



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 06:28 AM UTC

PDB ID : 8ZSO / pdb_00008zso
EMDB ID : EMD-60422
Title : Respirasome close state 2 in presence of metformin (SC-MetC2)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 3.11 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:

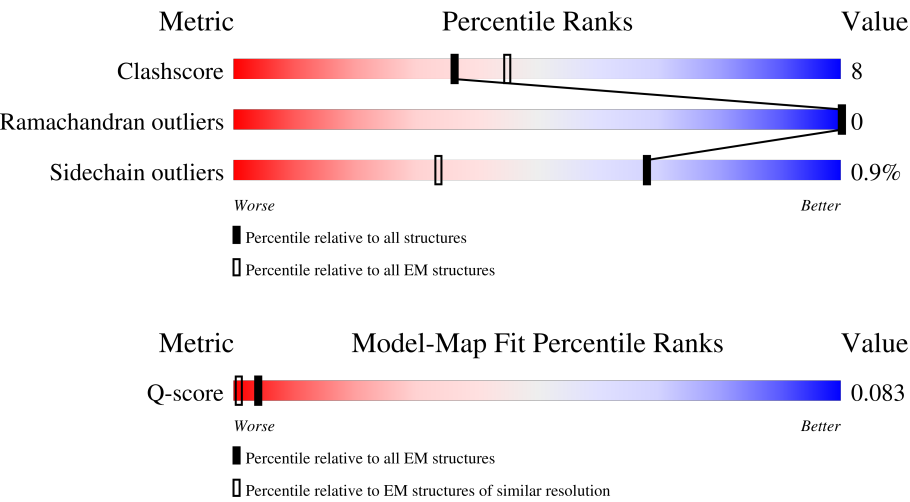
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	4L	98	11% 77% 23%
2	5A	102	78% 50% 47% .
3	5B	95	54% 68% 29% .
4	6A	73	53% 73% 26% .

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Mol	Chain	Length	Quality of chain
5	6B	82	
6	6C	70	
7	7A	57	
8	7B	50	
9	7C	47	
10	8B	43	
11	A1	70	
12	A2	85	
13	A3	83	
14	A5	112	
15	A6	114	
16	A7	112	
17	A8	171	
18	A9	341	
19	AB	87	
19	AC	87	
20	AK	321	
21	AL	140	
22	AM	144	
23	AN	142	
24	B1	56	
25	B2	67	
26	B3	80	
27	B4	128	
28	B5	138	

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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	176	
34	BL	102	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	174	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

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Mol	Chain	Length	Quality of chain
50	Qd	241	82% 90% 9%
51	QE	196	90% 74% 26%
51	Qe	196	93% 79% 21%
52	QF	67	88% 88% 12%
52	Qf	67	88% 81% 15%
53	QG	101	81% 87% 13%
53	Qg	101	79% 85% 15%
54	QH	79	82% 80% 19%
54	Qh	79	80% 86% 14%
55	QI	62	81% 89% 11%
55	Qi	62	77% 89% 8%
56	QJ	49	92% 92% 8%
57	QK	78	86% 79% 13% 6%
58	Qj	51	76% 92% 8%
59	S1	689	60% 83% 17%
60	S2	430	21% 77% 21% ..
61	S3	208	58% 86% 14%
62	S4	125	65% 86% 14%
63	S5	105	19% 82% 18%
64	S6	96	46% 84% 16%
65	S7	156	19% 71% 27%
66	S8	176	7% 75% 24%
67	V1	431	15% 76% 23%
68	V2	217	17% 79% 21%
69	V3	42	36% 62% 38%

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
84	FES	Qe	301	-	-	X	-

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 116635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	102	Total	C	N	O	S	0	0
			825	528	139	156	2		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	95	Total	C	N	O	S	0	0
			724	449	128	141	6		

- Molecule 4 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6A	73	Total	C	N	O	S	0	0
			609	395	116	97	1		

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6B	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6C	70	Total	C	N	O	S	0	0
			574	375	101	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7A	57	Total	C	N	O	S	0	0
			447	287	76	81	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7B	50	Total	C	N	O	S	0	0
			392	254	66	71	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7C	47	Total	C	N	O	S	0	0
			387	257	65	63	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8B	43	Total	C	N	O	0	0
			338	222	57	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 16 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	341	Total	C	N	O	S	0	0
			2743	1777	480	477	9		

- Molecule 19 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
19	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AK	321	Total	C	N	O	S	0	0
			2601	1655	444	492	10		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AM	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B3	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B4	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	101	Total	C	N	O	S	0	0
			861	562	153	145	1		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C1	514	Total	C	N	O	S	0	0
			4024	2692	625	675	32		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C2	228	Total	C	N	O	S	0	0
			1833	1193	282	340	18		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C3	260	Total	C	N	O	S	0	0
			2103	1403	337	353	10		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C4	138	Total	C	N	O	S	0	0
			1153	751	188	210	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N1	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	N3	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N6	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	QA	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		
47	Qa	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QB	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
48	Qb	433	Total	C	N	O	S	0	0
			3367	2103	592	653	19		

- Molecule 49 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QC	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
49	Qc	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 50 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	QD	241	Total	C	N	O	S	0	0
			1921	1225	330	350	16		
50	Qd	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QE	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		
51	Qe	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	QF	67	Total	C	N	O	S	0	0
			552	336	100	111	5		
52	Qf	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	QG	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
53	Qg	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	QH	78	Total	C	N	O	S	0	0
			662	432	121	107	2		
54	Qh	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 55 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	QI	62	Total	C	N	O	0	0
			507	331	90	86		
55	Qi	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	QJ	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Qj	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 59 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S2	427	Total	C	N	O	S	0	0
			3436	2198	591	623	24		

- Molecule 61 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S3	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S4	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S5	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 69 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

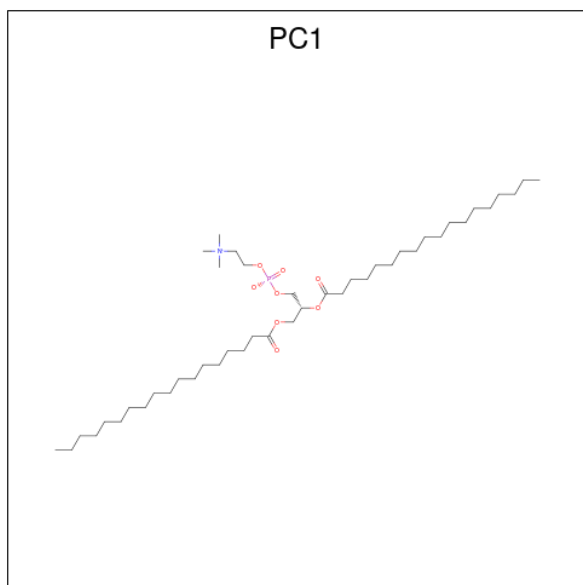
Mol	Chain	Residues	Atoms		AltConf
70	5B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
70	S6	1	Total	Zn	0
			1	1	

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



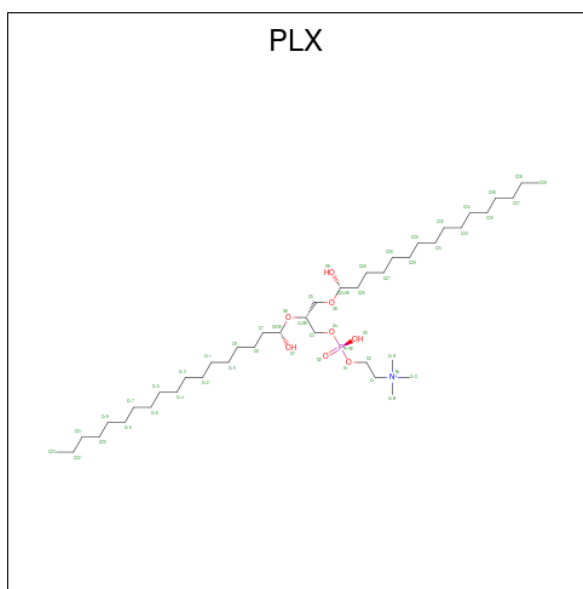
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
71	B4	1	Total	C	N	O	P	0
			50	40	1	8	1	
71	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	C3	1	Total	C	N	O	P	0
			50	40	1	8	1	
71	CB	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	N1	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	N4	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	QB	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qb	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qh	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qj	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	S7	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 72 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) (labeled as "Ligand of Interest" by depositor).



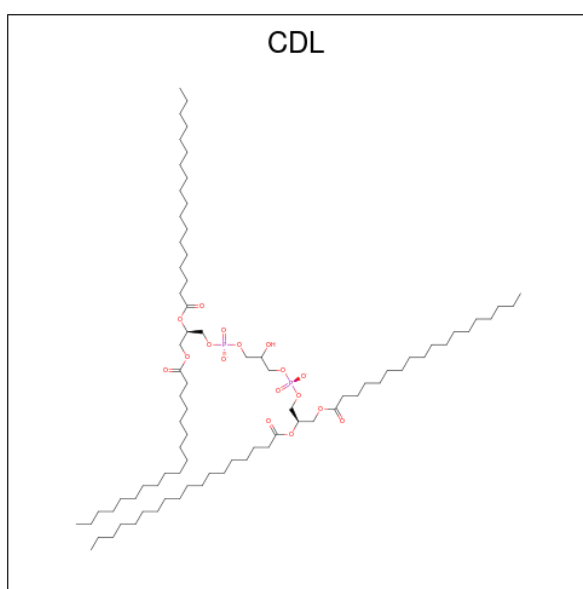
Mol	Chain	Residues	Atoms					AltConf
72	6C	1	Total	C	N	O	P	0
			31	21	1	8	1	
72	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
72	N2	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
72	QE	1	Total	C	N	O	P	0
			46	36	1	8	1	
72	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 73 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
73	A8	1	Total	C	O	P	0
			83	64	17	2	
73	AL	1	Total	C	O	P	0
			91	72	17	2	
73	AL	1	Total	C	O	P	0
			89	70	17	2	
73	B4	1	Total	C	O	P	0
			80	61	17	2	
73	B5	1	Total	C	O	P	0
			100	81	17	2	
73	CB	1	Total	C	O	P	0
			100	81	17	2	
73	N1	1	Total	C	O	P	0
			78	59	17	2	

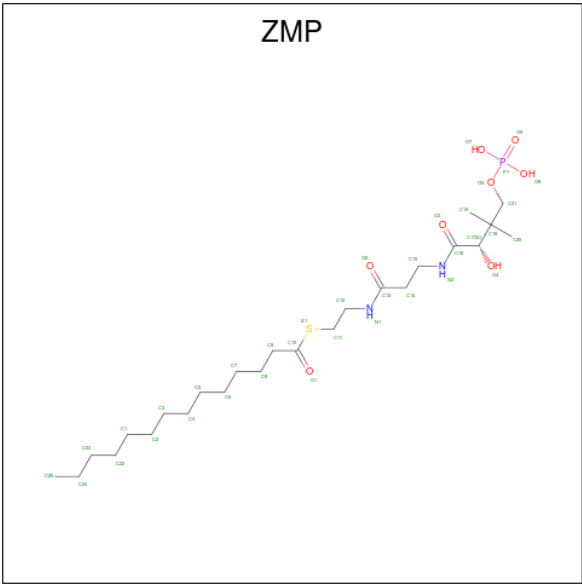
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Mol	Chain	Residues	Atoms				AltConf
73	N2	1	Total 68	C 49	O 17	P 2	0
73	N5	1	Total 89	C 70	O 17	P 2	0
73	N5	1	Total 100	C 81	O 17	P 2	0
73	QB	1	Total 62	C 43	O 17	P 2	0
73	QD	1	Total 64	C 45	O 17	P 2	0
73	QH	1	Total 61	C 42	O 17	P 2	0
73	QH	1	Total 64	C 45	O 17	P 2	0
73	Qb	1	Total 64	C 45	O 17	P 2	0
73	Qh	1	Total 55	C 36	O 17	P 2	0

- # NDP

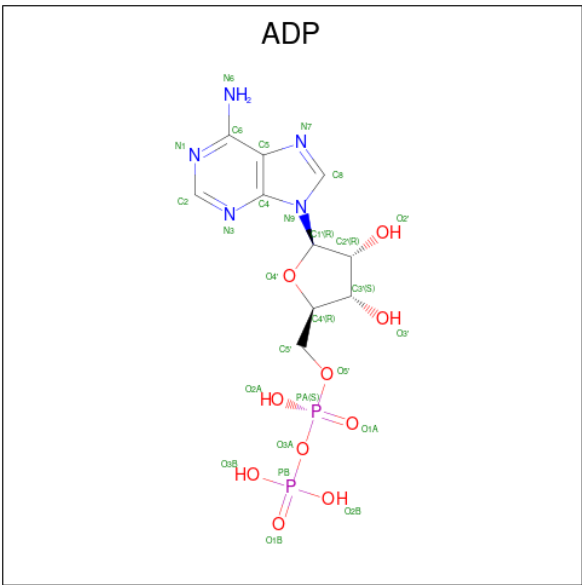
- Molecule 75 is S-[2-($\{N[(2S)-2\text{-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl}]\}$ -beta-alan

yl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



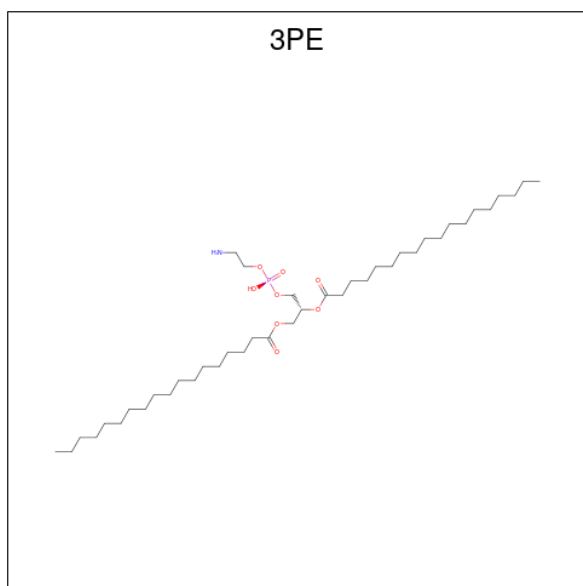
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
75	AB	1	36	25	2	7	1	1	0
75	AC	1	36	25	2	7	1	1	0

- Molecule 76 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



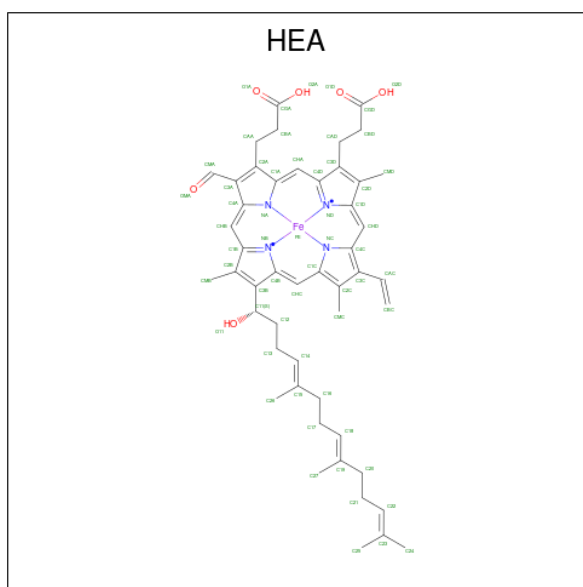
Mol	Chain	Residues	Atoms					AltConf
76	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 77 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
77	B8	1	Total	C	N	O	P	0
			32	22	1	8	1	
77	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
77	CB	1	Total	C	N	O	P	0
			51	41	1	8	1	
77	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	QC	1	Total	C	N	O	P	0
			34	24	1	8	1	
77	QE	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 78 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
78	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
78	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

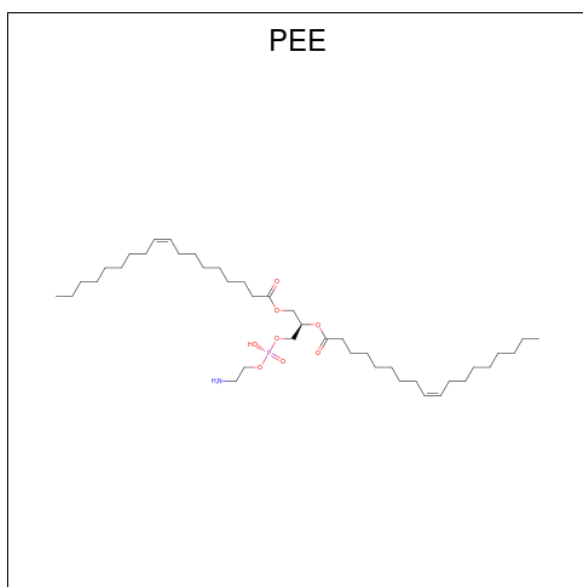
- Molecule 79 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
79	C1	1	Total	Cu	0
			1	1	
79	C2	2	Total	Cu	0
			2	2	

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

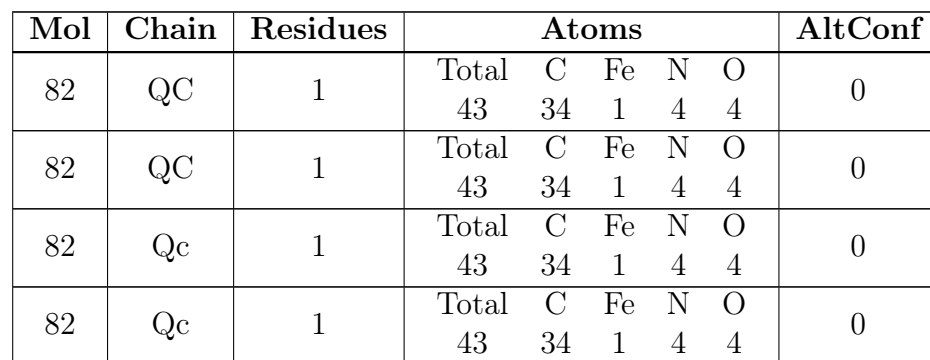
Mol	Chain	Residues	Atoms		AltConf
80	C1	1	Total	Mg	0
			1	1	
80	S1	1	Total	Mg	0
			1	1	

- Molecule 81 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).

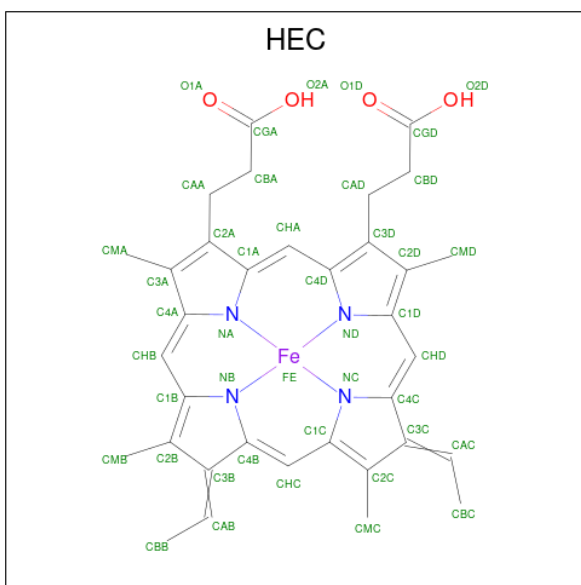


Mol	Chain	Residues	Atoms					AltConf
81	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
81	N4	1	Total	C	N	O	P	0
			46	36	1	8	1	
81	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
81	N5	1	Total	C	N	O	P	0
			51	41	1	8	1	
81	N6	1	Total	C	N	O	P	0
			51	41	1	8	1	
81	QC	1	Total	C	N	O	P	0
			40	30	1	8	1	
81	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
81	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
81	Qe	1	Total	C	N	O	P	0
			44	34	1	8	1	
81	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	
81	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

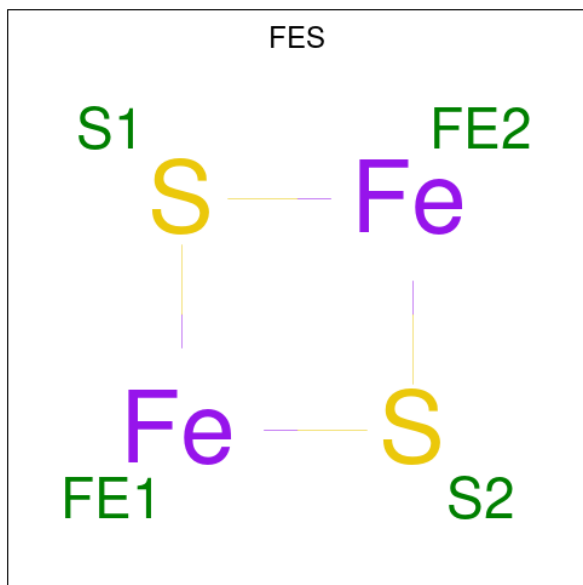


- Molecule 83 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



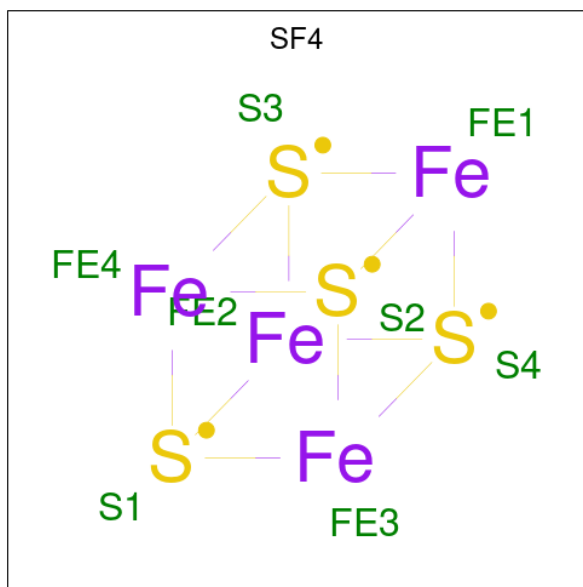
Mol	Chain	Residues	Atoms					AltConf
83	QD	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	Qd	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 84 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



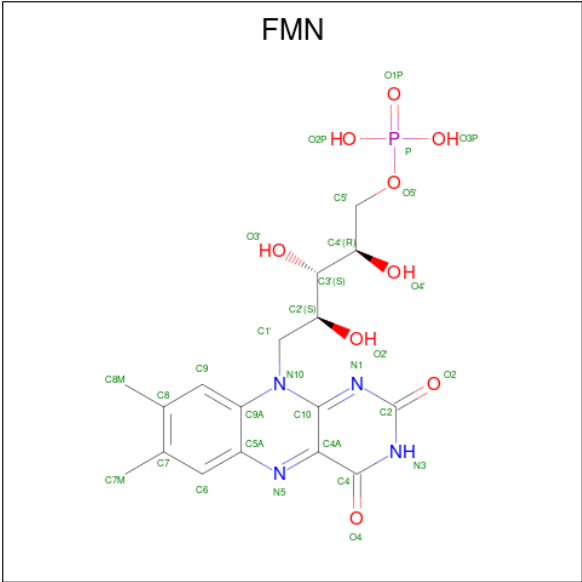
Mol	Chain	Residues	Atoms			AltConf
84	QE	1	Total	Fe	S	0
			4	2	2	
84	Qe	1	Total	Fe	S	0
			4	2	2	
84	S1	1	Total	Fe	S	0
			4	2	2	
84	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 85 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
85	S1	1	Total	Fe	S	0
			8	4	4	
85	S1	1	Total	Fe	S	0
			8	4	4	
85	S7	1	Total	Fe	S	0
			8	4	4	
85	S8	1	Total	Fe	S	0
			8	4	4	
85	S8	1	Total	Fe	S	0
			8	4	4	
85	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 86 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

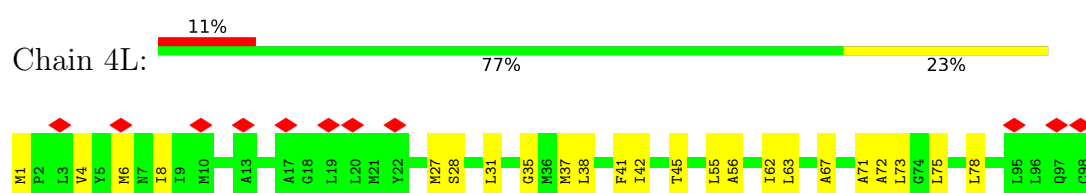


Mol	Chain	Residues	Atoms					AltConf
86	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

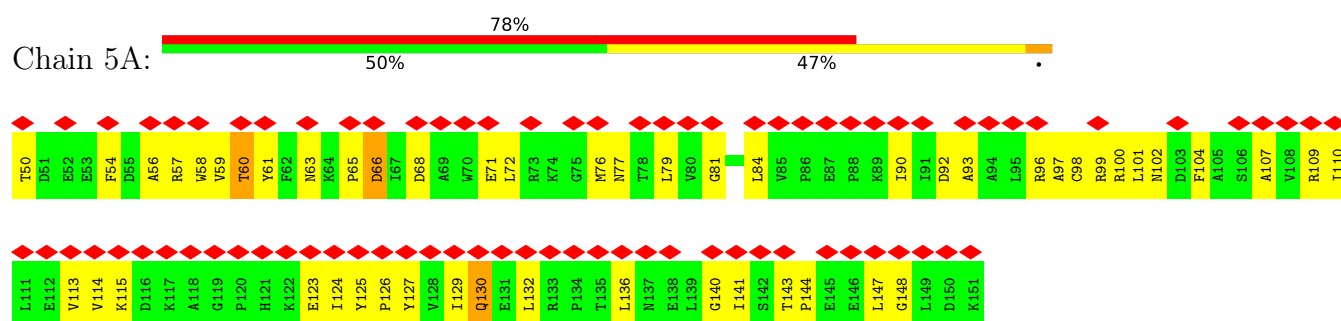
3 Residue-property plots [i](#)

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

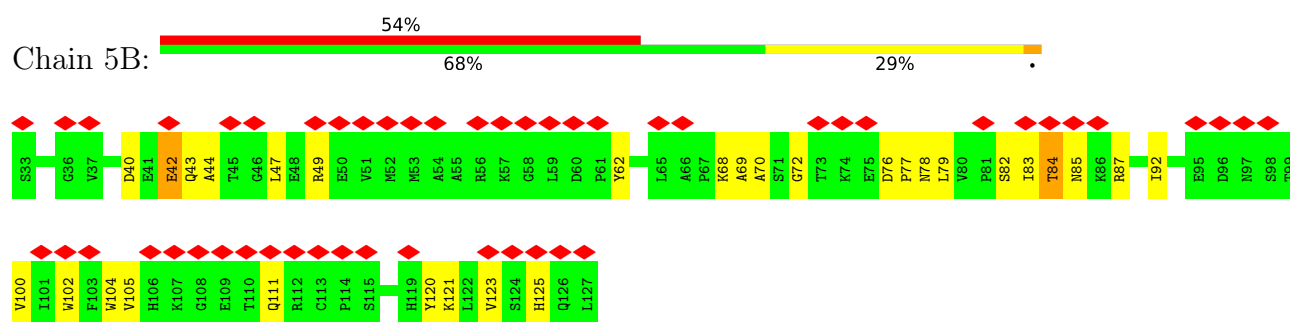
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



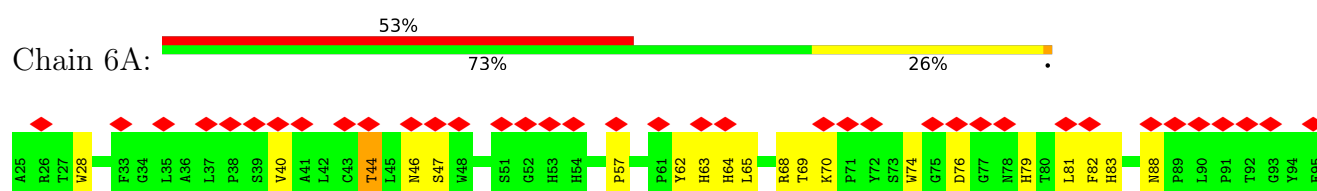
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

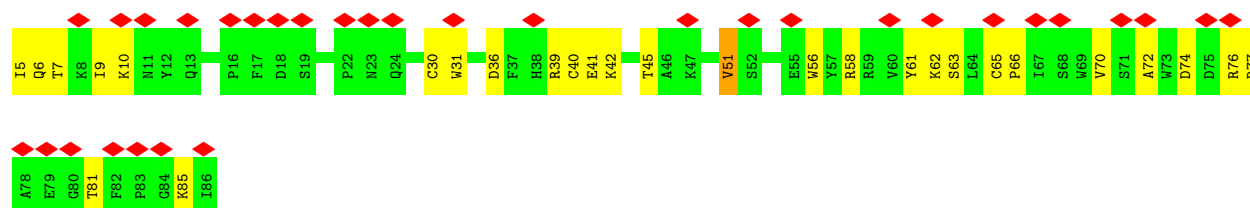


- Molecule 4: Cytochrome c oxidase subunit

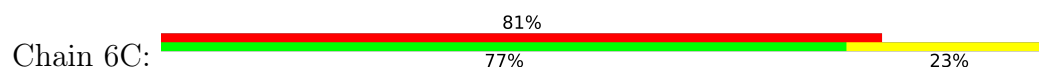




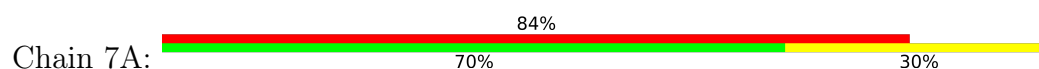
• Molecule 5: Cytochrome c oxidase subunit



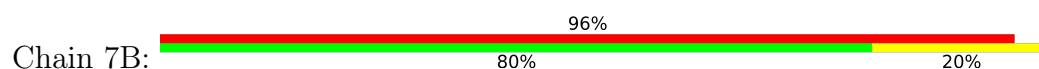
• Molecule 6: Cytochrome c oxidase subunit 6C



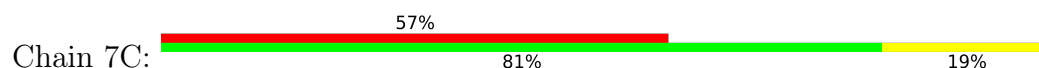
• Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



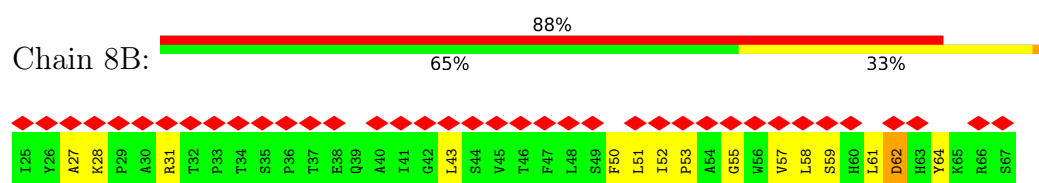
• Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



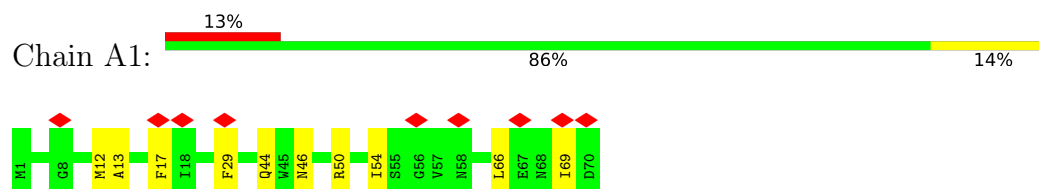
• Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



