



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 10:54 AM JST

PDB ID : 5XTI
EMDB ID : EMD-6776
Title : Cryo-EM architecture of human respiratory chain megacomplex-I2III2IV2
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 17.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

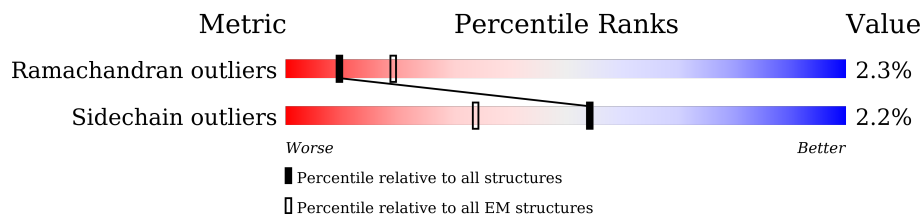
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 17.40 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	431	22% 98% .
1	BA	431	98% .
2	B	176	99% .
2	BB	176	99% .
3	BC	156	97% .
3	C	156	97% .
4	BE	113	97% .
4	E	113	97% .
5	BF	83	100%

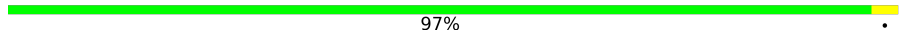
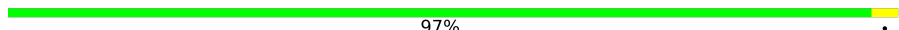
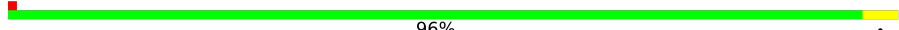
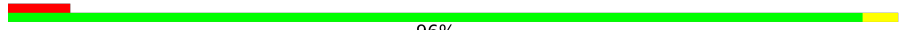
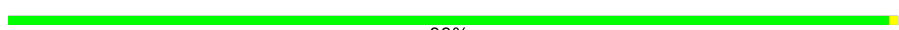





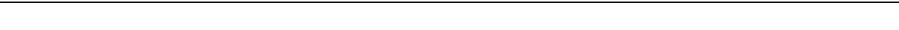

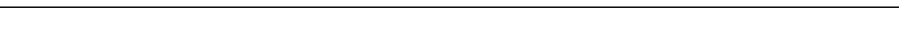
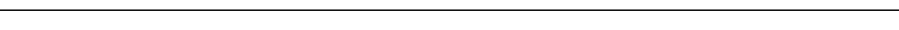
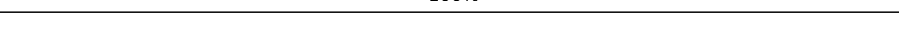
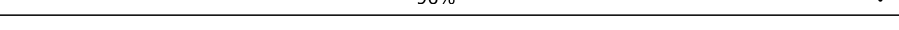
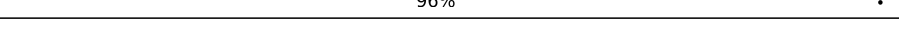


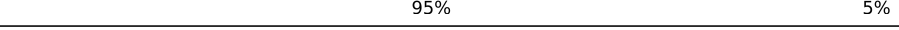
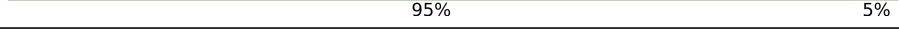
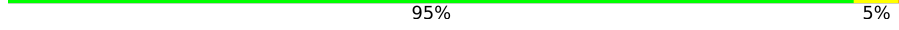
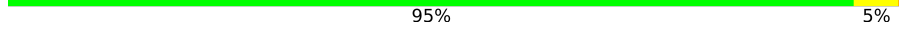
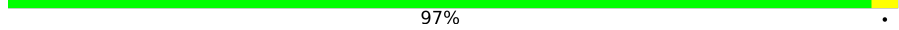
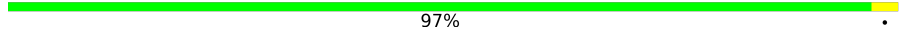
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Mol	Chain	Length	Quality of chain
5	F	83	100%
6	BG	85	26% 98%
6	BX	85	95% 5%
6	G	85	48% 98%
6	X	85	95% 5%
7	BH	112	96%
7	H	112	96%
8	BI	110	81% 5% 14%
8	I	110	81% 5% 14%
9	BJ	337	97%
9	J	337	97%
10	BK	33	91% 9%
10	K	33	91% 9%
11	BL	118	97%
11	L	118	97%
12	BM	687	96%
12	M	687	6% 96%
13	BN	143	95% 5%
13	N	143	95% 5%
14	BO	212	97%
14	O	212	10% 97%
15	BP	208	95% 5%
15	P	208	95% 5%
16	BQ	430	98%
16	Q	430	98%

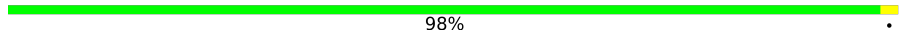
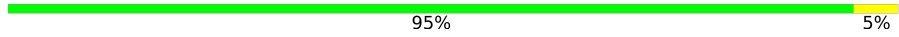
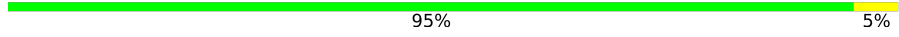
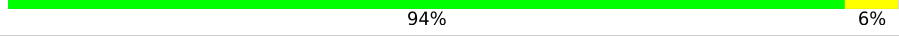
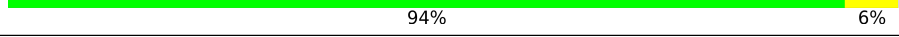
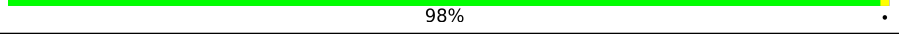
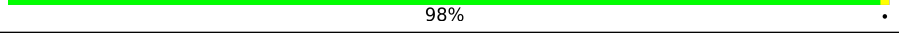
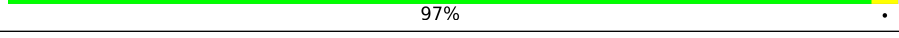
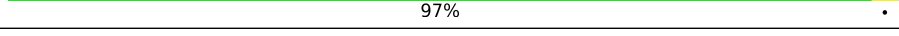
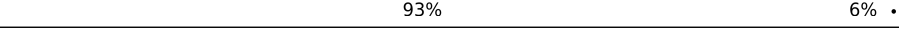
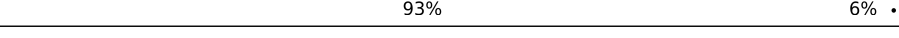
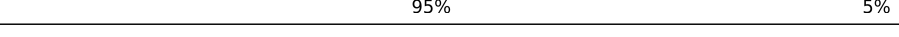
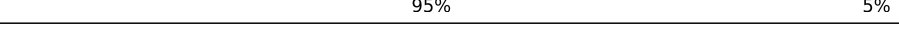
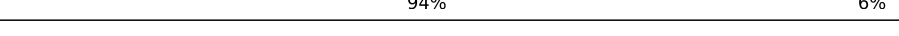
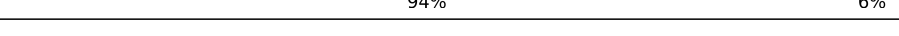
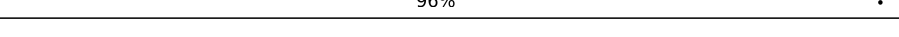
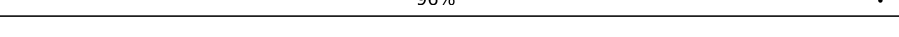
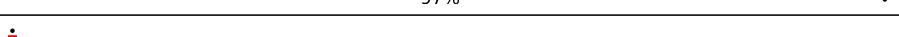
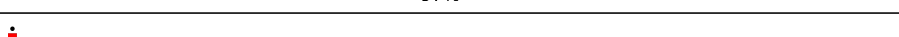






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Mol	Chain	Length	Quality of chain
17	BS	70	 97%
17	S	70	 97%
18	BT	95	 96%
18	T	95	 7% 96%
19	BU	83	 99%
19	U	83	 99%
20	BV	140	 98%
20	V	140	 98%
21	BW	138	 96%
21	W	138	 96%
22	BY	59	 75% 24%
22	Y	59	 75% 24%
23	BZ	80	 100%
23	Z	80	 100%
24	Ba	138	 96%
24	a	138	 96%
25	Bb	124	 90% 10%
25	b	124	 90% 10%
26	Bc	153	 95% 5%
26	c	153	 95% 5%
27	Bd	171	 95% 5%
27	d	171	 95% 5%
28	Be	97	 97%
28	e	97	 97%
29	Bf	47	 98%

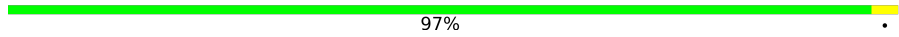
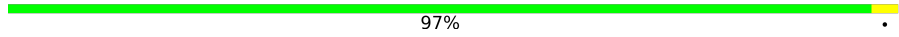


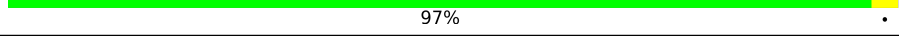
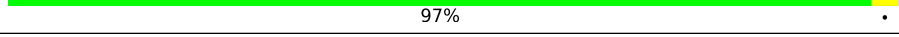
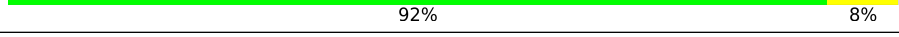
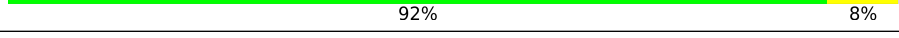
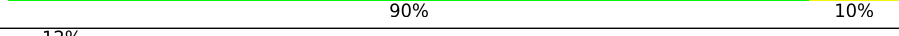

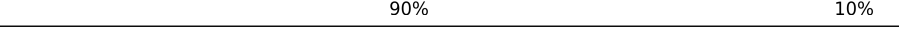
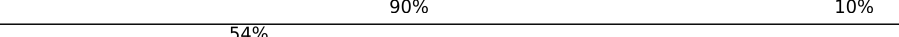
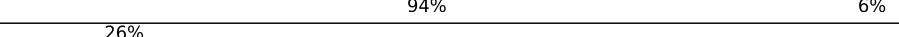
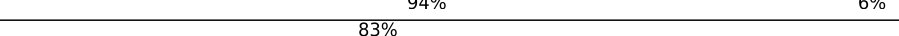
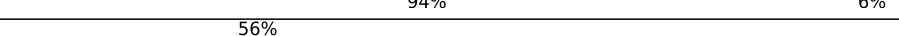
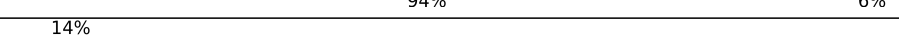
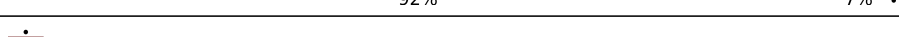
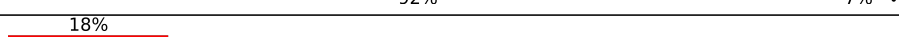
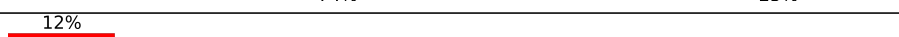






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Mol	Chain	Length	Quality of chain
29	f	47	 98% .
30	Bg	119	 95% 5% .
30	g	119	 95% 5% .
31	Bh	104	 94% 6% .
31	h	104	 94% 6% .
32	Bi	347	 98% .
32	i	347	 98% .
33	Bj	115	 97% .
33	j	115	 97% .
34	Bk	97	 93% 6% .
34	k	97	 93% 6% .
35	Bl	603	 95% 5% .
35	l	603	 95% 5% .
36	Bm	174	 94% 6% .
36	m	174	 94% 6% .
37	Bn	56	 96% .
37	n	56	 96% .
38	Bo	128	 97% .
38	o	128	 97% .
39	Bp	172	 98% .
39	p	172	 98% .
40	Br	459	 98% .
40	r	459	 98% .
41	Bs	318	 97% .
41	s	318	 97% .

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Mol	Chain	Length	Quality of chain
42	Bu	169	 97%
42	u	169	 97%
43	Bv	122	 86% 5% 9%
43	v	122	 86% 5% 9%
44	Bw	320	 97%
44	w	320	 97%
45	Bx	514	 92% 8%
45	x	514	 92% 8%
46	By	227	 90% 10%
46	y	227	 12% 90% 10%
47	Bz	261	 90% 10%
47	z	261	 90% 10%
48	0	144	 54% 94% 6%
48	B0	144	 26% 94% 6%
49	1	109	 83% 94% 6%
49	B1	109	 56% 94% 6%
50	2	98	 14% 92% 7%
50	B2	98	 14% 92% 7%
51	3	84	 18% 74% 25%
51	B3	84	 12% 74% 25%
52	4	75	 16% 87% 13%
52	B4	75	 11% 87% 13%
53	5	73	 51% 93% 7%
53	B5	73	 25% 93% 7%
54	6	56	 88% 9%

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Mol	Chain	Length	Quality of chain
54	B6	56	9% 88% 9%
55	7	49	39% 96%
55	B7	49	96%
56	8	47	96%
56	B8	47	96%
57	9	43	9% 93% 7%
57	B9	43	7% 93% 7%
58	AA	81	90% 10%
58	AN	81	99%
59	AB	57	93% 7%
59	AO	57	88% 12%
60	AC	196	97%
60	AP	196	98%
61	AD	62	100%
61	AQ	62	100%
62	AE	74	96%
62	AR	74	96%
63	AF	106	88% 12%
63	AS	106	100%
64	AG	51	100%
64	AT	51	96%
65	AH	241	99%
65	AU	241	99%
66	AJ	378	98%
66	AV	378	96%

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Mol	Chain	Length	Quality of chain
67	AK	419	 98%
67	AW	419	 98%
68	AL	446	 99%
68	AY	446	 96%

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
79	HEA	Bx	603	X	-	-	-
79	HEA	Bx	604	X	-	-	-
79	HEA	x	603	X	-	-	-
79	HEA	x	604	X	-	-	-

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 196753 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		
1	BA	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		
2	BB	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		
3	BC	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		
4	BE	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		
5	BF	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		
6	BG	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	BX	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		
7	BH	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		
8	BI	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BJ	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		
10	BK	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		
11	BL	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		
12	BM	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		
13	BN	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		
14	BO	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		
15	BP	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		
16	BQ	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		
17	BS	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		
18	BT	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		
19	BU	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		
20	BV	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		
21	BW	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		
22	BY	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		
23	BZ	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		
24	Ba	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		
25	Bb	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		
26	Bc	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		
27	Bd	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		
28	Be	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		
29	Bf	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		
30	Bg	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		
31	Bh	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		
32	Bi	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		
33	Bj	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Bk	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		
35	Bl	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		
36	Bm	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		
37	Bn	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	o	128	Total	C	N	O	S	0	0
			1063	684	191	186	2		
38	Bo	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		
39	Bp	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		
40	Br	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		
41	Bs	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		
42	Bu	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		
43	Bv	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		
44	Bw	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		
45	Bx	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		
46	By	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		
47	Bz	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		
48	B0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	B1	109	878	558	150	168	2	0	0

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	2	98	748	464	134	145	5	0	0
50	B2	98	748	464	134	145	5	0	0

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	3	84	672	431	129	111	1	0	0
51	B3	84	672	431	129	111	1	0	0

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	4	75	628	395	114	114	5	0	0
52	B4	75	628	395	114	114	5	0	0

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	5	73	598	388	107	99	4	0	0
53	B5	73	598	388	107	99	4	0	0

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	6	56	441	285	73	80	3	0	0
54	B6	56	441	285	73	80	3	0	0

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		
55	B7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		
56	B8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		
57	B9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AG	51	Total	C	N	O	0	0
			425	287	72	66		
64	AT	51	Total	C	N	O	0	0
			425	287	72	66		

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

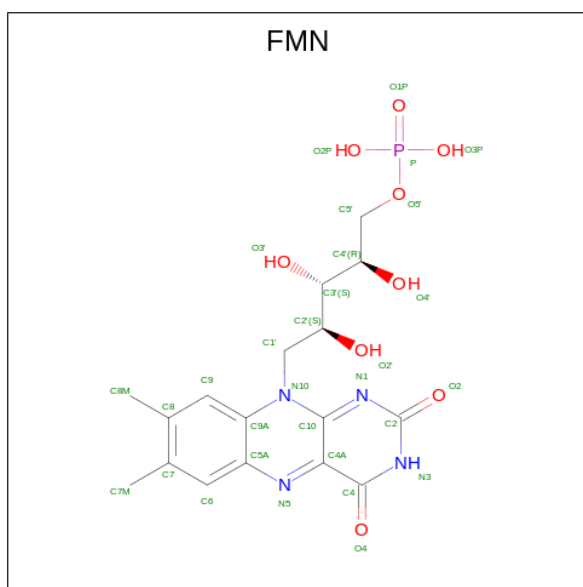
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AL	446	Total	C	N	O	S	0	0
			3442	2160	602	660	20		
68	AY	446	Total	C	N	O	S	0	0
			3428	2147	601	660	20		

- Molecule 69 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



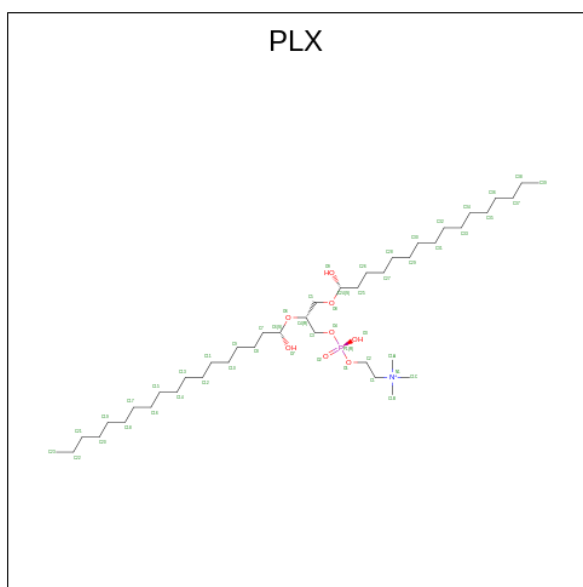
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
69	A	1	8	4	4	0
69	B	1	16	8	8	0
69	B	1	16	8	8	0
69	C	1	8	4	4	0
69	M	1	16	8	8	0
69	M	1	16	8	8	0
69	BA	1	8	4	4	0
69	BB	1	16	8	8	0
69	BB	1	16	8	8	0
69	BC	1	8	4	4	0
69	BM	1	16	8	8	0
69	BM	1	16	8	8	0

- Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					AltConf
70	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
70	BA	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



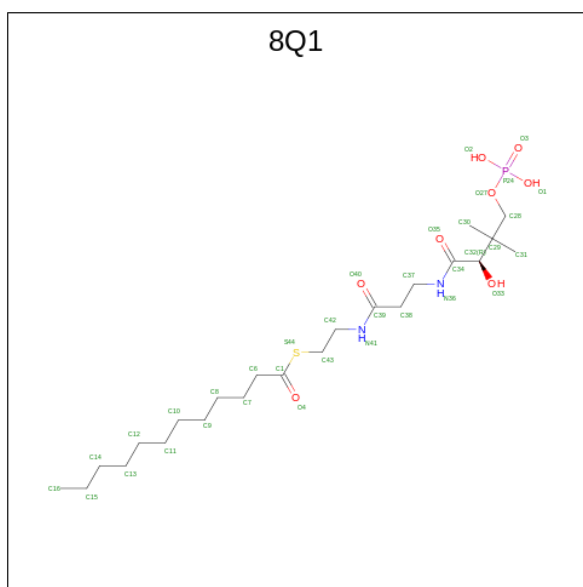
Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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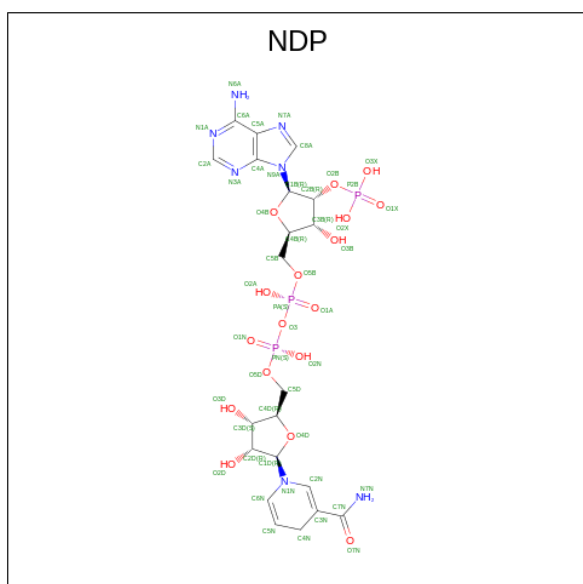
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
71	U	1	Total 52	C 42	N 1	O 8	P 1	0
71	b	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 156	C 126	N 3	O 24	P 3	0
71	g	1	Total 156	C 126	N 3	O 24	P 3	0
71	g	1	Total 156	C 126	N 3	O 24	P 3	0
71	r	1	Total 104	C 84	N 2	O 16	P 2	0
71	r	1	Total 104	C 84	N 2	O 16	P 2	0
71	AL	1	Total 52	C 42	N 1	O 8	P 1	0
71	AN	1	Total 52	C 42	N 1	O 8	P 1	0
71	AQ	1	Total 52	C 42	N 1	O 8	P 1	0
71	AT	1	Total 52	C 42	N 1	O 8	P 1	0
71	BB	1	Total 52	C 42	N 1	O 8	P 1	0
71	BU	1	Total 52	C 42	N 1	O 8	P 1	0
71	BV	1	Total 52	C 42	N 1	O 8	P 1	0
71	Bb	1	Total 52	C 42	N 1	O 8	P 1	0
71	Bg	1	Total 156	C 126	N 3	O 24	P 3	0
71	Bg	1	Total 156	C 126	N 3	O 24	P 3	0
71	Bg	1	Total 156	C 126	N 3	O 24	P 3	0
71	Br	1	Total 104	C 84	N 2	O 16	P 2	0
71	Br	1	Total 104	C 84	N 2	O 16	P 2	0

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



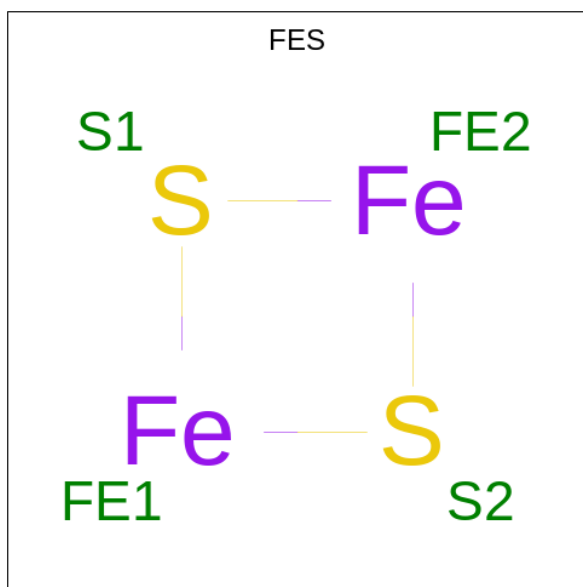
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
72	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	BE	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	Bp	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



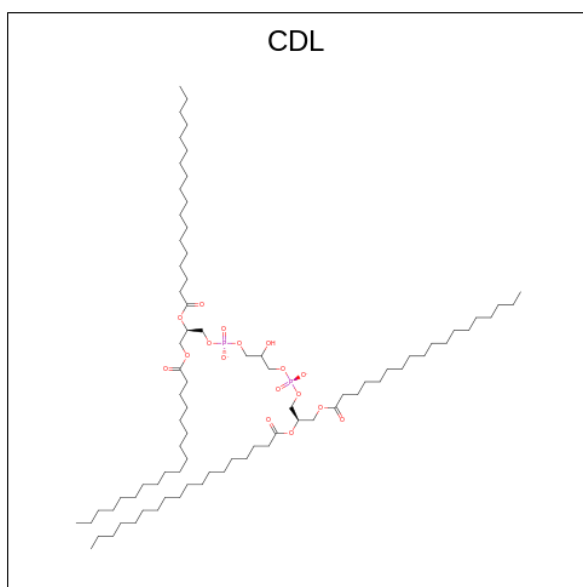
Mol	Chain	Residues	Atoms					AltConf
73	J	1	Total	C	N	O	P	0
			48	21	7	17	3	
73	BJ	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	
74	BM	1	Total	Fe	S	0
			4	2	2	
74	BO	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



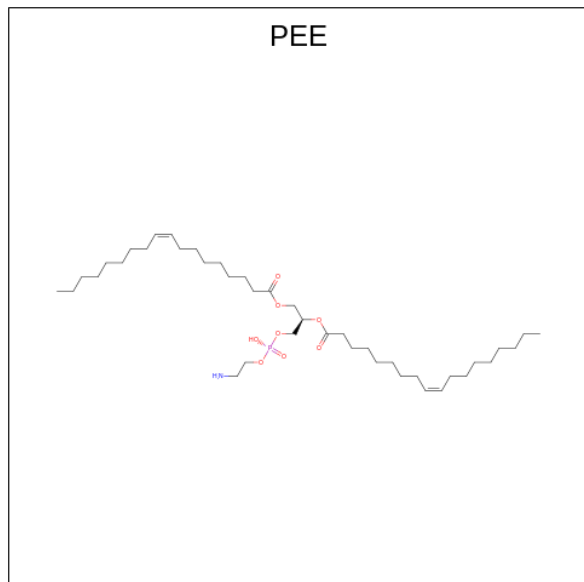
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	V	1	63	44	17	2	0
75	i	1	64	45	17	2	0
75	l	1	128	90	34	4	0
75	l	1	128	90	34	4	0
75	n	1	64	45	17	2	0
75	AA	1	64	45	17	2	0
75	AG	1	64	45	17	2	0
75	AH	1	64	45	17	2	0
75	AJ	1	128	90	34	4	0
75	AJ	1	128	90	34	4	0
75	AL	1	64	45	17	2	0
75	AN	1	64	45	17	2	0
75	AU	1	64	45	17	2	0
75	AY	1	64	45	17	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	BV	1	Total 63	C 44	O 17	P 2	0
75	Bi	1	Total 64	C 45	O 17	P 2	0
75	Bl	1	Total 128	C 90	O 34	P 4	0
75	Bl	1	Total 128	C 90	O 34	P 4	0
75	Bn	1	Total 64	C 45	O 17	P 2	0

- Molecule 76 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	V	1	Total 51	C 41	N 1	O 8	P 1	0
76	W	1	Total 51	C 41	N 1	O 8	P 1	0
76	l	1	Total 100	C 80	N 2	O 16	P 2	0
76	l	1	Total 100	C 80	N 2	O 16	P 2	0
76	AH	1	Total 49	C 39	N 1	O 8	P 1	0
76	AJ	1	Total 49	C 39	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
76	AL	1	Total 49	C 39	N 1	O 8	P 1	0
76	AU	1	Total 41	C 31	N 1	O 8	P 1	0
76	AV	1	Total 49	C 39	N 1	O 8	P 1	0
76	AY	1	Total 49	C 39	N 1	O 8	P 1	0
76	BV	1	Total 51	C 41	N 1	O 8	P 1	0
76	BW	1	Total 51	C 41	N 1	O 8	P 1	0
76	Bl	1	Total 100	C 80	N 2	O 16	P 2	0
76	Bl	1	Total 100	C 80	N 2	O 16	P 2	0

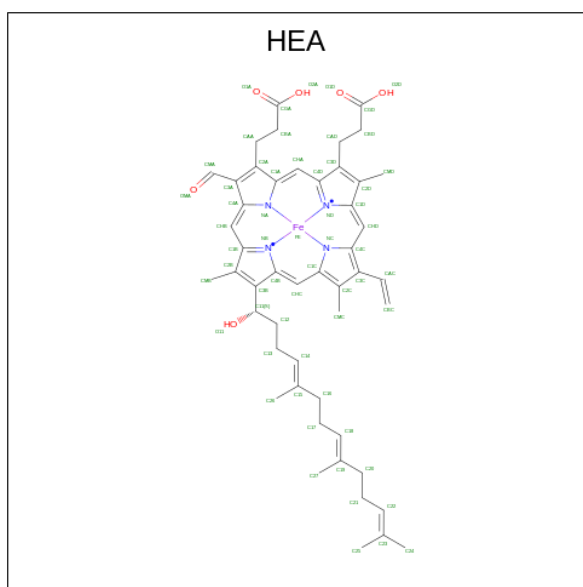
- Molecule 77 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
77	x	1	Total 1	Cu 1	0
77	y	2	Total 2	Cu 2	0
77	Bx	1	Total 1	Cu 1	0
77	By	2	Total 2	Cu 2	0

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
78	x	1	Total 1	Mg 1	0
78	Bx	1	Total 1	Mg 1	0

- Molecule 79 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

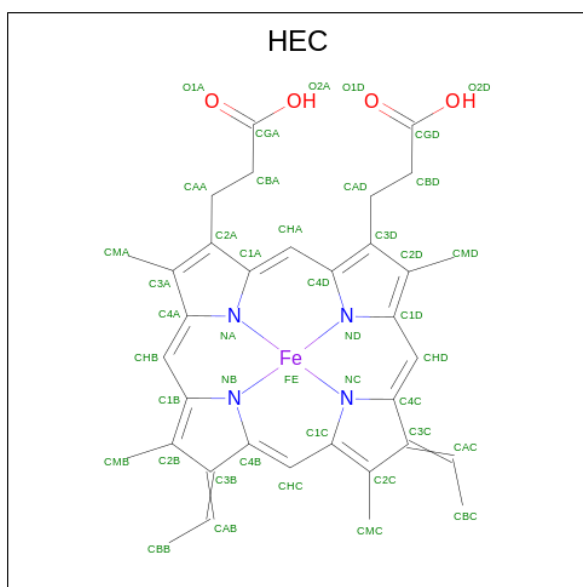


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
79	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	x	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	Bx	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
79	Bx	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

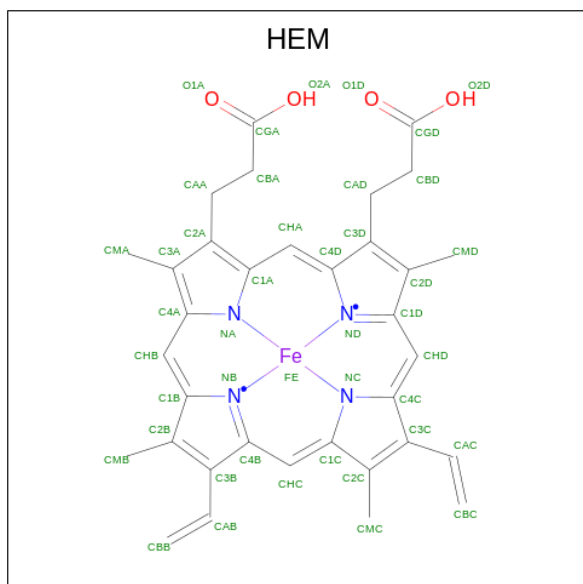
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	2	1	Total	Zn	0
			1	1	
80	B2	1	Total	Zn	0
			1	1	

- Molecule 81 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms				AltConf	
81	AH	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	AU	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				AltConf	
82	AJ	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

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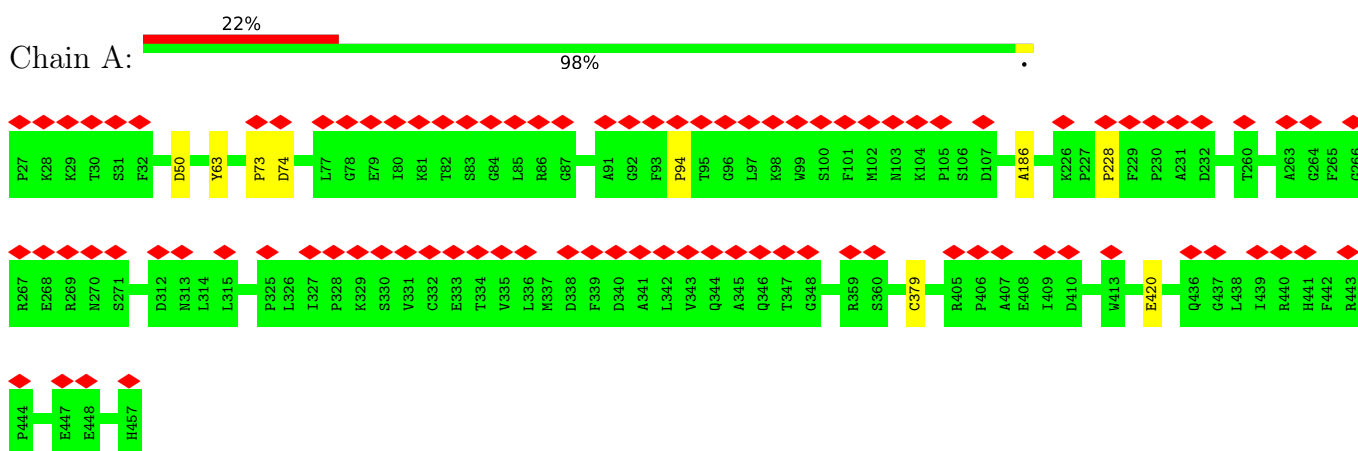
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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
82	AJ	1	Total 86	68	2	8	8	0
82	AV	1	Total 86	68	2	8	8	0
82	AV	1	Total 86	68	2	8	8	0

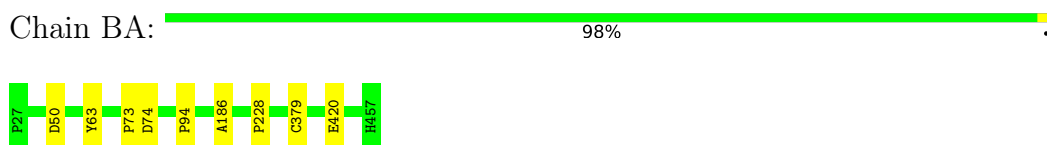
3 Residue-property plots

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

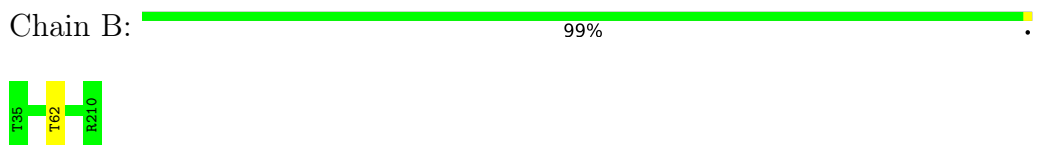
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



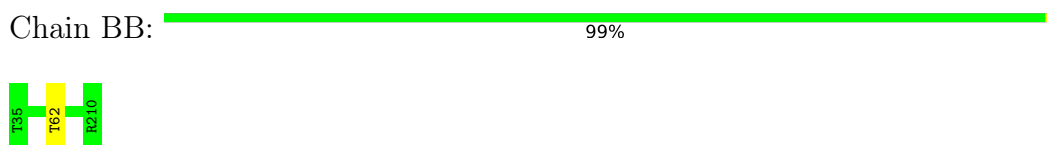
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



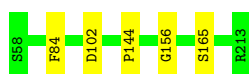
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:  97%



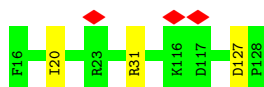
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain BC:  97%



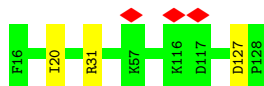
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:  97%



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain BE:  97%



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:  100%

There are no outlier residues recorded for this chain.

