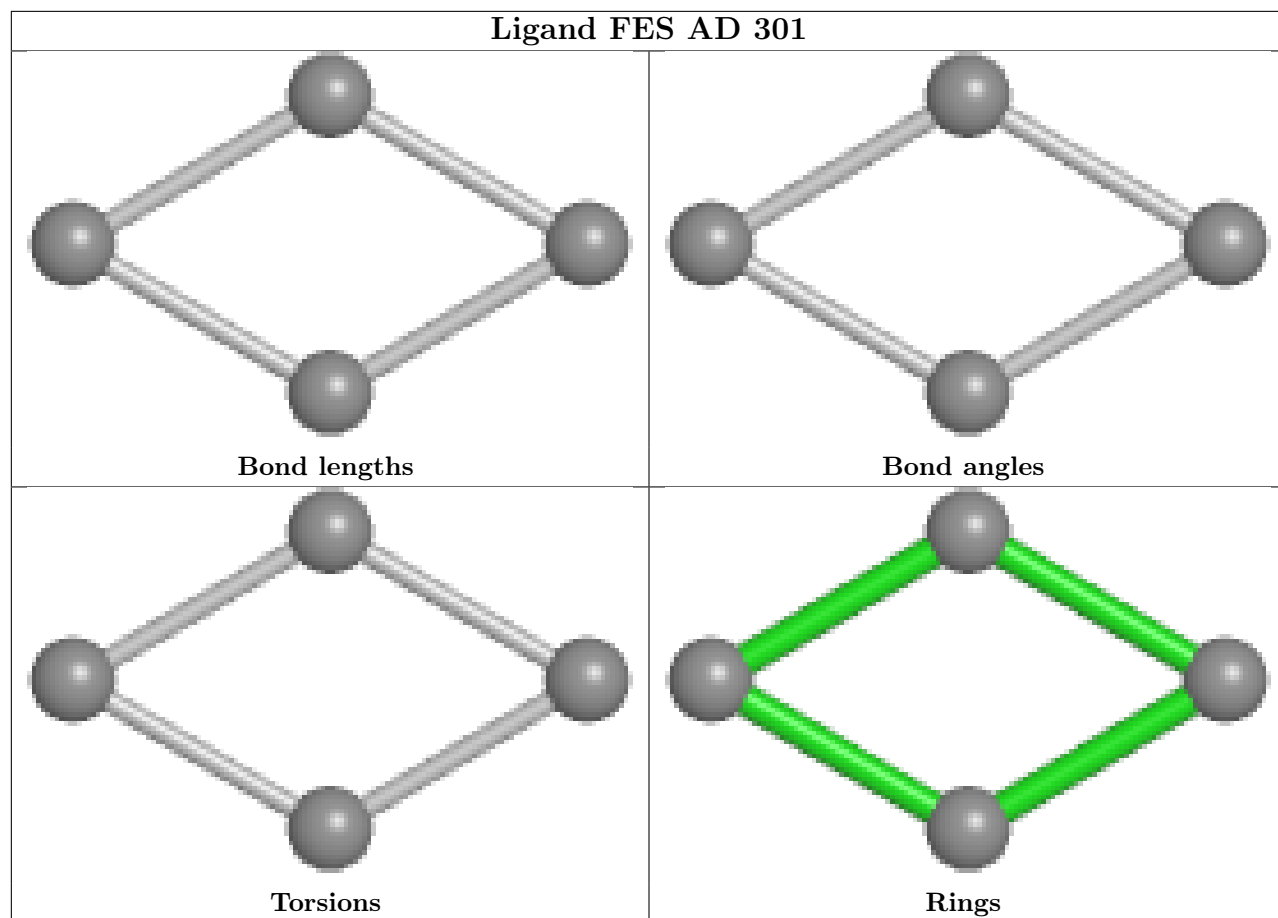


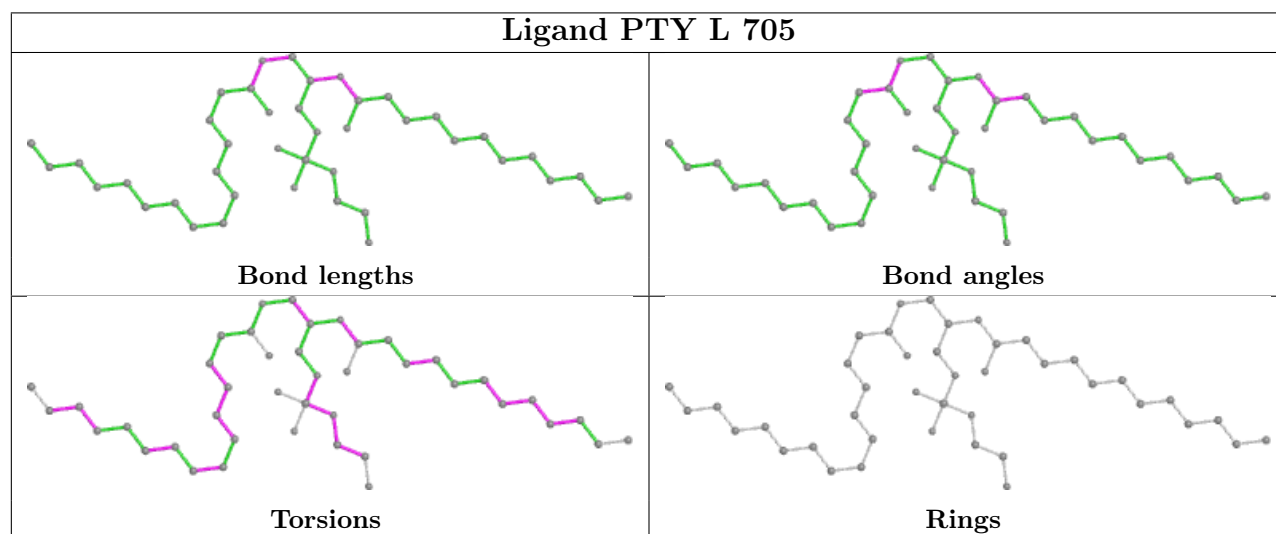
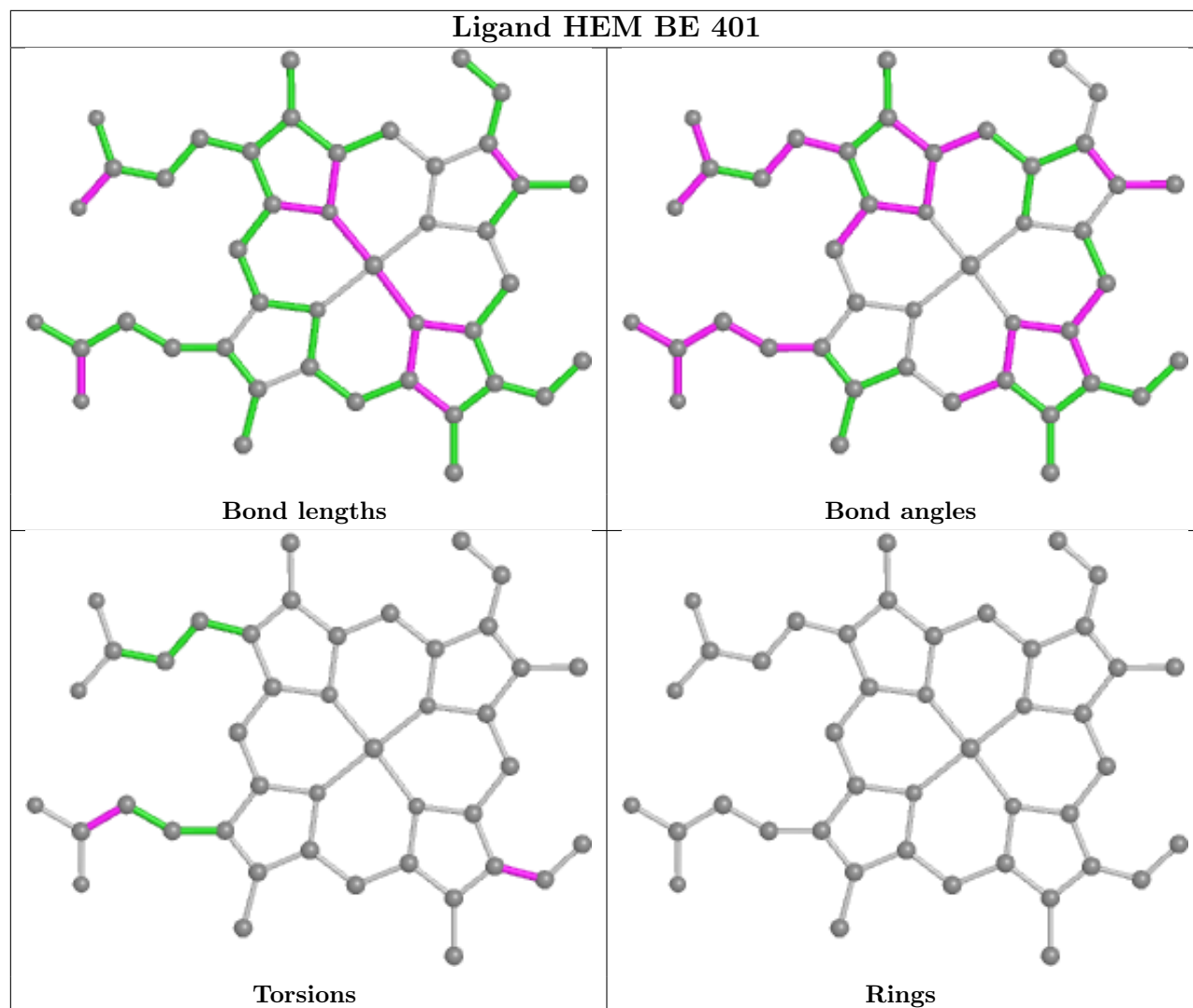