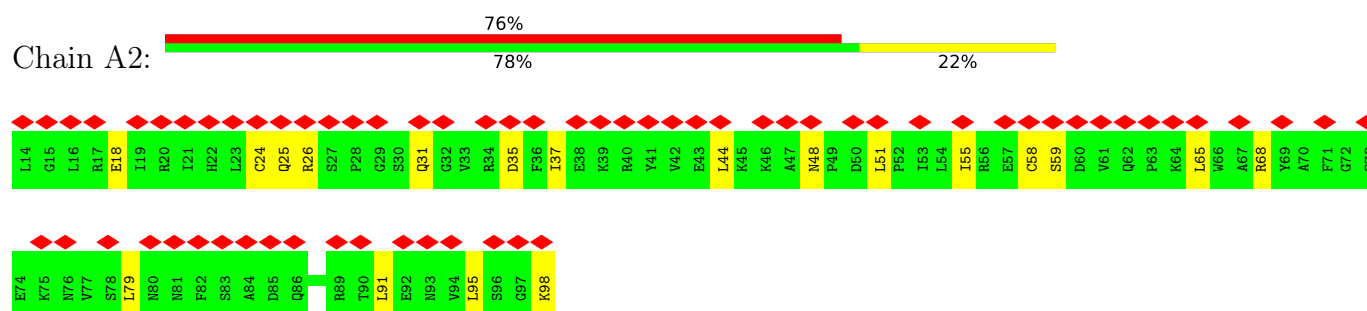
• Molecule 10: Cytochrome c oxidase subunit 8



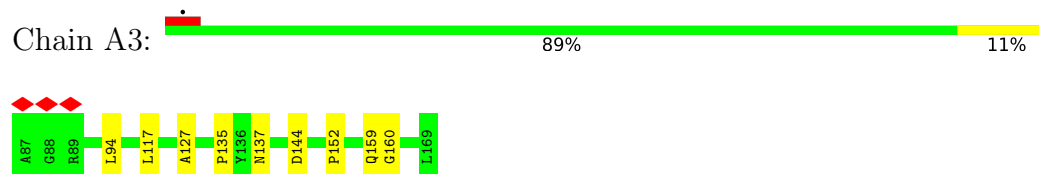
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



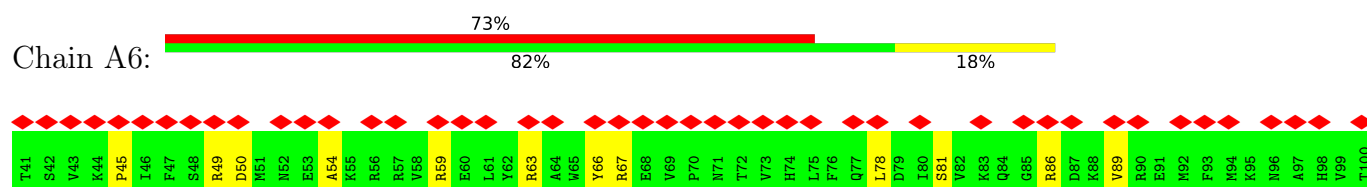
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

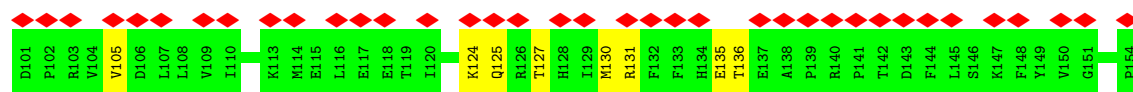


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

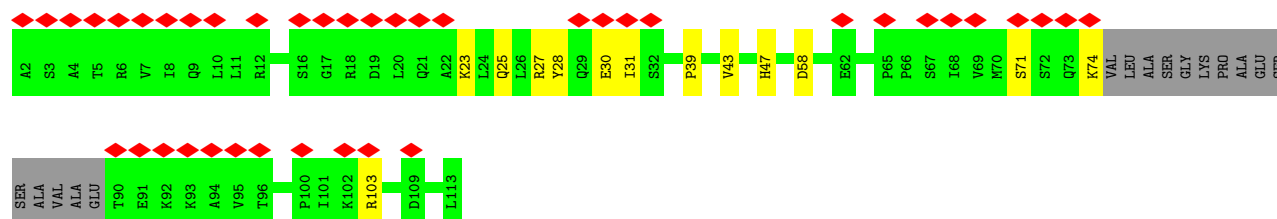
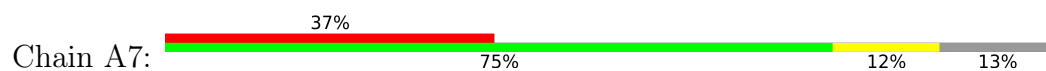


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

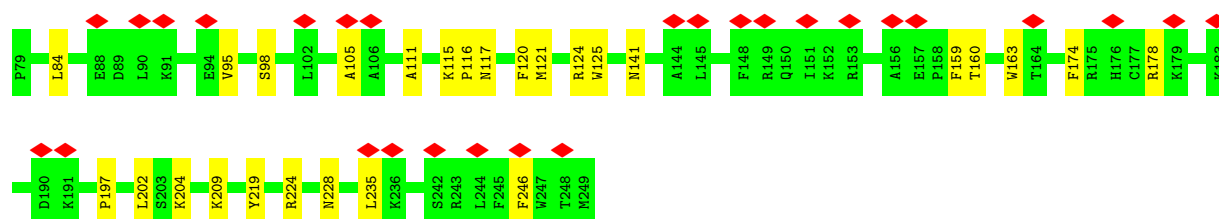
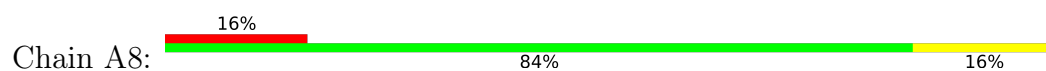




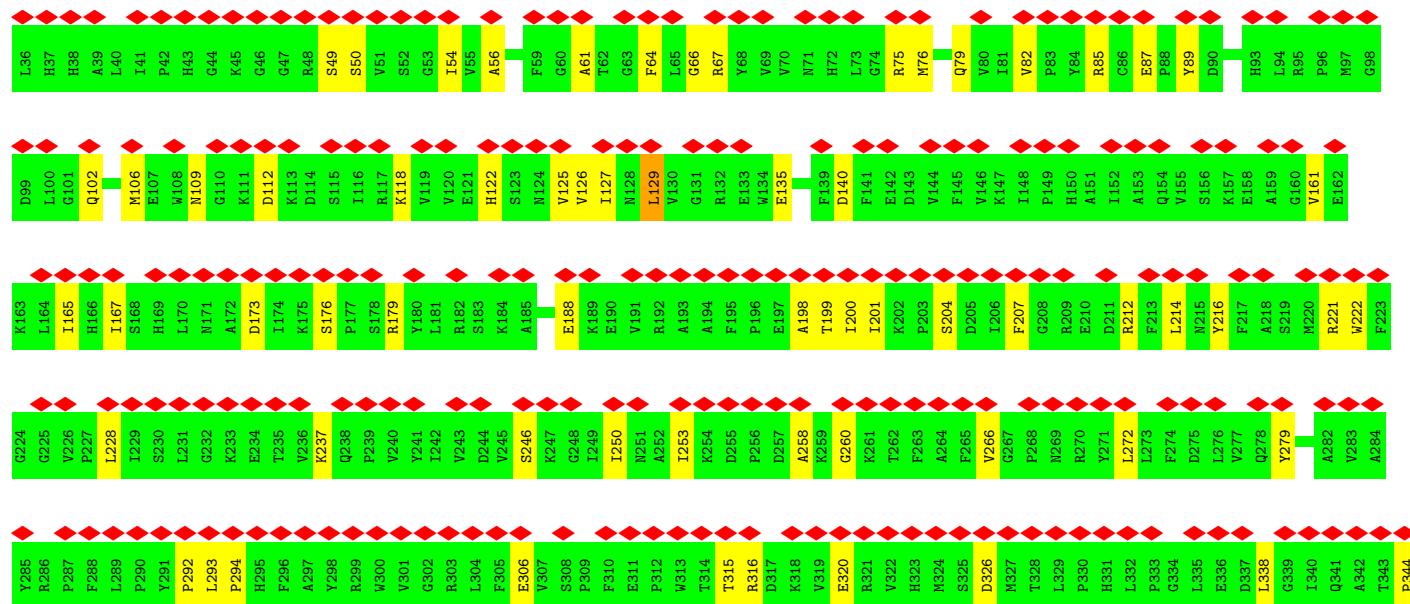
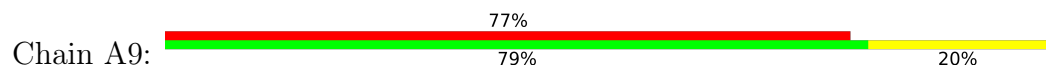
• Molecule 16: Complex I-B14.5a

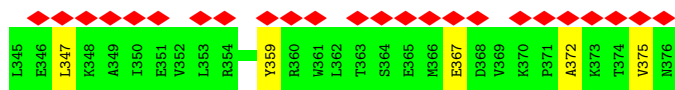


• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

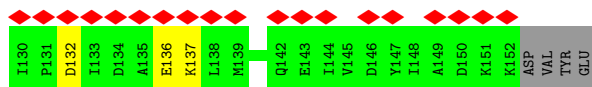
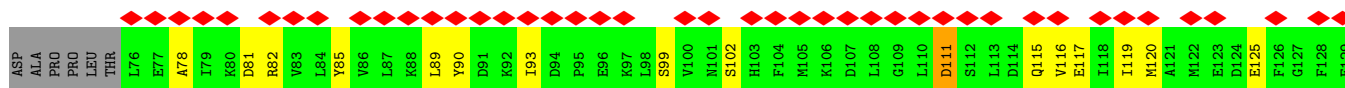
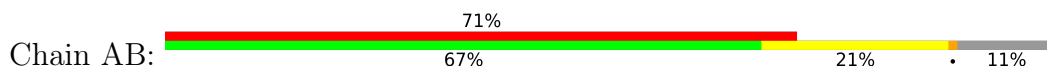


• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

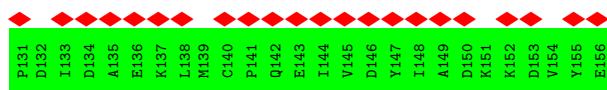
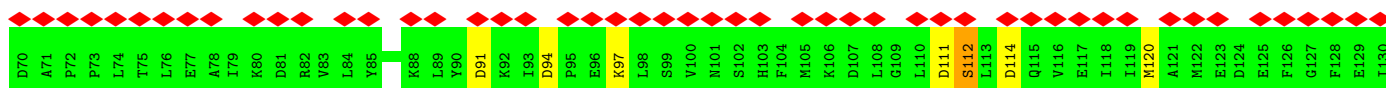
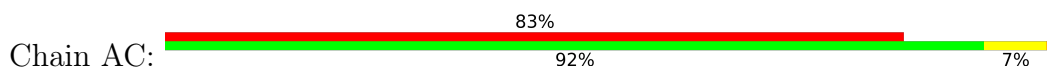




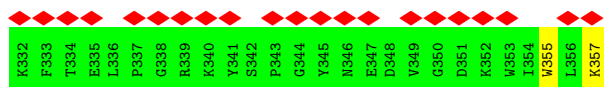
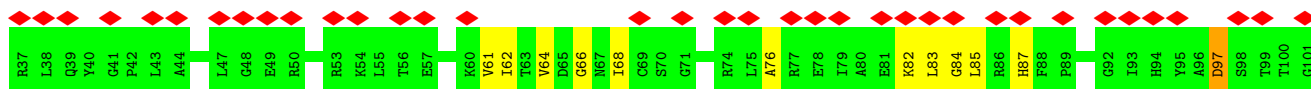
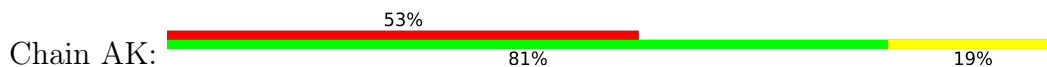
• Molecule 19: Acyl carrier protein



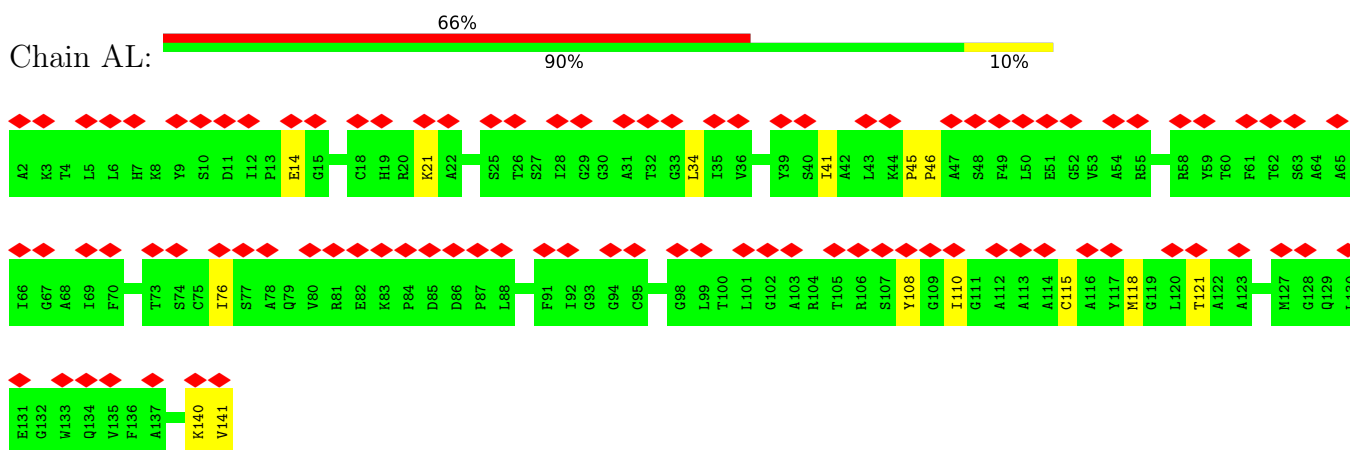
• Molecule 19: Acyl carrier protein



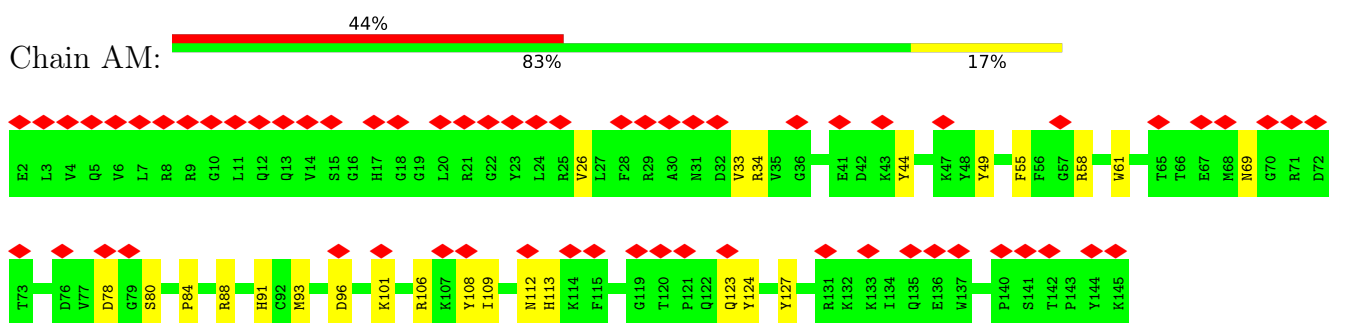
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



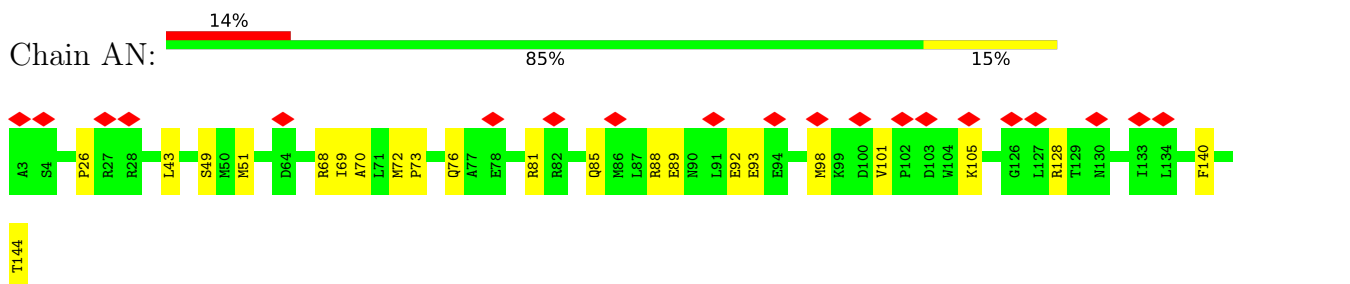
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



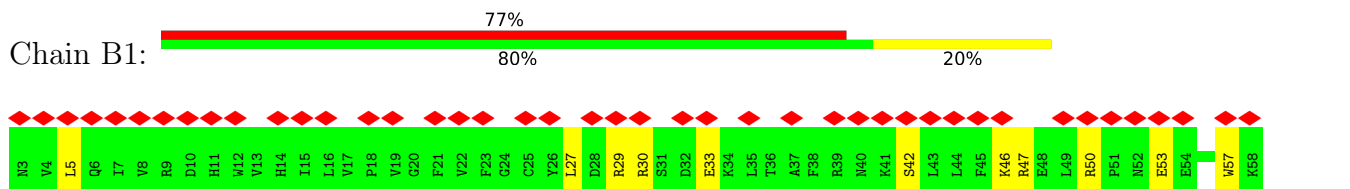
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



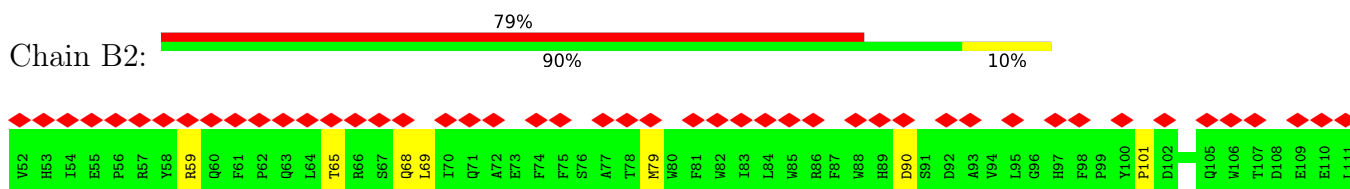
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

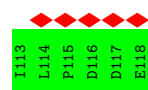


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

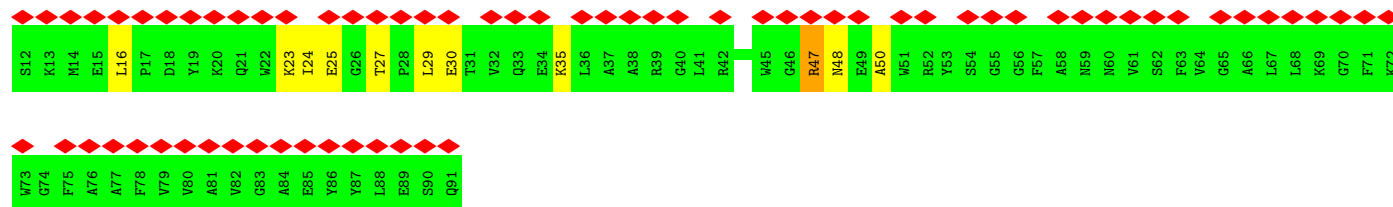
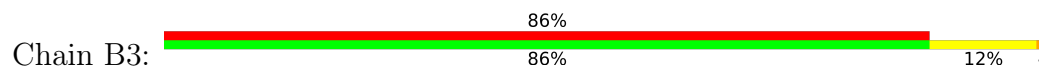


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

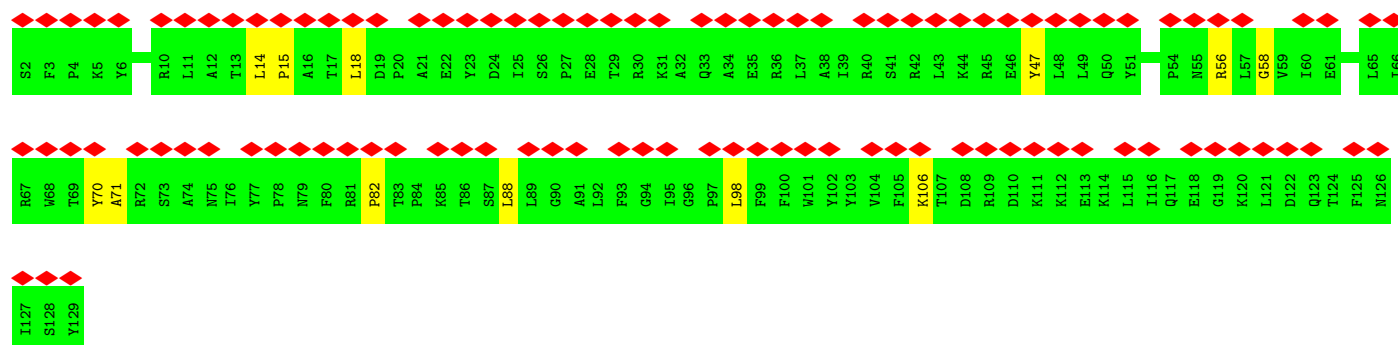
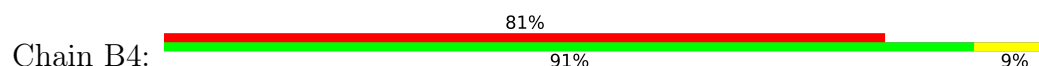




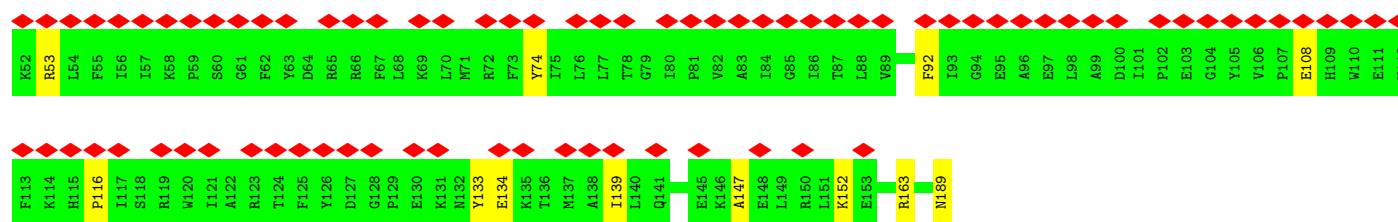
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

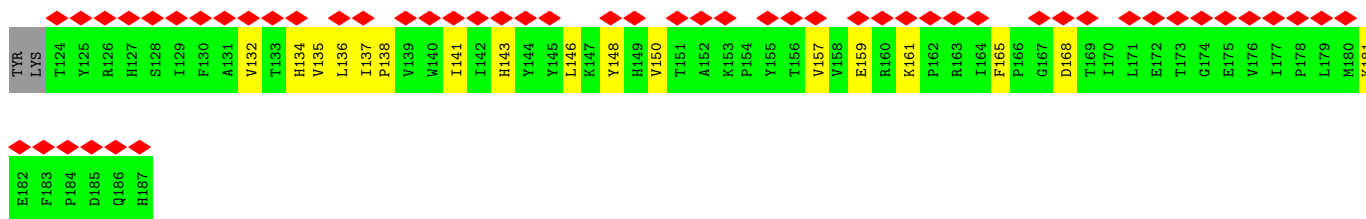


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

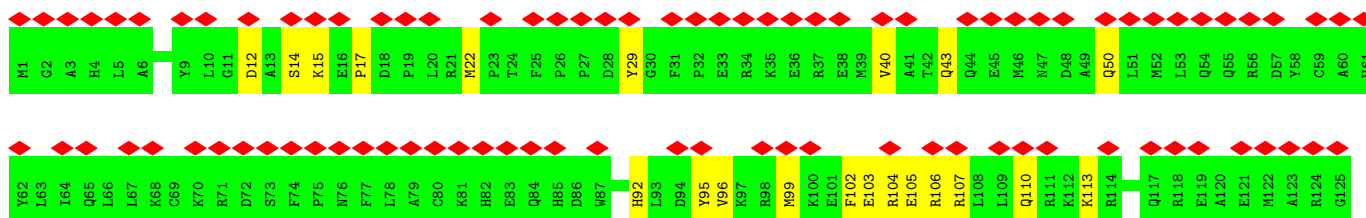
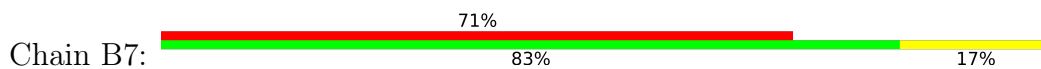


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

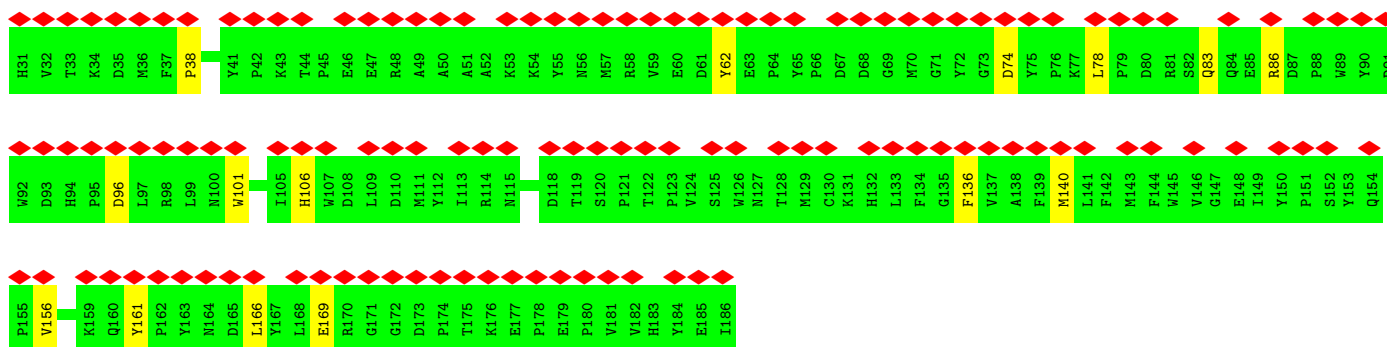
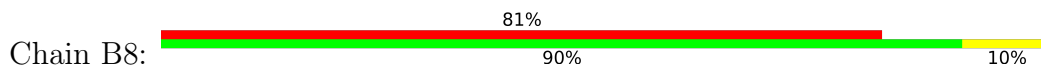




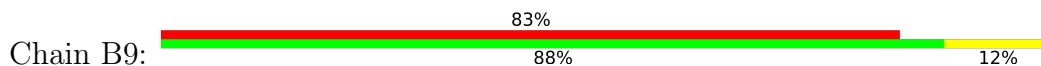
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



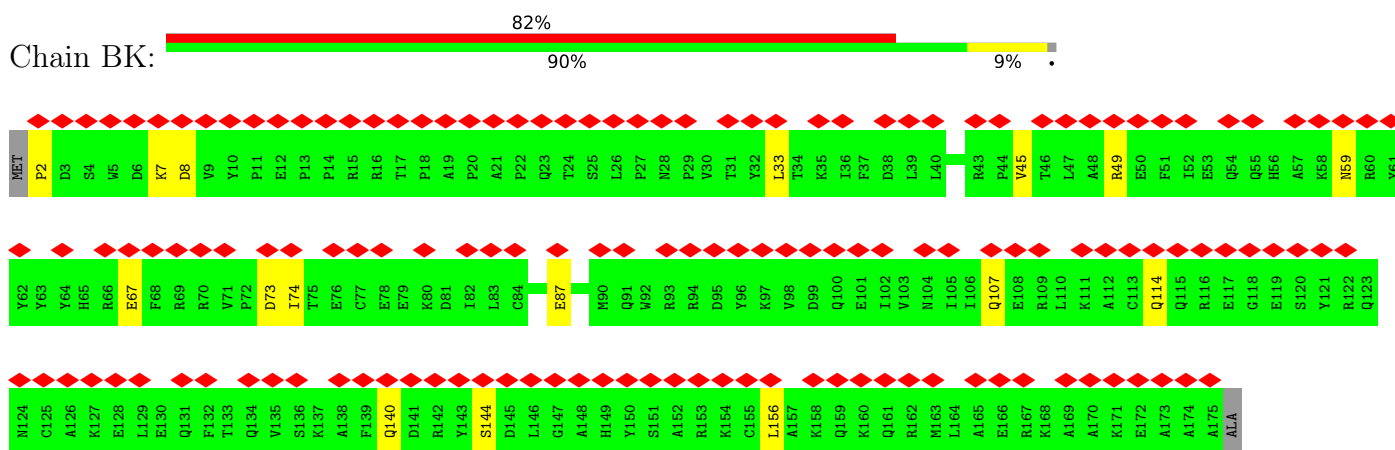
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



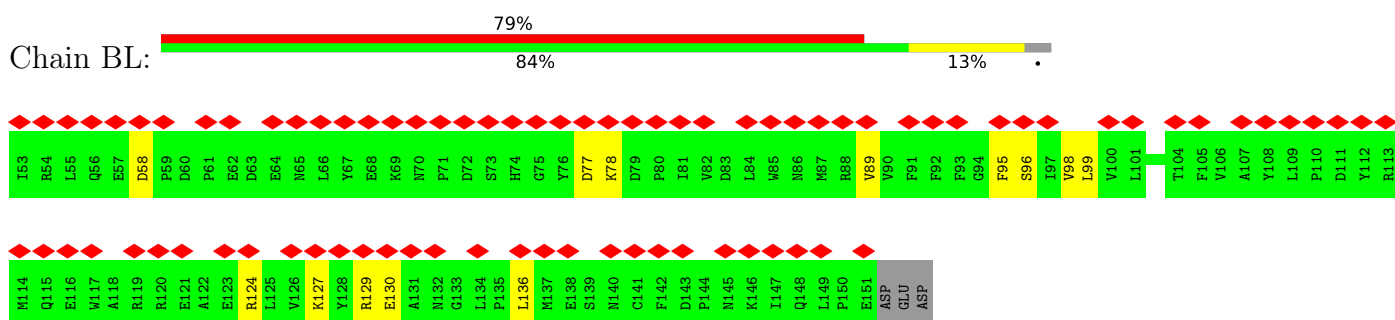
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



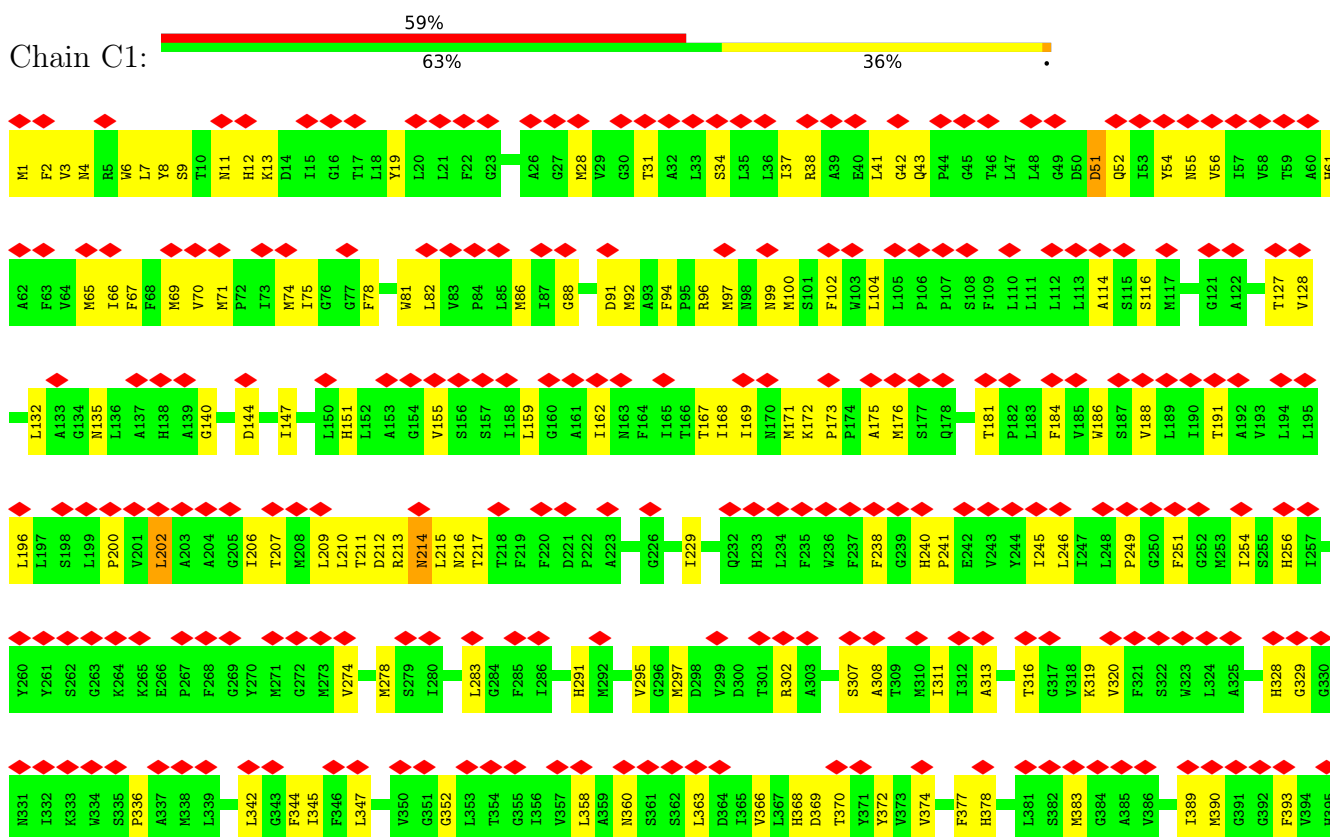
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