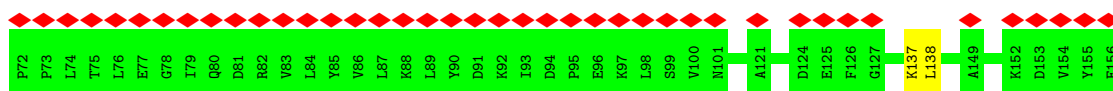
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain BF:  100%

There are no outlier residues recorded for this chain.

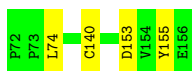
- Molecule 6: Acyl carrier protein, mitochondrial

Chain G:  48% 98%

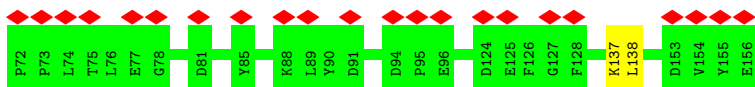


- Molecule 6: Acyl carrier protein, mitochondrial

Chain X:  95% 5%



- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



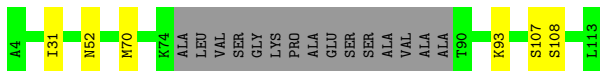
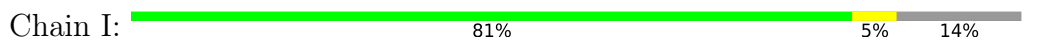
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



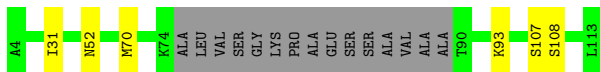
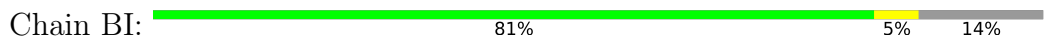
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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





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



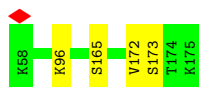
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



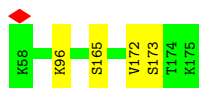
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



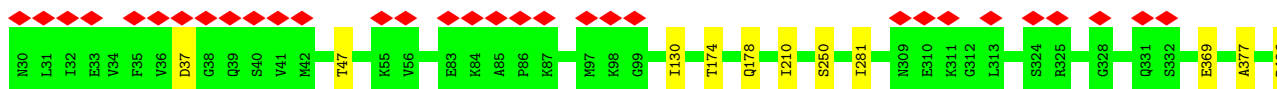
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

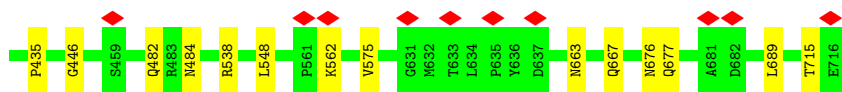


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



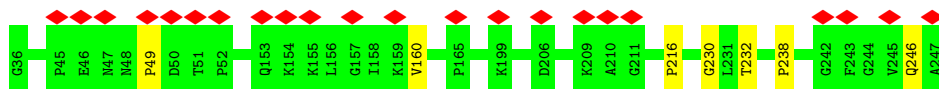
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



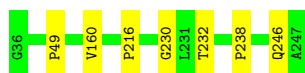
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain BP:  95% 5%



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:  98%



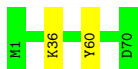
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain BQ:  98%



- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  97%



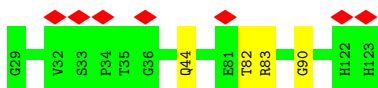
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain BS:  97%



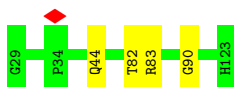
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  7% 96%



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

Chain BT:  96%



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  99%



- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain BU:  99%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  98%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain BV:  98%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  96%



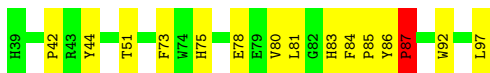
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain BW:  96%




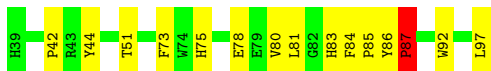
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  75%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain BY:  75% 24%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  100%

There are no outlier residues recorded for this chain.

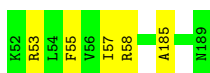
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain BZ:  100%

There are no outlier residues recorded for this chain.

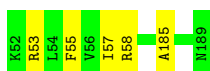
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  96%




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain Ba:  96%




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:  90% 10%



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain Bb:  90% 10%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  95% 5%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain Bc:  95% 5%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  95% 5%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain Bd:  95% 5%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  97%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain Be:  97%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  98%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain Bf:  98%



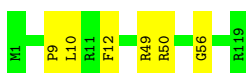
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  95% 5%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain Bg:  95% 5%



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

Chain h:  94% 6%



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

Chain Bh:  94% 6%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  98%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain Bi:  98%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  97%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain Bj:  97%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  93% 6%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain Bk:  93% 6%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  95% 5%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain Bl:  95% 5%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  94% 6%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain Bm:  94% 6%



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

Chain n:  96%



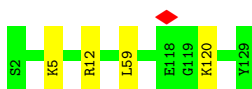
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain Bn:  96%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  97%



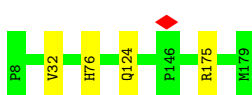
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain Bo:  97%



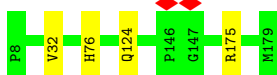
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:  98%



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

Chain Bp:  98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain Br:  98%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  97%



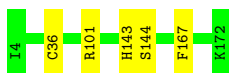
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain Bs:  97%



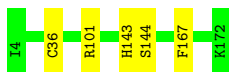
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  97%




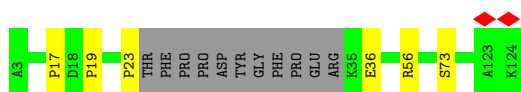
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Bu:  97%




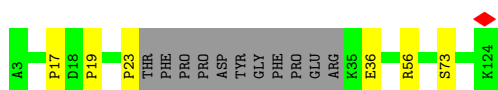
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  86% 5% 9%



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain Bv:  86% 5% 9%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w:  97%



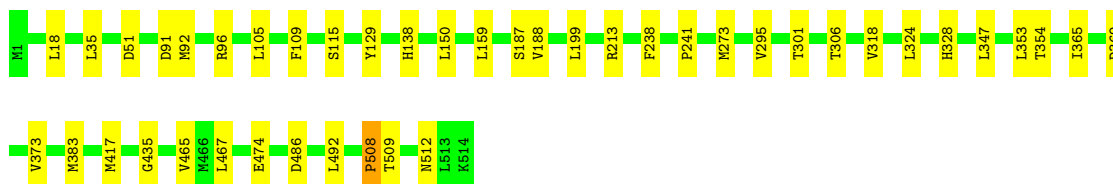
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain Bw:  97%



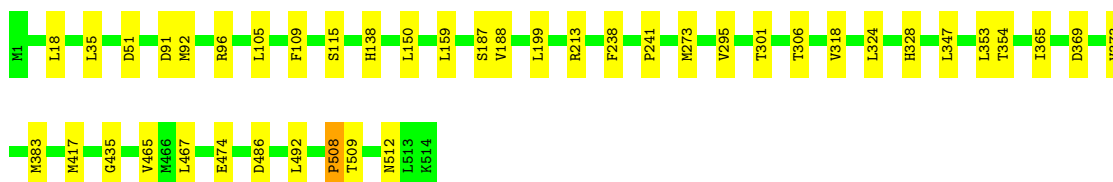
- Molecule 45: Cytochrome c oxidase subunit 1

Chain x:  92% 8%

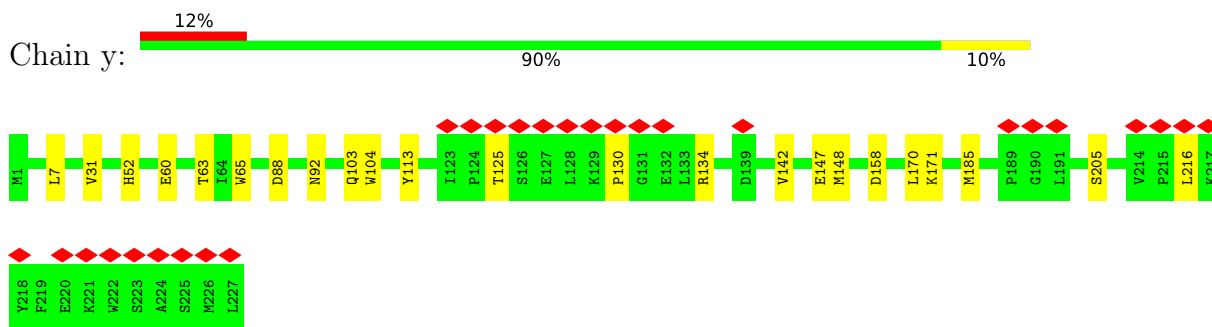


- Molecule 45: Cytochrome c oxidase subunit 1

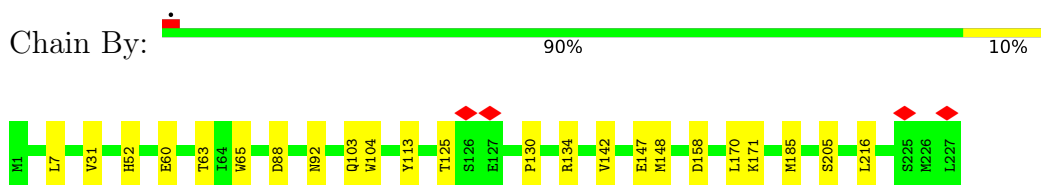
Chain Bx:  92% 8%



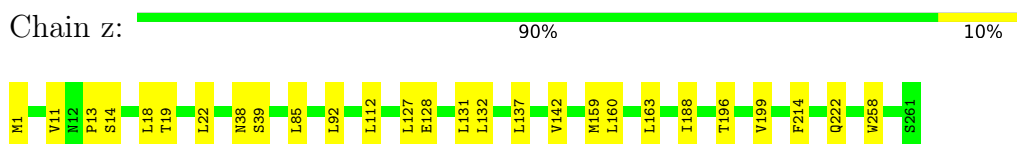
• Molecule 46: Cytochrome c oxidase subunit 2



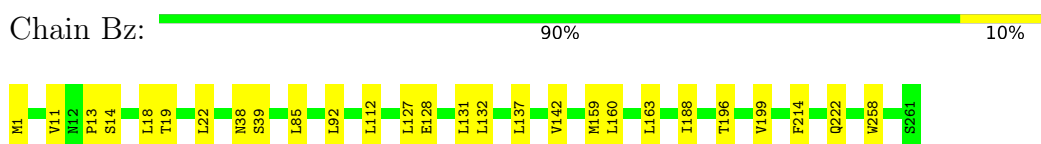
• Molecule 46: Cytochrome c oxidase subunit 2



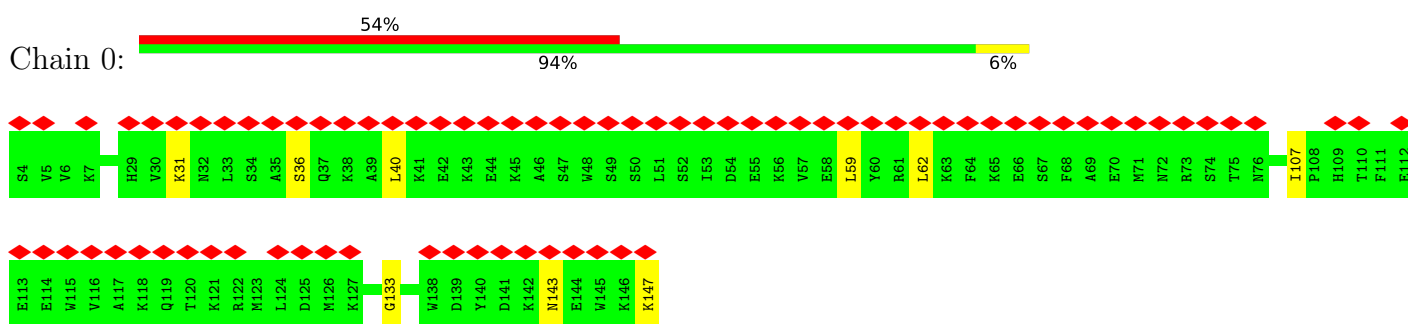
• Molecule 47: Cytochrome c oxidase subunit 3



• Molecule 47: Cytochrome c oxidase subunit 3

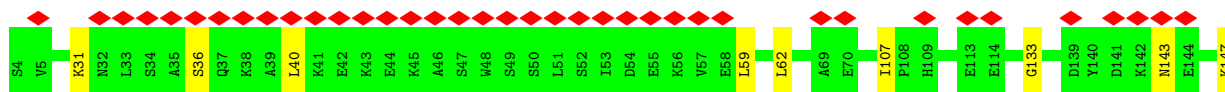


• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



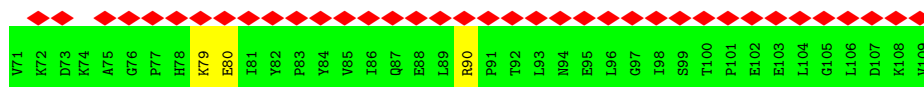
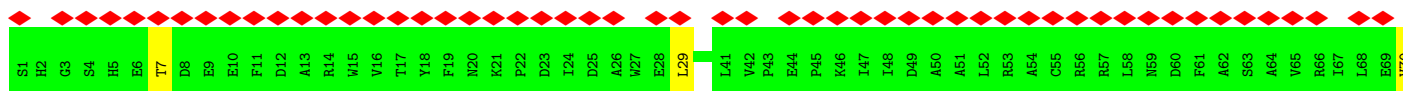
• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial





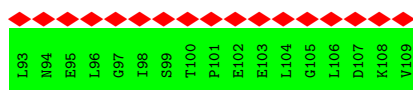
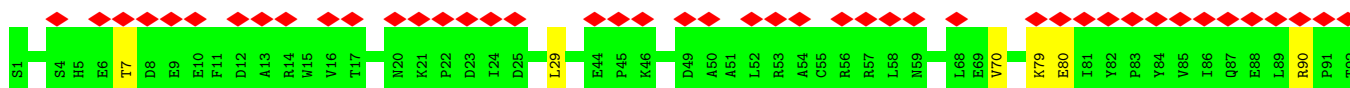
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 1:



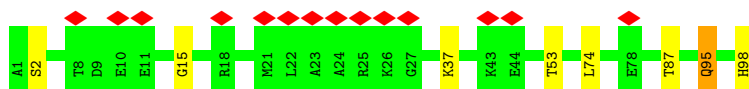
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial

Chain B1:



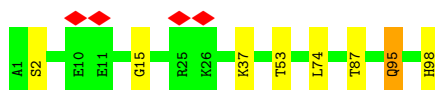
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 2:



- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial

Chain B2:

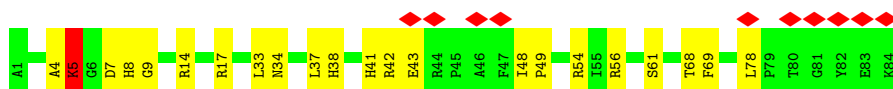
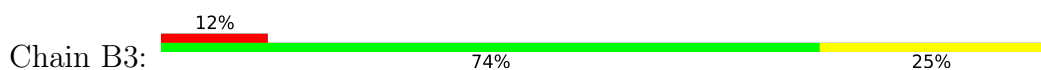


- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial

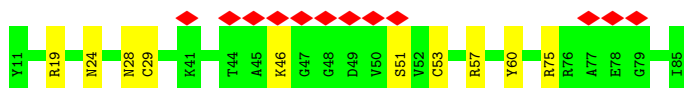
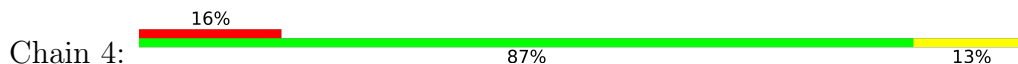
Chain 3:



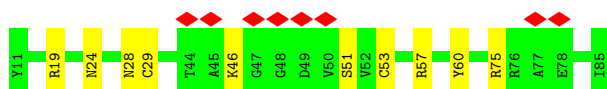
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



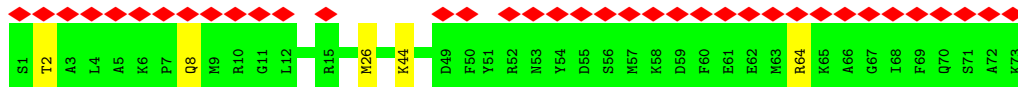
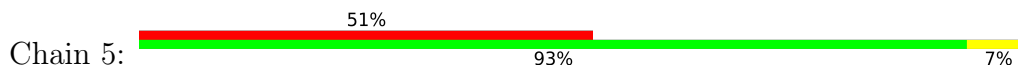
- Molecule 52: Cytochrome c oxidase subunit 6B1



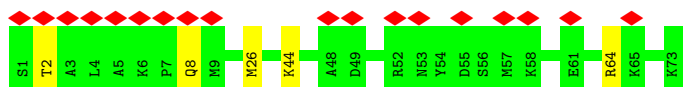
- Molecule 52: Cytochrome c oxidase subunit 6B1



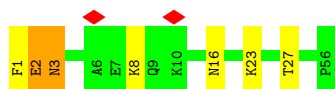
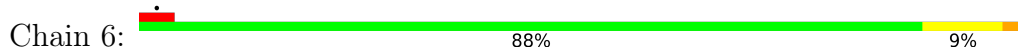
- Molecule 53: Cytochrome c oxidase subunit 6C



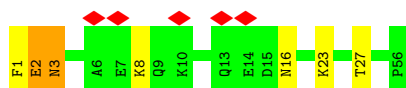
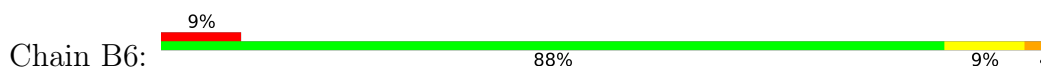
- Molecule 53: Cytochrome c oxidase subunit 6C



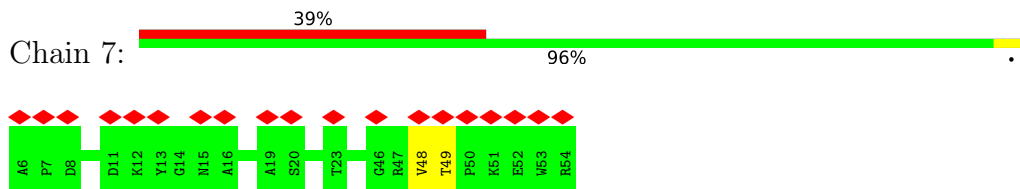
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



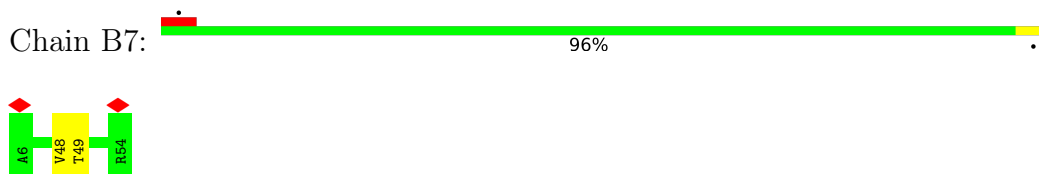
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



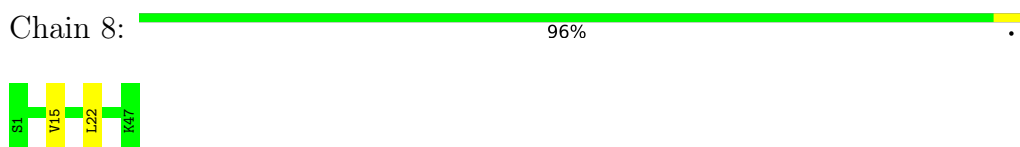
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



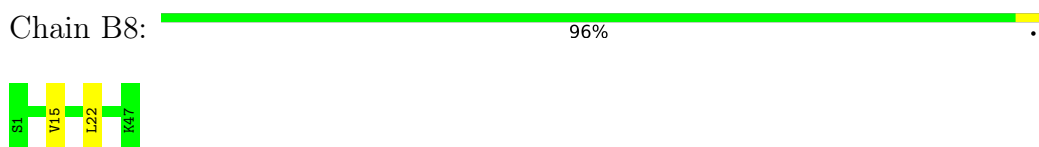
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



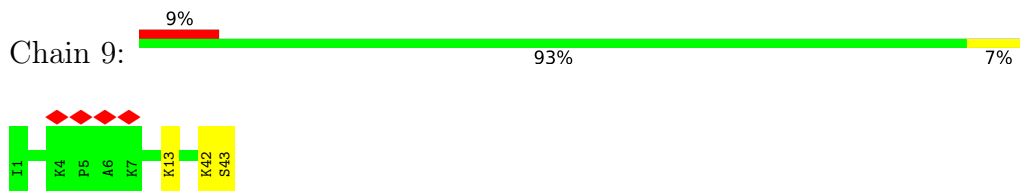
- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



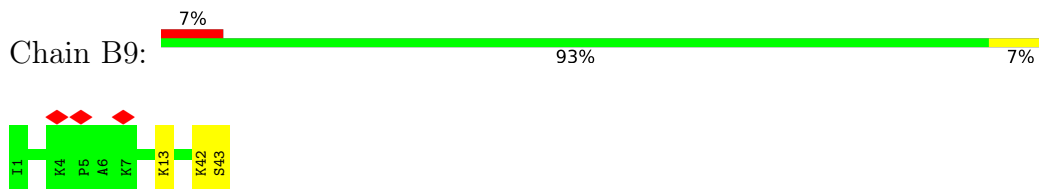
- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial

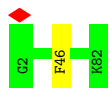


- Molecule 58: Cytochrome b-c1 complex subunit 8

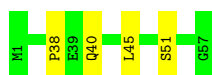




- Molecule 58: Cytochrome b-c1 complex subunit 8



- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 61: Cytochrome b-c1 complex subunit 9



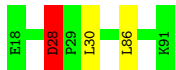
- Molecule 61: Cytochrome b-c1 complex subunit 9



There are no outlier residues recorded for this chain.

- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AE:  96%



- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AR:  96%



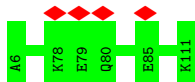
- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AF:  88% 12%



- Molecule 63: Cytochrome b-c1 complex subunit 7

Chain AS:  100%



- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AG:  100%

There are no outlier residues recorded for this chain.

