



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:28 PM UTC

PDB ID : 5XTI / pdb_00005xti
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:

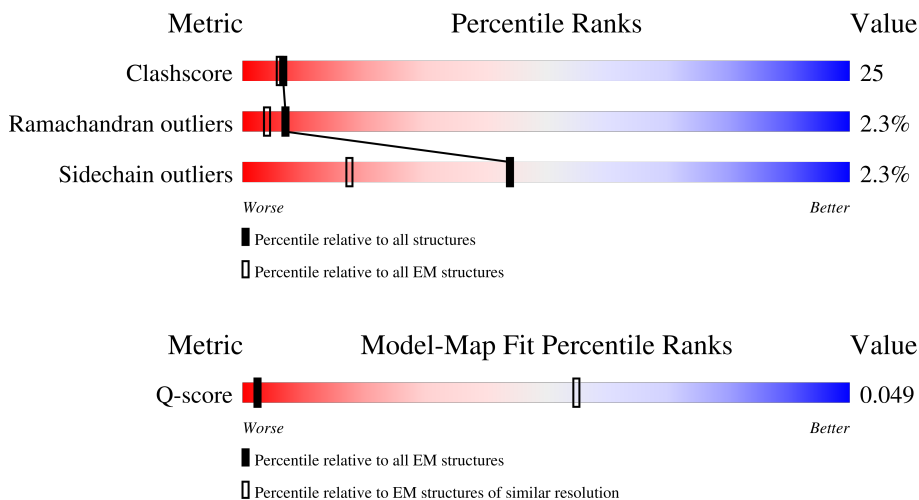
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.






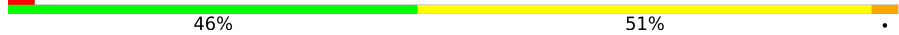


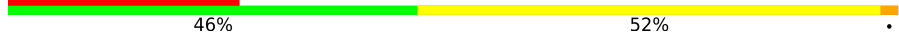





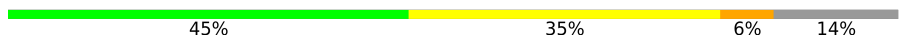
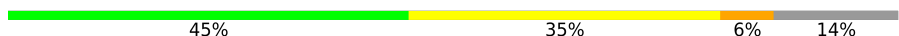











Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	31 (16.90 - 17.60)

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	
1	BA	431	
2	B	176	
2	BB	176	

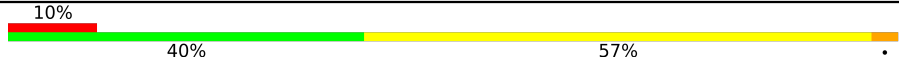


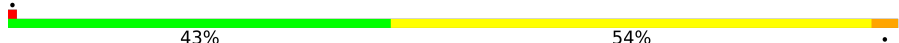
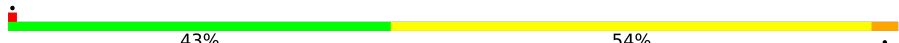



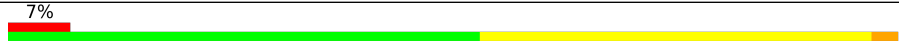

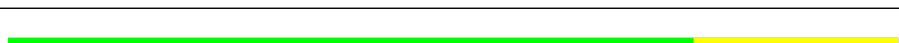


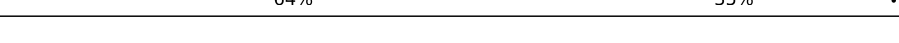
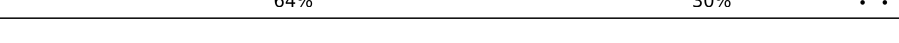
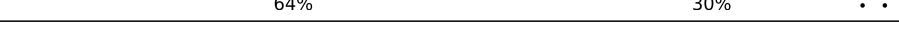
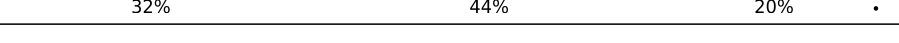
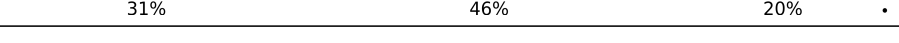
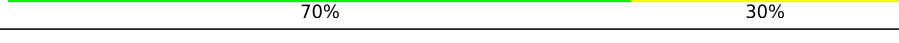






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Mol	Chain	Length	Quality of chain
3	BC	156	 52% 47%
3	C	156	 48% 51%
4	BE	113	 46% 51%
4	E	113	 46% 51%
5	BF	83	 48% 52%
5	F	83	 53% 47%
6	BG	85	 26% 46% 52%
6	BX	85	 51% 46%
6	G	85	 48% 46% 52%
6	X	85	 53% 45%
7	BH	112	 50% 46%
7	H	112	 51% 46%
8	BI	110	 45% 35% 6% 14%
8	I	110	 45% 35% 6% 14%
9	BJ	337	 45% 52%
9	J	337	 44% 53%
10	BK	33	 45% 45% 9%
10	K	33	 45% 52%
11	BL	118	 44% 54%
11	L	118	 44% 54%
12	BM	687	 46% 52%
12	M	687	 6% 46% 52%
13	BN	143	 57% 39%
13	N	143	 59% 38%
14	BO	212	 40% 57%








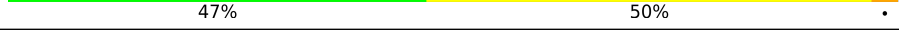
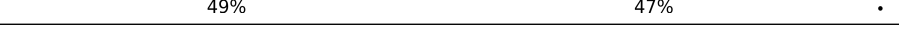
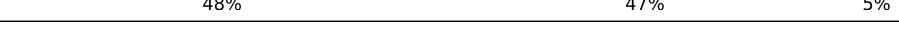

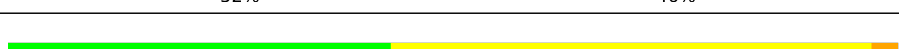
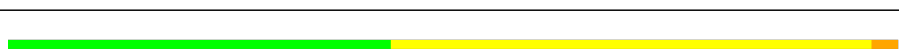
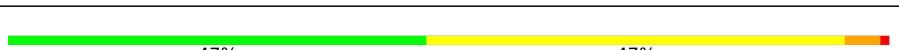
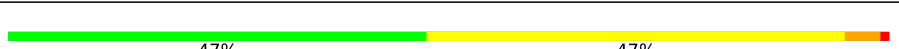





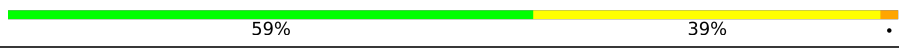
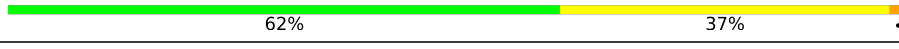



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Mol	Chain	Length	Quality of chain
14	O	212	
15	BP	208	
15	P	208	
16	BQ	430	
16	Q	430	
17	BS	70	
17	S	70	
18	BT	95	
18	T	95	
19	BU	83	
19	U	83	
20	BV	140	
20	V	140	
21	BW	138	
21	W	138	
22	BY	59	
22	Y	59	
23	BZ	80	
23	Z	80	
24	Ba	138	
24	a	138	
25	Bb	124	
25	b	124	
26	Bc	153	
26	c	153	

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Mol	Chain	Length	Quality of chain
27	Bd	171	 63% 33%
27	d	171	 62% 34%
28	Be	97	 69% 31%
28	e	97	 70% 30%
29	Bf	47	 66% 30%
29	f	47	 66% 30%
30	Bg	119	 49% 49%
30	g	119	 47% 50%
31	Bh	104	 49% 47%
31	h	104	 48% 47% 5%
32	Bi	347	 50% 47%
32	i	347	 52% 46%
33	Bj	115	 43% 54%
33	j	115	 43% 54%
34	Bk	97	 47% 47%
34	k	97	 47% 47%
35	Bl	603	 49% 45% 5%
35	l	603	 49% 45% 5%
36	Bm	174	 44% 52%
36	m	174	 45% 51%
37	Bn	56	 59% 39%
37	n	56	 59% 39%
38	Bo	128	 62% 37%
38	o	128	 62% 36%
39	Bp	172	 55% 40% 5%

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Mol	Chain	Length	Quality of chain
39	p	172	58% 38% 5%
40	Br	459	60% 39%
40	r	459	61% 39%
41	Bs	318	48% 49%
41	s	318	47% 49%
42	Bu	169	60% 38%
42	u	169	63% 35%
43	Bv	122	45% 43% 9%
43	v	122	47% 42% 9%
44	Bw	320	56% 41%
44	w	320	55% 42%
45	Bx	514	68% 27% 5%
45	x	514	68% 26% 5%
46	By	227	60% 35%
46	y	227	12% 60% 35%
47	Bz	261	70% 24% 5%
47	z	261	70% 24% 5%
48	0	144	54% 71% 26%
48	B0	144	26% 72% 25%
49	1	109	83% 74% 21% 5%
49	B1	109	56% 76% 22%
50	2	98	14% 62% 29% 9%
50	B2	98	59% 32% 9%
51	3	84	18% 62% 26% 11%
51	B3	84	12% 61% 27% 11%










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Mol	Chain	Length	Quality of chain
52	4	75	16% 63% 31% 7%
52	B4	75	11% 61% 33% 5%
53	5	73	51% 68% 26% 5%
53	B5	73	25% 73% 23% .
54	6	56	. 62% 25% 11% .
54	B6	56	9% 62% 29% 7% .
55	7	49	39% 65% 33% .
55	B7	49	. 65% 33% .
56	8	47	74% 23% .
56	B8	47	74% 23% .
57	9	43	9% 67% 30% .
57	B9	43	7% 67% 30% .
58	AA	81	. 63% 31% 6%
58	AN	81	. 74% 25% .
59	AB	57	49% 47% .
59	AO	57	51% 44% 5%
60	AC	196	68% 30% .
60	AP	196	62% 37% .
61	AD	62	. 74% 26%
61	AQ	62	61% 37% .
62	AE	74	68% 30% ..
62	AR	74	74% 22% .
63	AF	106	. 56% 30% 14%
63	AS	106	. 62% 38%
64	AG	51	73% 25% .

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Mol	Chain	Length	Quality of chain
64	AT	51	
65	AH	241	
65	AU	241	
66	AJ	378	
66	AV	378	
67	AK	419	
67	AW	419	
68	AL	446	
68	AY	446	

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
69	SF4	A	501	-	-	X	-
69	SF4	B	302	-	-	X	-
69	SF4	BA	501	-	-	X	-
69	SF4	BB	302	-	-	X	-
69	SF4	BM	801	-	-	X	-
69	SF4	M	801	-	-	X	-
70	FMN	A	502	-	-	X	-
70	FMN	BA	502	-	-	X	-
71	PLX	Bb	201	-	-	X	-
71	PLX	b	201	-	-	X	-
73	NDP	BJ	401	-	-	X	-
73	NDP	J	401	-	-	X	-
74	FES	AC	301	-	-	X	-
74	FES	AP	301	-	-	X	-
74	FES	BO	301	-	-	X	-
74	FES	O	301	-	-	X	-
75	CDL	AG	101	-	-	X	-
75	CDL	AL	502	-	-	X	-
76	PEE	AH	401	-	-	X	-
76	PEE	AL	503	-	-	X	-
76	PEE	AU	401	-	-	X	-
76	PEE	AV	403	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
76	PEE	AY	502	-	-	X	-
76	PEE	BV	202	-	-	X	-
76	PEE	B1	701	-	-	X	-
76	PEE	V	202	-	-	X	-
76	PEE	1	701	-	-	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	2712	1759	482	463	8	0	0

- 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	274	173	47	53	1	0	0
10	BK	33	274	173	47	53	1	0	0

- 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	964	608	173	179	4	0	0
11	BL	118	964	608	173	179	4	0	0

- 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	5274	3310	917	1009	38	0	0
12	BM	687	5274	3310	917	1009	38	0	0

- 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	1195	770	210	212	3	0	0
13	BN	143	1195	770	210	212	3	0	0

- 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	1924	1231	329	349	15	0	0

- Molecule 66 is a protein called Cytochrome b.

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

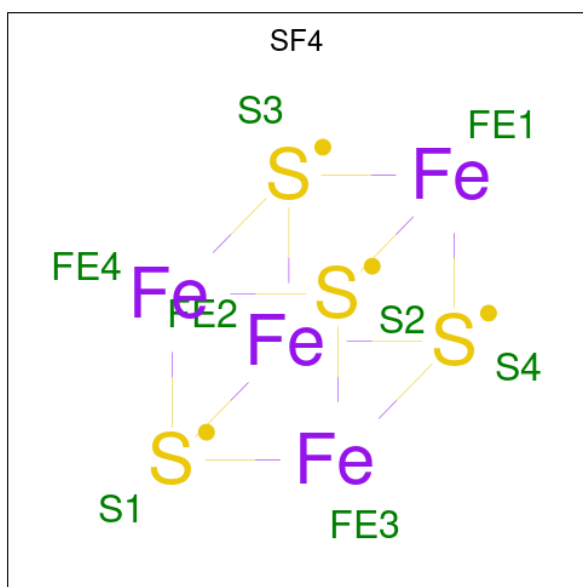
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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

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

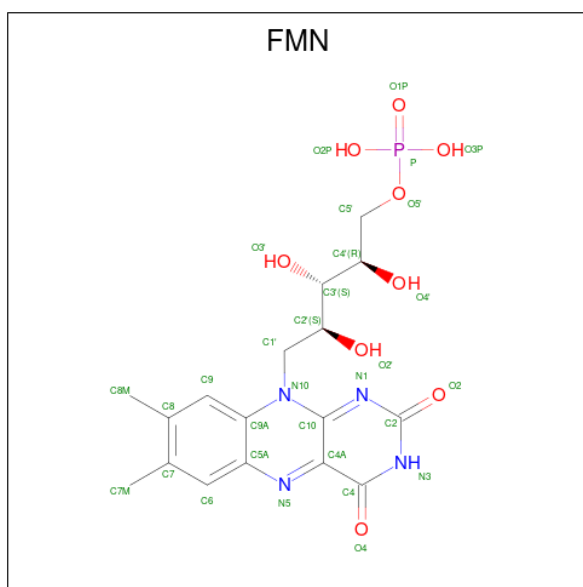
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AL	446	3442	2160	602	660	20	0	0
68	AY	446	3428	2147	601	660	20	0	0

- Molecule 69 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



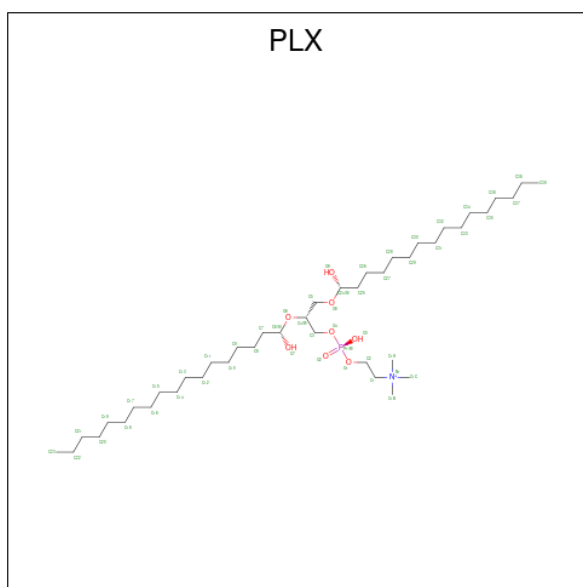
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
69	A	1	8	4	4	0
69	B	1	8	4	4	0
69	B	1	8	4	4	0
69	C	1	8	4	4	0
69	M	1	8	4	4	0
69	M	1	8	4	4	0
69	BA	1	8	4	4	0
69	BB	1	8	4	4	0
69	BB	1	8	4	4	0
69	BC	1	8	4	4	0
69	BM	1	8	4	4	0
69	BM	1	8	4	4	0

- Molecule 70 is FLAVIN MONONUCLEOTIDE (CCD ID: 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 (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



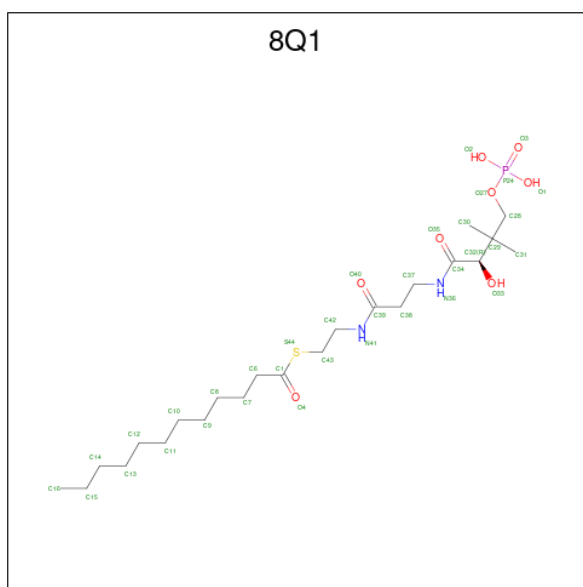
Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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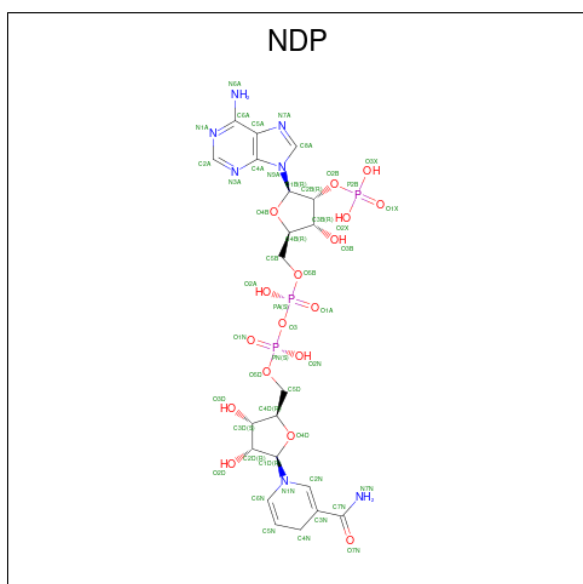
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
71	U	1	Total 52	C 42	N 1	O 8	P 1	0
71	b	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 52	C 42	N 1	O 8	P 1	0
71	g	1	Total 52	C 42	N 1	O 8	P 1	0
71	r	1	Total 52	C 42	N 1	O 8	P 1	0
71	r	1	Total 52	C 42	N 1	O 8	P 1	0
71	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 52	C 42	N 1	O 8	P 1	0
71	Bg	1	Total 52	C 42	N 1	O 8	P 1	0
71	Bg	1	Total 52	C 42	N 1	O 8	P 1	0
71	Br	1	Total 52	C 42	N 1	O 8	P 1	0
71	Br	1	Total 52	C 42	N 1	O 8	P 1	0

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



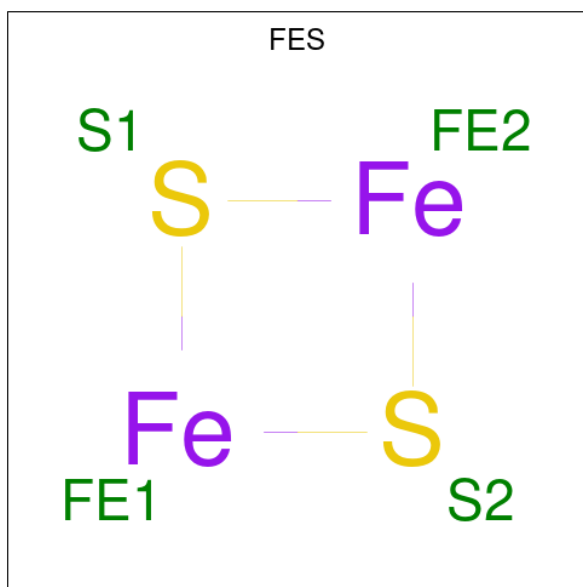
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
72	E	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	BE	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
72	Bp	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



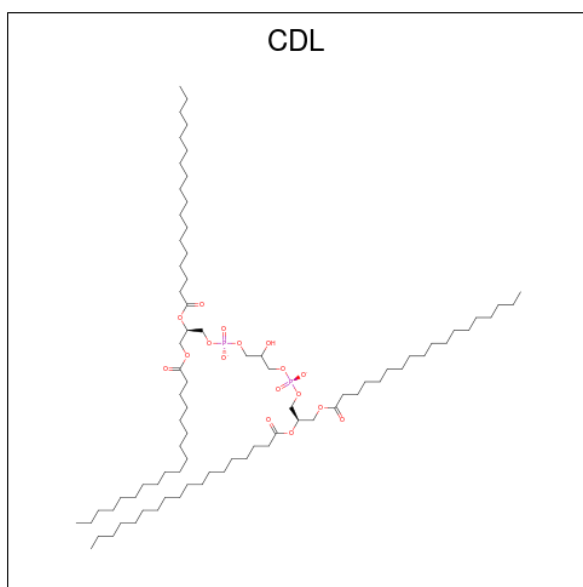
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
73	J	1	48	21	7	17	3	0
73	BJ	1	48	21	7	17	3	0

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



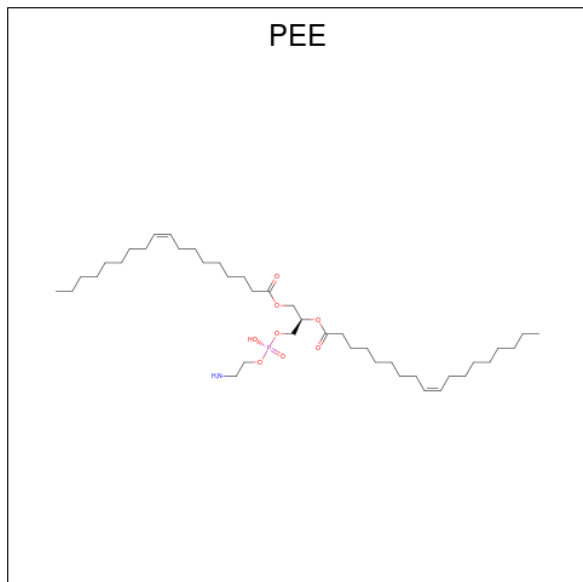
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
75	V	1	63	44	17	2	0
75	i	1	64	45	17	2	0
75	l	1	64	45	17	2	0
75	l	1	64	45	17	2	0
75	n	1	64	45	17	2	0
75	AA	1	64	45	17	2	0
75	AG	1	64	45	17	2	0
75	AH	1	64	45	17	2	0
75	AJ	1	64	45	17	2	0
75	AJ	1	64	45	17	2	0
75	AL	1	64	45	17	2	0
75	AN	1	64	45	17	2	0
75	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 64	C 45	O 17	P 2	0
75	Bl	1	Total 64	C 45	O 17	P 2	0
75	Bn	1	Total 64	C 45	O 17	P 2	0

- Molecule 76 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: 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 49	C 39	N 1	O 8	P 1	0
76	l	1	Total 51	C 41	N 1	O 8	P 1	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
76	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AU	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	AV	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AY	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	BV	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	BW	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	Bl	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	Bl	1	Total	C	N	O	P	0
			51	41	1	8	1	

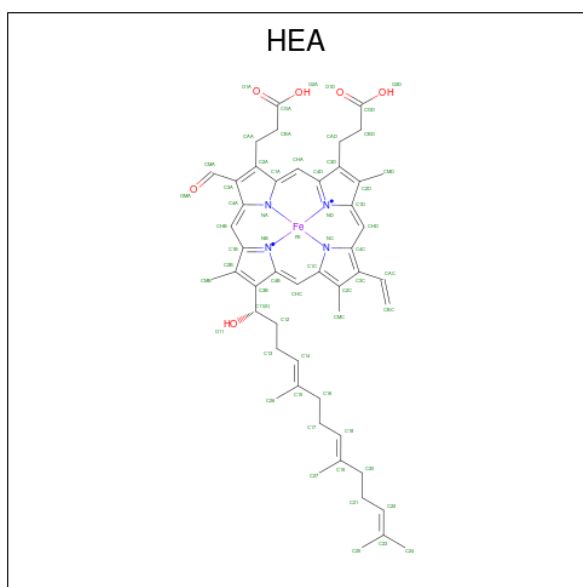
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

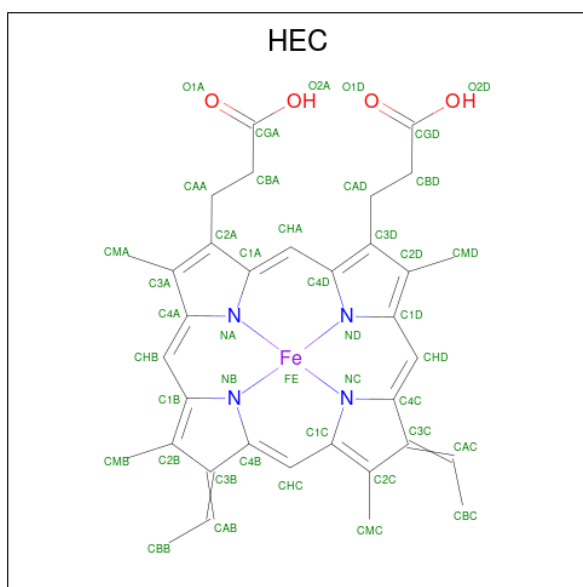


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
79	x	1	60	49	1	4	6	0
79	x	1	60	49	1	4	6	0
79	Bx	1	60	49	1	4	6	0
79	Bx	1	60	49	1	4	6	0

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

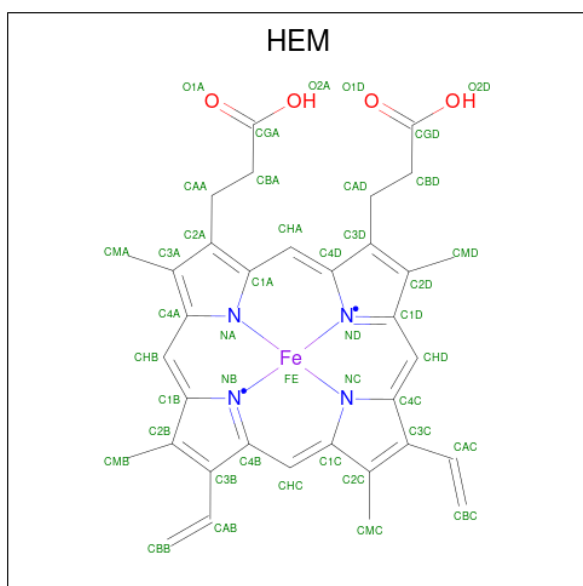
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	2	1	1	1	0
80	B2	1	1	1	0

- Molecule 81 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
82	AJ	1	43	34	1	4	4	0

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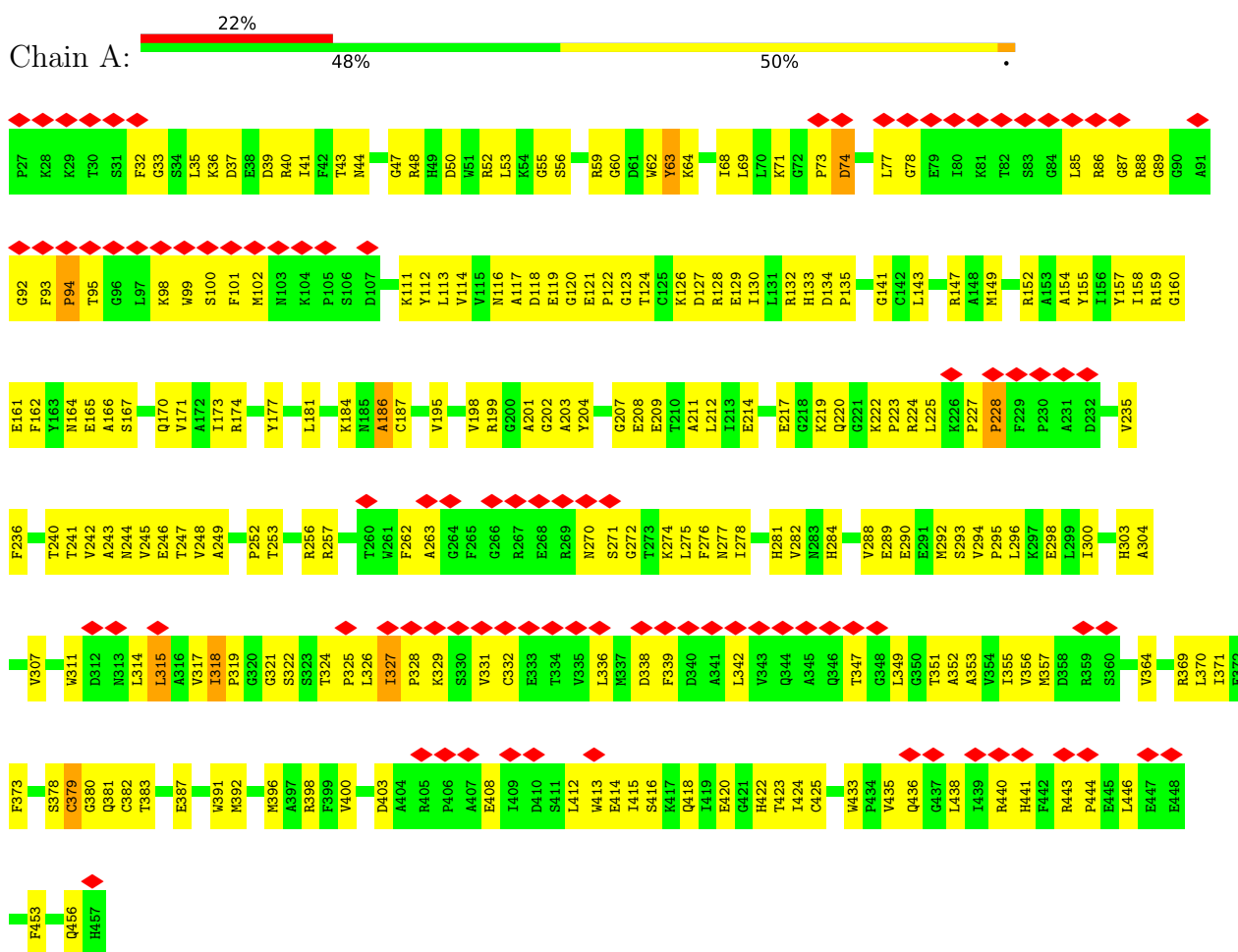
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
82	AJ	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0

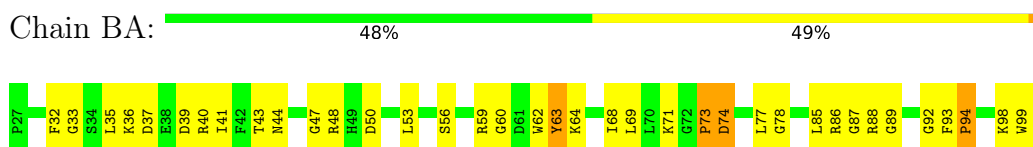
3 Residue-property plots

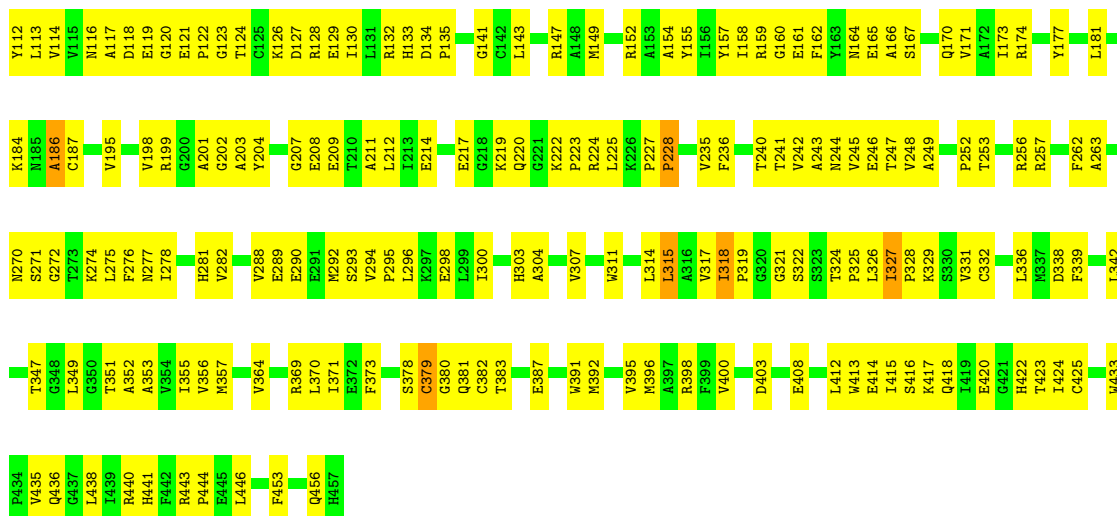
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

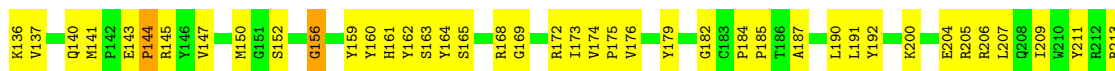


• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

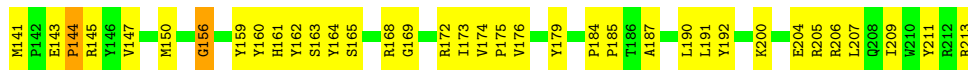


• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

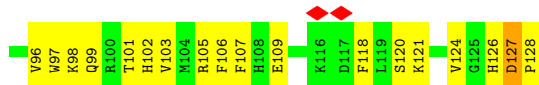




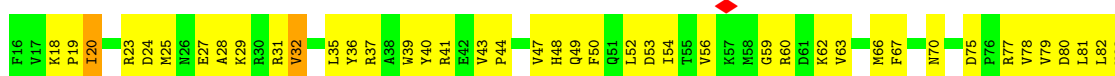
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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



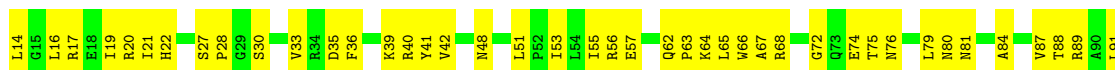
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

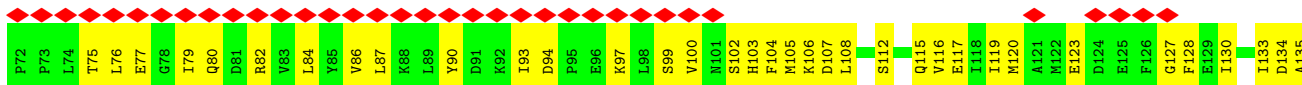


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2





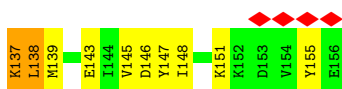
- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



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

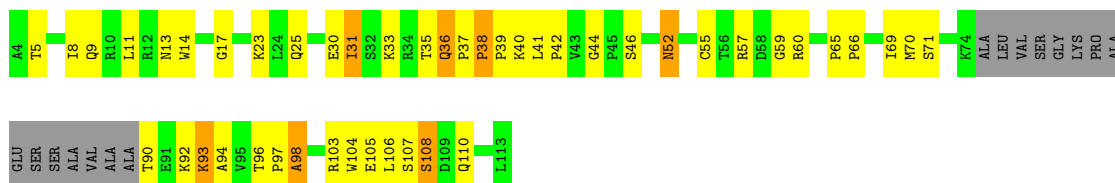




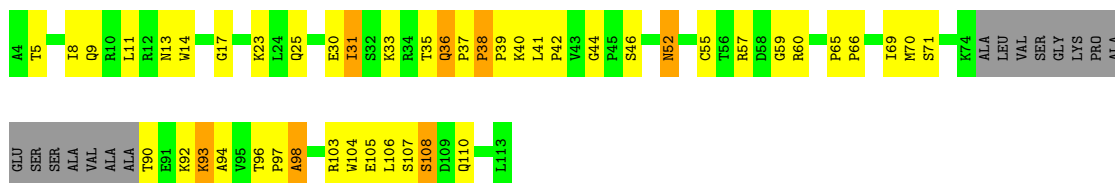
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



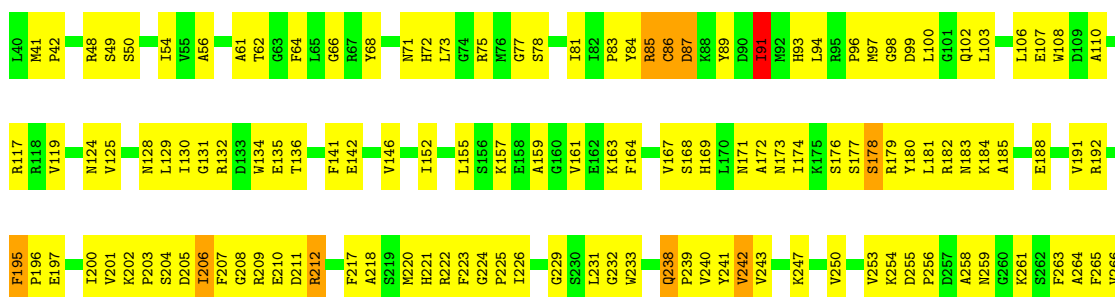
• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

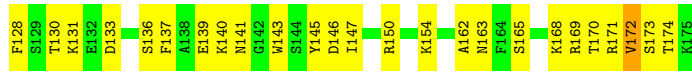


• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

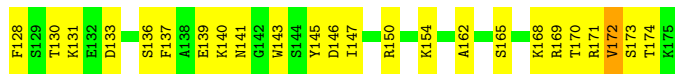
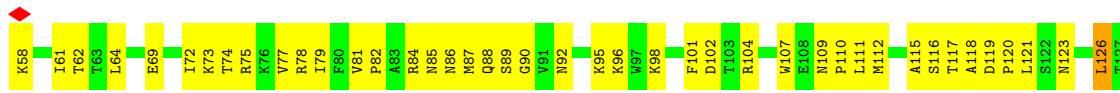