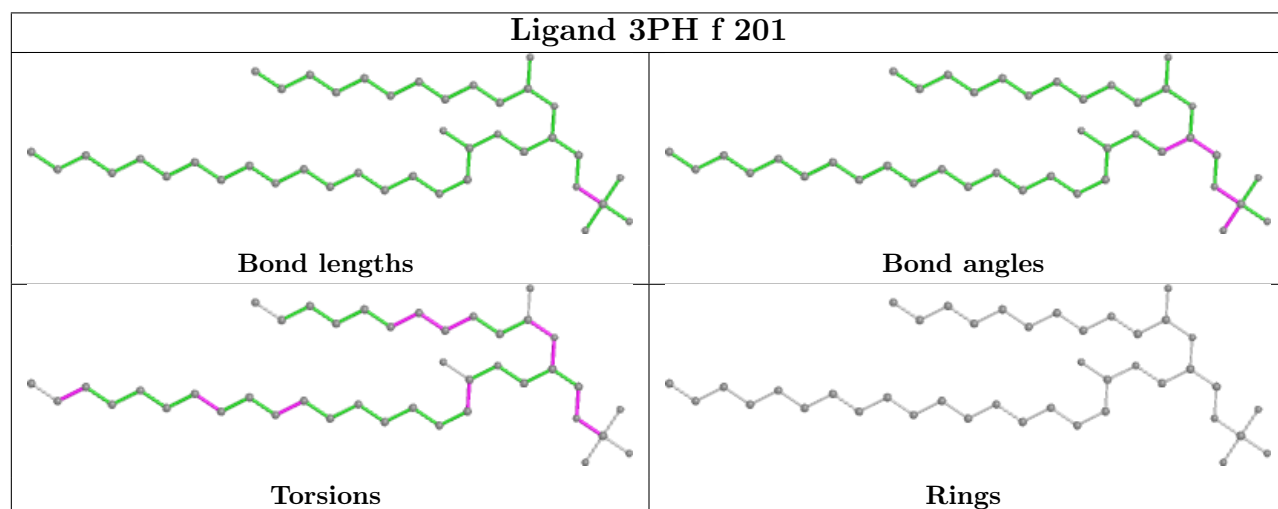
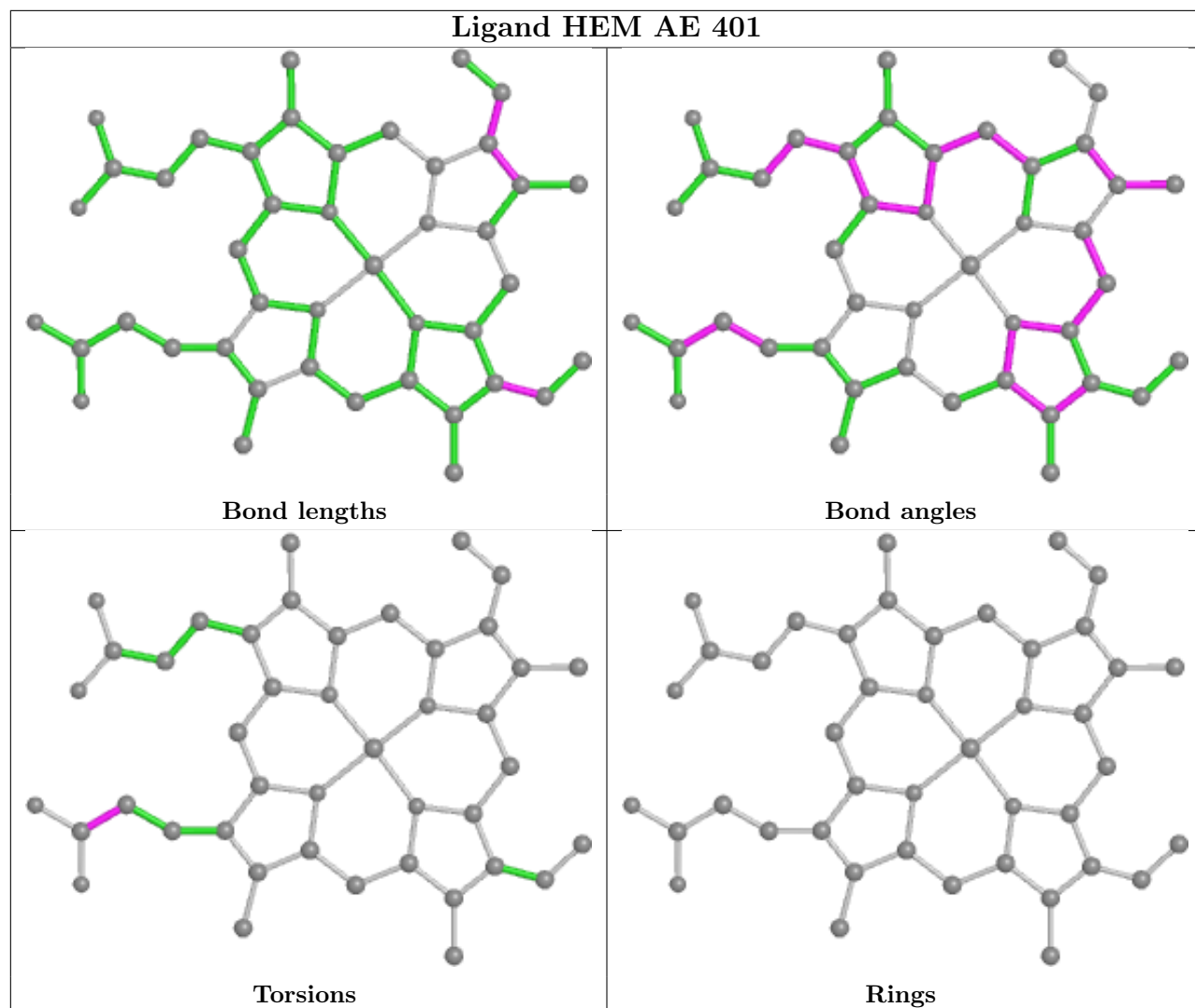