- Molecule 64: Cytochrome b-c1 complex subunit 10

Chain AT:  96%



- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AH:  99%



- Molecule 65: Cytochrome c1, heme protein, mitochondrial

Chain AU:  99%



- Molecule 66: Cytochrome b

Chain AJ:  98%



- Molecule 66: Cytochrome b

Chain AV:  96%



- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AK:  98%



- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AW:  98%



- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AL:  99%



- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AY:  96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0056	Depositor
Map size (\AA)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	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: SF4, 8Q1, PEE, NDP, HEM, HEA, HEC, FES, ZN, FMN, PLX, CU, MG, CDL

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	0/3398	0.49	0/4590
1	BA	0.30	0/3398	0.49	0/4590
2	B	0.50	0/1452	0.57	0/1964
2	BB	0.50	0/1452	0.57	0/1964
3	BC	0.58	0/1280	0.57	0/1732
3	C	0.58	0/1280	0.57	0/1732
4	BE	0.34	0/993	0.54	0/1335
4	E	0.34	0/993	0.54	0/1335
5	BF	0.28	0/682	0.53	0/922
5	F	0.28	0/682	0.53	0/922
6	BG	0.33	0/684	0.53	0/926
6	BX	0.57	0/698	0.61	0/942
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
7	BH	0.34	0/941	0.59	0/1275
7	H	0.34	0/941	0.59	0/1275
8	BI	0.29	0/788	0.54	0/1066
8	I	0.29	0/788	0.54	0/1066
9	BJ	0.35	0/2785	0.52	0/3771
9	J	0.35	0/2785	0.52	0/3771
10	BK	0.27	0/282	0.47	0/381
10	K	0.27	0/282	0.47	0/381
11	BL	0.33	0/987	0.53	0/1331
11	L	0.33	0/987	0.53	0/1331
12	BM	0.32	0/5362	0.53	0/7266
12	M	0.32	0/5362	0.53	0/7266
13	BN	0.37	0/1236	0.55	0/1681
13	N	0.37	0/1236	0.55	0/1681
14	BO	0.29	0/1682	0.51	0/2289
14	O	0.29	0/1682	0.51	0/2289
15	BP	0.38	0/1780	0.59	0/2424
15	P	0.38	0/1780	0.59	0/2424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BQ	0.43	0/3552	0.59	1/4815 (0.0%)
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	BS	0.60	0/583	0.64	0/785
17	S	0.60	0/583	0.64	0/785
18	BT	0.32	0/755	0.47	0/1017
18	T	0.32	0/755	0.47	0/1017
19	BU	0.52	0/670	0.63	0/920
19	U	0.52	0/670	0.63	0/920
20	BV	0.51	0/1065	0.61	0/1450
20	V	0.51	0/1065	0.61	0/1450
21	BW	0.57	0/1166	0.68	1/1579 (0.1%)
21	W	0.57	0/1166	0.68	1/1579 (0.1%)
22	BY	0.52	0/559	0.73	3/763 (0.4%)
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	BZ	0.45	0/669	0.53	0/899
23	Z	0.45	0/669	0.53	0/899
24	Ba	0.68	0/1209	0.65	0/1639
24	a	0.69	0/1209	0.65	0/1639
25	Bb	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	Bc	0.58	0/1287	0.59	0/1761
26	c	0.58	0/1287	0.58	0/1761
27	Bd	0.63	0/1445	0.65	1/1945 (0.1%)
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	Be	0.61	0/835	0.62	0/1134
28	e	0.61	0/835	0.62	0/1134
29	Bf	0.48	0/418	0.58	0/566
29	f	0.48	0/418	0.58	0/566
30	Bg	0.64	0/1035	0.63	0/1398
30	g	0.64	0/1035	0.63	0/1398
31	Bh	0.62	0/884	0.65	0/1182
31	h	0.62	0/884	0.65	0/1182
32	Bi	0.67	0/2808	0.77	2/3843 (0.1%)
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	Bj	0.55	0/945	0.70	1/1292 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	Bk	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	Bl	0.61	0/4840	0.70	3/6611 (0.0%)
35	l	0.61	1/4840 (0.0%)	0.70	3/6611 (0.0%)
36	Bm	0.68	0/1346	0.67	0/1832
36	m	0.68	0/1346	0.67	0/1832
37	Bn	0.49	0/484	0.62	0/652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	n	0.50	0/484	0.62	0/652
38	Bo	0.54	0/1093	0.61	0/1479
38	o	0.54	0/1090	0.61	0/1475
39	Bp	0.59	0/1549	0.59	0/2098
39	p	0.59	0/1549	0.59	0/2098
40	Br	0.71	0/3723	0.76	2/5089 (0.0%)
40	r	0.71	0/3723	0.76	2/5089 (0.0%)
41	Bs	0.62	0/2580	0.73	0/3539
41	s	0.62	0/2580	0.73	0/3539
42	Bu	0.57	0/1433	0.61	0/1937
42	u	0.57	0/1433	0.61	0/1937
43	Bv	0.49	0/934	0.67	3/1241 (0.2%)
43	v	0.49	0/934	0.67	3/1241 (0.2%)
44	Bw	0.44	0/2533	0.56	0/3440
44	w	0.44	0/2533	0.56	0/3440
45	Bx	0.60	0/4164	0.76	1/5688 (0.0%)
45	x	0.60	0/4164	0.76	2/5688 (0.0%)
46	By	0.58	0/1868	0.80	0/2544
46	y	0.58	0/1868	0.80	0/2544
47	Bz	0.56	0/2211	0.69	0/3023
47	z	0.56	0/2211	0.69	0/3023
48	0	0.57	0/1229	0.65	1/1658 (0.1%)
48	B0	0.57	0/1229	0.65	1/1658 (0.1%)
49	1	0.50	0/898	0.66	0/1218
49	B1	0.50	0/898	0.66	0/1218
50	2	0.56	0/765	0.81	0/1038
50	B2	0.56	0/765	0.81	0/1038
51	3	0.55	0/699	0.73	1/950 (0.1%)
51	B3	0.55	0/699	0.73	1/950 (0.1%)
52	4	0.55	0/648	0.73	0/877
52	B4	0.55	0/648	0.73	0/877
53	5	0.61	0/611	0.64	0/810
53	B5	0.60	0/611	0.65	0/810
54	6	0.60	0/451	0.72	0/610
54	B6	0.60	0/451	0.71	0/610
55	7	0.58	0/398	0.66	0/546
55	B7	0.58	0/398	0.66	0/546
56	8	0.63	0/399	0.62	0/534
56	B8	0.63	0/399	0.62	0/534
57	9	0.51	0/345	0.65	0/470
57	B9	0.52	0/345	0.65	0/470
58	AA	0.31	0/715	0.48	0/964
58	AN	0.27	0/707	0.49	0/953

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
59	AB	0.23	0/421	0.60	1/574 (0.2%)
59	AO	0.25	0/417	0.61	1/569 (0.2%)
60	AC	0.24	0/1554	0.43	0/2104
60	AP	0.24	0/1554	0.42	0/2104
61	AD	0.26	0/521	0.42	0/699
61	AQ	0.27	0/521	0.43	0/699
62	AE	0.35	0/587	0.54	1/789 (0.1%)
62	AR	0.27	0/587	0.46	0/789
63	AF	0.42	0/942	0.52	1/1263 (0.1%)
63	AS	0.27	0/942	0.44	0/1263
64	AG	0.27	0/442	0.48	0/608
64	AT	0.28	0/442	0.49	0/608
65	AH	0.26	0/1983	0.46	0/2691
65	AU	0.27	0/1983	0.45	0/2691
66	AJ	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)
66	AV	0.34	2/3108 (0.1%)	0.54	2/4254 (0.0%)
67	AK	0.27	0/3217	0.49	0/4361
67	AW	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)
68	AL	0.27	0/3514	0.47	0/4769
68	AY	0.30	1/3499 (0.0%)	0.51	2/4750 (0.0%)
All	All	0.49	10/197905 (0.0%)	0.62	61/268649 (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
44	Bw	0	1
44	w	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AW	448	PRO	N-CD	5.28	1.55	1.47
66	AJ	154	PRO	N-CD	5.24	1.55	1.47
66	AV	154	PRO	N-CD	5.23	1.55	1.47
25	b	118	PRO	N-CD	5.21	1.55	1.47
34	k	2	PRO	N-CD	5.20	1.55	1.47

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
32	Bi	323	THR	C-N-CD	-7.37	104.38	120.60
21	BW	31	SER	N-CA-C	-7.01	92.08	111.00
21	W	31	SER	N-CA-C	-7.00	92.09	111.00
22	BY	92	TRP	N-CA-C	-6.99	92.12	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	Bw	338	LYS	Peptide
44	w	338	LYS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	7 36
1	BA	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	7 36
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	25 66
2	BB	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	25 66
3	BC	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	4 26
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	4 26
4	BE	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	8 40
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	8 40
5	BF	81/83 (98%)	74 (91%)	7 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	BG	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	33
6	BX	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	21
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	6	33
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	21
7	BH	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	22
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	22
8	BI	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	16
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	16
9	BJ	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	7	36
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	7	36
10	BK	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	10
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	10
11	BL	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	26
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	26
12	BM	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	26
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	26
13	BN	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	20
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	20
14	BO	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	26
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	26
15	BP	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	19
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	19
16	BQ	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	9	44
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	9	44
17	BS	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	4	29
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	4	29
18	BT	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	22
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	22
19	BU	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	50
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	BV	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	35
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	35
21	BW	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	3	24
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	3	24
22	BY	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	8
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	8
23	BZ	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	Ba	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	6	35
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	6	35
25	Bb	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3	23
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3	23
26	Bc	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	21
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	21
27	Bd	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25	66
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	25	66
28	Be	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	4	26
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	4	26
29	Bf	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	35
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	35
30	Bg	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	19
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	19
31	Bh	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	17
31	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	17
32	Bi	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	9	42
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	9	42
33	Bj	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	31
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	5	31
34	Bk	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	26
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	26
35	Bl	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	9	42
36	Bm	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	18
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	18
37	Bn	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	3	24
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	3	24
38	Bo	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	26
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	4	26
39	Bp	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	40
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	8	40
40	Br	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	7	38
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	7	38
41	Bs	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	5	30
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	5	30
42	Bu	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	4	28
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	4	28
43	Bv	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	5	30
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	5	30
44	Bw	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	5	30
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	5	30
45	Bx	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	19	60
46	By	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	12	48
47	Bz	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
48	B0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
49	B1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	22
50	B2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	17
51	B3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	17
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	11	46
52	B4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	11	46
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
53	B5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	24
54	B6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	24
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
55	B7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
56	B8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
57	B9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	5	32
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	12	48
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	19
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	8
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	5	31
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	10	46
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	5	30
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	11	46
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	15	55
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	19	60
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	19	60
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	19	60
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	13	50
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	13	50
68	AL	444/446 (100%)	403 (91%)	35 (8%)	6 (1%)	11	46
68	AY	444/446 (100%)	414 (93%)	22 (5%)	8 (2%)	8	40
All	All	23880/24216 (99%)	21833 (91%)	1487 (6%)	560 (2%)	9	34

5 of 560 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

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	346/346 (100%)	346 (100%)	0	100	100
1	BA	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
2	BB	151/151 (100%)	151 (100%)	0	100	100
3	BC	132/132 (100%)	132 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	BE	106/106 (100%)	105 (99%)	1 (1%)	78	87
4	E	106/106 (100%)	105 (99%)	1 (1%)	78	87
5	BF	74/74 (100%)	74 (100%)	0	100	100
5	F	74/74 (100%)	74 (100%)	0	100	100
6	BG	74/79 (94%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BX	78/79 (99%)	78 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	BH	100/100 (100%)	100 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	BI	87/96 (91%)	87 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	BJ	292/292 (100%)	288 (99%)	4 (1%)	67	80
9	J	292/292 (100%)	288 (99%)	4 (1%)	67	80
10	BK	32/32 (100%)	32 (100%)	0	100	100
10	K	32/32 (100%)	32 (100%)	0	100	100
11	BL	107/107 (100%)	107 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	BM	576/577 (100%)	574 (100%)	2 (0%)	92	95
12	M	576/577 (100%)	574 (100%)	2 (0%)	92	95
13	BN	129/129 (100%)	129 (100%)	0	100	100
13	N	129/129 (100%)	129 (100%)	0	100	100
14	BO	181/181 (100%)	181 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	BP	190/190 (100%)	190 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	BQ	371/371 (100%)	369 (100%)	2 (0%)	88	93
16	Q	371/371 (100%)	369 (100%)	2 (0%)	88	93
17	BS	59/59 (100%)	59 (100%)	0	100	100
17	S	59/59 (100%)	59 (100%)	0	100	100
18	BT	79/79 (100%)	79 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	BU	72/72 (100%)	72 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	BV	102/102 (100%)	102 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	BW	119/119 (100%)	119 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	BY	57/57 (100%)	49 (86%)	8 (14%)	3	17
22	Y	57/57 (100%)	49 (86%)	8 (14%)	3	17
23	BZ	62/63 (98%)	62 (100%)	0	100	100
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	Ba	124/124 (100%)	122 (98%)	2 (2%)	62	79
24	a	124/124 (100%)	122 (98%)	2 (2%)	62	79
25	Bb	118/118 (100%)	114 (97%)	4 (3%)	37	60
25	b	118/118 (100%)	114 (97%)	4 (3%)	37	60
26	Bc	124/137 (90%)	124 (100%)	0	100	100
26	c	124/137 (90%)	124 (100%)	0	100	100
27	Bd	145/154 (94%)	137 (94%)	8 (6%)	21	47
27	d	145/154 (94%)	137 (94%)	8 (6%)	21	47
28	Be	90/90 (100%)	90 (100%)	0	100	100
28	e	90/90 (100%)	90 (100%)	0	100	100
29	Bf	43/43 (100%)	43 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	Bg	105/105 (100%)	105 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	Bh	90/90 (100%)	90 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	Bi	314/314 (100%)	314 (100%)	0	100	100
32	i	314/314 (100%)	314 (100%)	0	100	100
33	Bj	102/103 (99%)	102 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	Bk	85/85 (100%)	82 (96%)	3 (4%)	36	59
34	k	85/85 (100%)	82 (96%)	3 (4%)	36	59
35	Bl	531/532 (100%)	510 (96%)	21 (4%)	31	55
35	l	531/532 (100%)	510 (96%)	21 (4%)	31	55
36	Bm	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	m	137/137 (100%)	137 (100%)	0	100	100
37	Bn	53/53 (100%)	53 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	Bo	114/114 (100%)	114 (100%)	0	100	100
38	o	113/114 (99%)	113 (100%)	0	100	100
39	Bp	157/157 (100%)	156 (99%)	1 (1%)	86	92
39	p	157/157 (100%)	156 (99%)	1 (1%)	86	92
40	Br	416/416 (100%)	416 (100%)	0	100	100
40	r	416/416 (100%)	416 (100%)	0	100	100
41	Bs	278/278 (100%)	278 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	Bu	153/153 (100%)	153 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	Bv	89/111 (80%)	89 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	Bw	249/288 (86%)	249 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	Bx	427/427 (100%)	389 (91%)	38 (9%)	9	30
45	x	427/427 (100%)	389 (91%)	38 (9%)	9	30
46	By	211/211 (100%)	191 (90%)	20 (10%)	8	27
46	y	211/211 (100%)	191 (90%)	20 (10%)	8	27
47	Bz	226/226 (100%)	199 (88%)	27 (12%)	5	20
47	z	226/226 (100%)	199 (88%)	27 (12%)	5	20
48	0	128/128 (100%)	120 (94%)	8 (6%)	18	43
48	B0	128/128 (100%)	120 (94%)	8 (6%)	18	43
49	1	95/95 (100%)	89 (94%)	6 (6%)	18	43
49	B1	95/95 (100%)	89 (94%)	6 (6%)	18	43
50	2	81/81 (100%)	76 (94%)	5 (6%)	18	43
50	B2	81/81 (100%)	76 (94%)	5 (6%)	18	43
51	3	68/68 (100%)	50 (74%)	18 (26%)	0	3
51	B3	68/68 (100%)	50 (74%)	18 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	17
52	B4	67/67 (100%)	58 (87%)	9 (13%)	4	17
53	5	58/58 (100%)	53 (91%)	5 (9%)	10	32
53	B5	58/58 (100%)	53 (91%)	5 (9%)	10	32
54	6	47/47 (100%)	40 (85%)	7 (15%)	3	15
54	B6	47/47 (100%)	40 (85%)	7 (15%)	3	15
55	7	39/39 (100%)	37 (95%)	2 (5%)	24	48
55	B7	39/39 (100%)	37 (95%)	2 (5%)	24	48
56	8	40/40 (100%)	38 (95%)	2 (5%)	24	49
56	B8	40/40 (100%)	38 (95%)	2 (5%)	24	49
57	9	37/37 (100%)	34 (92%)	3 (8%)	11	35
57	B9	37/37 (100%)	34 (92%)	3 (8%)	11	35
58	AA	74/74 (100%)	68 (92%)	6 (8%)	11	35
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100
60	AC	166/166 (100%)	166 (100%)	0	100	100
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	52 (100%)	0	100	100
62	AE	61/71 (86%)	59 (97%)	2 (3%)	38	61
62	AR	61/71 (86%)	59 (97%)	2 (3%)	38	61
63	AF	95/95 (100%)	84 (88%)	11 (12%)	5	21
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	25	51
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	88	93
66	AJ	330/330 (100%)	327 (99%)	3 (1%)	78	87
66	AV	330/330 (100%)	322 (98%)	8 (2%)	49	69
67	AK	334/335 (100%)	331 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	AW	335/335 (100%)	332 (99%)	3 (1%)	78	87
68	AL	365/367 (100%)	365 (100%)	0	100	100
68	AY	362/367 (99%)	355 (98%)	7 (2%)	57	75
All	All	20773/21008 (99%)	20313 (98%)	460 (2%)	54	71

5 of 460 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	AR	78	ARG
53	B5	26	MET
34	Bk	3	LEU
52	B4	57	ARG
48	B0	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 413 such sidechains are listed below:

Mol	Chain	Res	Type
68	AY	87	ASN
16	BQ	147	ASN
50	B2	66	ASN
1	BA	116	ASN
8	BI	73	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 100 ligands modelled in this entry, 10 are monoatomic - leaving 90 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
76	PEE	AY	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
72	8Q1	Bp	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.56	5 (12%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
76	PEE	Bl	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
71	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
69	SF4	M	802	12	0,12,12	-	-	-		
69	SF4	BB	302	2	0,12,12	-	-	-		
72	8Q1	BE	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.38	7 (17%)
79	HEA	x	603	45	57,67,67	1.23	6 (10%)	61,103,103	1.47	11 (18%)
75	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.95	3 (4%)
71	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
71	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
76	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
69	SF4	BB	301	2	0,12,12	-	-	-		
76	PEE	AH	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
76	PEE	BW	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.97	2 (3%)
75	CDL	AA	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
73	NDP	BJ	401	-	45,52,52	0.95	2 (4%)	53,80,80	1.32	4 (7%)
81	HEC	AH	402	65	32,50,50	2.23	3 (9%)	24,82,82	1.35	1 (4%)
81	HEC	AU	402	65	32,50,50	2.28	3 (9%)	24,82,82	1.39	2 (8%)
69	SF4	C	301	3	0,12,12	-	-	-		
76	PEE	BV	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
75	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
71	PLX	AN	101	-	51,51,51	0.78	1 (1%)	55,59,59	0.60	1 (1%)
75	CDL	AH	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)
69	SF4	B	301	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	PLX	AQ	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
76	PEE	AU	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
70	FMN	A	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
71	PLX	AT	101	-	51,51,51	0.75	1 (1%)	55,59,59	0.60	1 (1%)
69	SF4	B	302	2	0,12,12	-	-	-	-	-
75	CDL	AN	102	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
79	HEA	Bx	603	45	57,67,67	1.23	6 (10%)	61,103,103	1.47	10 (16%)
71	PLX	g	201	-	51,51,51	0.81	1 (1%)	55,59,59	0.69	1 (1%)
74	FES	AC	301	60	0,4,4	-	-	-	-	-
71	PLX	Bb	201	-	51,51,51	0.57	0	55,59,59	0.63	0
76	PEE	Bl	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
75	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.08	4 (5%)
76	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
69	SF4	BA	501	1	0,12,12	-	-	-	-	-
69	SF4	BC	301	3	0,12,12	-	-	-	-	-
70	FMN	BA	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
69	SF4	BM	802	12	0,12,12	-	-	-	-	-
75	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
72	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
71	PLX	Br	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
79	HEA	Bx	604	45	57,67,67	1.48	6 (10%)	61,103,103	1.47	12 (19%)
71	PLX	BV	203	-	51,51,51	0.77	1 (1%)	55,59,59	0.60	1 (1%)
71	PLX	Br	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.66	1 (1%)
82	HEM	AJ	401	66	41,50,50	1.92	6 (14%)	45,82,82	1.60	5 (11%)
71	PLX	BB	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
82	HEM	AV	401	66	41,50,50	1.97	5 (12%)	45,82,82	1.55	5 (11%)
76	PEE	AJ	403	-	48,48,50	1.32	4 (8%)	51,53,55	0.99	2 (3%)
76	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
69	SF4	A	501	1	0,12,12	-	-	-	-	-
76	PEE	AV	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
75	CDL	Bn	101	-	63,63,99	1.23	5 (7%)	69,75,111	1.07	4 (5%)
72	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.56	5 (12%)
76	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
75	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
74	FES	O	301	14	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	Bl	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
75	CDL	AL	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
71	PLX	AL	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
74	FES	M	803	-	0,4,4	-	-	-	-	-
71	PLX	Bg	202	-	51,51,51	0.74	1 (1%)	55,59,59	0.61	1 (1%)
75	CDL	AJ	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.03	4 (5%)
79	HEA	x	604	45	57,67,67	1.47	6 (10%)	61,103,103	1.47	12 (19%)
71	PLX	Bg	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	55,59,59	0.61	1 (1%)
74	FES	BO	301	14	0,4,4	-	-	-	-	-
76	PEE	AL	503	-	48,48,50	1.37	4 (8%)	51,53,55	0.92	2 (3%)
82	HEM	AJ	402	66	41,50,50	1.89	6 (14%)	45,82,82	1.57	9 (20%)
71	PLX	BU	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
69	SF4	M	801	12	0,12,12	-	-	-	-	-
73	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.31	4 (7%)
82	HEM	AV	402	66	41,50,50	1.90	6 (14%)	45,82,82	1.60	8 (17%)
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.16	6 (8%)
71	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
75	CDL	BV	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
75	CDL	Bl	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
75	CDL	Bi	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
71	PLX	Bg	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
75	CDL	AU	403	-	63,63,99	1.24	6 (9%)	69,75,111	1.04	4 (5%)
74	FES	BM	803	-	0,4,4	-	-	-	-	-
74	FES	AP	301	60	0,4,4	-	-	-	-	-
69	SF4	BM	801	12	0,12,12	-	-	-	-	-
75	CDL	AY	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)

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
76	PEE	AY	502	-	-	20/52/52/54	-
72	8Q1	Bp	201	-	-	19/41/41/41	-
71	PLX	r	501	-	-	28/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	PEE	B1	702	-	-	27/54/54/54	-
71	PLX	U	101	-	-	22/55/55/55	-
69	SF4	M	802	12	-	-	0/6/5/5
69	SF4	BB	302	2	-	-	0/6/5/5
72	8Q1	BE	201	-	-	18/41/41/41	-
79	HEA	x	603	45	3/3/7/16	7/32/76/76	-
75	CDL	V	201	-	-	41/69/69/110	-
71	PLX	g	203	-	-	24/55/55/55	-
71	PLX	B	303	-	-	21/55/55/55	-
76	PEE	V	202	-	-	27/54/54/54	-
69	SF4	BB	301	2	-	-	0/6/5/5
76	PEE	AH	401	-	-	27/52/52/54	-
76	PEE	BW	201	-	-	31/54/54/54	-
75	CDL	AA	101	-	-	35/74/74/110	-
71	PLX	b	201	-	-	27/55/55/55	-
73	NDP	BJ	401	-	-	15/30/77/77	0/5/5/5
81	HEC	AH	402	65	-	2/10/54/54	-
81	HEC	AU	402	65	-	0/10/54/54	-
69	SF4	C	301	3	-	-	0/6/5/5
76	PEE	BV	202	-	-	27/54/54/54	-
75	CDL	n	101	-	-	33/74/74/110	-
71	PLX	AN	101	-	-	26/55/55/55	-
75	CDL	AH	403	-	-	42/74/74/110	-
69	SF4	B	301	2	-	-	0/6/5/5
71	PLX	AQ	101	-	-	25/55/55/55	-
76	PEE	AU	401	-	-	17/44/44/54	-
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
75	CDL	AJ	405	-	-	28/74/74/110	-
71	PLX	AT	101	-	-	23/55/55/55	-
69	SF4	B	302	2	-	-	0/6/5/5
75	CDL	AN	102	-	-	40/74/74/110	-
79	HEA	Bx	603	45	3/3/7/16	7/32/76/76	-
71	PLX	g	201	-	-	25/55/55/55	-
71	PLX	Bb	201	-	-	27/55/55/55	-
74	FES	AC	301	60	-	-	0/1/1/1
76	PEE	B1	701	-	-	32/52/52/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	l	703	-	-	38/74/74/110	-
76	PEE	W	201	-	-	32/54/54/54	-
69	SF4	BA	501	1	-	-	0/6/5/5
69	SF4	BC	301	3	-	-	0/6/5/5
70	FMN	BA	502	-	-	7/18/18/18	0/3/3/3
69	SF4	BM	802	12	-	-	0/6/5/5
75	CDL	l	704	-	-	44/74/74/110	-
72	8Q1	E	201	-	-	18/41/41/41	-
71	PLX	Br	502	-	-	36/55/55/55	-
79	HEA	Bx	604	45	3/3/7/16	5/32/76/76	-
71	PLX	BV	203	-	-	26/55/55/55	-
71	PLX	Br	501	-	-	28/55/55/55	-
82	HEM	AJ	401	66	-	1/12/54/54	-
71	PLX	BB	303	-	-	21/55/55/55	-
82	HEM	AV	401	66	-	3/12/54/54	-
76	PEE	AJ	403	-	-	20/52/52/54	-
76	PEE	l	702	-	-	27/54/54/54	-
69	SF4	A	501	1	-	-	0/6/5/5
76	PEE	AV	403	-	-	30/52/52/54	-
75	CDL	Bn	101	-	-	33/74/74/110	-
72	8Q1	p	201	-	-	20/41/41/41	-
76	PEE	l	701	-	-	32/52/52/54	-
75	CDL	i	401	-	-	39/74/74/110	-
74	FES	O	301	14	-	-	0/1/1/1
75	CDL	Bl	704	-	-	44/74/74/110	-
75	CDL	AL	502	-	-	43/74/74/110	-
71	PLX	AL	501	-	-	23/55/55/55	-
74	FES	M	803	-	-	-	0/1/1/1
71	PLX	Bg	202	-	-	25/55/55/55	-
75	CDL	AJ	404	-	-	33/74/74/110	-
79	HEA	x	604	45	3/3/7/16	5/32/76/76	-
71	PLX	Bg	203	-	-	24/55/55/55	-
71	PLX	g	202	-	-	25/55/55/55	-
74	FES	BO	301	14	-	-	0/1/1/1
76	PEE	AL	503	-	-	22/52/52/54	-
82	HEM	AJ	402	66	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	BU	101	-	-	22/55/55/55	-
69	SF4	M	801	12	-	-	0/6/5/5
73	NDP	J	401	-	-	15/30/77/77	0/5/5/5
82	HEM	AV	402	66	-	4/12/54/54	-
75	CDL	AG	101	-	-	38/74/74/110	-
71	PLX	r	502	-	-	36/55/55/55	-
75	CDL	BV	201	-	-	42/69/69/110	-
75	CDL	Bl	703	-	-	38/74/74/110	-
75	CDL	Bi	401	-	-	39/74/74/110	-
71	PLX	Bg	201	-	-	25/55/55/55	-
75	CDL	AU	403	-	-	48/74/74/110	-
74	FES	BM	803	-	-	-	0/1/1/1
74	FES	AP	301	60	-	-	0/1/1/1
69	SF4	BM	801	12	-	-	0/6/5/5
75	CDL	AY	501	-	-	36/74/74/110	-

The worst 5 of 270 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AV	402	HEM	C3D-C2D	7.86	1.53	1.36
82	AJ	401	HEM	C3D-C2D	7.86	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.81	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.73	1.53	1.36
81	AU	402	HEC	C3C-C2C	-6.99	1.33	1.40

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	AV	402	HEM	C4D-ND-C1D	6.19	111.46	105.07
82	AJ	401	HEM	C4D-ND-C1D	6.16	111.43	105.07
82	AJ	402	HEM	C4D-ND-C1D	6.05	111.32	105.07
72	p	201	8Q1	C6-C1-S44	6.01	120.45	113.46
72	Bp	201	8Q1	C6-C1-S44	6.00	120.44	113.46

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
79	x	603	HEA	NB
79	x	603	HEA	NA

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Mol	Chain	Res	Type	Atom
79	x	603	HEA	ND
79	x	604	HEA	NB
79	x	604	HEA	NA

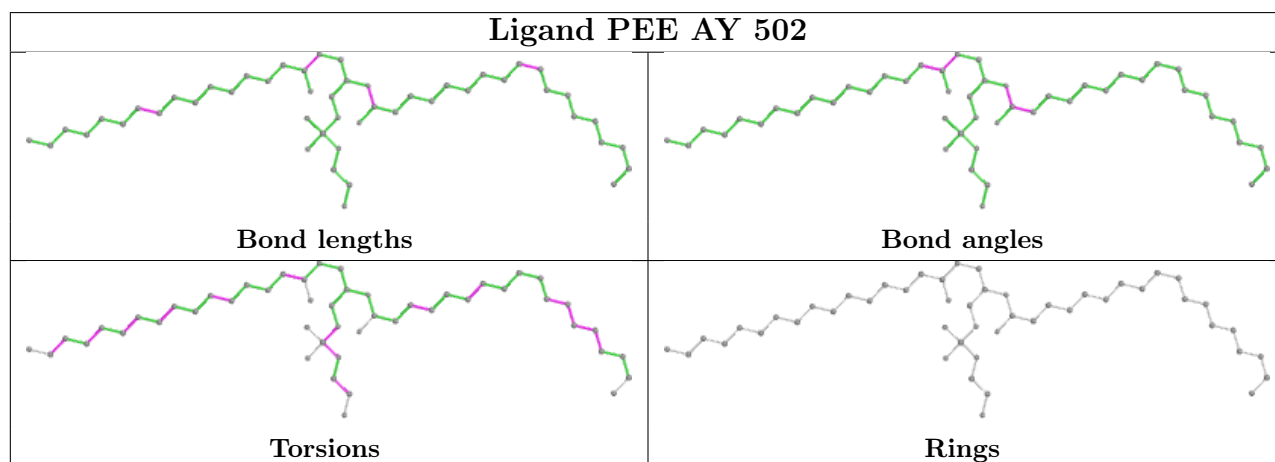
5 of 1799 torsion outliers are listed below:

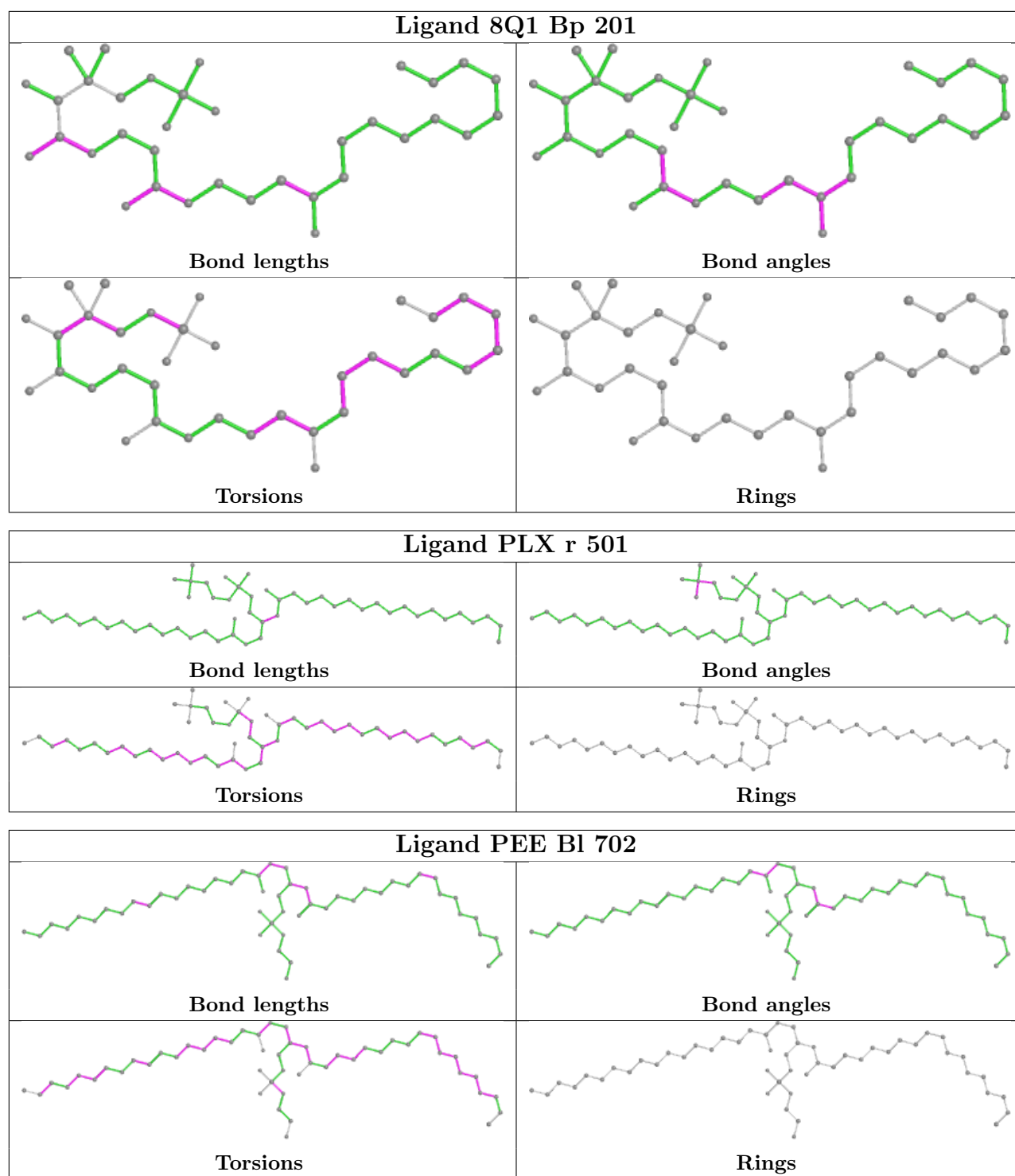
Mol	Chain	Res	Type	Atoms
70	A	502	FMN	C1'-C2'-C3'-O3'
70	A	502	FMN	C1'-C2'-C3'-C4'
70	A	502	FMN	C3'-C4'-C5'-O5'
70	A	502	FMN	O4'-C4'-C5'-O5'
70	BA	502	FMN	C1'-C2'-C3'-O3'

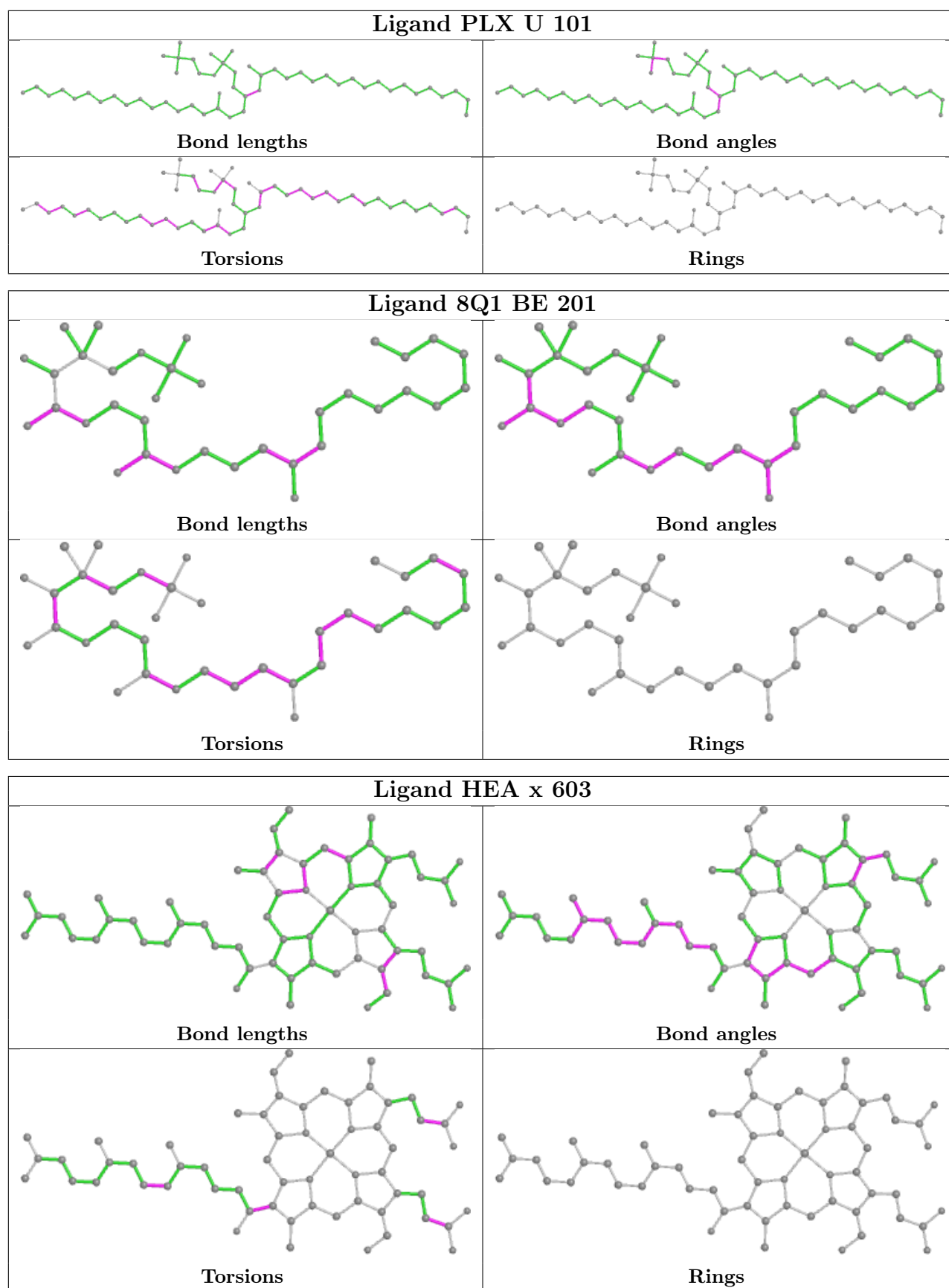
There are no ring outliers.