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

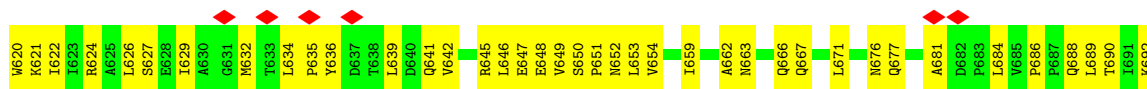
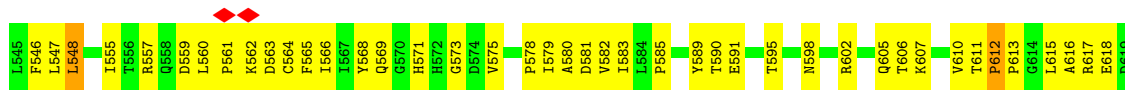
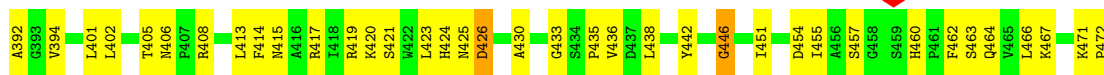
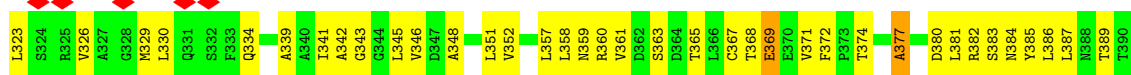
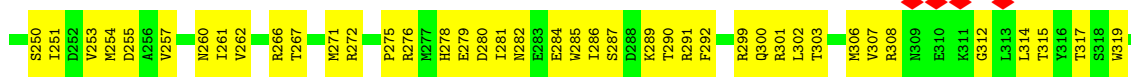
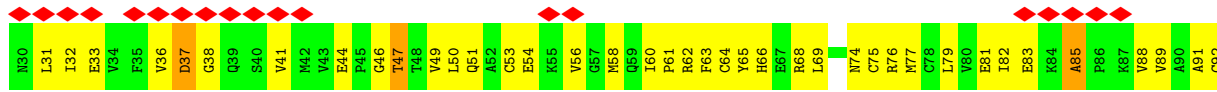




● Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

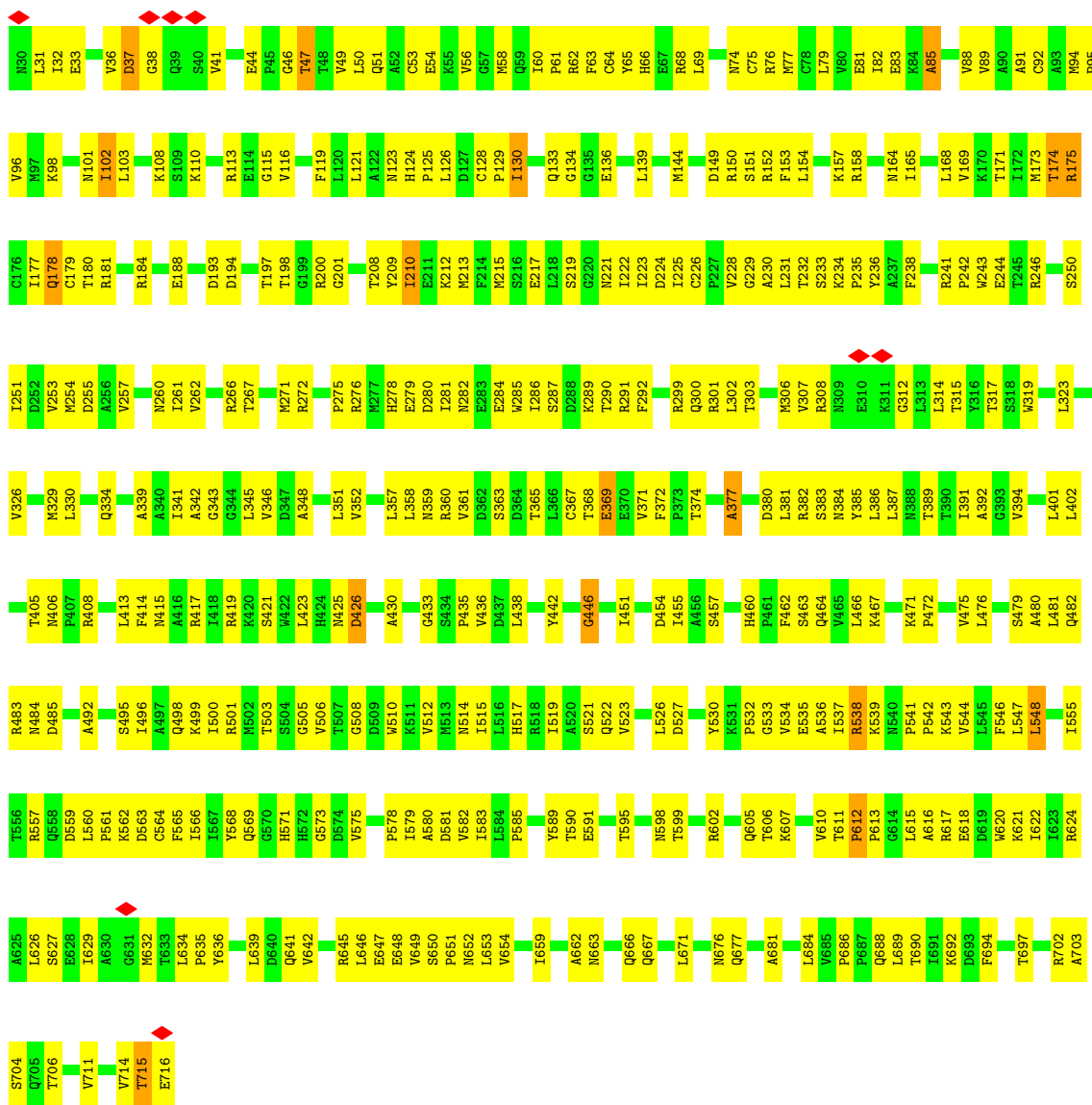


● Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





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

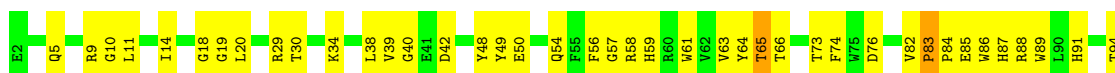


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

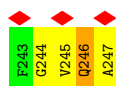
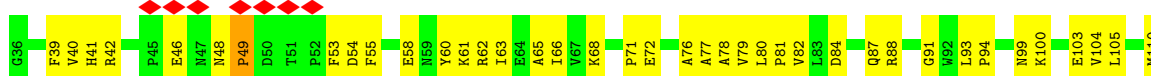




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

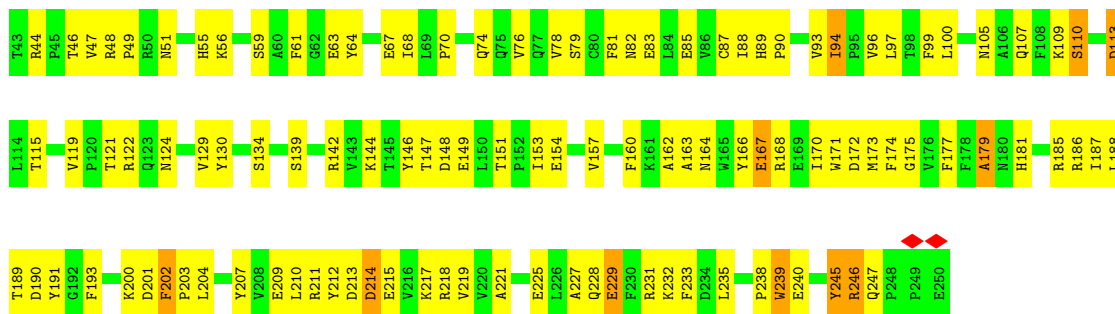


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

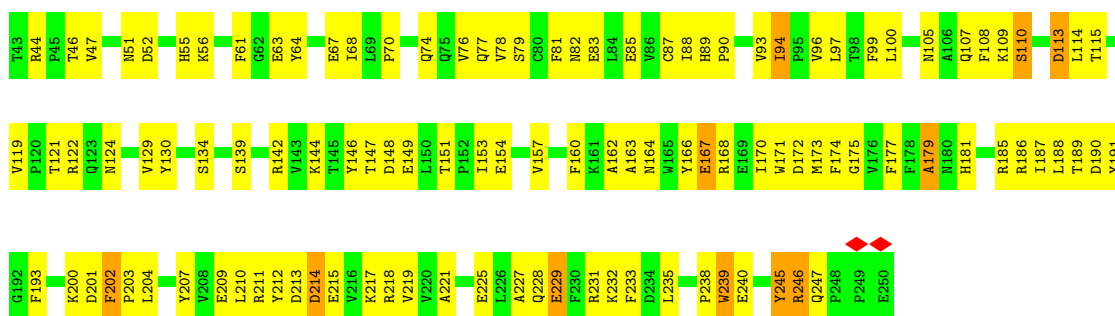


- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

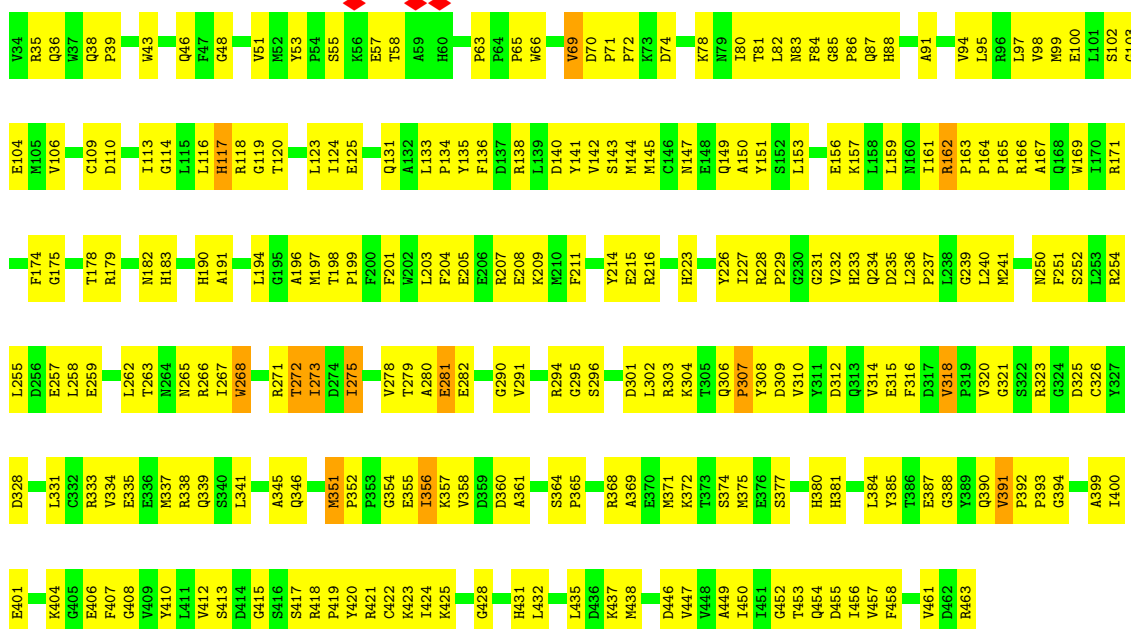




• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

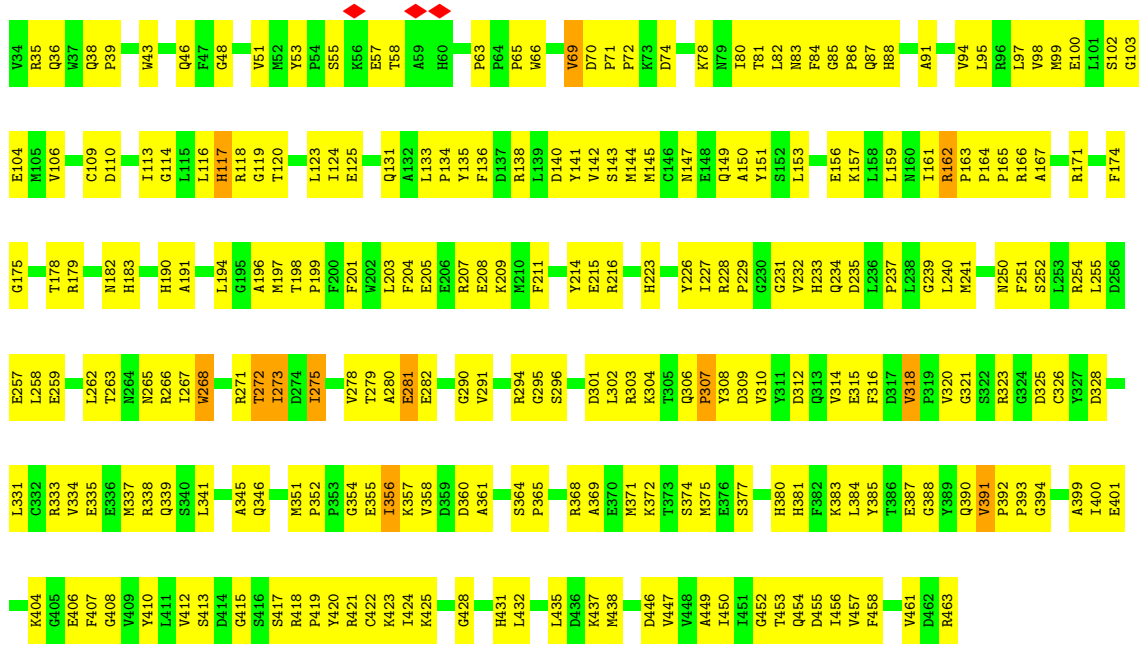


• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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





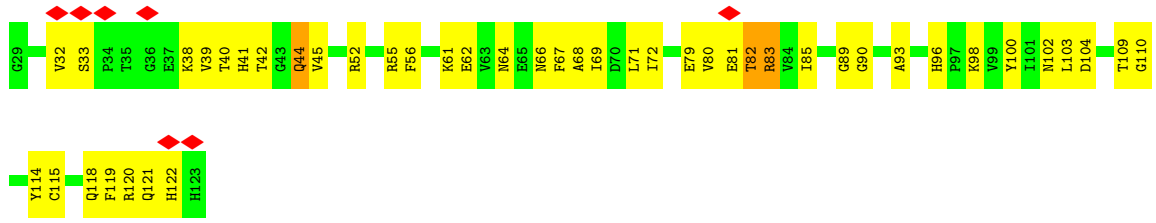
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

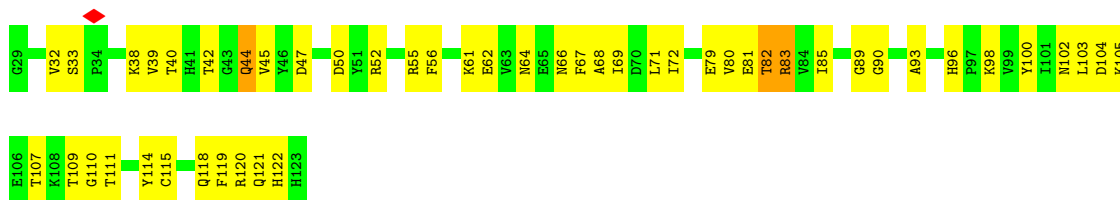


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

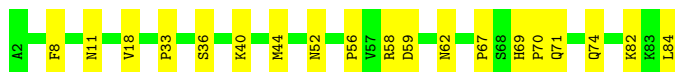


• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

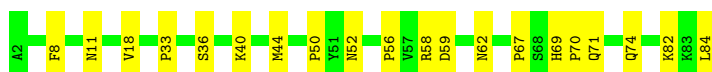
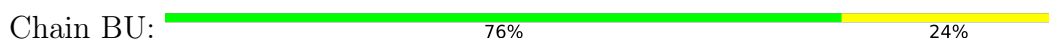




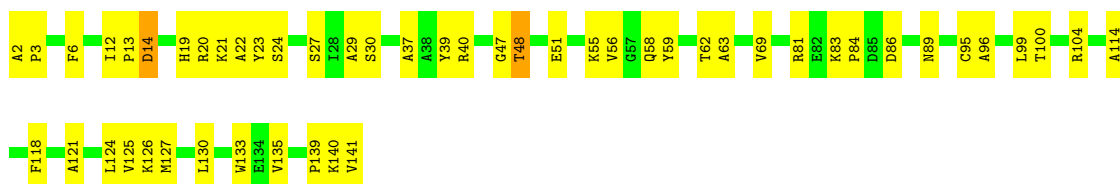
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



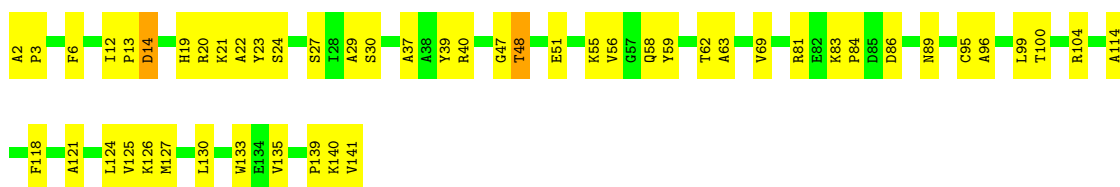
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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



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



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

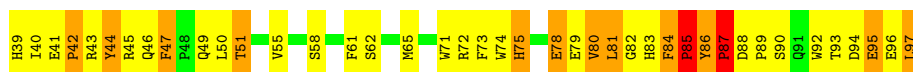




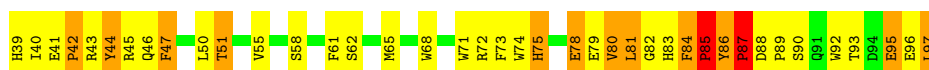
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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



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



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

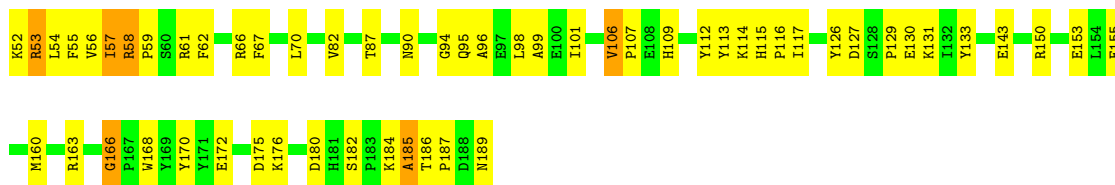


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



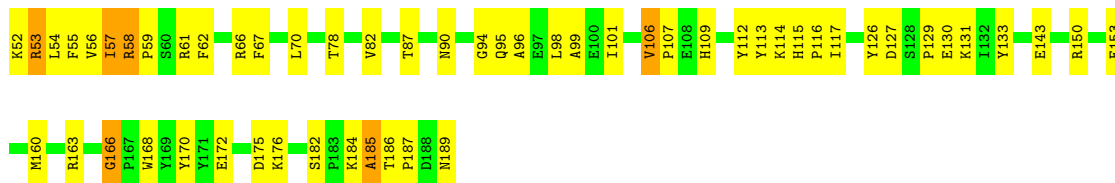
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial





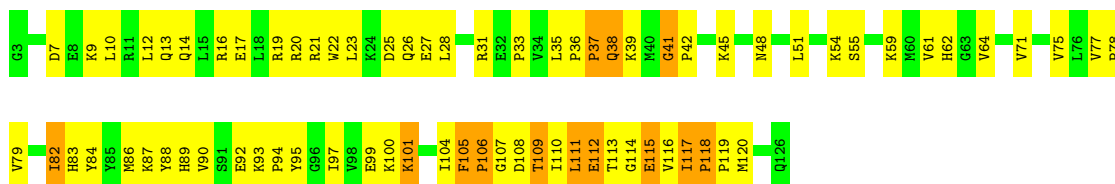
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain Ba: 60% 36%



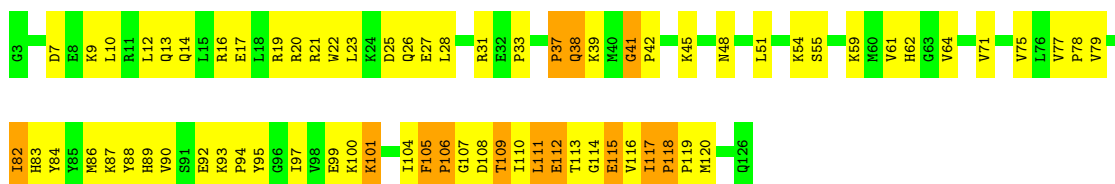
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 41% 48% 10%



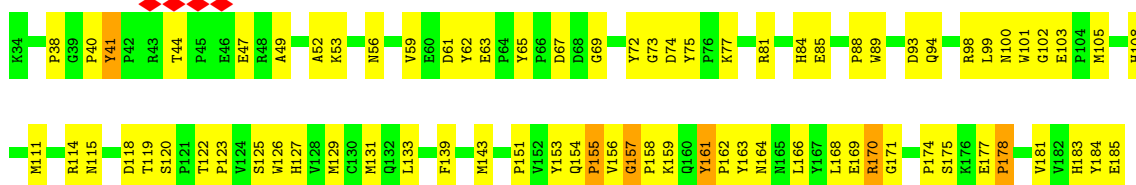
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain Bb: 43% 47% 10%



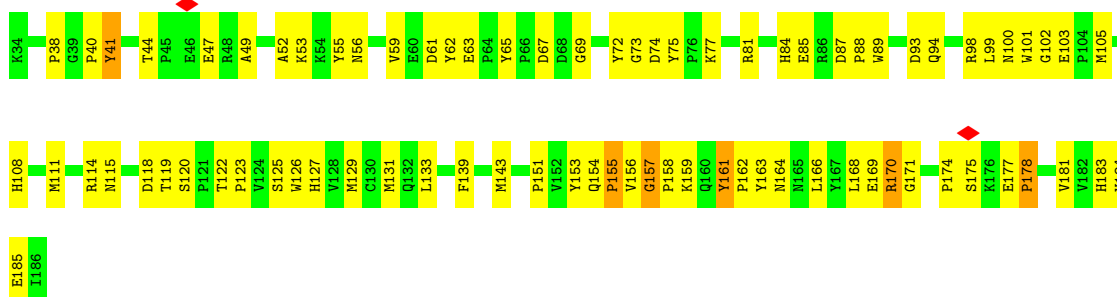
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 50% 46%

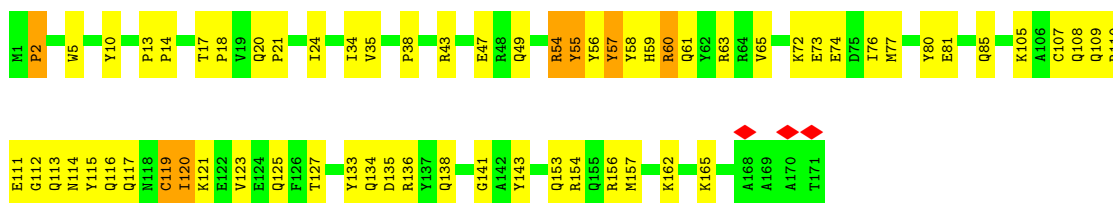


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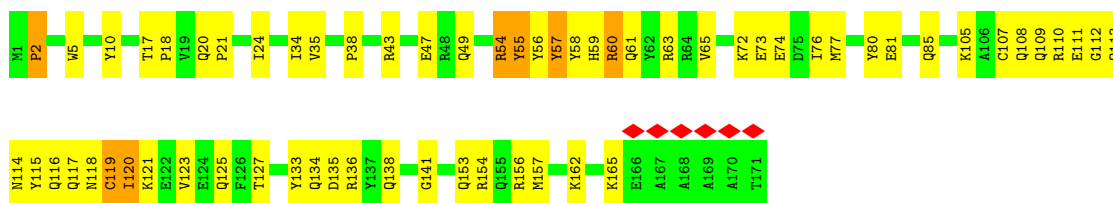
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain Bc:  48% 48%

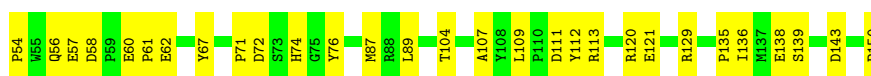
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  62% 34%

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

Chain Bd:  63% 33%

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

Chain e:  70% 30%

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

Chain Be:  69% 31%



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

Chain f:  66% 30%



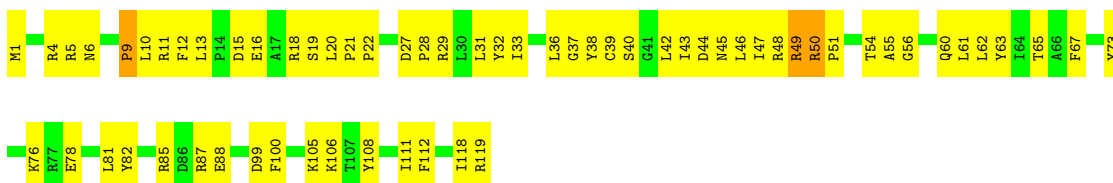
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain Bf:  66% 30%



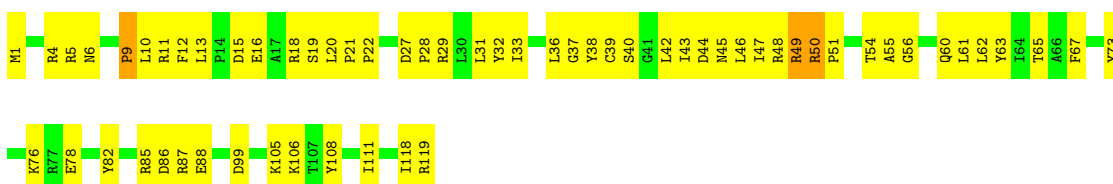
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  47% 50%



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

Chain Bg:  49% 49%

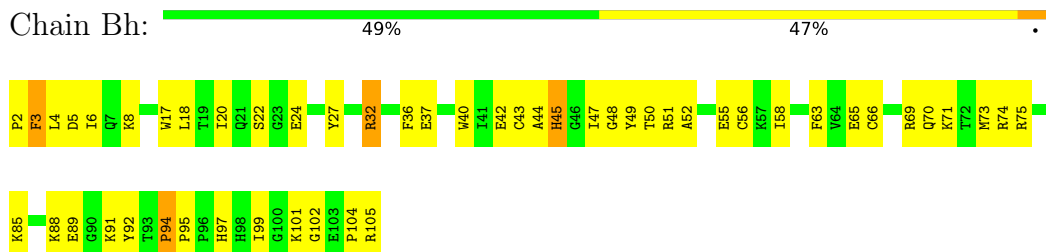


- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

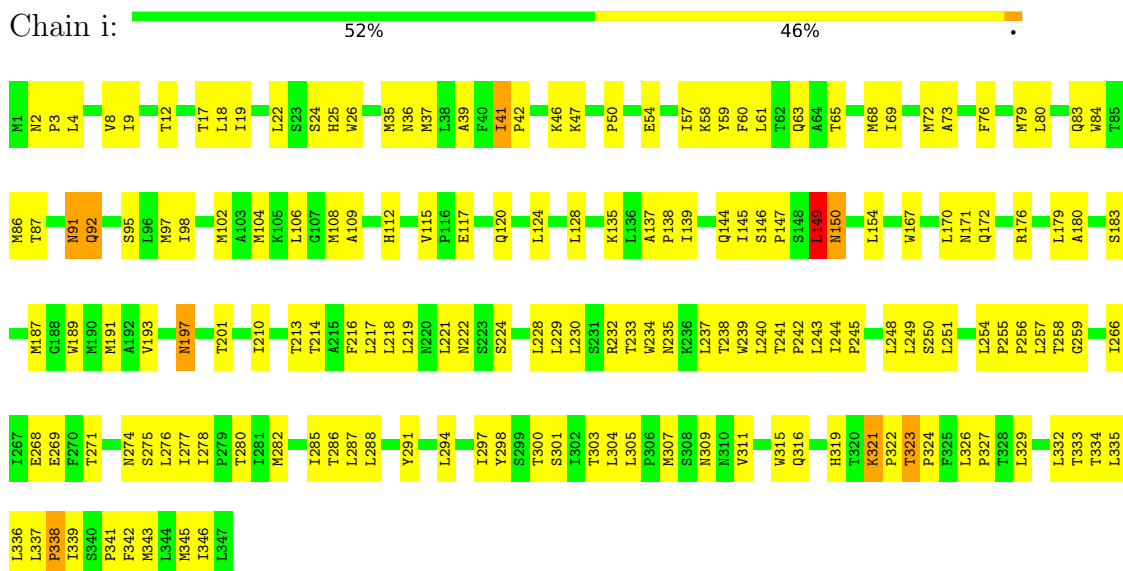
Chain h:  48% 47% 5%



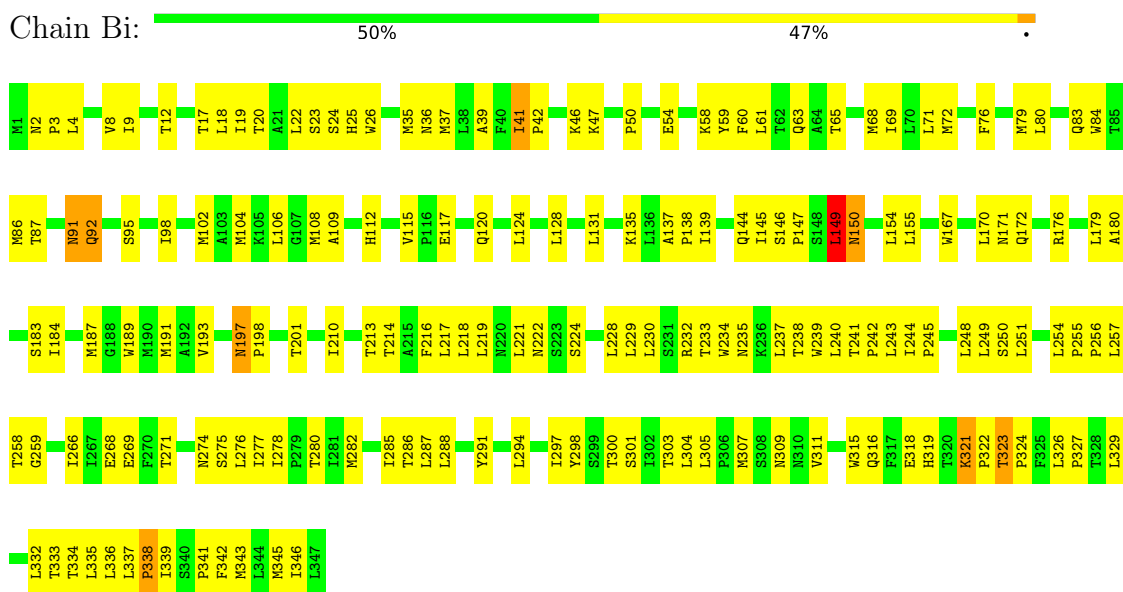
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

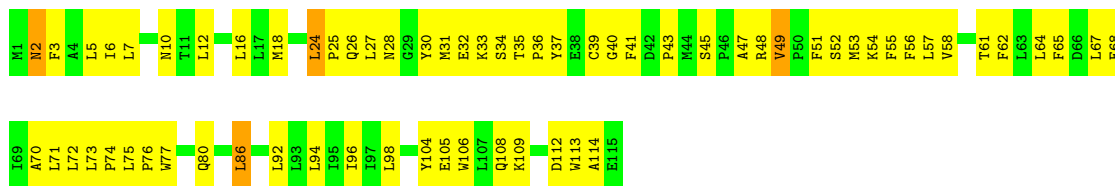


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



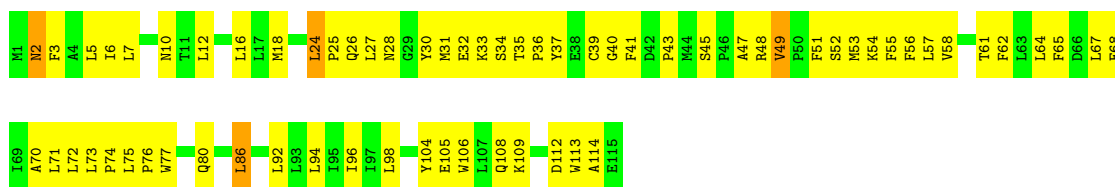
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 



• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain Bj: 



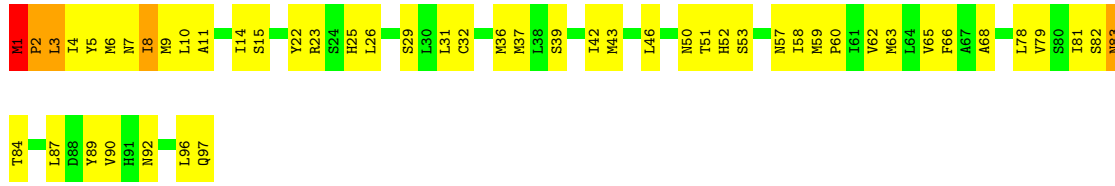
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 



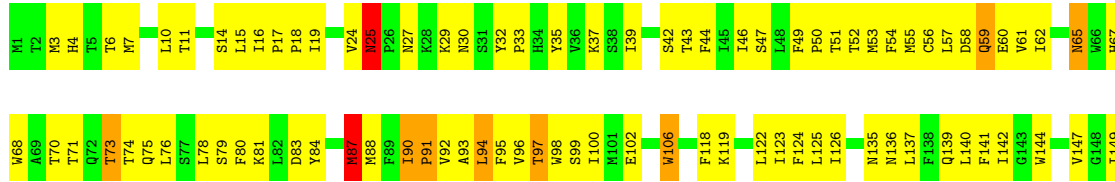
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

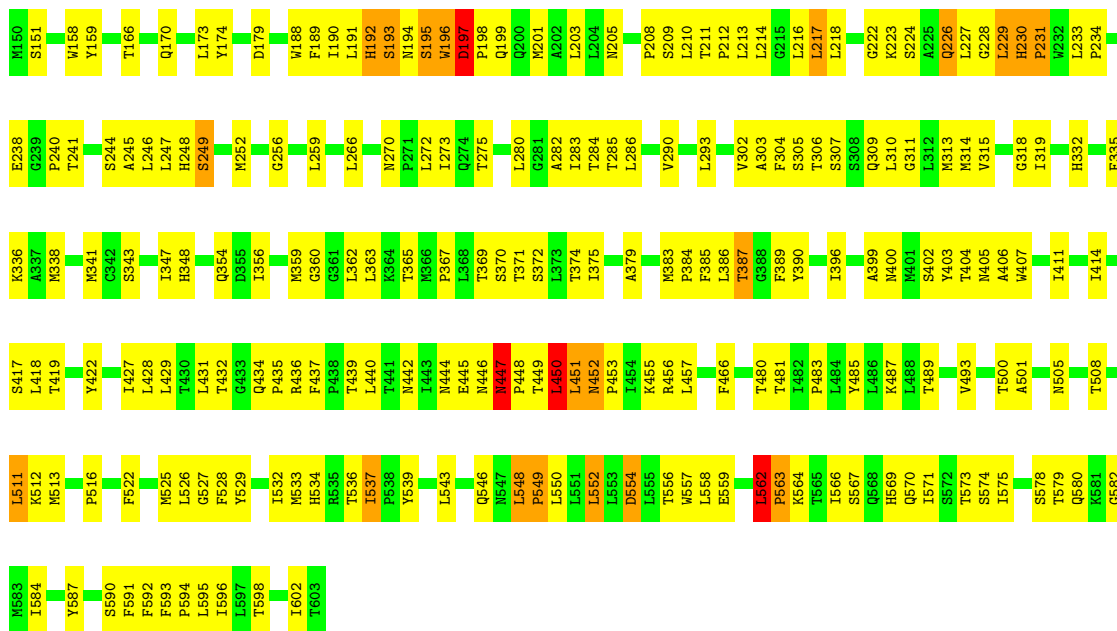
Chain Bk: 



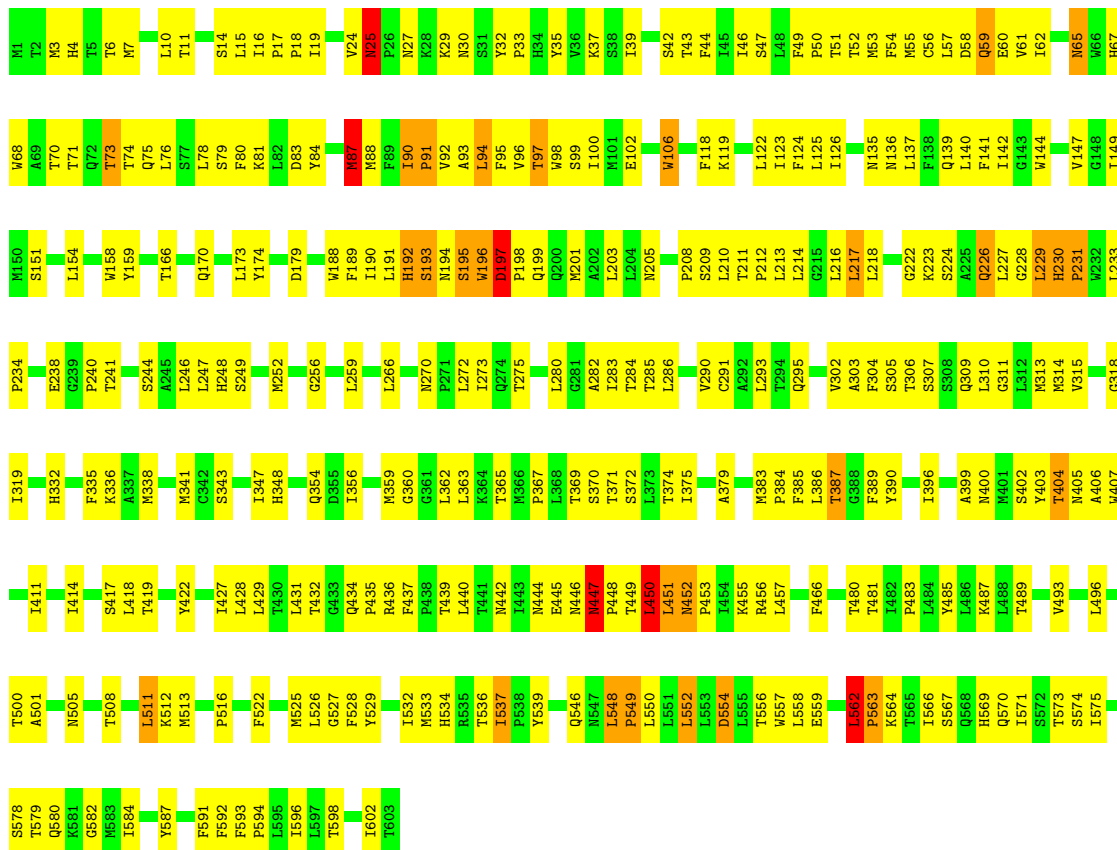
• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 