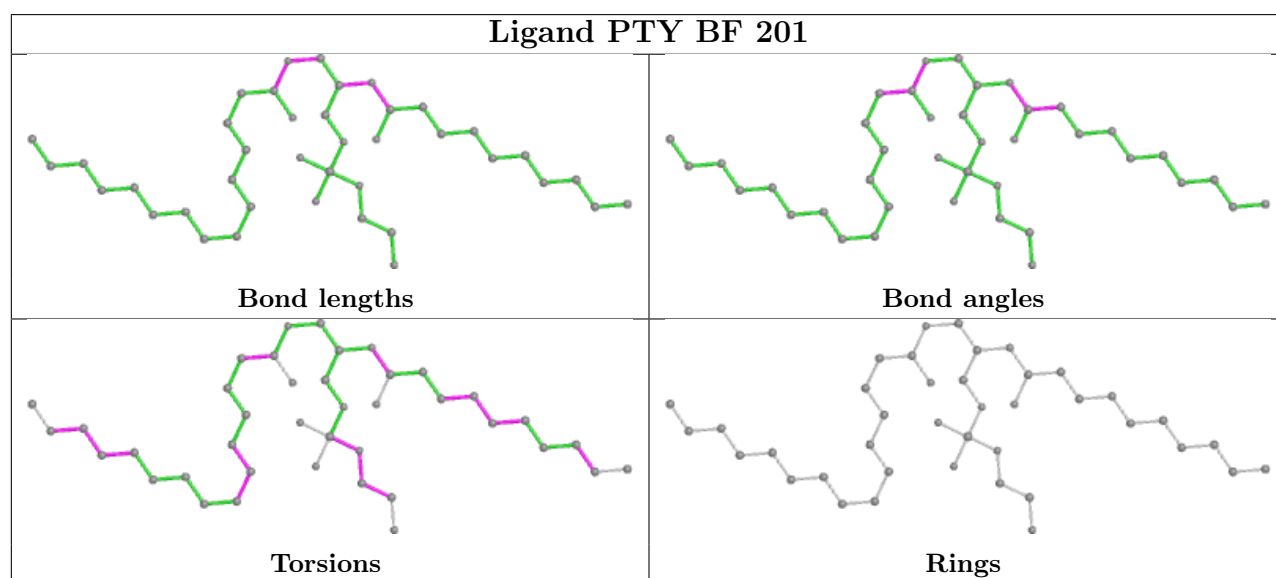
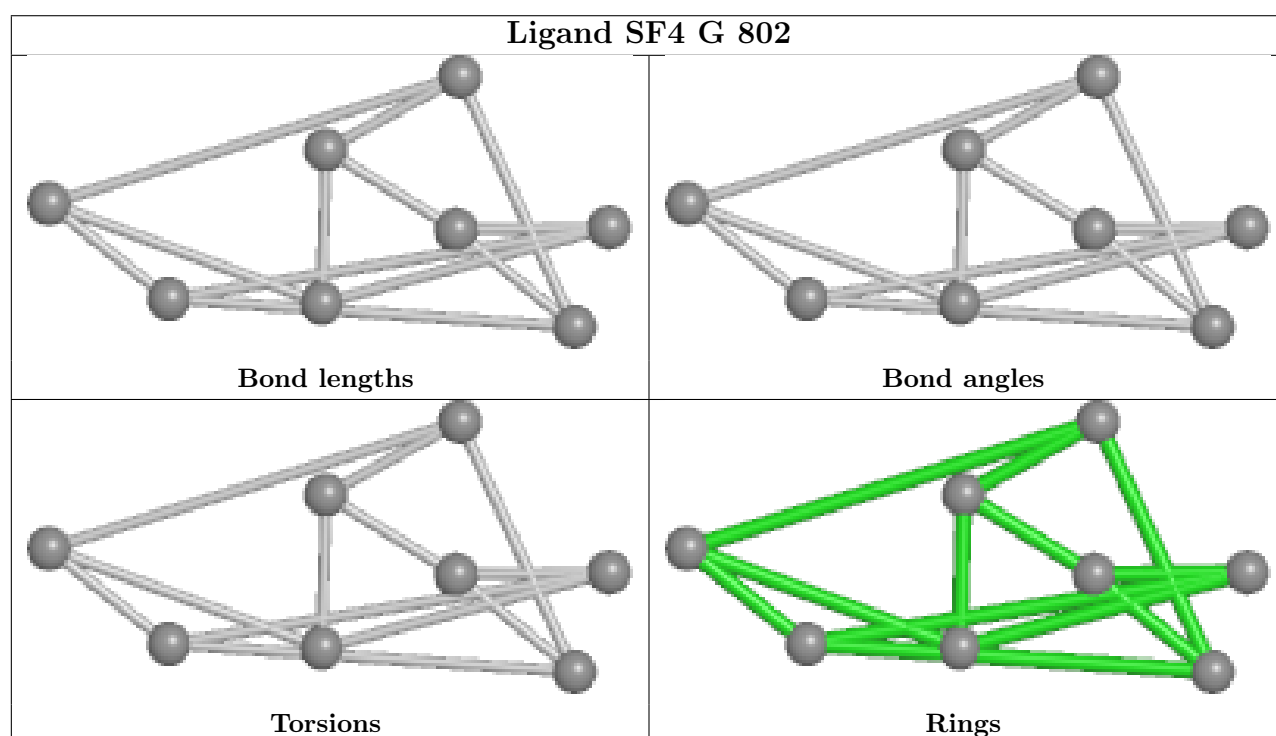
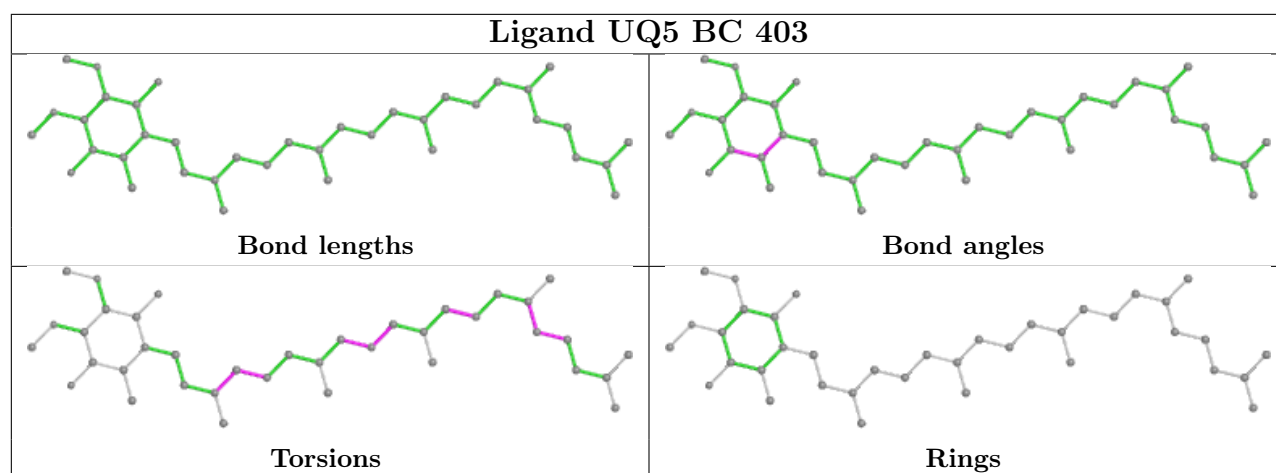


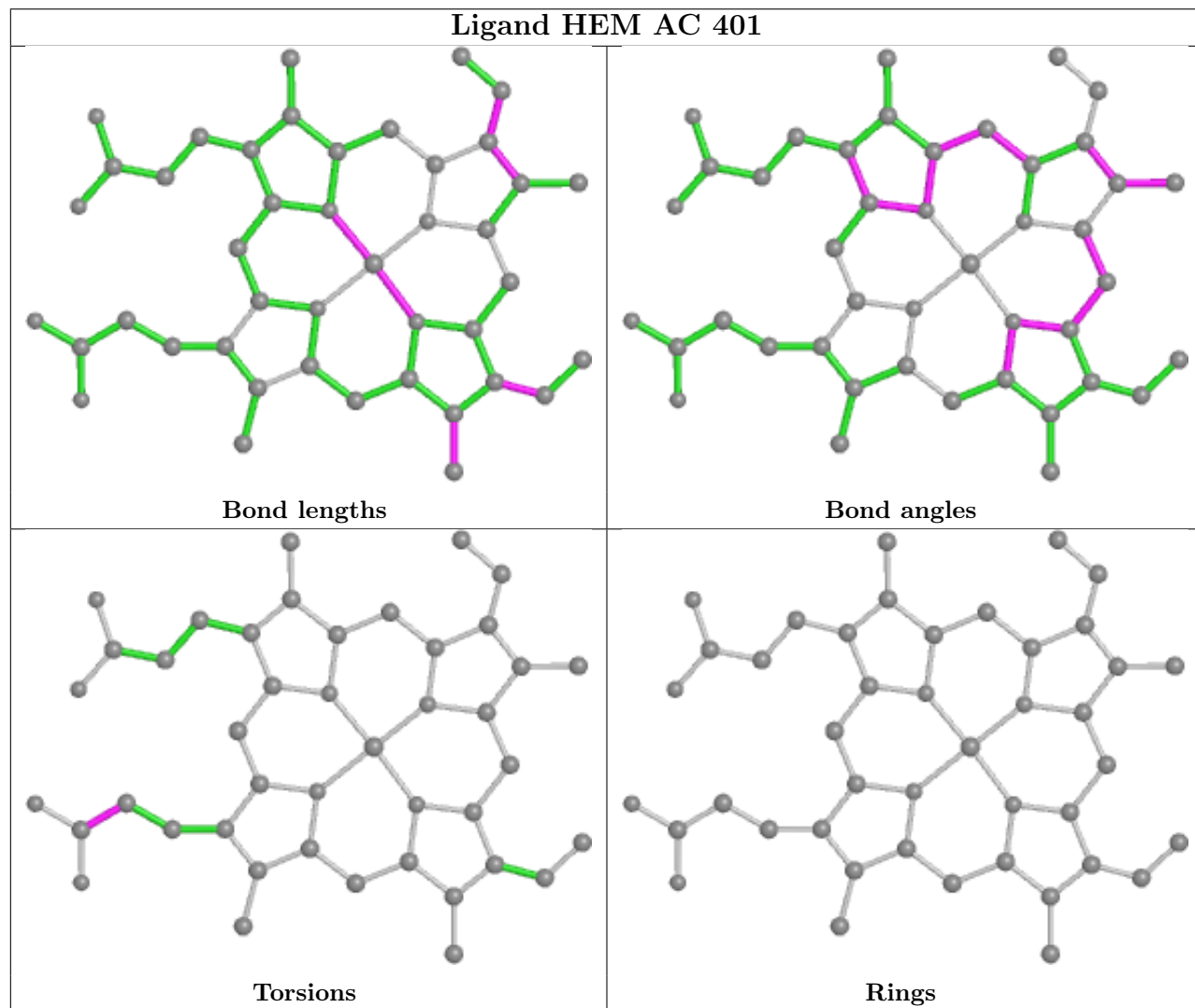
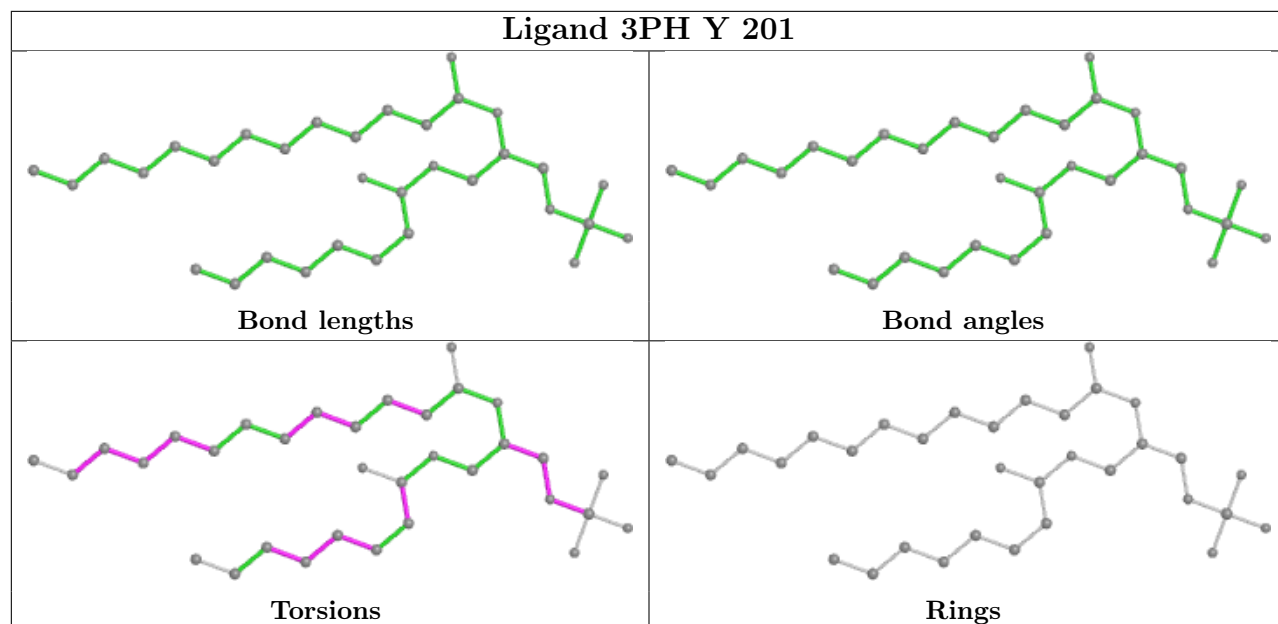