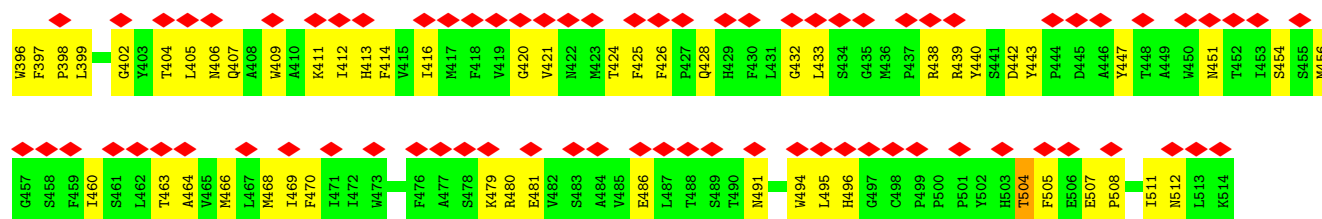


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

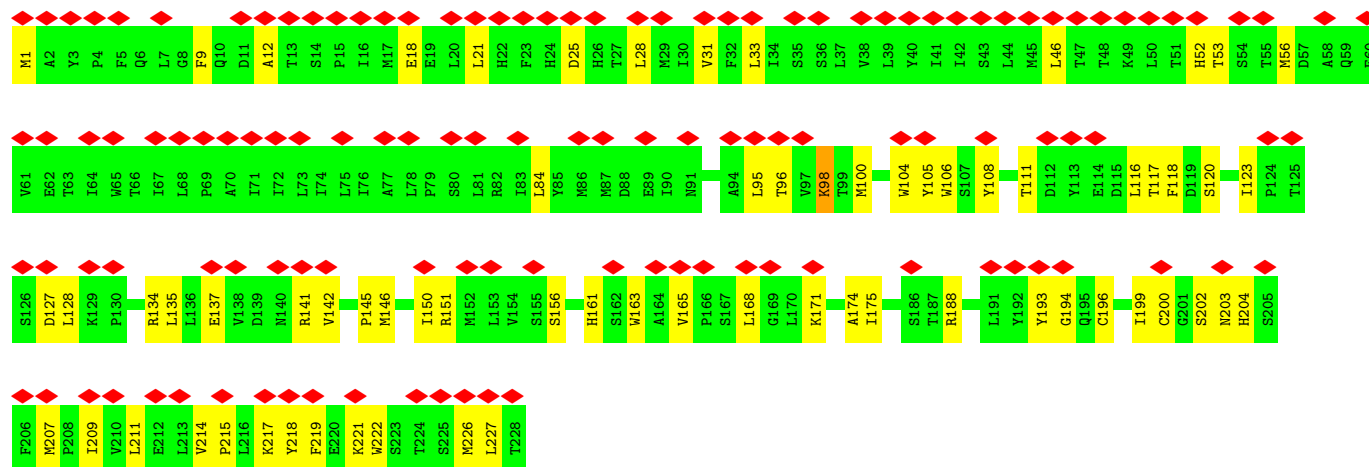
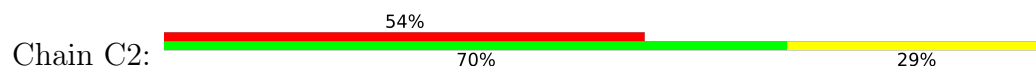


- Molecule 35: Cytochrome c oxidase subunit 1

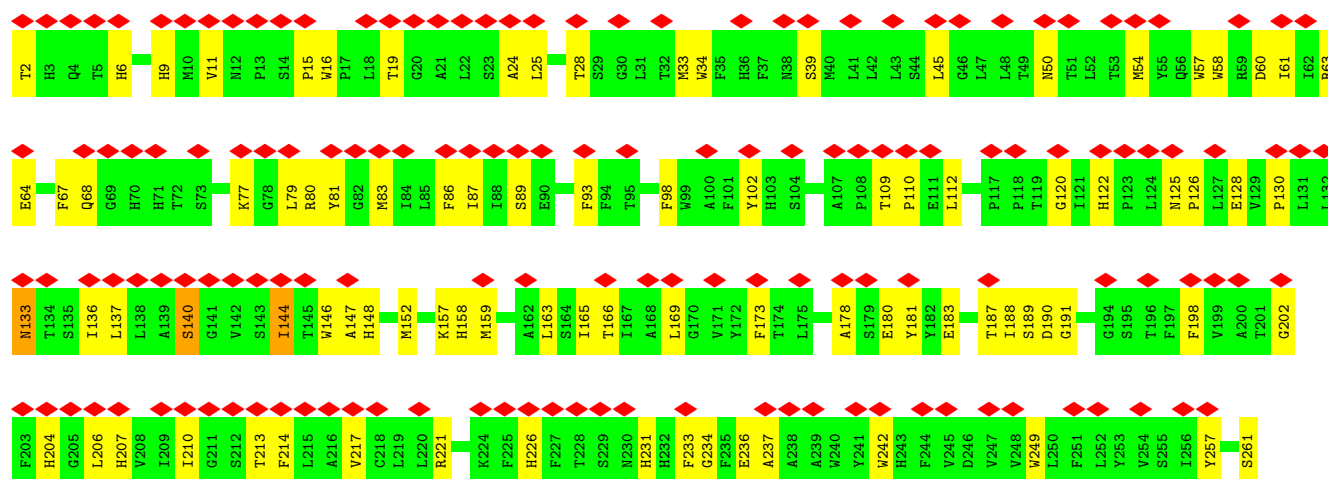




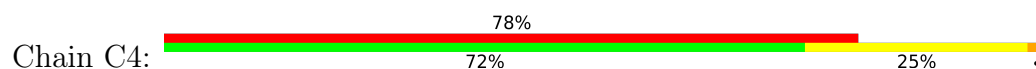
• Molecule 36: Cytochrome c oxidase subunit 2

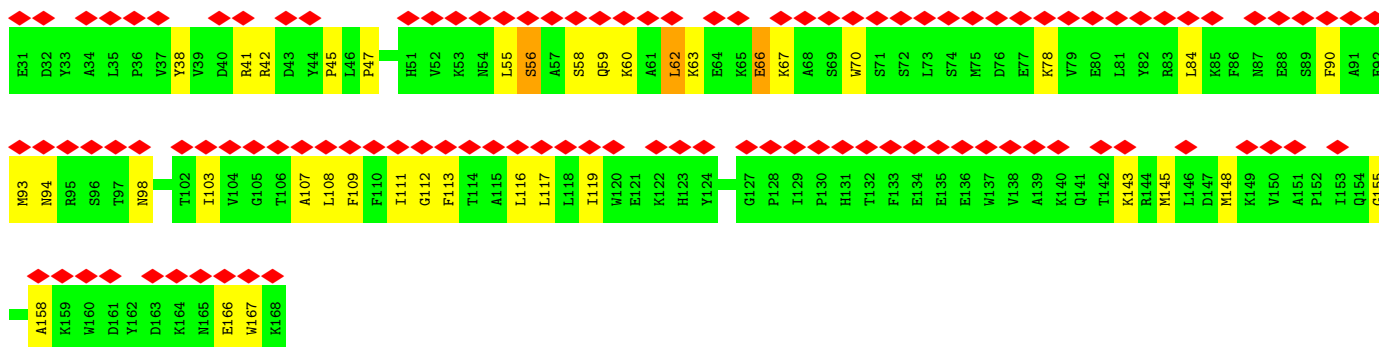


• Molecule 37: Cytochrome c oxidase subunit 3

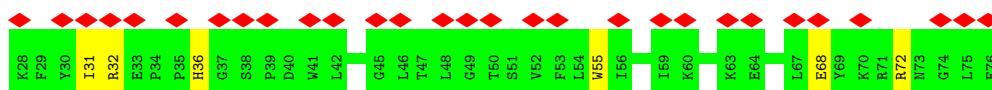
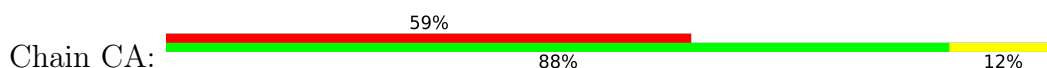


• Molecule 38: Cytochrome c oxidase subunit 4

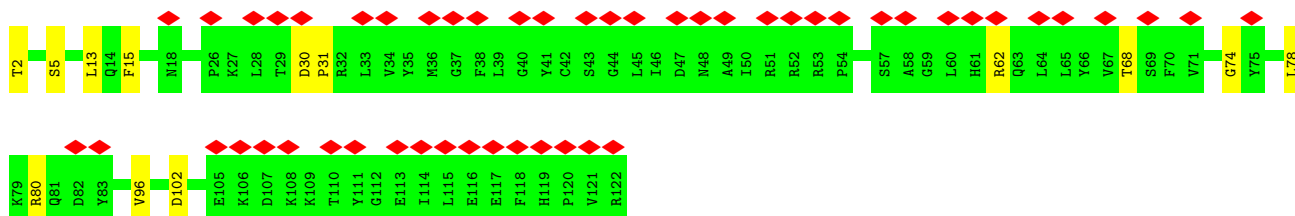
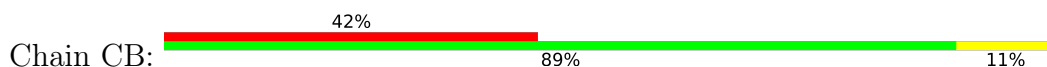




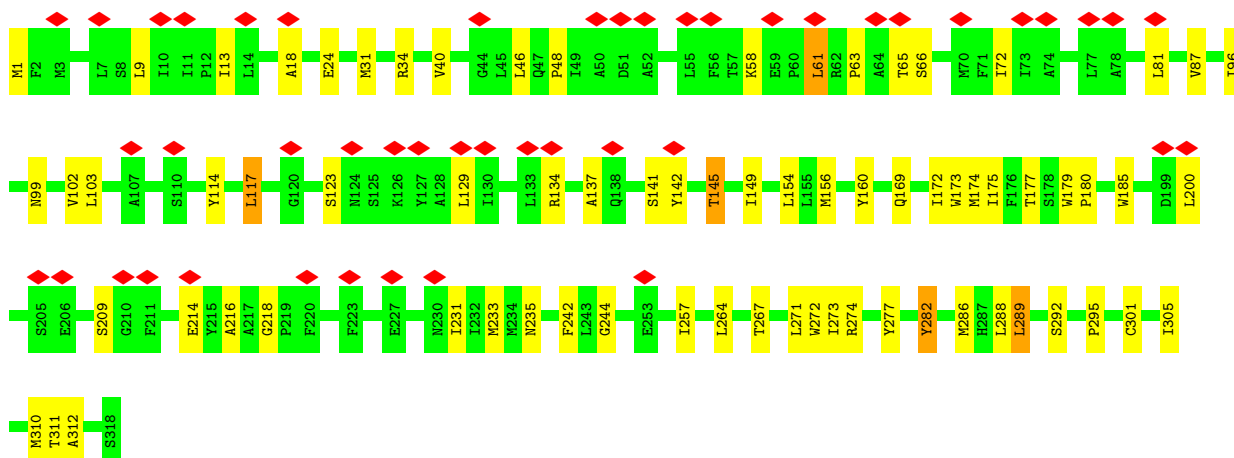
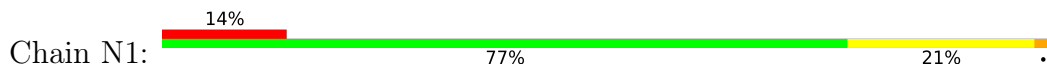
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



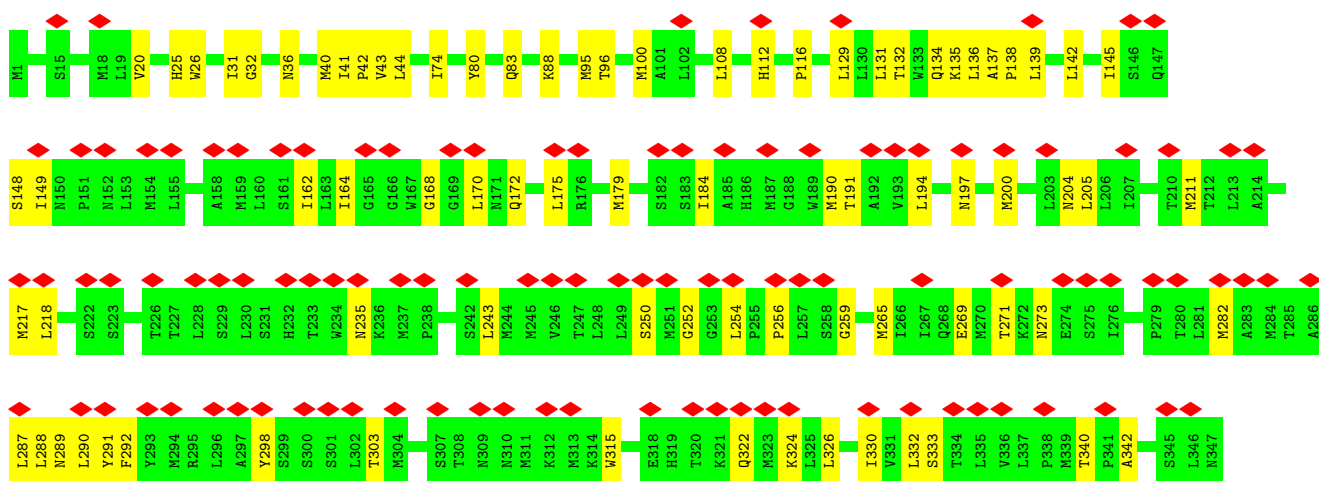
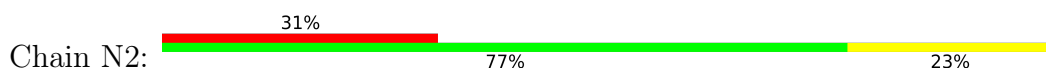
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2



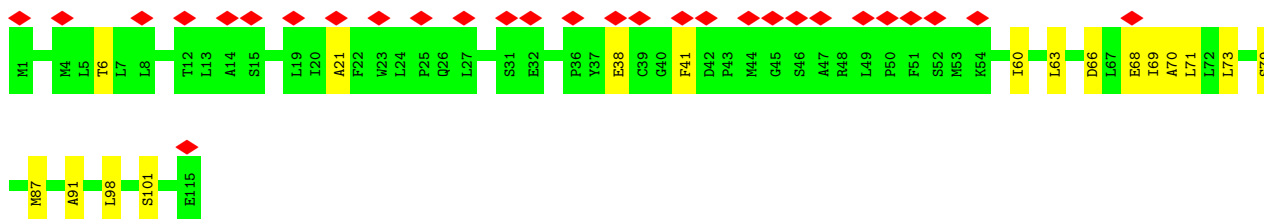
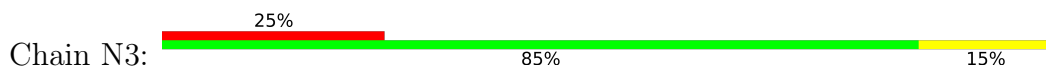
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



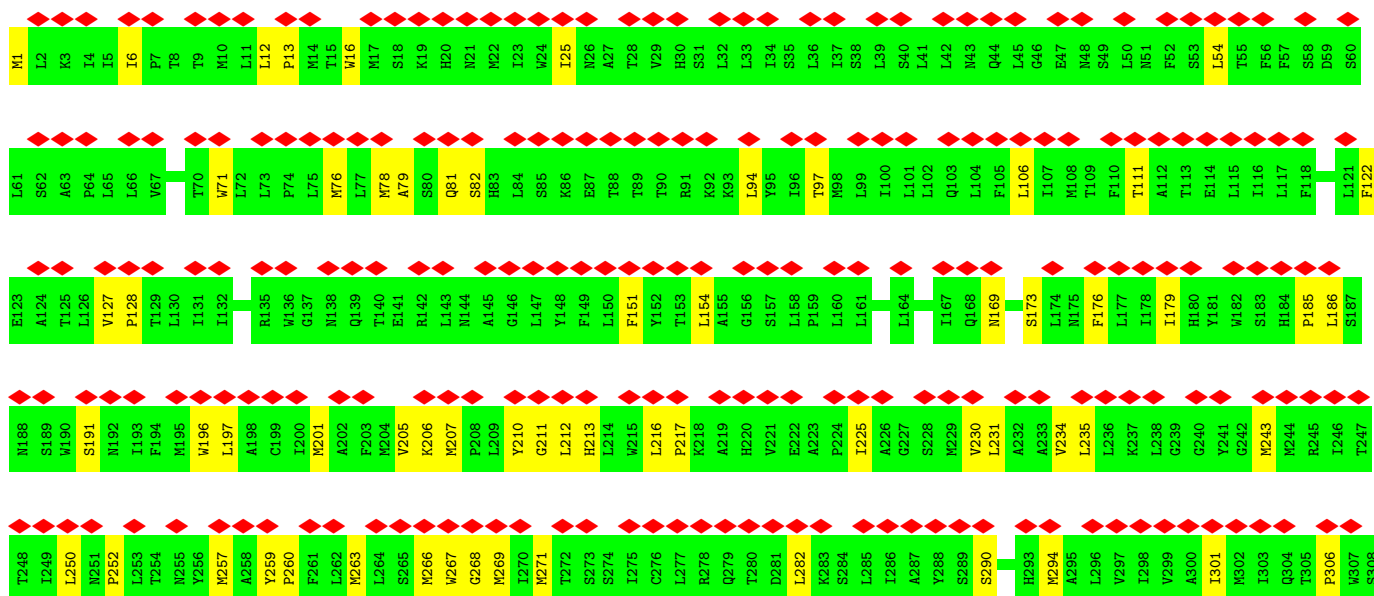
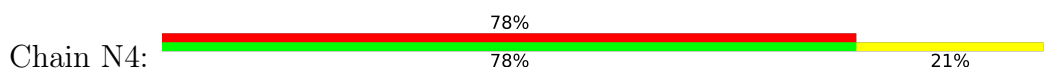
- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

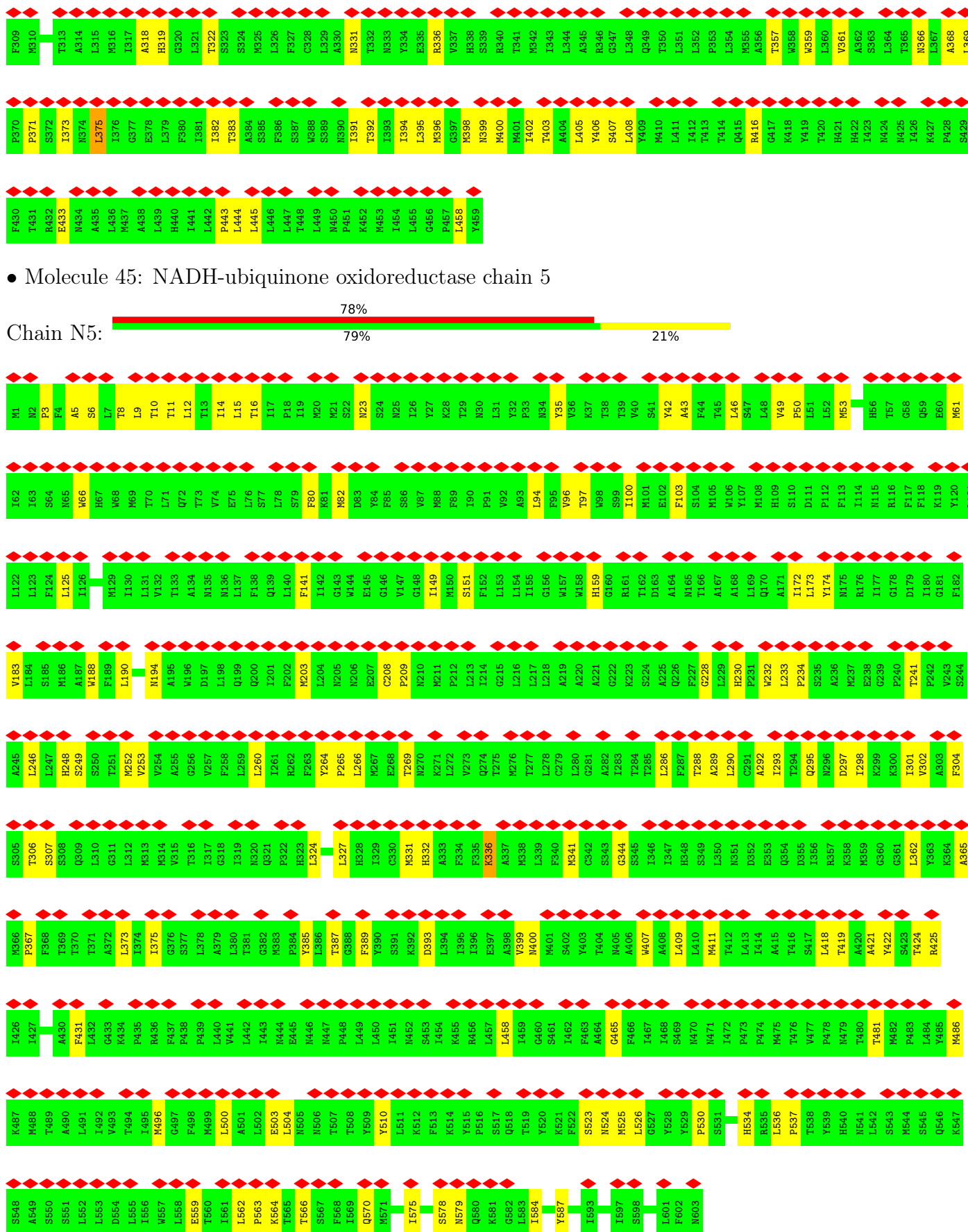


• Molecule 43: NADH-ubiquinone oxidoreductase chain 3

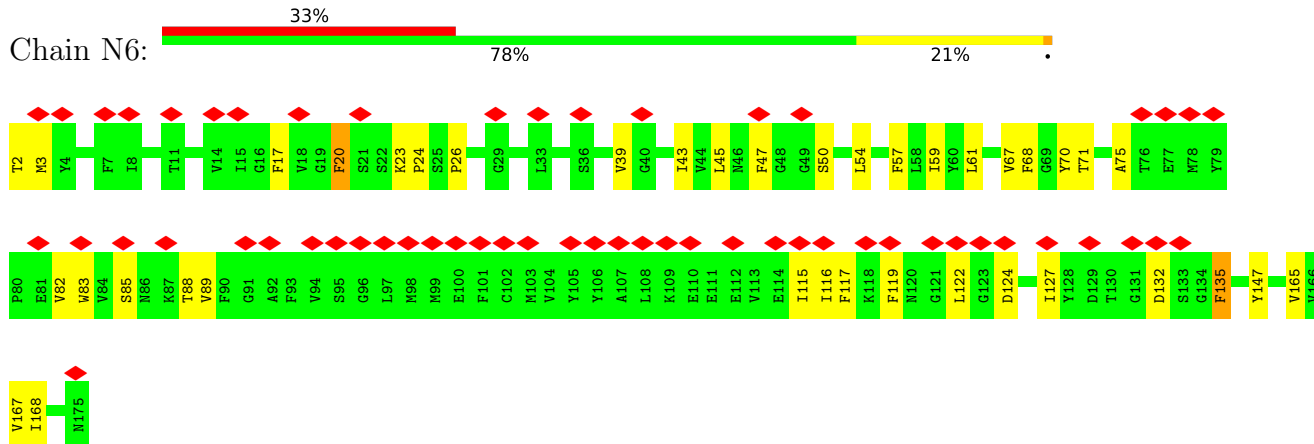


• Molecule 44: NADH-ubiquinone oxidoreductase chain 4

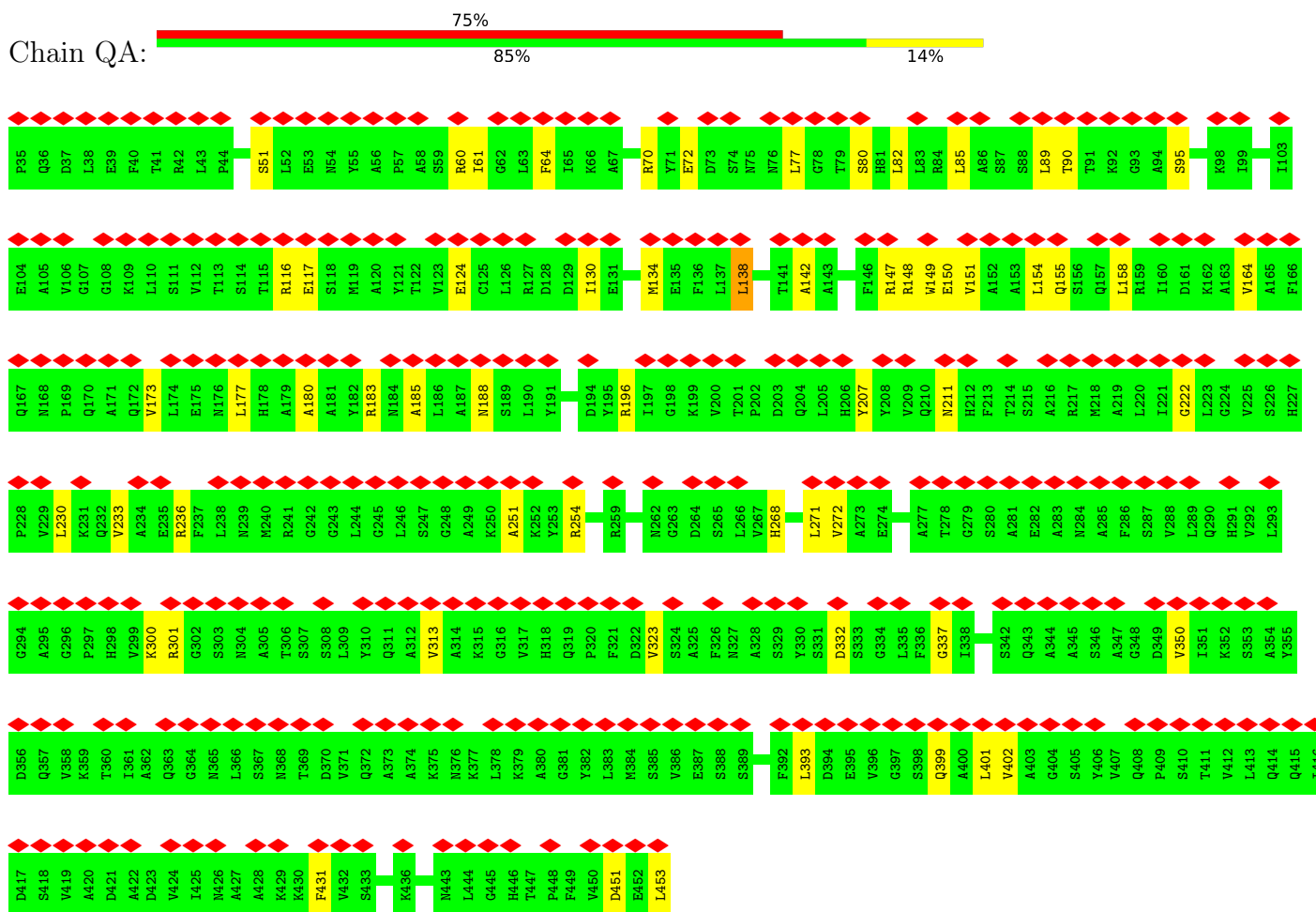




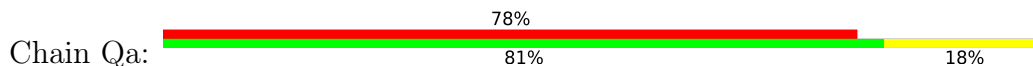
- Molecule 46: NADH-ubiquinone oxidoreductase chain 6