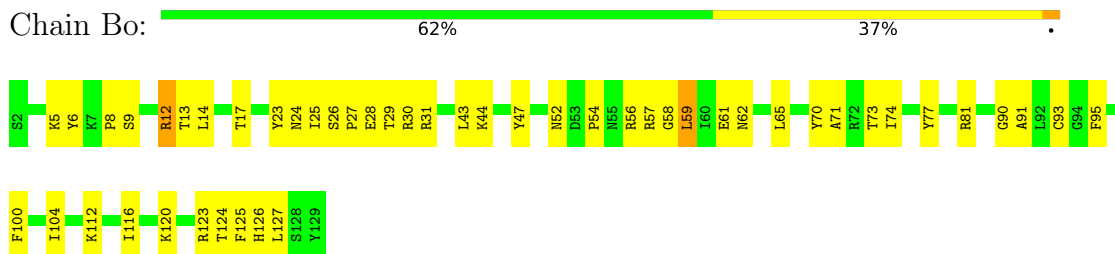


• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

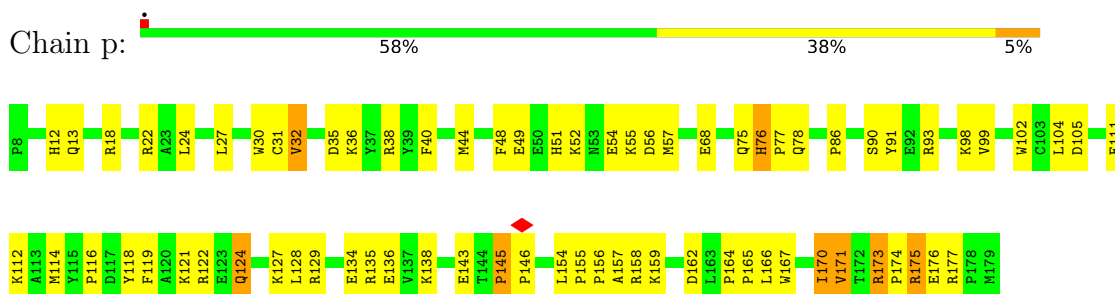


• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

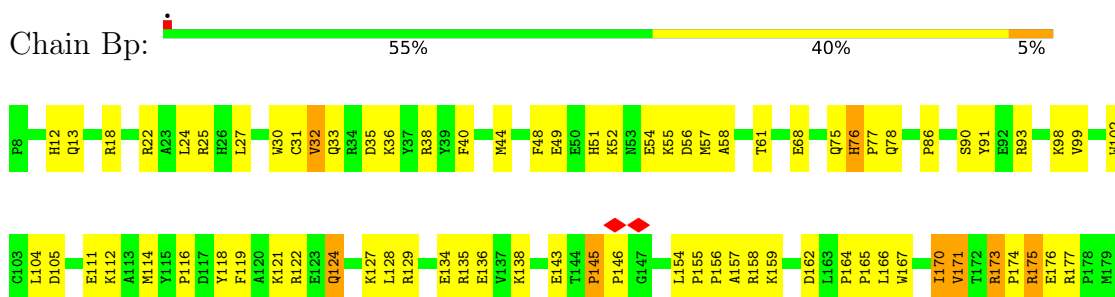
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



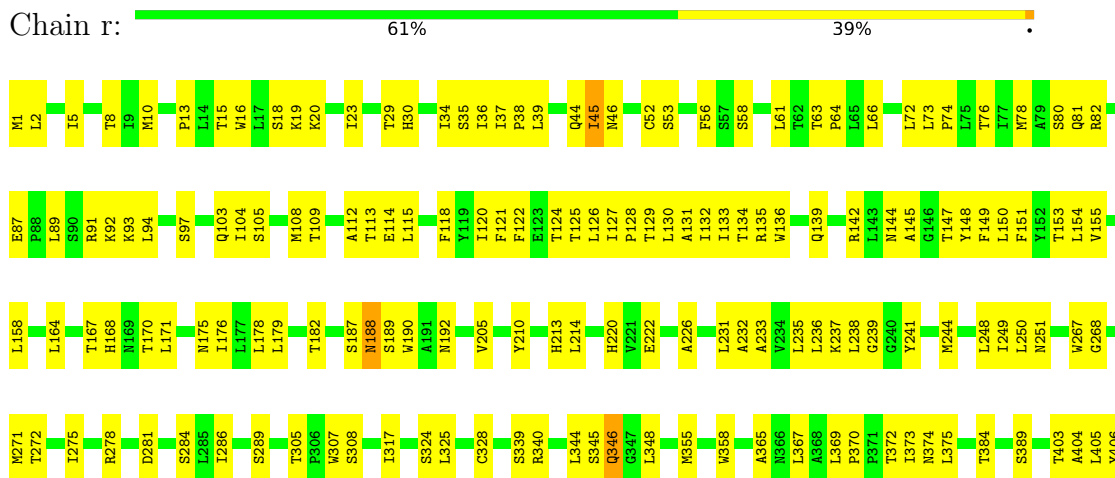
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

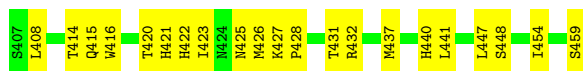


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



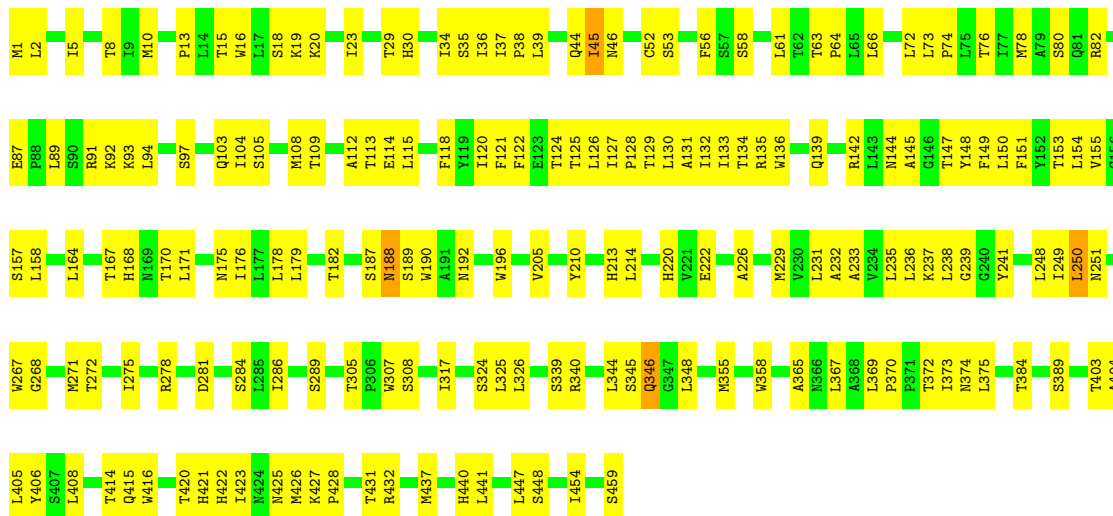
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4





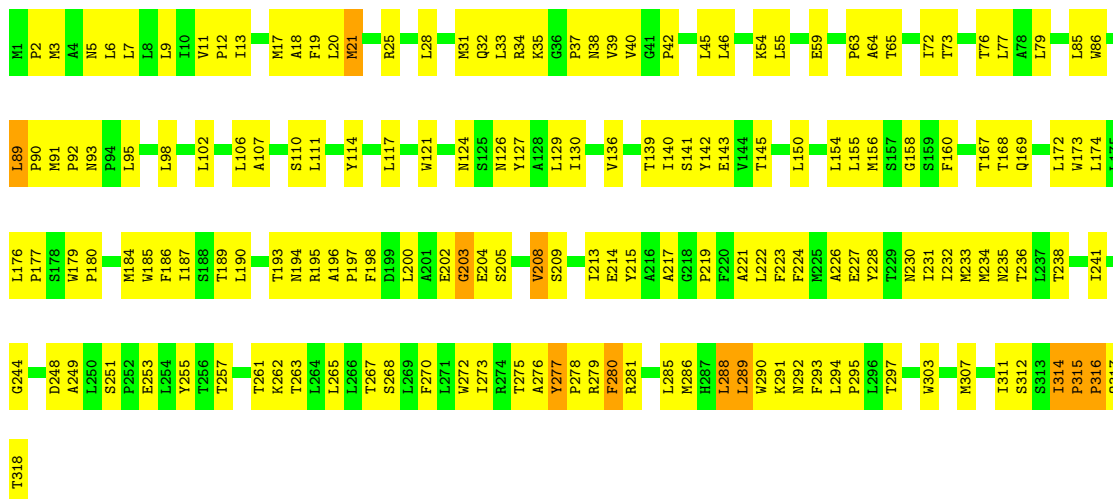
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain Br: 60% 39%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

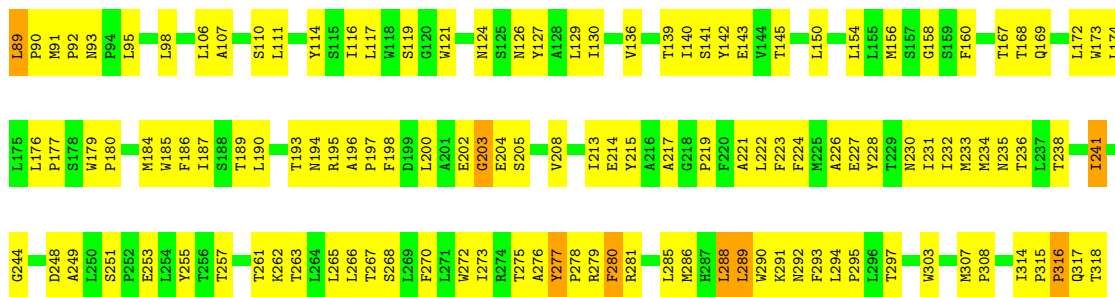
Chain s: 47% 49%



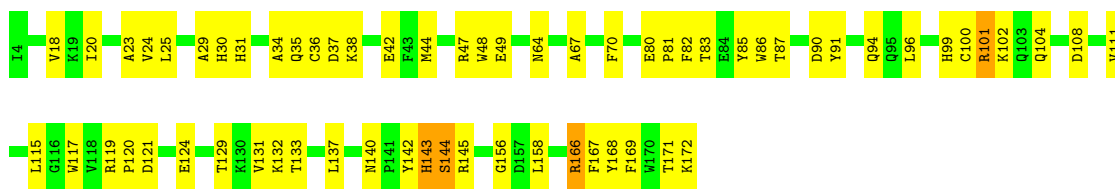
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain Bs: 48% 49%

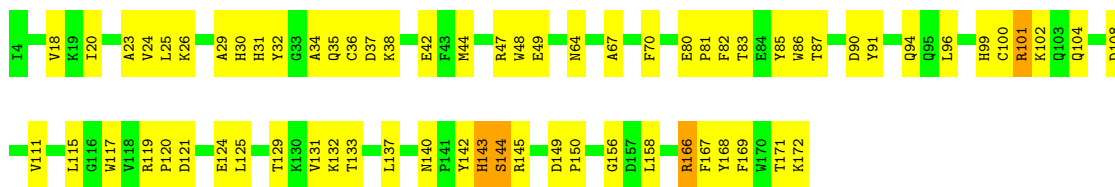




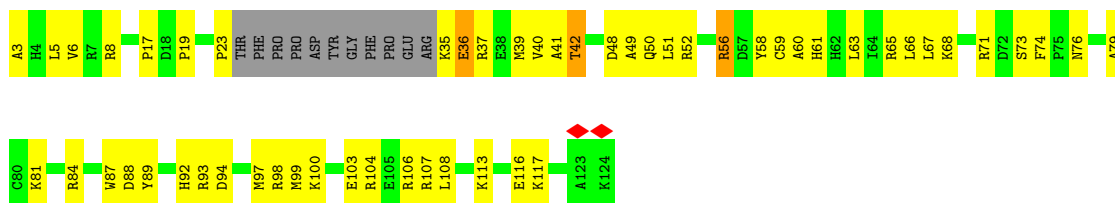
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



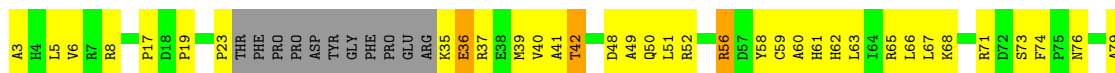
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

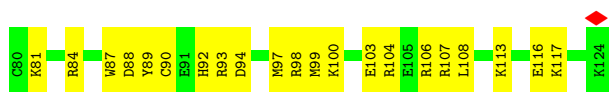


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



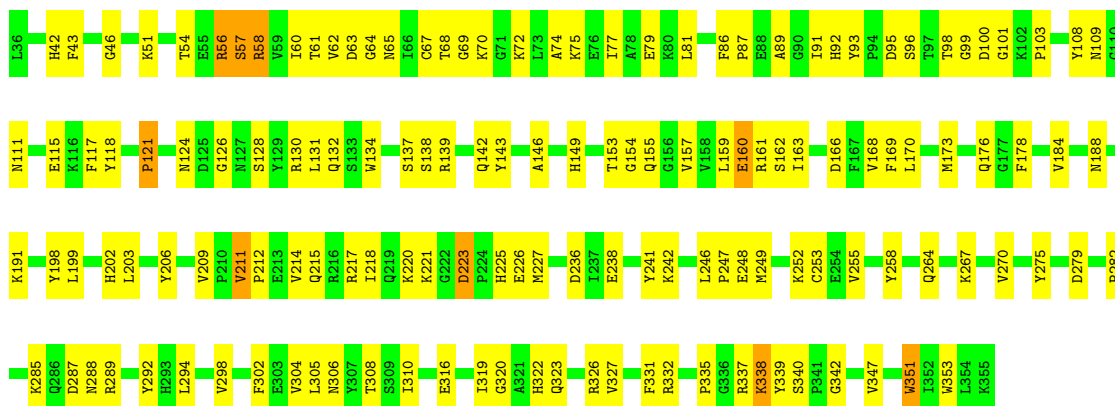
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7





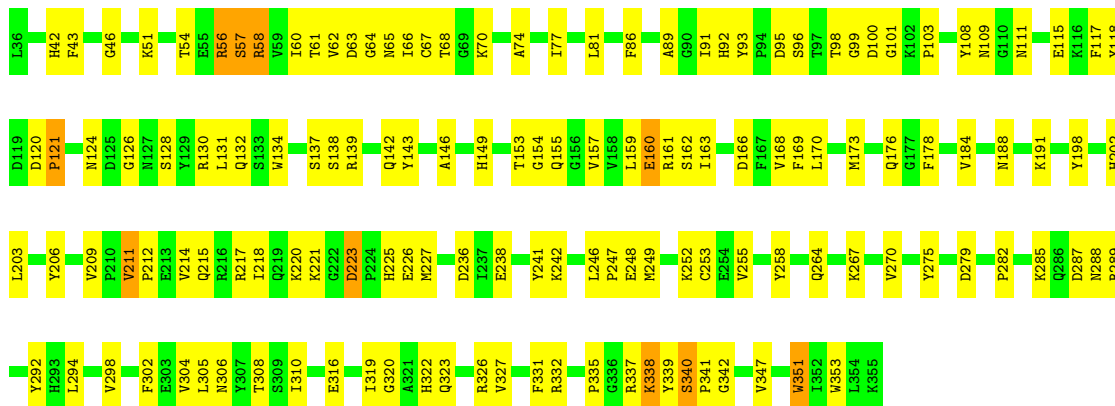
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w: 55% 42%



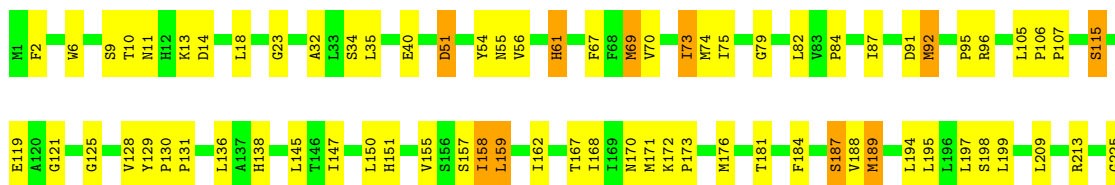
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain Bw: 56% 41%



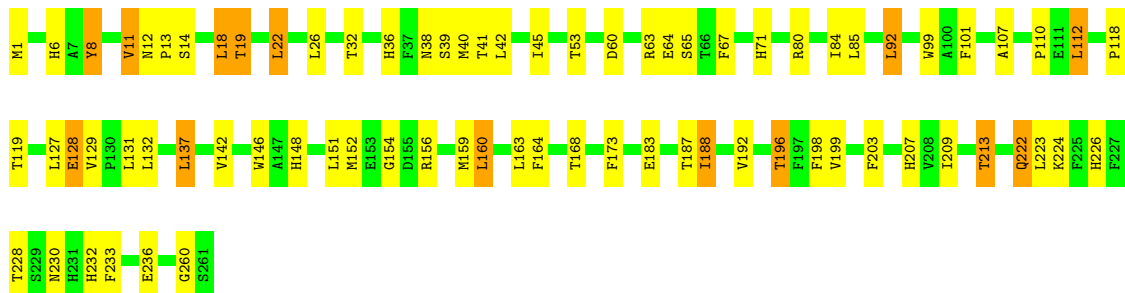
- Molecule 45: Cytochrome c oxidase subunit 1

Chain x: 68% 26% 5%

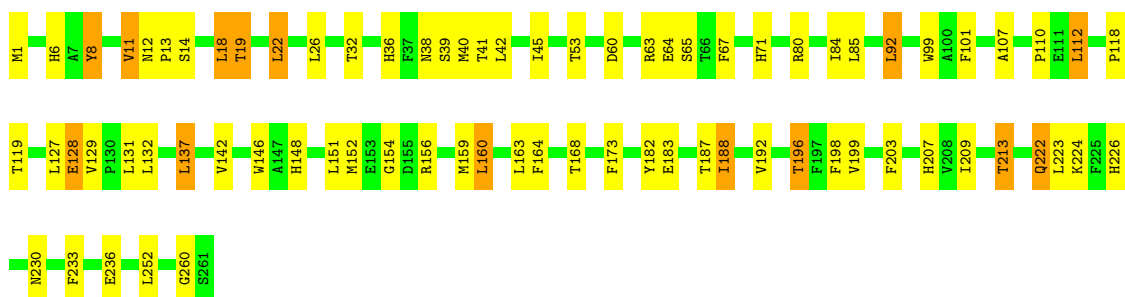




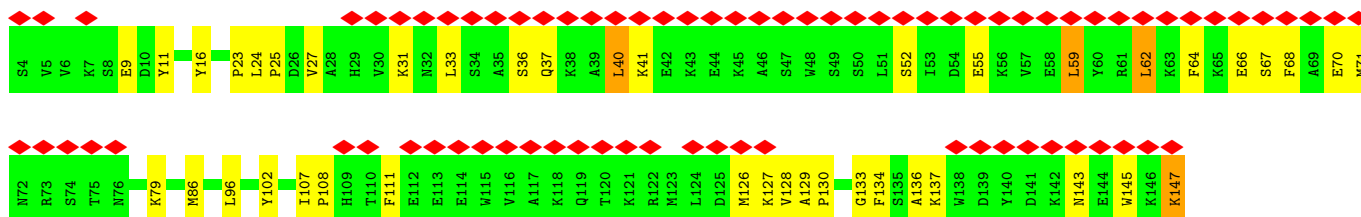
• Molecule 47: Cytochrome c oxidase subunit 3



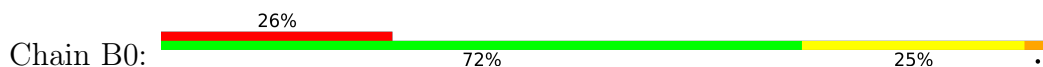
• Molecule 47: Cytochrome c oxidase subunit 3

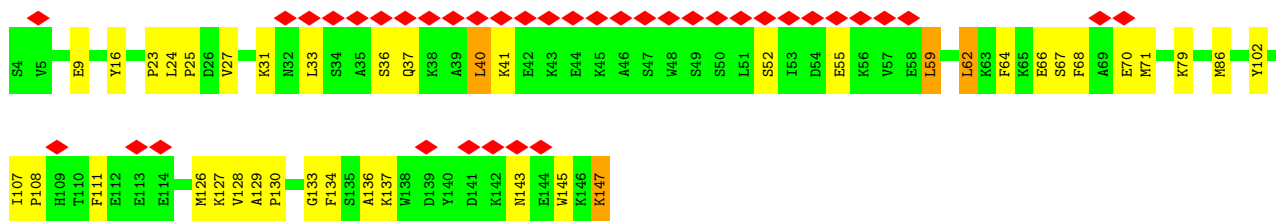


• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

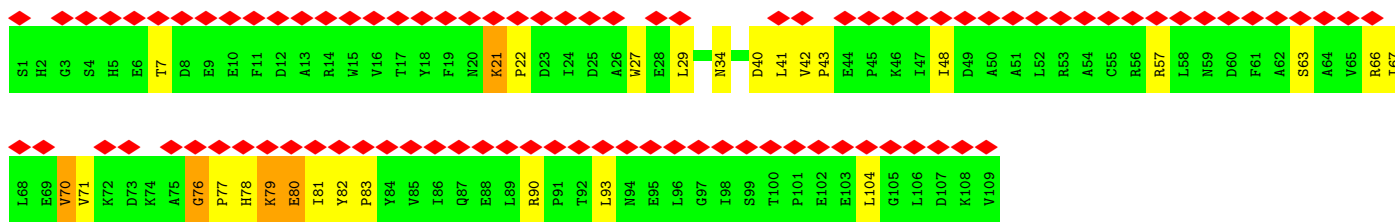
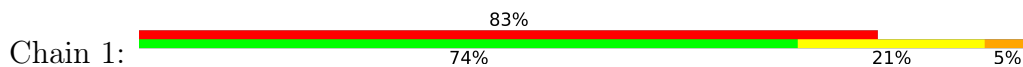


• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

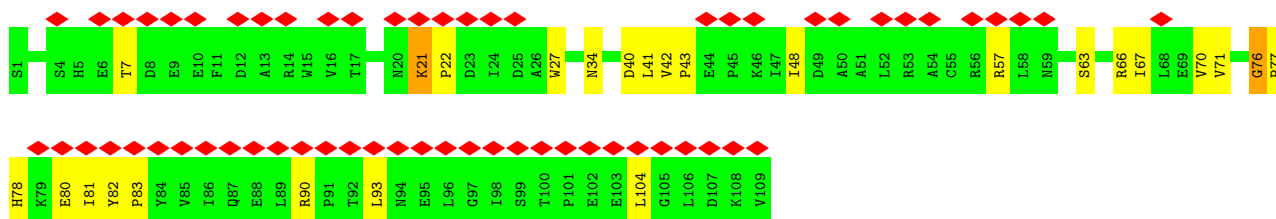
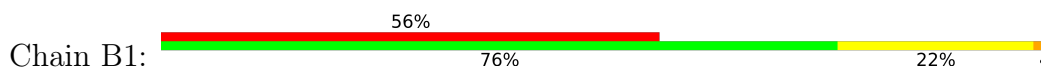




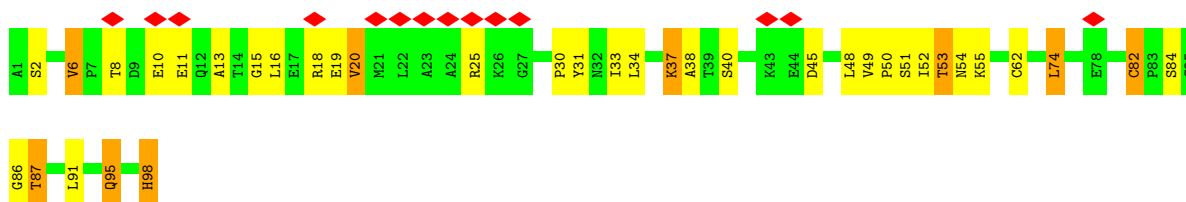
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



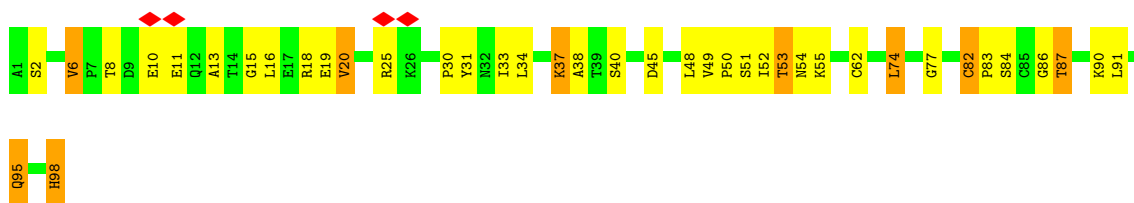
- Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial



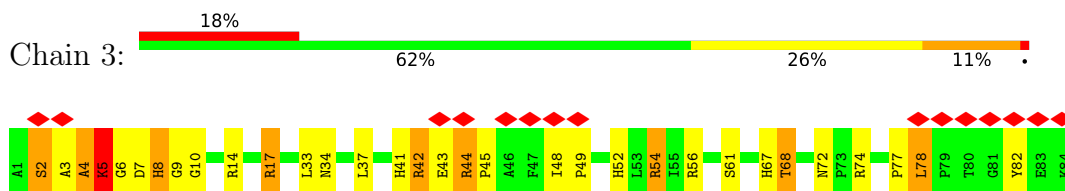
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



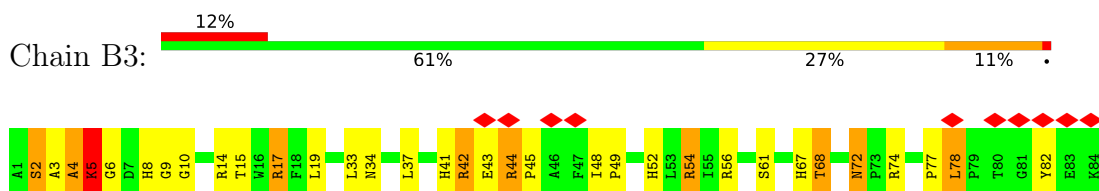
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



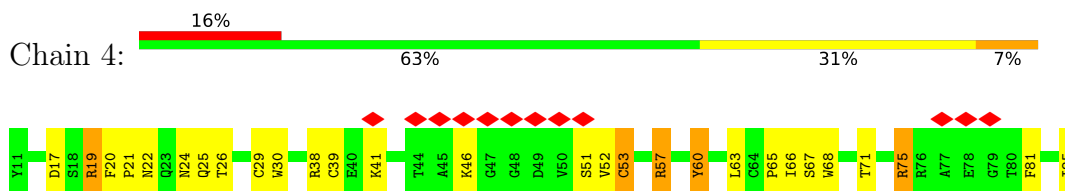
• Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



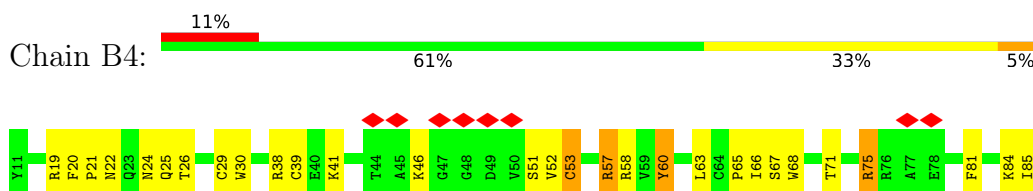
• Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



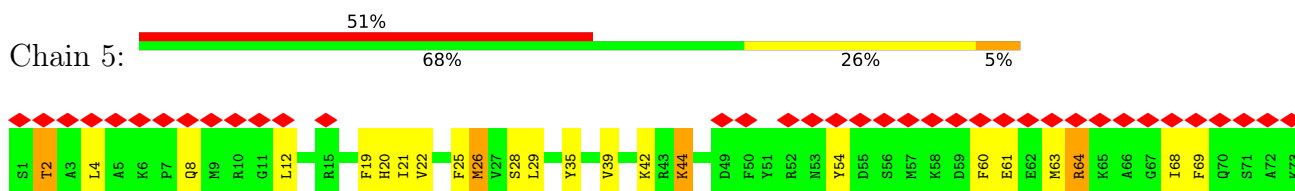
• Molecule 52: Cytochrome c oxidase subunit 6B1



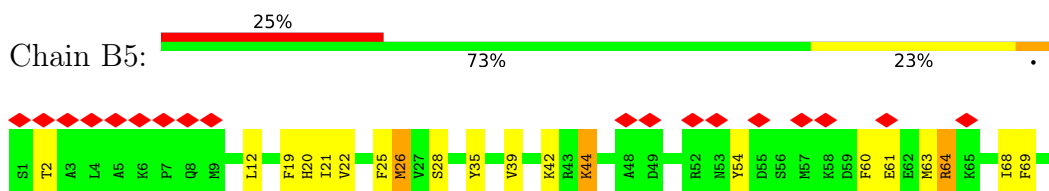
• Molecule 52: Cytochrome c oxidase subunit 6B1



• Molecule 53: Cytochrome c oxidase subunit 6C



• Molecule 53: Cytochrome c oxidase subunit 6C



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

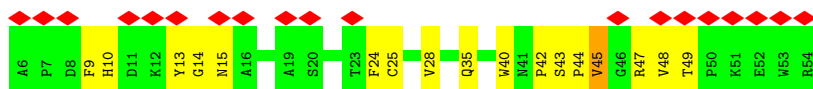




- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



- 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



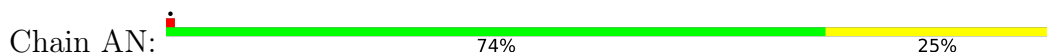
- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 58: Cytochrome b-c1 complex subunit 8



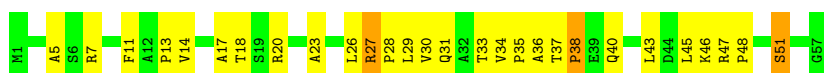
- Molecule 58: Cytochrome b-c1 complex subunit 8



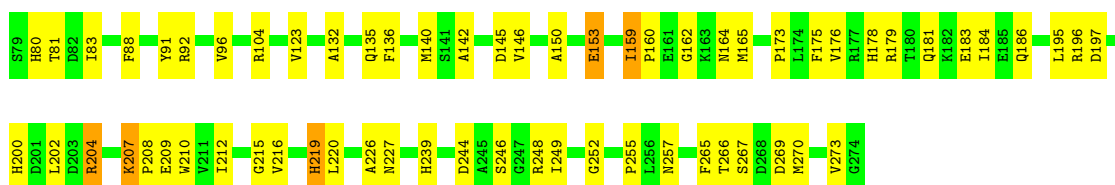
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

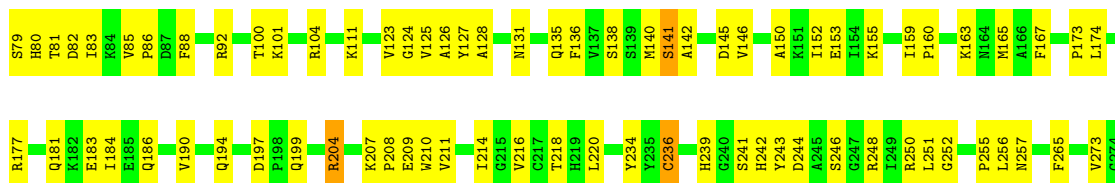


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

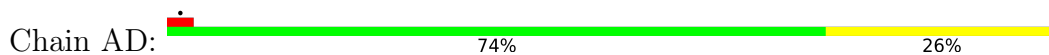


- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

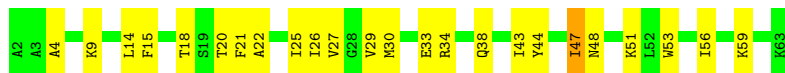




• Molecule 61: Cytochrome b-c1 complex subunit 9



• Molecule 61: Cytochrome b-c1 complex subunit 9



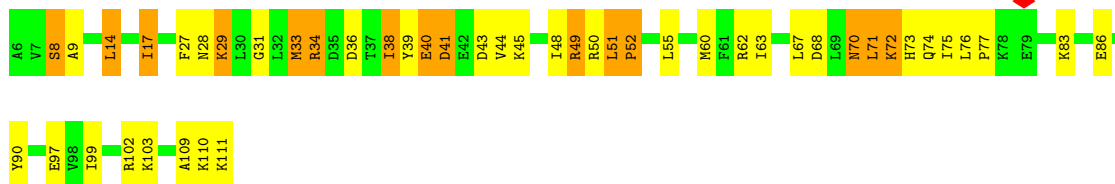
• Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



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

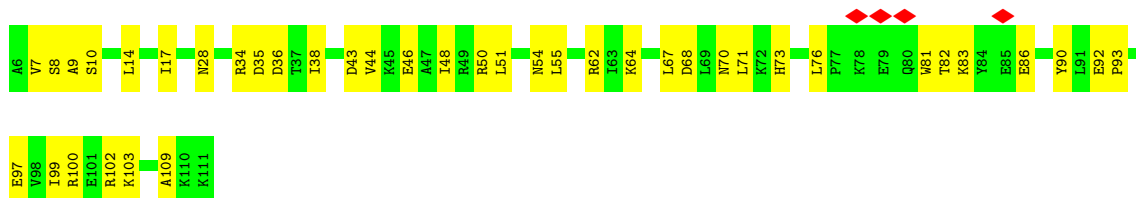


• Molecule 63: Cytochrome b-c1 complex subunit 7

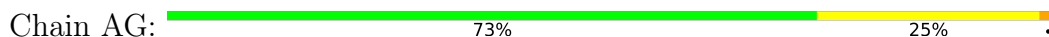


• Molecule 63: Cytochrome b-c1 complex subunit 7





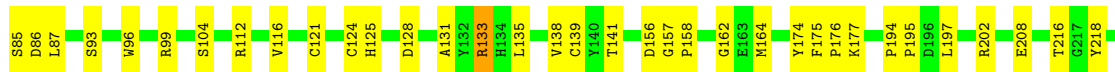
• Molecule 64: Cytochrome b-c1 complex subunit 10



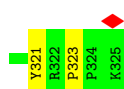
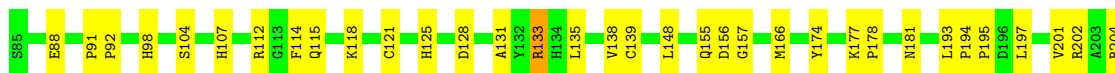
• Molecule 64: Cytochrome b-c1 complex subunit 10



• Molecule 65: Cytochrome c1, heme protein, mitochondrial



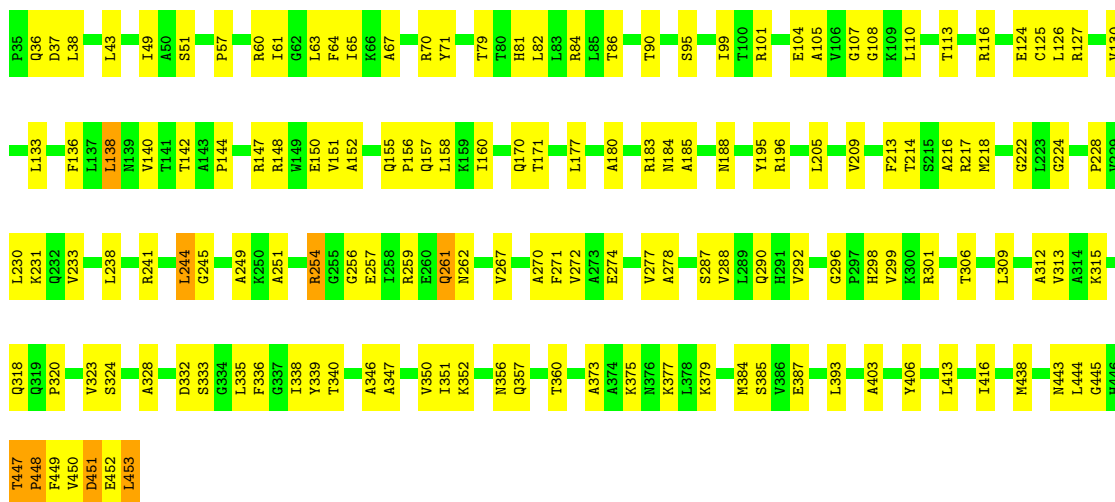
• Molecule 65: Cytochrome c1, heme protein, mitochondrial



• Molecule 66: Cytochrome b

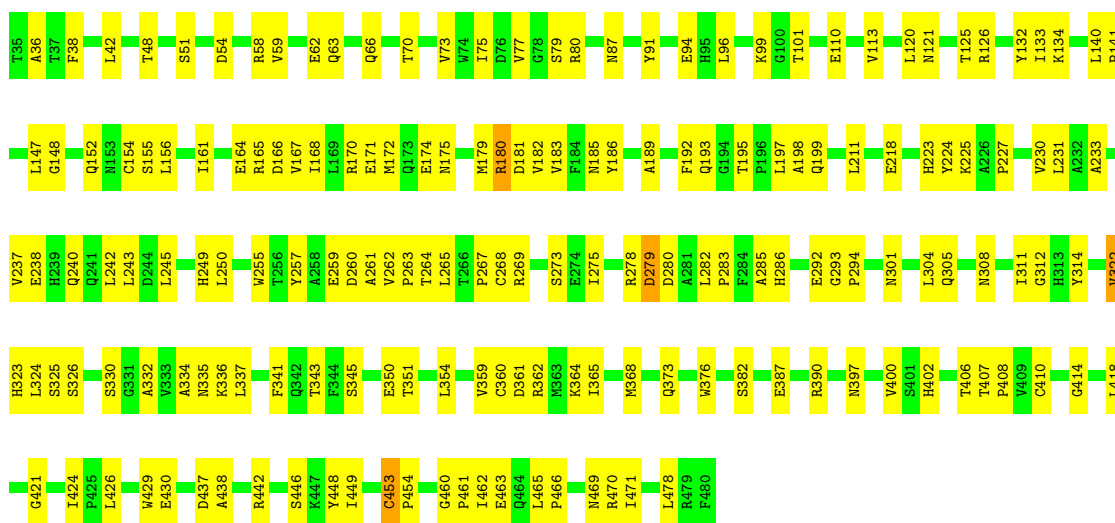


Chain AW: 64% 34%



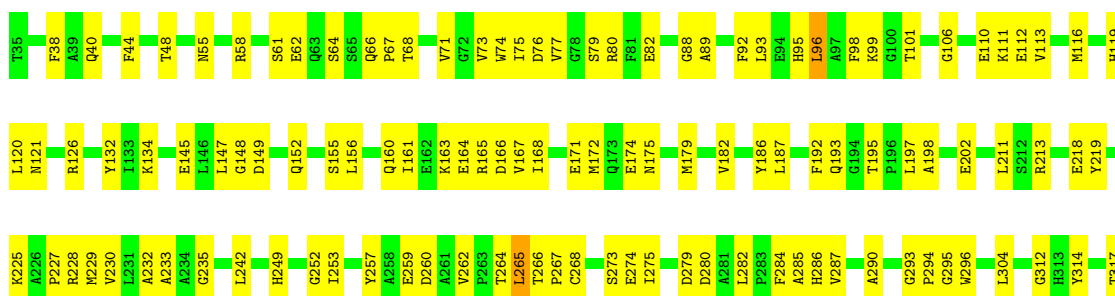
• Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