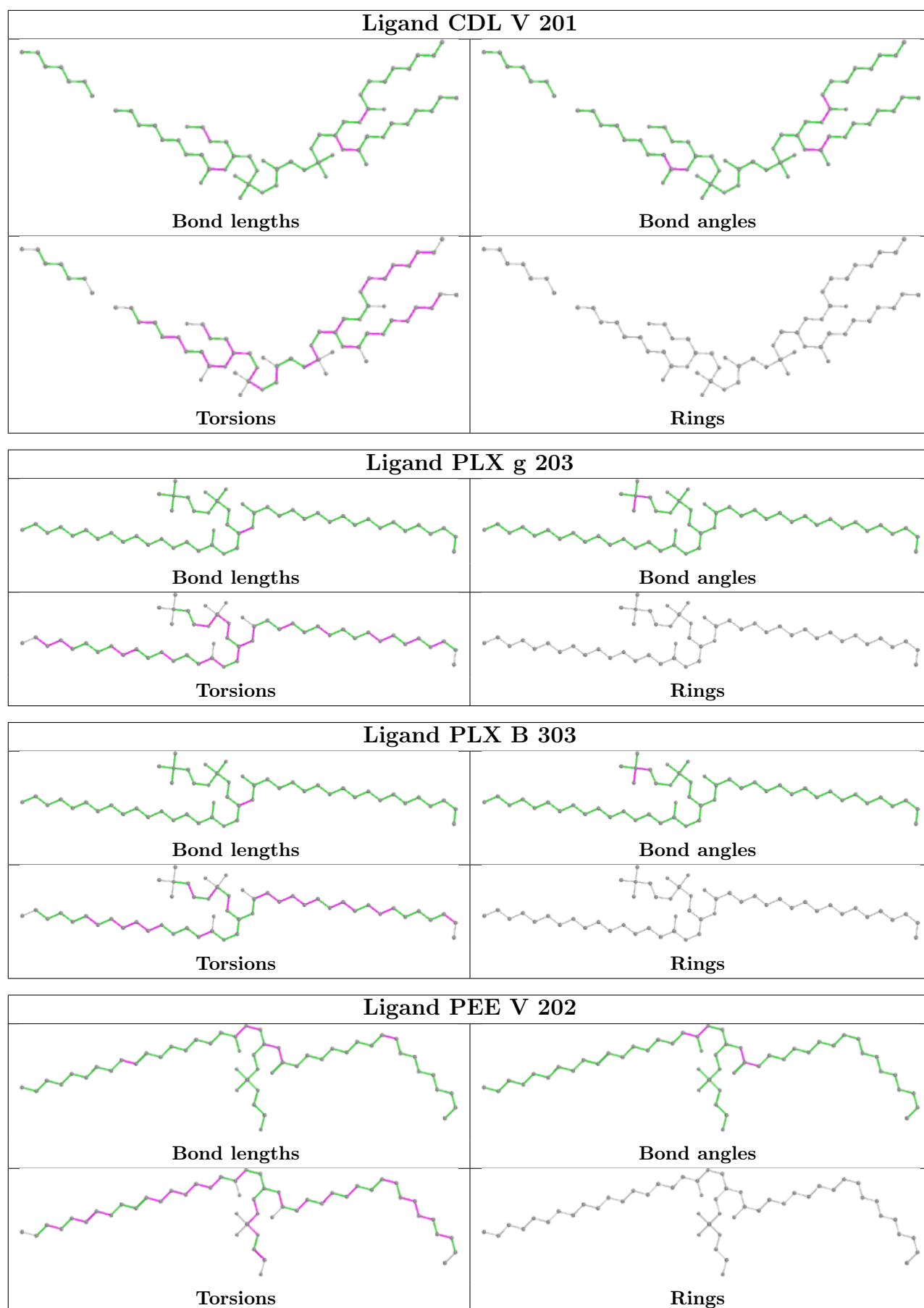
No monomer is involved in short contacts.

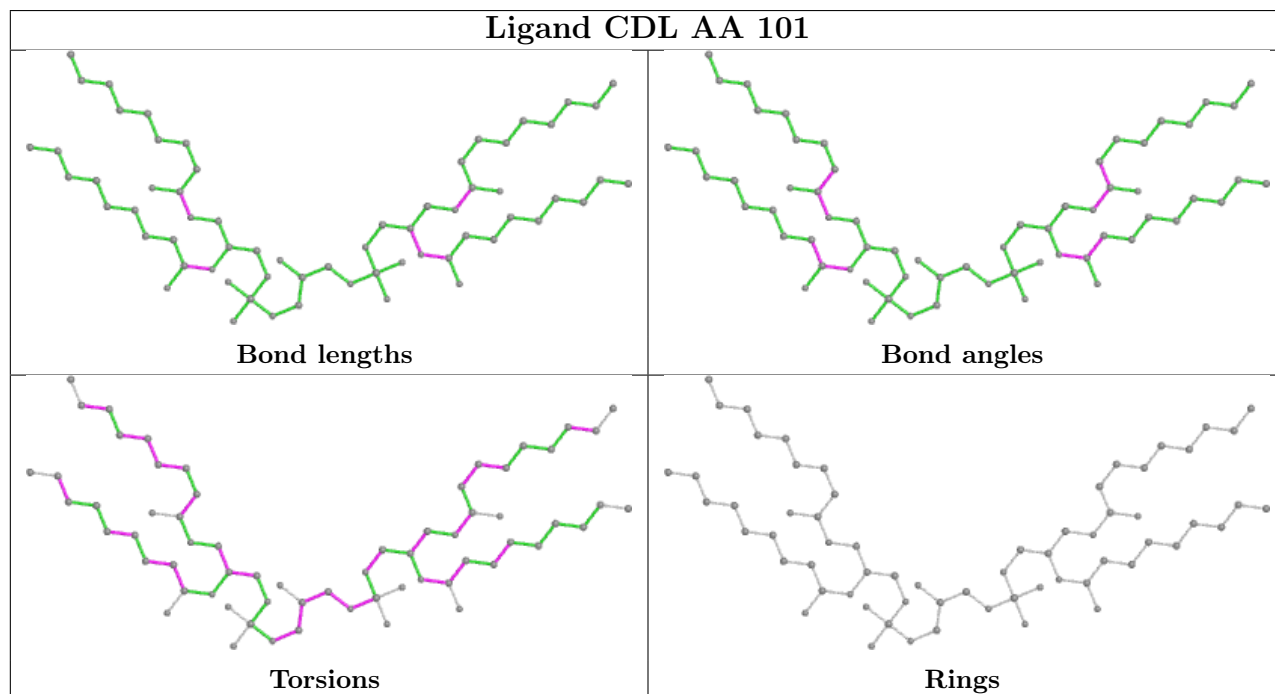
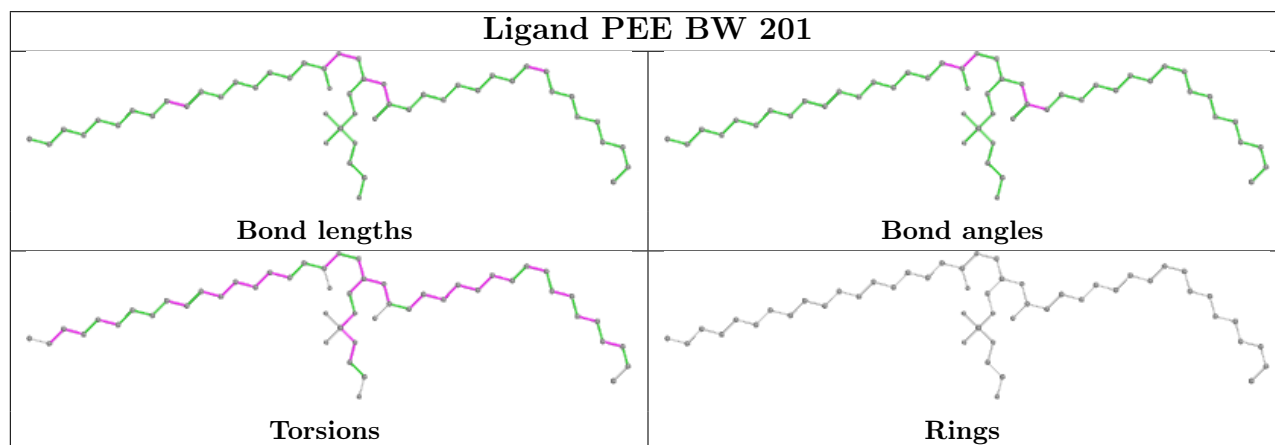
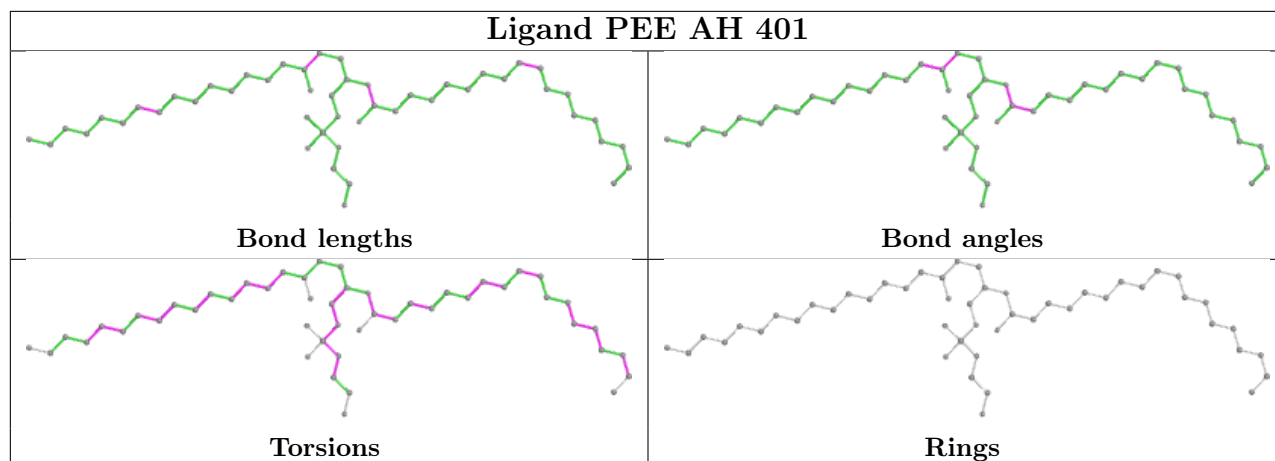
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

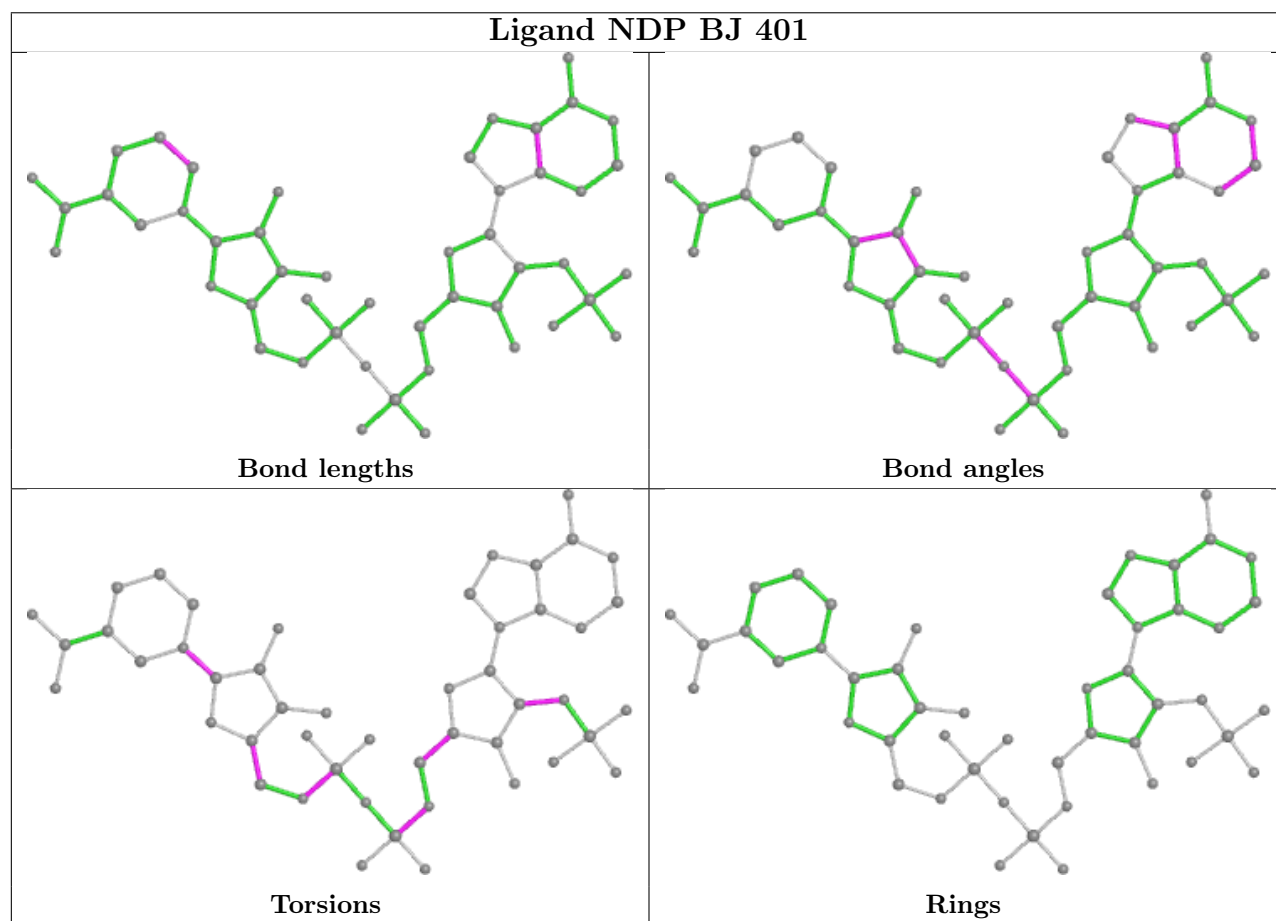
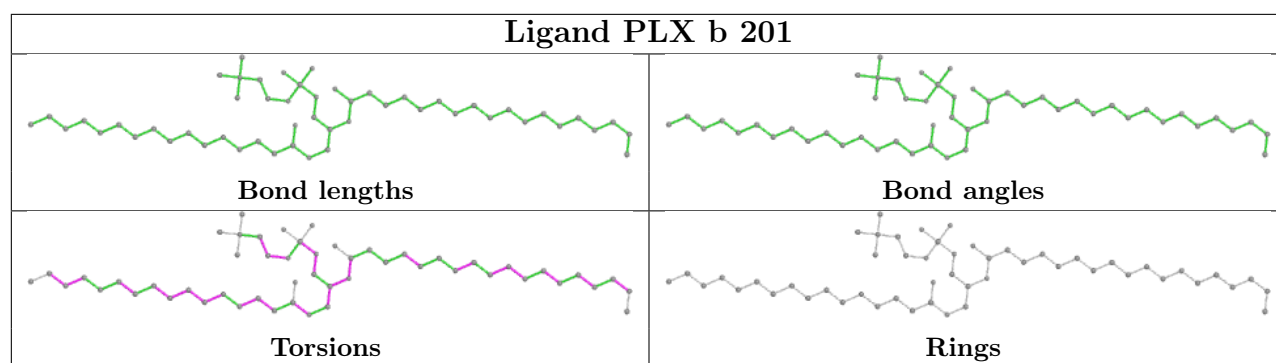


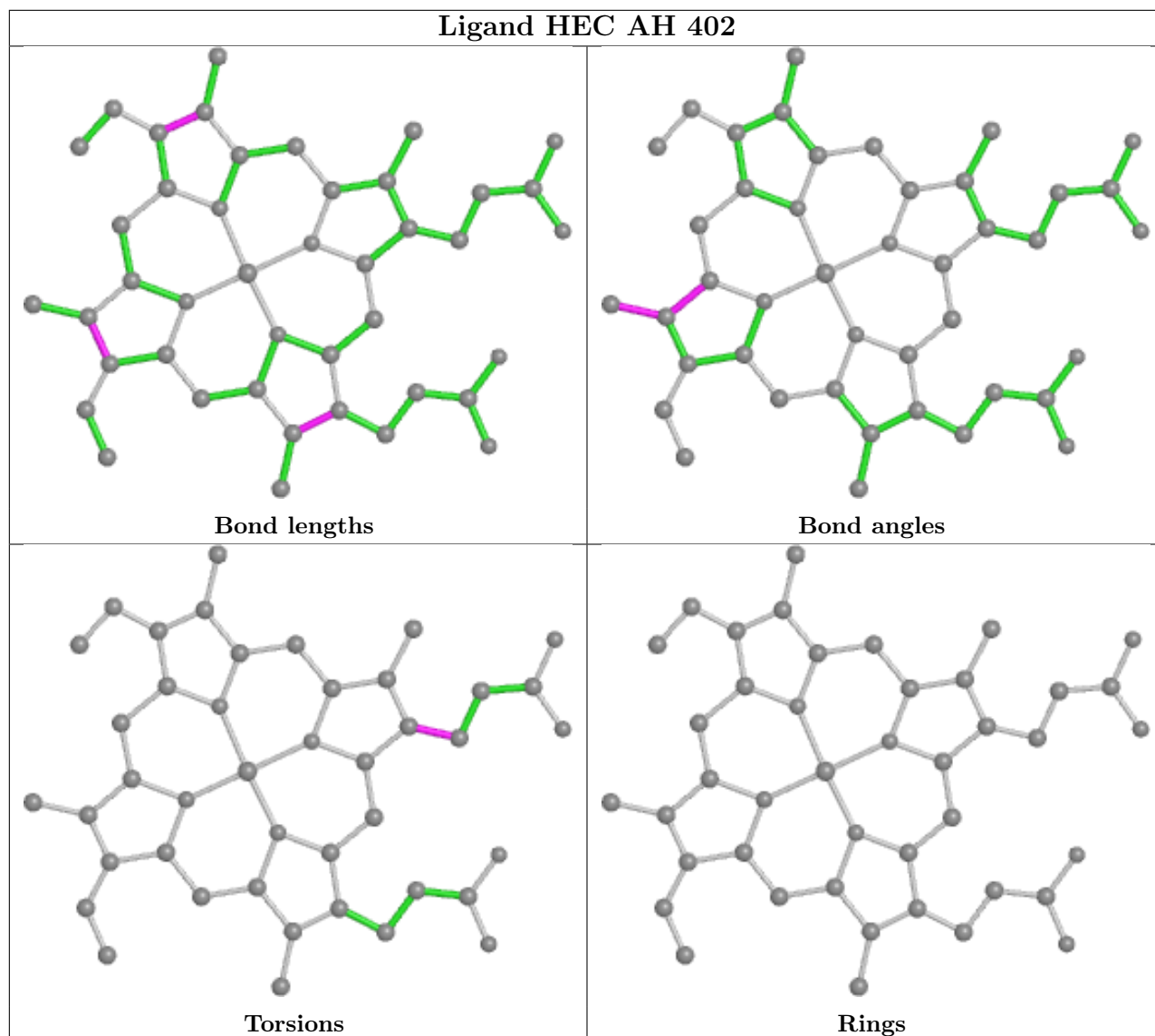


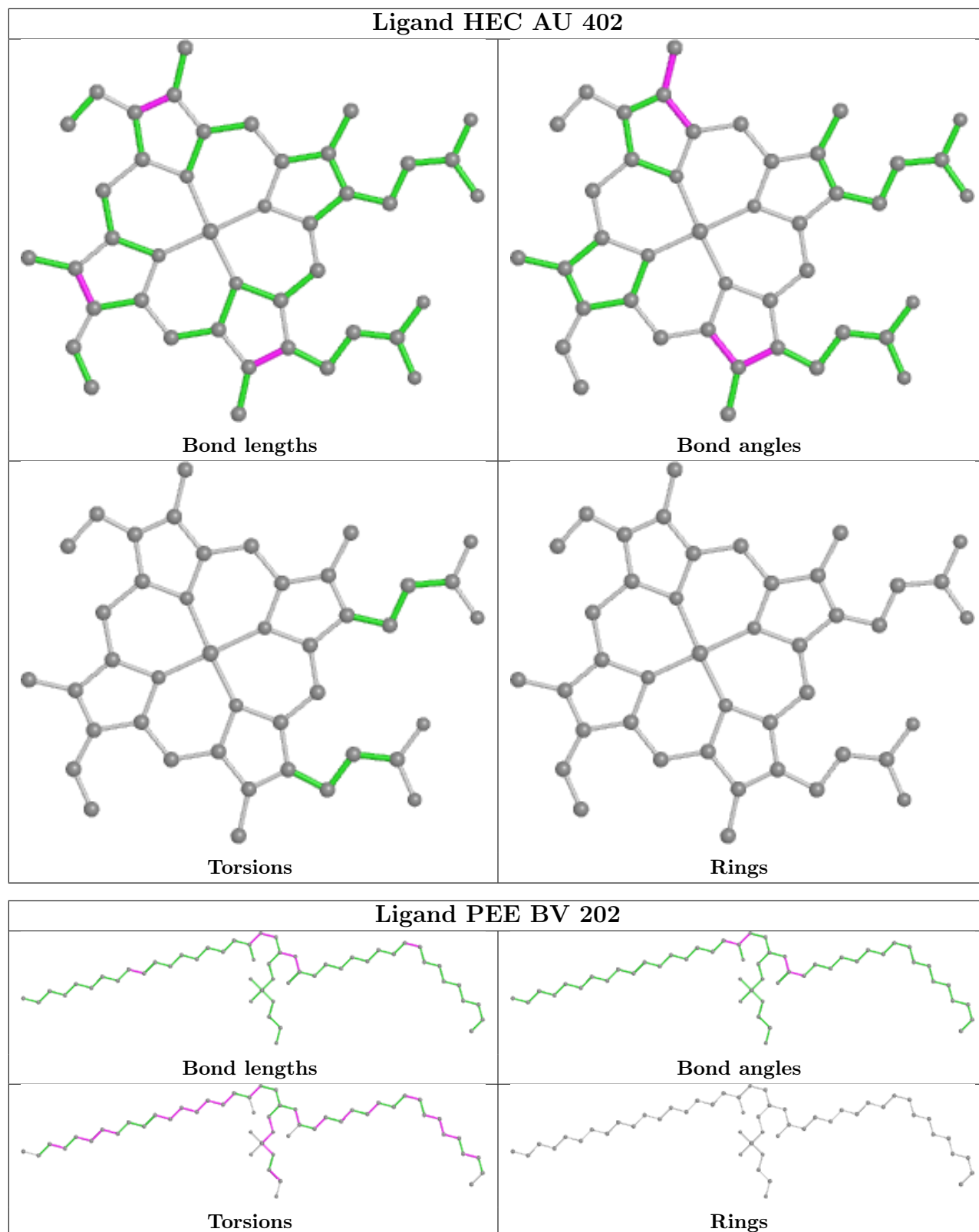


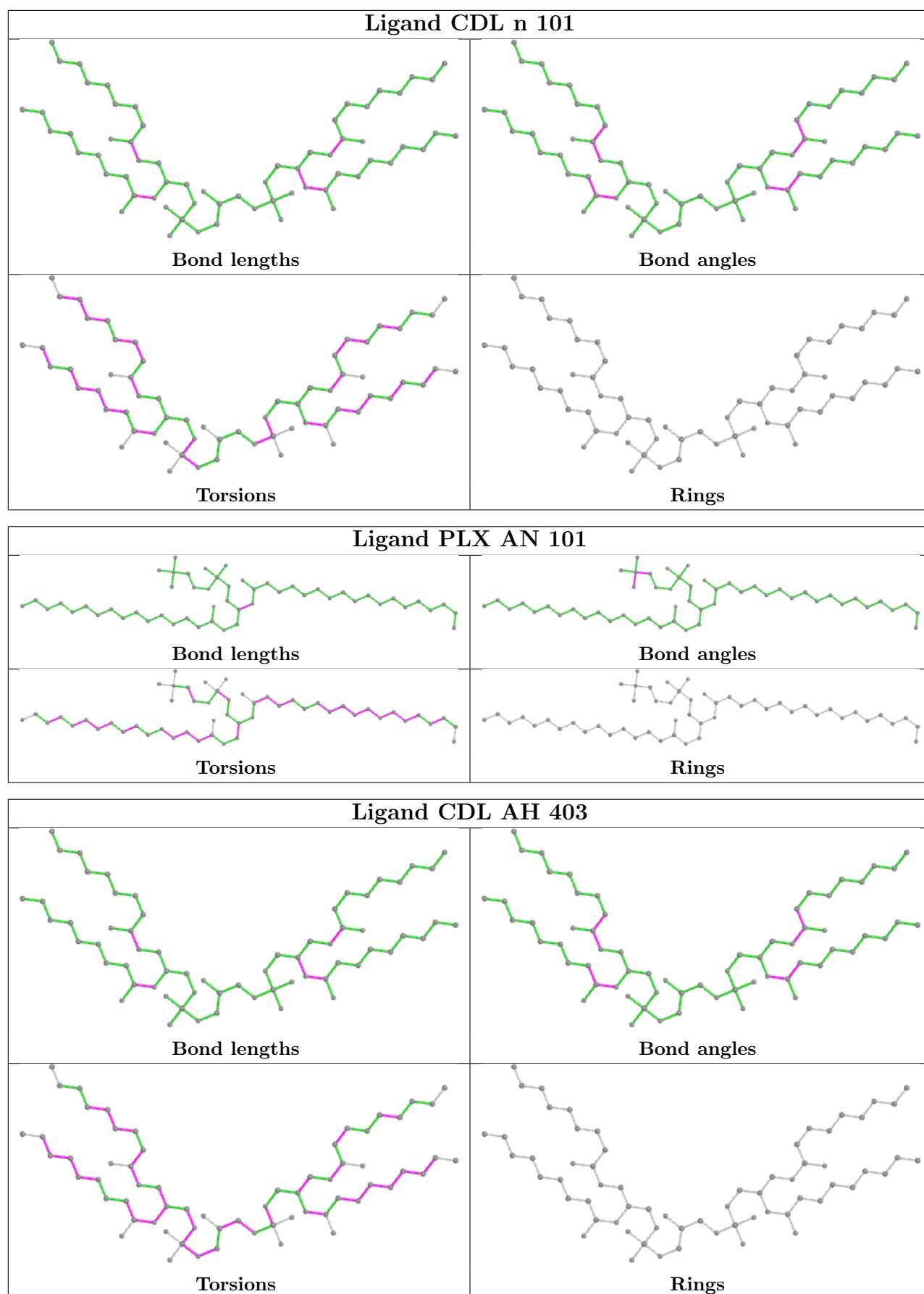


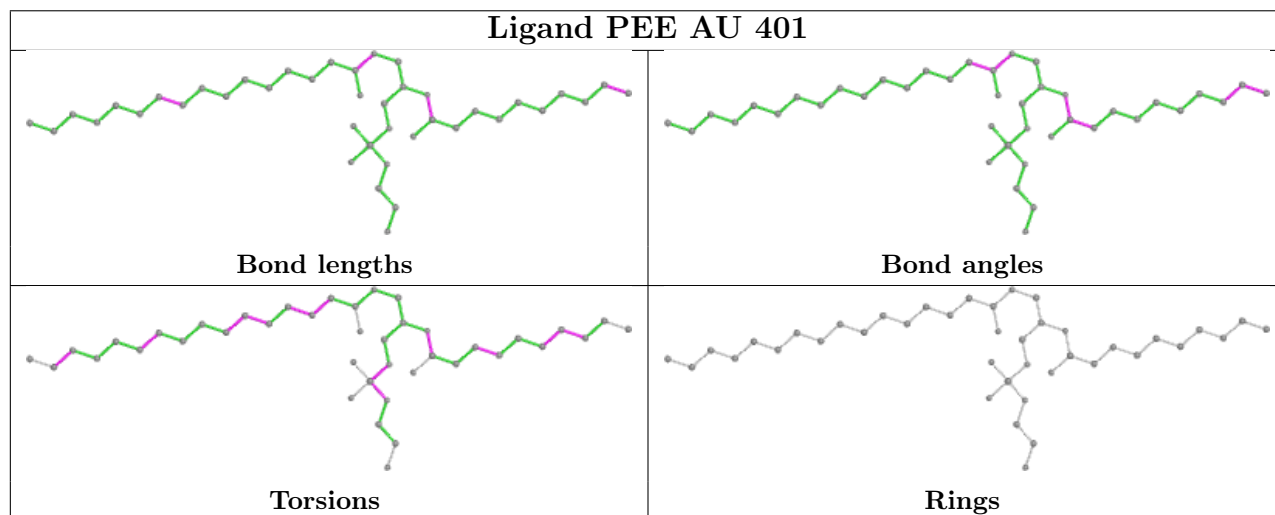
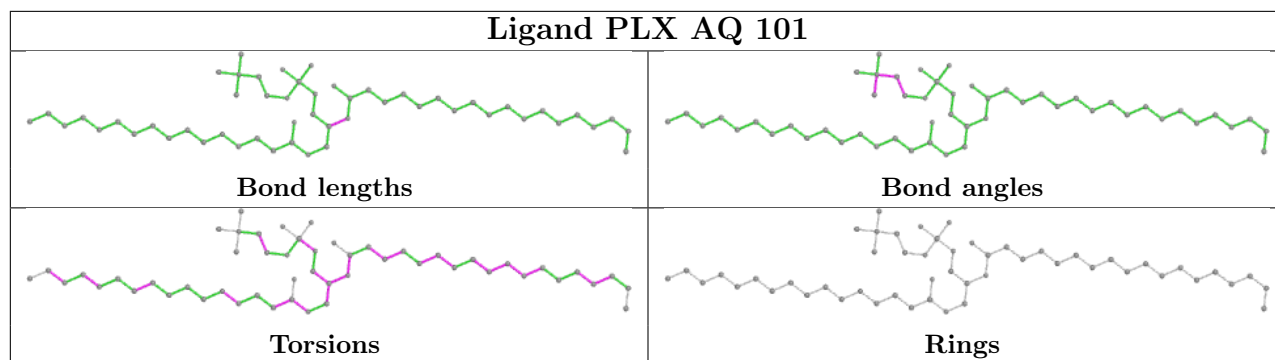