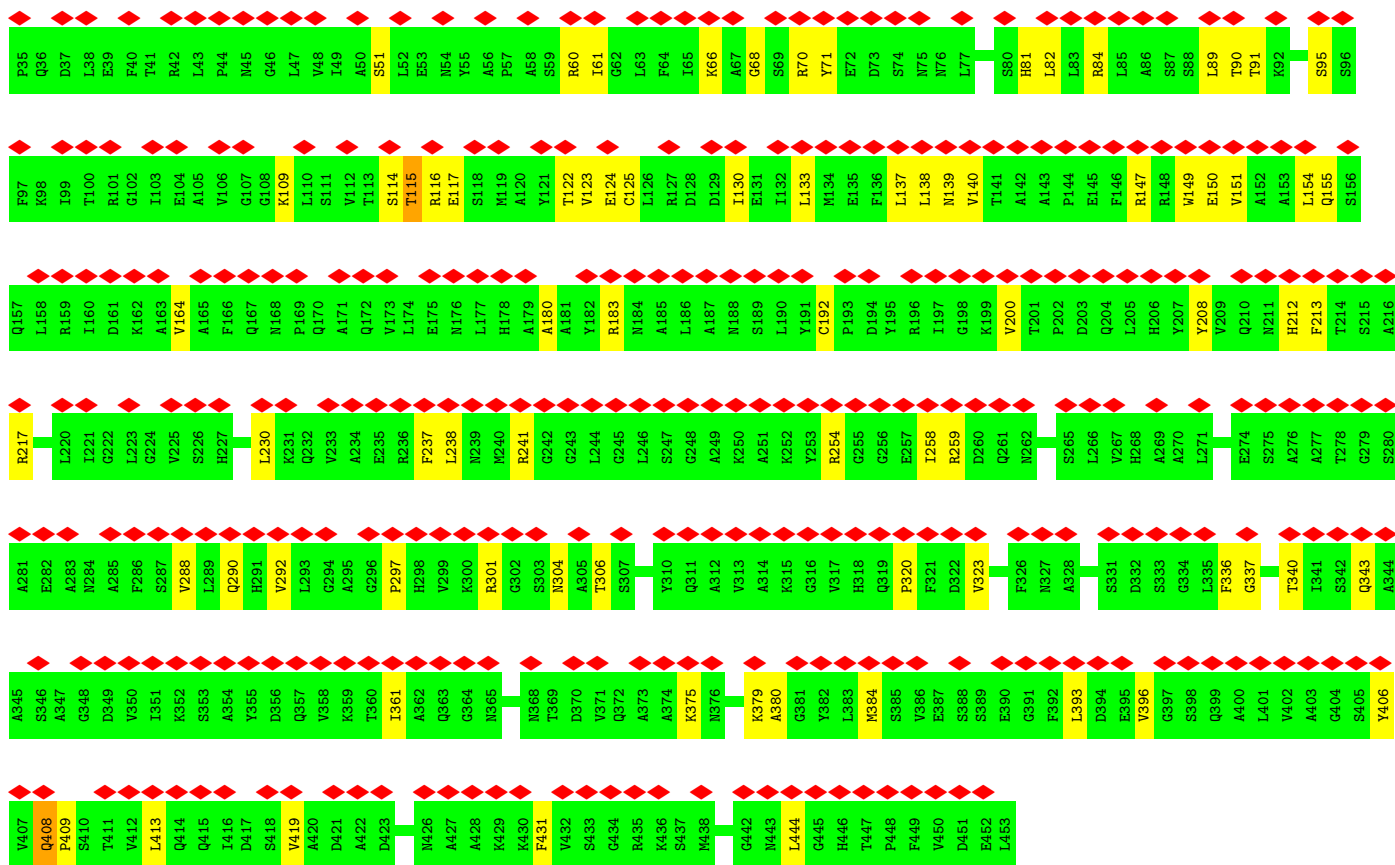


- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

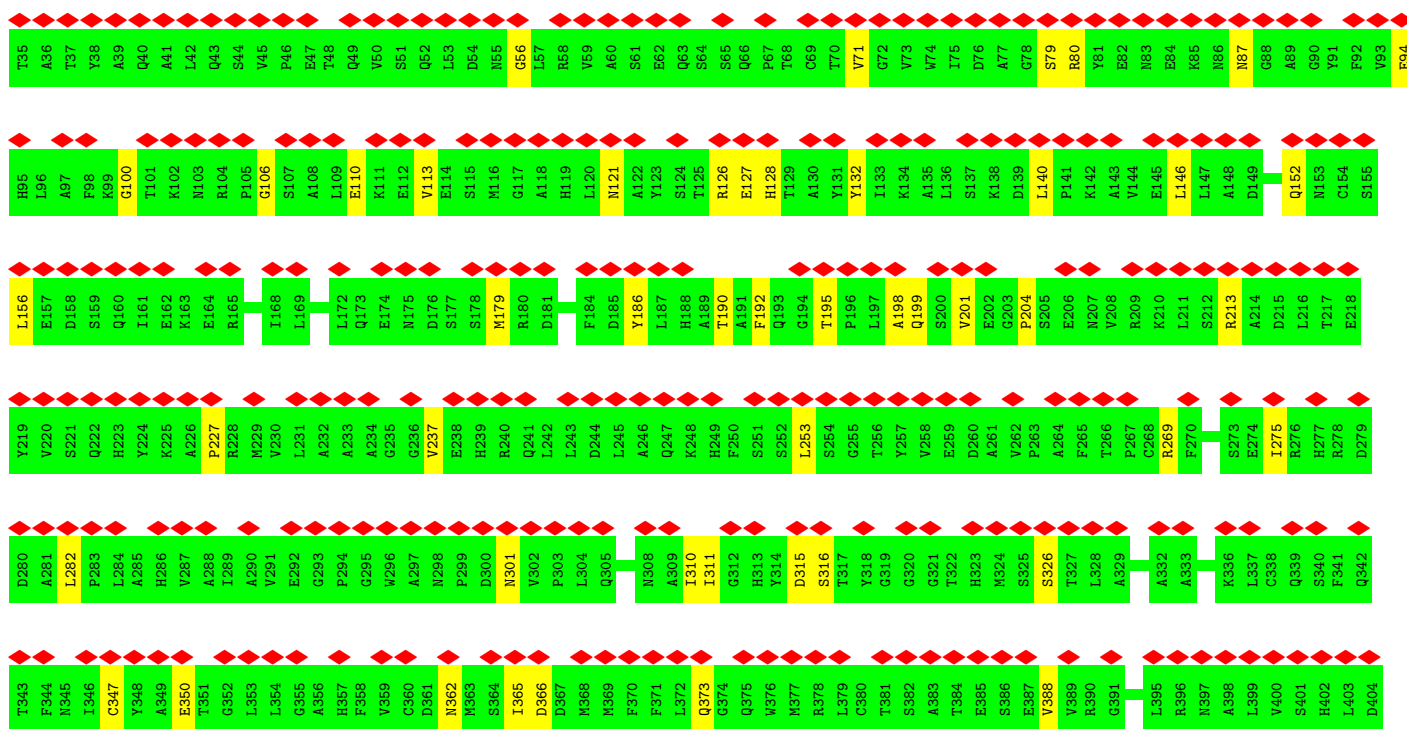
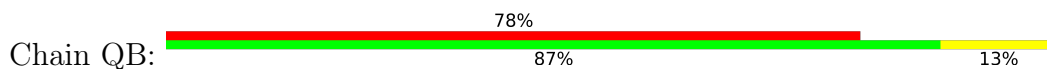


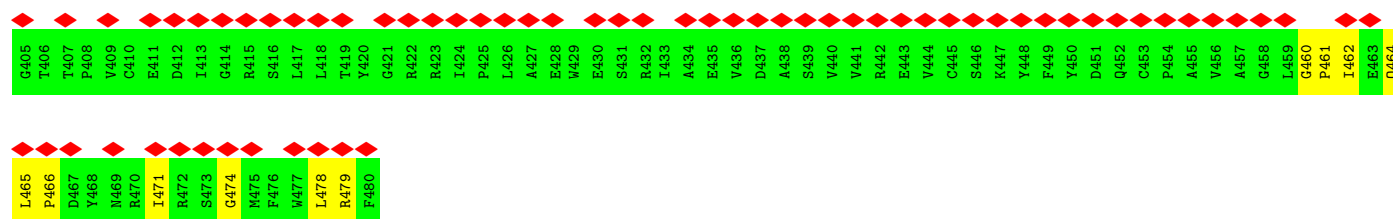
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial





• Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

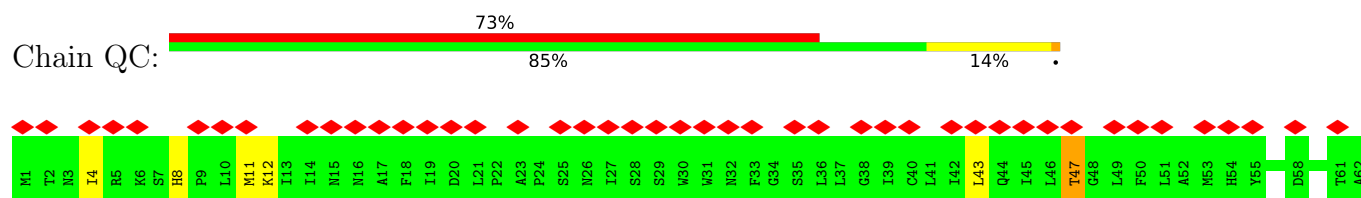


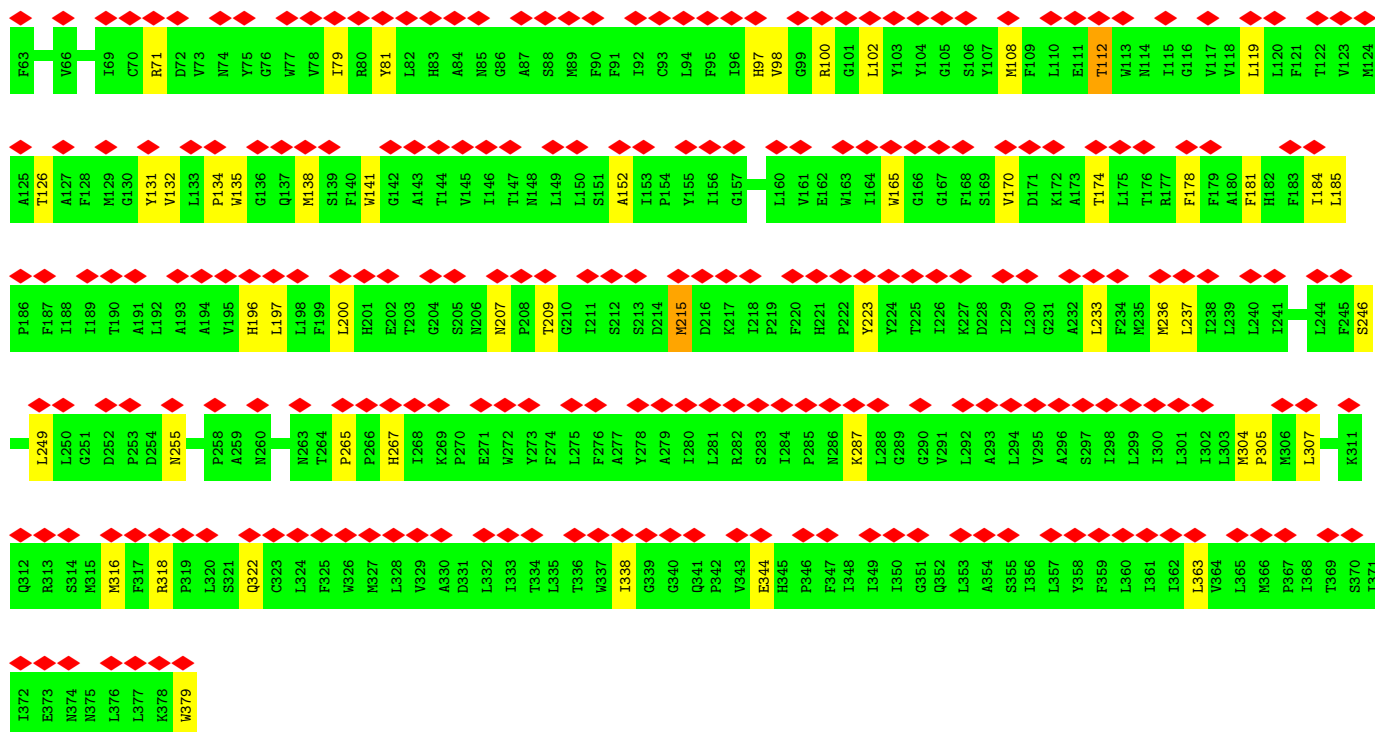


• Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

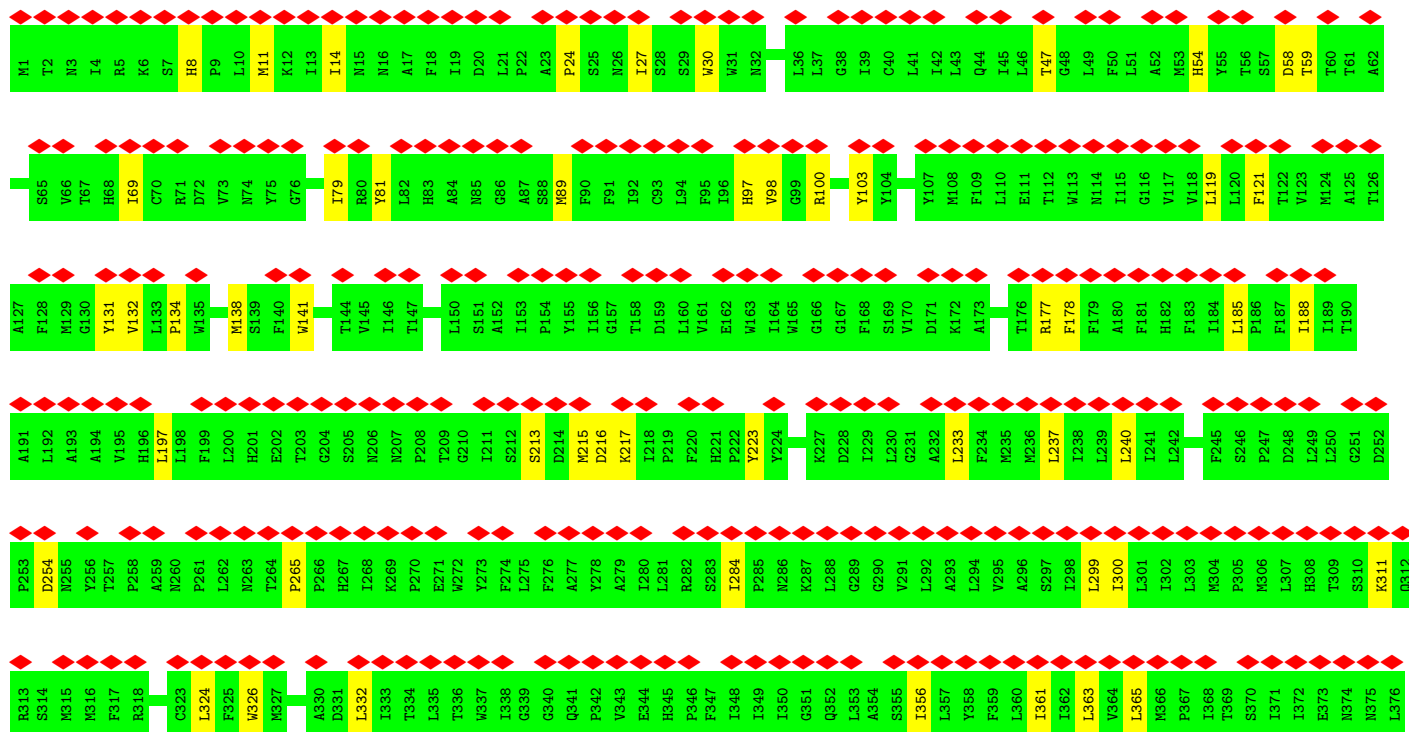
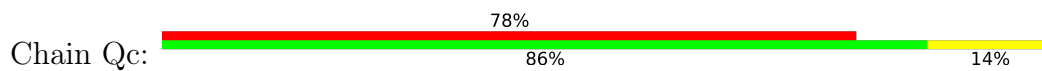


• Molecule 49: Cytochrome b



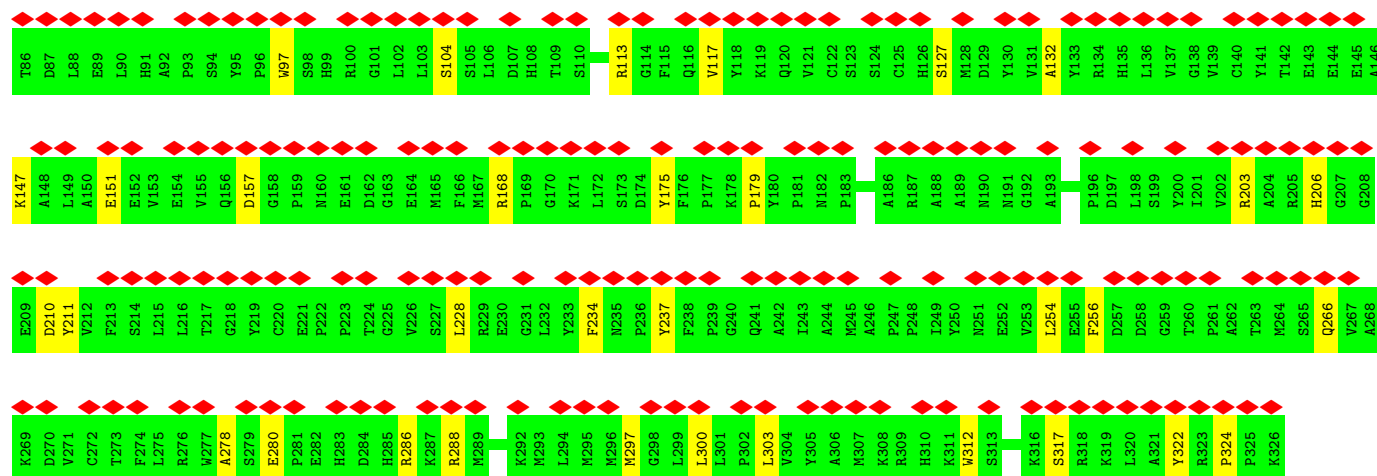
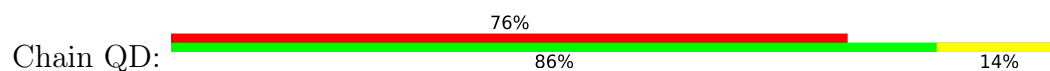


• Molecule 49: Cytochrome b

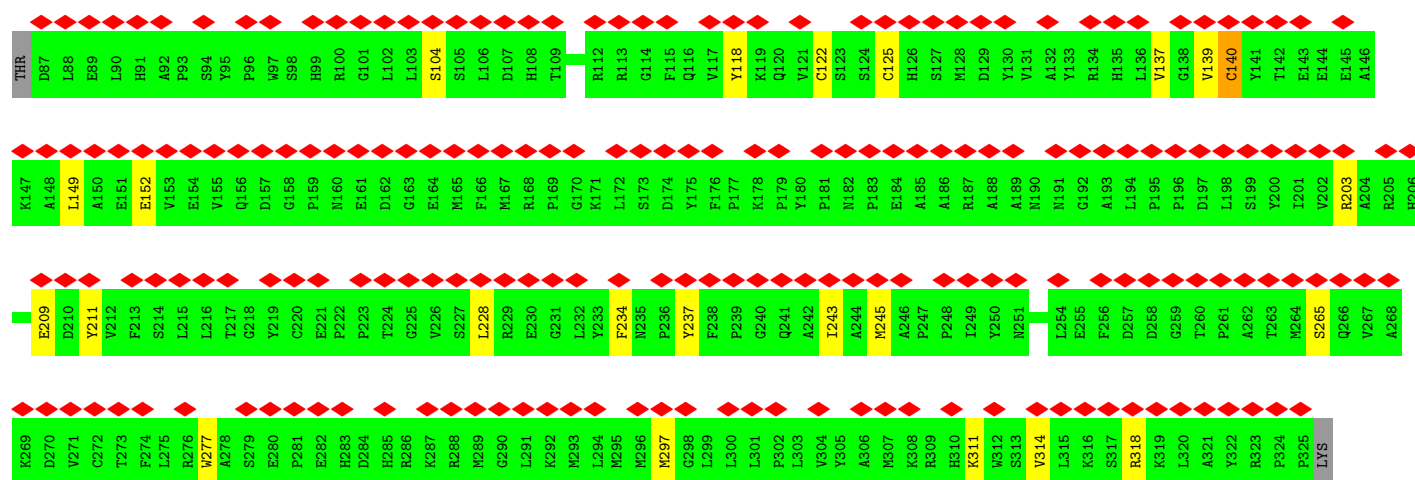
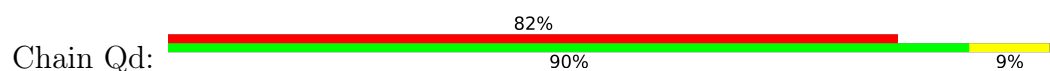




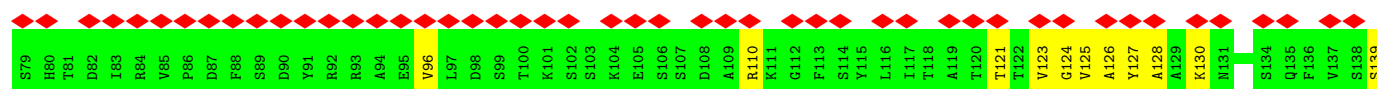
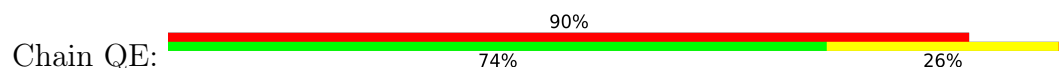
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

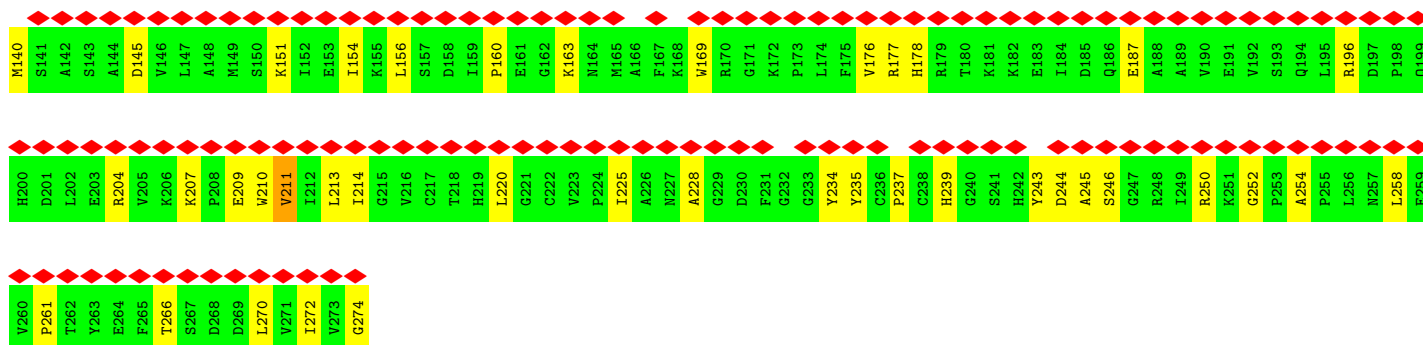


- Molecule 50: Cytochrome c1, heme protein, mitochondrial

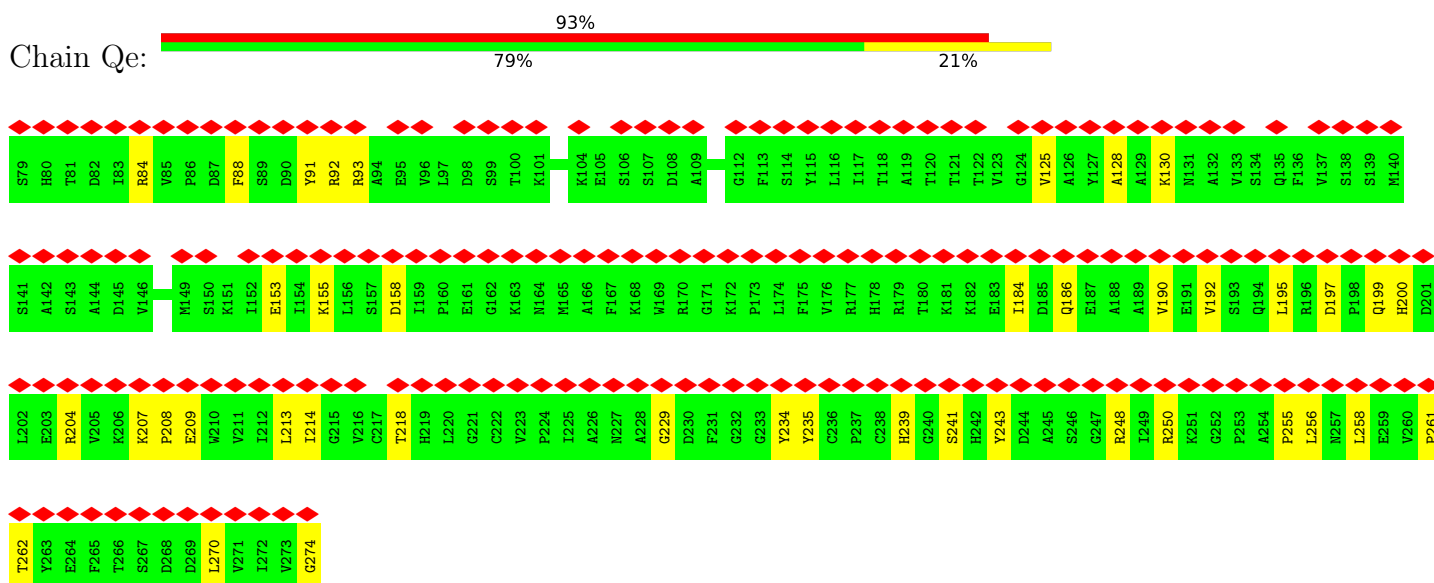


- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial

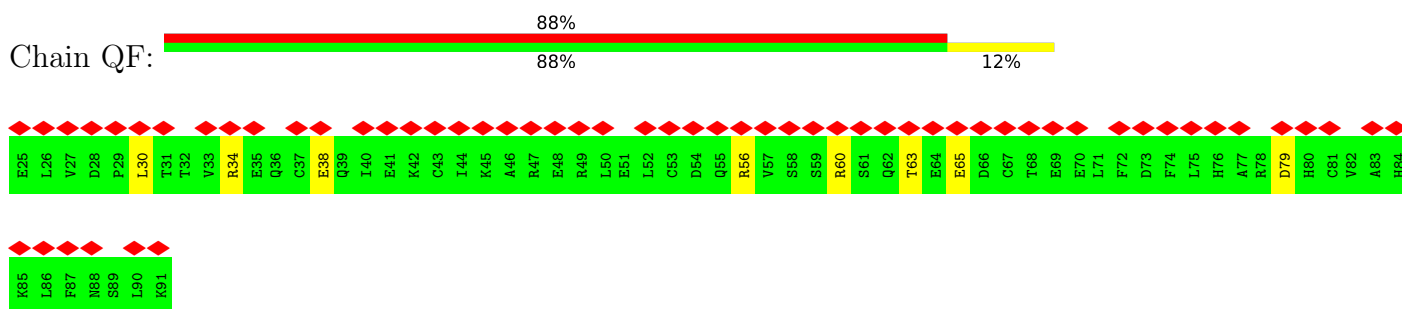




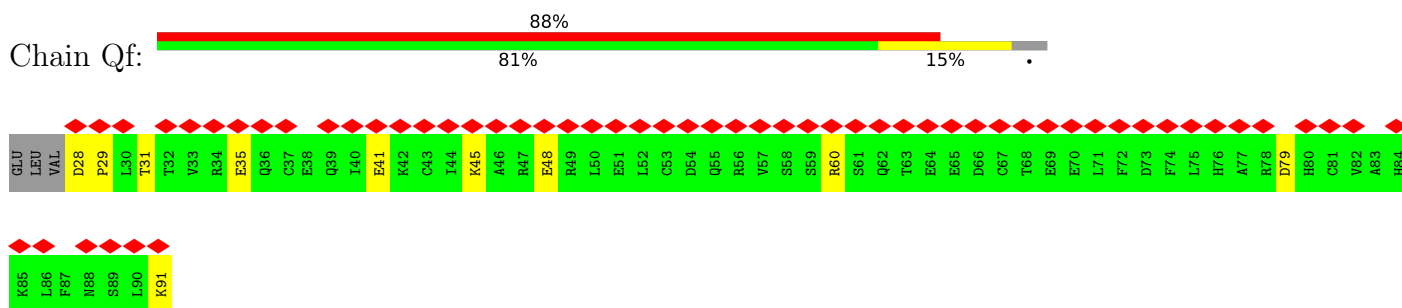
- Molecule 51: Cytochrome b-c1 complex subunit Rieske, mitochondrial



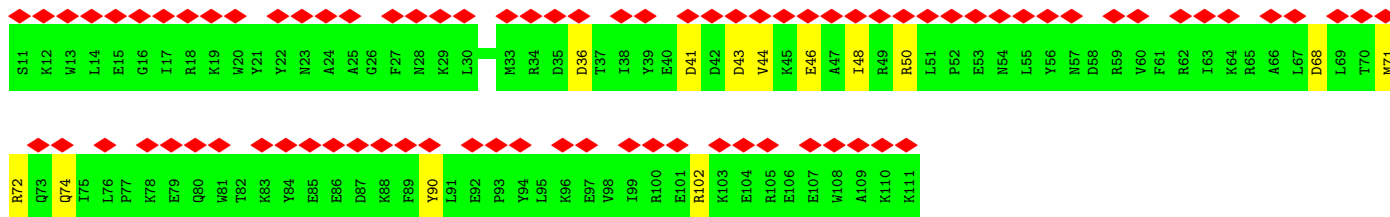
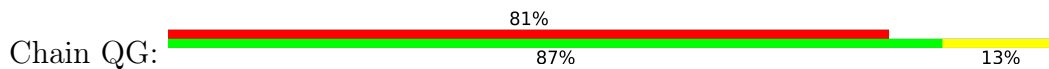
- Molecule 52: Cytochrome b-c1 complex subunit 6



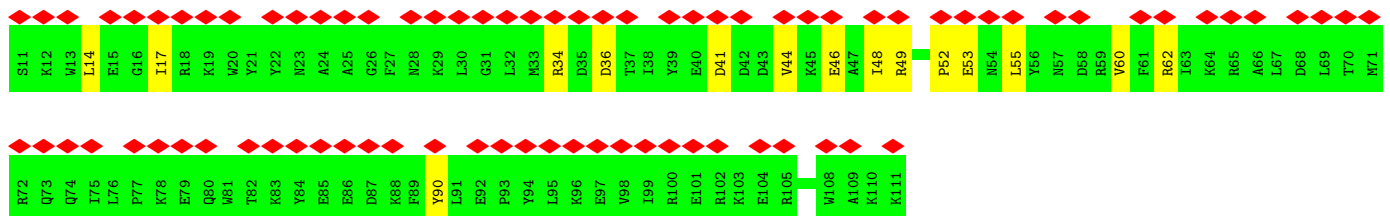
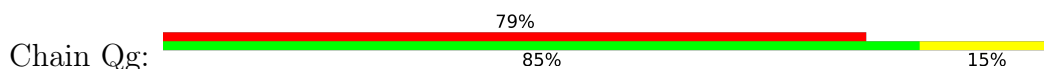
- Molecule 52: Cytochrome b-c1 complex subunit 6



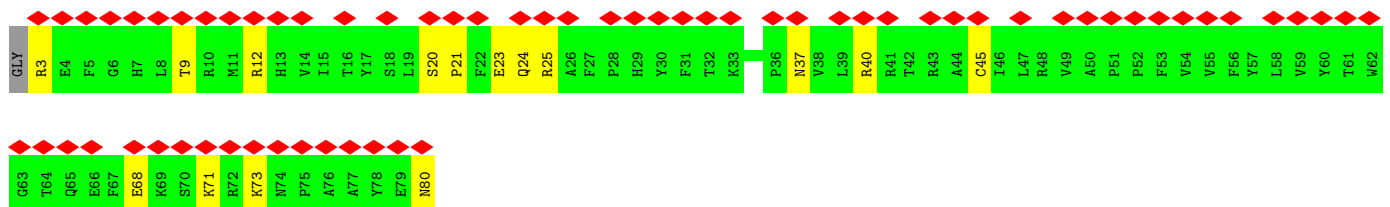
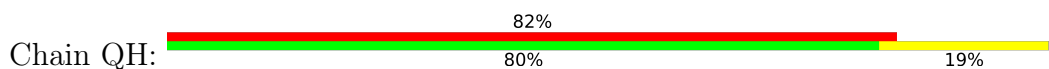
• Molecule 53: Cytochrome b-c1 complex subunit 7



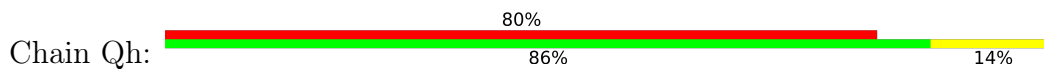
• Molecule 53: Cytochrome b-c1 complex subunit 7



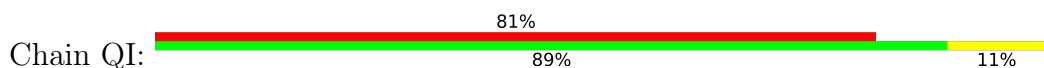
• Molecule 54: Cytochrome b-c1 complex subunit 8



• Molecule 54: Cytochrome b-c1 complex subunit 8

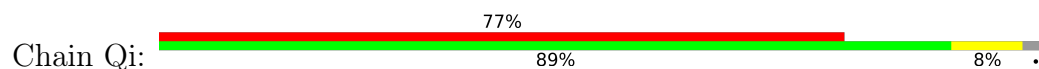


• Molecule 55: Complex III subunit 9

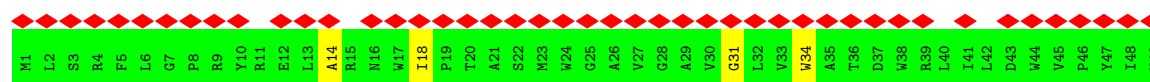




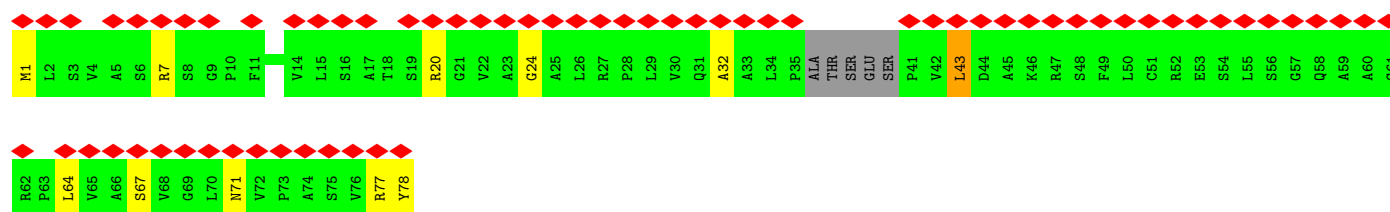
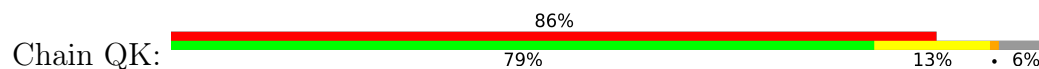
• Molecule 55: Complex III subunit 9