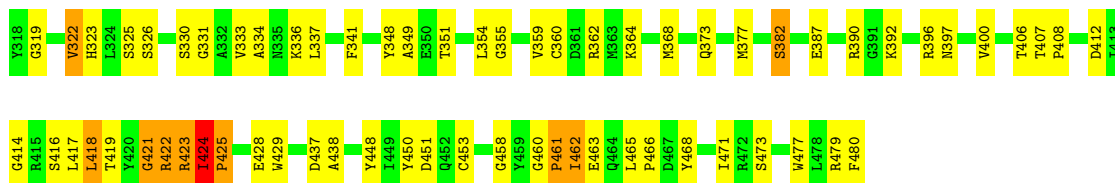
Chain AL: 61% 38%



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

Chain AY: 59% 38%





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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CDL, HEM, ZN, HEC, PEE, MG, SF4, CU, 8Q1, FMN, PLX, HEA, NDP

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	0.39	0/3398	0.87	6/4590 (0.1%)
1	BA	0.39	0/3398	0.87	6/4590 (0.1%)
2	B	0.59	0/1452	0.96	10/1964 (0.5%)
2	BB	0.59	0/1452	0.96	9/1964 (0.5%)
3	BC	0.74	0/1280	0.93	3/1732 (0.2%)
3	C	0.74	0/1280	0.93	3/1732 (0.2%)
4	BE	0.44	0/993	0.92	3/1335 (0.2%)
4	E	0.44	0/993	0.92	3/1335 (0.2%)
5	BF	0.37	0/682	0.87	0/922
5	F	0.37	0/682	0.87	0/922
6	BG	0.40	0/684	0.83	0/926
6	BX	0.71	0/698	0.89	0/942
6	G	0.40	0/684	0.83	0/926
6	X	0.71	0/698	0.89	0/942
7	BH	0.45	0/941	0.87	2/1275 (0.2%)
7	H	0.45	0/941	0.86	2/1275 (0.2%)
8	BI	0.45	0/788	1.10	7/1066 (0.7%)
8	I	0.45	0/788	1.10	7/1066 (0.7%)
9	BJ	0.44	0/2785	0.91	13/3771 (0.3%)
9	J	0.44	0/2785	0.91	13/3771 (0.3%)
10	BK	0.30	0/282	0.74	0/381
10	K	0.30	0/282	0.74	0/381
11	BL	0.42	0/987	0.83	1/1331 (0.1%)
11	L	0.42	0/987	0.83	1/1331 (0.1%)
12	BM	0.43	0/5362	0.87	11/7266 (0.2%)
12	M	0.43	0/5362	0.87	9/7266 (0.1%)
13	BN	0.44	0/1236	0.91	7/1681 (0.4%)
13	N	0.44	0/1236	0.91	6/1681 (0.4%)
14	BO	0.40	0/1682	0.87	4/2289 (0.2%)
14	O	0.40	0/1682	0.87	4/2289 (0.2%)
15	BP	0.48	0/1780	0.94	5/2424 (0.2%)
15	P	0.48	0/1780	0.94	5/2424 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BQ	0.55	0/3552	1.01	14/4815 (0.3%)
16	Q	0.55	0/3552	1.01	14/4815 (0.3%)
17	BS	0.81	0/583	0.94	1/785 (0.1%)
17	S	0.81	0/583	0.94	1/785 (0.1%)
18	BT	0.38	0/755	0.79	0/1017
18	T	0.37	0/755	0.79	0/1017
19	BU	0.69	0/670	1.05	4/920 (0.4%)
19	U	0.69	0/670	1.05	4/920 (0.4%)
20	BV	0.64	0/1065	0.89	4/1450 (0.3%)
20	V	0.64	0/1065	0.89	4/1450 (0.3%)
21	BW	0.74	1/1166 (0.1%)	1.12	8/1579 (0.5%)
21	W	0.74	1/1166 (0.1%)	1.12	8/1579 (0.5%)
22	BY	0.61	0/559	1.16	7/763 (0.9%)
22	Y	0.62	0/559	1.16	7/763 (0.9%)
23	BZ	0.56	0/669	0.82	0/899
23	Z	0.56	0/669	0.81	0/899
24	Ba	0.85	0/1209	0.98	6/1639 (0.4%)
24	a	0.85	0/1209	0.98	6/1639 (0.4%)
25	Bb	0.71	4/1095 (0.4%)	1.08	6/1480 (0.4%)
25	b	0.71	4/1095 (0.4%)	1.08	6/1480 (0.4%)
26	Bc	0.69	0/1287	0.99	10/1761 (0.6%)
26	c	0.69	0/1287	0.99	10/1761 (0.6%)
27	Bd	0.79	0/1445	0.97	3/1945 (0.2%)
27	d	0.79	0/1445	0.97	3/1945 (0.2%)
28	Be	0.76	0/835	0.95	2/1134 (0.2%)
28	e	0.76	0/835	0.95	2/1134 (0.2%)
29	Bf	0.66	0/418	0.87	1/566 (0.2%)
29	f	0.66	0/418	0.87	1/566 (0.2%)
30	Bg	0.78	0/1035	0.97	4/1398 (0.3%)
30	g	0.78	0/1035	0.97	4/1398 (0.3%)
31	Bh	0.79	0/884	0.98	3/1182 (0.3%)
31	h	0.79	0/884	0.98	3/1182 (0.3%)
32	Bi	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
32	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
33	Bj	0.76	0/945	1.01	3/1292 (0.2%)
33	j	0.76	0/945	1.01	3/1292 (0.2%)
34	Bk	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
34	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
35	Bl	0.84	6/4840 (0.1%)	1.04	29/6611 (0.4%)
35	l	0.84	6/4840 (0.1%)	1.04	29/6611 (0.4%)
36	Bm	0.82	0/1346	0.99	6/1832 (0.3%)
36	m	0.82	0/1346	0.99	6/1832 (0.3%)
37	Bn	0.63	0/484	0.99	0/652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	n	0.63	0/484	0.99	0/652
38	Bo	0.71	0/1093	0.89	0/1479
38	o	0.71	0/1090	0.89	0/1475
39	Bp	0.70	0/1549	1.01	11/2098 (0.5%)
39	p	0.70	0/1549	1.00	11/2098 (0.5%)
40	Br	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
40	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
41	Bs	0.83	0/2580	1.09	15/3539 (0.4%)
41	s	0.83	0/2580	1.09	15/3539 (0.4%)
42	Bu	0.70	0/1433	0.96	2/1937 (0.1%)
42	u	0.70	0/1433	0.96	2/1937 (0.1%)
43	Bv	0.64	0/934	1.00	4/1241 (0.3%)
43	v	0.64	0/934	1.00	4/1241 (0.3%)
44	Bw	0.54	1/2533 (0.0%)	0.91	7/3440 (0.2%)
44	w	0.54	1/2533 (0.0%)	0.91	9/3440 (0.3%)
45	Bx	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
45	x	0.86	7/4164 (0.2%)	1.16	36/5688 (0.6%)
46	By	0.78	0/1868	1.12	11/2544 (0.4%)
46	y	0.78	0/1868	1.12	11/2544 (0.4%)
47	Bz	0.75	0/2211	1.02	7/3023 (0.2%)
47	z	0.75	0/2211	1.02	7/3023 (0.2%)
48	0	0.68	0/1229	0.96	3/1658 (0.2%)
48	B0	0.68	0/1229	0.96	3/1658 (0.2%)
49	1	0.64	0/898	1.03	6/1218 (0.5%)
49	B1	0.64	0/898	1.02	6/1218 (0.5%)
50	2	0.72	0/765	1.13	3/1038 (0.3%)
50	B2	0.72	0/765	1.14	3/1038 (0.3%)
51	3	0.69	0/699	1.10	6/950 (0.6%)
51	B3	0.69	0/699	1.10	6/950 (0.6%)
52	4	0.67	0/648	1.17	5/877 (0.6%)
52	B4	0.67	0/648	1.17	5/877 (0.6%)
53	5	0.71	0/611	0.94	2/810 (0.2%)
53	B5	0.71	0/611	0.94	2/810 (0.2%)
54	6	0.70	0/451	1.04	3/610 (0.5%)
54	B6	0.70	0/451	1.04	3/610 (0.5%)
55	7	0.76	0/398	1.01	1/546 (0.2%)
55	B7	0.76	0/398	1.01	1/546 (0.2%)
56	8	0.78	0/399	0.97	2/534 (0.4%)
56	B8	0.78	0/399	0.97	2/534 (0.4%)
57	9	0.69	0/345	0.99	1/470 (0.2%)
57	B9	0.69	0/345	0.99	1/470 (0.2%)
58	AA	0.44	0/715	0.83	1/964 (0.1%)
58	AN	0.37	0/707	0.86	2/953 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
59	AB	0.37	0/421	0.91	0/574
59	AO	0.40	0/417	0.98	0/569
60	AC	0.32	0/1554	0.81	6/2104 (0.3%)
60	AP	0.30	0/1554	0.84	6/2104 (0.3%)
61	AD	0.30	0/521	0.63	0/699
61	AQ	0.31	0/521	0.68	0/699
62	AE	0.48	1/587 (0.2%)	0.84	2/789 (0.3%)
62	AR	0.37	0/587	0.77	2/789 (0.3%)
63	AF	0.61	2/942 (0.2%)	0.85	3/1263 (0.2%)
63	AS	0.34	0/942	0.66	0/1263
64	AG	0.38	0/442	0.82	4/608 (0.7%)
64	AT	0.40	0/442	0.80	1/608 (0.2%)
65	AH	0.35	0/1983	0.84	6/2691 (0.2%)
65	AU	0.35	0/1983	0.79	4/2691 (0.1%)
66	AJ	0.42	2/3108 (0.1%)	0.82	7/4254 (0.2%)
66	AV	0.46	4/3108 (0.1%)	0.86	11/4254 (0.3%)
67	AK	0.37	0/3217	0.79	0/4361
67	AW	0.39	2/3220 (0.1%)	0.81	4/4365 (0.1%)
68	AL	0.37	0/3514	0.82	8/4769 (0.2%)
68	AY	0.40	2/3499 (0.1%)	0.83	6/4750 (0.1%)
All	All	0.65	57/197905 (0.0%)	0.96	719/268649 (0.3%)

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 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	i	278	ILE	CA-CB	-7.62	1.50	1.54
32	Bi	278	ILE	CA-CB	-7.56	1.50	1.54
45	x	61	HIS	CG-CD2	7.46	1.44	1.35
45	Bx	61	HIS	CG-CD2	7.45	1.44	1.35
45	Bx	378	HIS	ND1-CE1	7.40	1.40	1.32

The worst 5 of 719 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	BW	31	SER	N-CA-C	-16.81	92.08	112.59
21	W	31	SER	N-CA-C	-16.81	92.09	112.59
21	W	10	MET	CA-C-N	-10.86	109.20	120.38
21	W	10	MET	C-N-CA	-10.86	109.20	120.38
21	BW	10	MET	CA-C-N	-10.85	109.21	120.38

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](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3289	214	0
1	BA	3322	0	3289	207	0
2	B	1420	0	1371	118	0
2	BB	1420	0	1371	123	0
3	BC	1249	0	1253	84	0
3	C	1249	0	1253	88	0
4	BE	968	0	982	64	0
4	E	968	0	982	64	0
5	BF	670	0	679	38	0
5	F	670	0	679	37	0
6	BG	672	0	650	31	0
6	BX	686	0	676	36	0
6	G	672	0	650	31	0
6	X	686	0	676	33	0
7	BH	922	0	950	58	0
7	H	922	0	950	58	0
8	BI	769	0	788	47	0
8	I	769	0	788	47	0
9	BJ	2712	0	2757	234	0
9	J	2712	0	2757	234	0
10	BK	274	0	257	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	274	0	257	22	0
11	BL	964	0	962	63	0
11	L	964	0	962	63	0
12	BM	5274	0	5312	338	0
12	M	5274	0	5312	334	0
13	BN	1195	0	1155	50	0
13	N	1195	0	1155	49	0
14	BO	1643	0	1646	110	0
14	O	1643	0	1646	113	0
15	BP	1730	0	1685	116	0
15	P	1730	0	1685	115	0
16	BQ	3460	0	3419	309	0
16	Q	3460	0	3419	309	0
17	BS	568	0	567	43	0
17	S	568	0	567	44	0
18	BT	742	0	723	43	0
18	T	742	0	723	42	0
19	BU	647	0	653	16	0
19	U	647	0	653	15	0
20	BV	1038	0	1027	36	0
20	V	1038	0	1027	36	0
21	BW	1135	0	1129	62	0
21	W	1135	0	1129	62	0
22	BY	533	0	475	102	0
22	Y	533	0	475	99	0
23	BZ	648	0	627	19	0
23	Z	648	0	627	18	0
24	Ba	1174	0	1177	103	0
24	a	1174	0	1177	102	0
25	Bb	1059	0	1079	123	0
25	b	1059	0	1079	126	0
26	Bc	1236	0	1092	87	0
26	c	1236	0	1092	82	0
27	Bd	1418	0	1375	119	0
27	d	1418	0	1375	118	0
28	Be	810	0	772	34	0
28	e	810	0	772	36	0
29	Bf	405	0	407	18	0
29	f	405	0	407	18	0
30	Bg	1004	0	1008	66	0
30	g	1004	0	1008	68	0
31	Bh	863	0	861	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	h	863	0	861	66	0
32	Bi	2735	0	2893	194	0
32	i	2735	0	2893	186	0
33	Bj	919	0	968	87	0
33	j	919	0	968	84	0
34	Bk	740	0	792	92	0
34	k	740	0	792	92	0
35	Bl	4717	0	4893	410	0
35	l	4717	0	4893	409	0
36	Bm	1313	0	1330	129	0
36	m	1313	0	1330	129	0
37	Bn	473	0	480	29	0
37	n	473	0	480	29	0
38	Bo	1066	0	1086	66	0
38	o	1063	0	1082	62	0
39	Bp	1495	0	1440	118	0
39	p	1495	0	1440	106	0
40	Br	3629	0	3825	162	0
40	r	3629	0	3825	161	0
41	Bs	2509	0	2617	168	0
41	s	2509	0	2617	168	0
42	Bu	1394	0	1367	64	0
42	u	1394	0	1367	60	0
43	Bv	921	0	892	91	0
43	v	921	0	892	89	0
44	Bw	2474	0	2304	120	0
44	w	2474	0	2304	119	0
45	Bx	4025	0	4003	88	0
45	x	4025	0	4003	87	0
46	By	1822	0	1834	73	0
46	y	1822	0	1834	72	0
47	Bz	2124	0	2042	52	0
47	z	2124	0	2042	52	0
48	0	1195	0	1183	33	0
48	B0	1195	0	1183	31	0
49	1	878	0	868	22	0
49	B1	878	0	868	23	0
50	2	748	0	728	23	0
50	B2	748	0	728	27	0
51	3	672	0	645	29	0
51	B3	672	0	645	29	0
52	4	628	0	582	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	628	0	582	21	0
53	5	598	0	612	17	0
53	B5	598	0	612	14	0
54	6	441	0	439	28	0
54	B6	441	0	439	27	0
55	7	384	0	366	12	0
55	B7	384	0	366	12	0
56	8	386	0	388	8	0
56	B8	386	0	388	8	0
57	9	335	0	352	14	0
57	B9	335	0	352	13	0
58	AA	694	0	683	47	0
58	AN	687	0	676	30	0
59	AB	413	0	438	25	0
59	AO	409	0	432	24	0
60	AC	1521	0	1505	56	0
60	AP	1521	0	1505	64	0
61	AD	509	0	511	15	0
61	AQ	509	0	511	23	0
62	AE	580	0	526	54	0
62	AR	580	0	526	33	0
63	AF	921	0	909	74	0
63	AS	921	0	910	30	0
64	AG	425	0	422	13	0
64	AT	425	0	422	30	0
65	AH	1924	0	1874	62	0
65	AU	1924	0	1874	80	0
66	AJ	3009	0	3065	114	0
66	AV	3009	0	3065	178	0
67	AK	3159	0	3130	160	0
67	AW	3162	0	3139	124	0
68	AL	3442	0	3357	174	0
68	AY	3428	0	3326	206	0
69	A	8	0	0	6	0
69	B	16	0	0	3	0
69	BA	8	0	0	6	0
69	BB	16	0	0	3	0
69	BC	8	0	0	0	0
69	BM	16	0	0	3	0
69	C	8	0	0	0	0
69	M	16	0	0	4	0
70	A	31	0	19	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	BA	31	0	19	16	0
71	AL	52	0	88	4	0
71	AN	52	0	88	10	0
71	AQ	52	0	88	9	0
71	AT	52	0	88	2	0
71	B	52	0	88	4	0
71	BB	52	0	88	4	0
71	BU	52	0	88	2	0
71	BV	52	0	88	4	0
71	Bb	52	0	88	35	0
71	Bg	156	0	264	14	0
71	Br	104	0	176	24	0
71	U	52	0	88	2	0
71	b	52	0	88	36	0
71	g	156	0	264	13	0
71	r	104	0	176	23	0
72	BE	35	0	0	4	0
72	Bp	35	0	0	13	0
72	E	35	0	0	4	0
72	p	35	0	0	12	0
73	BJ	48	0	26	26	0
73	J	48	0	26	26	0
74	AC	4	0	0	3	0
74	AP	4	0	0	2	0
74	BM	4	0	0	1	0
74	BO	4	0	0	2	0
74	M	4	0	0	1	0
74	O	4	0	0	2	0
75	AA	64	0	72	3	0
75	AG	64	0	72	29	0
75	AH	64	0	72	8	0
75	AJ	128	0	144	23	0
75	AL	64	0	72	24	0
75	AN	64	0	72	9	0
75	AU	64	0	72	11	0
75	AY	64	0	72	6	0
75	BV	63	0	68	6	0
75	Bi	64	0	72	2	0
75	Bl	128	0	144	5	0
75	Bn	64	0	72	10	0
75	V	63	0	68	8	0
75	i	64	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	l	128	0	144	4	0
75	n	64	0	72	10	0
76	AH	49	0	75	32	0
76	AJ	49	0	75	8	0
76	AL	49	0	75	39	0
76	AU	41	0	56	24	0
76	AV	49	0	75	23	0
76	AY	49	0	75	21	0
76	BV	51	0	82	21	0
76	BW	51	0	82	20	0
76	Bl	100	0	157	67	0
76	V	51	0	82	22	0
76	W	51	0	82	20	0
76	l	100	0	157	66	0
77	Bx	1	0	0	0	0
77	By	2	0	0	0	0
77	x	1	0	0	0	0
77	y	2	0	0	0	0
78	Bx	1	0	0	0	0
78	x	1	0	0	0	0
79	Bx	120	0	108	4	0
79	x	120	0	108	4	0
80	2	1	0	0	0	0
80	B2	1	0	0	0	0
81	AH	43	0	32	5	0
81	AU	43	0	32	7	0
82	AJ	86	0	60	8	0
82	AV	86	0	60	13	0
All	All	196753	0	197037	9753	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 9753 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bl:533:MET:CE	76:Bl:702:PEE:H36	1.25	1.65
24:a:55:PHE:CE2	39:p:118:TYR:CE2	1.82	1.64
35:l:533:MET:CE	76:l:702:PEE:H36	1.25	1.64
24:Ba:55:PHE:CE2	39:BP:118:TYR:CE2	1.82	1.64
63:AF:29:LYS:CG	63:AF:75:ILE:HD11	1.16	1.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	30
1	BA	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	30
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	59
2	BB	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	21	59
3	BC	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	21
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	21
4	BE	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	6	34
5	BF	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	BG	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	27
6	BX	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	16
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	4	27
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	16
7	BH	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	17
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	17
8	BI	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	12
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	12
9	BJ	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	30
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	30
10	BK	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	BL	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	21
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	21
12	BM	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	21
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	21
13	BN	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	16
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	16
14	BO	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	21
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	21
15	BP	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	15
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	15
16	BQ	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	7	38
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	7	38
17	BS	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	23
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	23
18	BT	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	17
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	17
19	BU	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	44
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	44
20	BV	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	29
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	29
21	BW	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	20
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	20
22	BY	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	6
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%)	5	29
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	29
25	Bb	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	18
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	18
26	Bc	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	17
27	Bd	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	59
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	59
28	Be	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	21
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	21
29	Bf	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	29
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	29
30	Bg	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	15
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	15
31	Bh	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	13
31	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	13
32	Bi	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	36
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	36
33	Bj	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	25
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	25
34	Bk	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	21
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	21
35	Bl	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	36
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	36
36	Bm	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	14
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	14
37	Bn	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	20
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	20
38	Bo	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	21
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	21
39	Bp	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	6	34
40	Br	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	31
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	31
41	Bs	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	24
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Bu	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	23
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	23
43	Bv	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	24
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	24
44	Bw	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	24
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	24
45	Bx	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	54
46	By	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	42
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%)	2	17
50	B2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
51	B3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	13
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	40
52	B4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	40
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%)	2	20
54	B6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	2	20
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	B9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4	26
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	9	42
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	15
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	6
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4	25
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8	40
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%)	4	24
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	9	40
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	12	49
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%)	16	54
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	54
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16	54
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16	54
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	10	44
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	10	44
68	AL	444/446 (100%)	403 (91%)	35 (8%)	6 (1%)	9	40
68	AY	444/446 (100%)	414 (93%)	22 (5%)	8 (2%)	6	34
All	All	23880/24216 (99%)	21833 (91%)	1487 (6%)	560 (2%)	7	28

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%)	106 (100%)	0	100	100
4	E	106/106 (100%)	106 (100%)	0	100	100
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
6	BX	78/79 (99%)	77 (99%)	1 (1%)	61	74
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%)	99 (99%)	1 (1%)	68	78
7	H	100/100 (100%)	99 (99%)	1 (1%)	68	78
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%)	59	72
9	J	292/292 (100%)	288 (99%)	4 (1%)	59	72
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%)	86	86
12	M	576/577 (100%)	574 (100%)	2 (0%)	86	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	368 (99%)	3 (1%)	73	80
16	Q	371/371 (100%)	368 (99%)	3 (1%)	73	80
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
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%)	50 (88%)	7 (12%)	4	17
22	Y	57/57 (100%)	50 (88%)	7 (12%)	4	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%)	123 (99%)	1 (1%)	73	80
24	a	124/124 (100%)	123 (99%)	1 (1%)	73	80
25	Bb	118/118 (100%)	113 (96%)	5 (4%)	26	48
25	b	118/118 (100%)	113 (96%)	5 (4%)	26	48
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%)	19	41
27	d	145/154 (94%)	137 (94%)	8 (6%)	19	41
28	Be	90/90 (100%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	313 (100%)	1 (0%)	86	86
32	i	314/314 (100%)	313 (100%)	1 (0%)	86	86
33	Bj	102/103 (99%)	101 (99%)	1 (1%)	68	78
33	j	102/103 (99%)	101 (99%)	1 (1%)	68	78
34	Bk	85/85 (100%)	81 (95%)	4 (5%)	23	45
34	k	85/85 (100%)	81 (95%)	4 (5%)	23	45
35	Bl	531/532 (100%)	511 (96%)	20 (4%)	29	50
35	l	531/532 (100%)	511 (96%)	20 (4%)	29	50
36	Bm	137/137 (100%)	137 (100%)	0	100	100
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%)	155 (99%)	2 (1%)	61	74
39	p	157/157 (100%)	155 (99%)	2 (1%)	61	74
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	387 (91%)	40 (9%)	8	26
45	x	427/427 (100%)	387 (91%)	40 (9%)	8	26
46	By	211/211 (100%)	191 (90%)	20 (10%)	8	25
46	y	211/211 (100%)	192 (91%)	19 (9%)	9	27
47	Bz	226/226 (100%)	199 (88%)	27 (12%)	5	18
47	z	226/226 (100%)	199 (88%)	27 (12%)	5	18
48	0	128/128 (100%)	118 (92%)	10 (8%)	11	32
48	B0	128/128 (100%)	118 (92%)	10 (8%)	11	32
49	1	95/95 (100%)	89 (94%)	6 (6%)	16	37
49	B1	95/95 (100%)	94 (99%)	1 (1%)	65	76
50	2	81/81 (100%)	73 (90%)	8 (10%)	7	24
50	B2	81/81 (100%)	73 (90%)	8 (10%)	7	24
51	3	68/68 (100%)	52 (76%)	16 (24%)	1	5
51	B3	68/68 (100%)	55 (81%)	13 (19%)	1	8
52	4	67/67 (100%)	58 (87%)	9 (13%)	4	14
52	B4	67/67 (100%)	58 (87%)	9 (13%)	4	14
53	5	58/58 (100%)	51 (88%)	7 (12%)	5	17
53	B5	58/58 (100%)	54 (93%)	4 (7%)	14	36
54	6	47/47 (100%)	41 (87%)	6 (13%)	4	15
54	B6	47/47 (100%)	44 (94%)	3 (6%)	16	37
55	7	39/39 (100%)	36 (92%)	3 (8%)	12	32
55	B7	39/39 (100%)	36 (92%)	3 (8%)	12	32
56	8	40/40 (100%)	37 (92%)	3 (8%)	12	33
56	B8	40/40 (100%)	37 (92%)	3 (8%)	12	33
57	9	37/37 (100%)	34 (92%)	3 (8%)	11	31
57	B9	37/37 (100%)	34 (92%)	3 (8%)	11	31
58	AA	74/74 (100%)	68 (92%)	6 (8%)	11	31
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	51 (98%)	1 (2%)	50	67
62	AE	61/71 (86%)	59 (97%)	2 (3%)	33	55
62	AR	61/71 (86%)	58 (95%)	3 (5%)	22	43
63	AF	95/95 (100%)	82 (86%)	13 (14%)	3	14
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%)	23	44
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	81	83
66	AJ	330/330 (100%)	326 (99%)	4 (1%)	63	75
66	AV	330/330 (100%)	321 (97%)	9 (3%)	39	61
67	AK	334/335 (100%)	330 (99%)	4 (1%)	63	75
67	AW	335/335 (100%)	331 (99%)	4 (1%)	63	75
68	AL	365/367 (100%)	365 (100%)	0	100	100
68	AY	362/367 (99%)	356 (98%)	6 (2%)	53	69
All	All	20773/21008 (99%)	20298 (98%)	475 (2%)	44	64

5 of 475 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	AF	41	ASP
51	B3	42	ARG
22	BY	87	PRO
51	B3	17	ARG
57	B9	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 482 such sidechains are listed below:

Mol	Chain	Res	Type
67	AK	290	GLN

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Mol	Chain	Res	Type
45	Bx	256	HIS
1	BA	313	ASN
45	Bx	12	HIS
52	B4	37	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
72	8Q1	p	201	-	32,34,34	1.60	5 (15%)	39,43,43	1.59	6 (15%)
74	FES	AP	301	60	0,4,4	-	-	-		
75	CDL	AA	101	-	63,63,99	1.26	5 (7%)	69,75,111	1.08	5 (7%)
72	8Q1	BE	201	-	32,34,34	1.58	6 (18%)	39,43,43	1.42	7 (17%)
71	PLX	b	201	-	51,51,51	0.55	0	53,59,59	0.64	0
71	PLX	Bg	202	-	51,51,51	0.76	1 (1%)	53,59,59	0.62	1 (1%)
75	CDL	Bn	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.08	4 (5%)
71	PLX	AN	101	-	51,51,51	0.80	1 (1%)	53,59,59	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	HEA	Bx	603	45	67,67,67	1.20	4 (5%)	81,103,103	1.33	10 (12%)
71	PLX	AQ	101	-	51,51,51	0.79	1 (1%)	53,59,59	0.63	2 (3%)
71	PLX	BU	101	-	51,51,51	0.77	1 (1%)	53,59,59	0.71	2 (3%)
69	SF4	BM	802	12	0,12,12	-	-	-	-	-
71	PLX	U	101	-	51,51,51	0.77	1 (1%)	53,59,59	0.71	2 (3%)
74	FES	M	803	-	0,4,4	-	-	-	-	-
69	SF4	C	301	3	0,12,12	-	-	-	-	-
69	SF4	M	802	12	0,12,12	-	-	-	-	-
69	SF4	BC	301	3	0,12,12	-	-	-	-	-
69	SF4	BB	302	2	0,12,12	-	-	-	-	-
75	CDL	Bl	703	-	63,63,99	1.22	5 (7%)	69,75,111	1.09	4 (5%)
76	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
70	FMN	BA	502	-	33,33,33	1.42	5 (15%)	48,50,50	1.35	9 (18%)
74	FES	BM	803	-	0,4,4	-	-	-	-	-
75	CDL	AH	403	-	63,63,99	1.27	5 (7%)	69,75,111	1.05	4 (5%)
69	SF4	M	801	12	0,12,12	-	-	-	-	-
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.24	5 (7%)
75	CDL	n	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.08	4 (5%)
71	PLX	Br	502	-	51,51,51	0.62	0	53,59,59	0.67	1 (1%)
82	HEM	AJ	401	66	50,50,50	1.81	9 (18%)	67,82,82	1.19	2 (2%)
69	SF4	B	301	2	0,12,12	-	-	-	-	-
75	CDL	AJ	404	-	63,63,99	1.26	5 (7%)	69,75,111	1.04	4 (5%)
79	HEA	x	604	45	67,67,67	1.20	7 (10%)	81,103,103	1.35	11 (13%)
76	PEE	W	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
69	SF4	BM	801	12	0,12,12	-	-	-	-	-
72	8Q1	E	201	-	32,34,34	1.57	6 (18%)	39,43,43	1.42	7 (17%)
75	CDL	l	704	-	63,63,99	1.27	5 (7%)	69,75,111	1.02	4 (5%)
76	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)
75	CDL	AU	403	-	63,63,99	1.26	6 (9%)	69,75,111	1.06	4 (5%)
73	NDP	BJ	401	-	51,52,52	1.15	6 (11%)	71,80,80	1.57	10 (14%)
71	PLX	g	201	-	51,51,51	0.84	1 (1%)	53,59,59	0.70	1 (1%)
75	CDL	AN	102	-	63,63,99	1.25	5 (7%)	69,75,111	1.04	4 (5%)
76	PEE	AH	401	-	48,48,50	1.37	4 (8%)	51,53,55	0.97	2 (3%)
76	PEE	Bl	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
74	FES	BO	301	14	0,4,4	-	-	-	-	-
82	HEM	AV	402	66	50,50,50	1.79	8 (16%)	67,82,82	1.25	6 (8%)
76	PEE	AU	401	-	40,40,50	1.47	4 (10%)	43,45,55	0.95	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	l	703	-	63,63,99	1.22	5 (7%)	69,75,111	1.09	4 (5%)
71	PLX	g	202	-	51,51,51	0.76	1 (1%)	53,59,59	0.62	1 (1%)
75	CDL	V	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.96	3 (4%)
71	PLX	r	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
76	PEE	l	702	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
74	FES	AC	301	60	0,4,4	-	-	-		
79	HEA	x	603	45	67,67,67	1.20	4 (5%)	81,103,103	1.34	11 (13%)
75	CDL	i	401	-	63,63,99	1.23	5 (7%)	69,75,111	1.06	5 (7%)
71	PLX	AL	501	-	51,51,51	0.80	1 (1%)	53,59,59	0.64	1 (1%)
74	FES	O	301	14	0,4,4	-	-	-		
71	PLX	g	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.59	1 (1%)
71	PLX	Bb	201	-	51,51,51	0.55	0	53,59,59	0.64	0
82	HEM	AV	401	66	50,50,50	1.82	9 (18%)	67,82,82	1.21	3 (4%)
71	PLX	Bg	201	-	51,51,51	0.84	1 (1%)	53,59,59	0.70	1 (1%)
76	PEE	AJ	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.00	2 (3%)
75	CDL	AY	501	-	63,63,99	1.26	5 (7%)	69,75,111	1.03	4 (5%)
76	PEE	AY	502	-	48,48,50	1.41	4 (8%)	51,53,55	0.97	2 (3%)
76	PEE	AV	403	-	48,48,50	1.36	4 (8%)	51,53,55	1.05	2 (3%)
75	CDL	Bl	704	-	63,63,99	1.28	5 (7%)	69,75,111	1.02	4 (5%)
71	PLX	Bg	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.60	1 (1%)
76	PEE	BV	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)
73	NDP	J	401	-	51,52,52	1.15	5 (9%)	71,80,80	1.56	10 (14%)
70	FMN	A	502	-	33,33,33	1.42	5 (15%)	48,50,50	1.35	8 (16%)
71	PLX	r	502	-	51,51,51	0.62	0	53,59,59	0.66	1 (1%)
71	PLX	BB	303	-	51,51,51	0.80	1 (1%)	53,59,59	0.69	1 (1%)
82	HEM	AJ	402	66	50,50,50	1.82	8 (16%)	67,82,82	1.23	6 (8%)
69	SF4	BA	501	1	0,12,12	-	-	-		
69	SF4	A	501	1	0,12,12	-	-	-		
76	PEE	Bl	702	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
75	CDL	AL	502	-	63,63,99	1.26	5 (7%)	69,75,111	1.07	4 (5%)
75	CDL	BV	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.96	3 (4%)
81	HEC	AU	402	65	46,50,50	1.84	5 (10%)	58,82,82	1.84	4 (6%)
69	SF4	BB	301	2	0,12,12	-	-	-		
71	PLX	B	303	-	51,51,51	0.80	1 (1%)	53,59,59	0.69	1 (1%)
76	PEE	BW	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
71	PLX	AT	101	-	51,51,51	0.78	1 (1%)	53,59,59	0.61	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
79	HEA	Bx	604	45	67,67,67	1.20	7 (10%)	81,103,103	1.35	11 (13%)
75	CDL	Bi	401	-	63,63,99	1.23	5 (7%)	69,75,111	1.06	5 (7%)
81	HEC	AH	402	65	46,50,50	1.82	5 (10%)	58,82,82	1.86	5 (8%)
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.18	6 (8%)
71	PLX	Br	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
76	PEE	AL	503	-	48,48,50	1.39	4 (8%)	51,53,55	0.94	2 (3%)
72	8Q1	Bp	201	-	32,34,34	1.60	5 (15%)	39,43,43	1.59	6 (15%)
69	SF4	B	302	2	0,12,12	-	-	-	-	-
71	PLX	BV	203	-	51,51,51	0.80	1 (1%)	53,59,59	0.61	1 (1%)

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
72	8Q1	p	201	-	-	21/41/41/41	-
74	FES	AP	301	60	-	-	0/1/1/1
75	CDL	AA	101	-	-	35/74/74/110	-
72	8Q1	BE	201	-	-	18/41/41/41	-
71	PLX	b	201	-	-	26/55/55/55	-
71	PLX	Bg	202	-	-	26/55/55/55	-
75	CDL	Bn	101	-	-	32/74/74/110	-
71	PLX	AN	101	-	-	26/55/55/55	-
71	PLX	BV	203	-	-	26/55/55/55	-
79	HEA	Bx	603	45	-	7/36/76/76	-
71	PLX	AQ	101	-	-	24/55/55/55	-
71	PLX	BU	101	-	-	22/55/55/55	-
69	SF4	BM	802	12	-	-	0/6/5/5
71	PLX	U	101	-	-	22/55/55/55	-
74	FES	M	803	-	-	-	0/1/1/1
69	SF4	C	301	3	-	-	0/6/5/5
69	SF4	M	802	12	-	-	0/6/5/5
69	SF4	BC	301	3	-	-	0/6/5/5
69	SF4	BB	302	2	-	-	0/6/5/5
75	CDL	Bl	703	-	-	36/74/74/110	-
76	PEE	l	701	-	-	31/52/52/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	FMN	BA	502	-	-	7/18/18/18	0/3/3/3
74	FES	BM	803	-	-	-	0/1/1/1
75	CDL	AH	403	-	-	41/74/74/110	-
69	SF4	M	801	12	-	-	0/6/5/5
75	CDL	AJ	405	-	-	25/74/74/110	-
75	CDL	n	101	-	-	32/74/74/110	-
71	PLX	Br	502	-	-	36/55/55/55	-
82	HEM	AJ	401	66	-	1/14/54/54	-
69	SF4	B	301	2	-	-	0/6/5/5
75	CDL	AJ	404	-	-	31/74/74/110	-
79	HEA	x	604	45	-	7/36/76/76	-
76	PEE	W	201	-	-	29/54/54/54	-
69	SF4	BM	801	12	-	-	0/6/5/5
72	8Q1	E	201	-	-	18/41/41/41	-
75	CDL	l	704	-	-	42/74/74/110	-
76	PEE	V	202	-	-	26/54/54/54	-
75	CDL	AU	403	-	-	46/74/74/110	-
73	NDP	BJ	401	-	-	15/34/77/77	0/5/5/5
71	PLX	g	201	-	-	24/55/55/55	-
75	CDL	AN	102	-	-	39/74/74/110	-
76	PEE	AH	401	-	-	25/52/52/54	-
76	PEE	Bl	701	-	-	31/52/52/54	-
74	FES	BO	301	14	-	-	0/1/1/1
82	HEM	AV	402	66	-	4/14/54/54	-
76	PEE	AU	401	-	-	17/44/44/54	-
75	CDL	l	703	-	-	36/74/74/110	-
71	PLX	g	202	-	-	26/55/55/55	-
75	CDL	V	201	-	-	40/69/69/110	-
71	PLX	r	501	-	-	27/55/55/55	-
76	PEE	l	702	-	-	26/54/54/54	-
74	FES	AC	301	60	-	-	0/1/1/1
79	HEA	x	603	45	-	7/36/76/76	-
75	CDL	i	401	-	-	39/74/74/110	-
71	PLX	AL	501	-	-	23/55/55/55	-
74	FES	O	301	14	-	-	0/1/1/1
71	PLX	g	203	-	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	Bb	201	-	-	26/55/55/55	-
82	HEM	AV	401	66	-	5/14/54/54	-
71	PLX	Bg	201	-	-	24/55/55/55	-
76	PEE	AJ	403	-	-	18/52/52/54	-
75	CDL	AY	501	-	-	35/74/74/110	-
76	PEE	AY	502	-	-	18/52/52/54	-
76	PEE	AV	403	-	-	29/52/52/54	-
75	CDL	Bl	704	-	-	42/74/74/110	-
71	PLX	Bg	203	-	-	22/55/55/55	-
76	PEE	BV	202	-	-	26/54/54/54	-
73	NDP	J	401	-	-	15/34/77/77	0/5/5/5
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
71	PLX	r	502	-	-	36/55/55/55	-
71	PLX	BB	303	-	-	22/55/55/55	-
82	HEM	AJ	402	66	-	2/14/54/54	-
69	SF4	BA	501	1	-	-	0/6/5/5
76	PEE	Bl	702	-	-	27/54/54/54	-
69	SF4	A	501	1	-	-	0/6/5/5
75	CDL	AL	502	-	-	42/74/74/110	-
75	CDL	BV	201	-	-	40/69/69/110	-
81	HEC	AU	402	65	-	4/14/54/54	-
69	SF4	BB	301	2	-	-	0/6/5/5
71	PLX	B	303	-	-	22/55/55/55	-
71	PLX	AT	101	-	-	22/55/55/55	-
79	HEA	Bx	604	45	-	7/36/76/76	-
75	CDL	Bi	401	-	-	39/74/74/110	-
81	HEC	AH	402	65	-	6/14/54/54	-
75	CDL	AG	101	-	-	37/74/74/110	-
71	PLX	Br	501	-	-	27/55/55/55	-
76	PEE	AL	503	-	-	21/52/52/54	-
72	8Q1	Bp	201	-	-	19/41/41/41	-
69	SF4	B	302	2	-	-	0/6/5/5
76	PEE	BW	201	-	-	29/54/54/54	-

The worst 5 of 288 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AV	402	HEM	C3D-C2D	7.74	1.53	1.36
82	AJ	401	HEM	C3D-C2D	7.74	1.53	1.36
82	AJ	402	HEM	C3D-C2D	7.69	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.61	1.53	1.36
81	AU	402	HEC	CAB-C3B	6.22	1.55	1.35

The worst 5 of 262 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AU	402	HEC	CBC-CAC-C3C	-8.69	110.07	127.43
81	AH	402	HEC	CBC-CAC-C3C	-7.92	111.60	127.43
81	AH	402	HEC	CBB-CAB-C3B	-7.83	111.78	127.43
81	AU	402	HEC	CBB-CAB-C3B	-7.08	113.28	127.43
72	p	201	8Q1	C6-C1-S44	5.92	120.45	113.40

There are no chirality outliers.