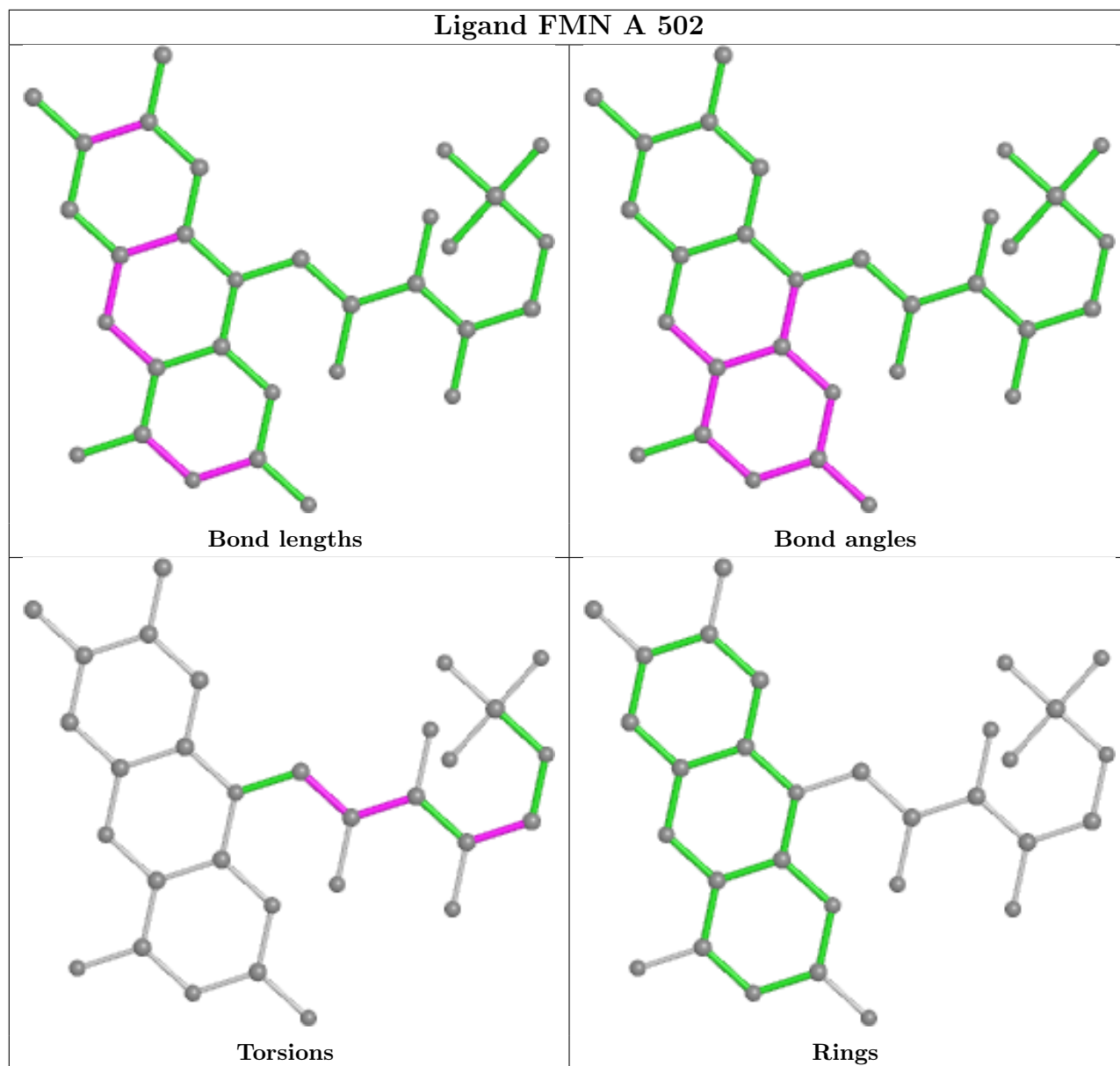


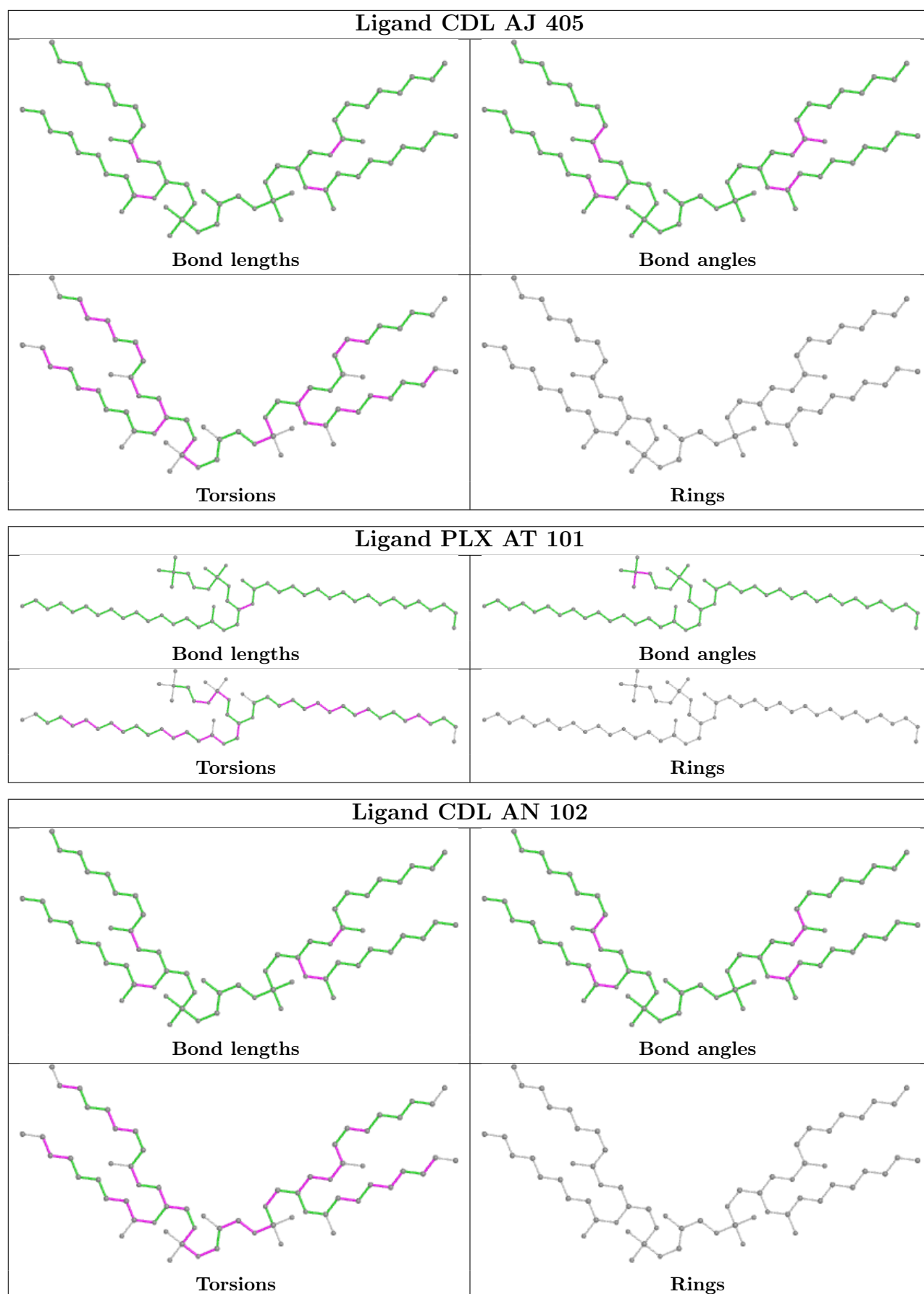


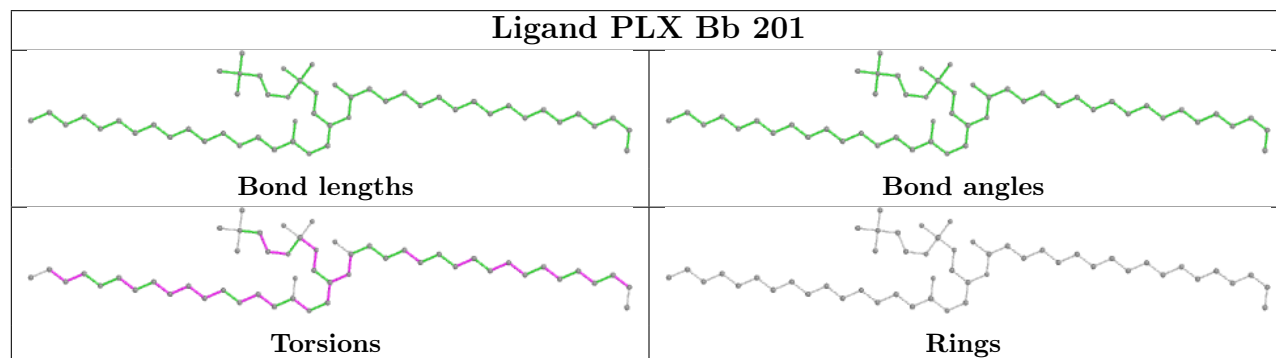
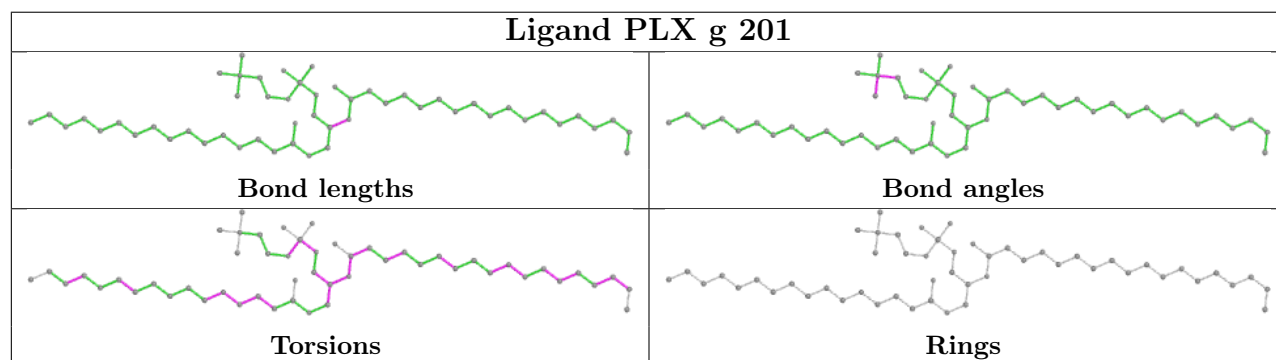
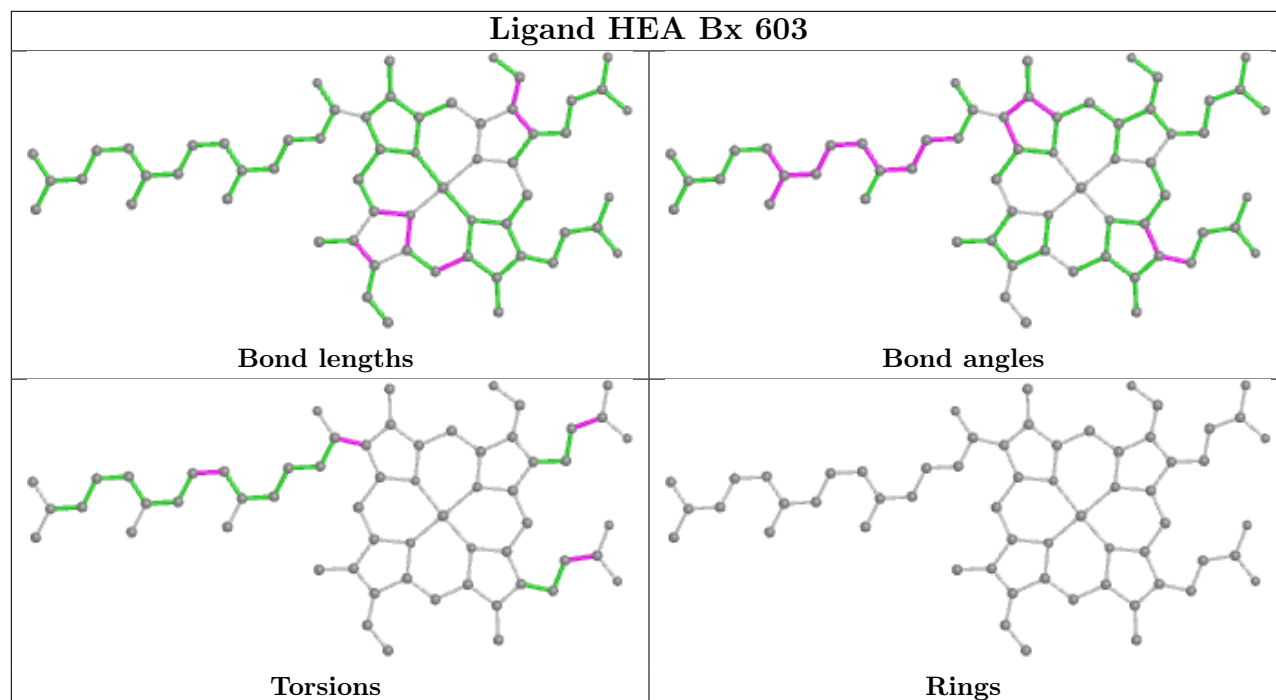


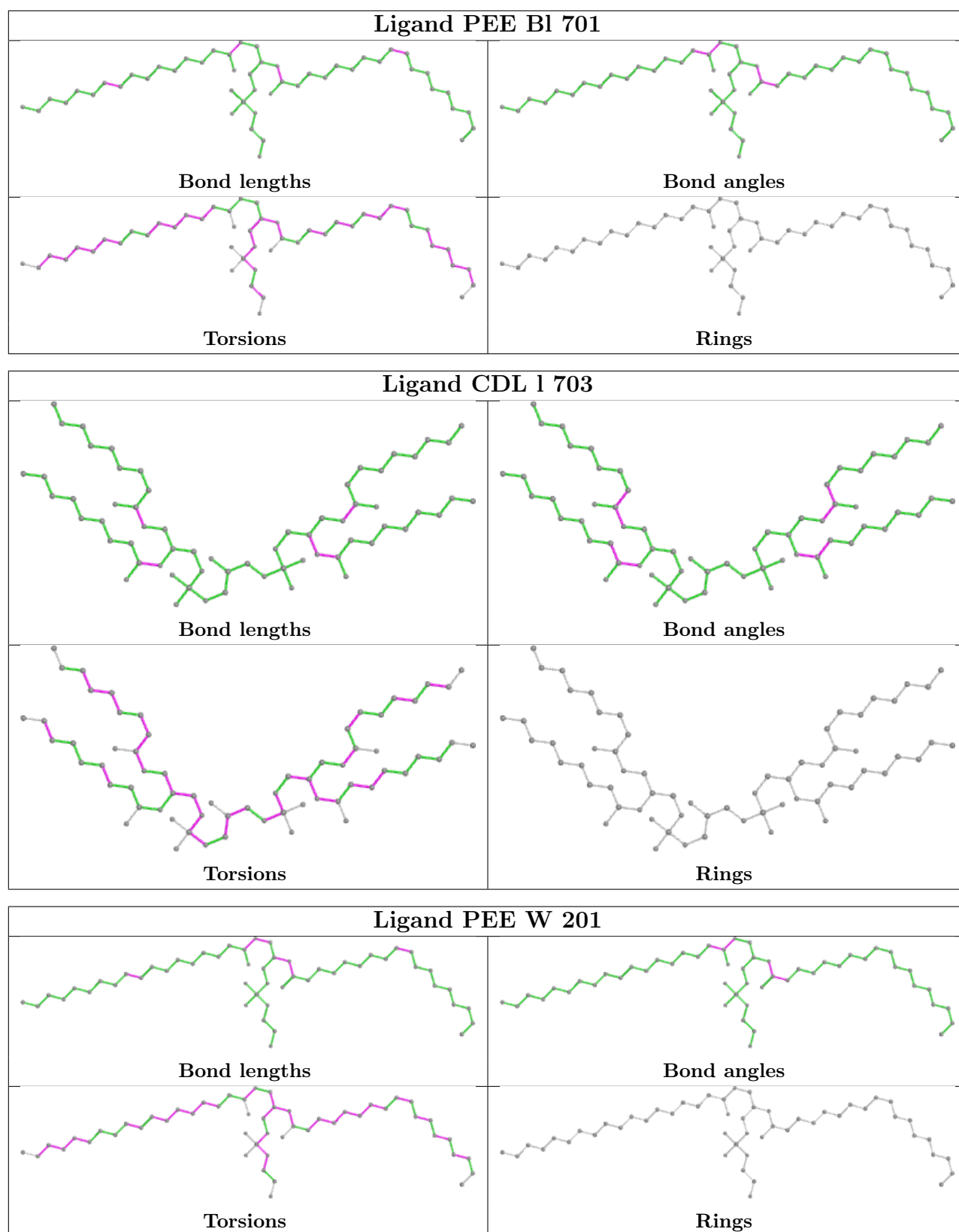


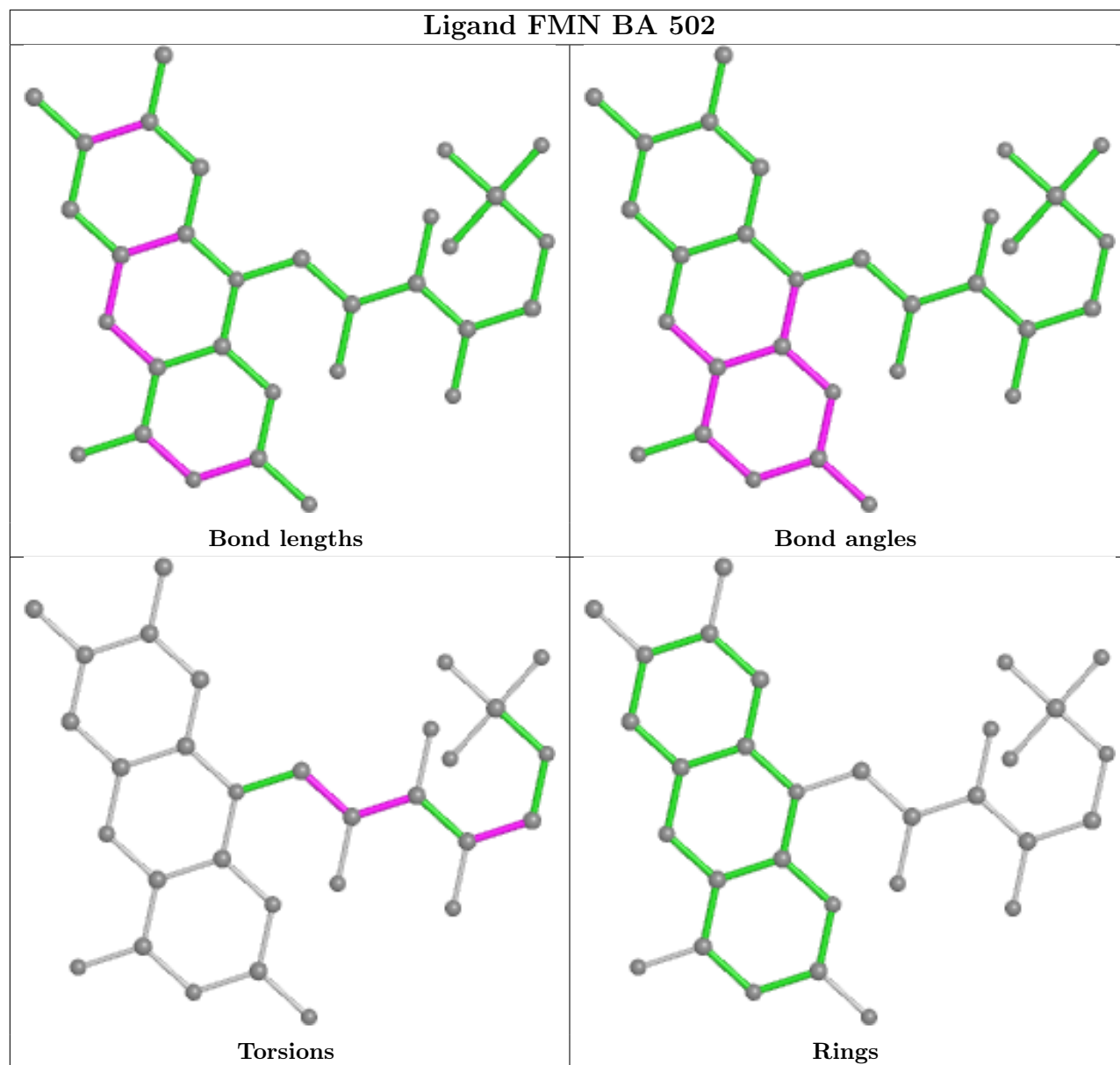


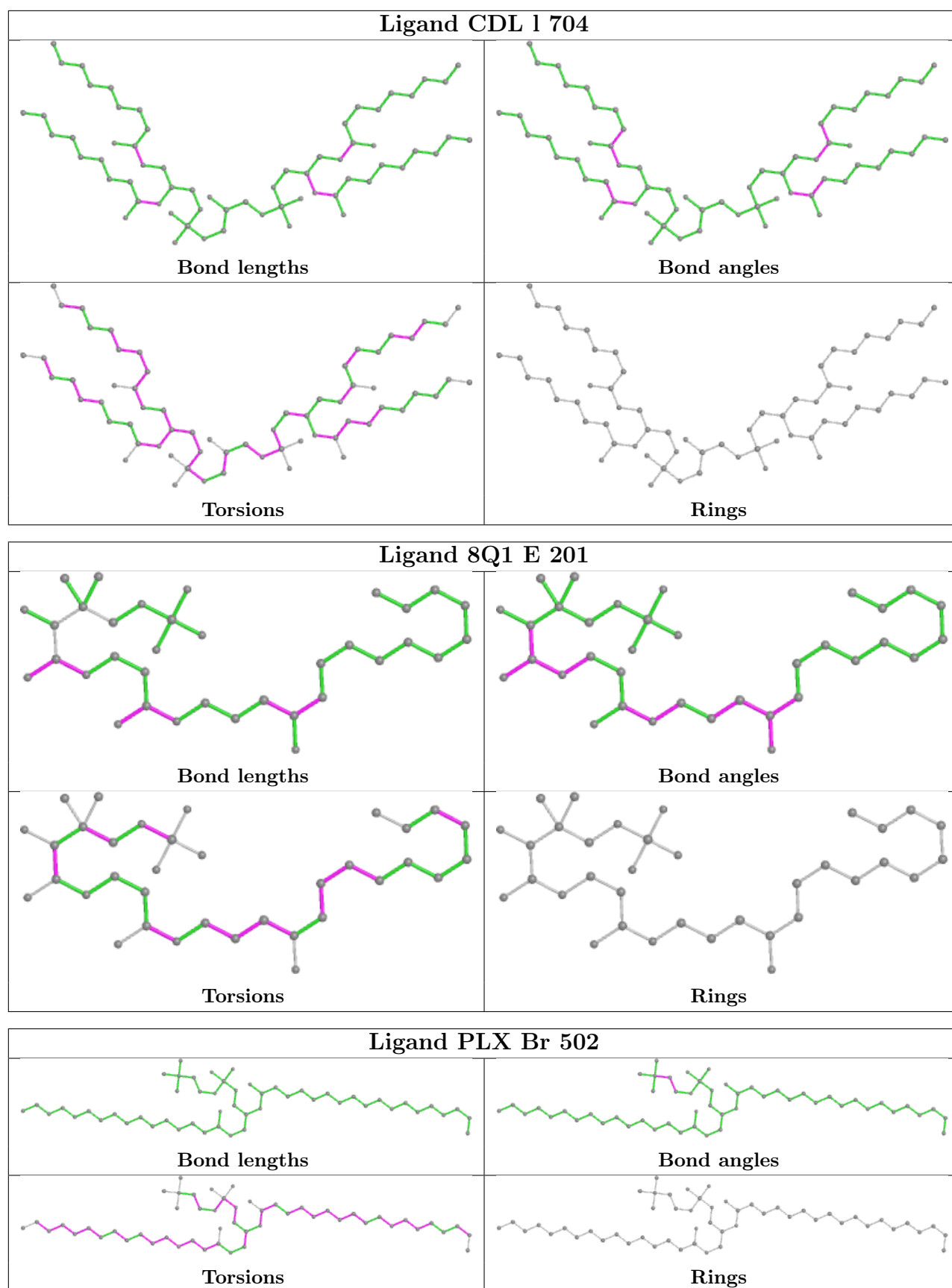


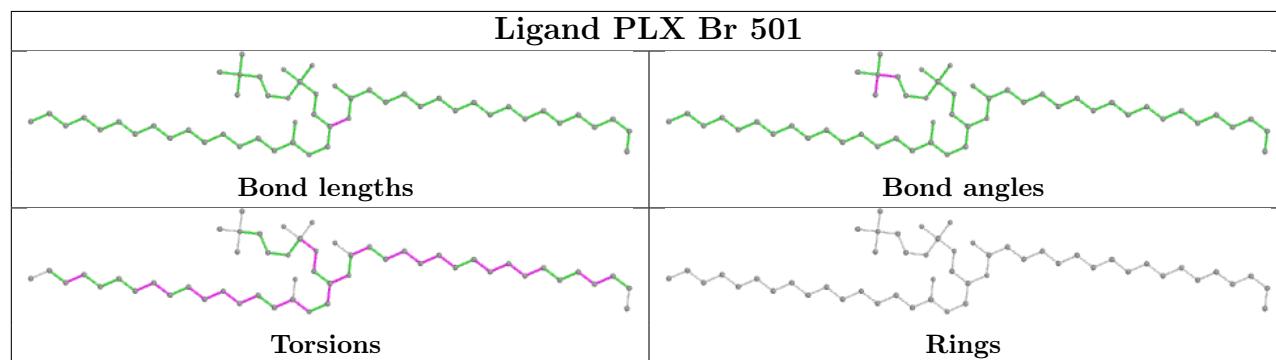
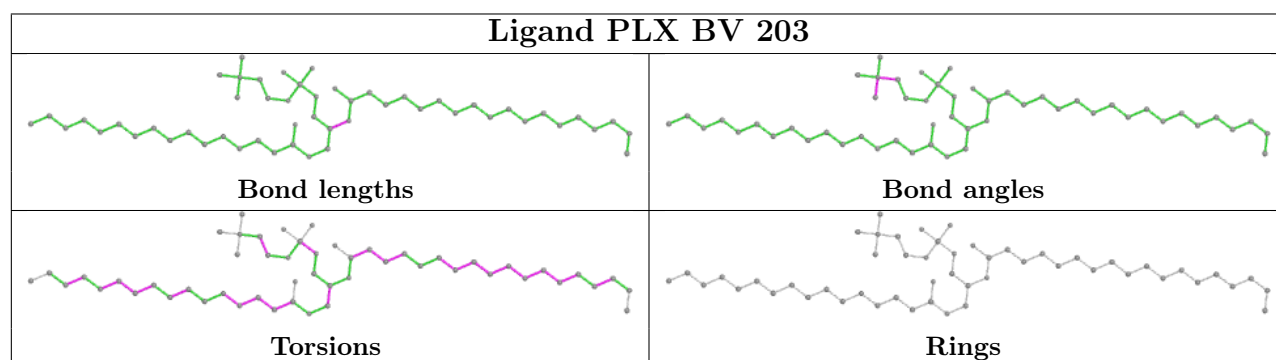
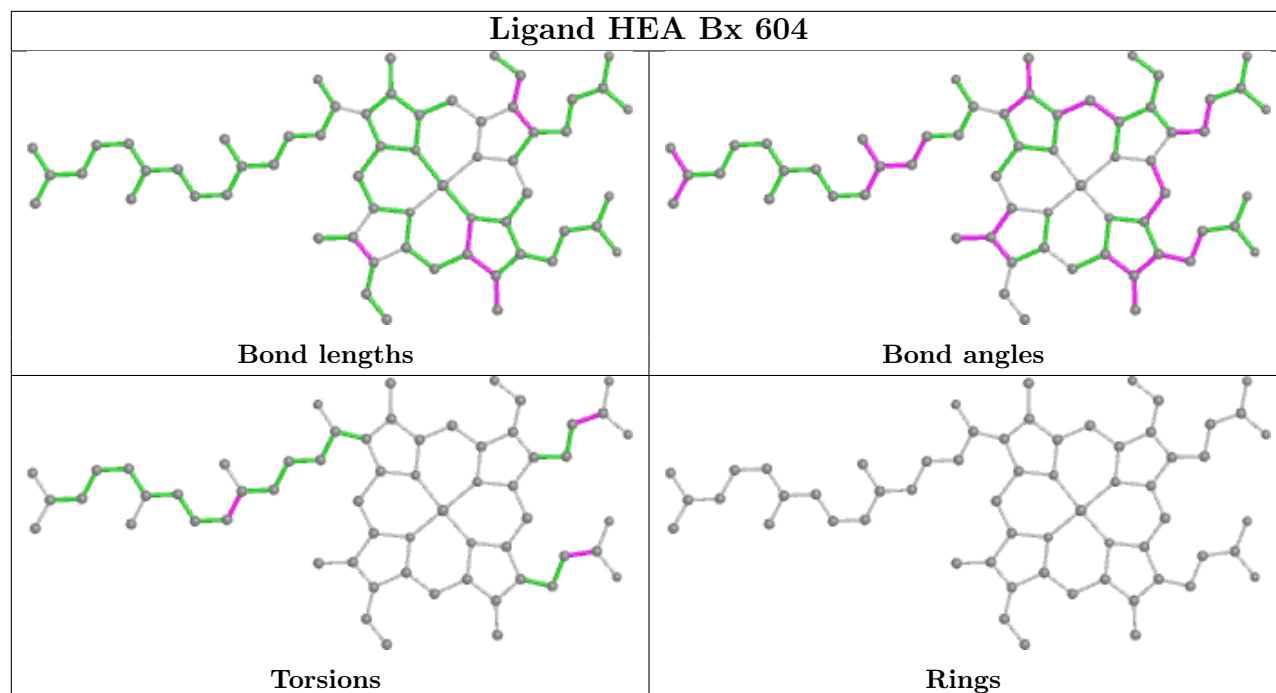