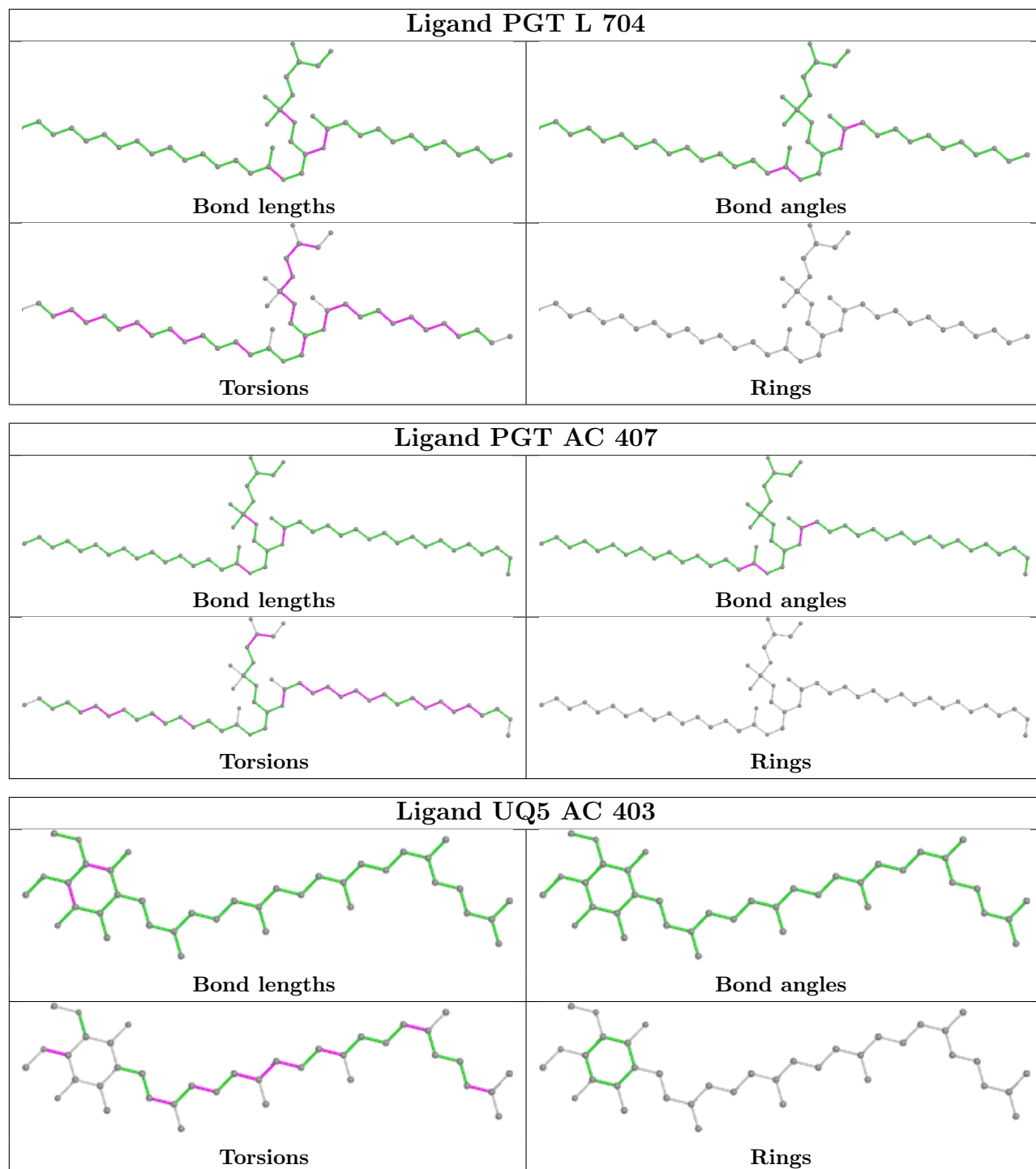


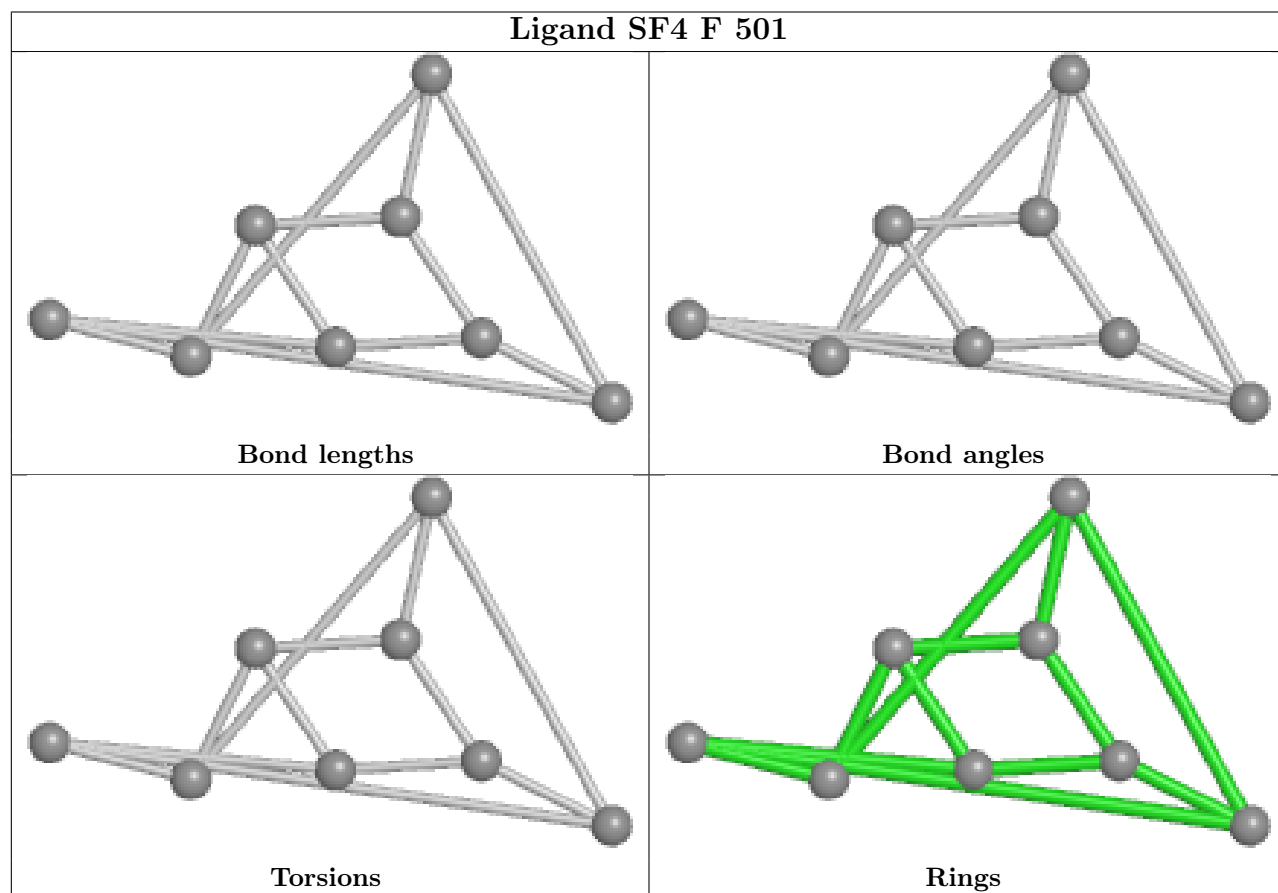
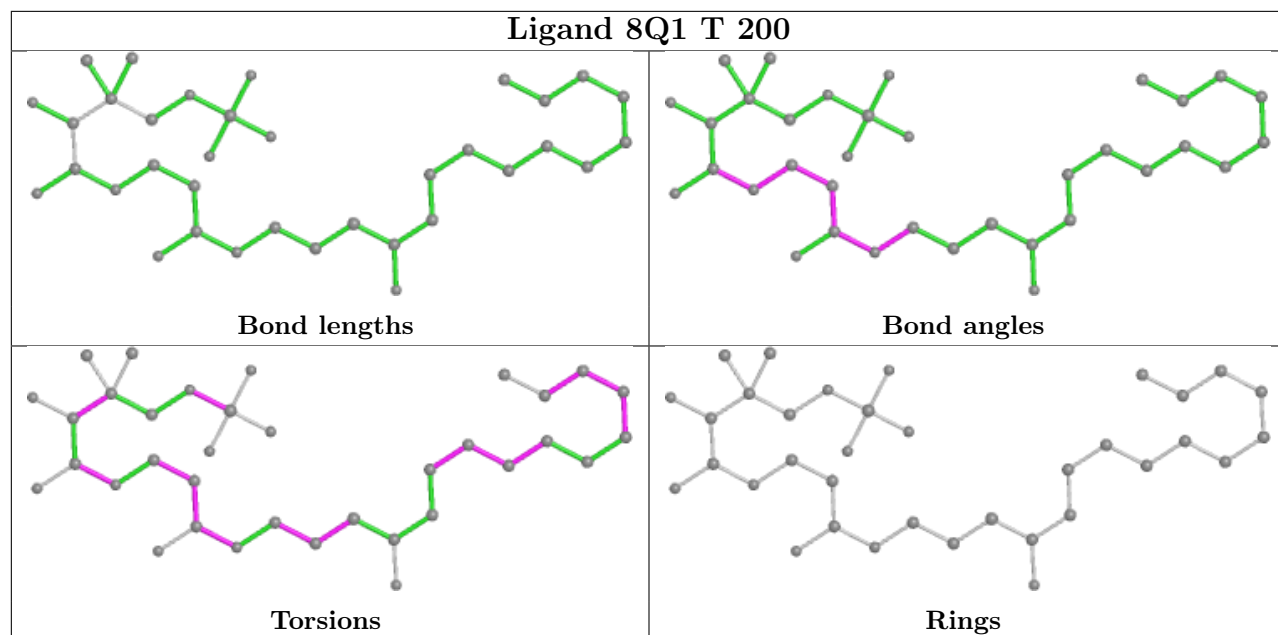