5 of 1763 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.

86 monomers are involved in 860 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	p	201	8Q1	12	0
74	AP	301	FES	2	0
75	AA	101	CDL	3	0
72	BE	201	8Q1	4	0
71	b	201	PLX	36	0
71	Bg	202	PLX	3	0
75	Bn	101	CDL	10	0
71	AN	101	PLX	10	0
79	Bx	603	HEA	1	0
71	AQ	101	PLX	9	0
71	BU	101	PLX	2	0
71	U	101	PLX	2	0
74	M	803	FES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	BB	302	SF4	2	0
75	Bl	703	CDL	2	0
76	l	701	PEE	48	0
70	BA	502	FMN	16	0
74	BM	803	FES	1	0
75	AH	403	CDL	8	0
69	M	801	SF4	4	0
75	AJ	405	CDL	17	0
75	n	101	CDL	10	0
71	Br	502	PLX	16	0
82	AJ	401	HEM	4	0
69	B	301	SF4	1	0
75	AJ	404	CDL	6	0
79	x	604	HEA	3	0
76	W	201	PEE	20	0
69	BM	801	SF4	3	0
72	E	201	8Q1	4	0
75	l	704	CDL	2	0
76	V	202	PEE	22	0
75	AU	403	CDL	11	0
73	BJ	401	NDP	26	0
71	g	201	PLX	2	0
75	AN	102	CDL	9	0
76	AH	401	PEE	32	0
76	Bl	701	PEE	49	0
74	BO	301	FES	2	0
82	AV	402	HEM	6	0
76	AU	401	PEE	24	0
75	l	703	CDL	2	0
71	g	202	PLX	3	0
75	V	201	CDL	8	0
71	r	501	PLX	7	0
76	l	702	PEE	18	0
74	AC	301	FES	3	0
79	x	603	HEA	1	0
75	i	401	CDL	2	0
71	AL	501	PLX	4	0
74	O	301	FES	2	0
71	g	203	PLX	8	0
71	Bb	201	PLX	35	0
82	AV	401	HEM	7	0
71	Bg	201	PLX	2	0

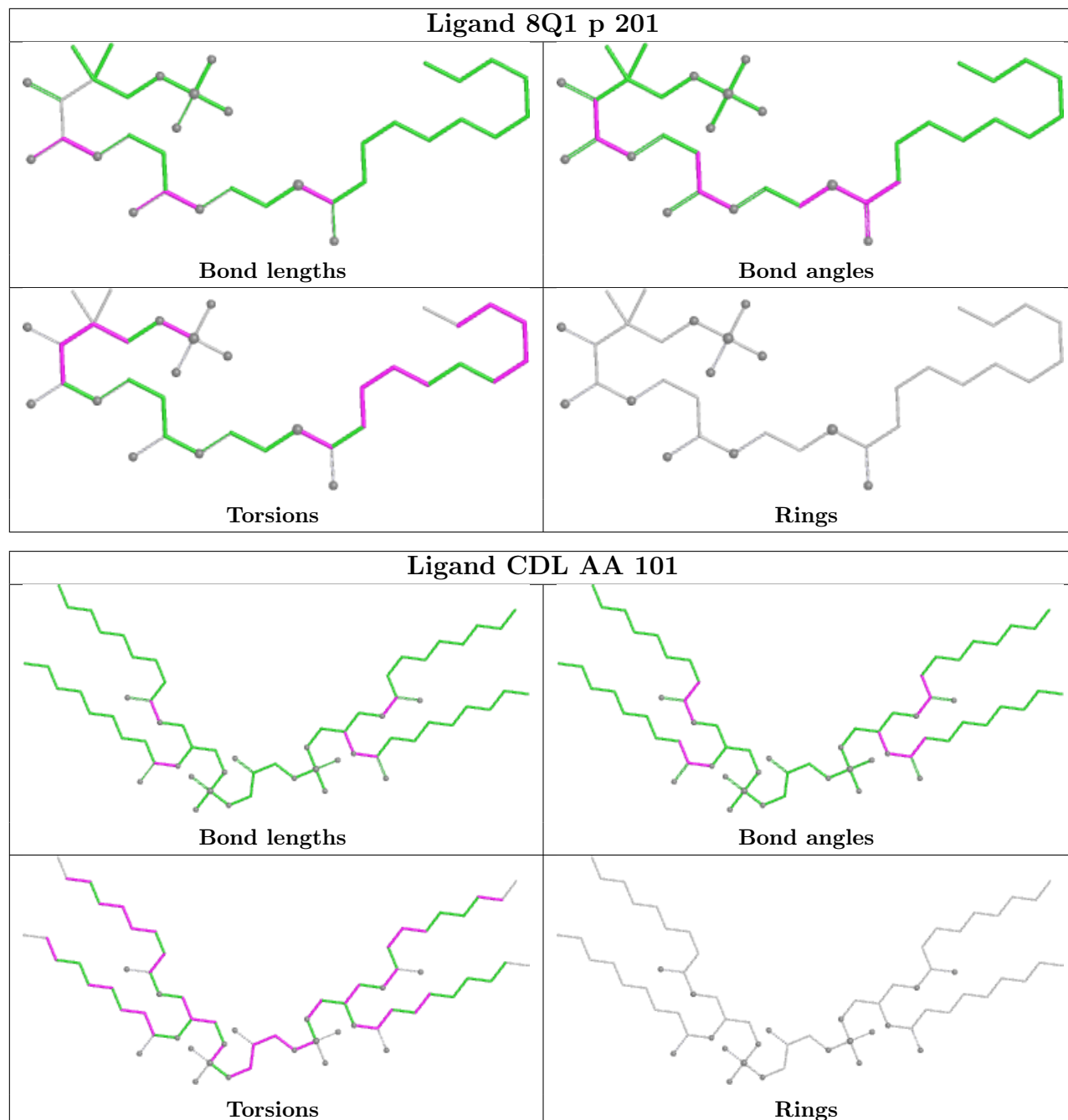
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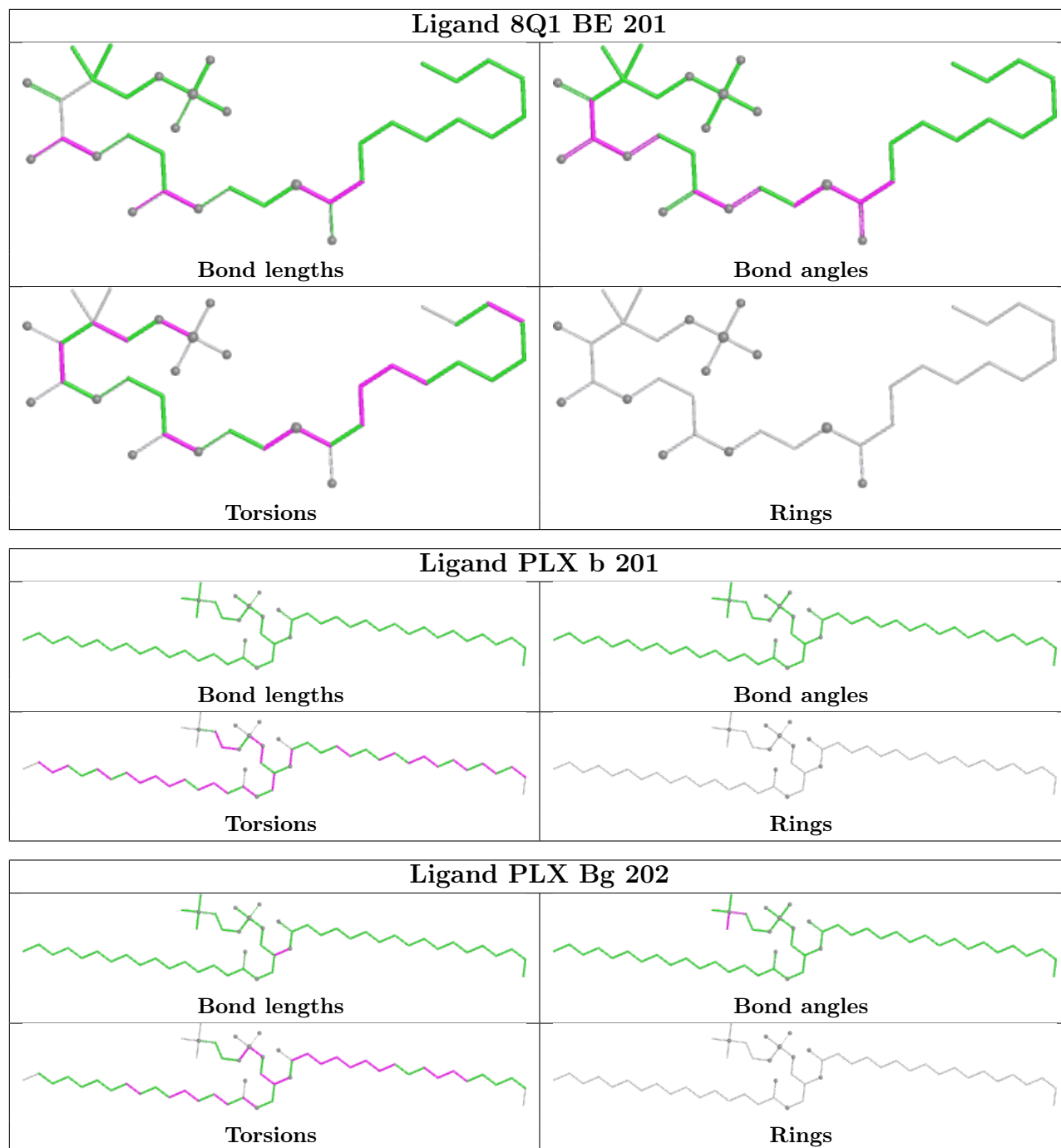
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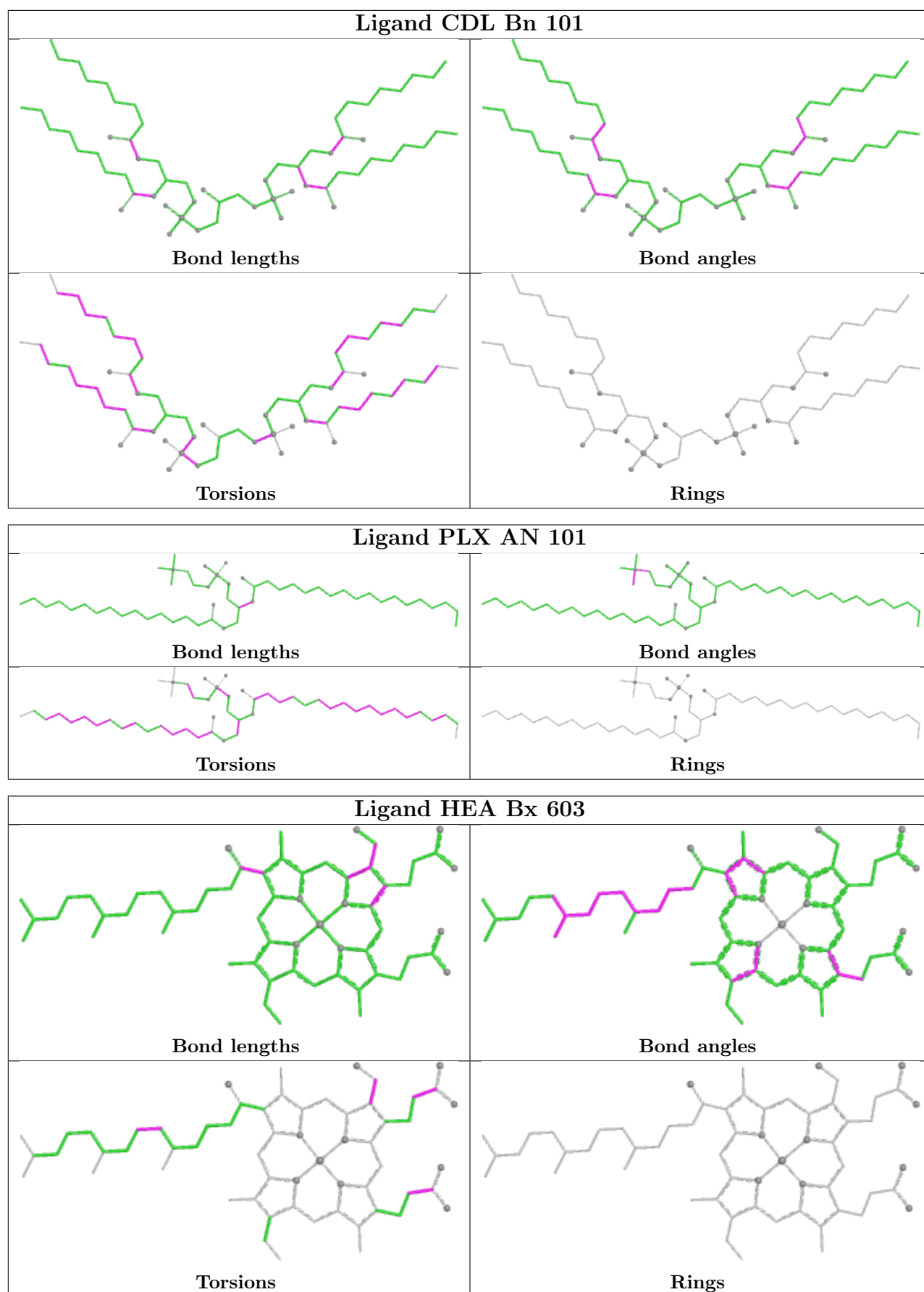
Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	AJ	403	PEE	8	0
75	AY	501	CDL	6	0
76	AY	502	PEE	21	0
76	AV	403	PEE	23	0
75	Bl	704	CDL	3	0
71	Bg	203	PLX	9	0
76	BV	202	PEE	21	0
73	J	401	NDP	26	0
70	A	502	FMN	17	0
71	r	502	PLX	16	0
71	BB	303	PLX	4	0
82	AJ	402	HEM	4	0
69	BA	501	SF4	6	0
69	A	501	SF4	6	0
76	Bl	702	PEE	18	0
75	AL	502	CDL	24	0
75	BV	201	CDL	6	0
81	AU	402	HEC	7	0
69	BB	301	SF4	1	0
71	B	303	PLX	4	0
76	BW	201	PEE	20	0
71	AT	101	PLX	2	0
79	Bx	604	HEA	3	0
75	Bi	401	CDL	2	0
81	AH	402	HEC	5	0
75	AG	101	CDL	29	0
71	Br	501	PLX	8	0
76	AL	503	PEE	39	0
72	Bp	201	8Q1	13	0
69	B	302	SF4	2	0
71	BV	203	PLX	4	0

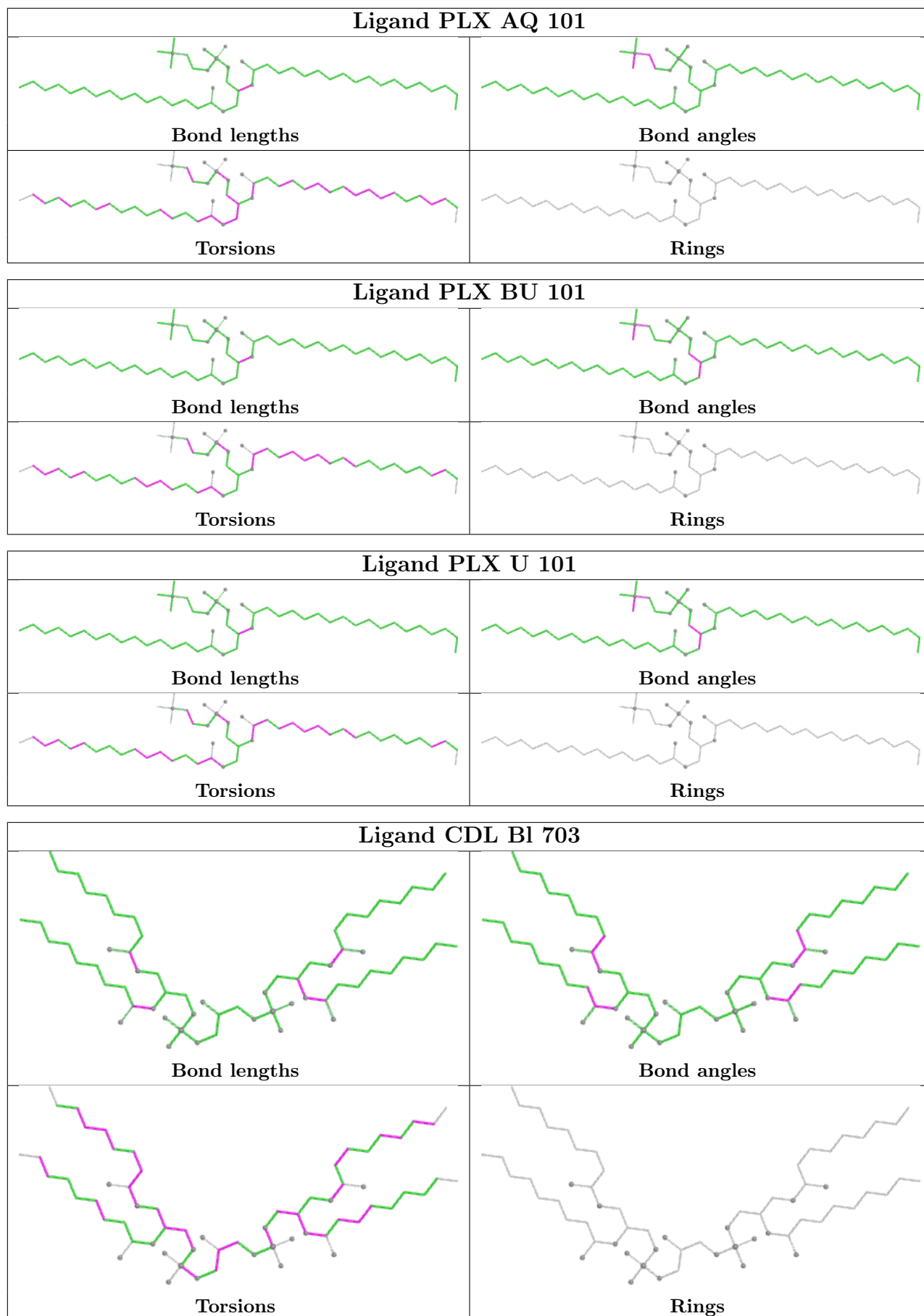
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

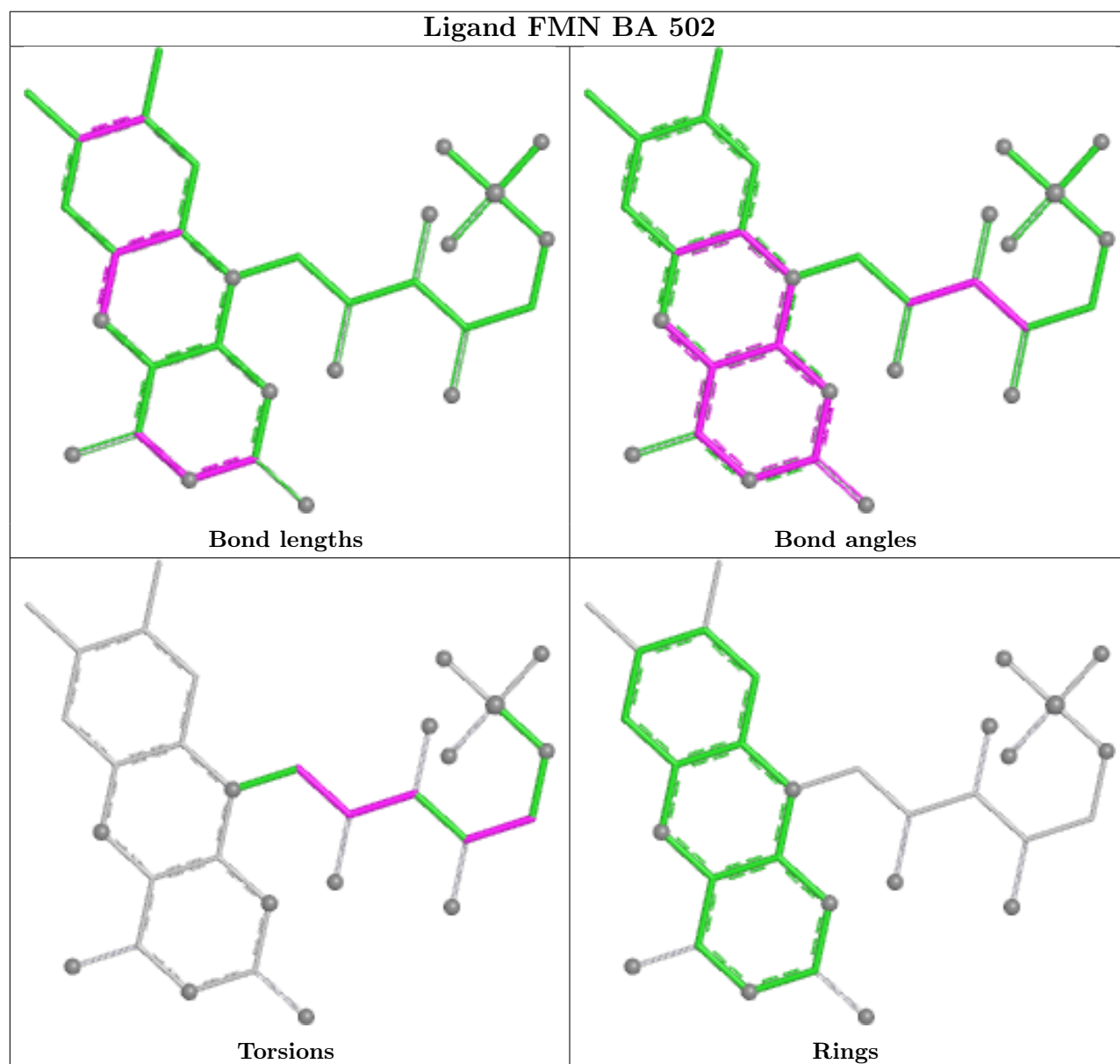
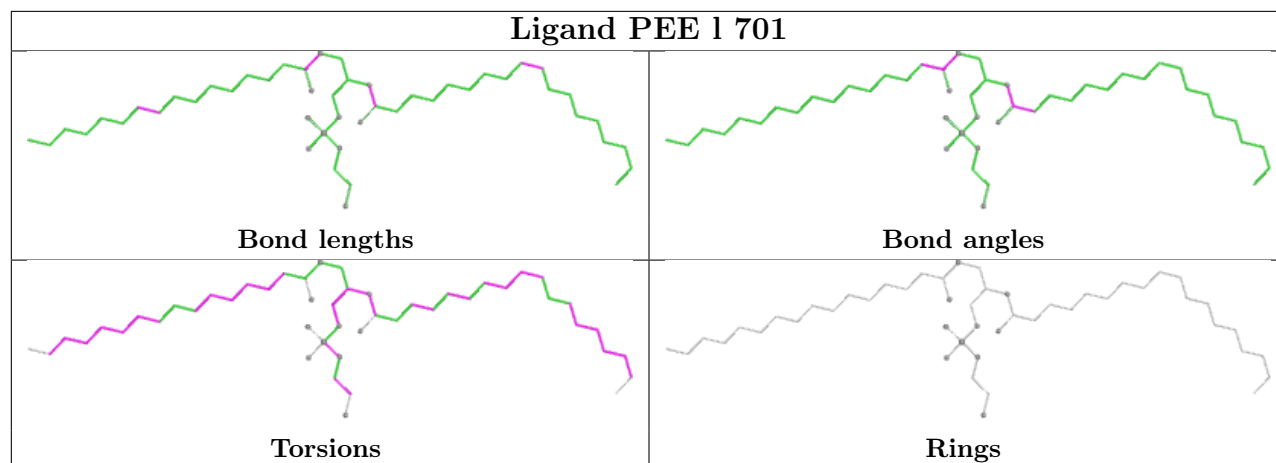
equivalents in the CSD to analyse the geometry.