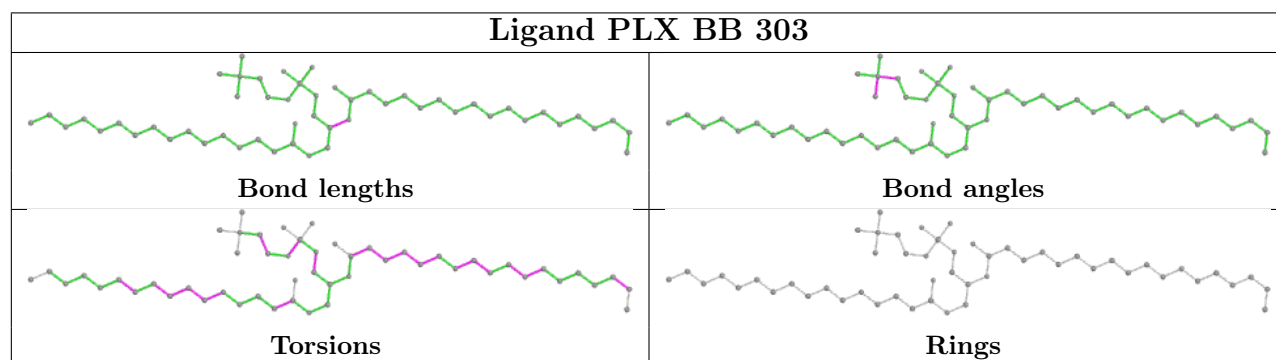
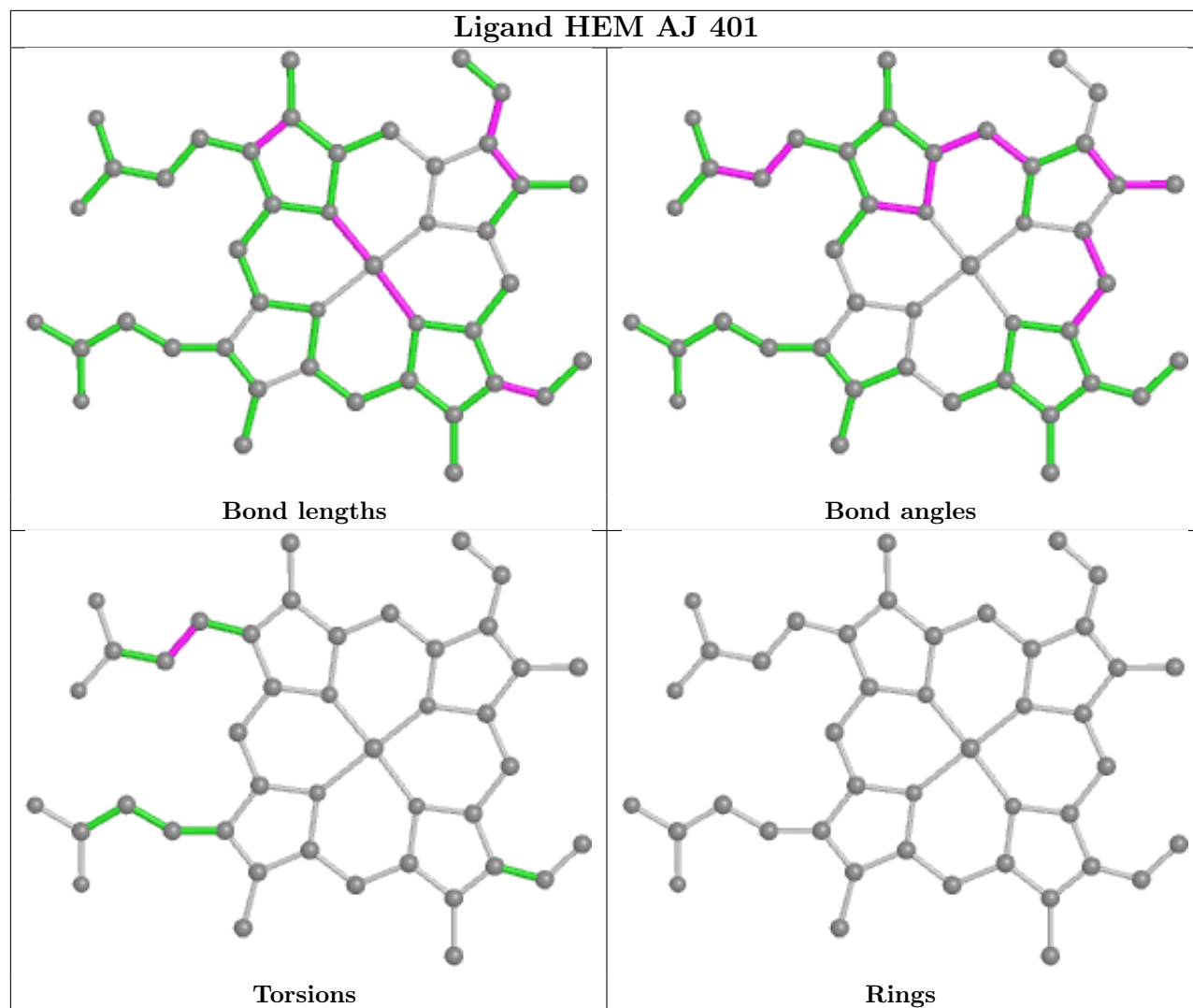


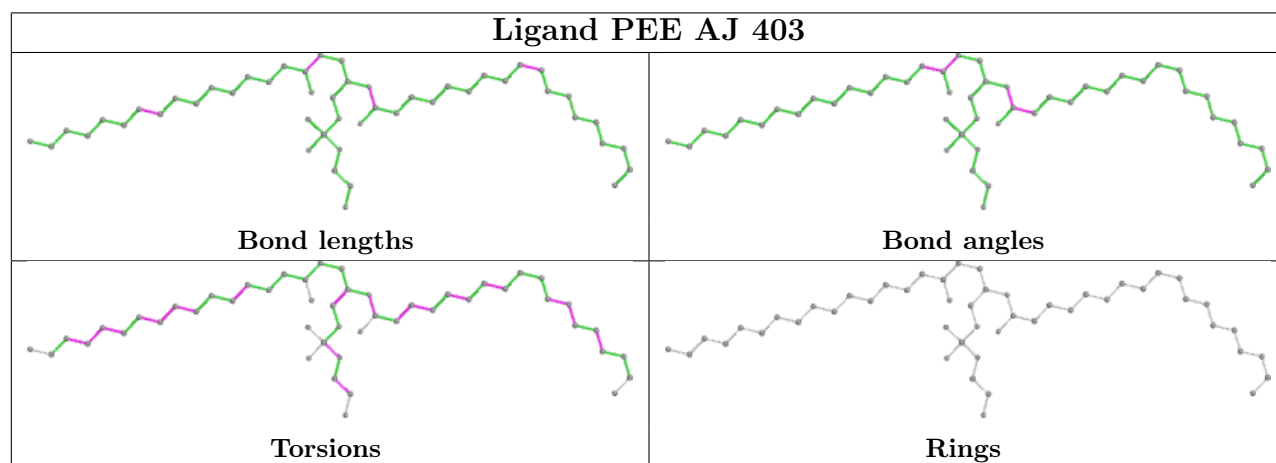
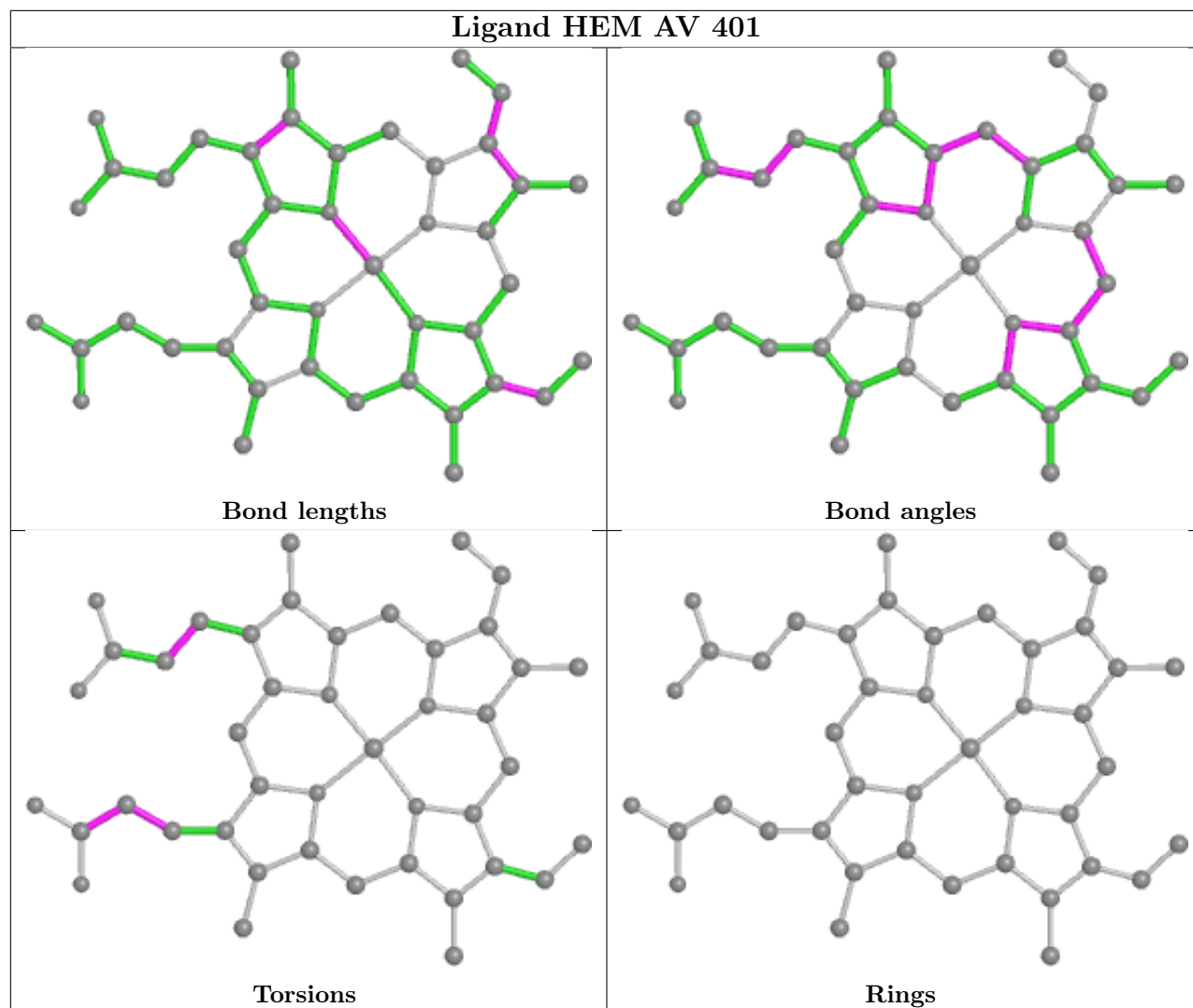


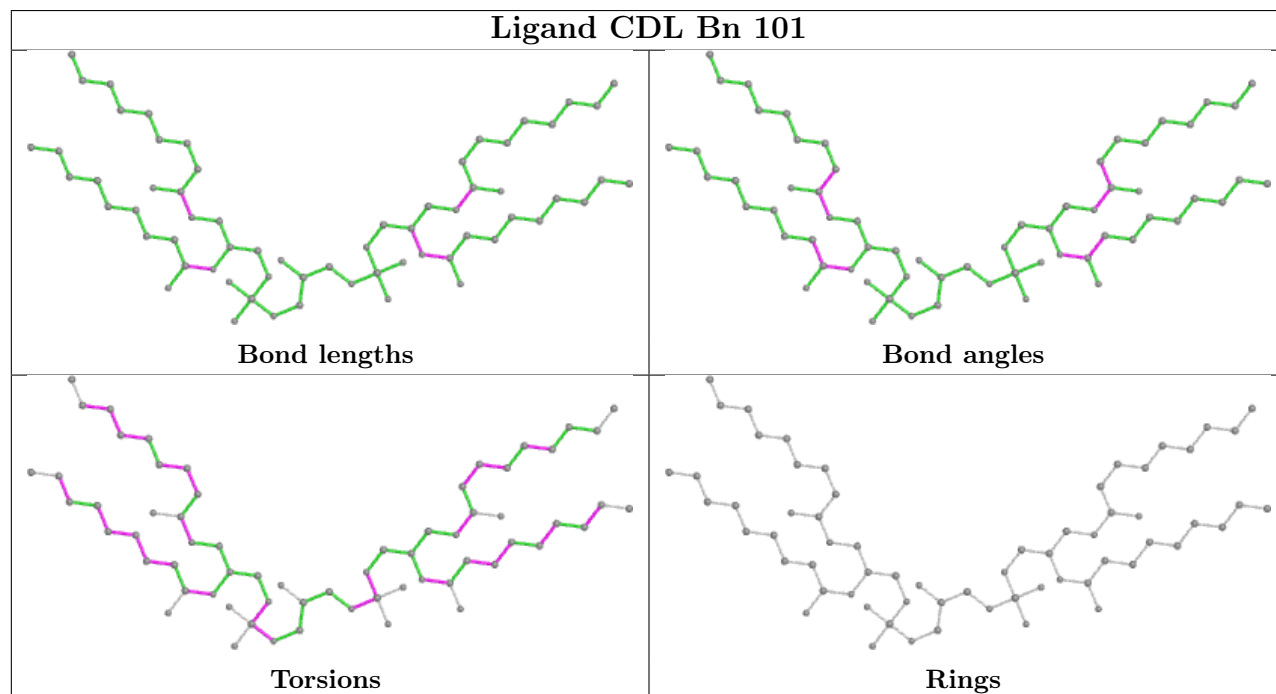
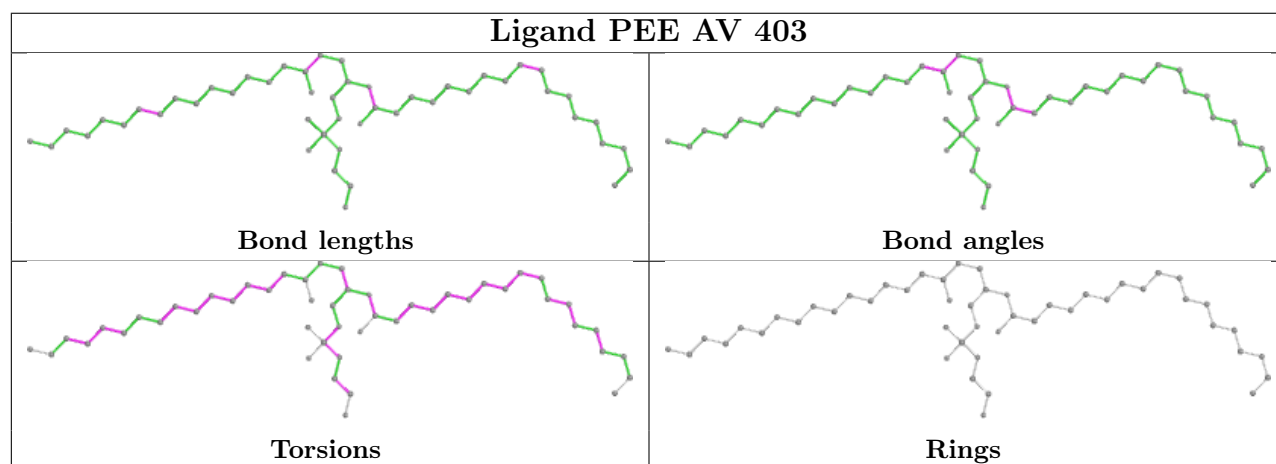
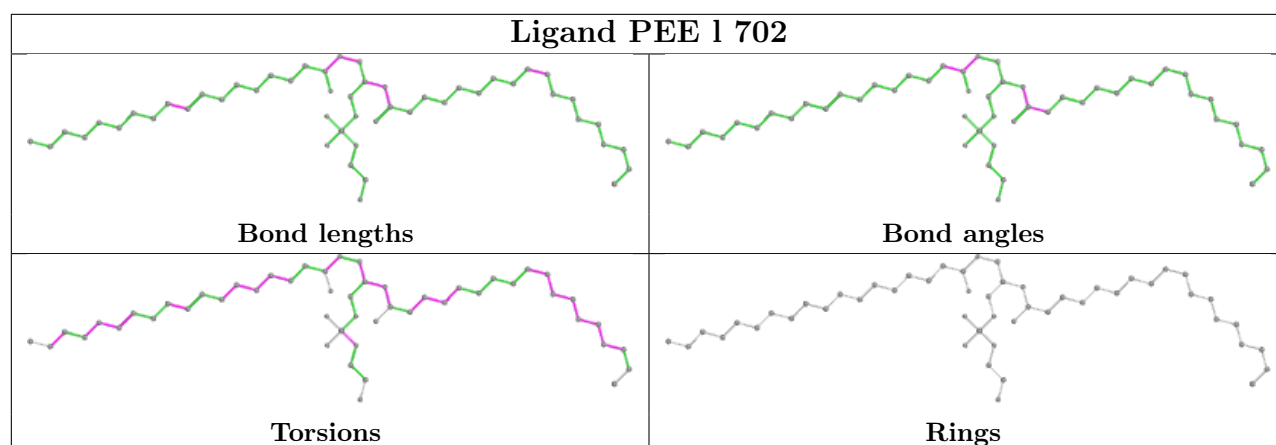


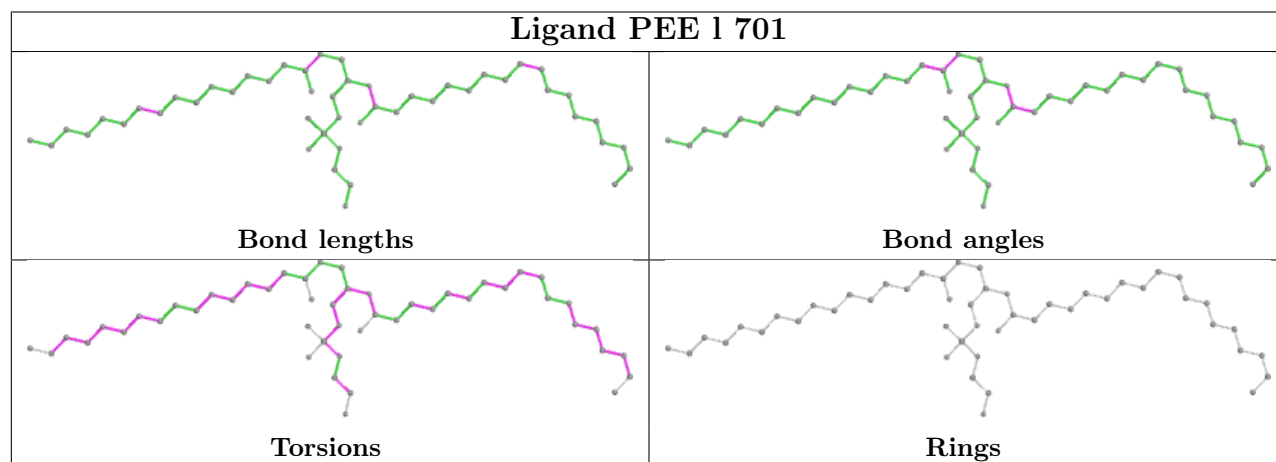
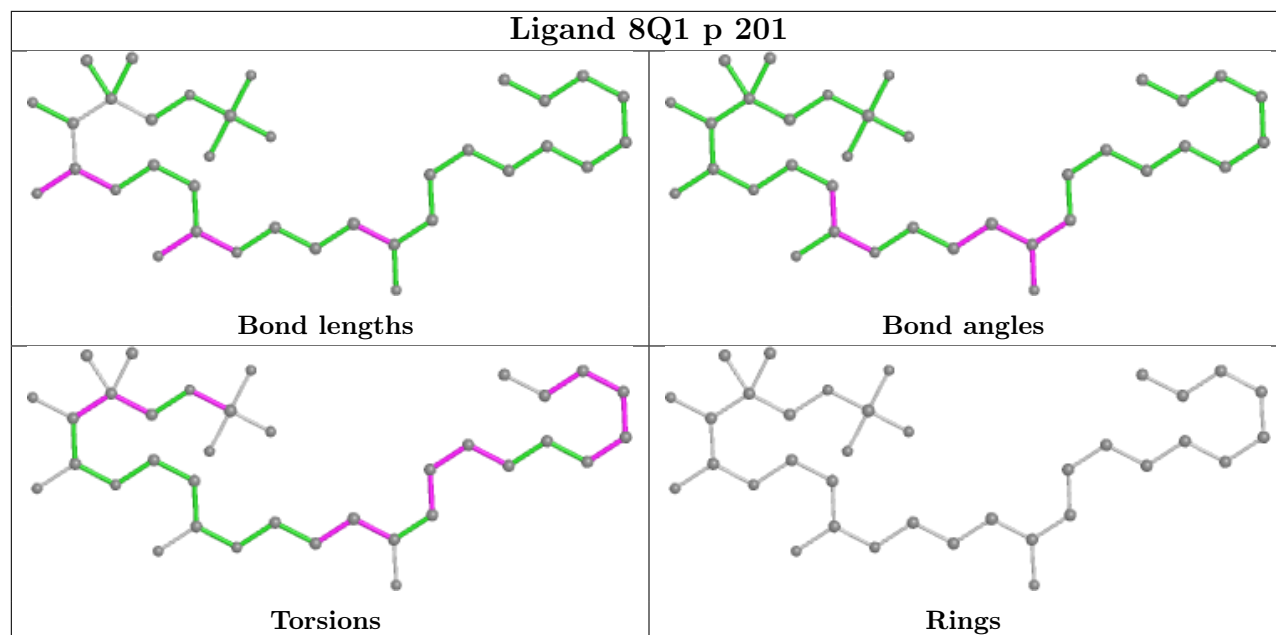