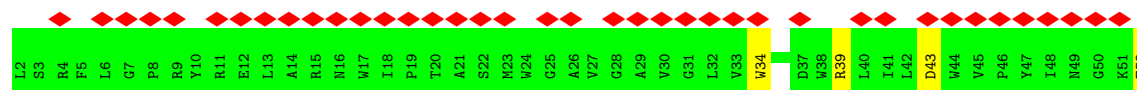
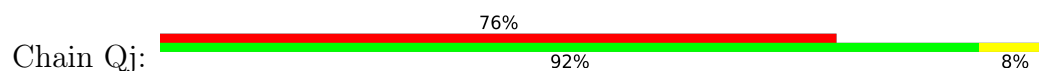
• Molecule 56: Cytochrome b-c1 complex subunit 10



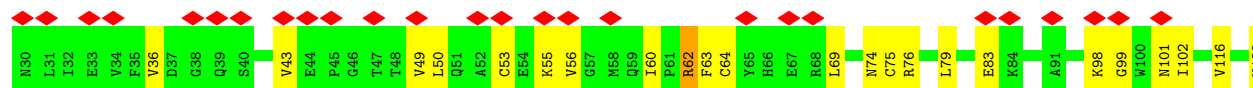
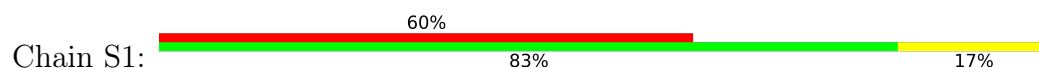
• Molecule 57: Cytochrome b-c1 complex subunit Rieske, mitochondrial

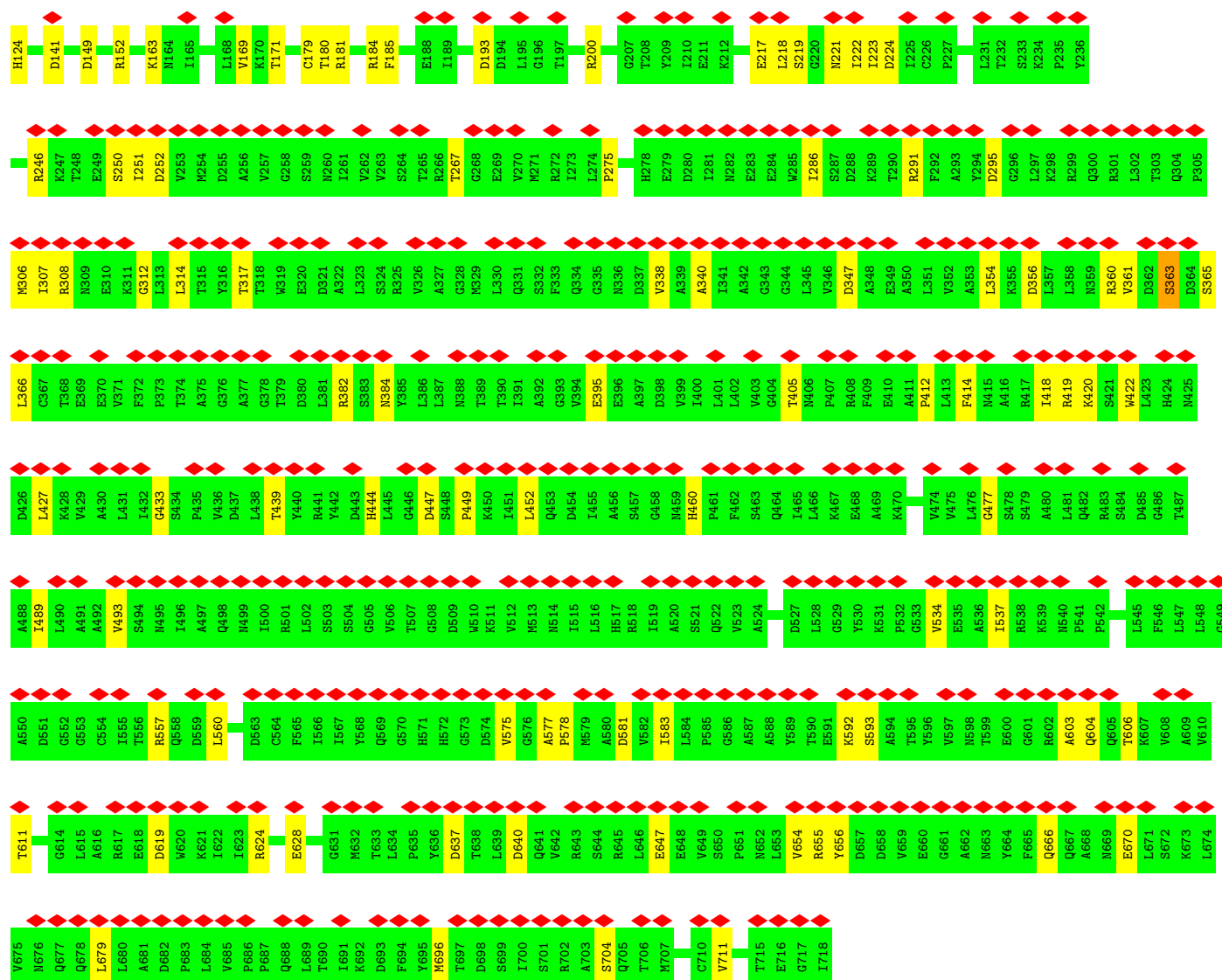


• Molecule 58: Cytochrome b-c1 complex subunit 10

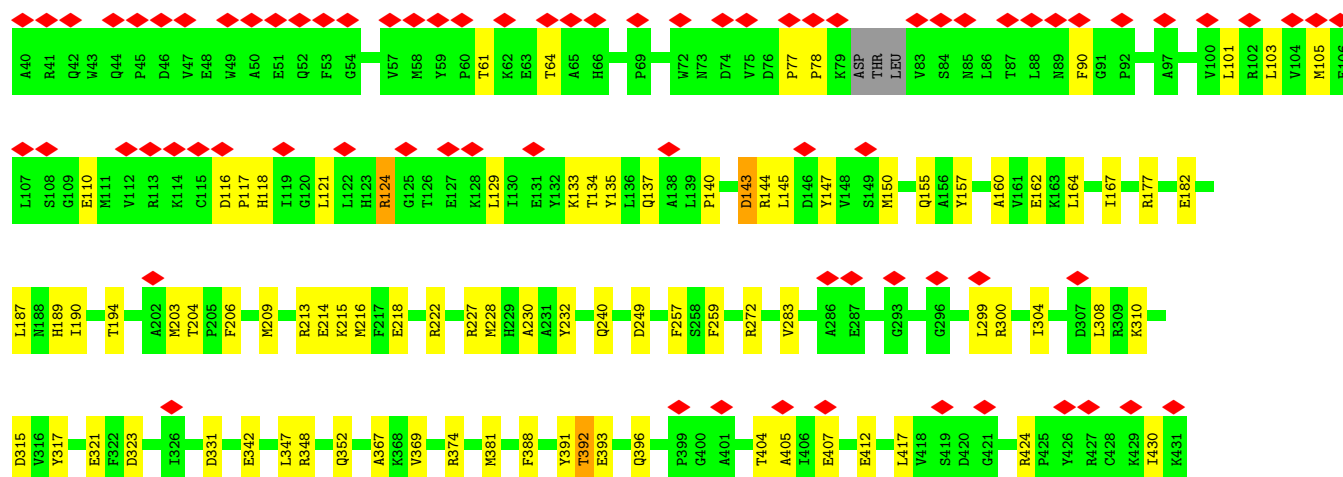
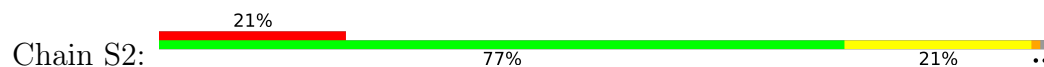


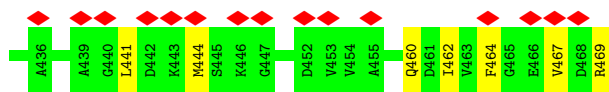
• Molecule 59: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



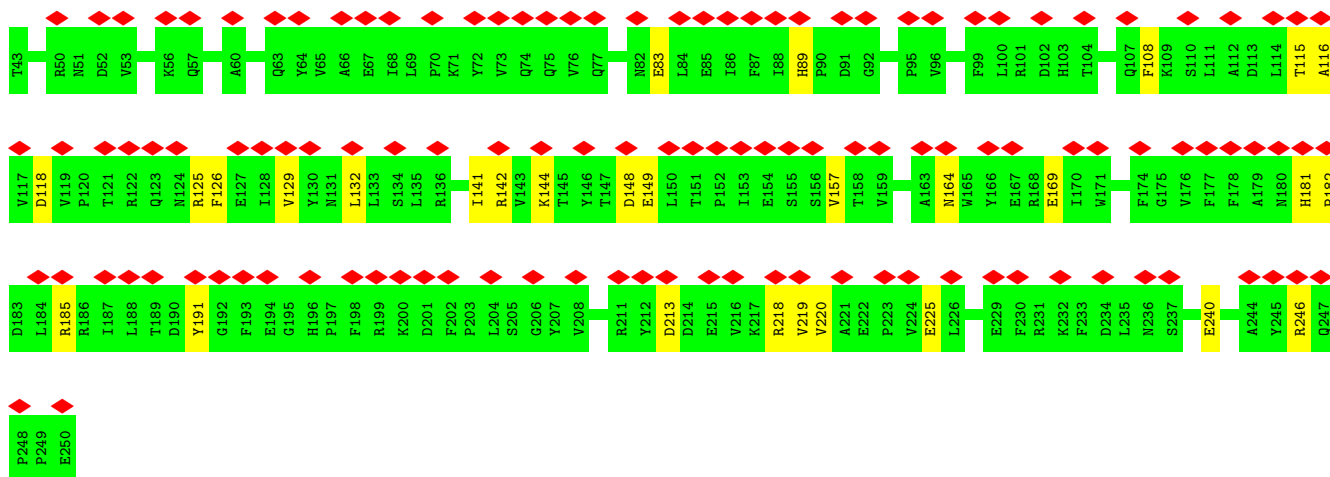
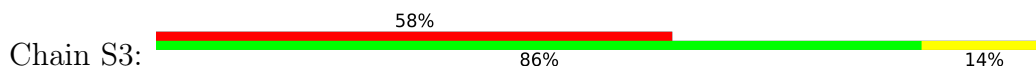


• Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

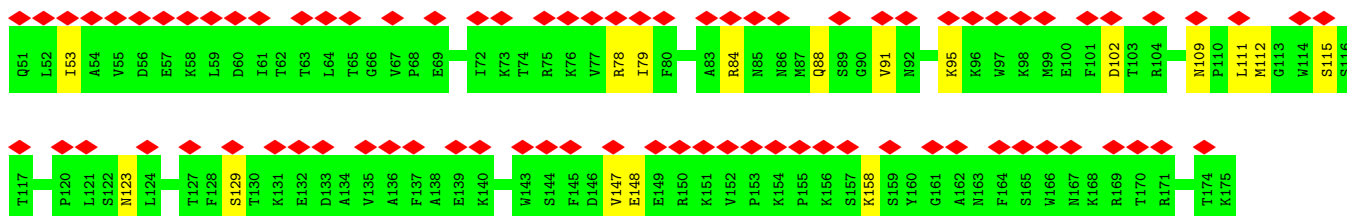
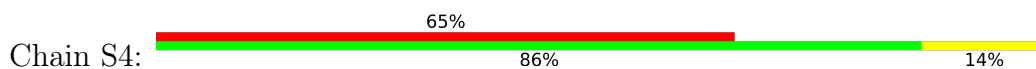




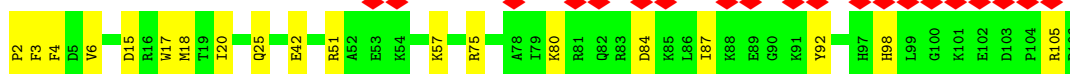
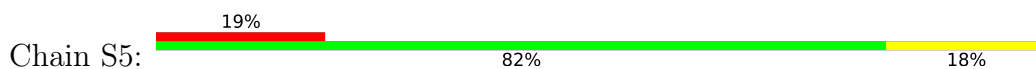
• Molecule 61: Complex I-30kD



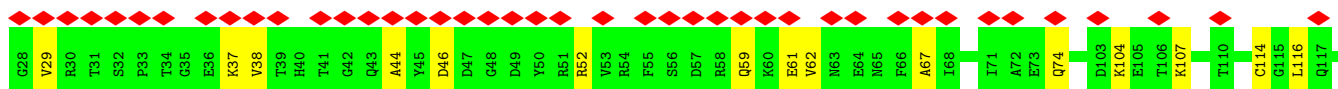
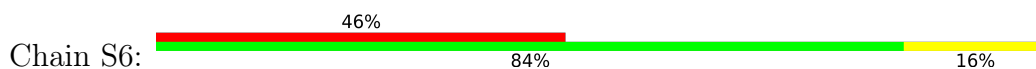
• Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



• Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

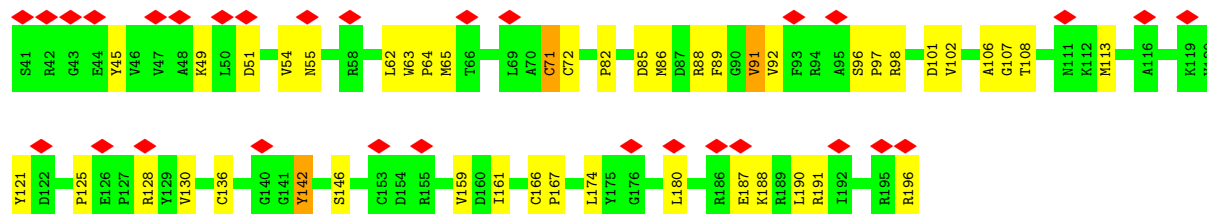
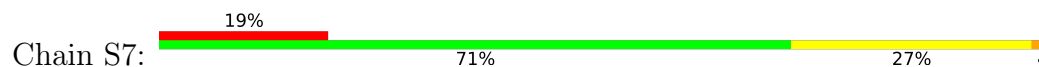


• Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

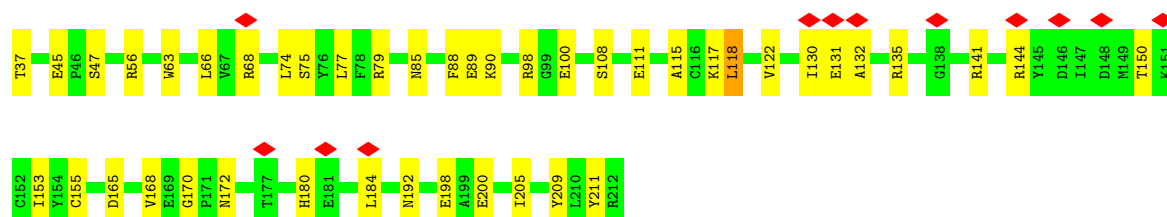
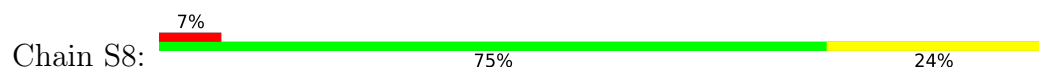




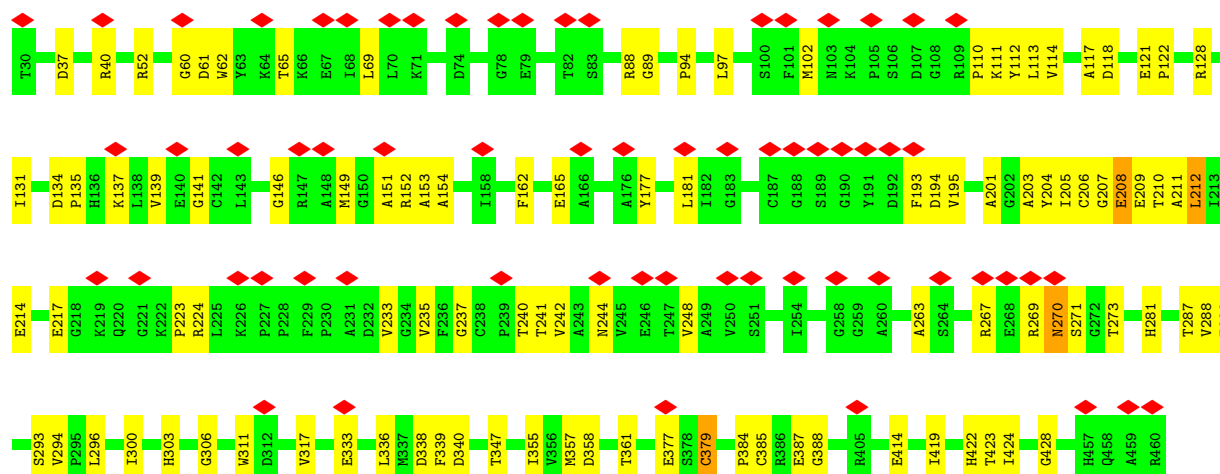
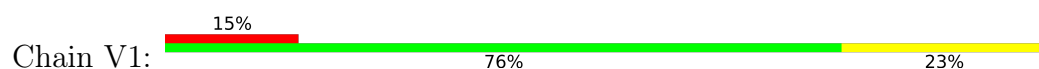
- Molecule 65: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



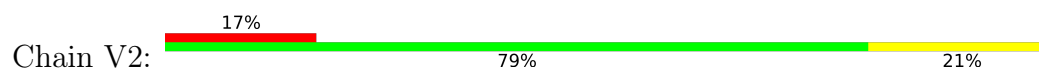
- Molecule 66: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

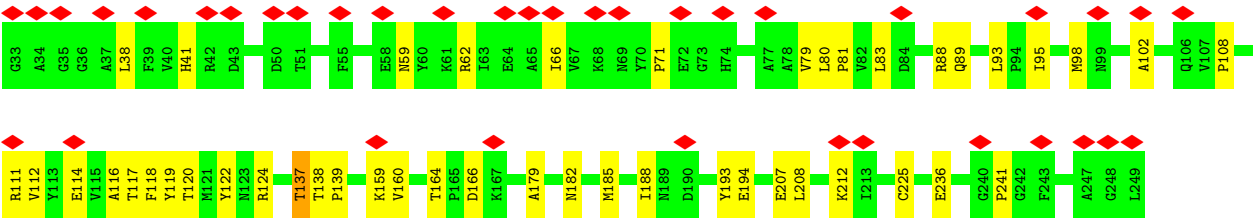


- Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

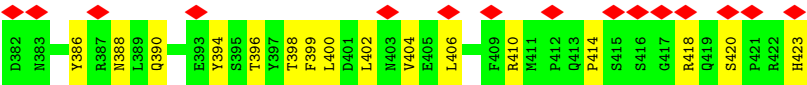


- Molecule 68: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





• Molecule 69: NADH:ubiquinone oxidoreductase subunit V3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89819	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	131.693	Depositor
Minimum map value	-54.678	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.161	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, CU, HEC, FES, ZMP, 3PE, ADP, 2MR, PLX, FMN, ZN, HEM, NDP, HEA, MG, SF4, CDL, PC1

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	4L	0.13	0/759	0.27	0/1029
2	5A	0.13	0/843	0.32	0/1145
3	5B	0.11	0/739	0.28	0/1002
4	6A	0.11	0/637	0.27	0/873
5	6B	0.14	0/704	0.32	0/951
6	6C	0.09	0/587	0.23	0/781
7	7A	0.09	0/457	0.23	0/620
8	7B	0.09	0/405	0.26	0/555
9	7C	0.11	0/400	0.22	0/536
10	8B	0.09	0/349	0.23	0/477
11	A1	0.12	0/577	0.27	0/777
12	A2	0.09	0/697	0.26	0/938
13	A3	0.09	0/664	0.23	0/912
14	A5	0.11	0/929	0.23	0/1258
15	A6	0.11	0/991	0.26	0/1335
16	A7	0.09	0/798	0.23	0/1079
17	A8	0.09	0/1436	0.24	0/1938
18	A9	0.10	0/2820	0.25	0/3823
19	AB	0.08	0/633	0.23	0/851
19	AC	0.11	0/714	0.24	0/965
20	AK	0.10	0/2661	0.26	0/3602
21	AL	0.10	0/1042	0.22	0/1411
22	AM	0.08	0/1245	0.21	0/1694
23	AN	0.12	0/1204	0.26	0/1624
24	B1	0.10	0/491	0.23	0/663
25	B2	0.12	0/610	0.24	0/836
26	B3	0.11	0/660	0.25	0/892
27	B4	0.12	0/1092	0.25	0/1481
28	B5	0.12	0/1184	0.27	0/1603
29	B6	0.13	0/888	0.30	0/1208
30	B7	0.11	0/1092	0.24	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	B8	0.10	0/1371	0.25	0/1875
32	B9	0.11	0/1590	0.26	0/2155
33	BK	0.12	0/1489	0.24	0/2008
34	BL	0.12	0/851	0.27	0/1155
35	C1	0.13	0/4164	0.30	0/5689
36	C2	0.11	0/1880	0.28	0/2564
37	C3	0.11	0/2186	0.26	0/2991
38	C4	0.12	0/1187	0.30	0/1606
39	CA	0.10	0/430	0.20	0/581
40	CB	0.12	0/1031	0.24	0/1394
41	N1	0.14	0/2581	0.32	0/3529
42	N2	0.15	0/2773	0.31	0/3768
43	N3	0.11	0/938	0.26	0/1281
44	N4	0.16	0/3723	0.33	0/5078
45	N5	0.15	0/4914	0.33	0/6683
46	N6	0.13	0/1364	0.30	0/1850
47	QA	0.12	0/3200	0.28	0/4333
47	Qa	0.11	0/3200	0.27	0/4333
48	QB	0.12	0/3531	0.29	0/4793
48	Qb	0.11	0/3436	0.26	0/4659
49	QC	0.14	0/3123	0.30	0/4269
49	Qc	0.15	0/3123	0.30	0/4269
50	QD	0.11	0/1979	0.26	0/2684
50	Qd	0.12	0/1962	0.26	0/2663
51	QE	0.10	0/1550	0.24	0/2098
51	Qe	0.11	0/1550	0.26	0/2098
52	QF	0.09	0/558	0.21	0/747
52	Qf	0.10	0/534	0.22	0/714
53	QG	0.11	0/913	0.25	0/1223
53	Qg	0.11	0/913	0.24	0/1223
54	QH	0.12	0/684	0.28	0/926
54	Qh	0.13	0/688	0.28	0/931
55	QI	0.08	0/520	0.19	0/701
55	Qi	0.12	0/506	0.24	0/683
56	QJ	0.08	0/420	0.21	0/576
57	QK	0.09	0/528	0.26	0/716
58	Qj	0.12	0/437	0.29	0/598
59	S1	0.13	0/5378	0.31	0/7287
60	S2	0.14	0/3514	0.28	0/4761
61	S3	0.12	0/1789	0.28	0/2436
62	S4	0.11	0/1039	0.28	0/1403
63	S5	0.10	0/889	0.22	0/1190
64	S6	0.11	0/755	0.27	0/1018

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
65	S7	0.14	0/1279	0.28	0/1730
66	S8	0.13	0/1443	0.26	0/1952
67	V1	0.13	0/3391	0.30	0/4583
68	V2	0.11	0/1711	0.29	0/2328
69	V3	0.08	0/365	0.29	0/493
All	All	0.12	0/115688	0.28	0/156943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4L	748	0	799	22	0
2	5A	825	0	823	39	0
3	5B	724	0	705	26	0
4	6A	609	0	579	22	0
5	6B	684	0	649	25	0
6	6C	574	0	590	13	0
7	7A	447	0	443	11	0
8	7B	392	0	372	10	0
9	7C	387	0	385	8	0
10	8B	338	0	342	13	0
11	A1	562	0	557	10	0
12	A2	686	0	699	10	0
13	A3	643	0	642	9	0
14	A5	910	0	950	15	0
15	A6	967	0	972	17	0
16	A7	780	0	808	9	0
17	A8	1398	0	1372	27	0
18	A9	2743	0	2762	42	0
19	AB	624	0	625	13	0
19	AC	702	0	694	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AK	2601	0	2566	42	0
21	AL	1021	0	1025	10	0
22	AM	1204	0	1162	19	0
23	AN	1173	0	1166	21	0
24	B1	479	0	486	7	0
25	B2	584	0	529	6	0
26	B3	641	0	620	9	0
27	B4	1062	0	1072	10	0
28	B5	1151	0	1164	12	0
29	B6	861	0	877	19	0
30	B7	1068	0	1043	17	0
31	B8	1315	0	1208	12	0
32	B9	1534	0	1470	15	0
33	BK	1456	0	1426	14	0
34	BL	828	0	788	10	0
35	C1	4024	0	4005	160	0
36	C2	1833	0	1843	59	0
37	C3	2103	0	2034	82	0
38	C4	1153	0	1130	35	0
39	CA	417	0	422	4	0
40	CB	1000	0	994	10	0
41	N1	2508	0	2607	60	0
42	N2	2710	0	2874	58	0
43	N3	914	0	951	13	0
44	N4	3631	0	3839	69	0
45	N5	4785	0	4933	93	0
46	N6	1329	0	1326	37	0
47	QA	3147	0	3129	37	0
47	Qa	3147	0	3129	48	0
48	QB	3459	0	3350	37	0
48	Qb	3367	0	3262	31	0
49	QC	3025	0	3090	43	0
49	Qc	3025	0	3090	41	0
50	QD	1921	0	1867	26	0
50	Qd	1904	0	1849	18	0
51	QE	1517	0	1500	38	0
51	Qe	1517	0	1500	31	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	8	0
53	QG	893	0	888	8	0
53	Qg	893	0	888	12	0
54	QH	662	0	660	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	Qh	666	0	663	9	0
55	QI	507	0	509	4	0
55	Qi	493	0	491	6	0
56	QJ	405	0	405	3	0
57	QK	520	0	554	9	0
58	Qj	421	0	418	3	0
59	S1	5290	0	5321	76	0
60	S2	3436	0	3373	70	0
61	S3	1738	0	1693	21	0
62	S4	1016	0	1016	15	0
63	S5	867	0	871	19	0
64	S6	741	0	701	11	0
65	S7	1248	0	1254	33	0
66	S8	1412	0	1363	38	0
67	V1	3316	0	3272	67	0
68	V2	1671	0	1673	30	0
69	V3	355	0	329	13	0
70	5B	1	0	0	0	0
70	S6	1	0	0	0	0
71	6A	45	0	64	10	0
71	B4	50	0	77	4	0
71	B5	54	0	88	1	0
71	C3	99	0	152	24	0
71	CB	54	0	88	0	0
71	N1	48	0	73	5	0
71	N4	100	0	154	7	0
71	QB	105	0	167	6	0
71	Qb	48	0	73	2	0
71	Qc	108	0	176	5	0
71	Qh	54	0	88	1	0
71	Qj	43	0	63	0	0
71	S7	54	0	88	2	0
72	6C	31	0	40	3	0
72	AM	52	0	88	4	0
72	B5	52	0	88	1	0
72	N2	52	0	88	4	0
72	N4	52	0	88	3	0
72	QE	46	0	73	6	0
72	QI	52	0	88	4	0
73	A8	83	0	113	6	0
73	AL	180	0	257	5	0
73	B4	80	0	107	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	B5	100	0	156	8	0
73	CB	100	0	156	10	0
73	N1	78	0	103	5	0
73	N2	68	0	80	1	0
73	N5	189	0	284	15	0
73	QB	62	0	68	3	0
73	QD	64	0	72	0	0
73	QH	125	0	138	4	0
73	Qb	64	0	72	3	0
73	Qh	55	0	54	1	0
74	A9	48	0	26	0	0
75	AB	36	0	47	2	0
75	AC	36	0	47	4	0
76	AK	27	0	12	4	0
77	B8	32	0	38	0	0
77	C1	51	0	82	8	0
77	CB	51	0	82	4	0
77	N5	46	0	69	0	0
77	QC	34	0	42	1	0
77	QE	43	0	63	3	0
78	C1	120	0	108	23	0
79	C1	1	0	0	0	0
79	C2	2	0	0	0	0
80	C1	1	0	0	0	0
80	S1	1	0	0	0	0
81	N3	51	0	82	3	0
81	N4	46	0	66	2	0
81	N5	97	0	151	8	0
81	N6	51	0	82	1	0
81	QC	40	0	54	2	0
81	QE	47	0	71	2	0
81	Qc	42	0	61	4	0
81	Qe	44	0	65	4	0
81	S2	48	0	73	3	0
81	S8	51	0	82	2	0
82	QC	86	0	60	8	0
82	Qc	86	0	60	8	0
83	QD	43	0	30	1	0
83	Qd	43	0	32	3	0
84	QE	4	0	0	0	0
84	Qe	4	0	0	2	0
84	S1	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	V2	4	0	0	0	0
85	S1	16	0	0	0	0
85	S7	8	0	0	1	0
85	S8	16	0	0	1	0
85	V1	8	0	0	0	0
86	V1	31	0	19	4	0
All	All	116635	0	117650	1806	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 8.