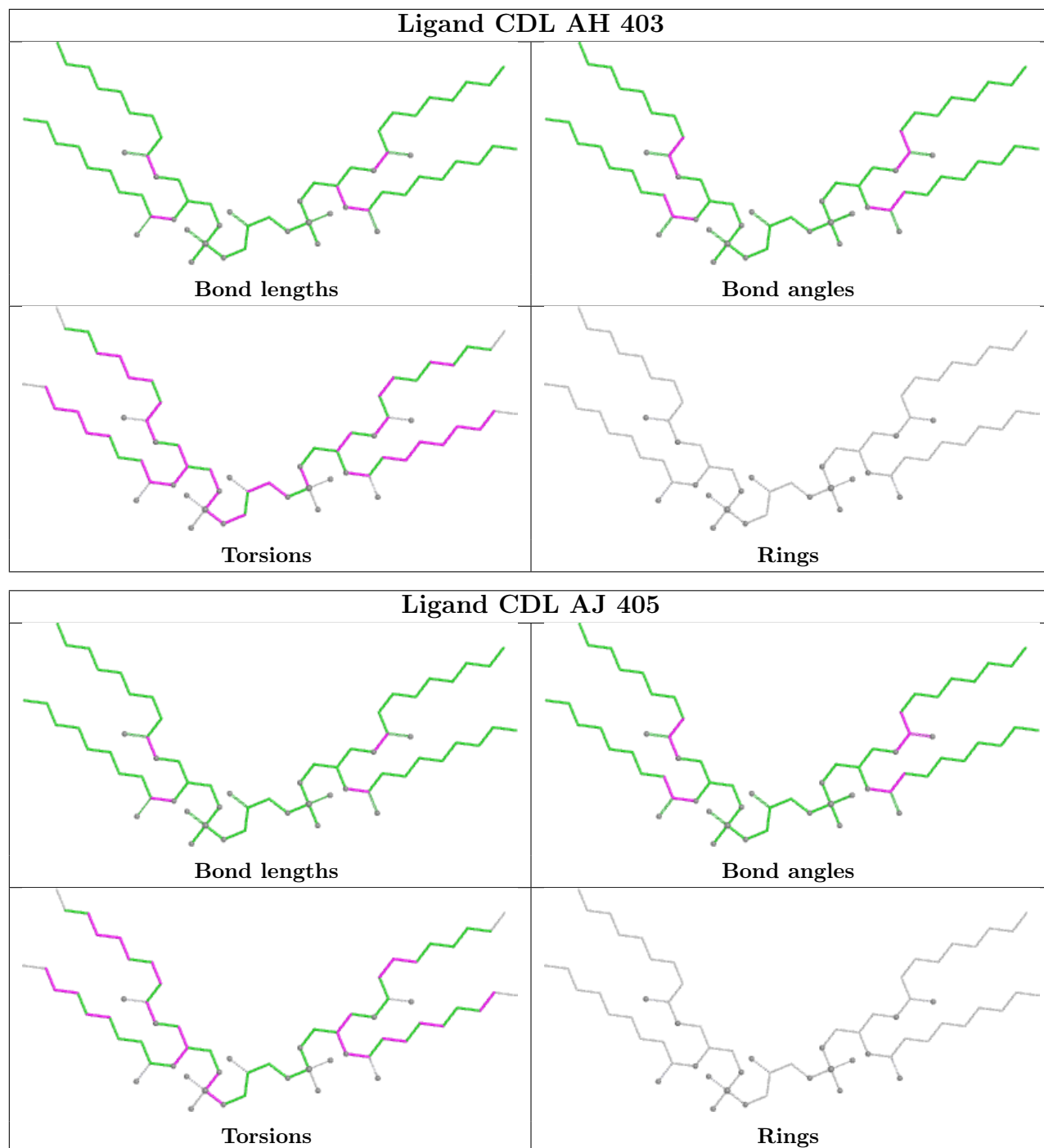


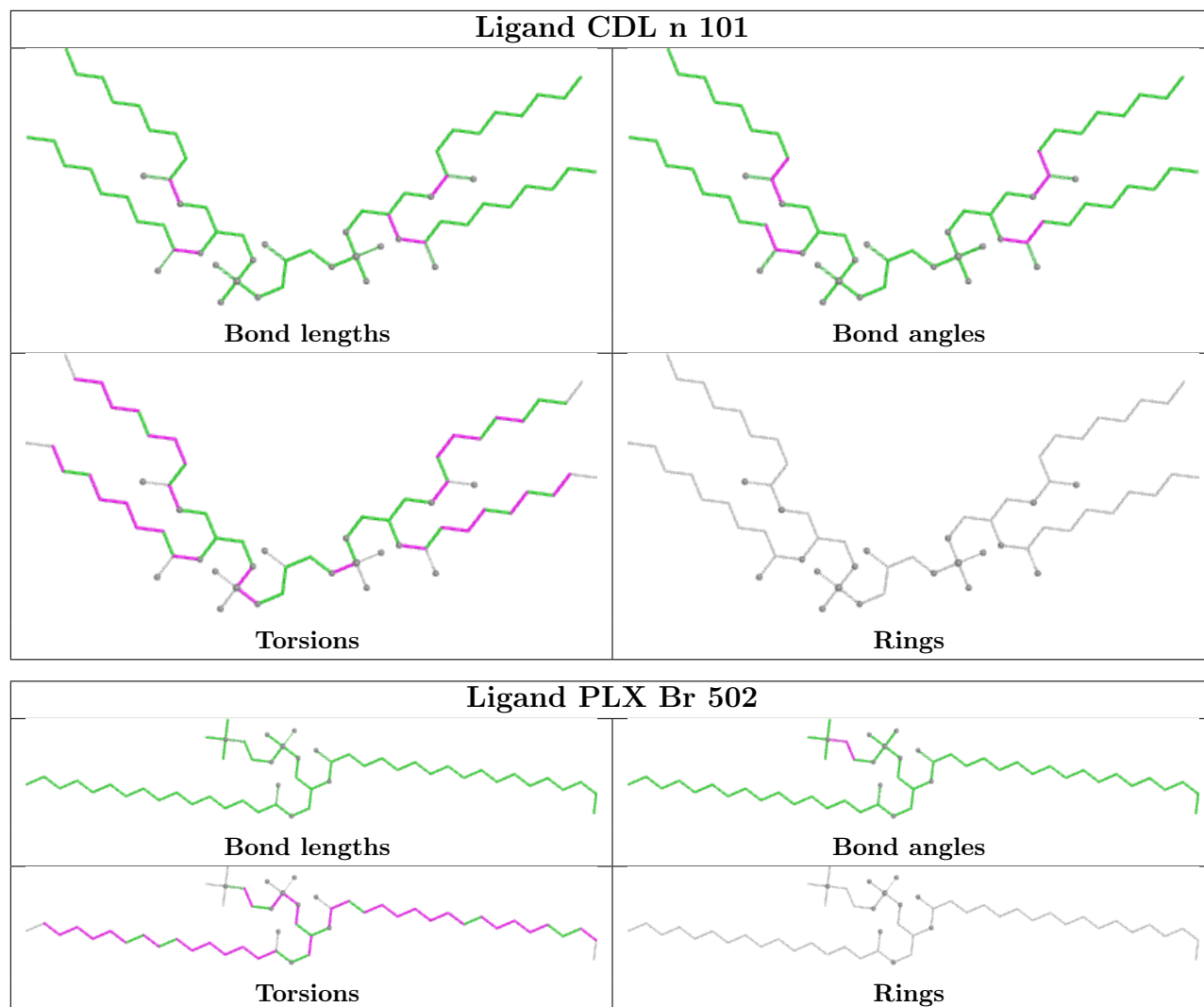


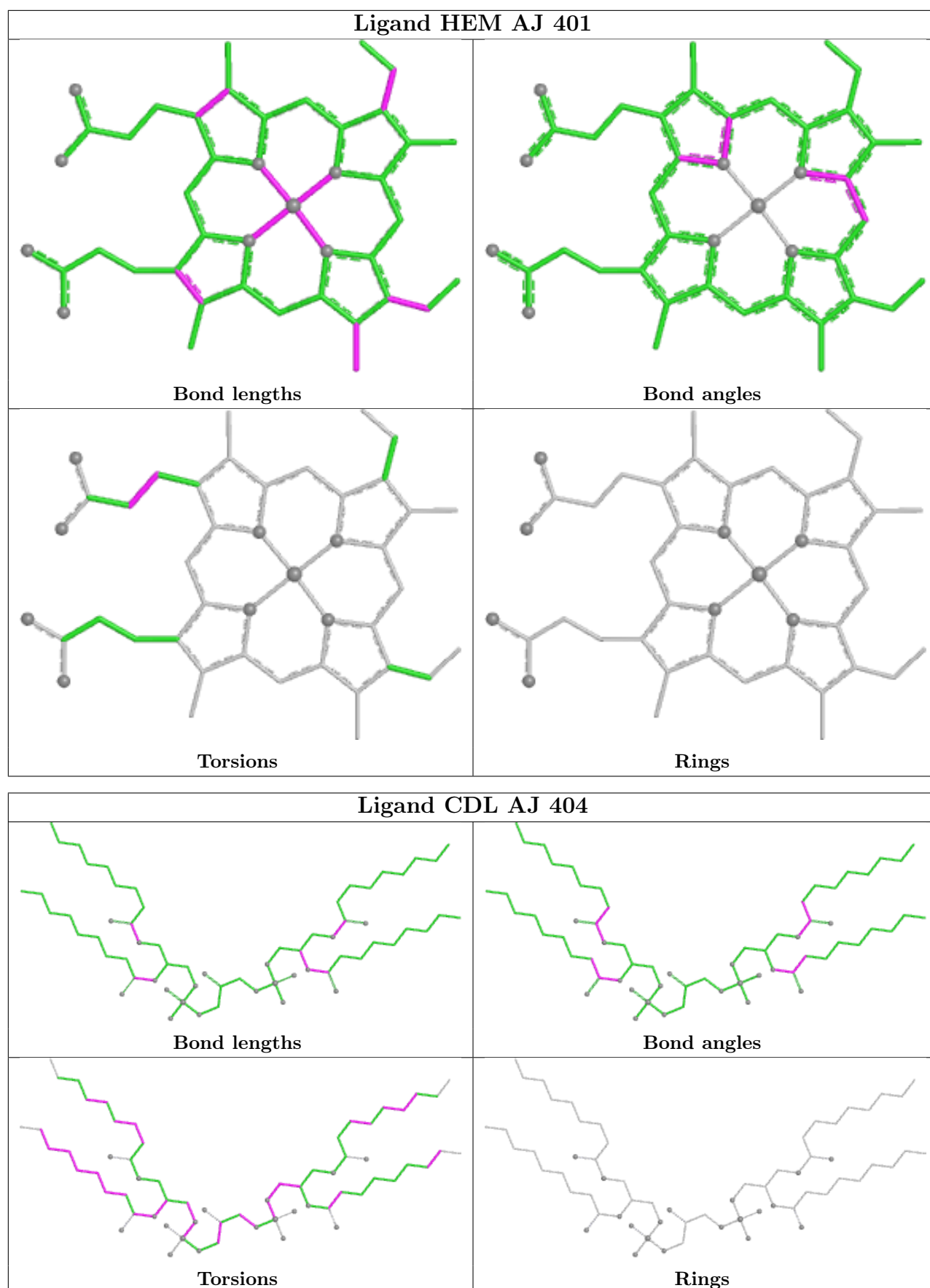


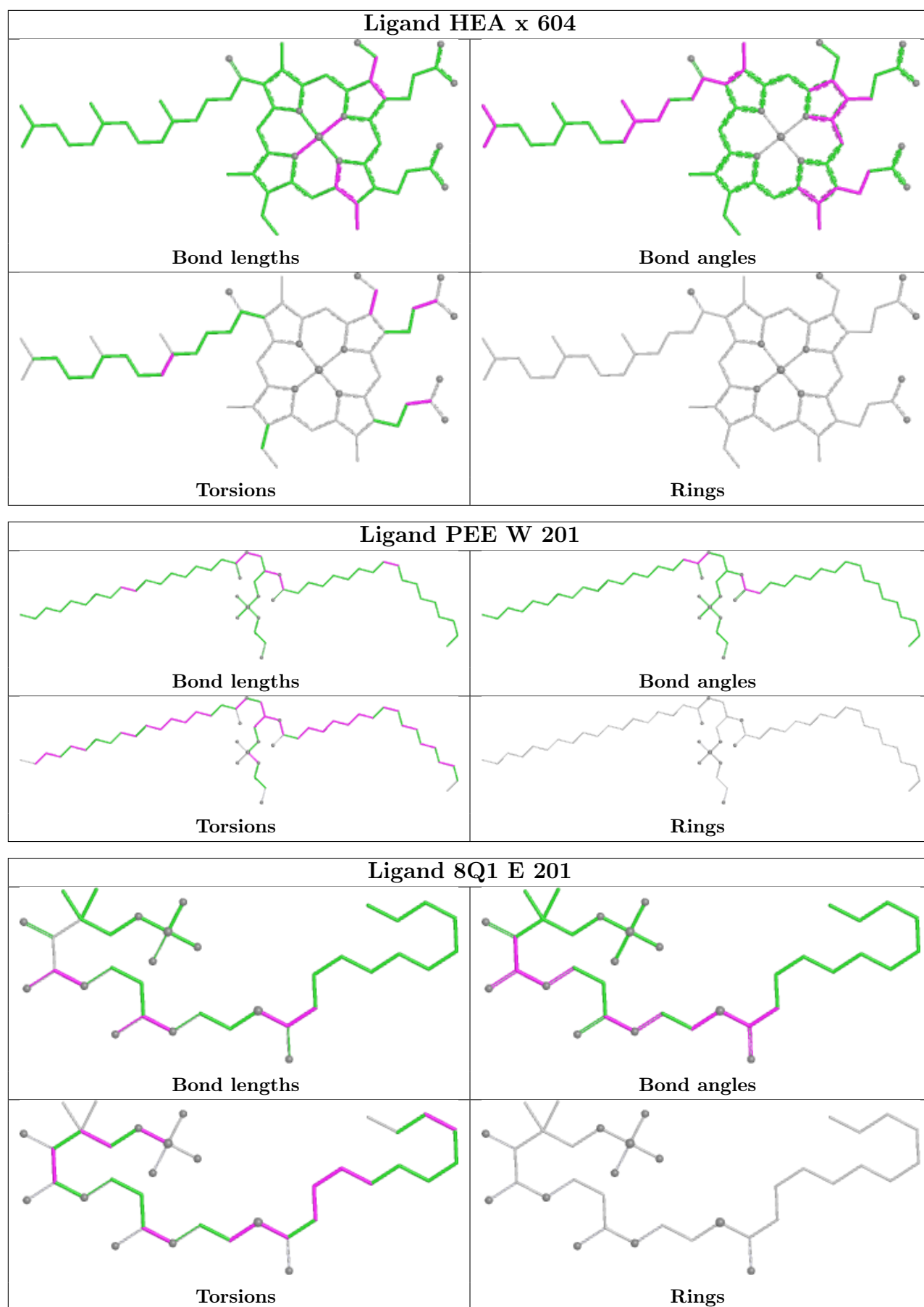


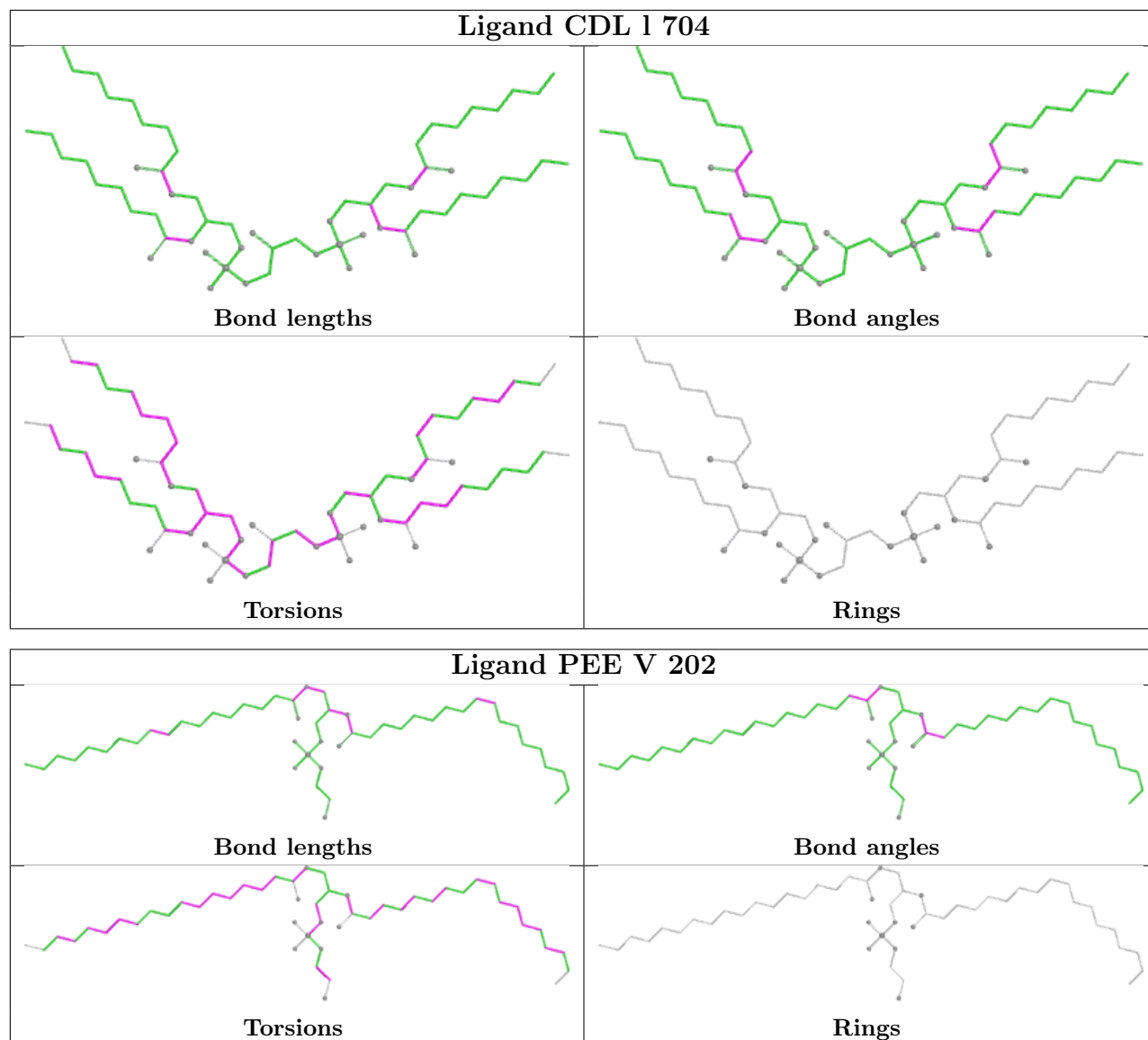


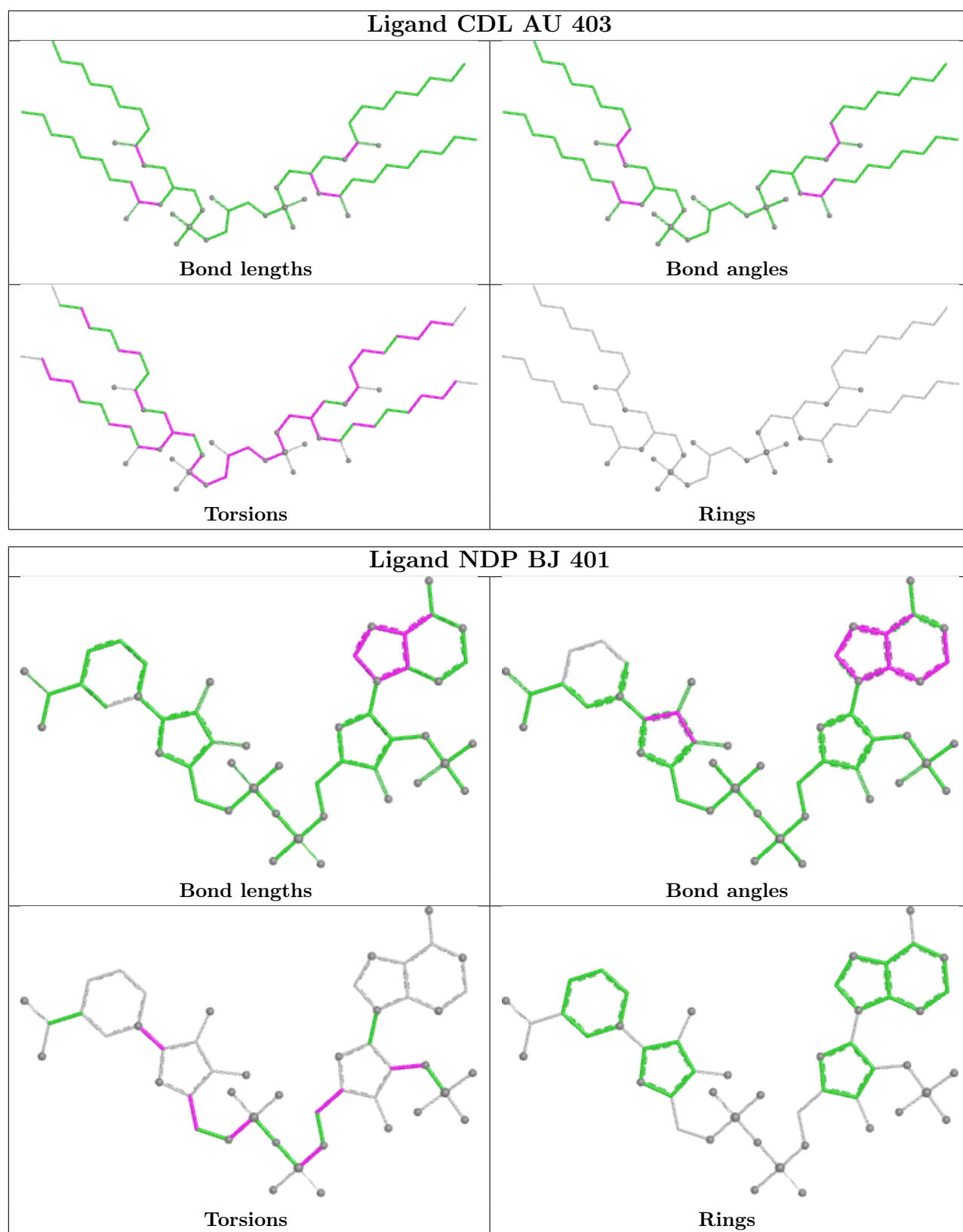


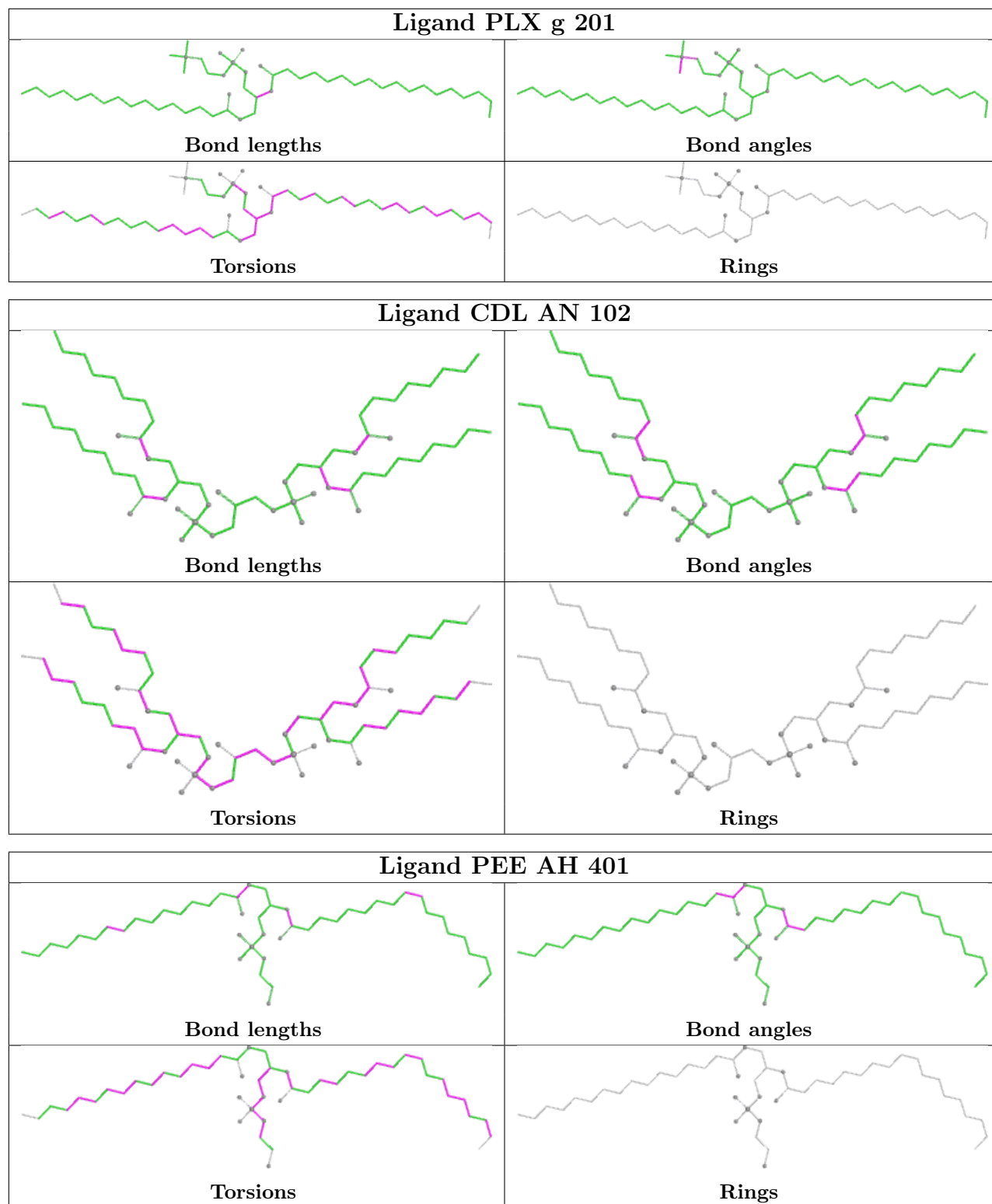


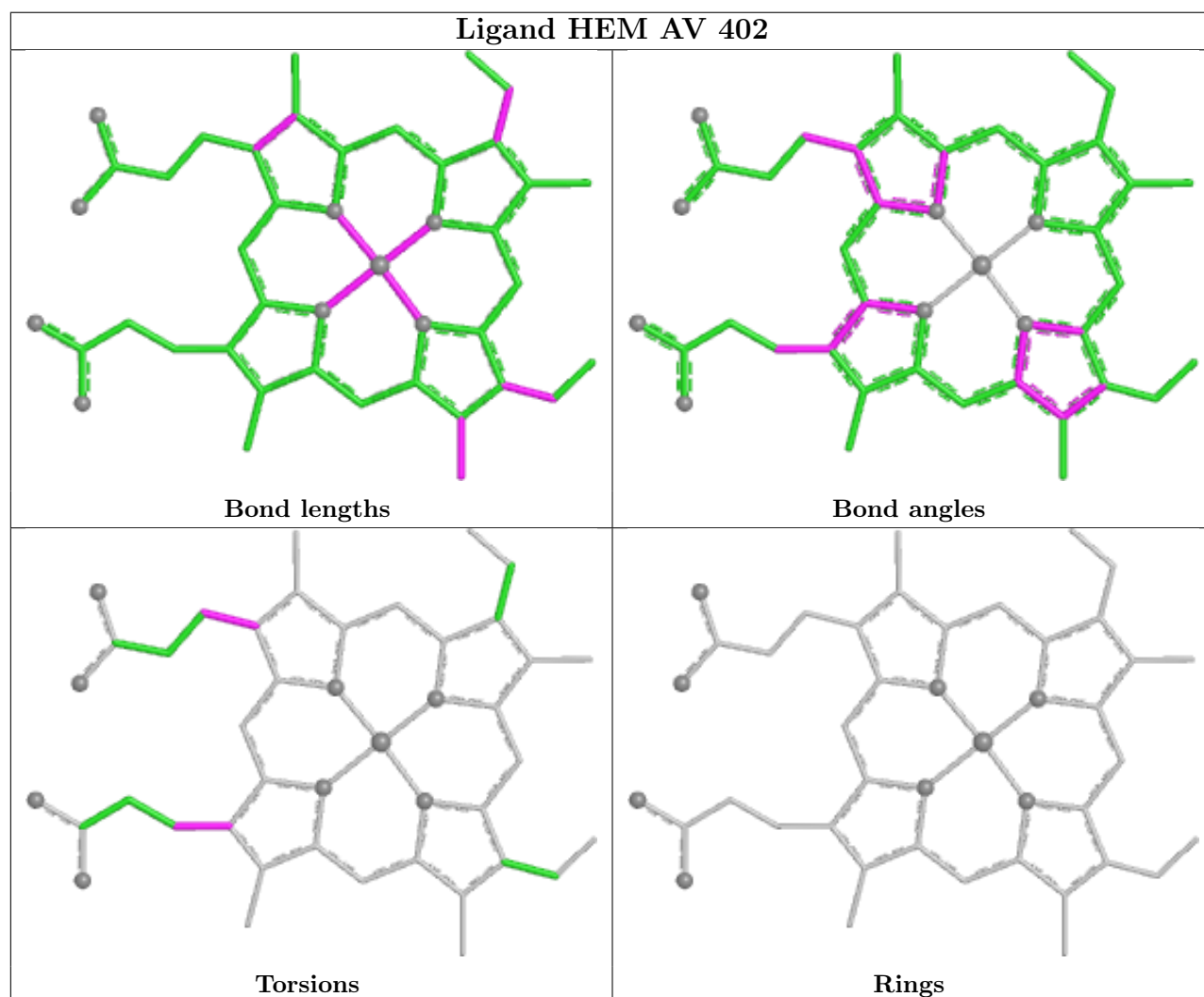
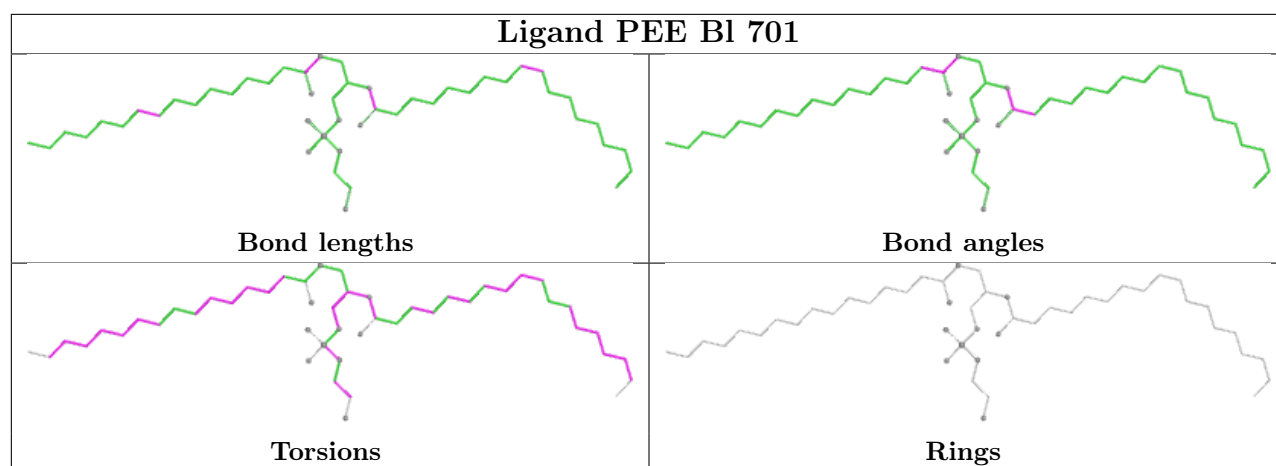


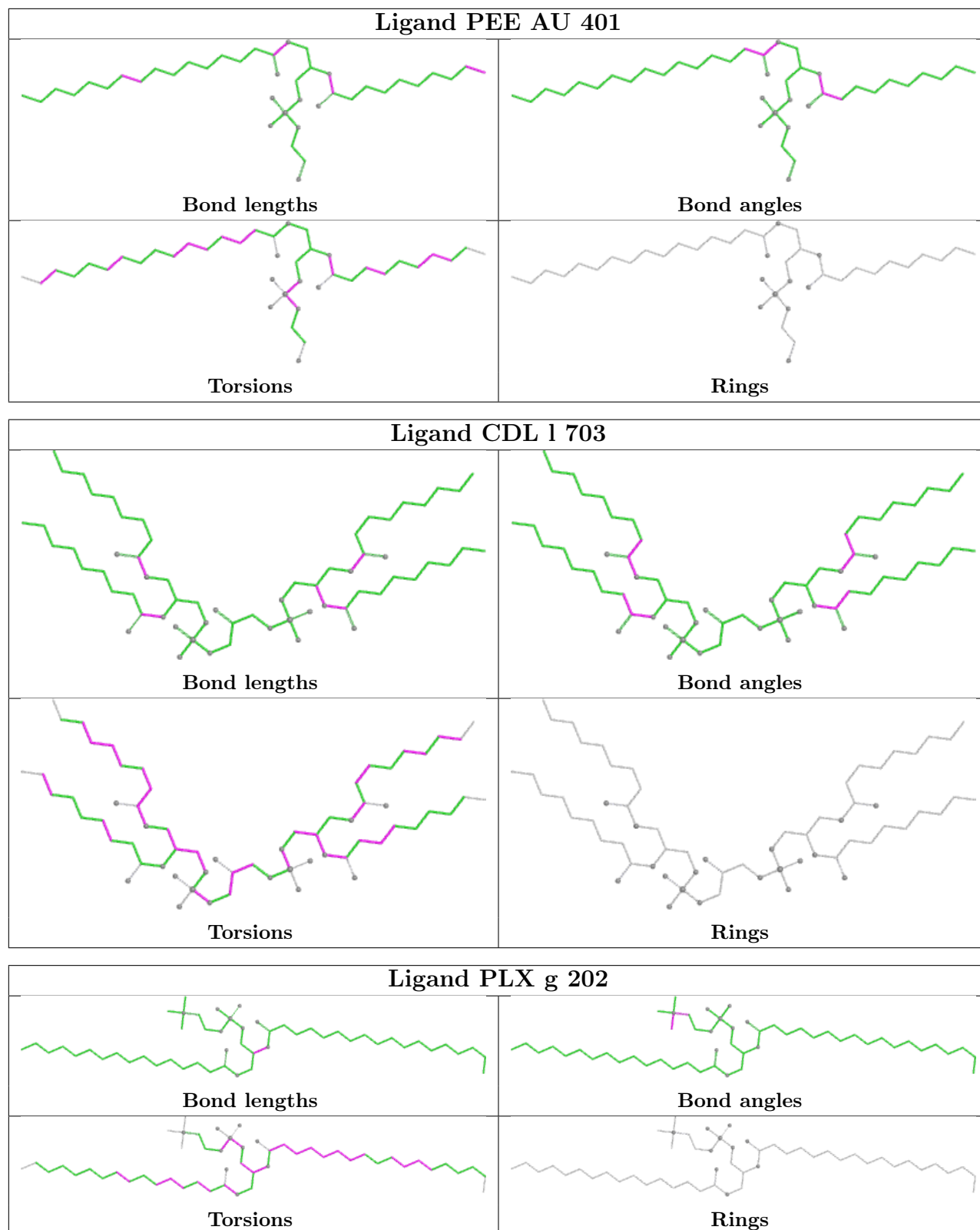


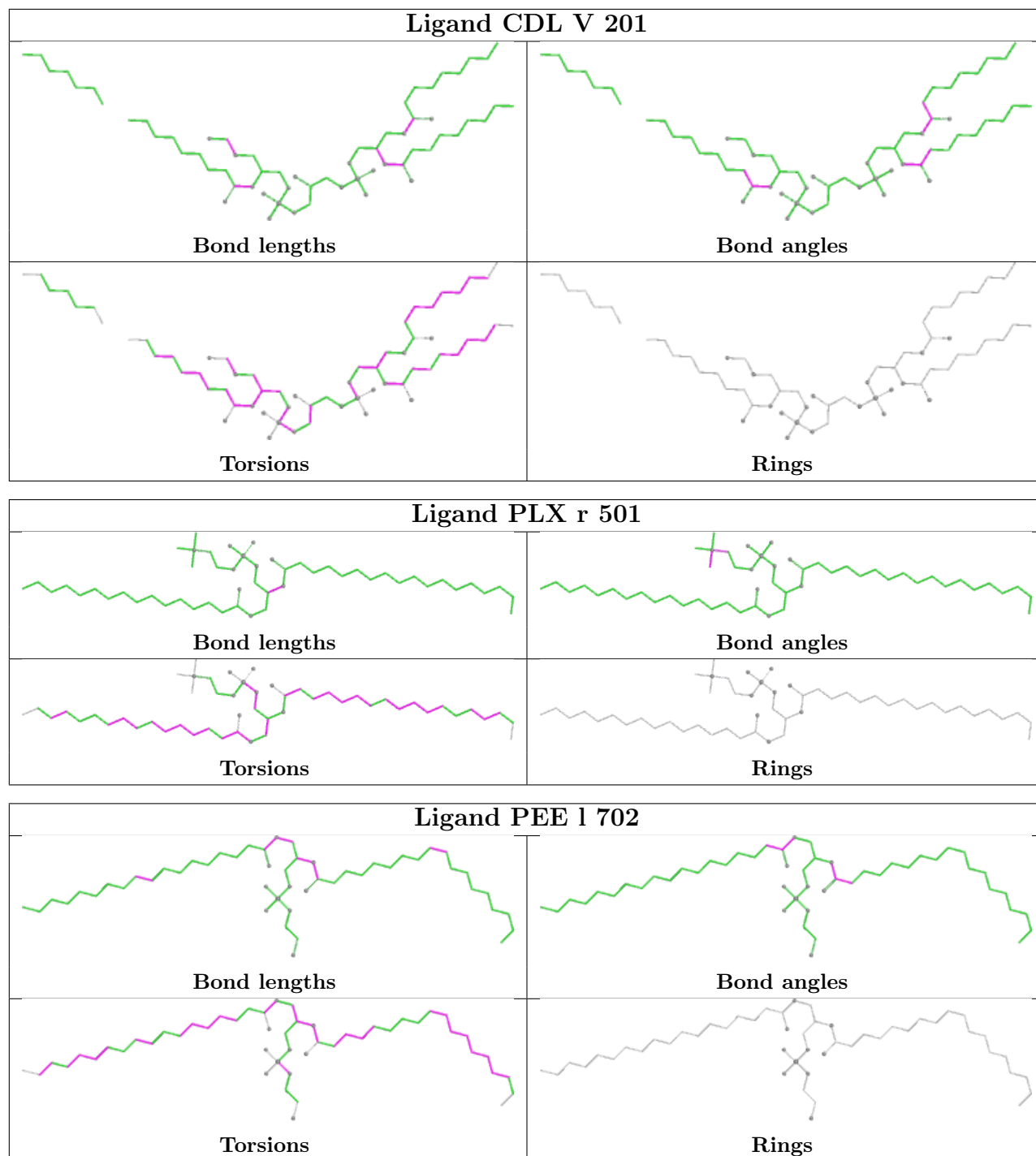


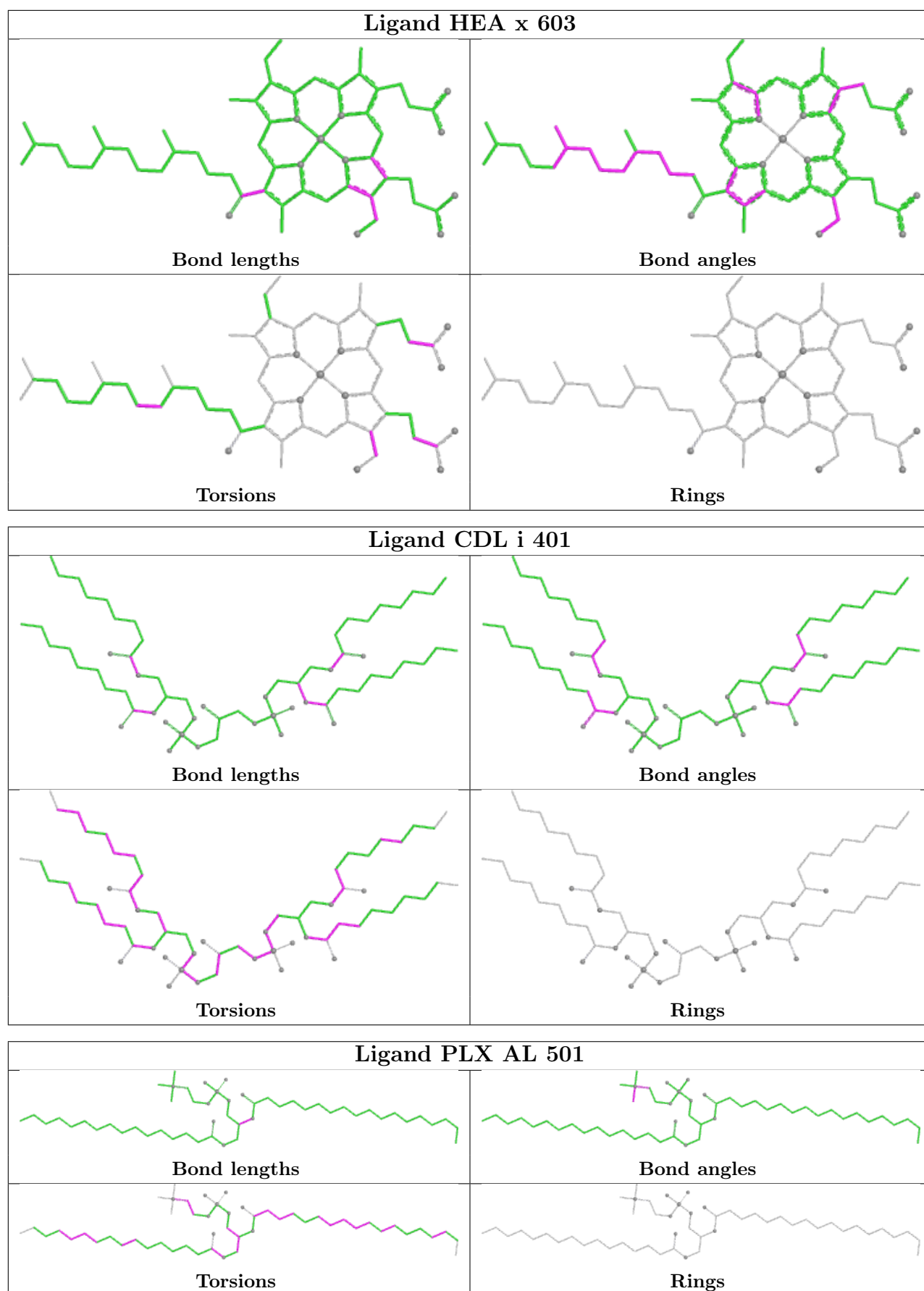


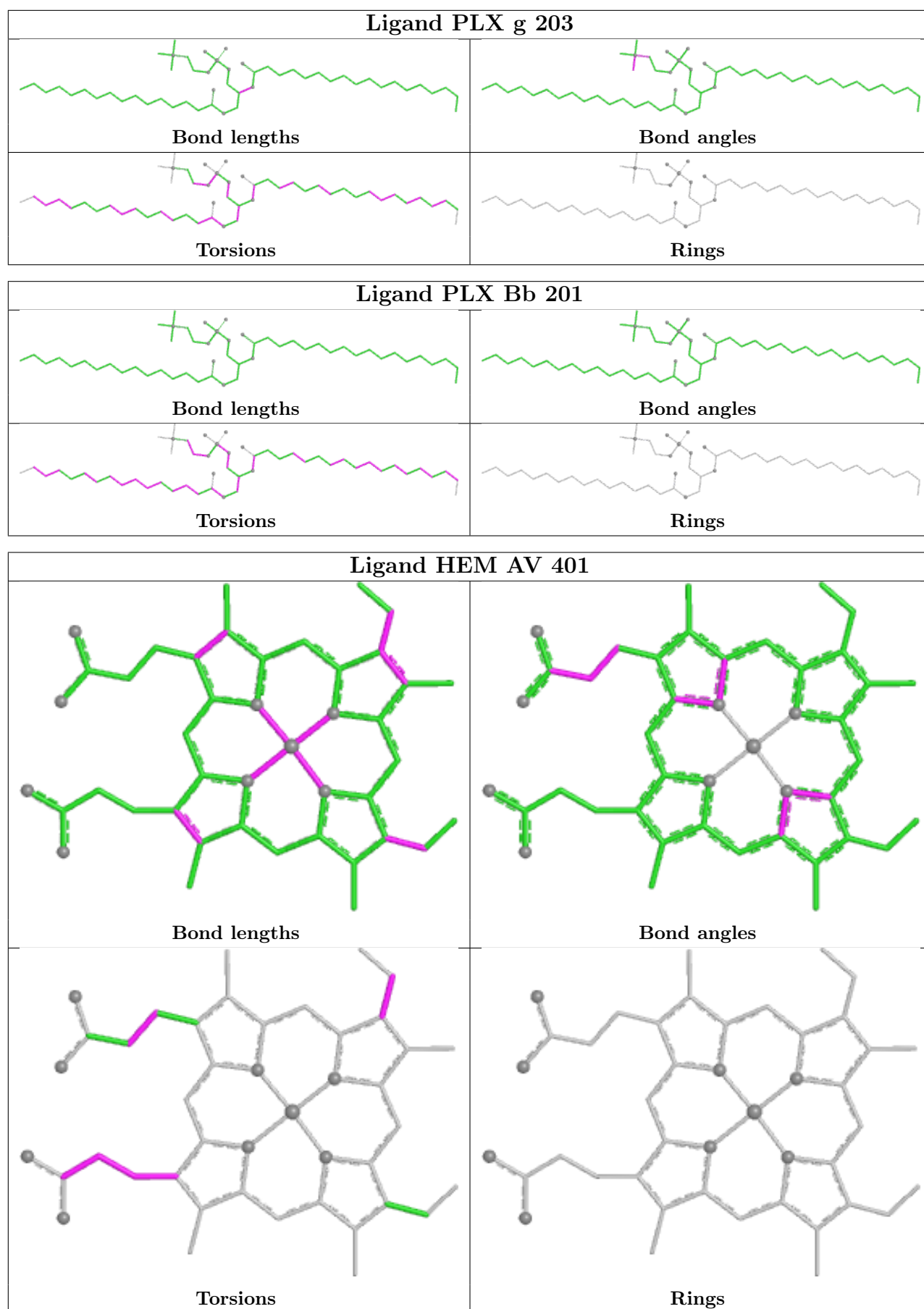


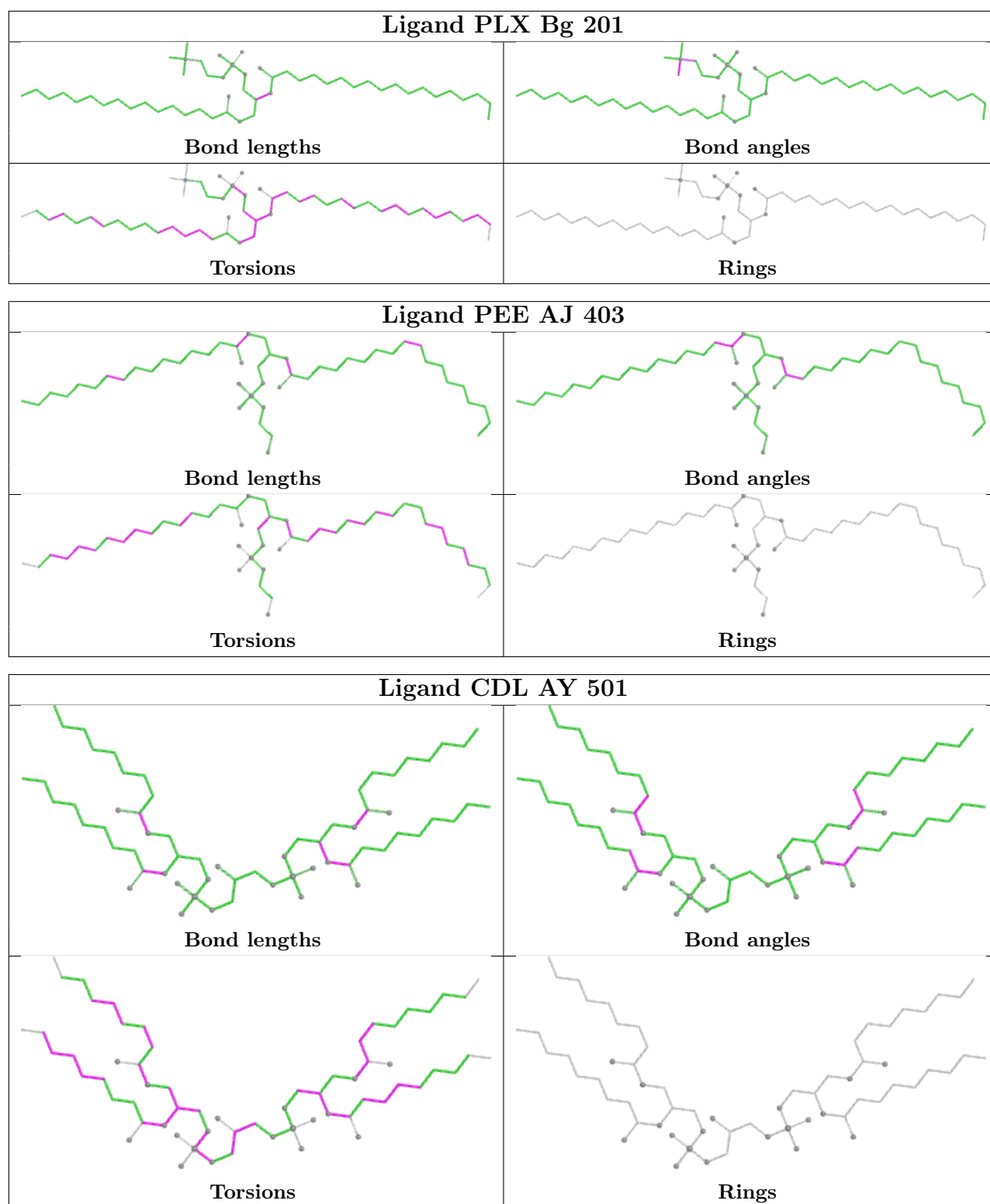


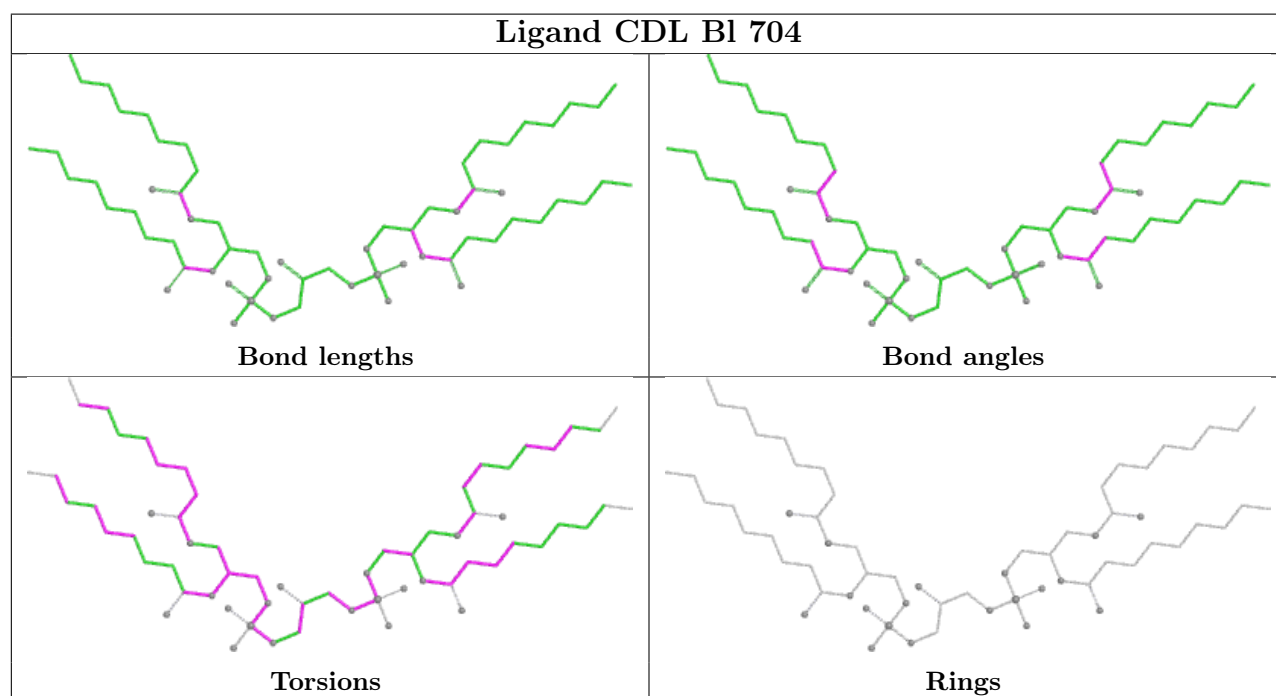
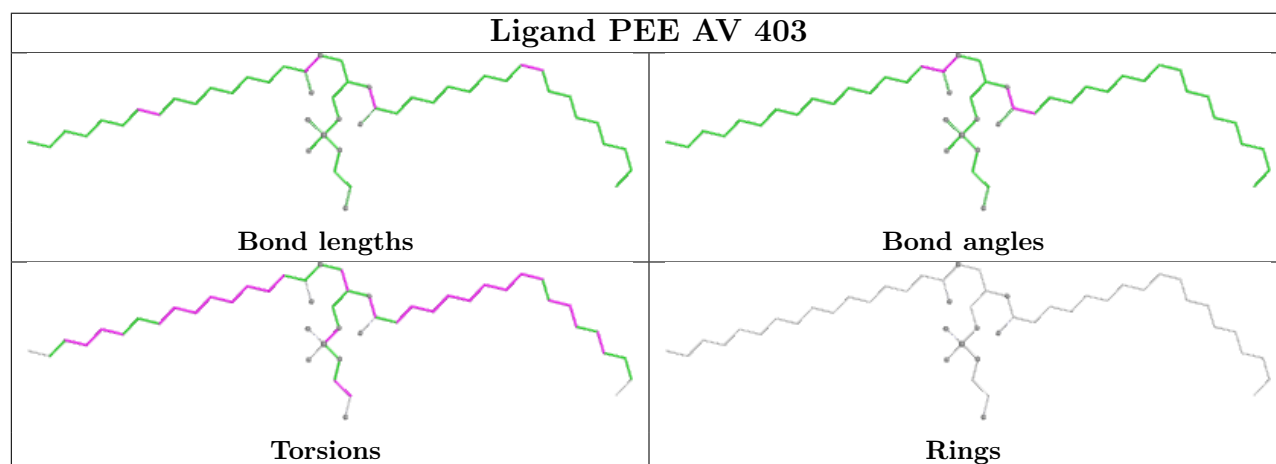
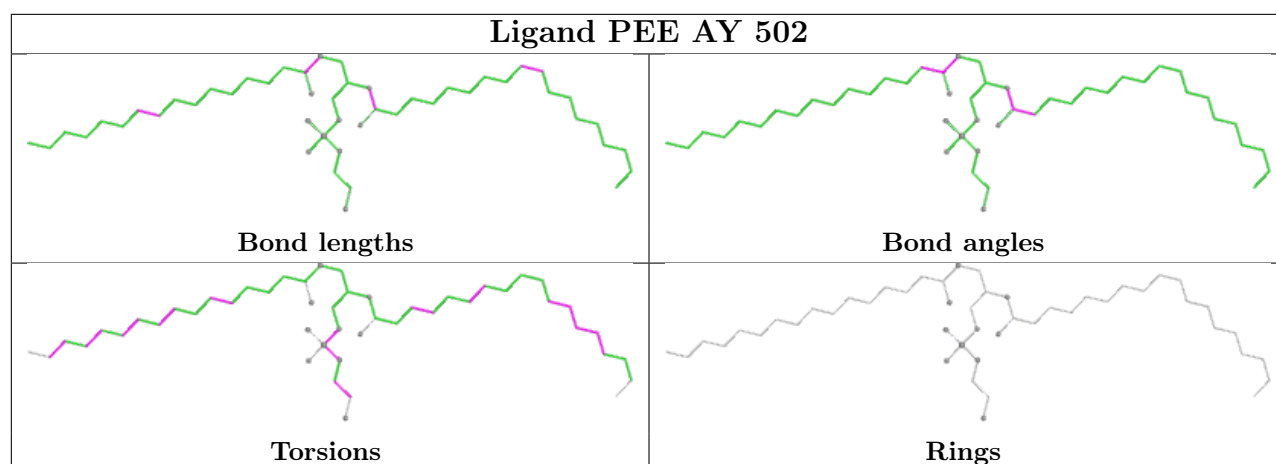