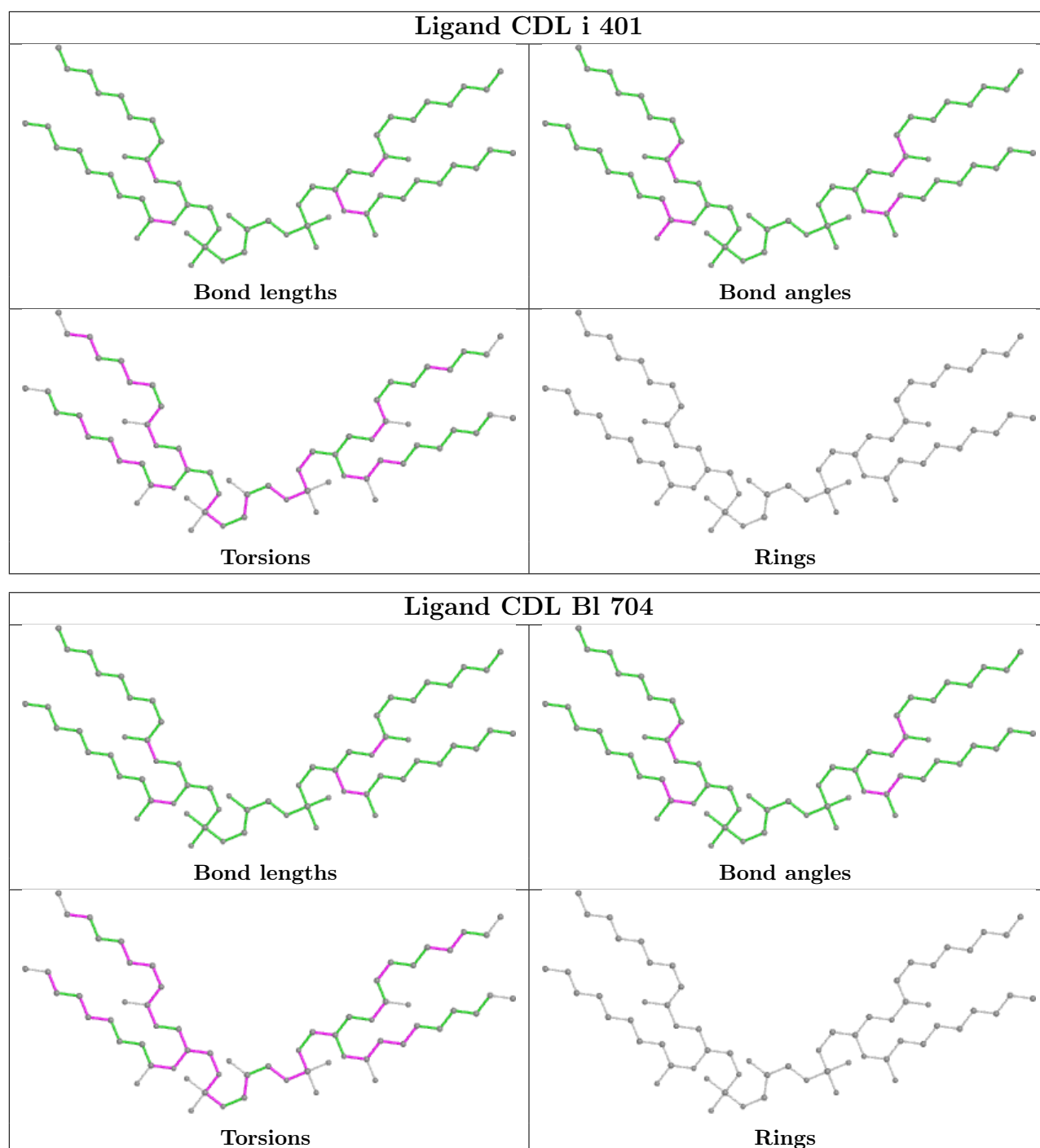


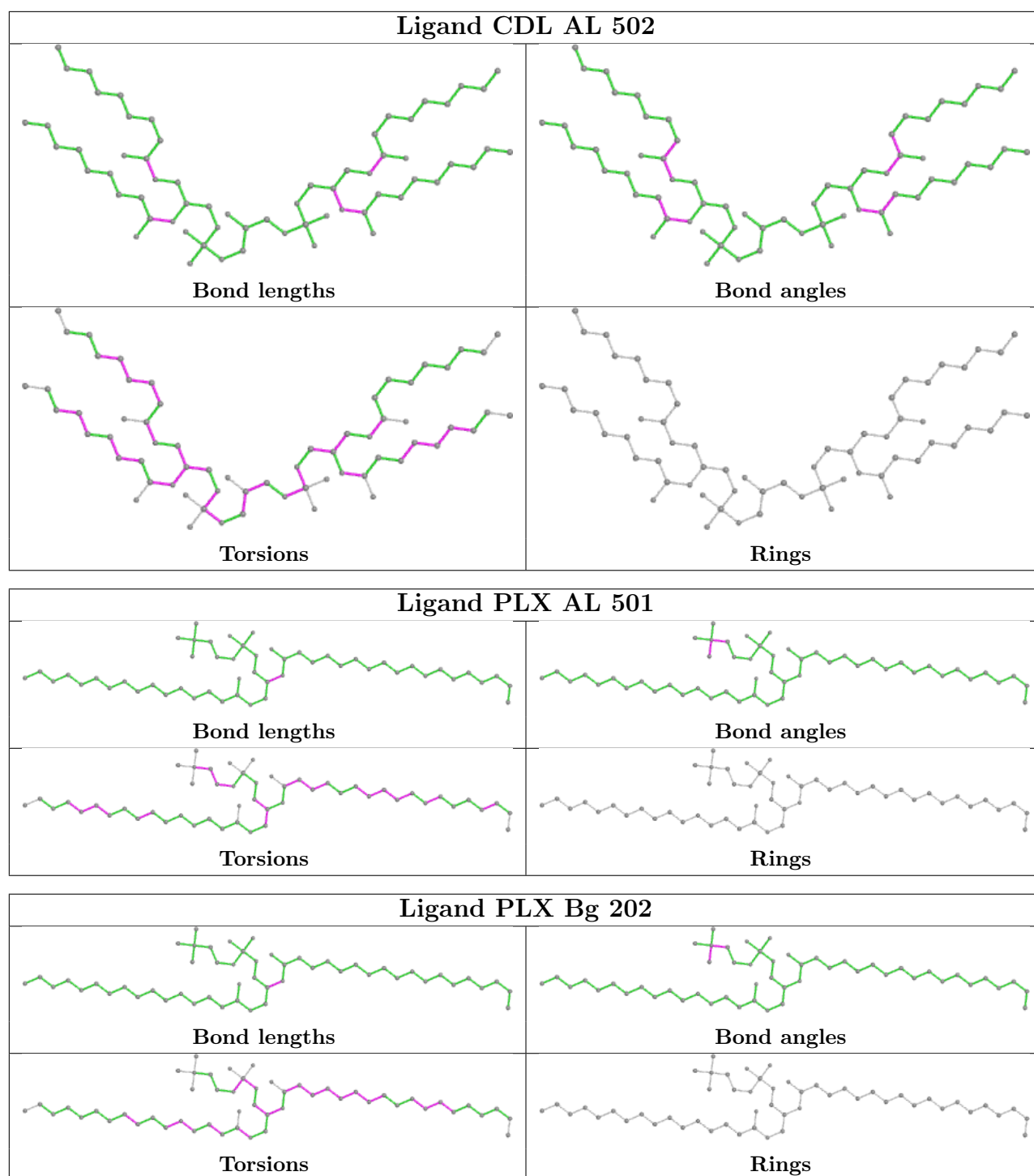


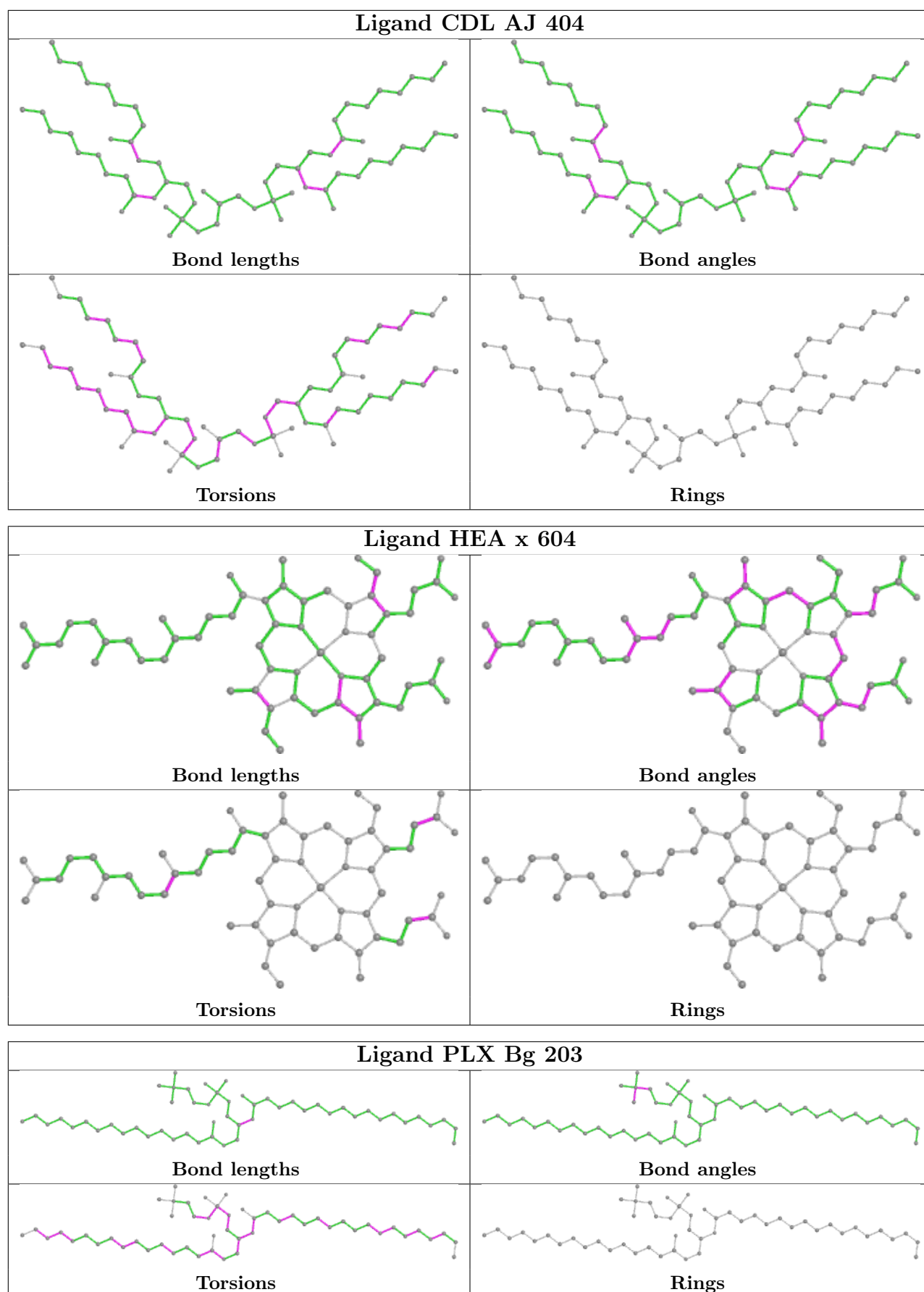


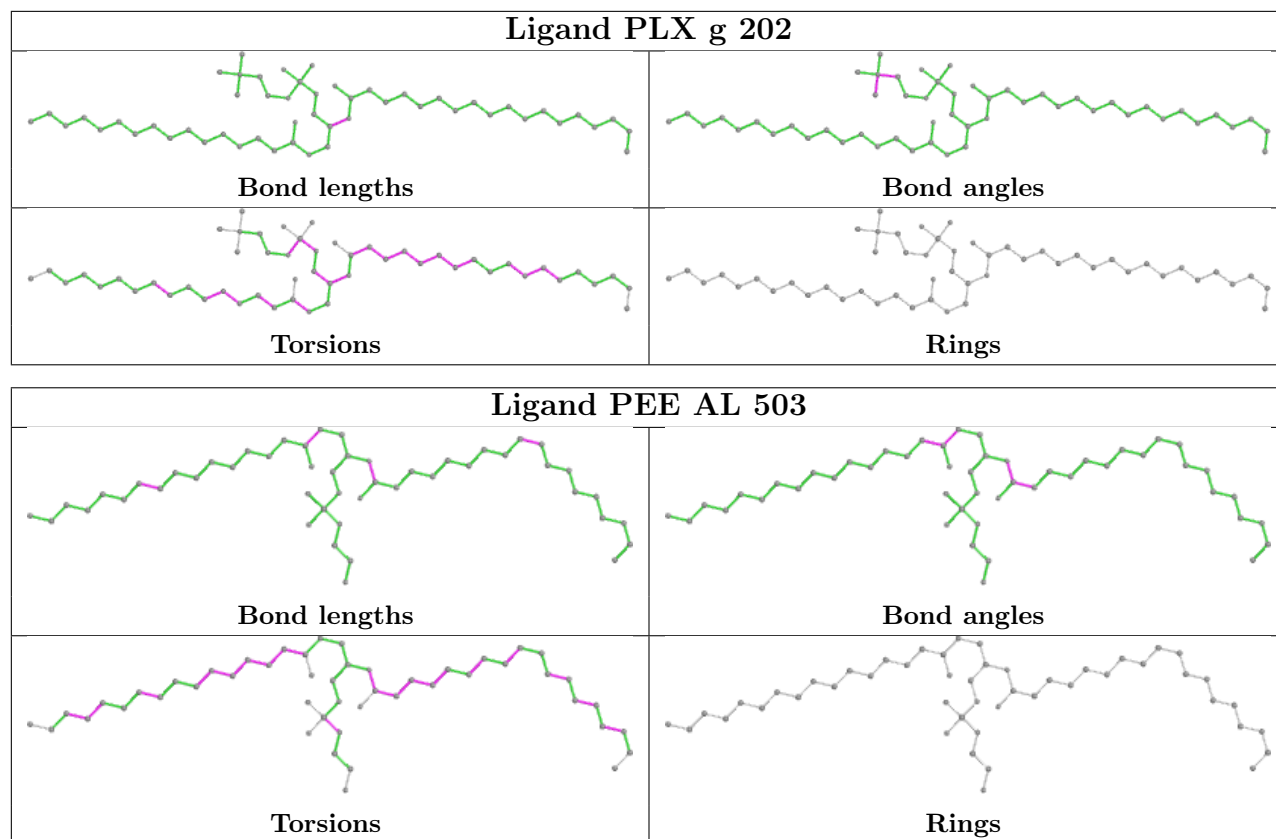


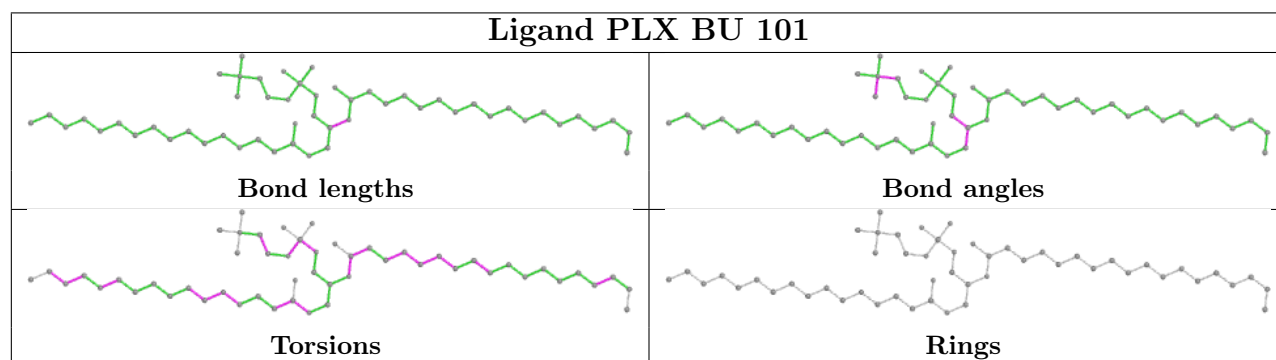
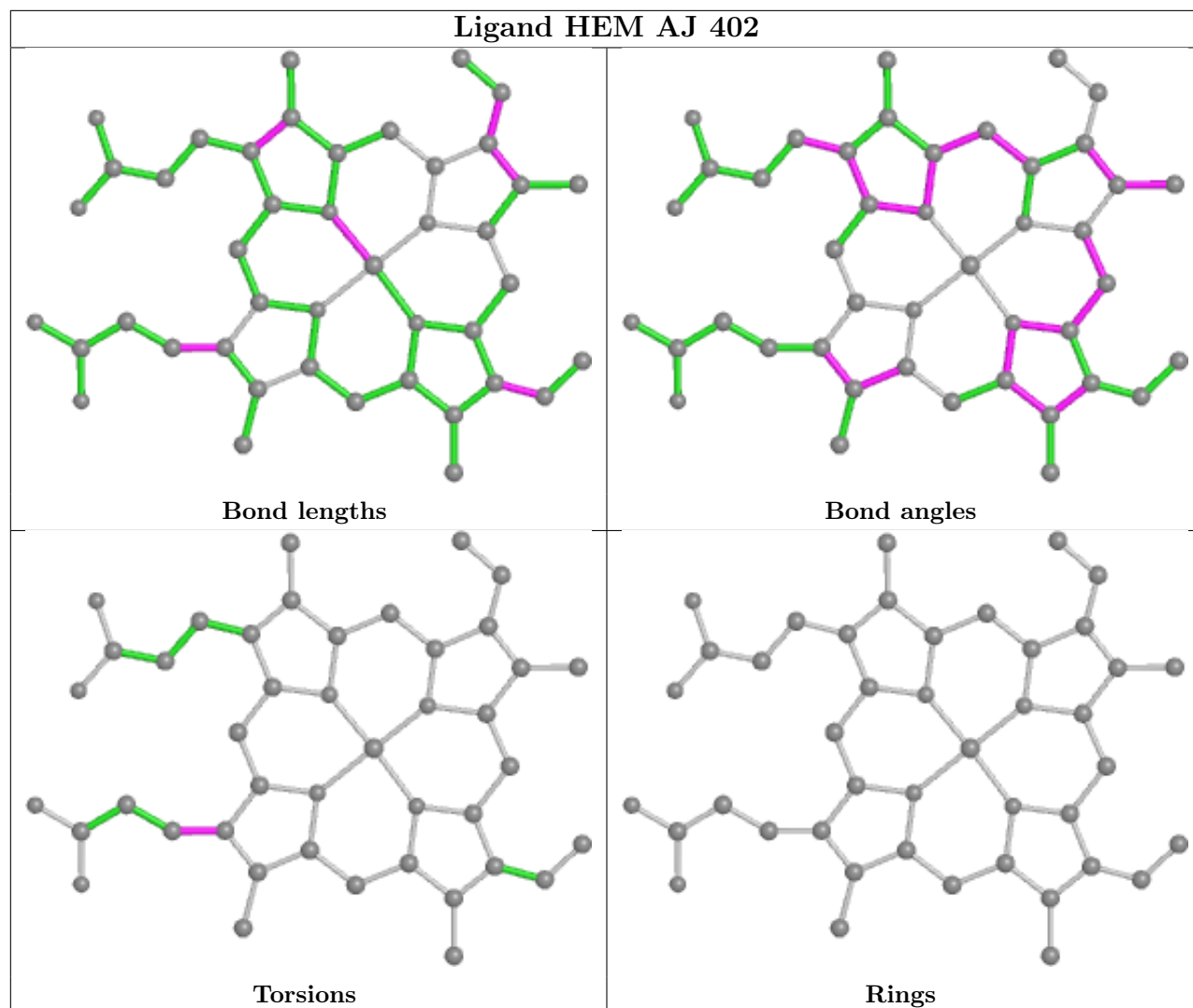


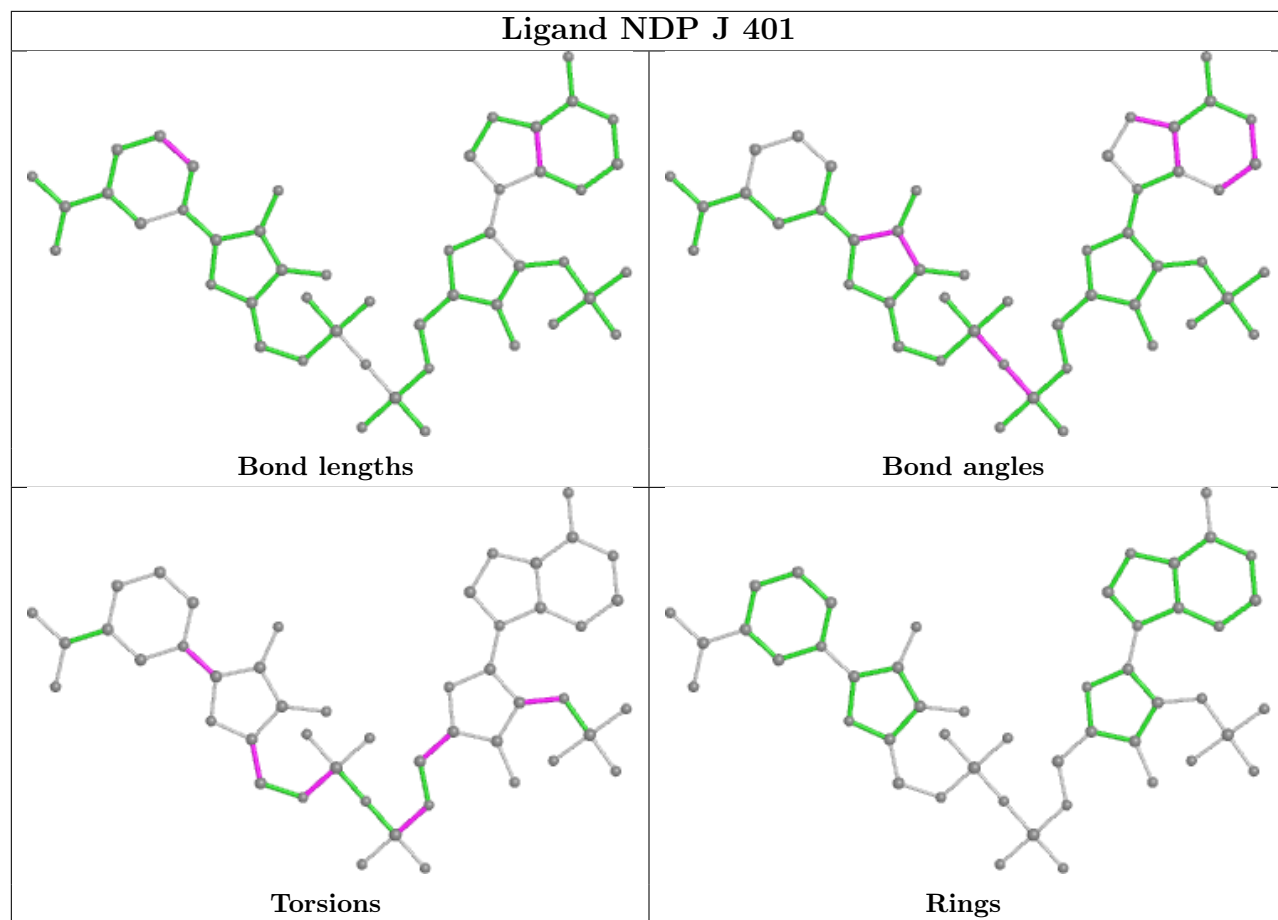


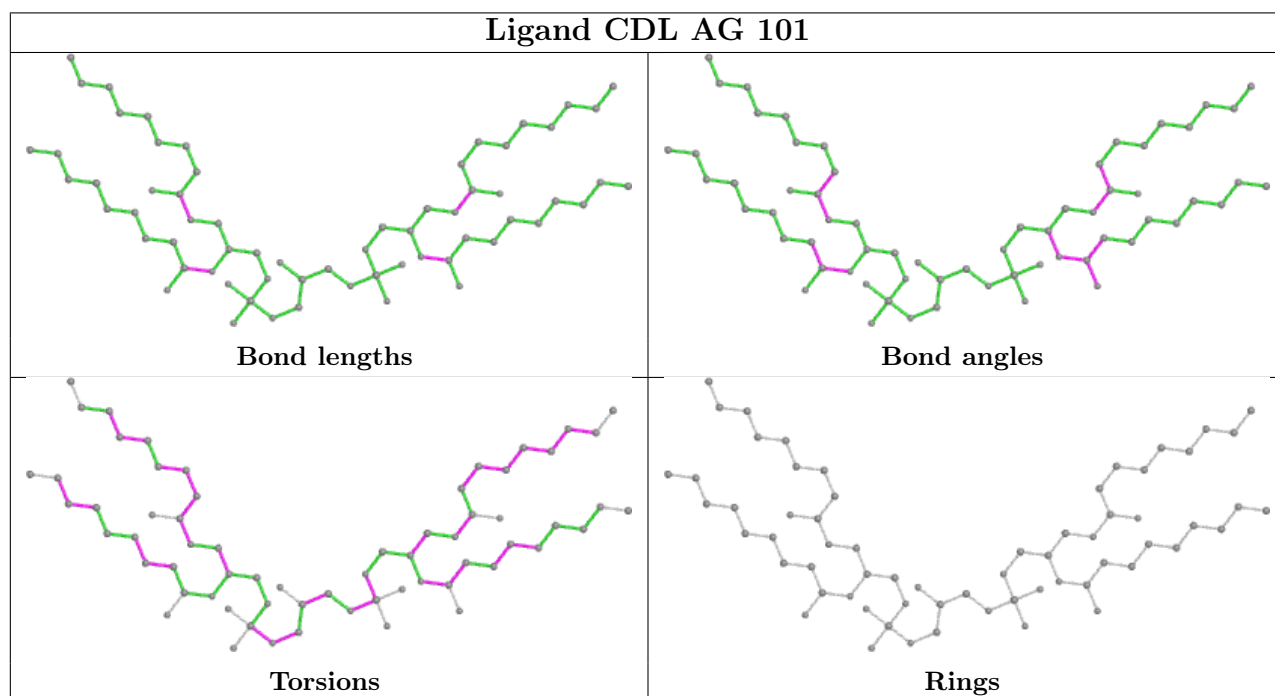
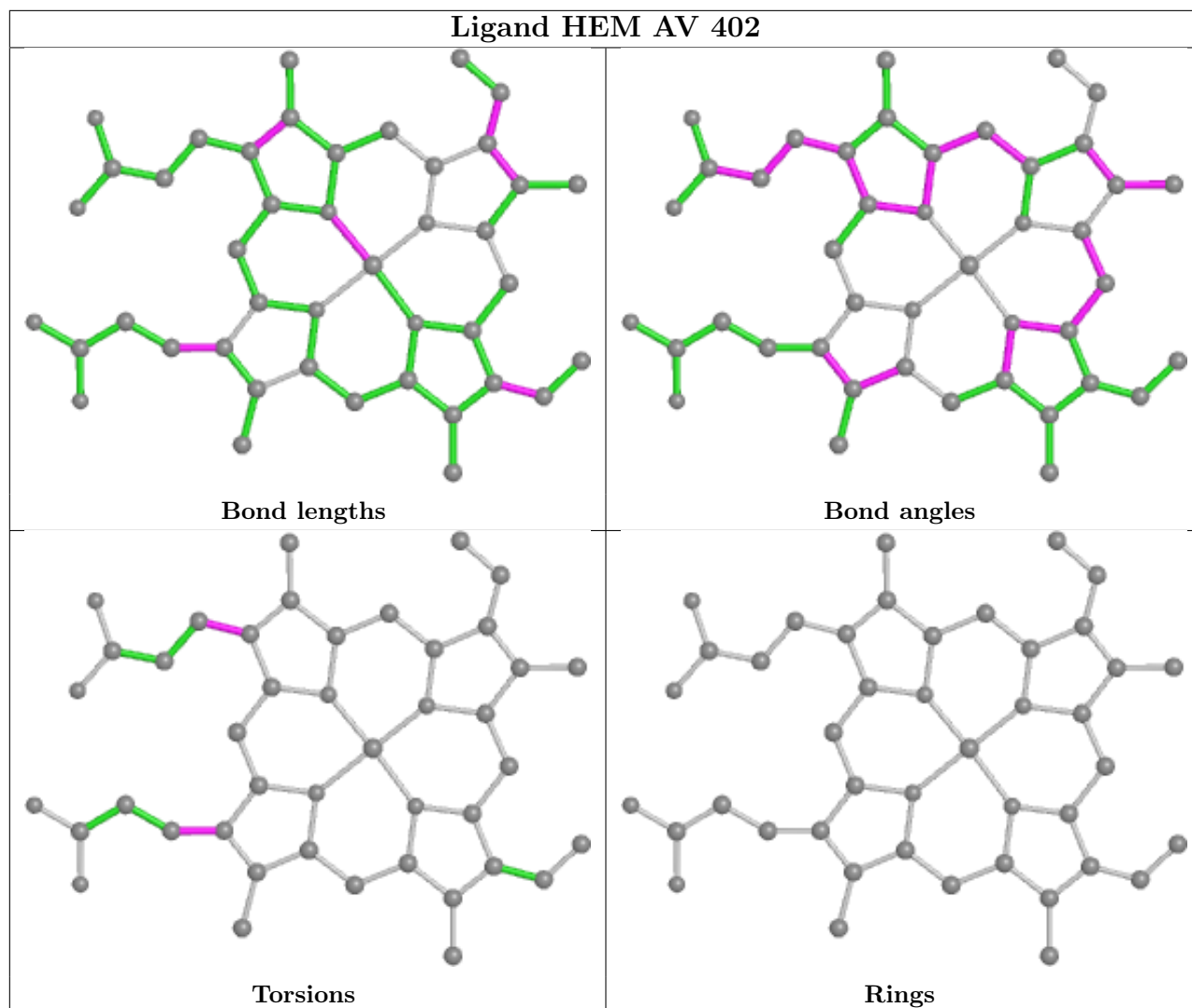


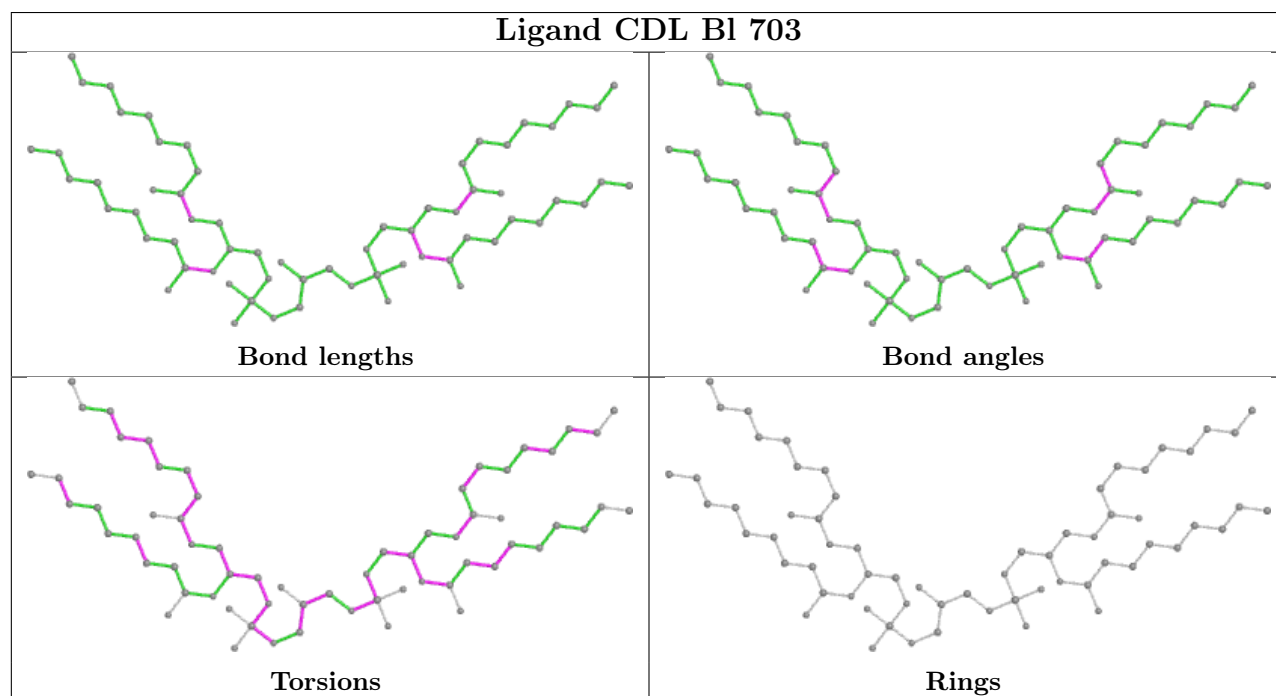
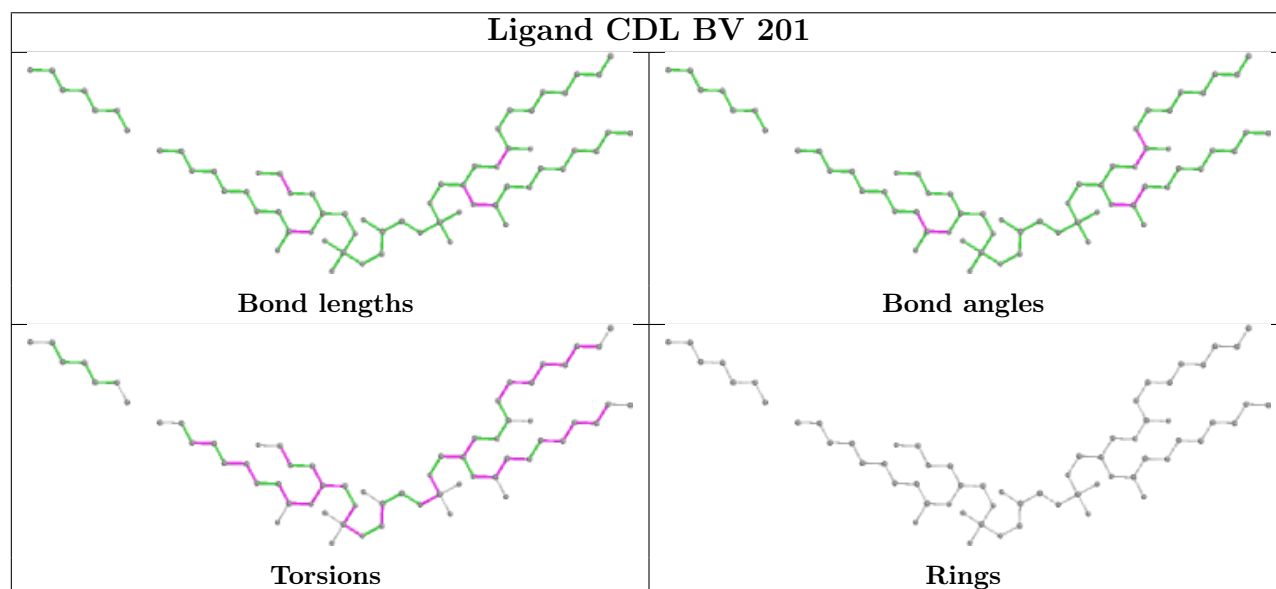
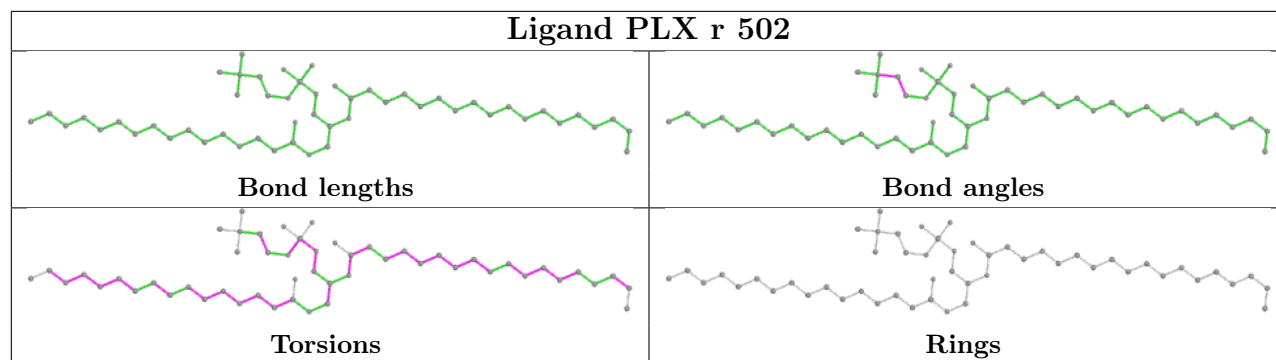


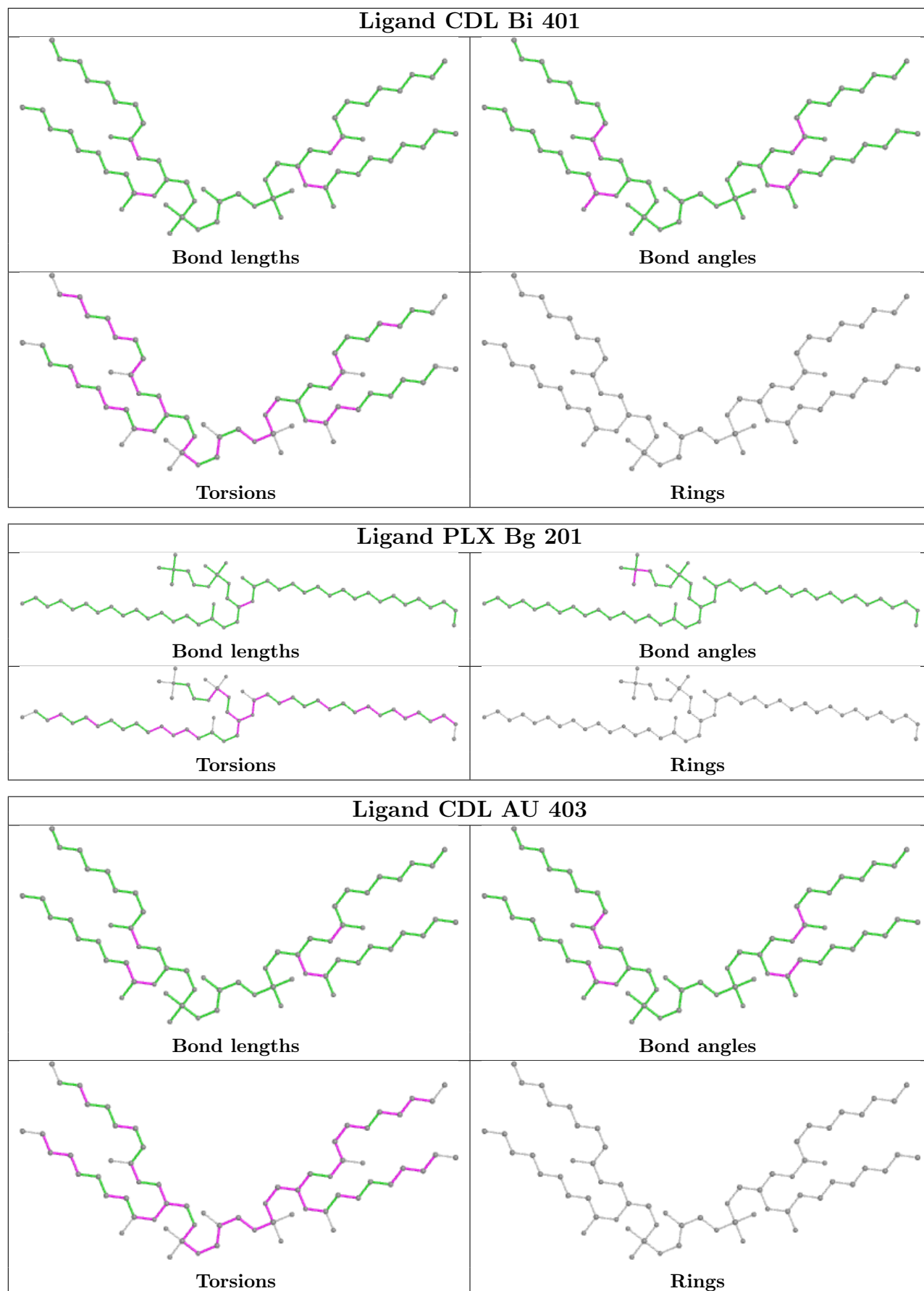


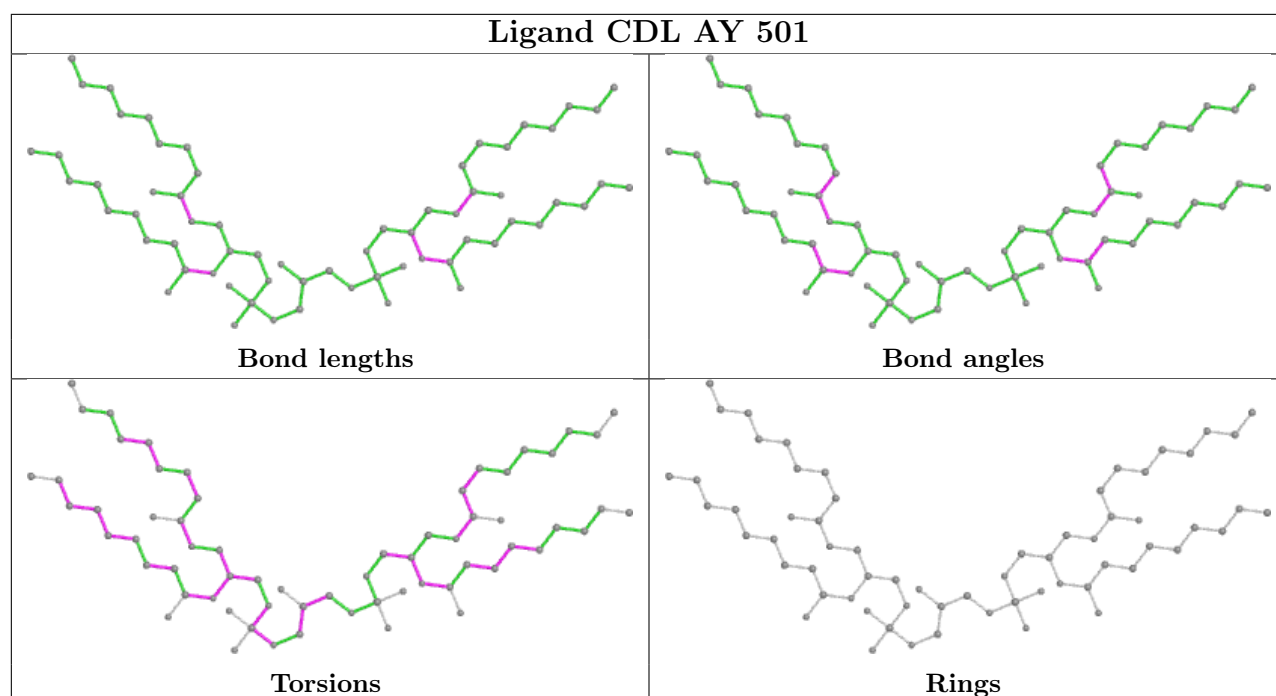












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

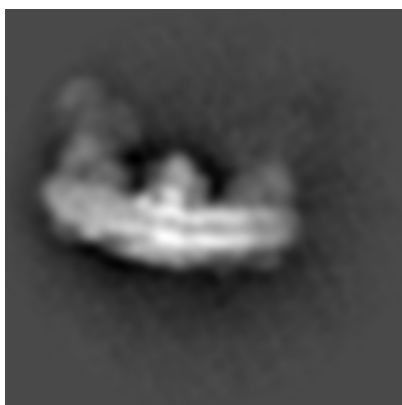
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6776. These allow visual inspection of the internal detail of the map and identification of artifacts.