The worst 5 of 1806 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)
36:C2:200:CYS:SG	36:C2:207:MET:HE1	1.69	1.33
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.60	1.00
30:B7:92:HIS:HD1	45:N5:481:THR:HG1	1.23	0.87
49:Qc:98:VAL:HG22	82:Qc:403:HEM:HBC2	1.60	0.84
51:Qe:200:HIS:HA	51:Qe:204:ARG:HG3	1.58	0.83

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	4L	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
2	5A	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
3	5B	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
4	6A	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
5	6B	80/82 (98%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6C	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
7	7A	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
8	7B	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
9	7C	45/47 (96%)	45 (100%)	0	0	100	100
10	8B	41/43 (95%)	41 (100%)	0	0	100	100
11	A1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
12	A2	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
13	A3	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
14	A5	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
15	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
16	A7	93/112 (83%)	92 (99%)	1 (1%)	0	100	100
17	A8	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
18	A9	339/341 (99%)	329 (97%)	10 (3%)	0	100	100
19	AB	75/87 (86%)	74 (99%)	1 (1%)	0	100	100
19	AC	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
20	AK	319/321 (99%)	313 (98%)	6 (2%)	0	100	100
21	AL	138/140 (99%)	138 (100%)	0	0	100	100
22	AM	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
23	AN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100
25	B2	65/67 (97%)	65 (100%)	0	0	100	100
26	B3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
29	B6	97/126 (77%)	94 (97%)	3 (3%)	0	100	100
30	B7	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
31	B8	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
32	B9	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
33	BK	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
34	BL	97/102 (95%)	88 (91%)	9 (9%)	0	100	100
35	C1	512/514 (100%)	495 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	C2	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
37	C3	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
38	C4	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
39	CA	47/49 (96%)	47 (100%)	0	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
42	N2	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
43	N3	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
44	N4	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
45	N5	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
46	N6	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
47	QA	417/419 (100%)	410 (98%)	7 (2%)	0	100	100
47	Qa	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
48	QB	444/446 (100%)	430 (97%)	14 (3%)	0	100	100
48	Qb	429/446 (96%)	419 (98%)	10 (2%)	0	100	100
49	QC	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
49	Qc	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
50	QD	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
50	Qd	237/241 (98%)	230 (97%)	7 (3%)	0	100	100
51	QE	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
51	Qe	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	62 (100%)	0	0	100	100
53	QG	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
53	Qg	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
54	QH	76/79 (96%)	72 (95%)	4 (5%)	0	100	100
54	Qh	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
55	QI	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/62 (94%)	58 (100%)	0	0	100	100
56	QJ	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
57	QK	69/78 (88%)	68 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Qj	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
59	S1	687/689 (100%)	656 (96%)	31 (4%)	0	100	100
60	S2	422/430 (98%)	405 (96%)	17 (4%)	0	100	100
61	S3	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
62	S4	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
63	S5	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
64	S6	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
65	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
66	S8	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
67	V1	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
68	V2	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
69	V3	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
All	All	13964/14217 (98%)	13550 (97%)	414 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	85 (96%)	4 (4%)	24	54
3	5B	80/80 (100%)	78 (98%)	2 (2%)	42	66
4	6A	65/65 (100%)	62 (95%)	3 (5%)	24	53
5	6B	73/73 (100%)	72 (99%)	1 (1%)	59	74
6	6C	57/57 (100%)	57 (100%)	0	100	100
7	7A	48/48 (100%)	45 (94%)	3 (6%)	16	43
8	7B	39/39 (100%)	39 (100%)	0	100	100
9	7C	40/40 (100%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	8B	37/37 (100%)	36 (97%)	1 (3%)	39	65
11	A1	58/58 (100%)	58 (100%)	0	100	100
12	A2	76/76 (100%)	75 (99%)	1 (1%)	61	75
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	98 (99%)	1 (1%)	68	77
15	A6	107/107 (100%)	107 (100%)	0	100	100
16	A7	87/97 (90%)	86 (99%)	1 (1%)	65	76
17	A8	153/153 (100%)	153 (100%)	0	100	100
18	A9	295/295 (100%)	294 (100%)	1 (0%)	86	86
19	AB	71/80 (89%)	70 (99%)	1 (1%)	59	74
19	AC	80/80 (100%)	79 (99%)	1 (1%)	61	75
20	AK	284/284 (100%)	282 (99%)	2 (1%)	76	80
21	AL	101/101 (100%)	100 (99%)	1 (1%)	68	77
22	AM	130/130 (100%)	130 (100%)	0	100	100
23	AN	123/123 (100%)	123 (100%)	0	100	100
24	B1	53/53 (100%)	52 (98%)	1 (2%)	50	71
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	62/62 (100%)	61 (98%)	1 (2%)	55	73
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	96/119 (81%)	95 (99%)	1 (1%)	68	77
30	B7	112/112 (100%)	112 (100%)	0	100	100
31	B8	141/141 (100%)	141 (100%)	0	100	100
32	B9	159/159 (100%)	158 (99%)	1 (1%)	78	81
33	BK	155/156 (99%)	155 (100%)	0	100	100
34	BL	91/94 (97%)	91 (100%)	0	100	100
35	C1	425/425 (100%)	410 (96%)	15 (4%)	32	60
36	C2	212/212 (100%)	209 (99%)	3 (1%)	59	74
37	C3	224/224 (100%)	219 (98%)	5 (2%)	45	68
38	C4	123/123 (100%)	119 (97%)	4 (3%)	33	61
39	CA	45/45 (100%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	275/275 (100%)	269 (98%)	6 (2%)	45	68
42	N2	311/311 (100%)	310 (100%)	1 (0%)	86	86
43	N3	100/100 (100%)	99 (99%)	1 (1%)	68	77
44	N4	410/410 (100%)	408 (100%)	2 (0%)	81	83
45	N5	537/537 (100%)	535 (100%)	2 (0%)	84	85
46	N6	140/140 (100%)	137 (98%)	3 (2%)	47	69
47	QA	330/330 (100%)	328 (99%)	2 (1%)	78	81
47	Qa	330/330 (100%)	327 (99%)	3 (1%)	70	78
48	QB	372/372 (100%)	371 (100%)	1 (0%)	86	86
48	Qb	362/372 (97%)	360 (99%)	2 (1%)	78	81
49	QC	332/332 (100%)	328 (99%)	4 (1%)	63	76
49	Qc	332/332 (100%)	332 (100%)	0	100	100
50	QD	206/206 (100%)	206 (100%)	0	100	100
50	Qd	204/206 (99%)	201 (98%)	3 (2%)	57	73
51	QE	166/166 (100%)	164 (99%)	2 (1%)	63	76
51	Qe	166/166 (100%)	166 (100%)	0	100	100
52	QF	64/64 (100%)	64 (100%)	0	100	100
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	93 (100%)	0	100	100
53	Qg	93/93 (100%)	93 (100%)	0	100	100
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	70 (100%)	0	100	100
55	QI	50/50 (100%)	50 (100%)	0	100	100
55	Qi	49/50 (98%)	49 (100%)	0	100	100
56	QJ	40/40 (100%)	40 (100%)	0	100	100
57	QK	55/59 (93%)	54 (98%)	1 (2%)	51	71
58	Qj	41/41 (100%)	41 (100%)	0	100	100
59	S1	579/579 (100%)	573 (99%)	6 (1%)	68	77
60	S2	367/370 (99%)	364 (99%)	3 (1%)	73	80
61	S3	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	S4	113/113 (100%)	113 (100%)	0	100	100
63	S5	93/93 (100%)	93 (100%)	0	100	100
64	S6	79/79 (100%)	78 (99%)	1 (1%)	61	75
65	S7	132/132 (100%)	127 (96%)	5 (4%)	29	58
66	S8	151/151 (100%)	150 (99%)	1 (1%)	76	80
67	V1	344/344 (100%)	337 (98%)	7 (2%)	48	70
68	V2	183/183 (100%)	179 (98%)	4 (2%)	45	68
69	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12179/12248 (99%)	12065 (99%)	114 (1%)	68	78

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	N1	145	THR
68	V2	117	THR
48	QB	71	VAL
67	V1	385	CYS
65	S7	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 254 such sidechains are listed below:

Mol	Chain	Res	Type
44	N4	366	ASN
59	S1	425	ASN
48	QB	160	GLN
59	S1	336	ASN
63	S5	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	2MR	S2	124	60	10,12,13	2.50	2 (20%)	5,13,15	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	2MR	S2	124	60	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	S2	124	2MR	CZ-NH2	5.37	1.44	1.33
60	S2	124	2MR	CZ-NE	5.13	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	S2	124	2MR	NE-CD-CG-CB
60	S2	124	2MR	CA-CB-CG-CD
60	S2	124	2MR	CG-CD-NE-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	S2	124	2MR	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 87 ligands modelled in this entry, 7 are monoatomic - leaving 80 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
71	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.35	0
72	PLX	B5	201	-	51,51,51	1.14	4 (7%)	53,59,59	0.91	1 (1%)
72	PLX	QI	301	-	51,51,51	1.15	5 (9%)	53,59,59	0.91	1 (1%)
72	PLX	AM	201	-	51,51,51	1.14	5 (9%)	53,59,59	0.90	1 (1%)
81	PEE	QE	302	-	46,46,50	1.40	5 (10%)	49,51,55	1.22	6 (12%)
71	PC1	C3	301	-	48,48,53	0.31	0	54,56,61	0.50	0
81	PEE	N5	701	-	45,45,50	1.41	5 (11%)	48,50,55	1.22	6 (12%)
73	CDL	N2	402	-	67,67,99	0.35	0	73,79,111	0.35	0
81	PEE	N5	704	-	50,50,50	1.35	5 (10%)	53,55,55	1.16	5 (9%)
84	FES	Qe	301	51	0,4,4	-	-	-	-	-
71	PC1	CB	202	-	53,53,53	0.28	0	59,61,61	0.29	0
73	CDL	QH	102	-	63,63,99	0.36	0	69,75,111	0.31	0
72	PLX	N2	401	-	51,51,51	1.14	4 (7%)	53,59,59	0.88	1 (1%)
73	CDL	QD	402	-	63,63,99	0.37	0	69,75,111	0.37	0
71	PC1	N1	402	-	47,47,53	0.30	0	53,55,61	0.32	0
73	CDL	QB	501	-	61,61,99	0.38	0	67,73,111	0.43	0
85	SF4	S1	801	59	0,12,12	-	-	-	-	-
78	HEA	C1	602	35	67,67,67	2.25	25 (37%)	81,103,103	2.48	29 (35%)
84	FES	QE	304	51	0,4,4	-	-	-	-	-
71	PC1	QB	503	-	53,53,53	0.29	0	59,61,61	0.31	0
71	PC1	B4	202	-	49,49,53	0.30	0	55,57,61	0.32	0
78	HEA	C1	603	35	67,67,67	2.27	25 (37%)	81,103,103	2.49	30 (37%)
73	CDL	N1	401	-	77,77,99	0.33	0	83,89,111	0.30	0
77	3PE	C1	601	-	50,50,50	0.31	0	53,55,55	0.28	0
85	SF4	S7	301	65	0,12,12	-	-	-	-	-
85	SF4	S8	301	66	0,12,12	-	-	-	-	-
73	CDL	N5	703	-	99,99,99	0.30	0	105,111,111	0.29	0
73	CDL	AL	201	-	90,90,99	0.32	0	96,102,111	0.39	0
82	HEM	QC	402	49	50,50,50	1.31	7 (14%)	67,82,82	1.58	12 (17%)
71	PC1	QB	502	-	50,50,53	0.30	0	56,58,61	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	PC1	Qb	502	-	47,47,53	0.31	0	53,55,61	0.39	0
81	PEE	N3	201	-	50,50,50	1.34	5 (10%)	53,55,55	1.18	5 (9%)
81	PEE	Qc	401	-	41,41,50	1.31	4 (9%)	44,46,55	1.20	4 (9%)
71	PC1	Qc	405	-	53,53,53	0.28	0	59,61,61	0.33	0
73	CDL	B5	202	-	99,99,99	0.30	0	105,111,111	0.27	0
73	CDL	CB	203	-	99,99,99	0.29	0	105,111,111	0.26	0
73	CDL	Qh	101	-	54,54,99	0.39	0	60,66,111	0.34	0
81	PEE	N6	201	-	50,50,50	1.35	5 (10%)	53,55,55	1.19	4 (7%)
85	SF4	V1	501	67	0,12,12	-	-	-	-	-
71	PC1	N4	503	-	47,47,53	0.31	0	53,55,61	0.33	0
82	HEM	QC	401	49	50,50,50	1.30	7 (14%)	67,82,82	1.60	10 (14%)
73	CDL	B4	201	-	79,79,99	0.32	0	85,91,111	0.31	0
71	PC1	S7	302	-	53,53,53	0.29	0	59,61,61	0.29	0
81	PEE	N4	501	-	45,45,50	1.41	5 (11%)	48,50,55	1.24	7 (14%)
73	CDL	AL	202	-	88,88,99	0.32	0	94,100,111	0.34	0
75	ZMP	AC	201	19	30,35,36	0.68	1 (3%)	34,42,45	0.75	0
71	PC1	N4	504	-	51,51,53	0.30	0	57,59,61	0.30	0
73	CDL	A8	301	-	82,82,99	0.32	0	88,94,111	0.36	0
73	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.38	0
77	3PE	CB	201	-	50,50,50	0.30	0	53,55,55	0.30	0
84	FES	S1	803	59	0,4,4	-	-	-	-	-
74	NDP	A9	401	-	51,52,52	0.31	0	71,80,80	0.35	0
72	PLX	QE	301	-	45,45,51	1.20	5 (11%)	47,53,59	0.90	1 (2%)
72	PLX	N4	502	-	51,51,51	1.15	4 (7%)	53,59,59	0.90	1 (1%)
81	PEE	Qe	302	-	43,43,50	1.41	5 (11%)	46,48,55	1.27	6 (13%)
73	CDL	N5	702	-	88,88,99	0.31	0	94,100,111	0.29	0
82	HEM	Qc	402	49	50,50,50	1.29	7 (14%)	67,82,82	1.61	10 (14%)
71	PC1	Qc	404	-	53,53,53	0.30	0	59,61,61	0.30	0
72	PLX	6C	101	-	30,30,51	1.36	4 (13%)	32,38,59	0.83	1 (3%)
71	PC1	Qj	101	-	42,42,53	0.32	0	48,50,61	0.32	0
77	3PE	N5	705	-	45,45,50	0.32	0	48,50,55	0.29	0
77	3PE	QE	303	-	42,42,50	0.32	0	45,47,55	0.36	0
83	HEC	Qd	401	50	46,50,50	1.92	10 (21%)	58,82,82	1.82	6 (10%)
71	PC1	Qh	102	-	53,53,53	0.29	0	59,61,61	0.30	0
83	HEC	QD	401	50	46,50,50	1.91	9 (19%)	58,82,82	1.85	8 (13%)
86	FMN	V1	502	-	33,33,33	0.21	0	48,50,50	0.40	0
73	CDL	QH	101	-	60,60,99	0.37	0	66,72,111	0.33	0
71	PC1	B5	203	-	53,53,53	0.28	0	59,61,61	0.29	0
77	3PE	QC	404	-	33,33,50	0.36	0	36,38,55	0.34	0
81	PEE	S2	501	-	47,47,50	1.38	5 (10%)	50,52,55	1.18	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	HEM	Qc	403	49	50,50,50	1.30	5 (10%)	67,82,82	1.60	13 (19%)
85	SF4	S1	802	59	0,12,12	-	-	-	-	-
71	PC1	C3	302	-	49,49,53	0.30	0	55,57,61	0.31	0
84	FES	V2	301	68	0,4,4	-	-	-	-	-
85	SF4	S8	302	66	0,12,12	-	-	-	-	-
75	ZMP	AB	201	19	30,35,36	0.69	1 (3%)	34,42,45	0.74	1 (2%)
81	PEE	S8	303	-	50,50,50	1.34	5 (10%)	53,55,55	1.17	5 (9%)
77	3PE	B8	201	-	31,31,50	0.37	0	34,36,55	0.35	0
81	PEE	QC	403	-	39,39,50	1.35	4 (10%)	42,44,55	1.14	3 (7%)
76	ADP	AK	401	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)

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
71	PC1	6A	101	-	-	9/48/48/57	-
72	PLX	B5	201	-	-	20/55/55/55	-
72	PLX	QI	301	-	-	21/55/55/55	-
72	PLX	AM	201	-	-	23/55/55/55	-
81	PEE	QE	302	-	-	16/50/50/54	-
71	PC1	C3	301	-	-	12/52/52/57	-
81	PEE	N5	701	-	-	20/49/49/54	-
73	CDL	N2	402	-	-	19/78/78/110	-
81	PEE	N5	704	-	-	25/54/54/54	-
84	FES	Qe	301	51	-	-	0/1/1/1
71	PC1	CB	202	-	-	5/57/57/57	-
73	CDL	QH	102	-	-	17/74/74/110	-
72	PLX	N2	401	-	-	27/55/55/55	-
73	CDL	QD	402	-	-	13/74/74/110	-
71	PC1	N1	402	-	-	12/51/51/57	-
73	CDL	QB	501	-	-	16/72/72/110	-
85	SF4	S1	801	59	-	-	0/6/5/5
78	HEA	C1	602	35	-	13/36/76/76	-
84	FES	QE	304	51	-	-	0/1/1/1
71	PC1	QB	503	-	-	9/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PC1	B4	202	-	-	10/53/53/57	-
78	HEA	C1	603	35	-	12/36/76/76	-
73	CDL	N1	401	-	-	15/88/88/110	-
77	3PE	C1	601	-	-	14/54/54/54	-
85	SF4	S7	301	65	-	-	0/6/5/5
85	SF4	S8	301	66	-	-	0/6/5/5
73	CDL	N5	703	-	-	24/110/110/110	-
73	CDL	AL	201	-	-	17/101/101/110	-
82	HEM	QC	402	49	-	8/14/54/54	-
71	PC1	QB	502	-	-	16/54/54/57	-
71	PC1	Qb	502	-	-	11/51/51/57	-
81	PEE	N3	201	-	-	28/54/54/54	-
81	PEE	Qc	401	-	-	24/45/45/54	-
71	PC1	Qc	405	-	-	10/57/57/57	-
73	CDL	B5	202	-	-	18/110/110/110	-
73	CDL	CB	203	-	-	20/110/110/110	-
73	CDL	Qh	101	-	-	5/65/65/110	-
81	PEE	N6	201	-	-	22/54/54/54	-
85	SF4	V1	501	67	-	-	0/6/5/5
71	PC1	N4	503	-	-	24/51/51/57	-
82	HEM	QC	401	49	-	7/14/54/54	-
73	CDL	B4	201	-	-	16/90/90/110	-
71	PC1	S7	302	-	-	8/57/57/57	-
81	PEE	N4	501	-	-	25/49/49/54	-
73	CDL	AL	202	-	-	16/99/99/110	-
75	ZMP	AC	201	19	-	16/40/42/43	-
71	PC1	N4	504	-	-	5/55/55/57	-
73	CDL	A8	301	-	-	20/93/93/110	-
73	CDL	Qb	501	-	-	20/74/74/110	-
77	3PE	CB	201	-	-	15/54/54/54	-
84	FES	S1	803	59	-	-	0/1/1/1
74	NDP	A9	401	-	-	6/34/77/77	0/5/5/5
72	PLX	QE	301	-	-	23/49/49/55	-
72	PLX	N4	502	-	-	19/55/55/55	-
81	PEE	Qe	302	-	-	21/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	CDL	N5	702	-	-	24/99/99/110	-
82	HEM	Qc	402	49	-	7/14/54/54	-
71	PC1	Qc	404	-	-	11/57/57/57	-
72	PLX	6C	101	-	-	15/34/34/55	-
71	PC1	Qj	101	-	-	14/46/46/57	-
77	3PE	N5	705	-	-	11/49/49/54	-
77	3PE	QE	303	-	-	9/46/46/54	-
83	HEC	Qd	401	50	-	7/14/54/54	-
71	PC1	Qh	102	-	-	11/57/57/57	-
83	HEC	QD	401	50	-	6/14/54/54	-
86	FMN	V1	502	-	-	6/18/18/18	0/3/3/3
73	CDL	QH	101	-	-	13/71/71/110	-
71	PC1	B5	203	-	-	14/57/57/57	-
77	3PE	QC	404	-	-	3/37/37/54	-
81	PEE	S2	501	-	-	30/51/51/54	-
82	HEM	Qc	403	49	-	10/14/54/54	-
85	SF4	S1	802	59	-	-	0/6/5/5
71	PC1	C3	302	-	-	13/53/53/57	-
84	FES	V2	301	68	-	-	0/1/1/1
85	SF4	S8	302	66	-	-	0/6/5/5
75	ZMP	AB	201	19	-	22/40/42/43	-
81	PEE	S8	303	-	-	25/54/54/54	-
77	3PE	B8	201	-	-	5/35/35/54	-
81	PEE	QC	403	-	-	18/43/43/54	-
76	ADP	AK	401	-	-	0/16/32/32	0/3/3/3

The worst 5 of 185 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	Qd	401	HEC	CAC-C3C	7.15	1.58	1.35
83	QD	401	HEC	CAC-C3C	7.11	1.58	1.35
83	Qd	401	HEC	CAB-C3B	6.76	1.56	1.35
83	QD	401	HEC	CAB-C3B	6.72	1.56	1.35
78	C1	602	HEA	C3B-C2B	5.38	1.47	1.34

The worst 5 of 191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	Qd	401	HEC	CBB-CAB-C3B	-8.72	110.01	127.43
83	QD	401	HEC	CBB-CAB-C3B	-8.56	110.32	127.43
78	C1	602	HEA	CAD-CBD-CGD	-7.46	93.88	113.67
78	C1	603	HEA	CAD-CBD-CGD	-6.94	95.25	113.67
83	QD	401	HEC	CBC-CAC-C3C	-6.91	113.63	127.43

There are no chirality outliers.

5 of 1046 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
71	6A	101	PC1	C11-O13-P-O12
71	6A	101	PC1	C11-O13-P-O11
71	6A	101	PC1	C1-O11-P-O12
71	6A	101	PC1	C1-O11-P-O13
71	6A	101	PC1	C12-C11-O13-P

There are no ring outliers.

67 monomers are involved in 251 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	6A	101	PC1	10	0
72	B5	201	PLX	1	0
72	QI	301	PLX	4	0
72	AM	201	PLX	4	0
81	QE	302	PEE	2	0
71	C3	301	PC1	13	0
81	N5	701	PEE	7	0
73	N2	402	CDL	1	0
81	N5	704	PEE	1	0
84	Qe	301	FES	2	0
73	QH	102	CDL	3	0
72	N2	401	PLX	4	0
71	N1	402	PC1	5	0
73	QB	501	CDL	3	0
78	C1	602	HEA	16	0
71	QB	503	PC1	4	0
71	B4	202	PC1	4	0
78	C1	603	HEA	7	0
73	N1	401	CDL	5	0
77	C1	601	3PE	8	0
85	S7	301	SF4	1	0
73	N5	703	CDL	5	0

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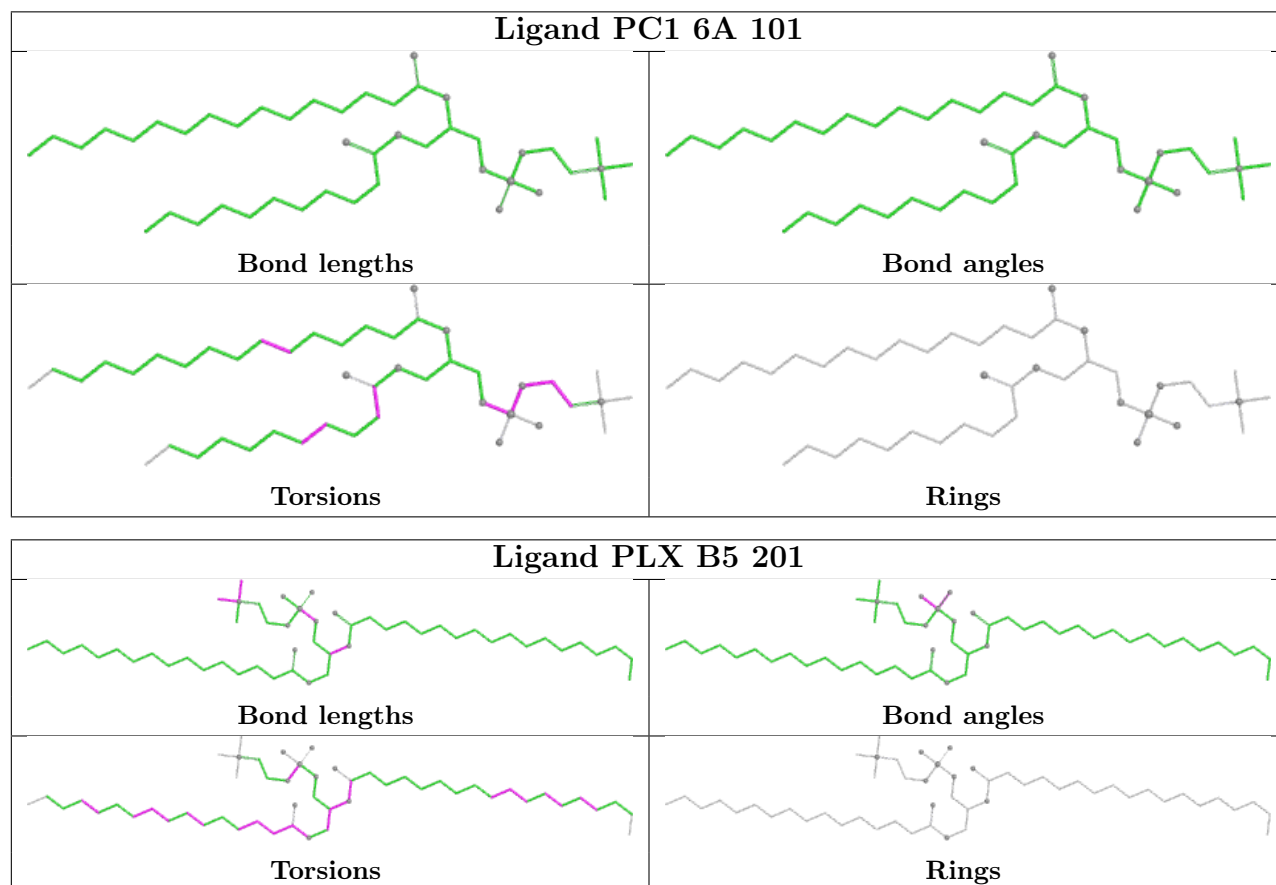
Mol	Chain	Res	Type	Clashes	Symm-Clashes
73	AL	201	CDL	1	0
82	QC	402	HEM	6	0
71	QB	502	PC1	2	0
71	Qb	502	PC1	2	0
81	N3	201	PEE	3	0
81	Qc	401	PEE	4	0
71	Qc	405	PC1	2	0
73	B5	202	CDL	8	0
73	CB	203	CDL	10	0
73	Qh	101	CDL	1	0
81	N6	201	PEE	1	0
71	N4	503	PC1	5	0
82	QC	401	HEM	2	0
73	B4	201	CDL	4	0
71	S7	302	PC1	2	0
81	N4	501	PEE	2	0
73	AL	202	CDL	4	0
75	AC	201	ZMP	4	0
71	N4	504	PC1	3	0
73	A8	301	CDL	6	0
73	Qb	501	CDL	3	0
77	CB	201	3PE	4	0
72	QE	301	PLX	6	0
72	N4	502	PLX	3	0
81	Qe	302	PEE	4	0
73	N5	702	CDL	10	0
82	Qc	402	HEM	2	0
71	Qc	404	PC1	3	0
72	6C	101	PLX	3	0
77	QE	303	3PE	3	0
83	Qd	401	HEC	3	0
71	Qh	102	PC1	1	0
83	QD	401	HEC	1	0
86	V1	502	FMN	4	0
73	QH	101	CDL	2	0
71	B5	203	PC1	1	0
77	QC	404	3PE	1	0
81	S2	501	PEE	3	0
82	Qc	403	HEM	6	0
71	C3	302	PC1	12	0
85	S8	302	SF4	1	0
75	AB	201	ZMP	2	0

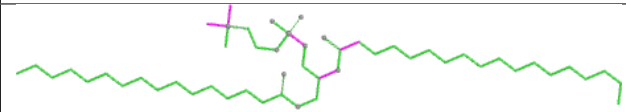
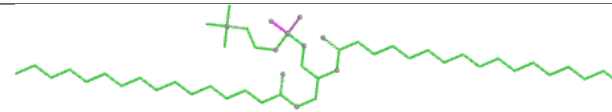
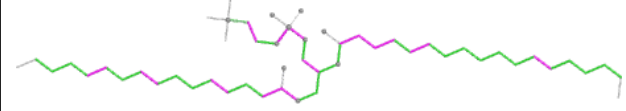
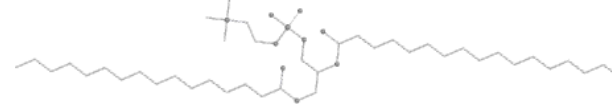
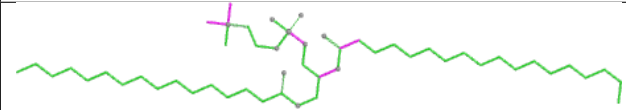
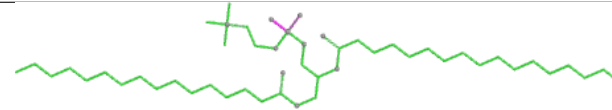
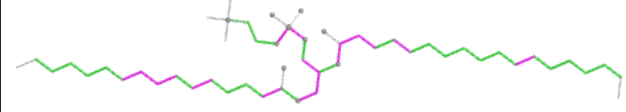
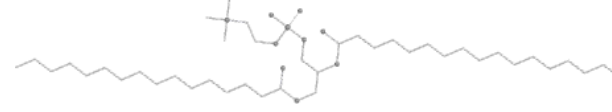
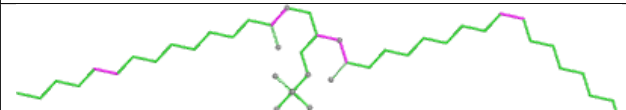
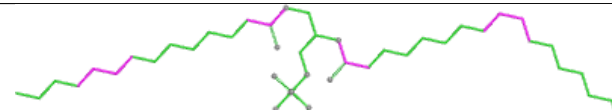
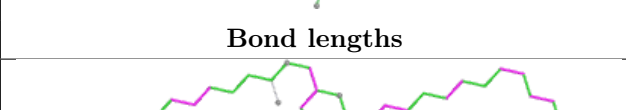
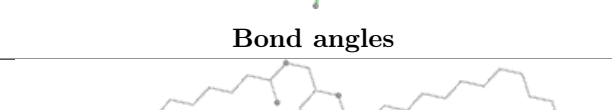
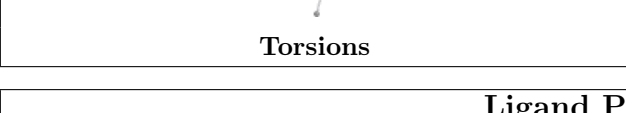
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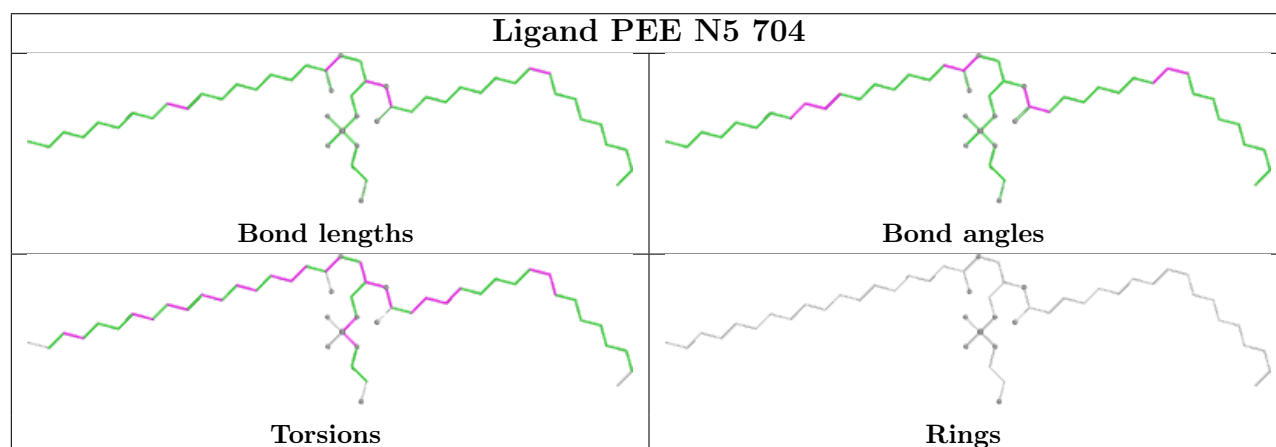
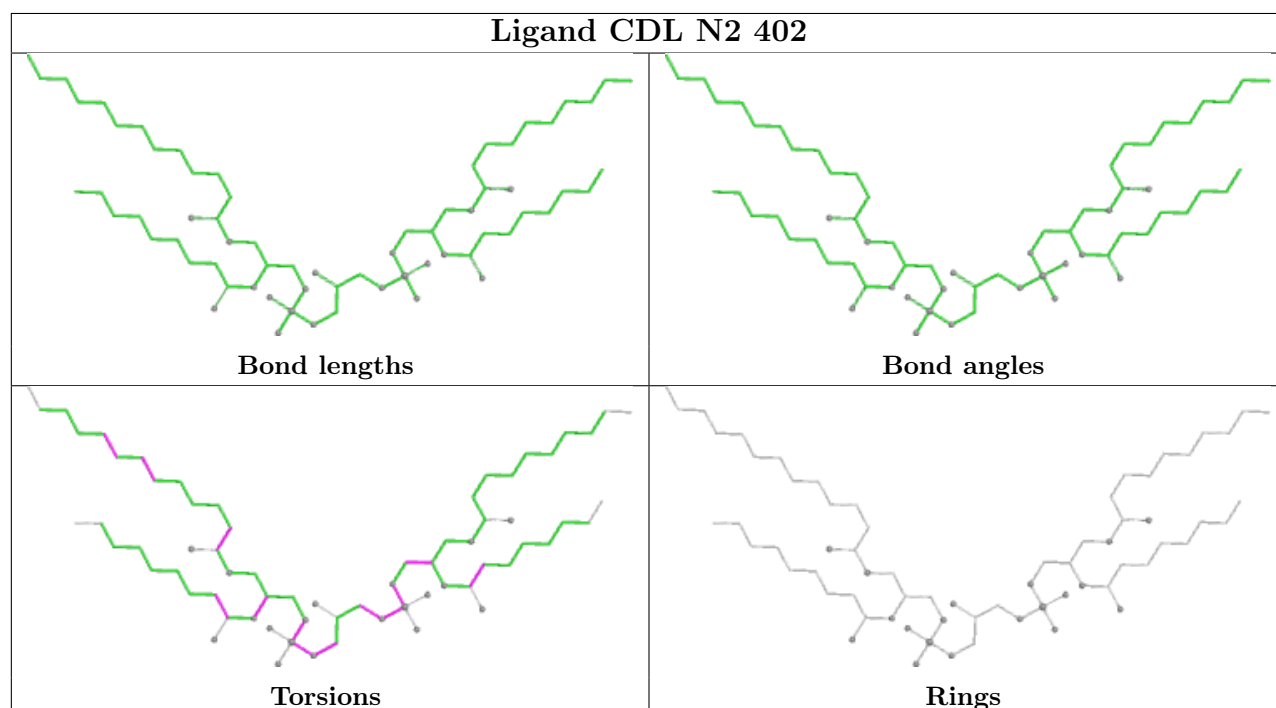
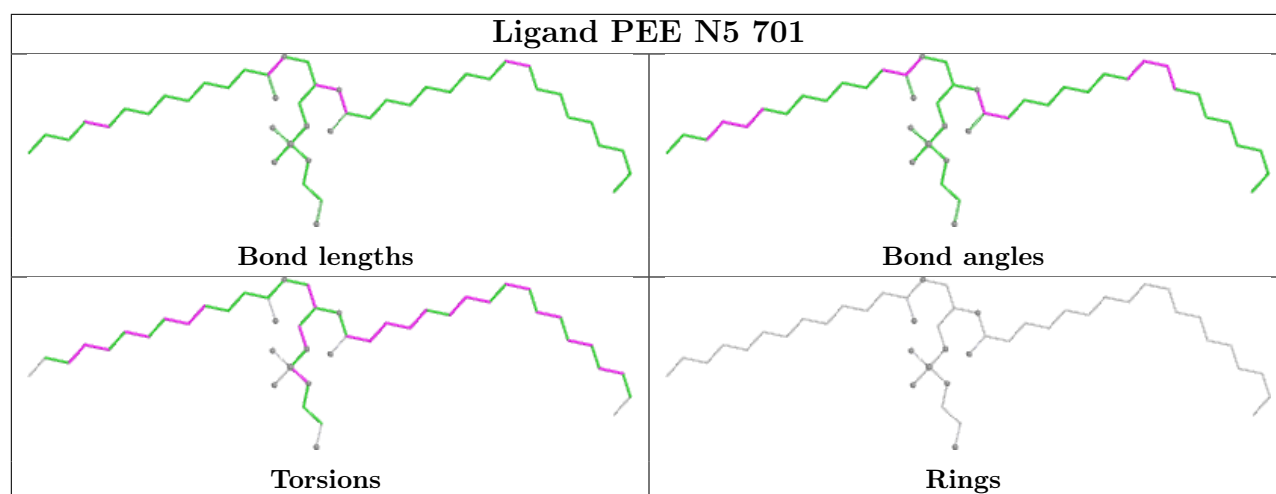
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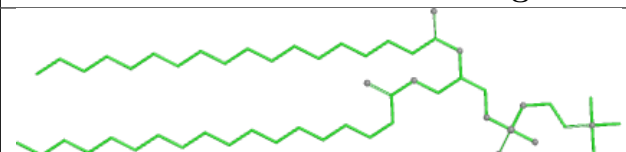
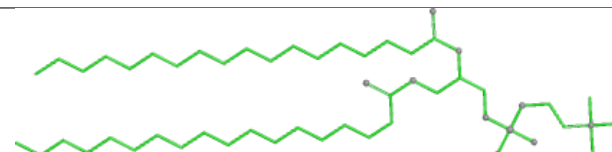
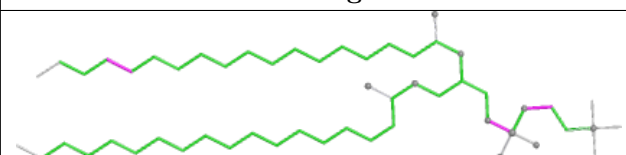
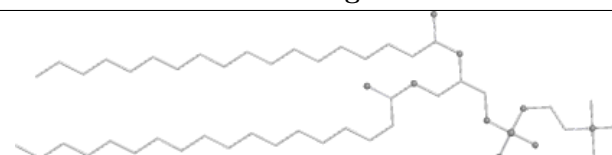
Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	S8	303	PEE	2	0
81	QC	403	PEE	2	0
76	AK	401	ADP	4	0