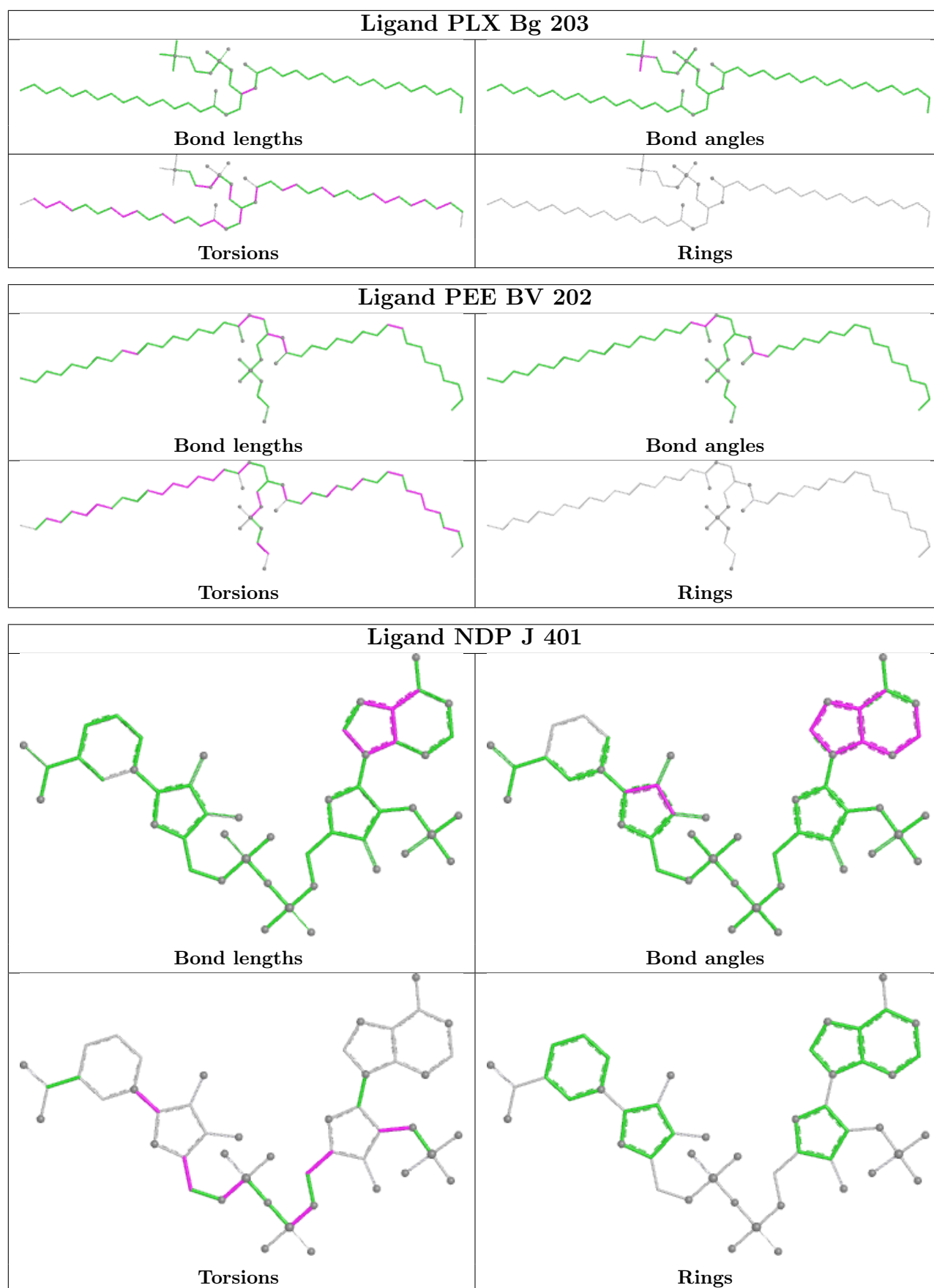


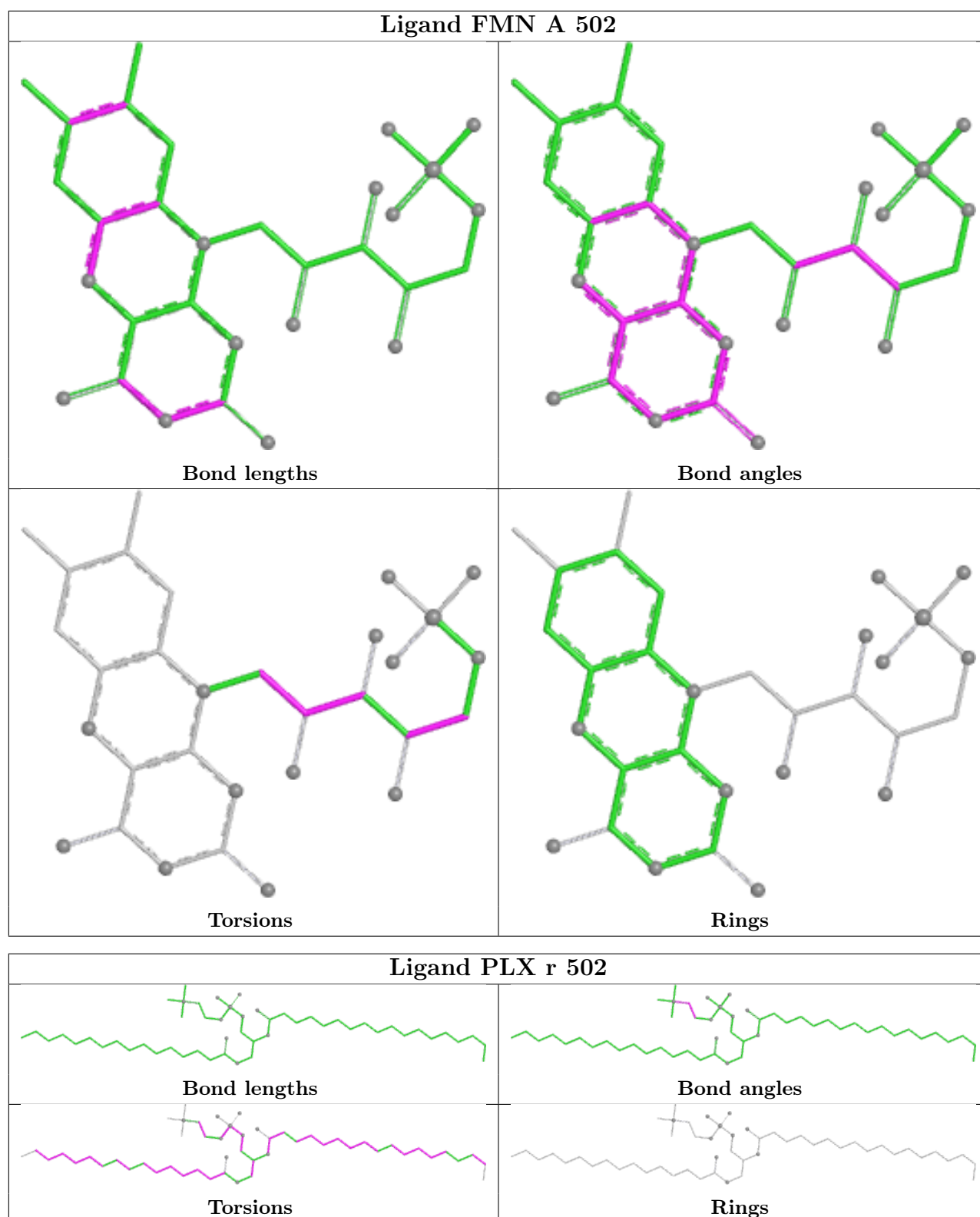


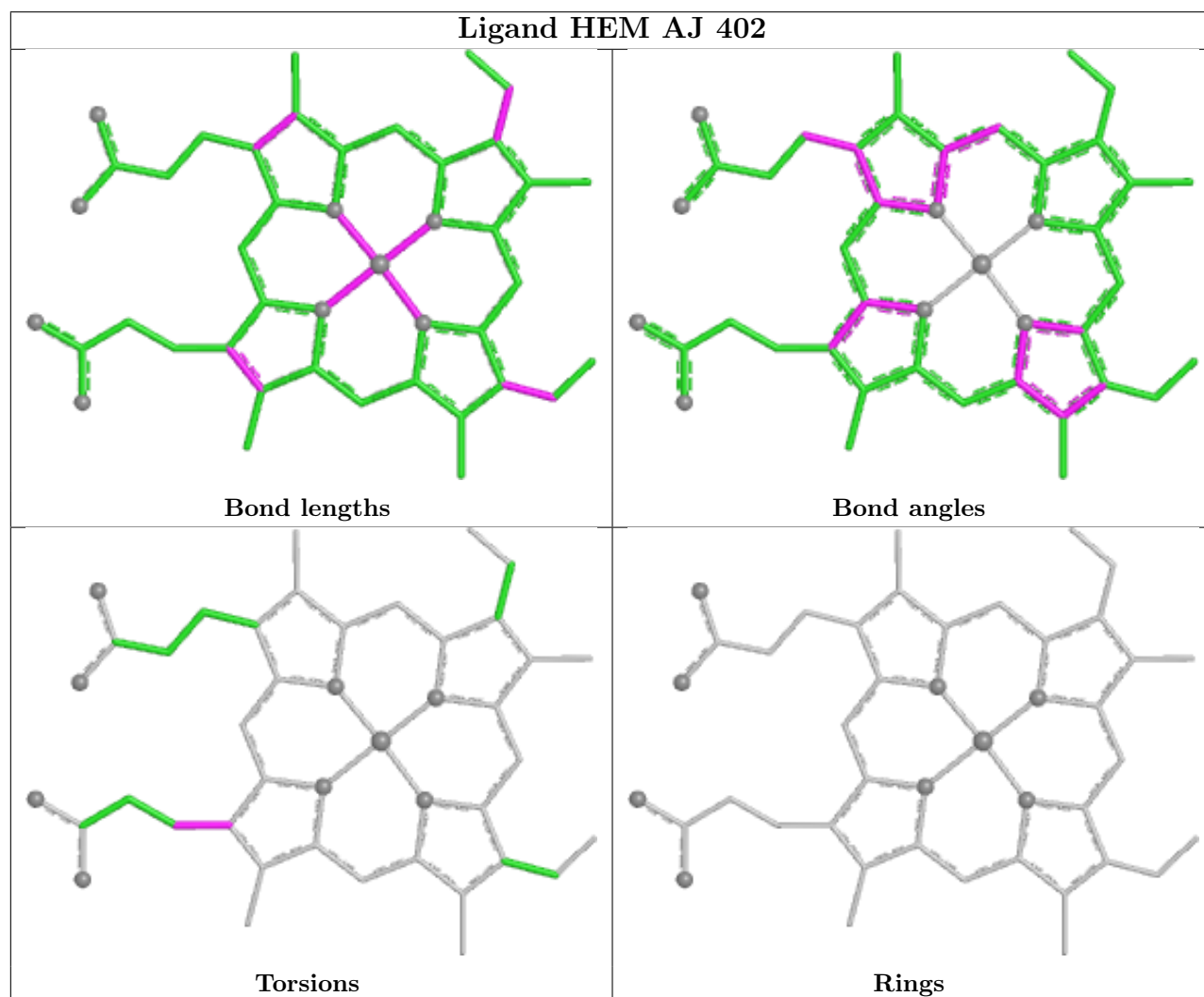


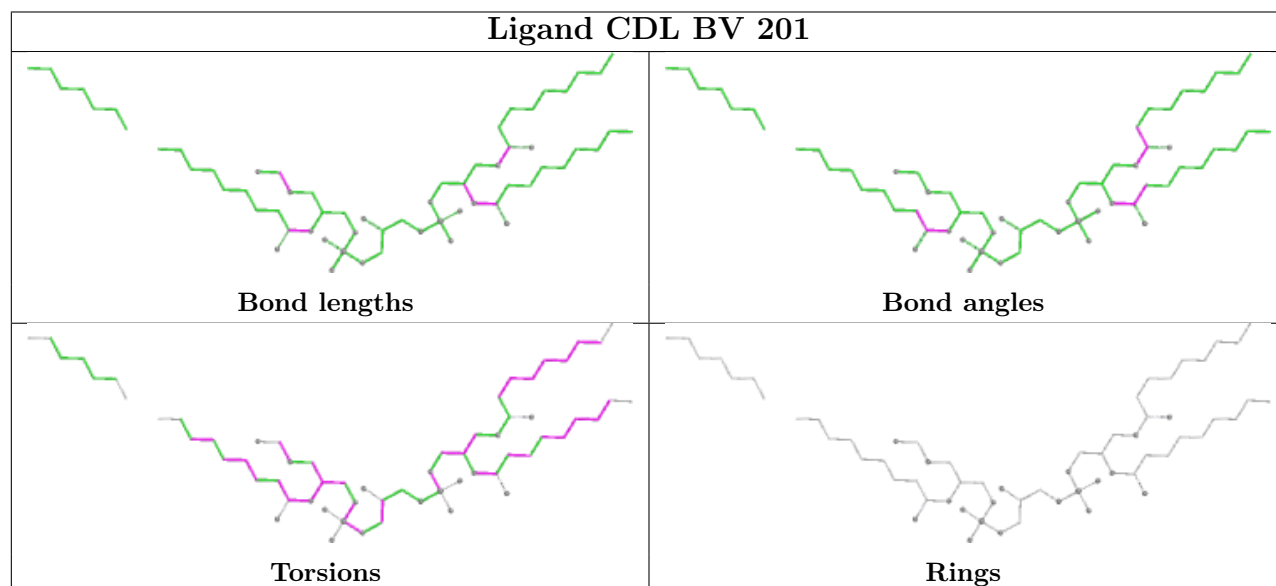
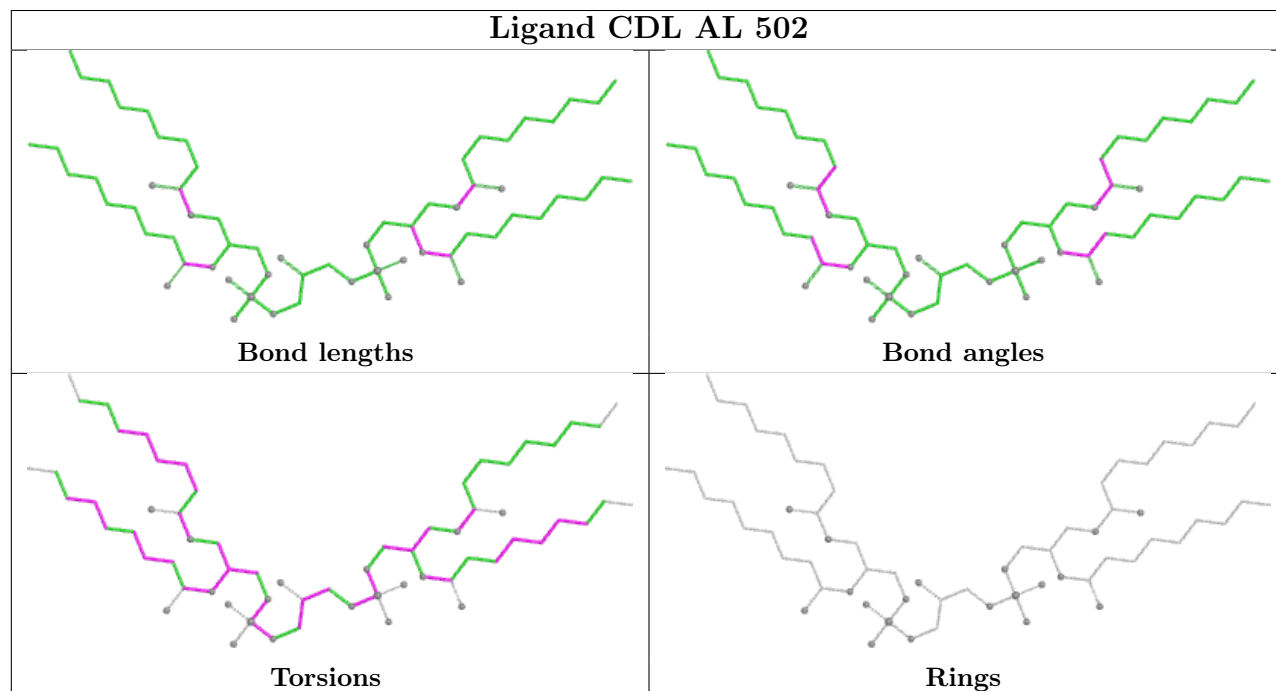
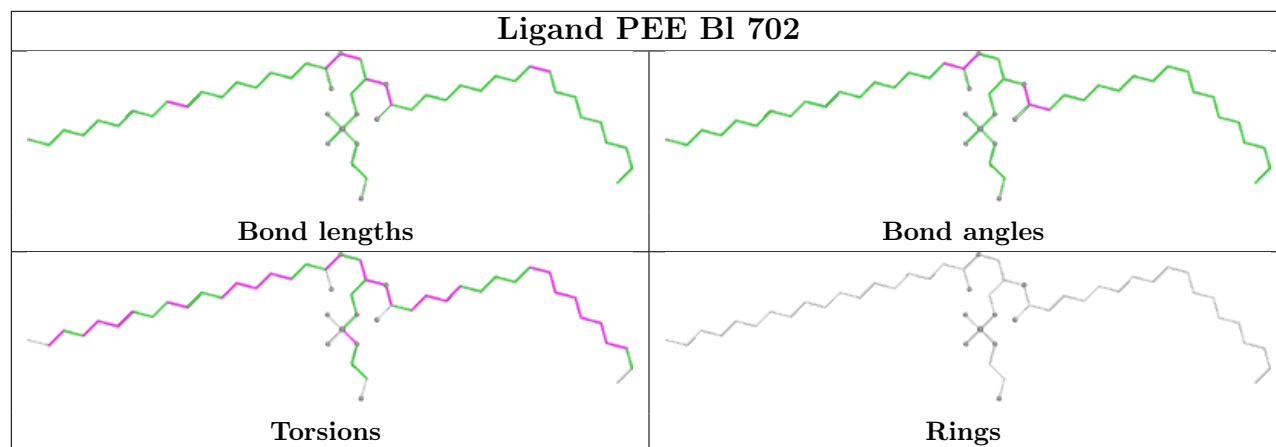