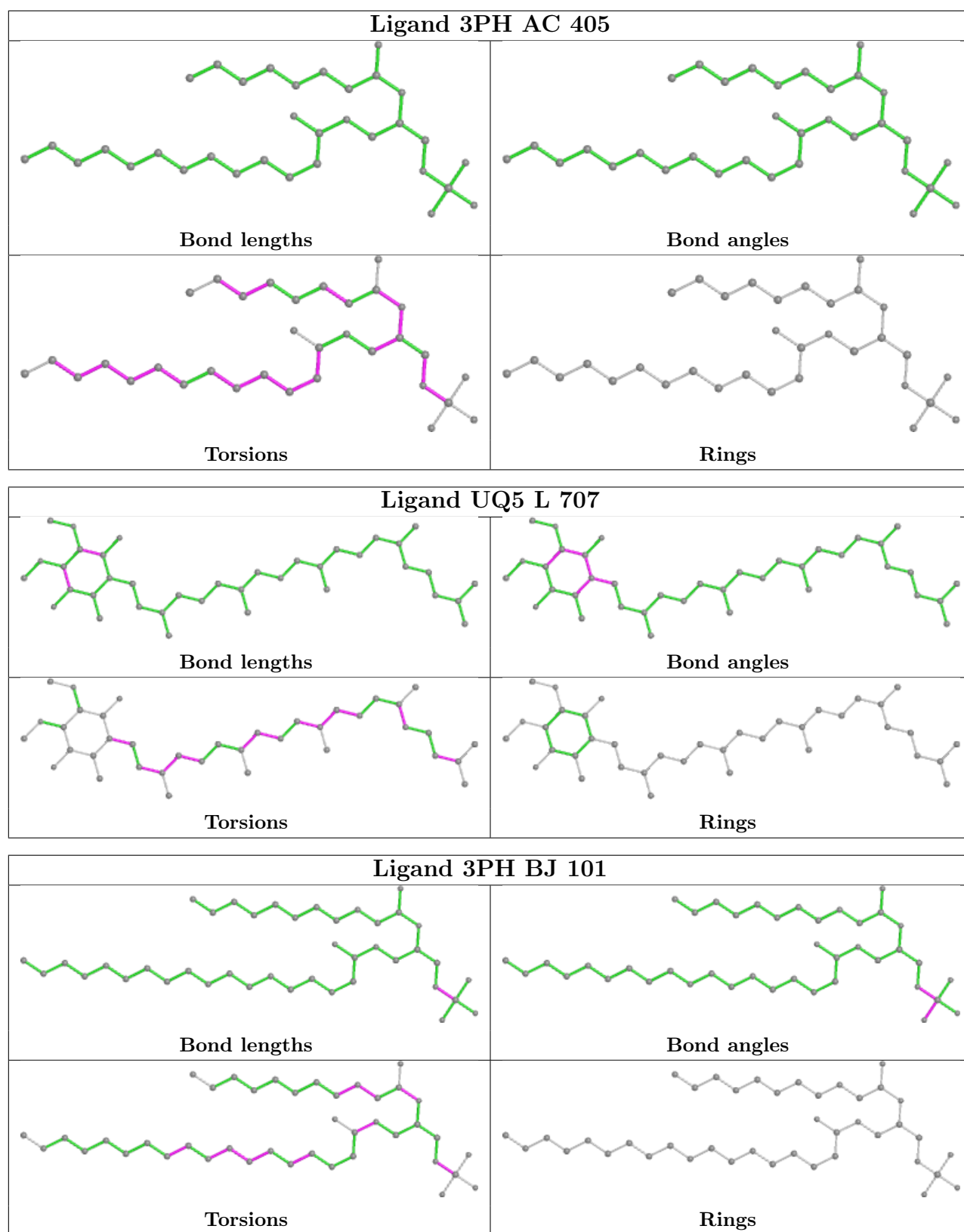












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

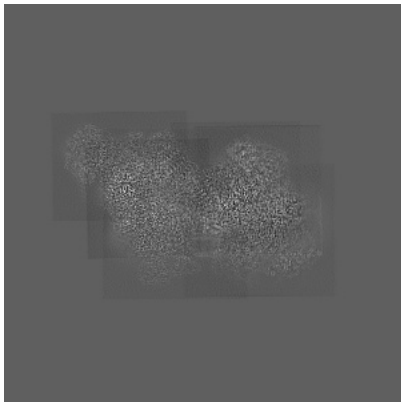
6 Map visualisation [i](#)

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

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

6.1 Orthogonal projections [i](#)

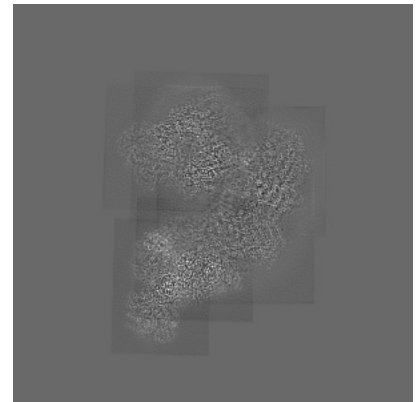
6.1.1 Primary map



X



Y

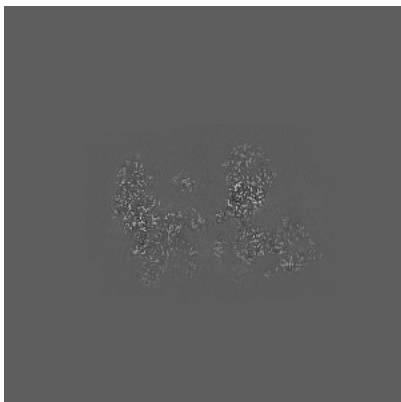


Z

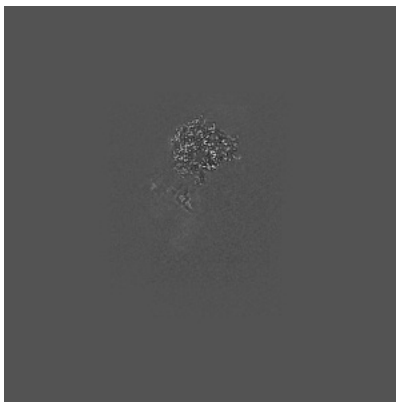
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

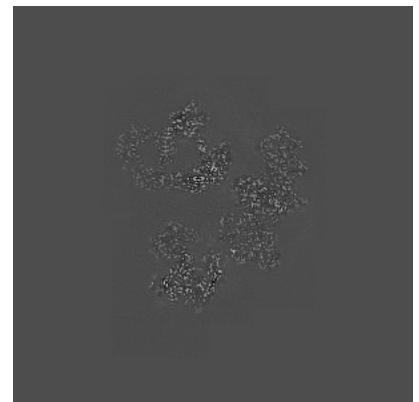
6.2.1 Primary map



X Index: 375



Y Index: 375

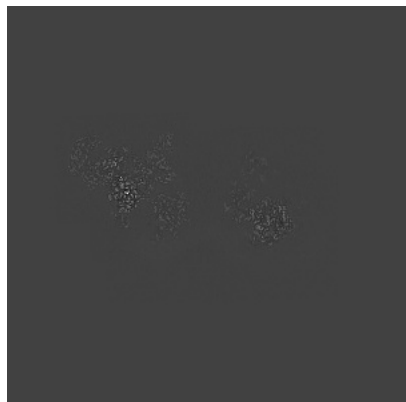


Z Index: 375

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

6.3 Largest variance slices [i](#)

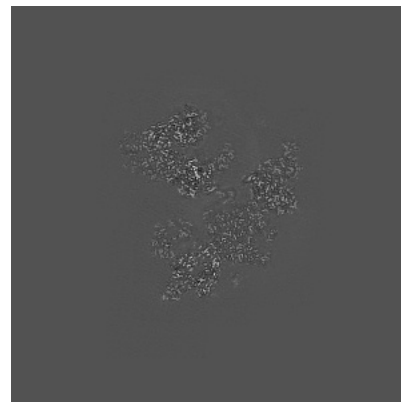
6.3.1 Primary map



X Index: 289



Y Index: 236

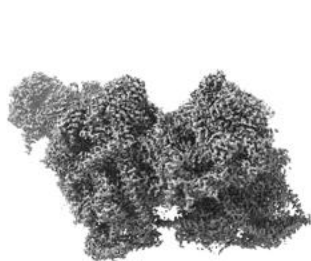


Z Index: 355

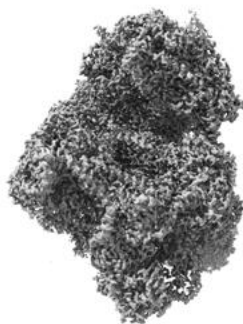
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