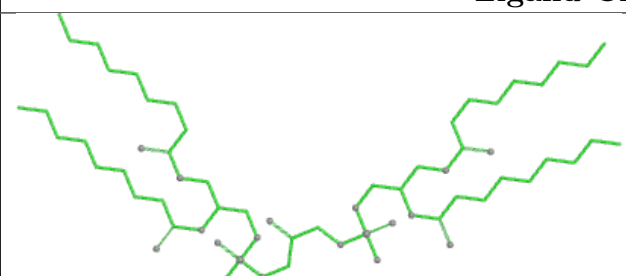
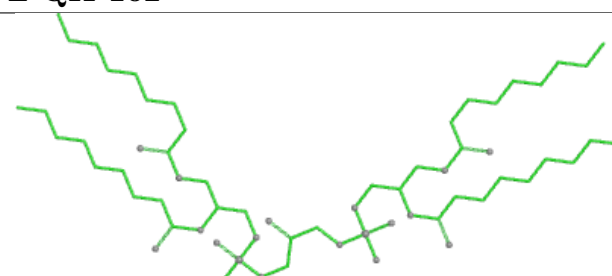
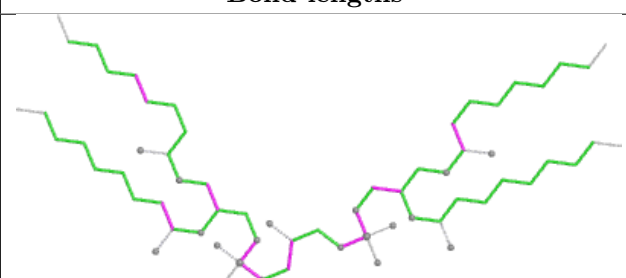
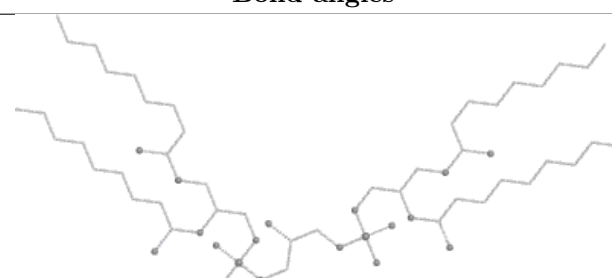
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

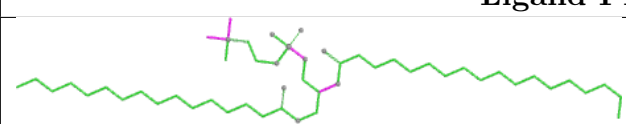
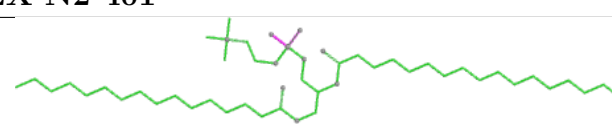
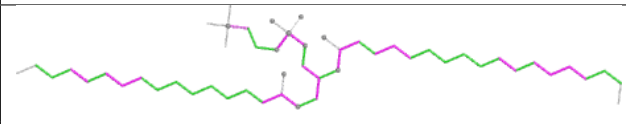
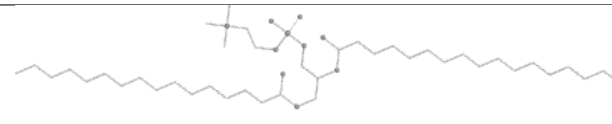


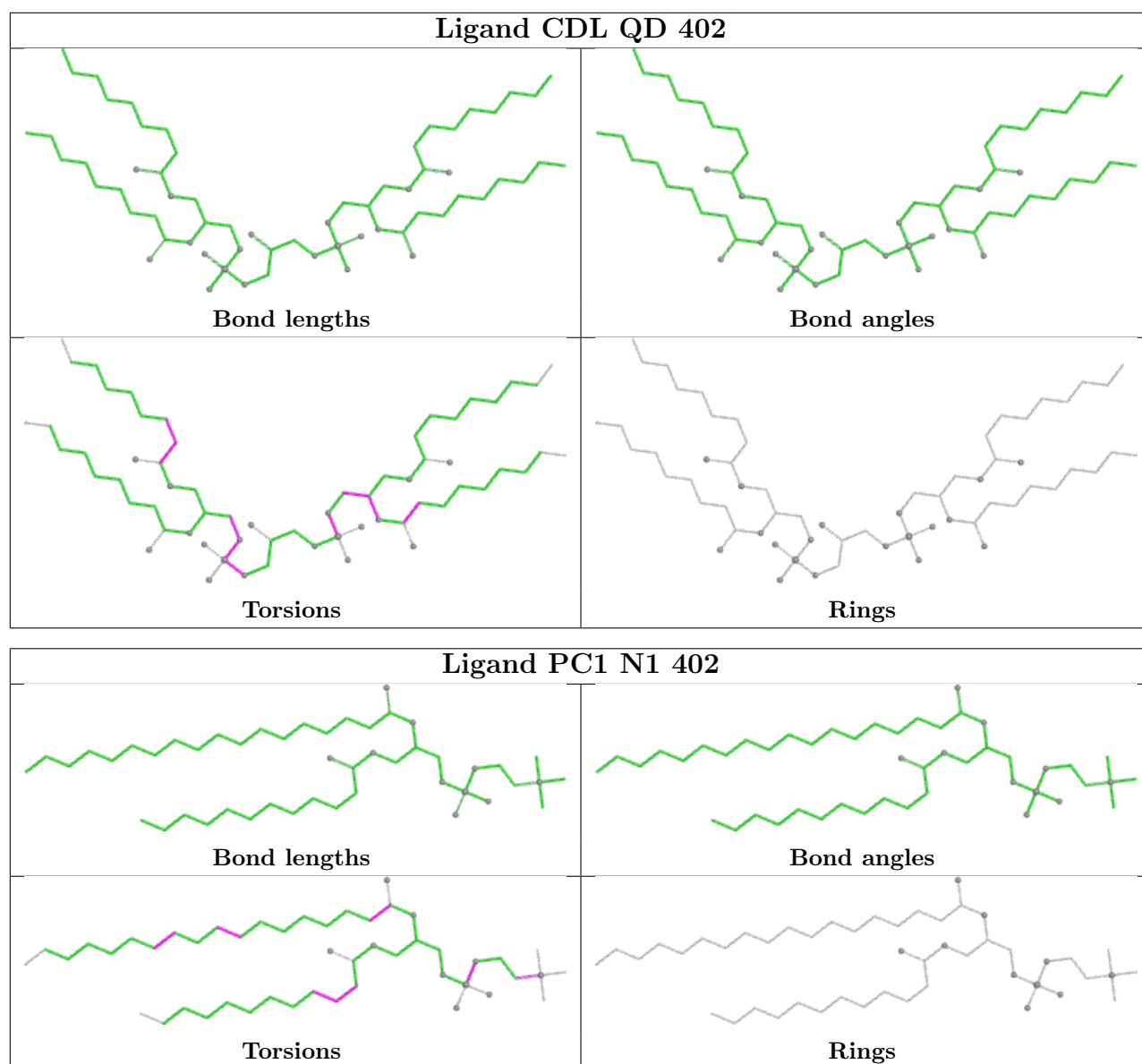
Ligand PLX QI 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX AM 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE QE 302	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 C3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

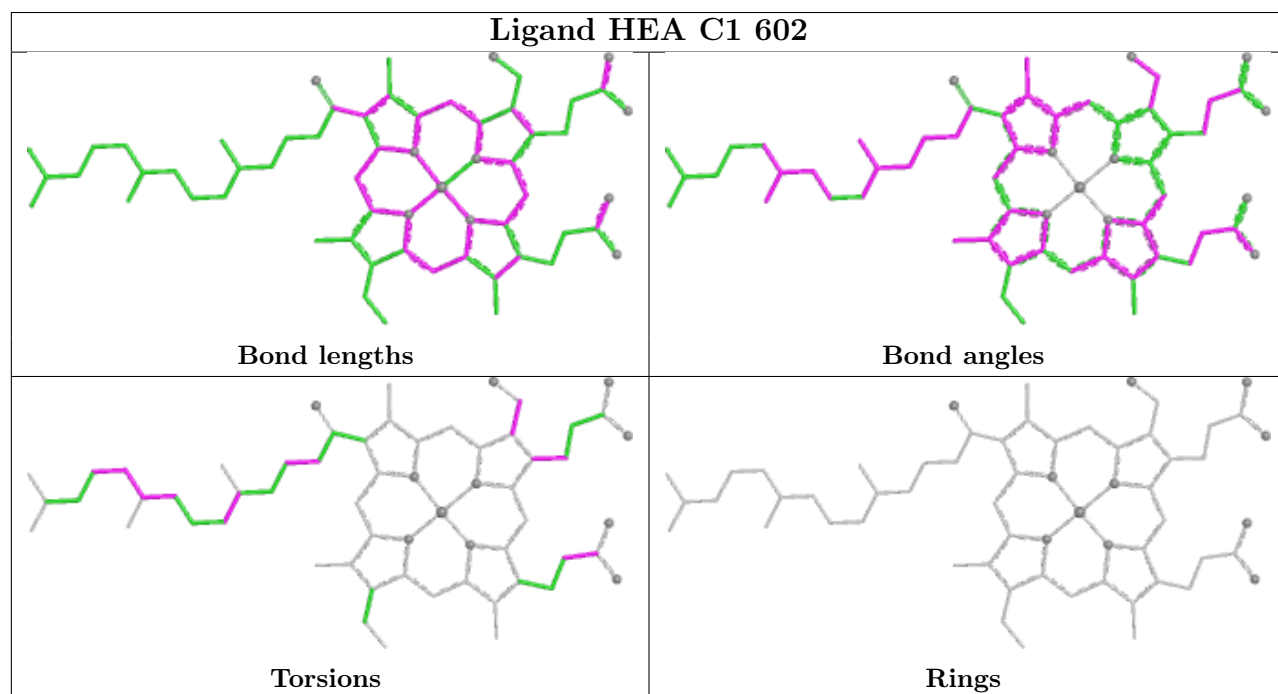
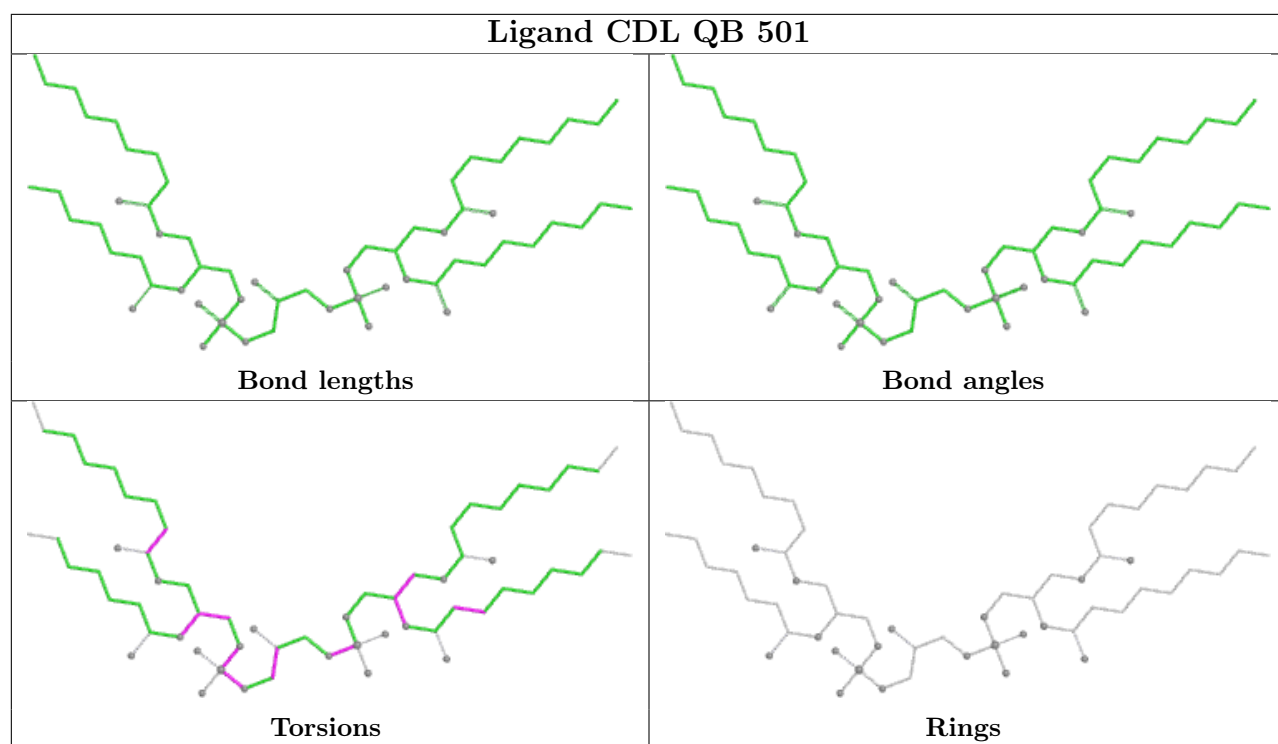


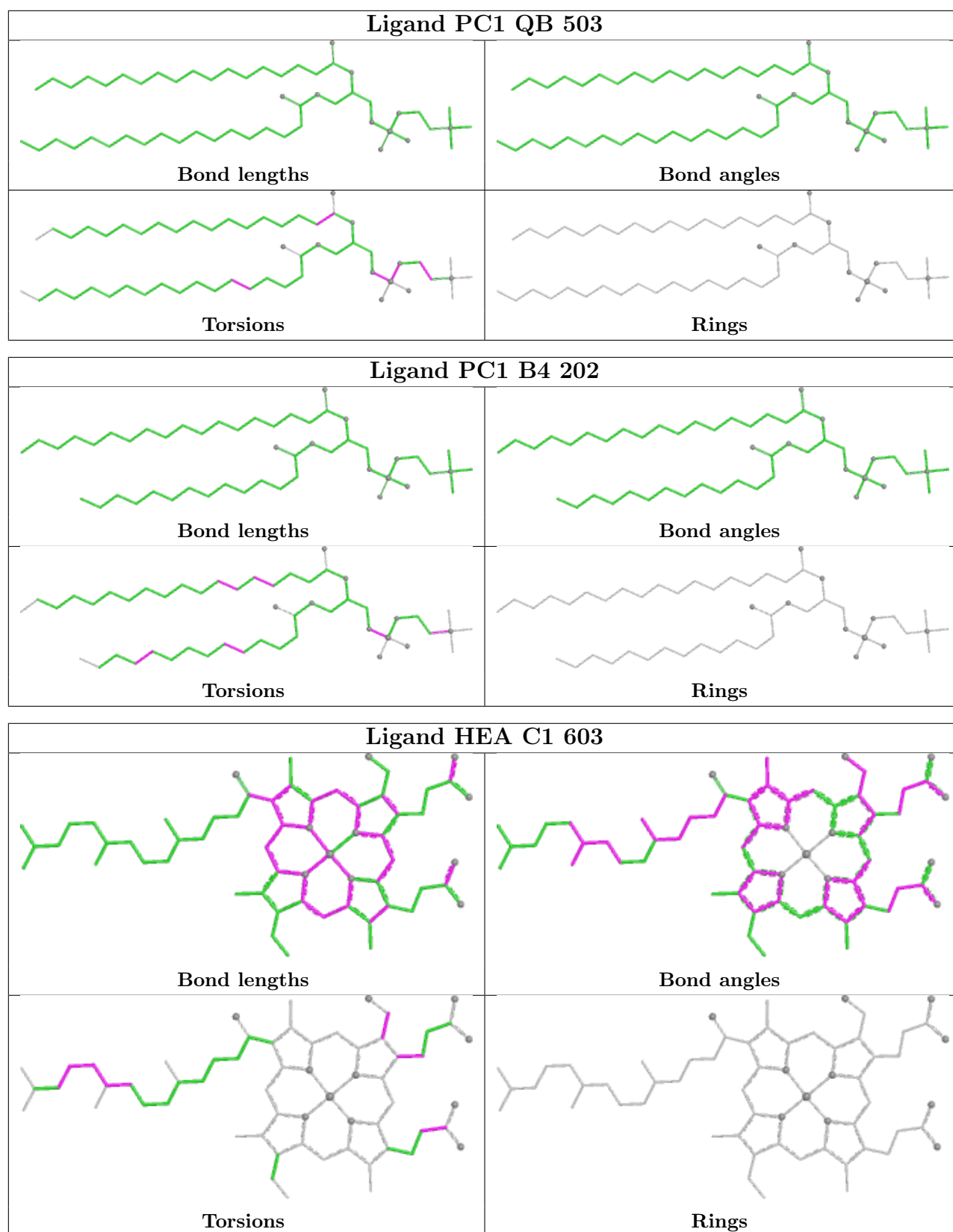
Ligand PC1 CB 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

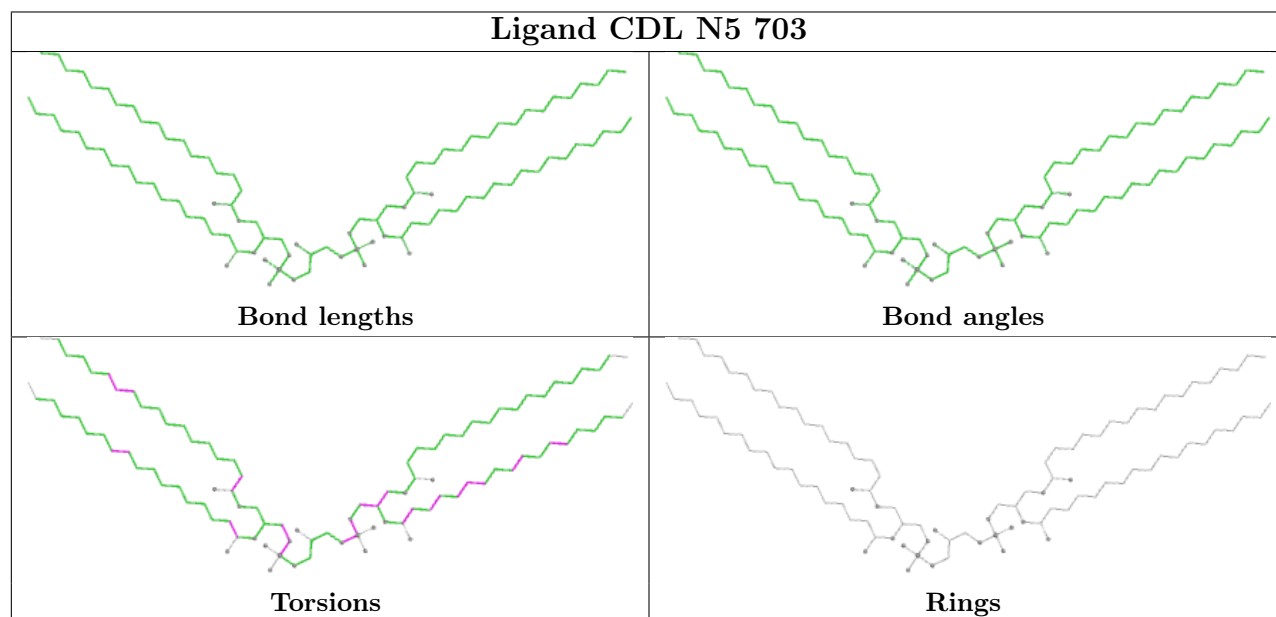
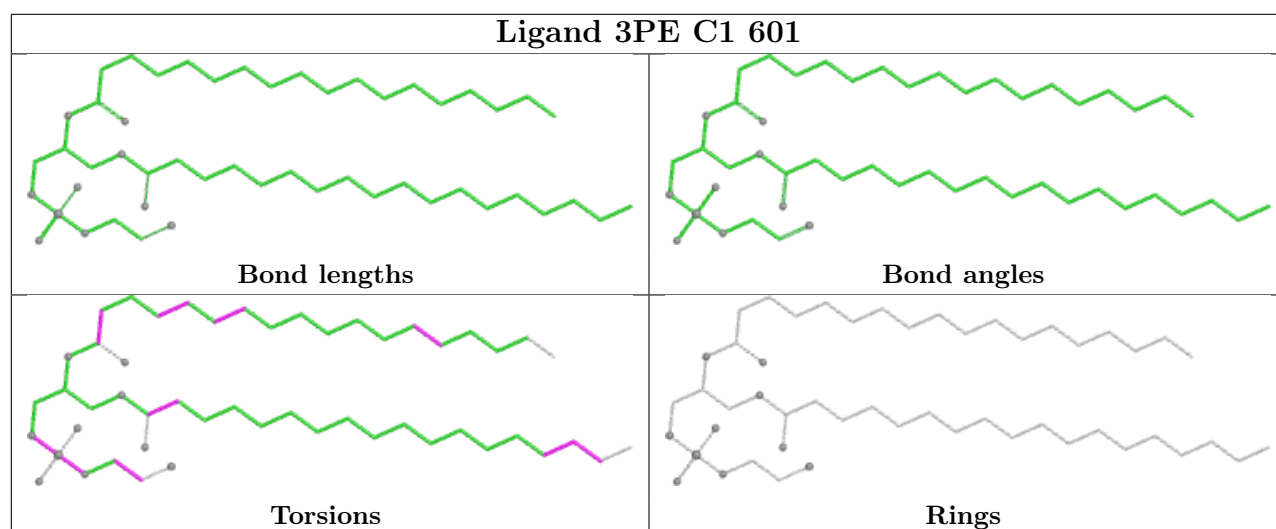
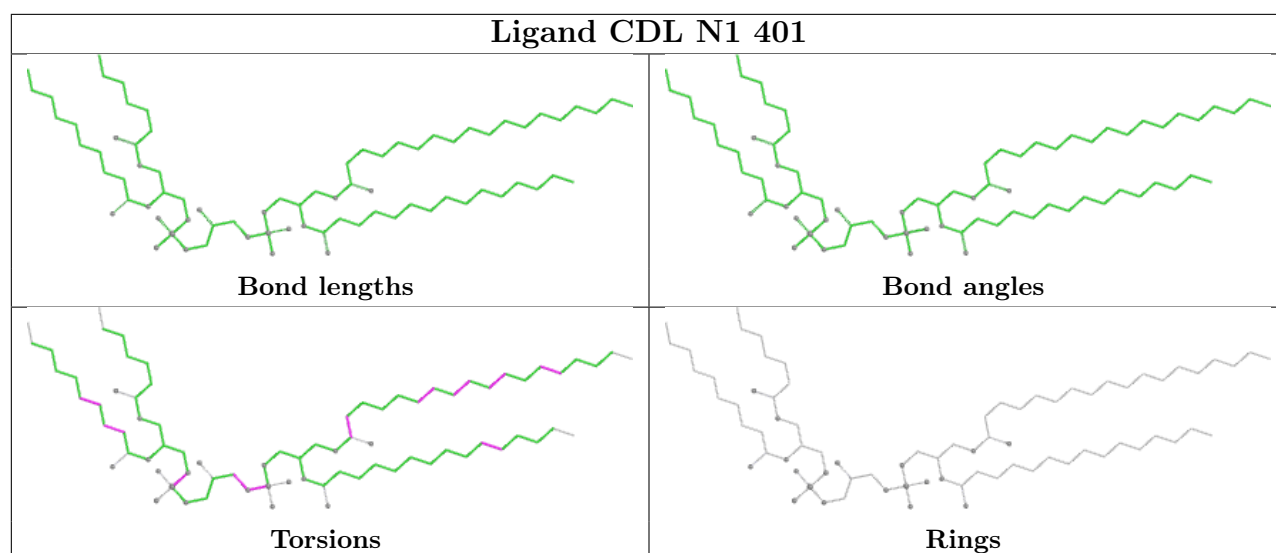
Ligand CDL QH 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

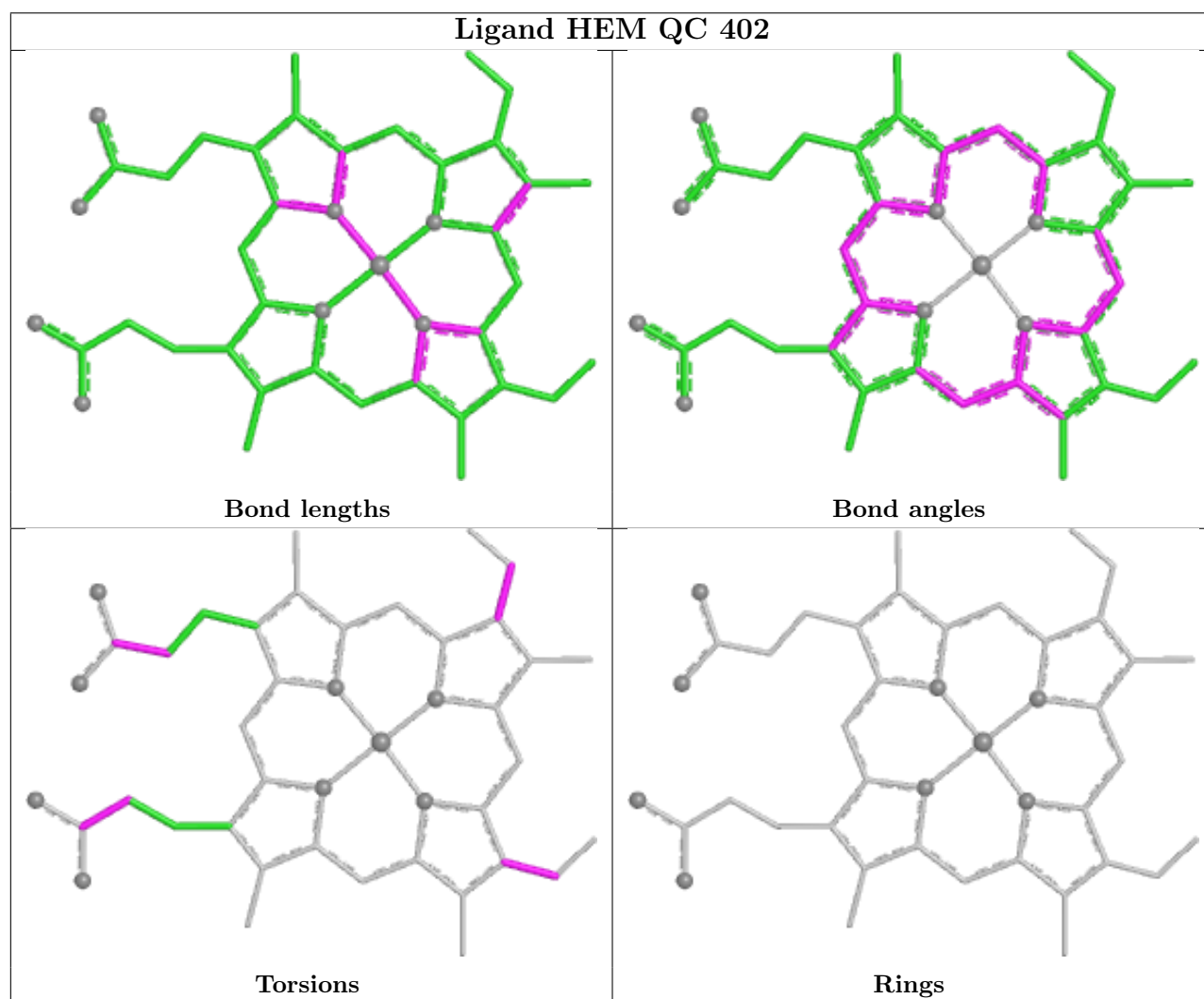
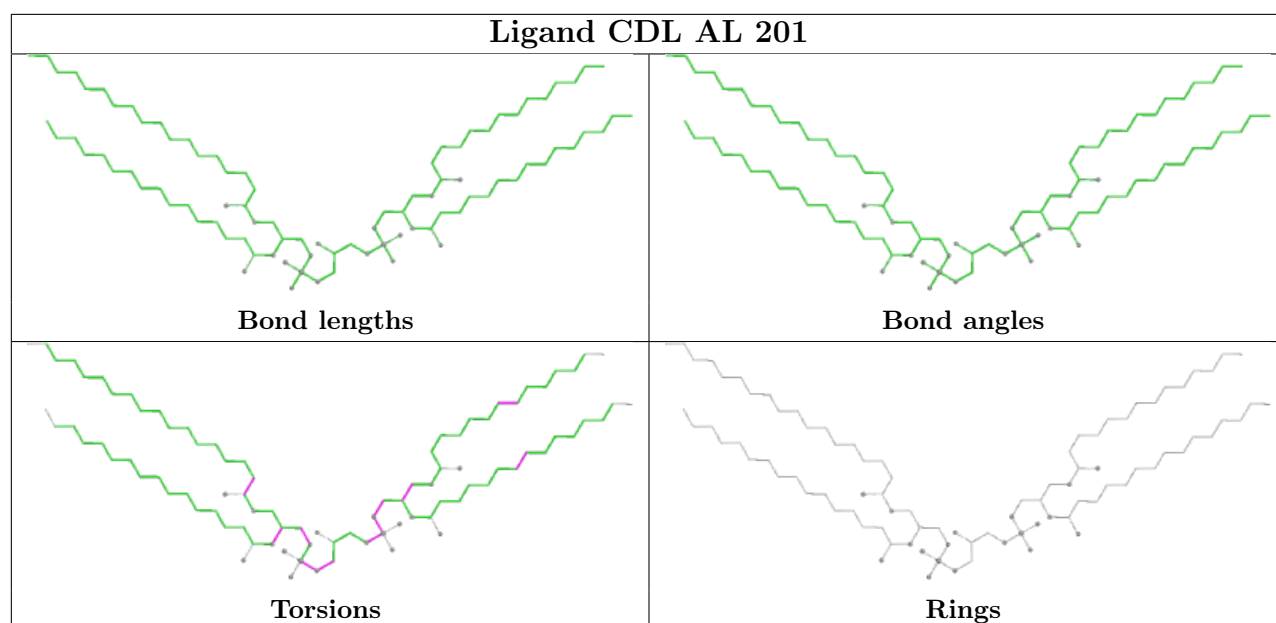
Ligand PLX N2 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