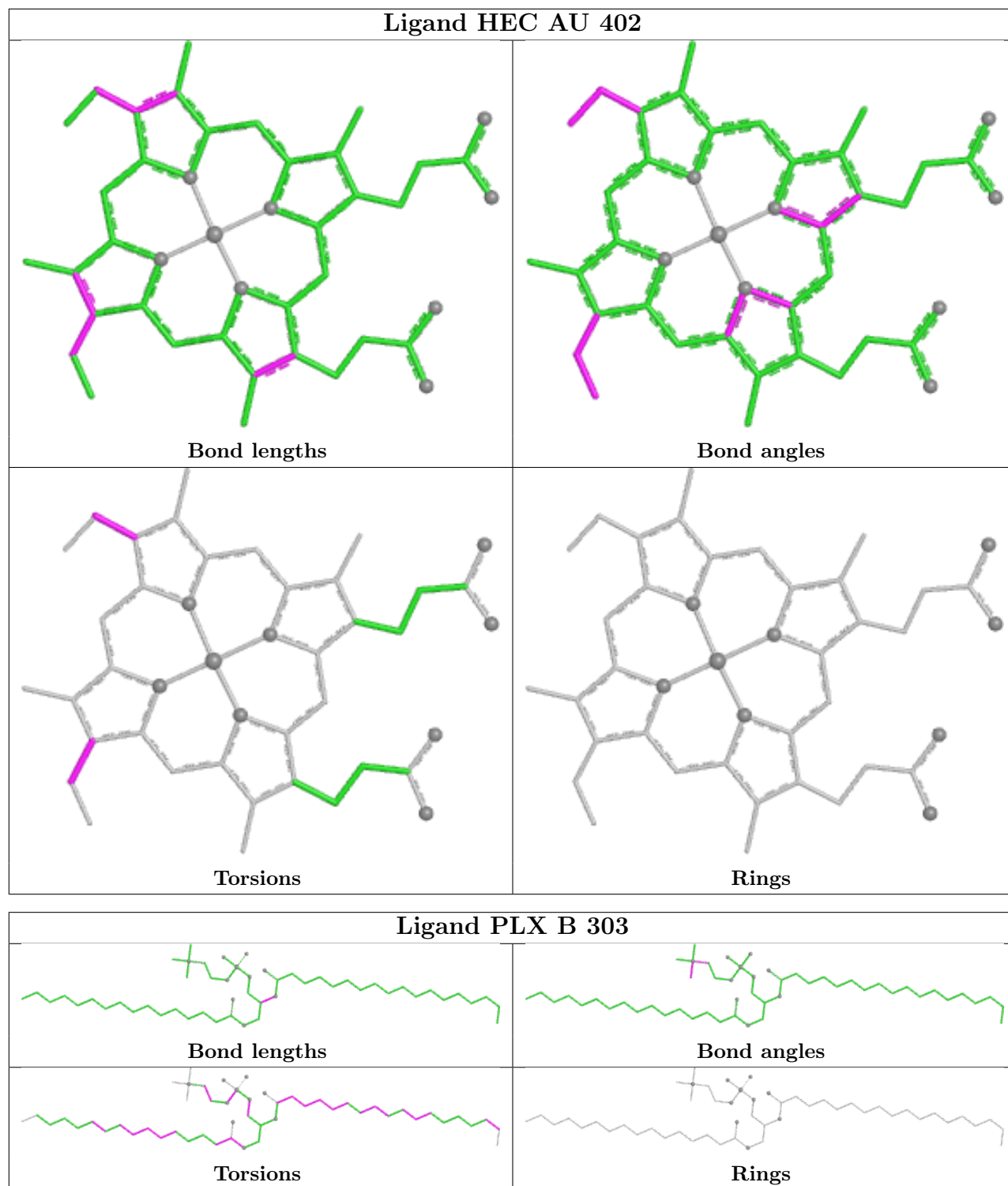


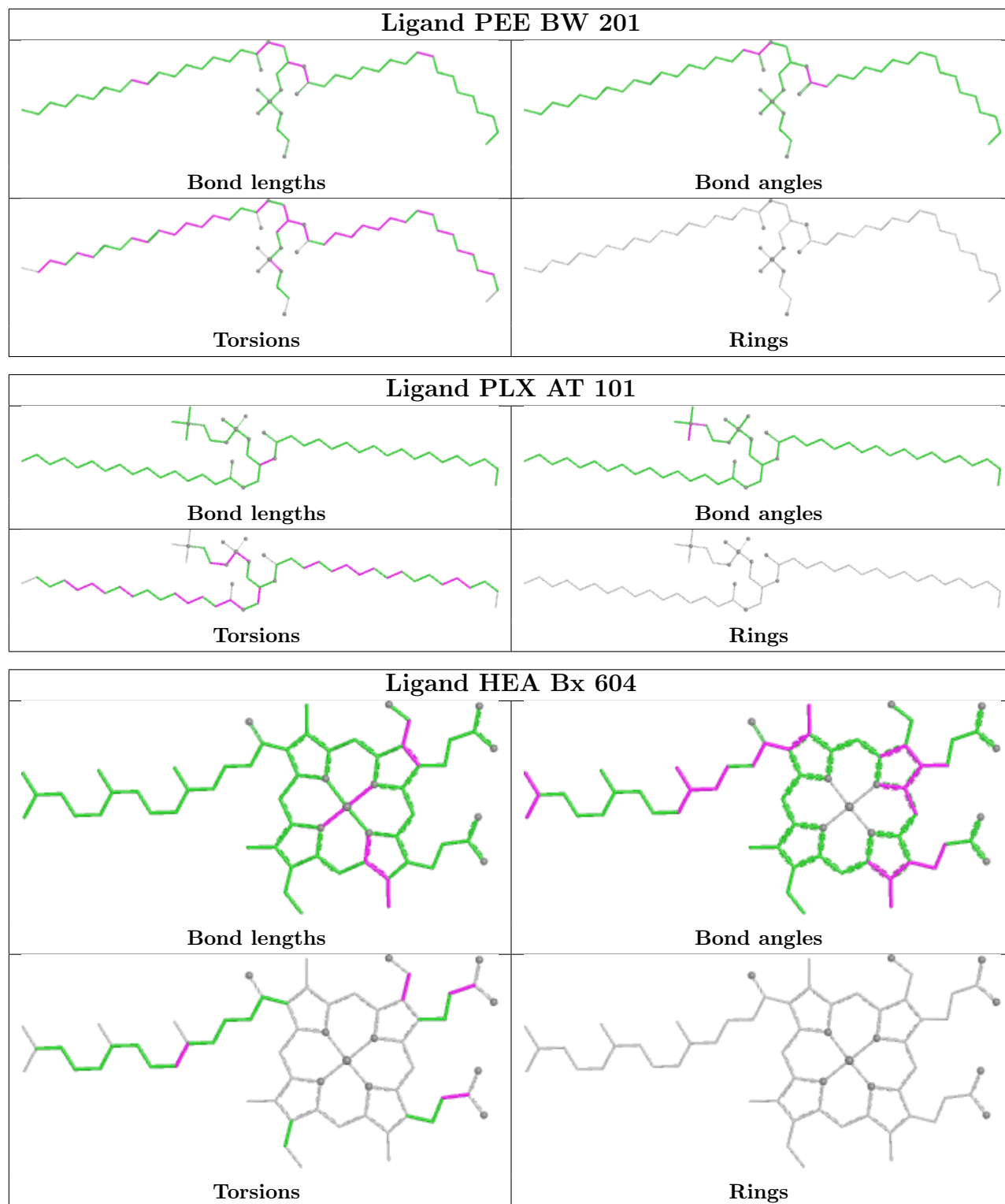


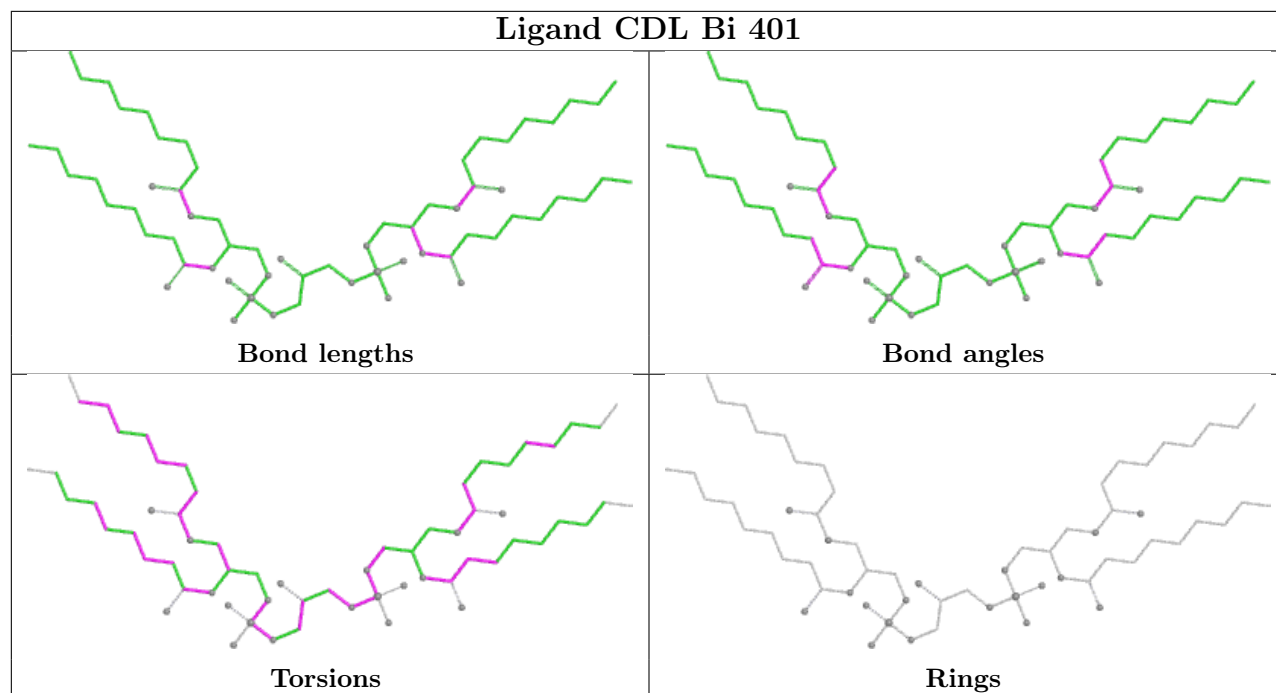


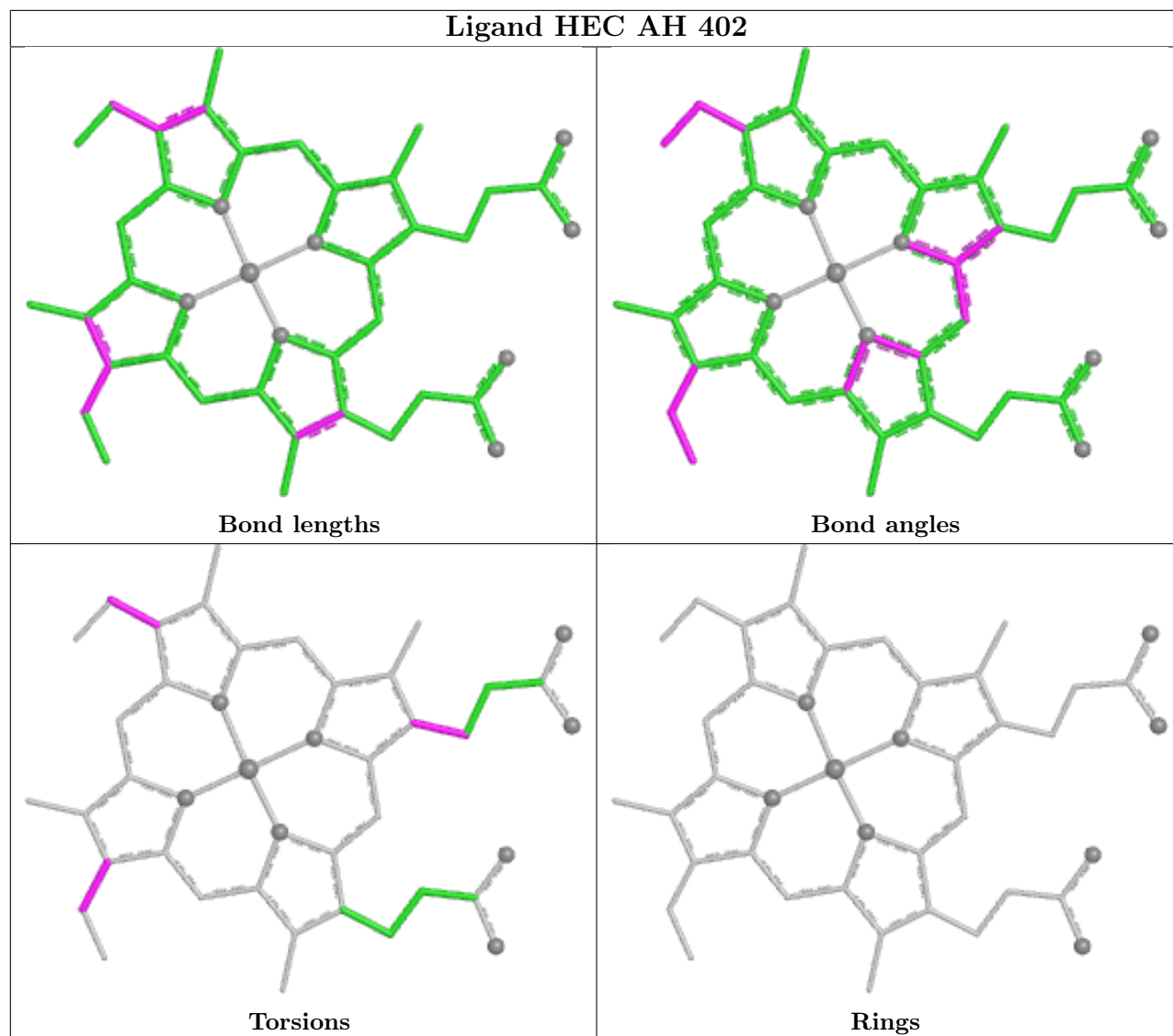


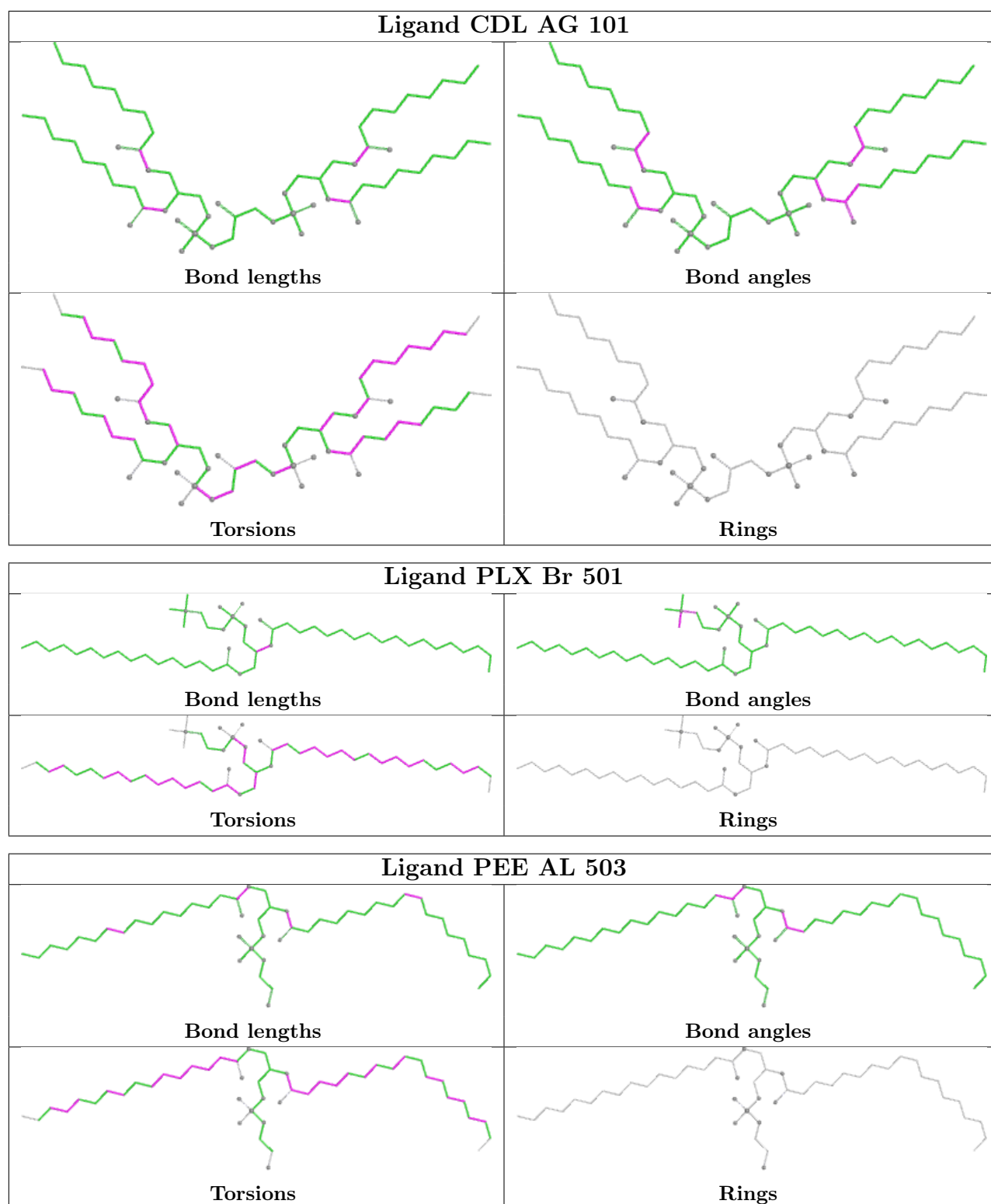


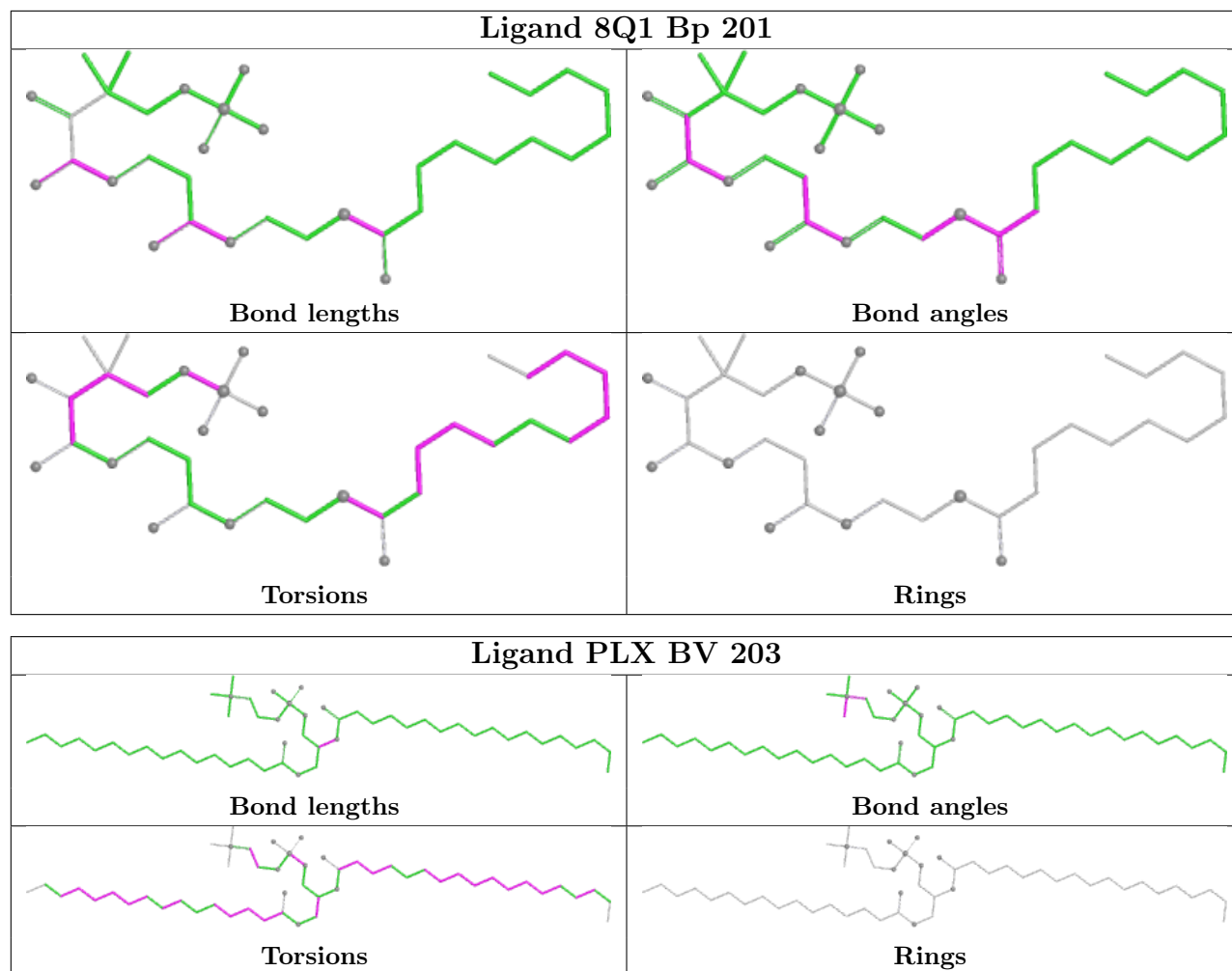












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

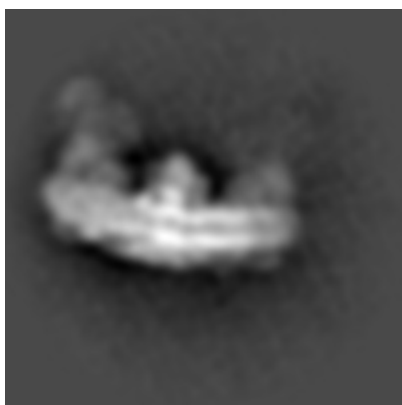
6 Map visualisation [i](#)

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.

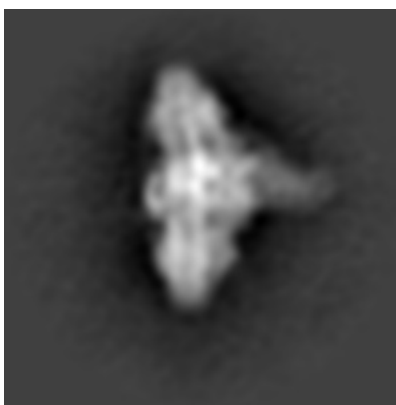
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

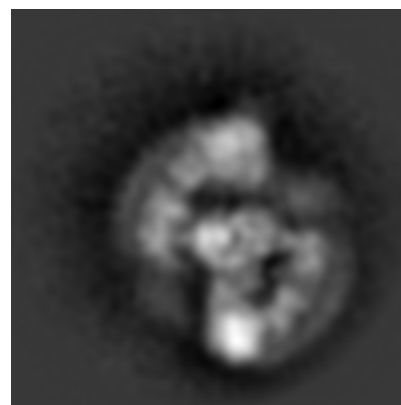
6.1.1 Primary map



X



Y



Z

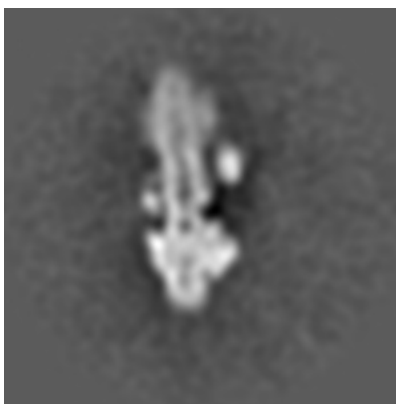
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

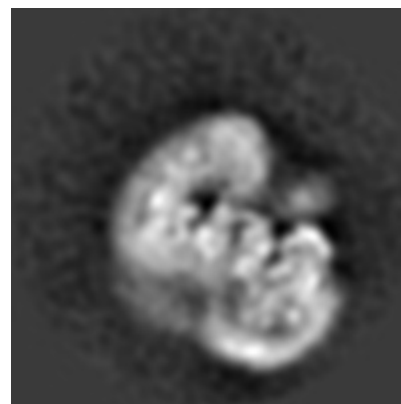
6.2.1 Primary map



X Index: 240



Y Index: 240

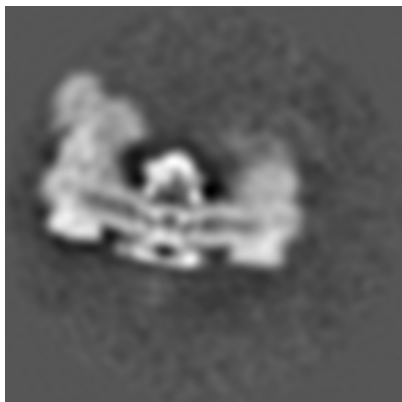


Z Index: 240

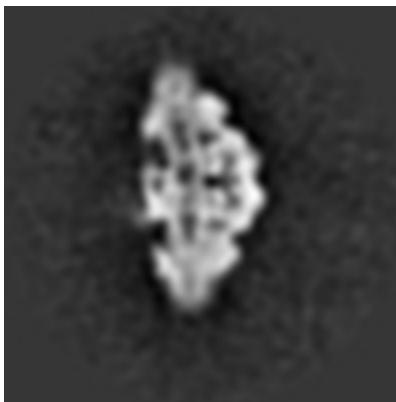
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

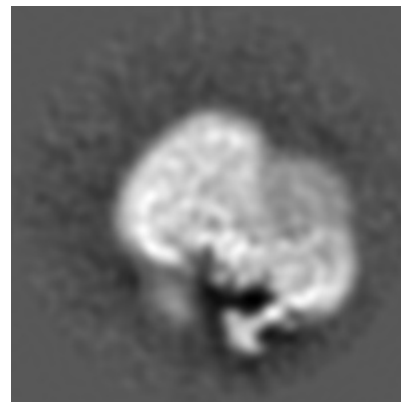
6.3.1 Primary map



X Index: 266



Y Index: 204

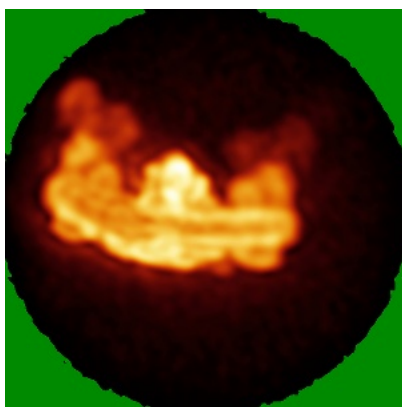


Z Index: 202

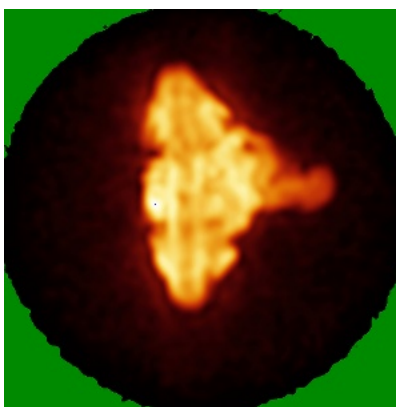
The images above show the largest variance slices of the map in three orthogonal directions.

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

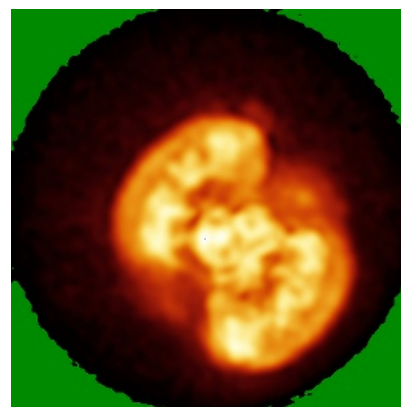
6.4.1 Primary map



X



Y

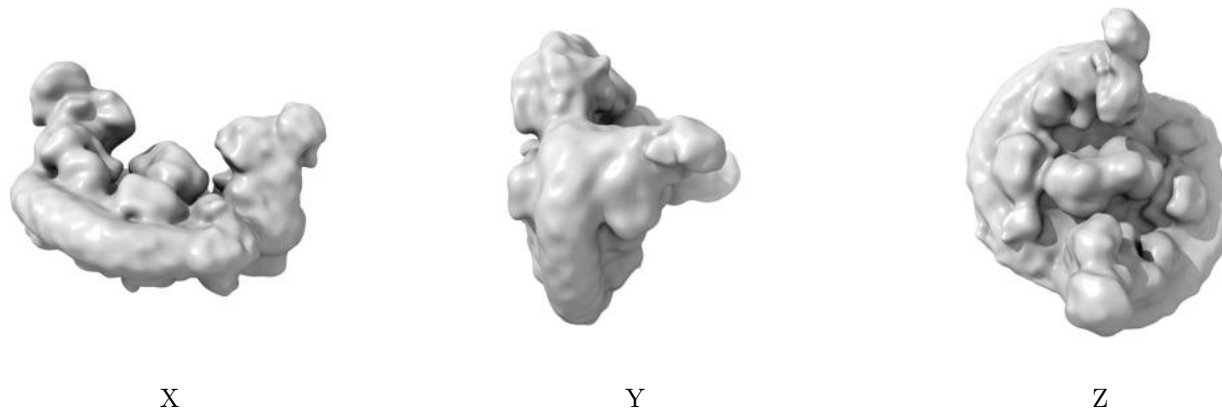


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

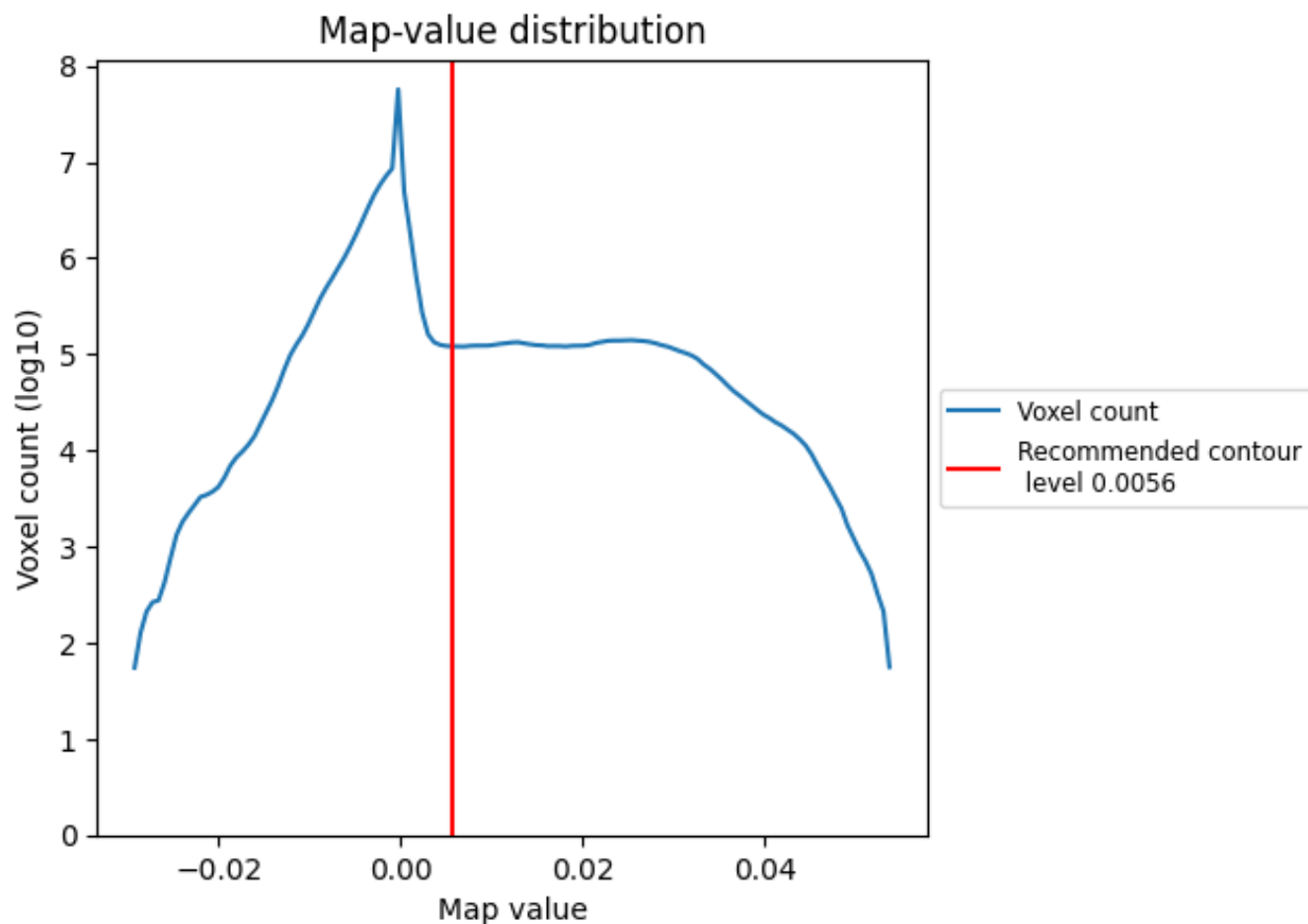
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

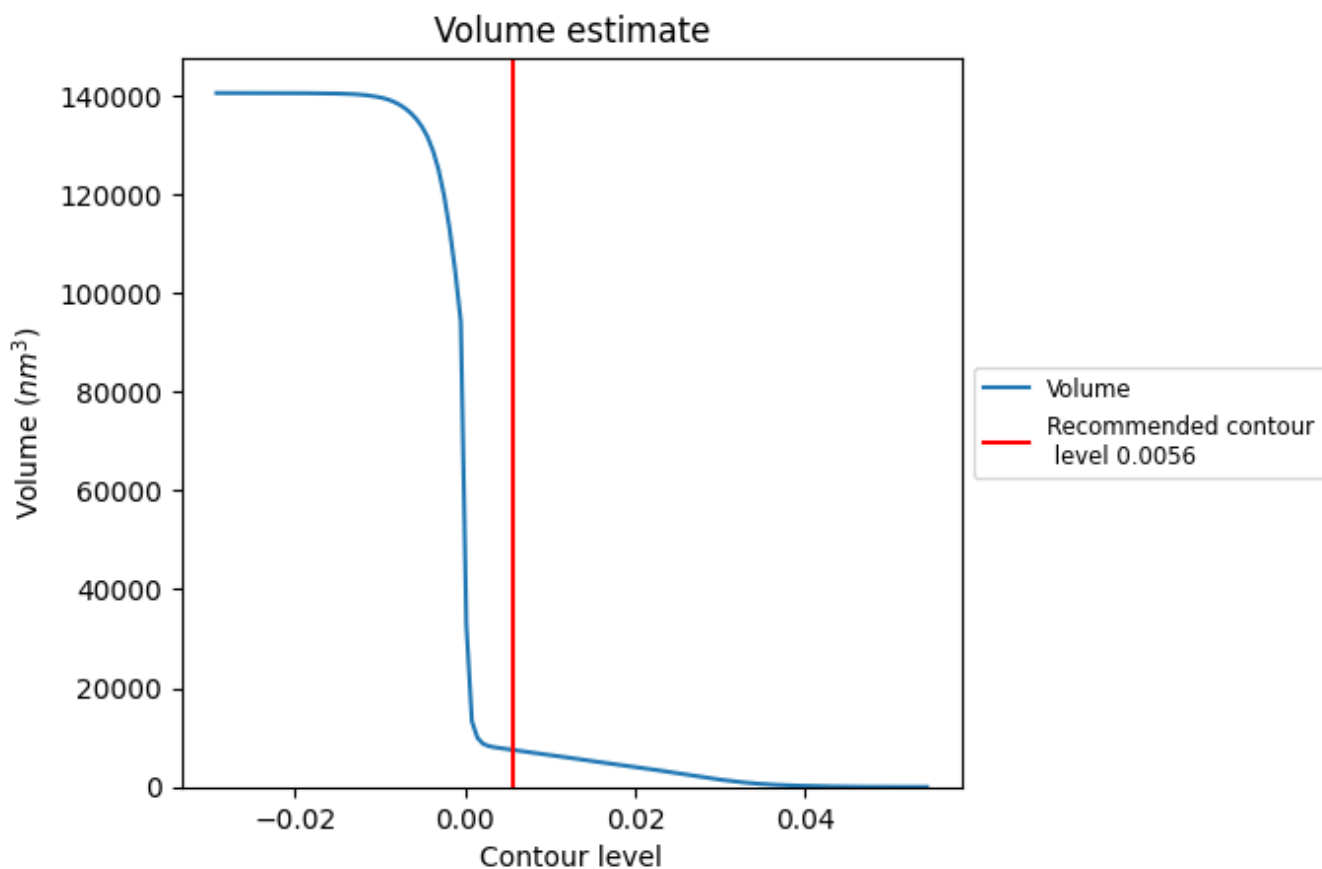
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

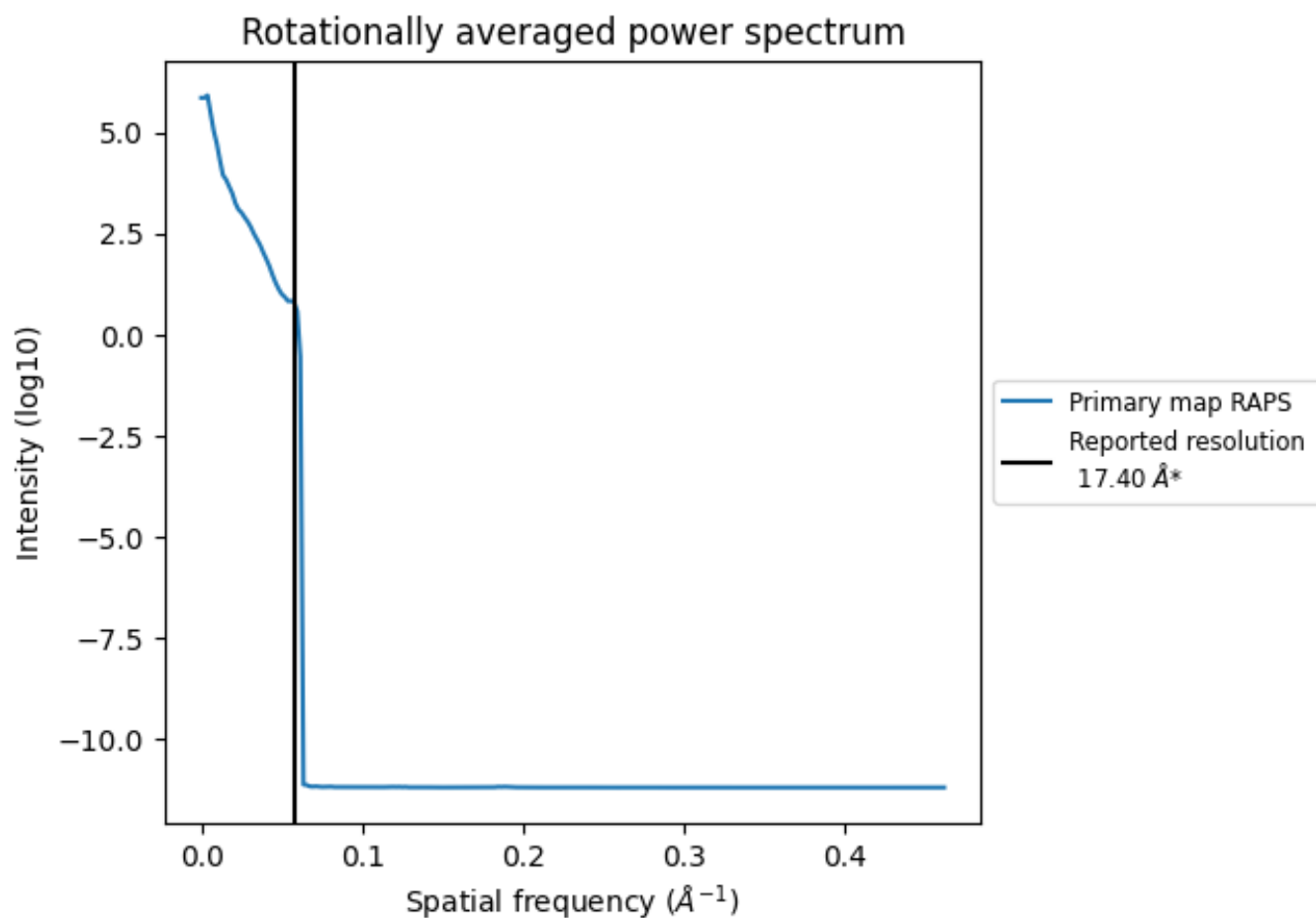
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 7506 nm³; 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

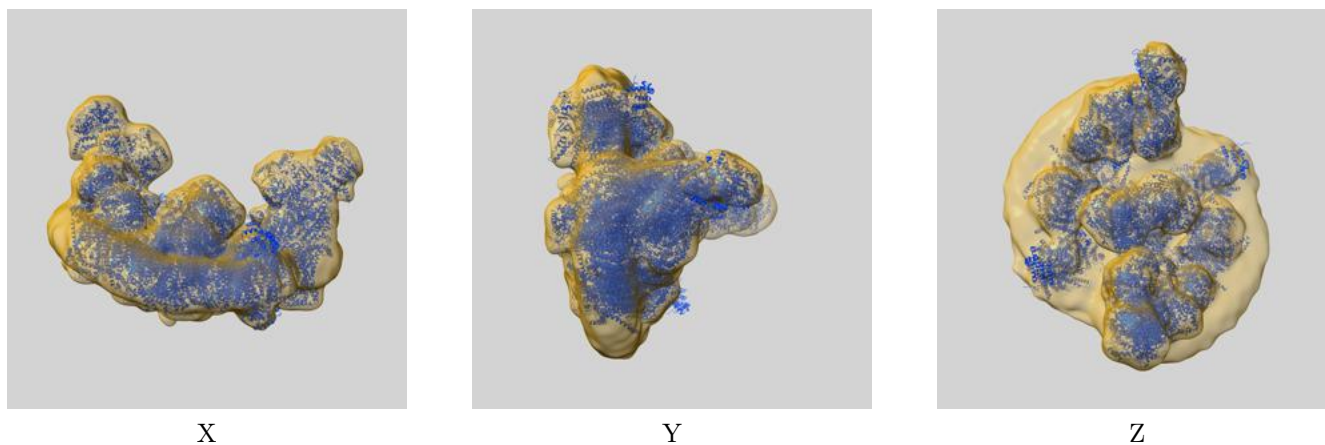
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

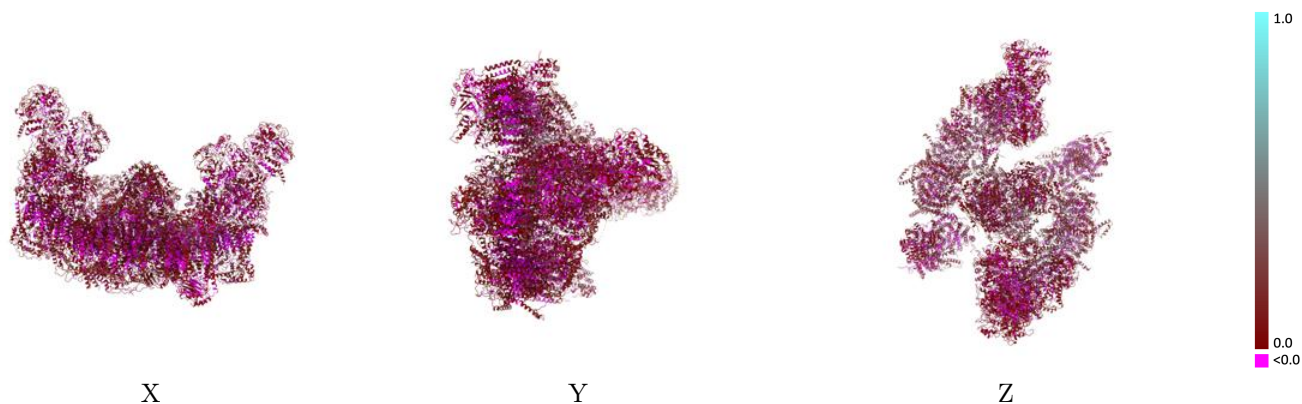
This section contains information regarding the fit between EMDB map EMD-6776 and PDB model 5XTI. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)



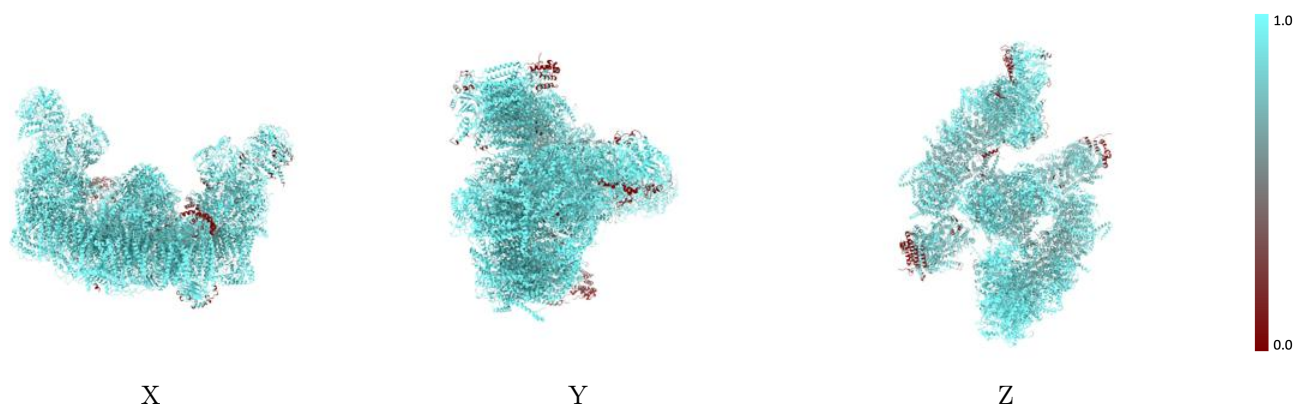
The images above show the 3D surface view of the map at the recommended contour level 0.0056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



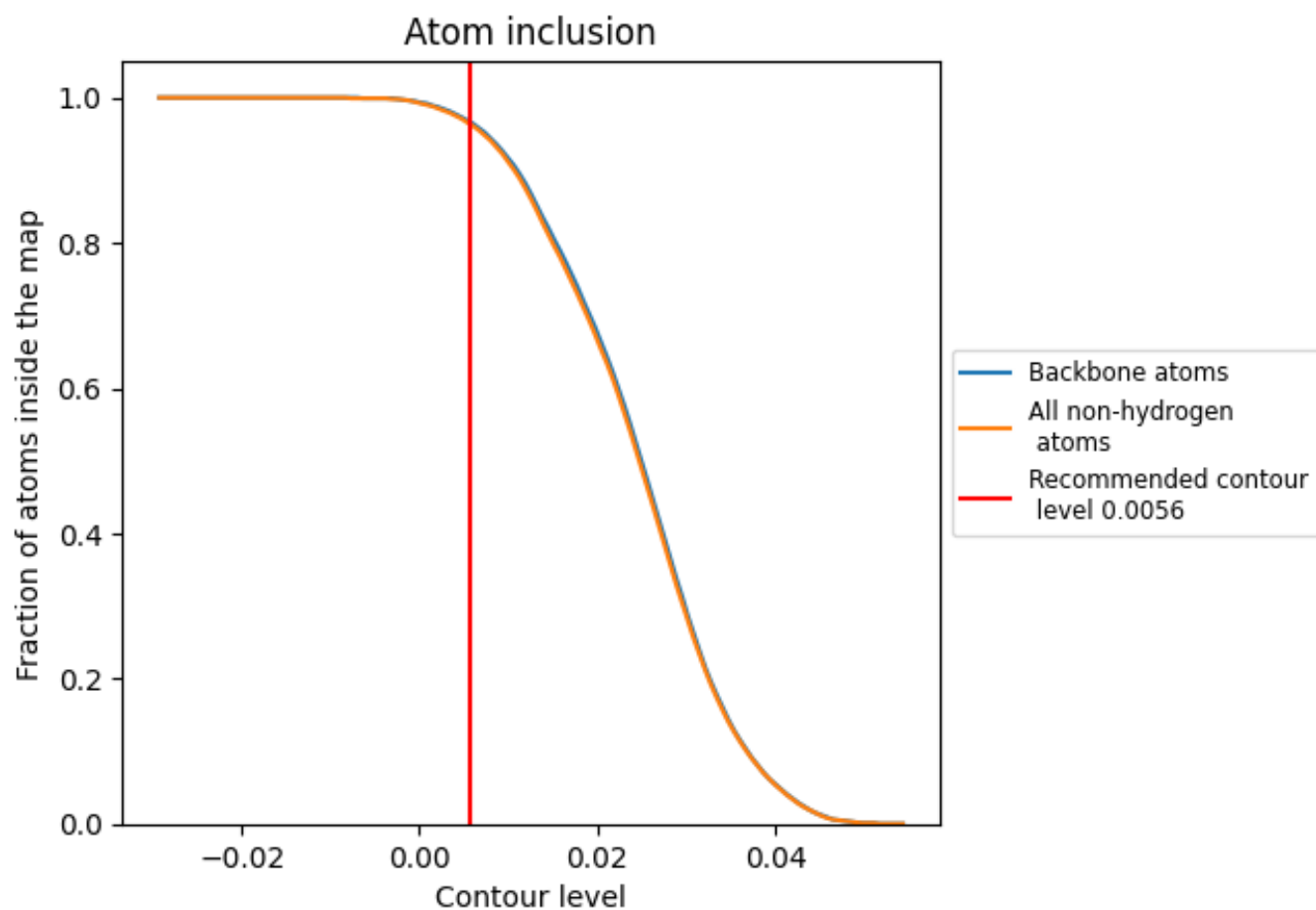
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0056).







































































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	Q-score
All	 0.9640	 0.0490
0	 0.4390	 0.0310
1	 0.1490	 0.0480
2	 0.8350	 0.0570
3	 0.8150	 0.0140
4	 0.8660	 0.0570
5	 0.4740	 0.0160
6	 0.9610	 0.0080
7	 0.5870	 0.0110
8	 1.0000	 0.0130
9	 0.8980	 0.0270
A	 0.7550	 0.0440
AA	 0.9860	 0.0800
AB	 1.0000	 -0.0640
AC	 0.9950	 0.0580
AD	 0.9660	 0.1020
AE	 0.9980	 0.0910
AF	 0.9830	 0.0910
AG	 0.9940	 0.0930
AH	 0.9960	 0.0670
AJ	 0.9990	 0.0520
AK	 0.9990	 0.0770
AL	 0.9960	 0.0590
AN	 0.9950	 0.0710
AO	 1.0000	 -0.0730
AP	 0.9900	 0.0620
AQ	 0.9860	 0.0800
AR	 1.0000	 0.0990
AS	 0.9460	 0.0730
AT	 1.0000	 0.0850
AU	 0.9960	 0.0700
AV	 0.9980	 0.0540
AW	 0.9990	 0.0750
AY	 0.9980	 0.0610
B	 1.0000	 0.0610























































































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Chain	Atom inclusion	Q-score
B0	 0.7250	 0.0280
B1	 0.4010	 0.0380
B2	 0.9040	 0.0640
B3	 0.8590	 0.0230
B4	 0.8980	 0.0540
B5	 0.7100	 0.0380
B6	 0.8980	 0.0250
B7	 0.9280	 0.0540
B8	 0.9920	 0.0530
B9	 0.9370	 0.0260
BA	 0.9940	 0.0540
BB	 1.0000	 0.0520
BC	 1.0000	 0.0320
BE	 0.9470	 0.0410
BF	 0.9970	 0.0800
BG	 0.7100	 0.0790
BH	 0.9990	 0.0570
BI	 0.9930	 0.0470
BJ	 0.9800	 0.0510
BK	 1.0000	 0.0830
BL	 0.9860	 0.0100
BM	 0.9860	 0.0460
BN	 0.9850	 0.0570
BO	 0.9960	 0.0580
BP	 0.9890	 0.0530
BQ	 0.9890	 0.0240
BS	 1.0000	 0.0600
BT	 0.9780	 0.0630
BU	 0.9990	 0.0510
BV	 0.9990	 0.0900
BW	 0.9950	 0.0800
BX	 0.9880	 0.0580
BY	 1.0000	 0.1000
BZ	 1.0000	 0.0880
Ba	 0.9970	 0.0780
Bb	 1.0000	 0.0850
Bc	 0.9750	 0.0800
Bd	 0.9720	 0.1000
Be	 0.9850	 0.0430
Bf	 0.9980	 0.0650
Bg	 0.9950	 0.0640
Bh	 0.9980	 0.0780









































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Chain	Atom inclusion	Q-score
Bi	 1.0000	 0.0420
Bj	 1.0000	 -0.0070
Bk	 1.0000	 0.0160
Bl	 1.0000	 0.0250
Bm	 1.0000	 0.0300
Bn	 0.9910	 0.0680
Bo	 0.9890	 0.0680
Bp	 0.9900	 0.0740
Br	 0.9990	 0.0200
Bs	 1.0000	 0.0340
Bu	 0.9930	 0.0710
Bv	 0.9880	 0.1100
Bw	 0.9960	 0.0650
Bx	 1.0000	 0.0300
By	 0.9770	 0.0100
Bz	 1.0000	 0.0450
C	 1.0000	 0.0540
E	 0.9510	 0.0410
F	 0.9710	 0.0720
G	 0.4850	 0.0550
H	 0.9990	 0.0500
I	 0.9870	 0.0350
J	 0.9730	 0.0400
K	 0.9780	 0.0470
L	 0.9840	 -0.0060
M	 0.9240	 0.0390
N	 0.9740	 0.0270
O	 0.8670	 0.0510
P	 0.9880	 0.0530
Q	 0.9920	 0.0310
S	 1.0000	 0.0550
T	 0.9060	 0.0120
U	 1.0000	 0.0630
V	 0.9990	 0.0830
W	 0.9990	 0.0710
X	 1.0000	 0.0630
Y	 1.0000	 0.0930
Z	 1.0000	 0.0890
a	 0.9970	 0.0830
b	 1.0000	 0.0860
c	 0.9760	 0.0760
d	 0.9880	 0.1000

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Chain	Atom inclusion	Q-score
e	 1.0000	 0.0470
f	 1.0000	 0.0610
g	 0.9970	 0.0540
h	 1.0000	 0.0700
i	 1.0000	 0.0490
j	 1.0000	 -0.0020
k	 1.0000	 0.0210
l	 1.0000	 0.0240
m	 1.0000	 0.0370
n	 0.9870	 0.0570
o	 0.9870	 0.0480
p	 0.9950	 0.0570
r	 0.9990	 0.0240
s	 1.0000	 0.0240
u	 0.9970	 0.0630
v	 0.9850	 0.1040
w	 0.9990	 0.0660
x	 0.9990	 0.0280
y	 0.8650	 0.0330
z	 1.0000	 0.0310