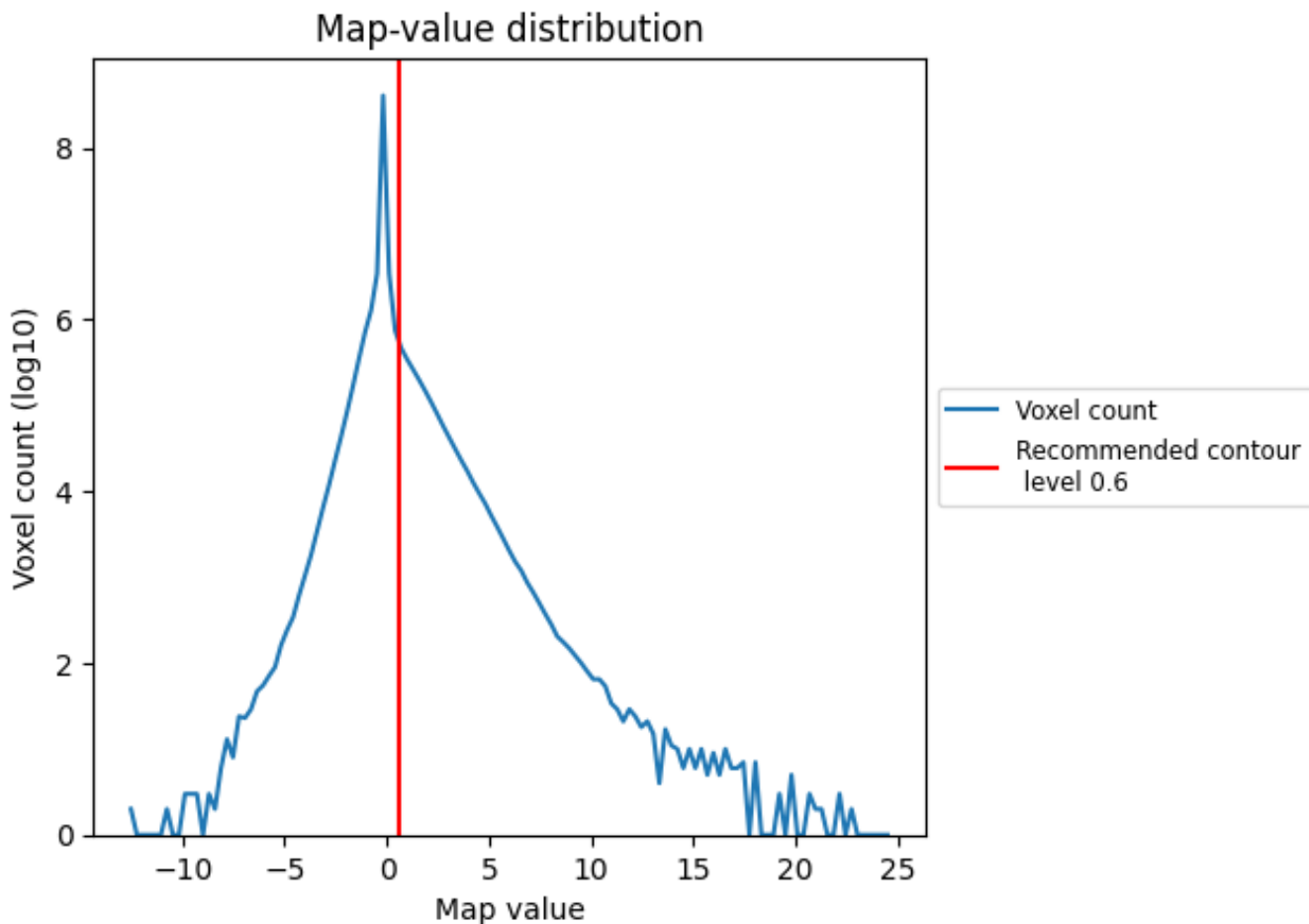
6.5 Mask visualisation

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

7 Map analysis [i](#)

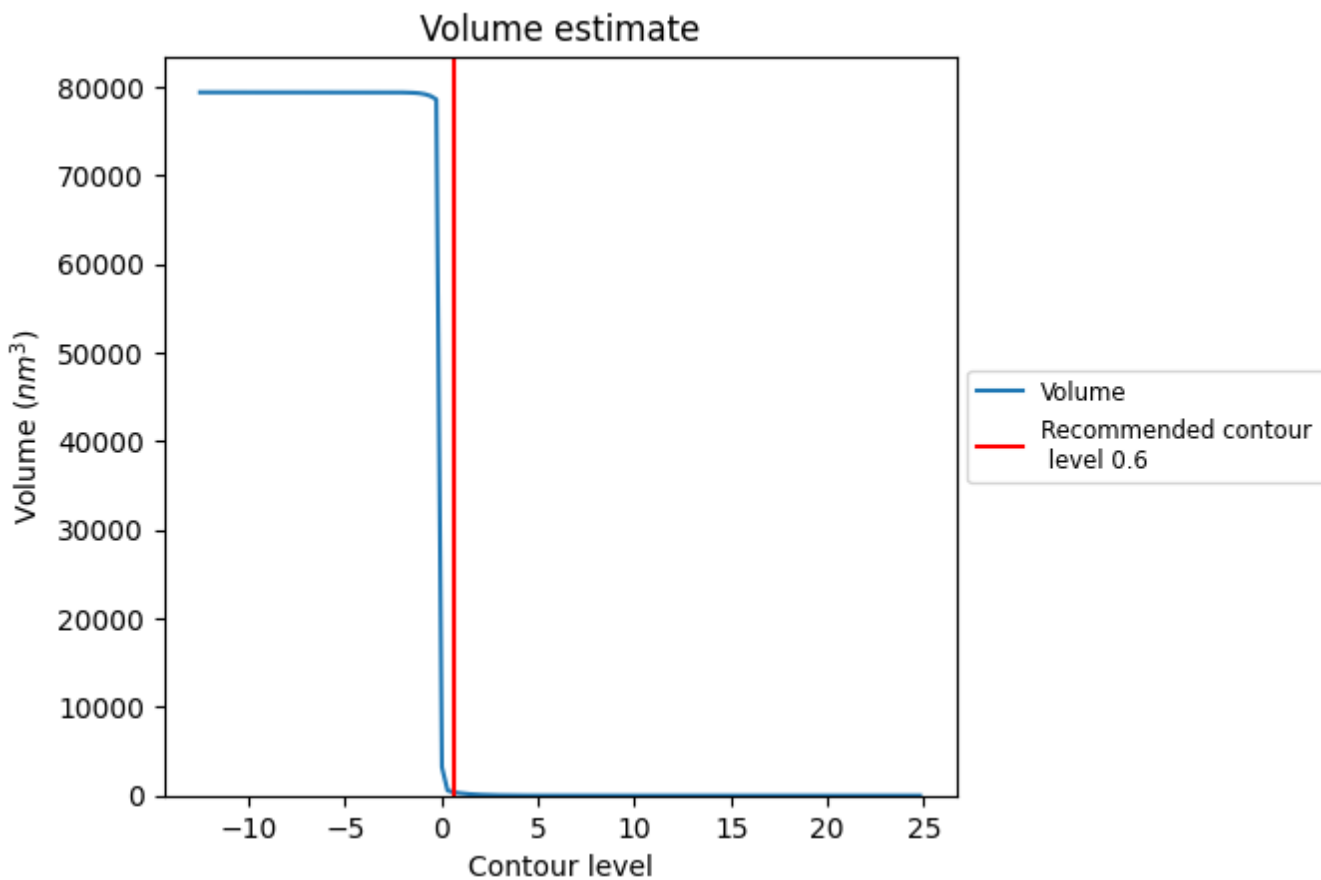
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