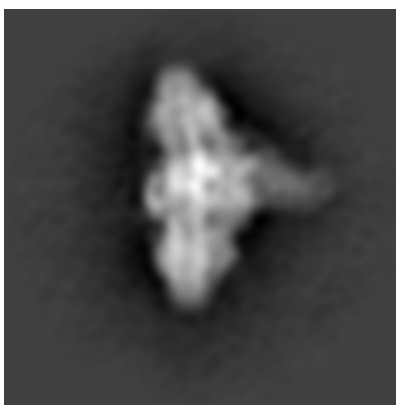
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

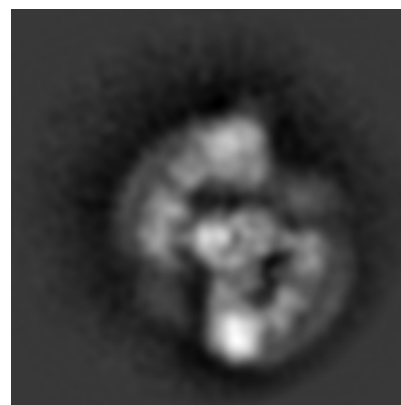
6.1.1 Primary map



X



Y



Z

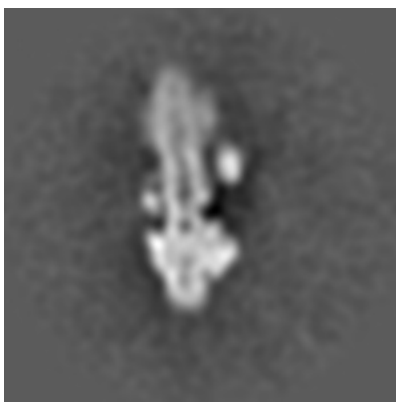
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

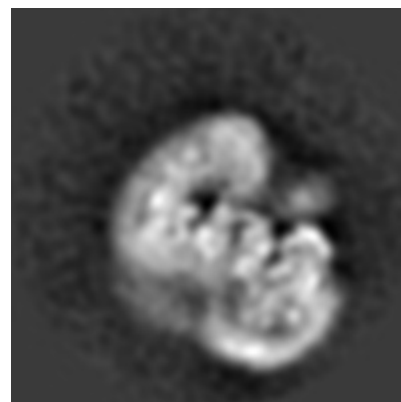
6.2.1 Primary map



X Index: 240



Y Index: 240

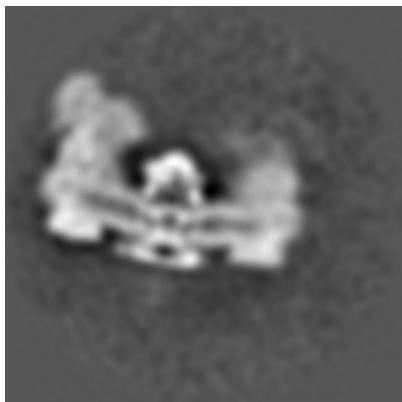


Z Index: 240

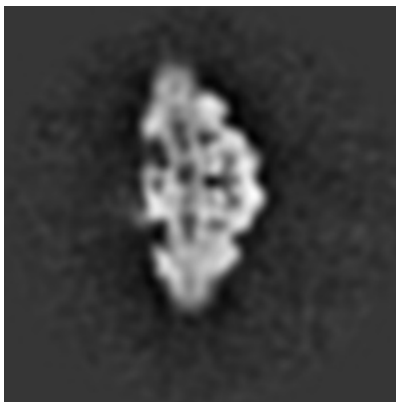
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

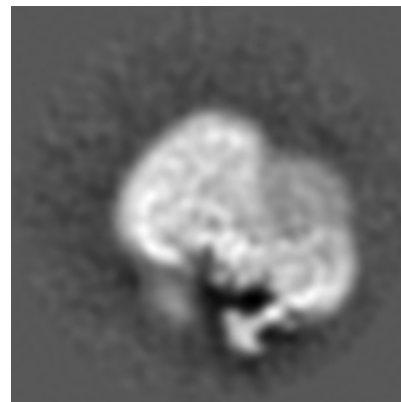
6.3.1 Primary map



X Index: 266



Y Index: 204

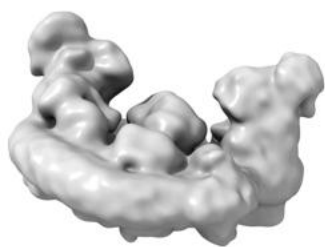


Z Index: 202

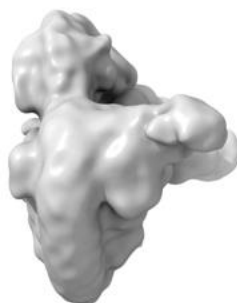
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

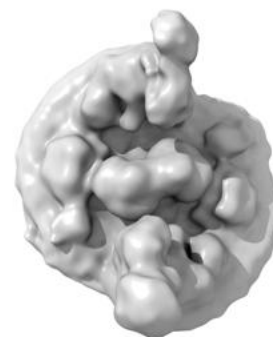
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

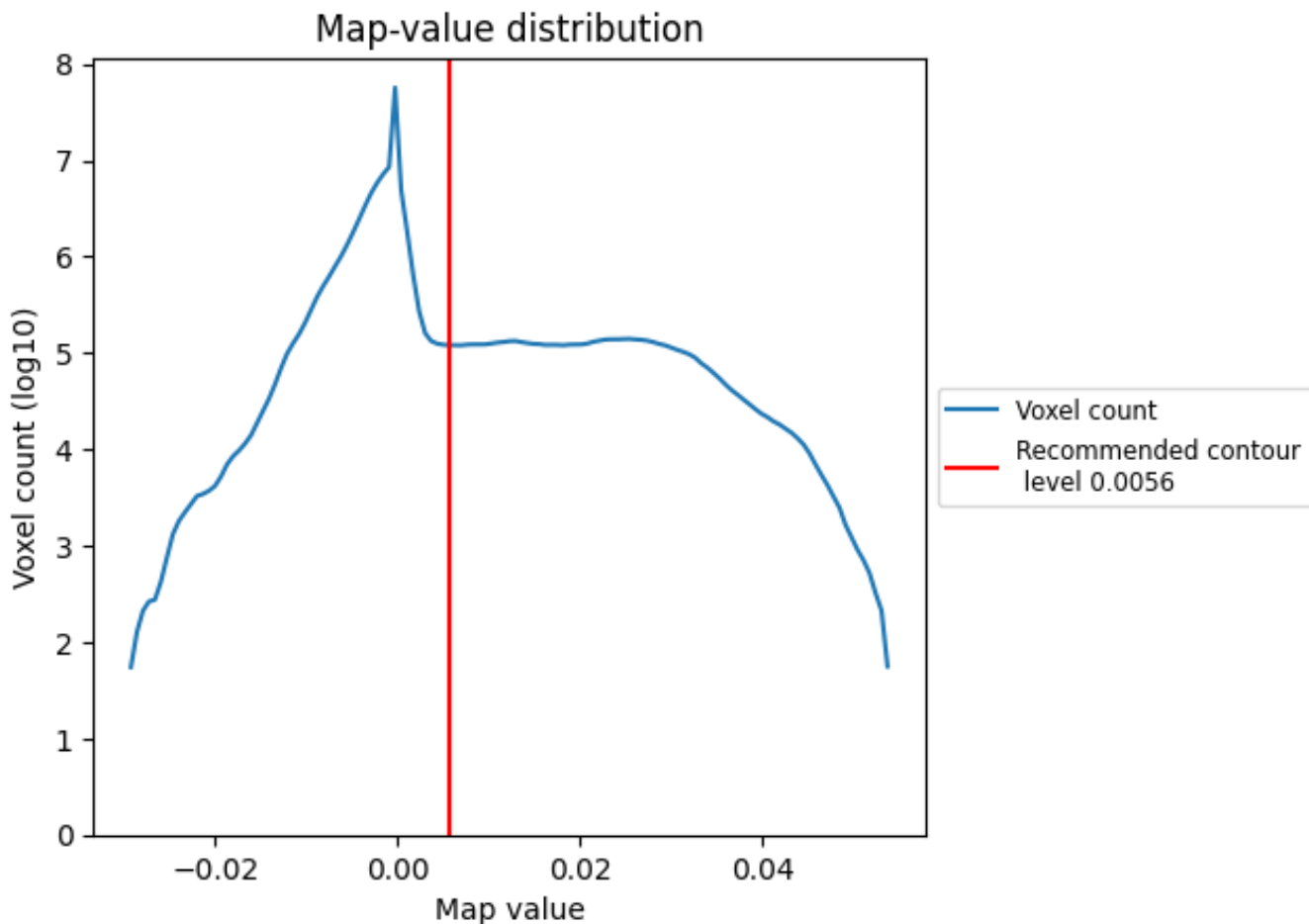
6.5 Mask visualisation

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

7 Map analysis [i](#)

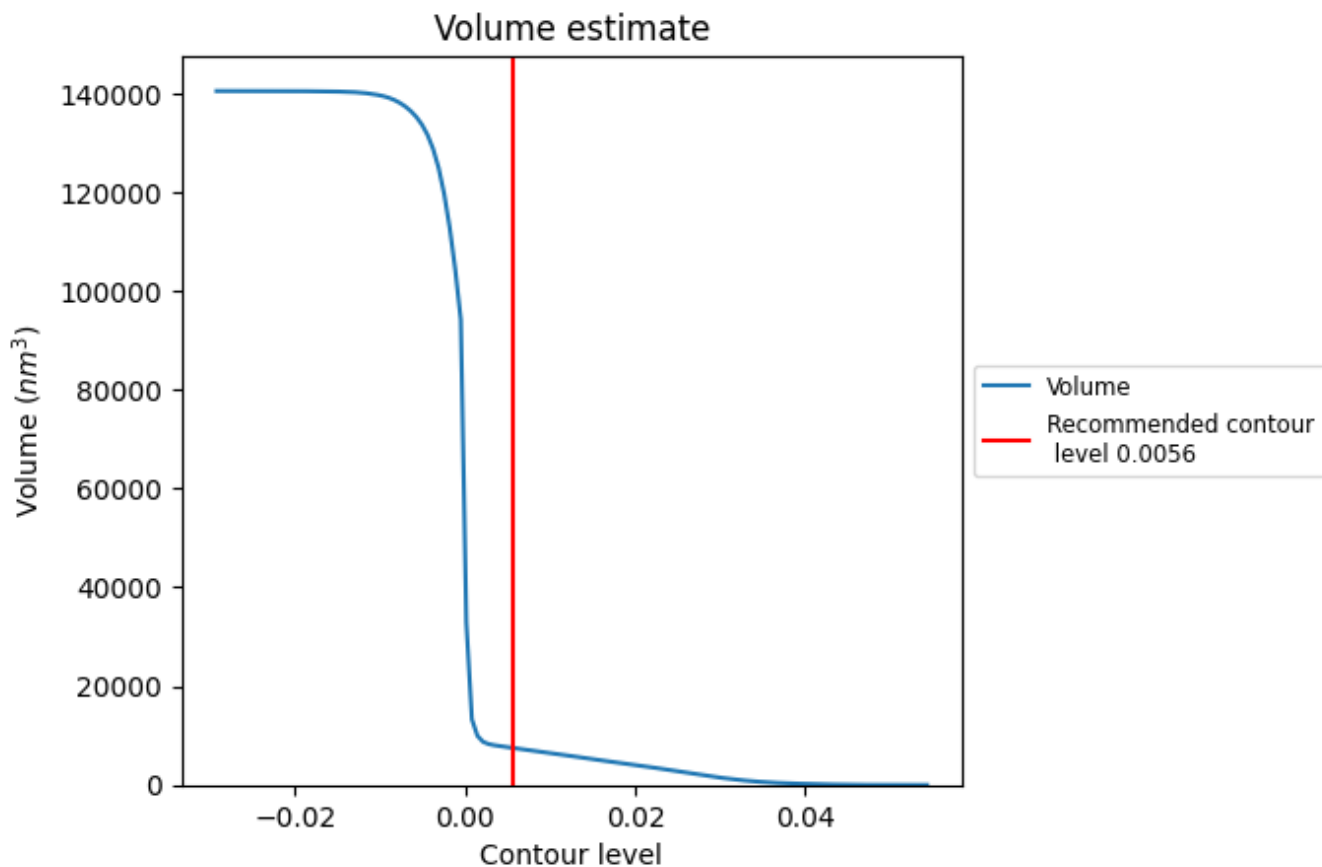
This section contains the results of statistical analysis of the map.

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.

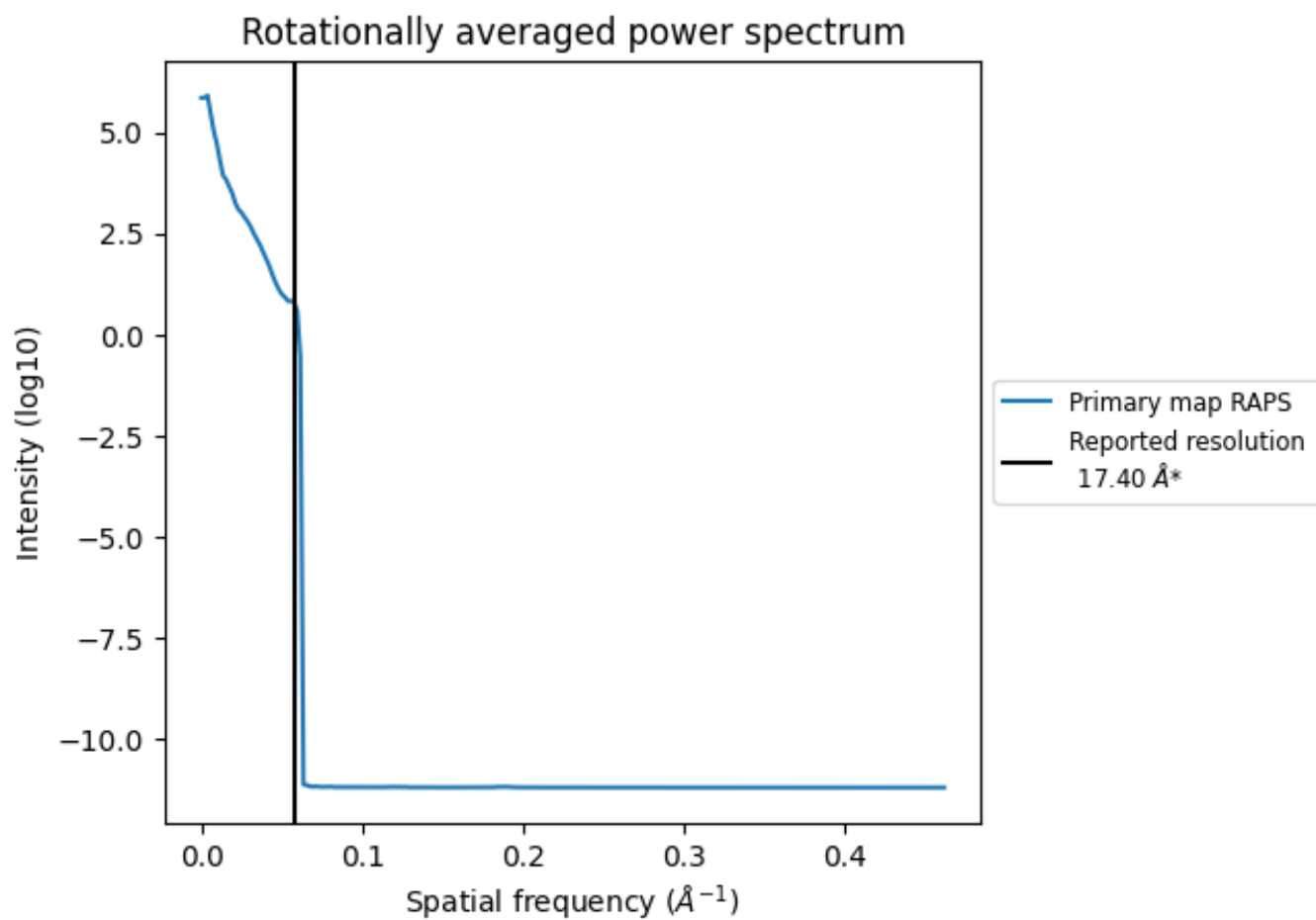
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 7506 nm^3 ; this corresponds to an approximate mass of 6780 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 0.057 Å⁻¹

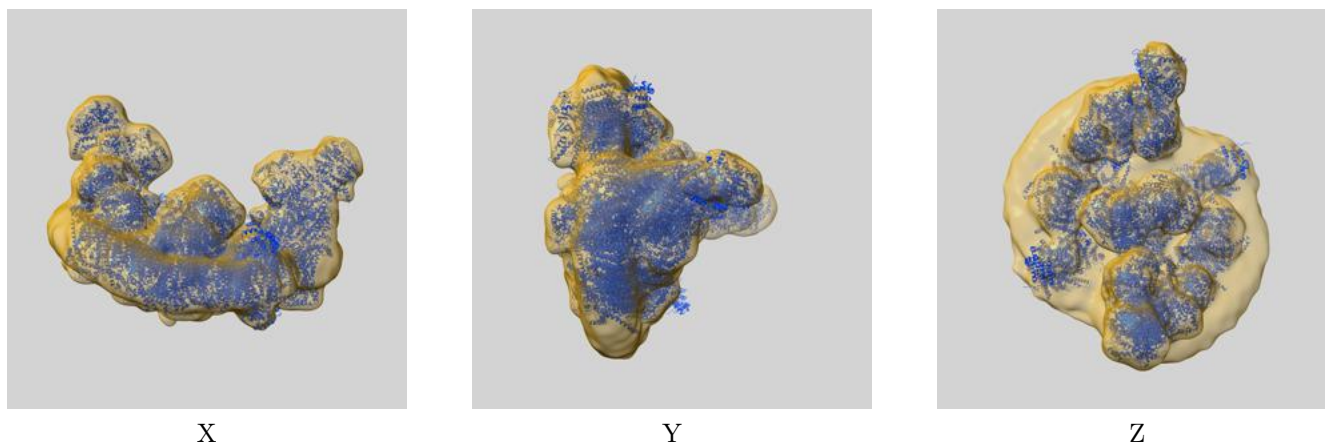
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6776 and PDB model 5XTI. Per-residue inclusion information can be found in section 3 on page 34.

9.1 Map-model overlay [i](#)

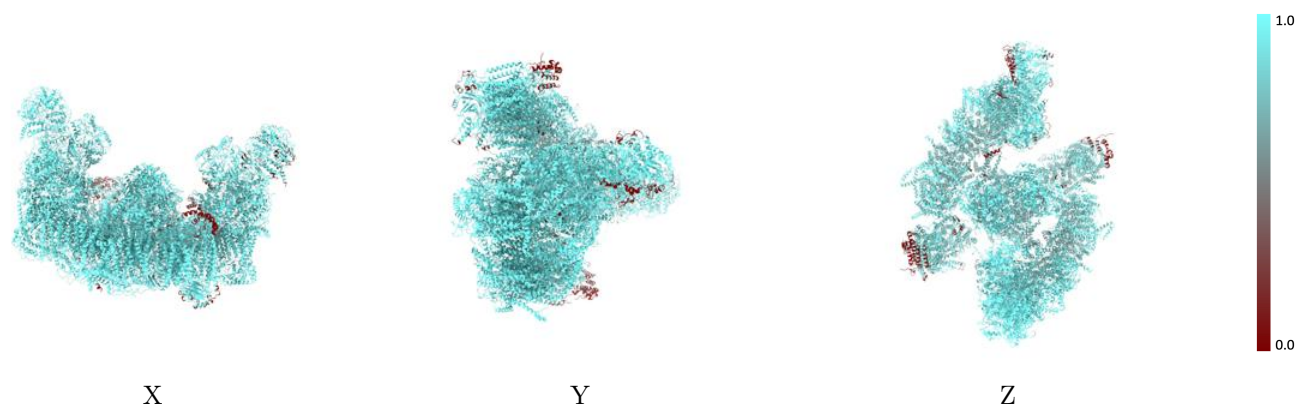


The images above show the 3D surface view of the map at the recommended contour level 0.0056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

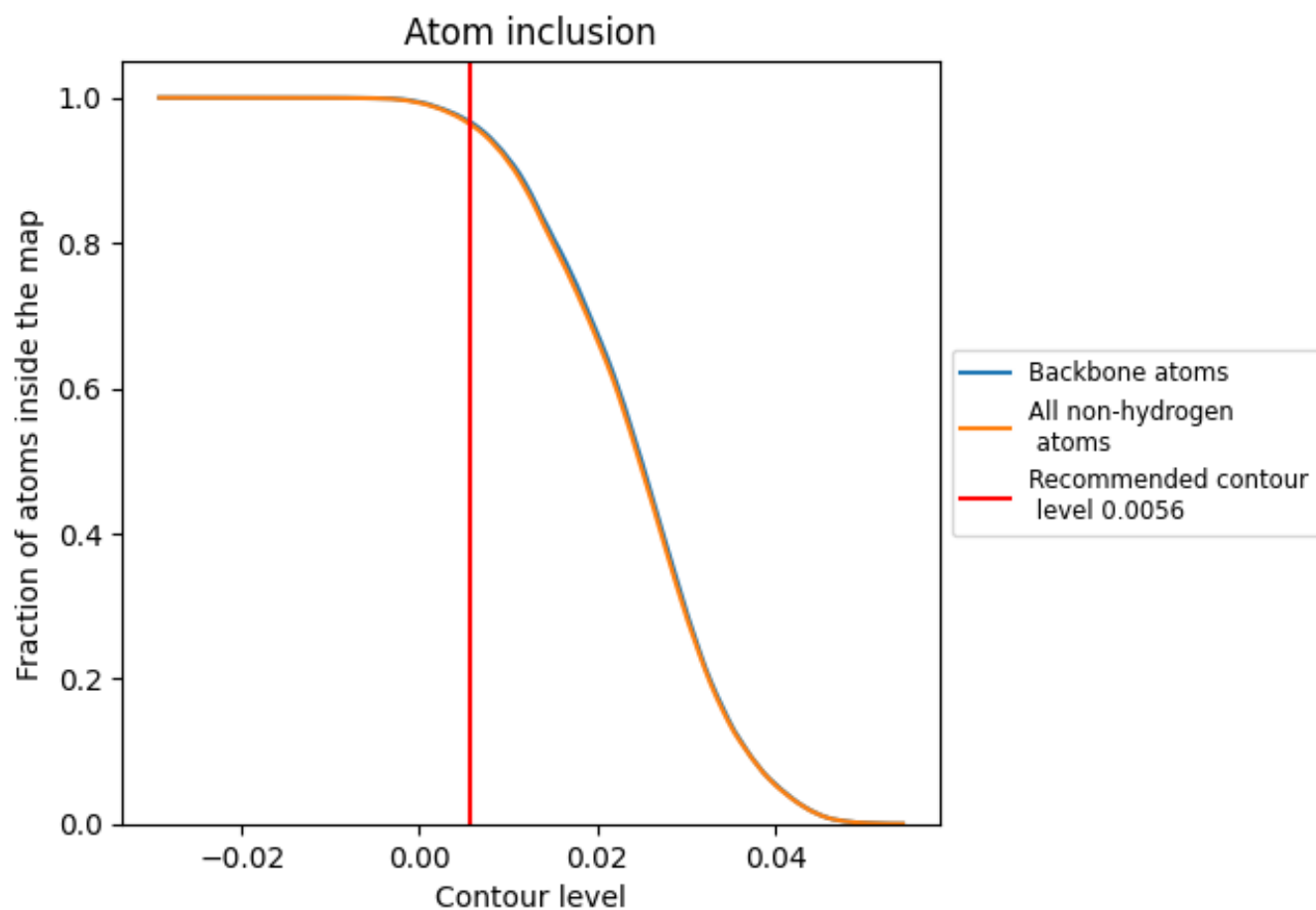
This section was not generated.

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 (0.0056).




































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.9643
0	 0.4386
1	 0.1492
2	 0.8345
3	 0.8147
4	 0.8663
5	 0.4741
6	 0.9607
7	 0.5867
8	 1.0000
9	 0.8976
A	 0.7546
AA	 0.9863
AB	 1.0000
AC	 0.9946
AD	 0.9659
AE	 0.9982
AF	 0.9831
AG	 0.9937
AH	 0.9956
AJ	 0.9988
AK	 0.9994
AL	 0.9958
AN	 0.9949
AO	 1.0000
AP	 0.9900
AQ	 0.9855
AR	 1.0000
AS	 0.9461
AT	 1.0000
AU	 0.9955
AV	 0.9984
AW	 0.9990
AY	 0.9983
B	 1.0000













































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Chain	Atom inclusion
B0	 0.7253
B1	 0.4009
B2	 0.9037
B3	 0.8591
B4	 0.8977
B5	 0.7103
B6	 0.8984
B7	 0.9280
B8	 0.9921
B9	 0.9367
BA	 0.9942
BB	 1.0000
BC	 1.0000
BE	 0.9466
BF	 0.9969
BG	 0.7102
BH	 0.9989
BI	 0.9933
BJ	 0.9800
BK	 1.0000
BL	 0.9862
BM	 0.9856
BN	 0.9845
BO	 0.9963
BP	 0.9887
BQ	 0.9893
BS	 1.0000
BT	 0.9779
BU	 0.9985
BV	 0.9992
BW	 0.9948
BX	 0.9882
BY	 1.0000
BZ	 1.0000
Ba	 0.9974
Bb	 1.0000
Bc	 0.9750
Bd	 0.9715
Be	 0.9848
Bf	 0.9975
Bg	 0.9947
Bh	 0.9976





















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Chain	Atom inclusion
Bi	 1.0000
Bj	 1.0000
Bk	 1.0000
Bl	 0.9998
Bm	 1.0000
Bn	 0.9905
Bo	 0.9893
Bp	 0.9898
Br	 0.9986
Bs	 1.0000
Bu	 0.9934
Bv	 0.9876
Bw	 0.9963
Bx	 0.9998
By	 0.9772
Bz	 1.0000
C	 1.0000
E	 0.9507
F	 0.9708
G	 0.4850
H	 0.9989
I	 0.9866
J	 0.9725
K	 0.9776
L	 0.9841
M	 0.9238
N	 0.9742
O	 0.8668
P	 0.9881
Q	 0.9923
S	 1.0000
T	 0.9061
U	 1.0000
V	 0.9991
W	 0.9991
X	 1.0000
Y	 1.0000
Z	 1.0000
a	 0.9965
b	 1.0000
c	 0.9758
d	 0.9876

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Chain	Atom inclusion
e	 1.0000
f	 1.0000
g	 0.9973
h	 1.0000
i	 1.0000
j	 1.0000
k	 1.0000
l	 1.0000
m	 1.0000
n	 0.9866
o	 0.9873
p	 0.9946
r	 0.9989
s	 1.0000
u	 0.9971
v	 0.9853
w	 0.9992
x	 0.9985
y	 0.8653
z	 1.0000