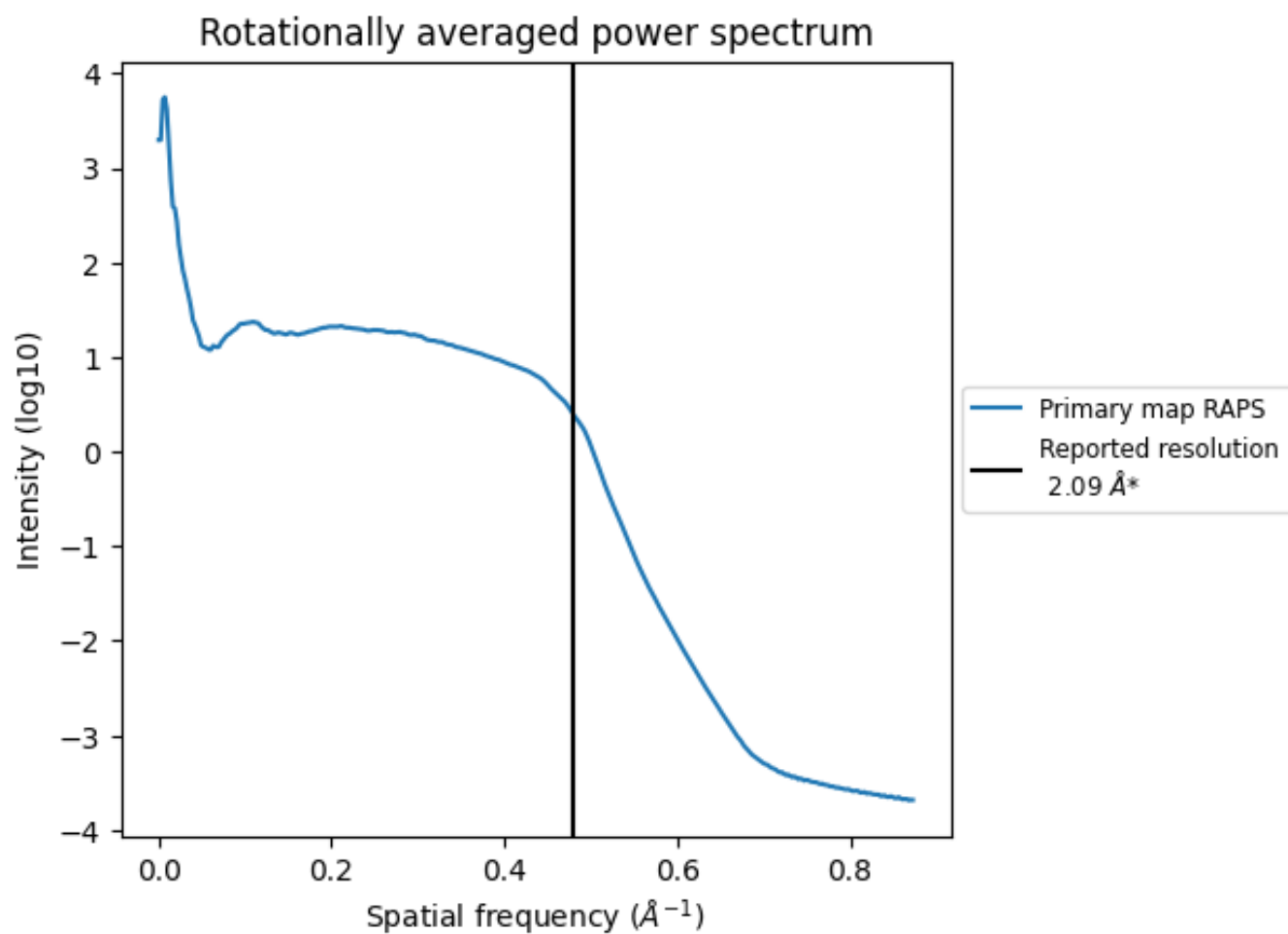
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

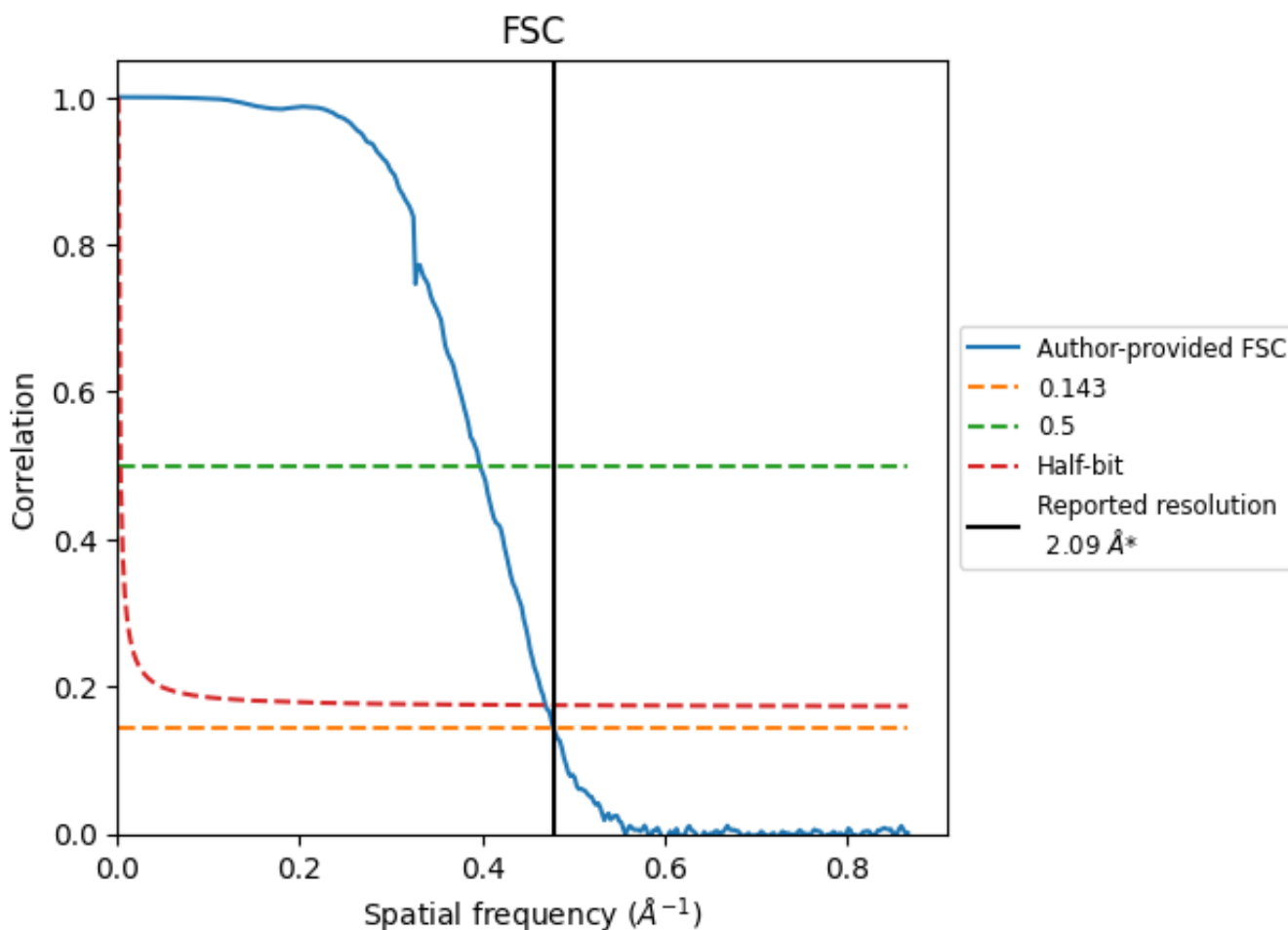


*Reported resolution corresponds to spatial frequency of 0.478\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

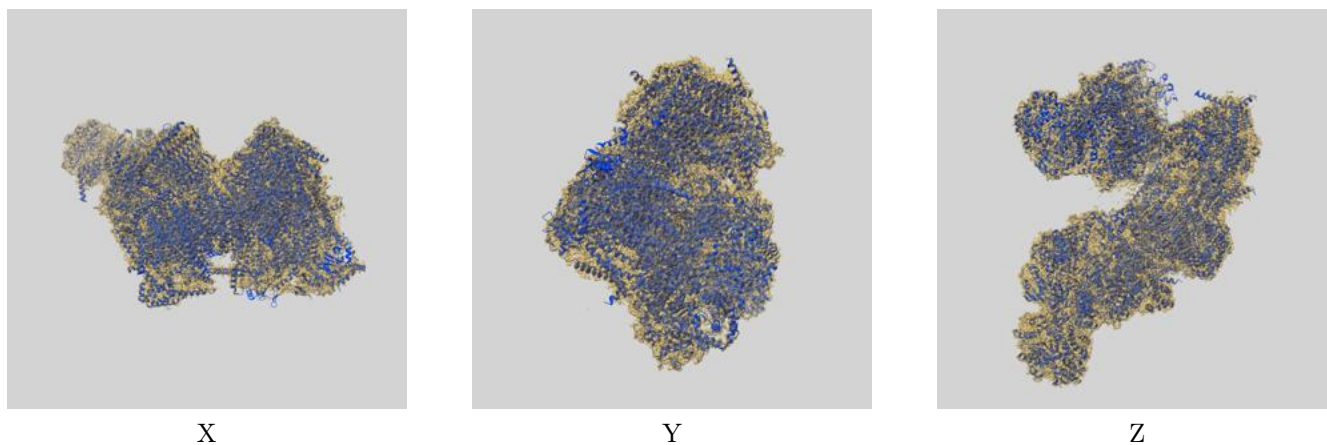
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.09	2.51	2.13
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

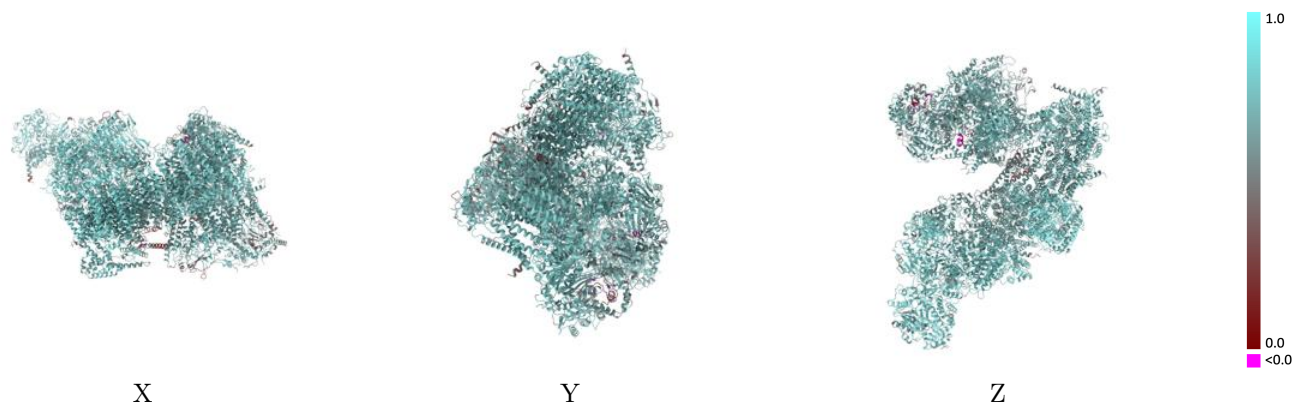
This section contains information regarding the fit between EMDB map EMD-16168 and PDB model 8BPX. Per-residue inclusion information can be found in section 3 on page 33.

9.1 Map-model overlay [i](#)



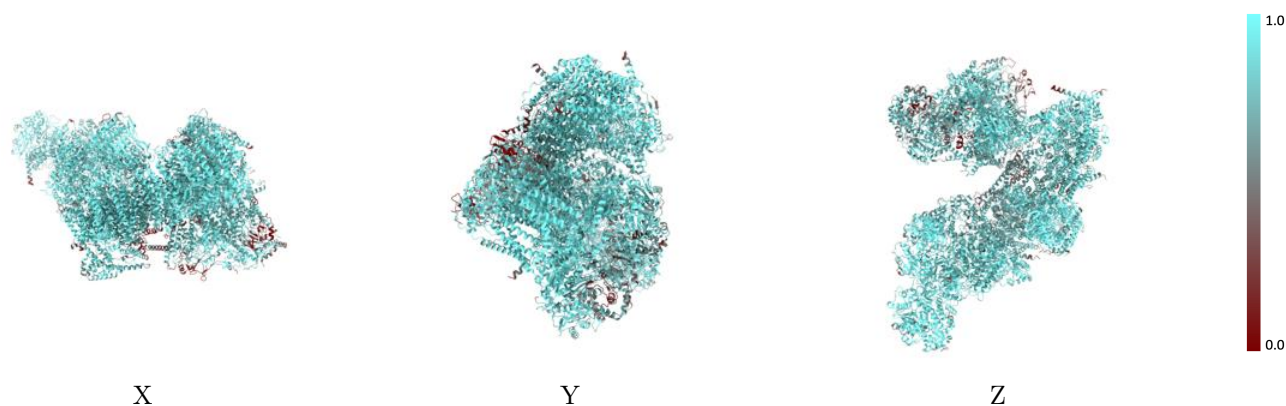
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



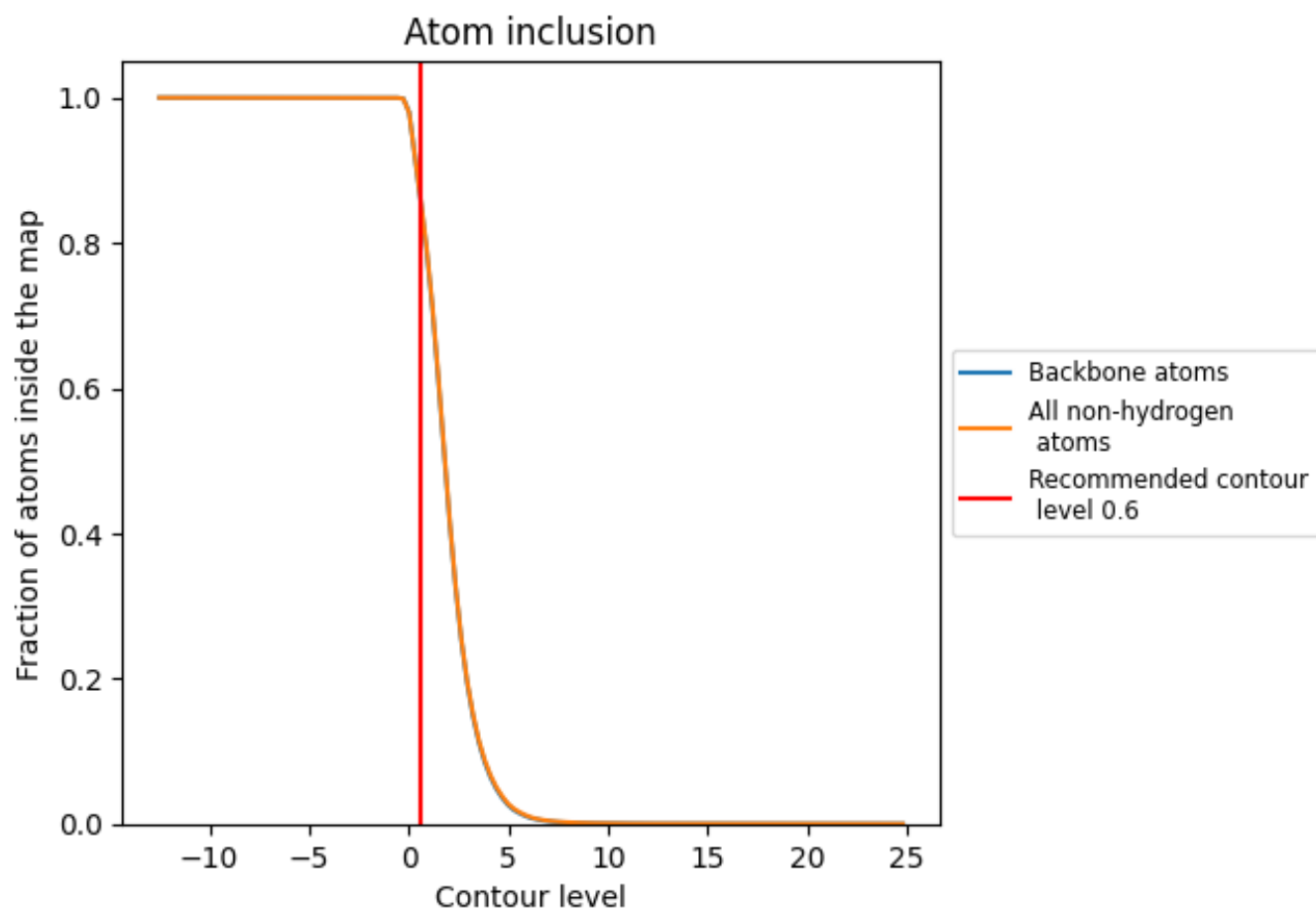
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



































































The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8589	 0.7070
A	 0.9393	 0.7560
AA	 0.6669	 0.5930
AB	 0.8814	 0.7020
AC	 0.9065	 0.7190
AD	 0.5257	 0.5880
AE	 0.9124	 0.7220
AF	 0.9331	 0.7300
AG	 0.8574	 0.6890
AH	 0.7710	 0.6450
AI	 0.8330	 0.6880
AJ	 0.5700	 0.5930
B	 0.9786	 0.8060
BA	 0.6824	 0.6050
BB	 0.8731	 0.7010
BC	 0.8884	 0.7010
BD	 0.5724	 0.5910
BE	 0.8805	 0.6940
BF	 0.9169	 0.6960
BG	 0.7867	 0.6430
BH	 0.6091	 0.5780
BI	 0.7821	 0.6380
BJ	 0.5729	 0.5980
C	 0.9579	 0.7940
D	 0.9525	 0.7910
E	 0.8472	 0.6810
F	 0.9333	 0.7460
G	 0.9218	 0.7420
H	 0.9246	 0.7710
I	 0.9646	 0.7850
J	 0.9062	 0.7450
K	 0.9170	 0.7600
L	 0.9237	 0.7200
M	 0.9275	 0.7270
N	 0.9418	 0.7730



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Chain	Atom inclusion	Q-score
O	 0.9364	 0.7570
P	 0.8674	 0.6930
Q	 0.8187	 0.6700
R	 0.8845	 0.7270
S	 0.9100	 0.7020
T	 0.8285	 0.6560
U	 0.6241	 0.5640
V	 0.8693	 0.7290
W	 0.8388	 0.6900
X	 0.8102	 0.7000
Y	 0.5887	 0.5500
Z	 0.8416	 0.7090
a	 0.8431	 0.7150
b	 0.7524	 0.6610
c	 0.9218	 0.7100
d	 0.7725	 0.6850
e	 0.8672	 0.7180
f	 0.8854	 0.7520
g	 0.7840	 0.6390
i	 0.6432	 0.5780
j	 0.8416	 0.6610
k	 0.8081	 0.6400
l	 0.8102	 0.6520
m	 0.8627	 0.6840
n	 0.9133	 0.6840
o	 0.8274	 0.6800
p	 0.8610	 0.6780
q	 0.9186	 0.7380
u	 0.5846	 0.5480
v	 0.8835	 0.7440
x	 0.9598	 0.7990
y	 0.9117	 0.7580
z	 0.9049	 0.7460