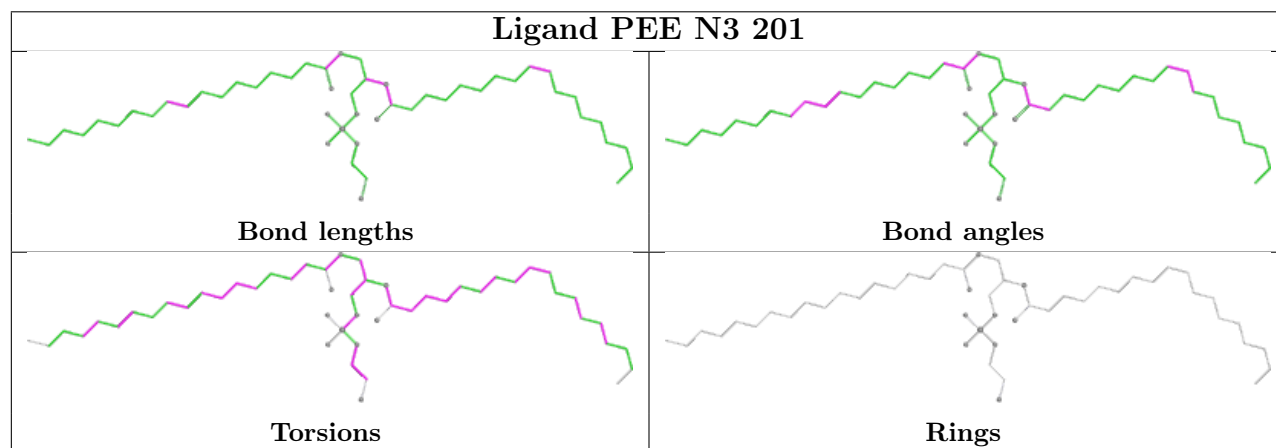
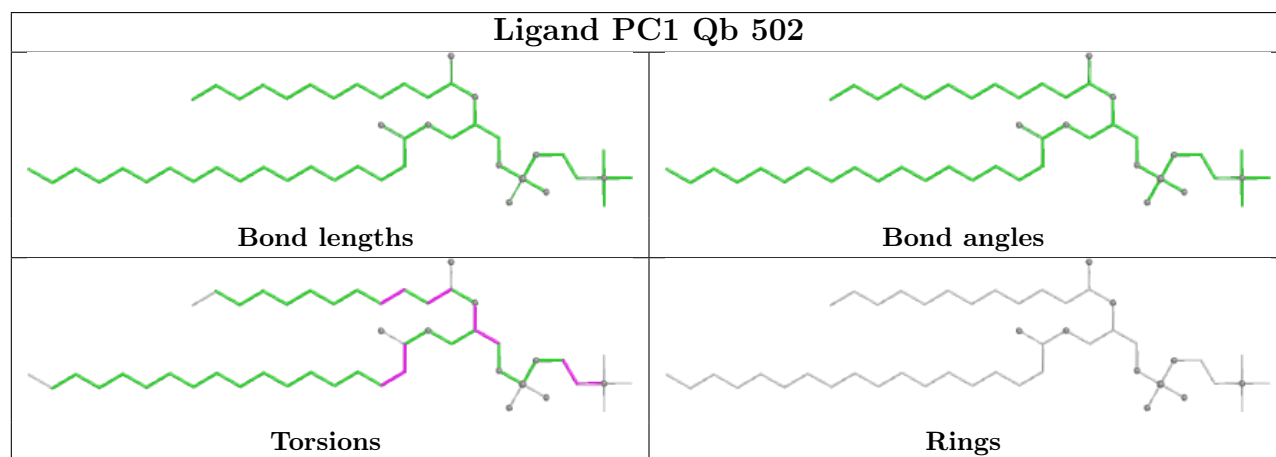
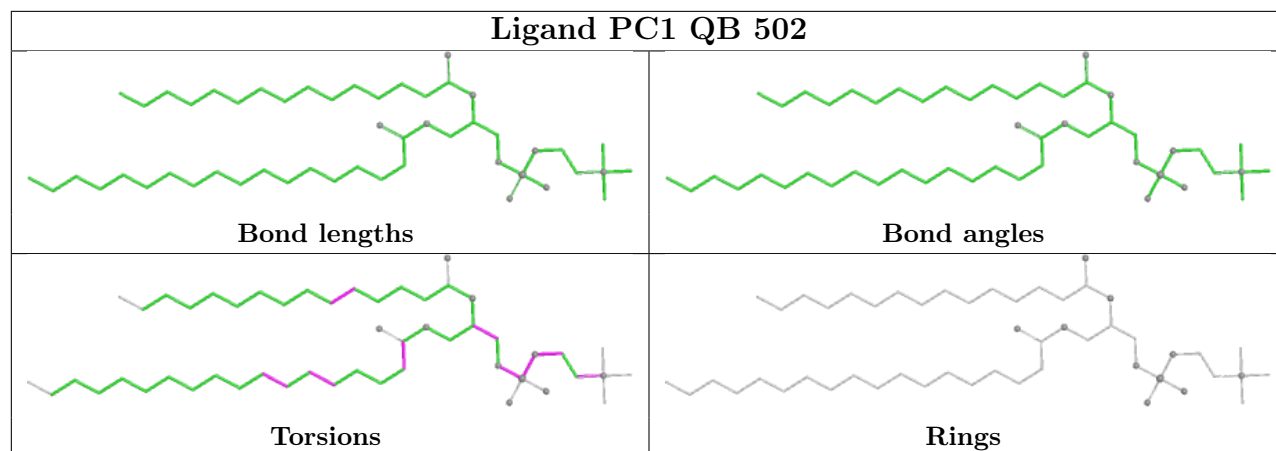


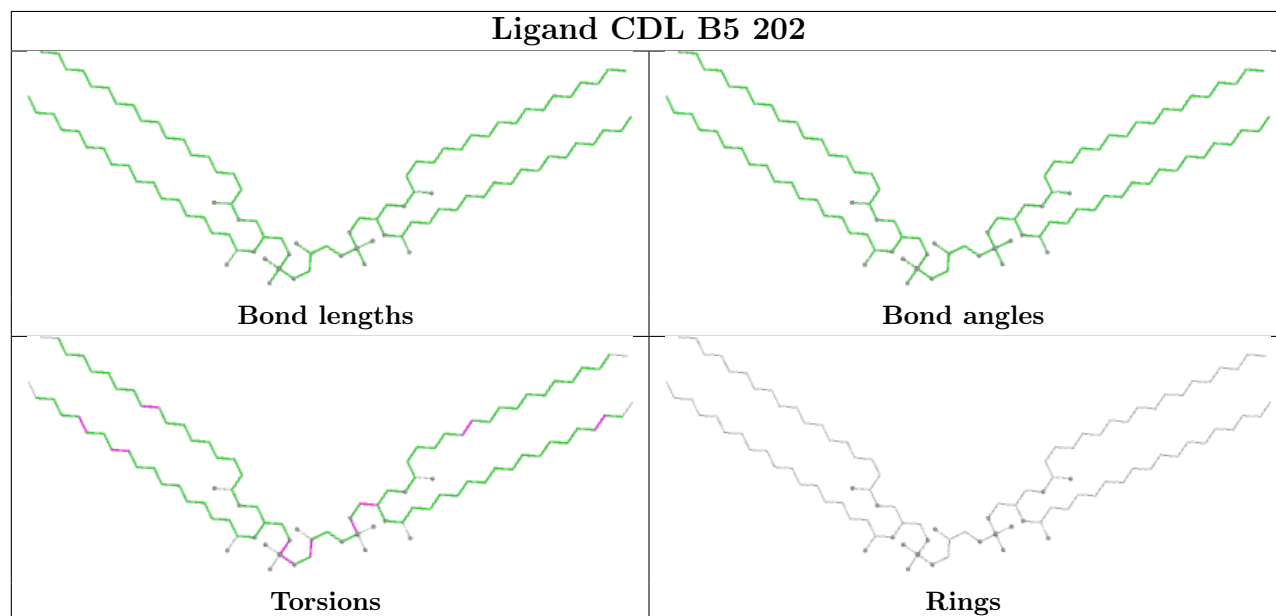
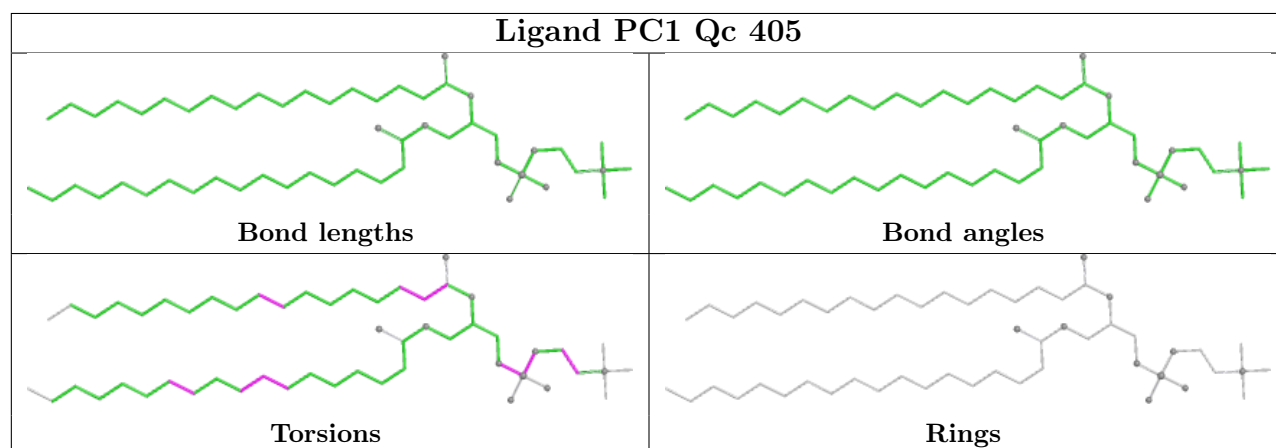
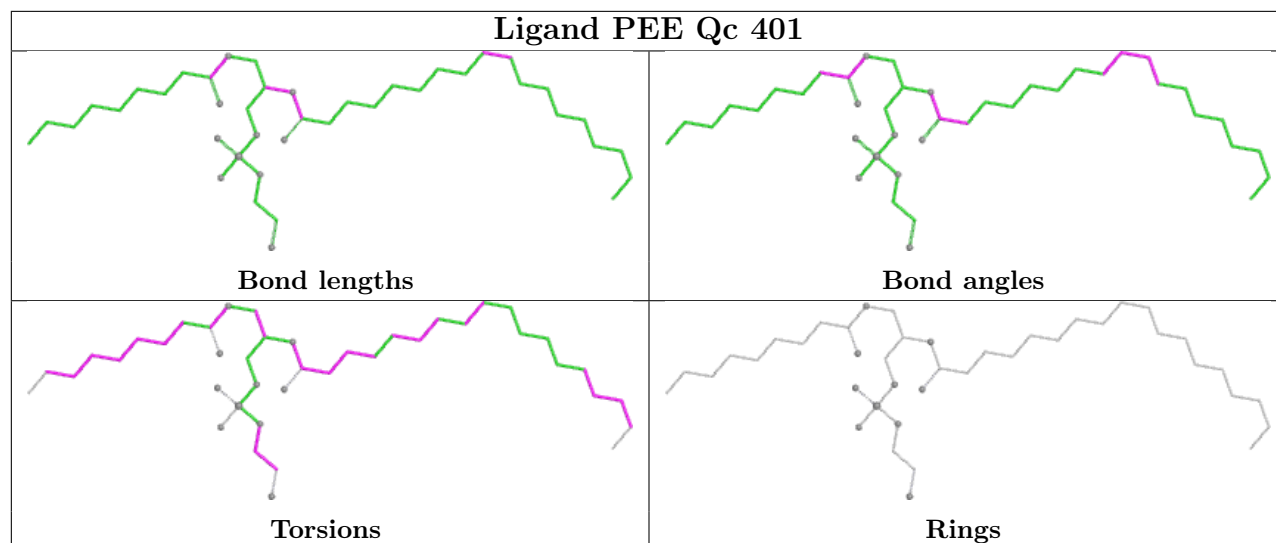


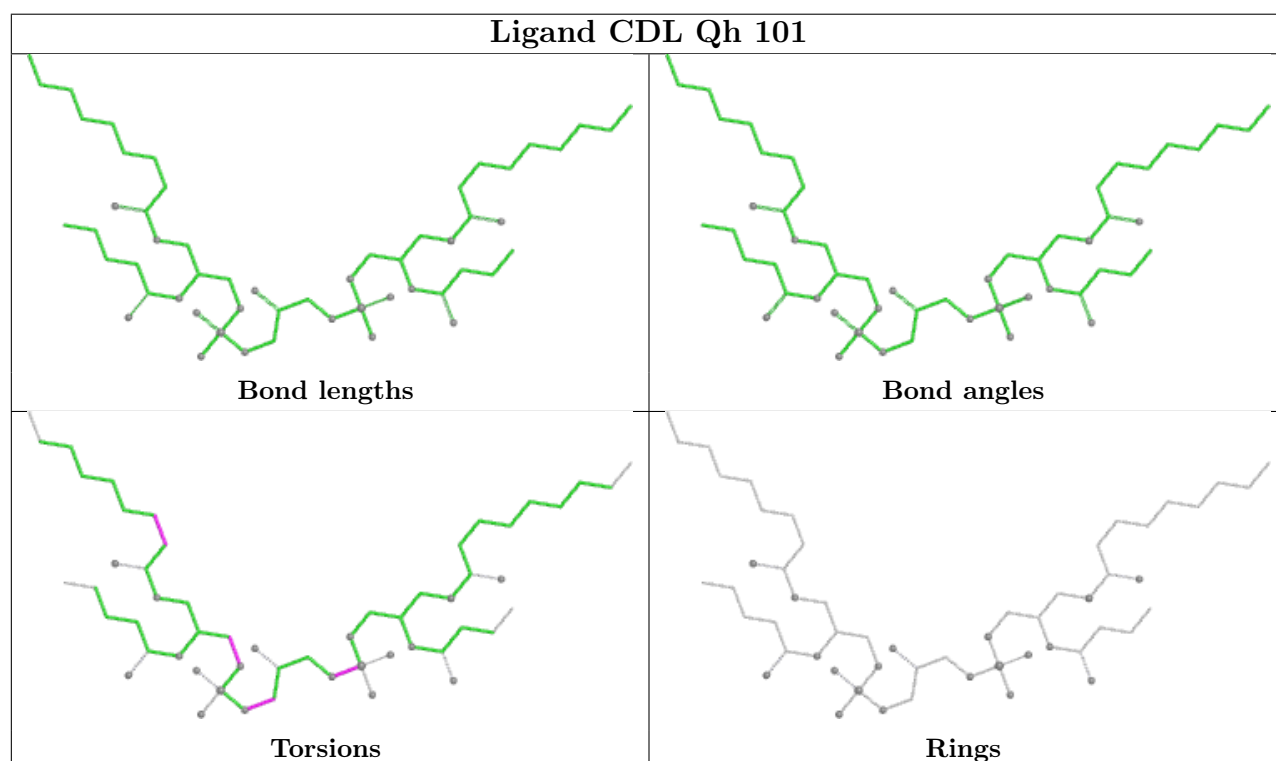
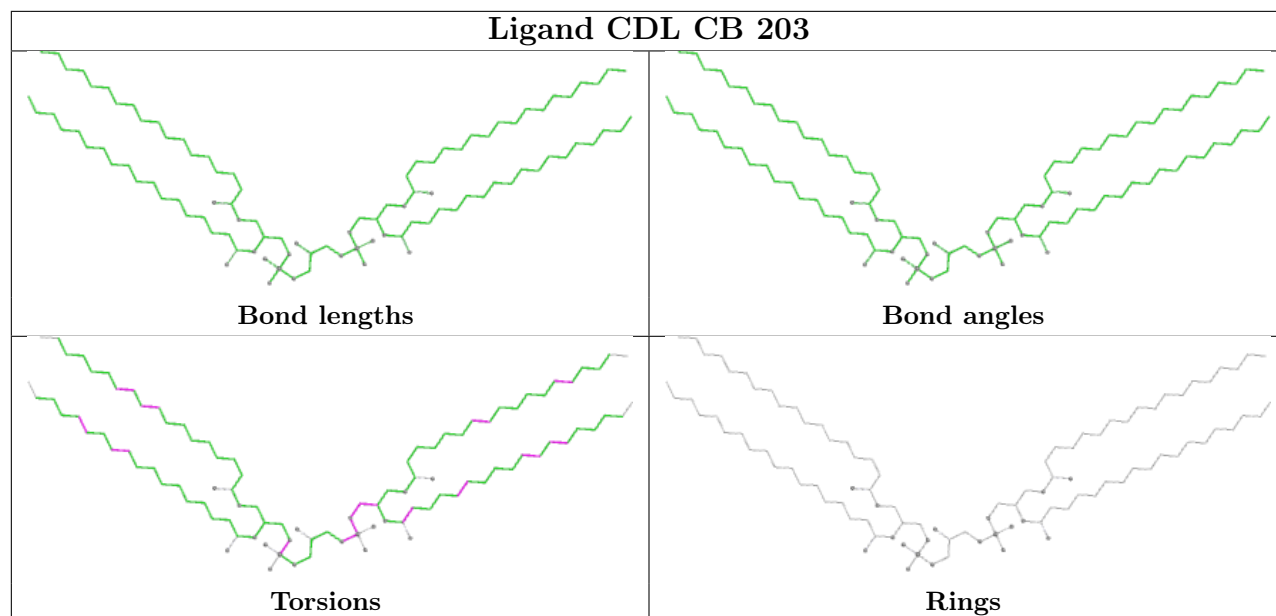


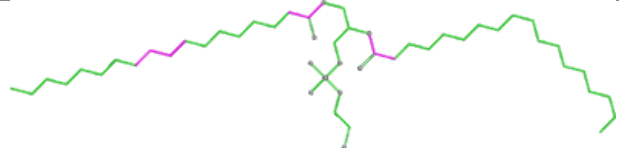
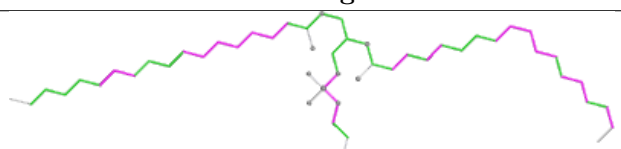
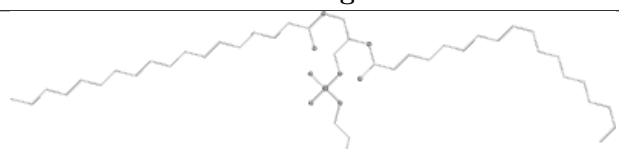
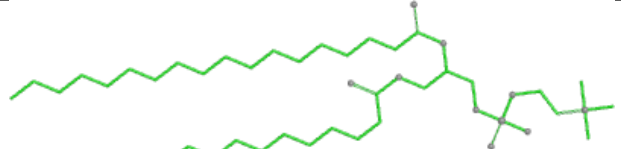
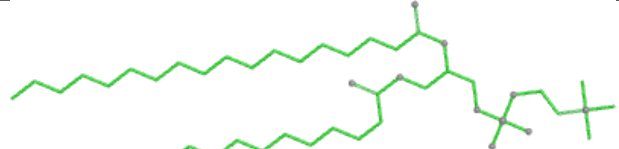
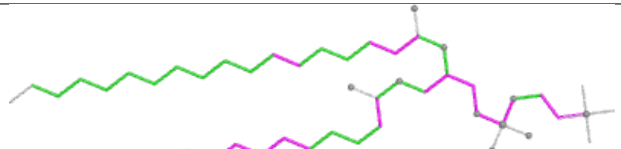
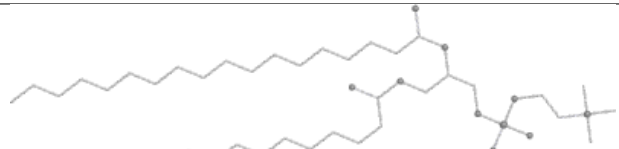




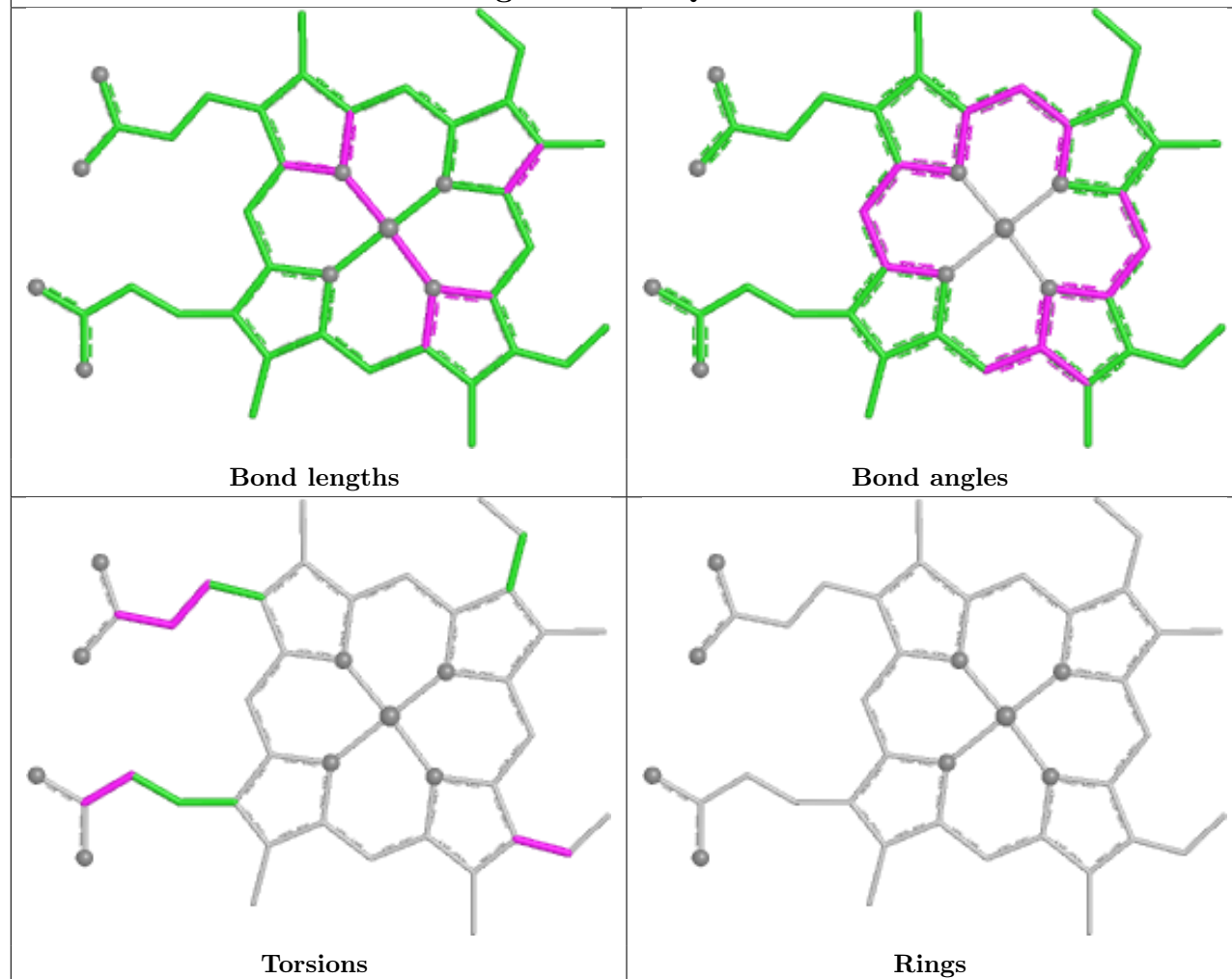




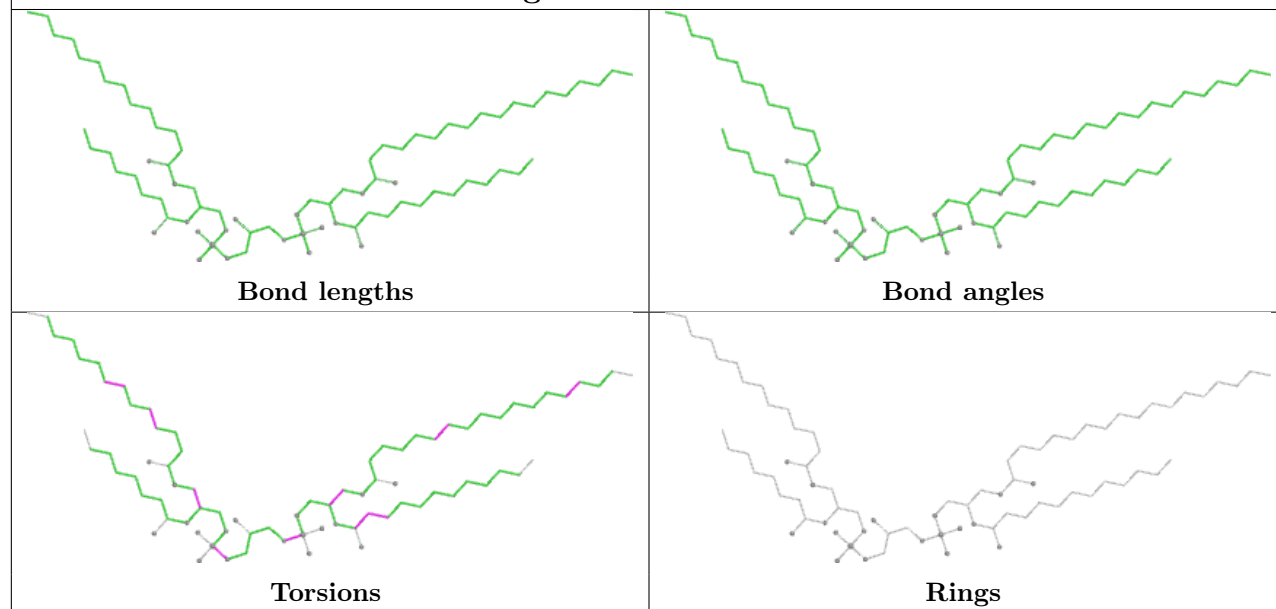


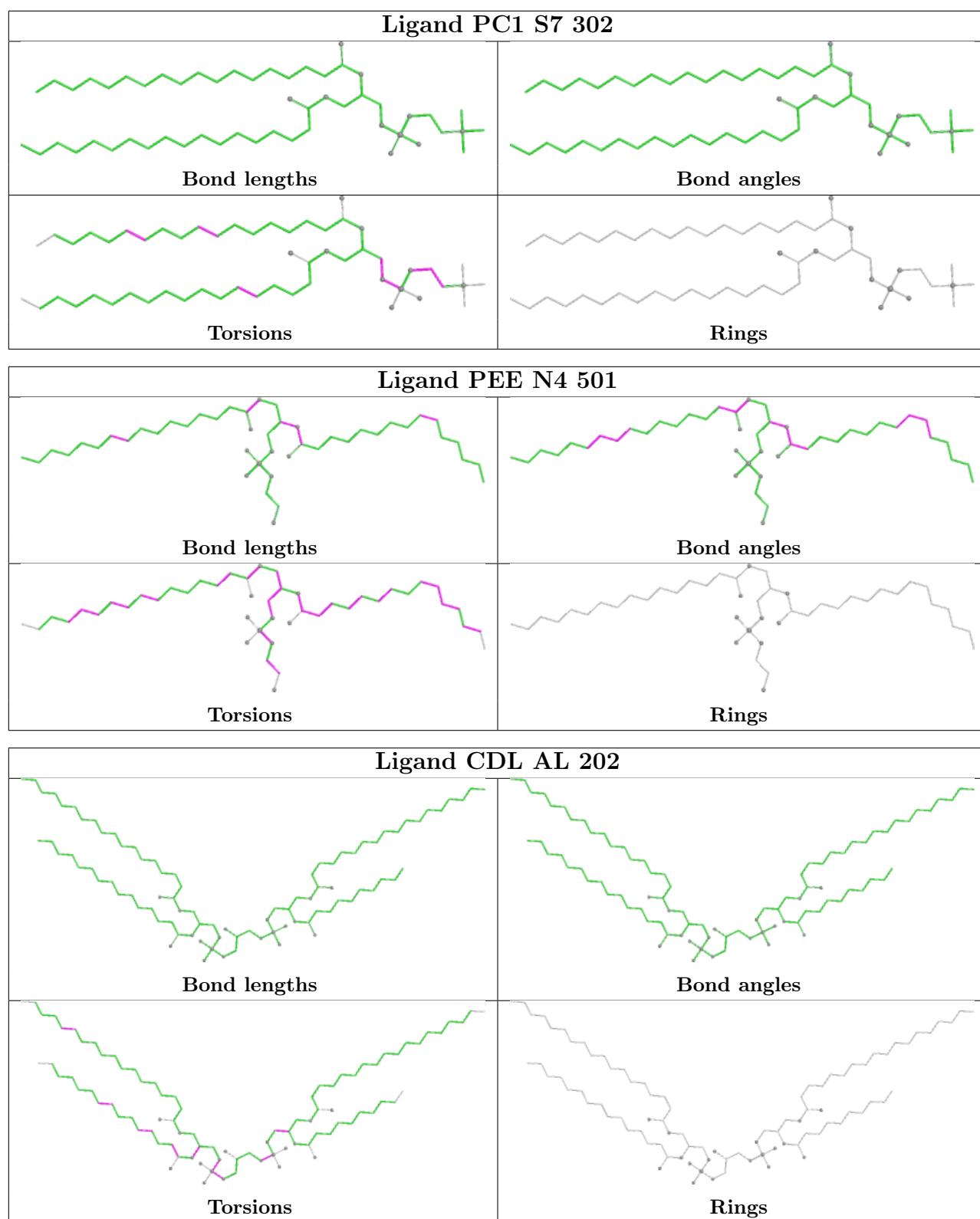
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 N4 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

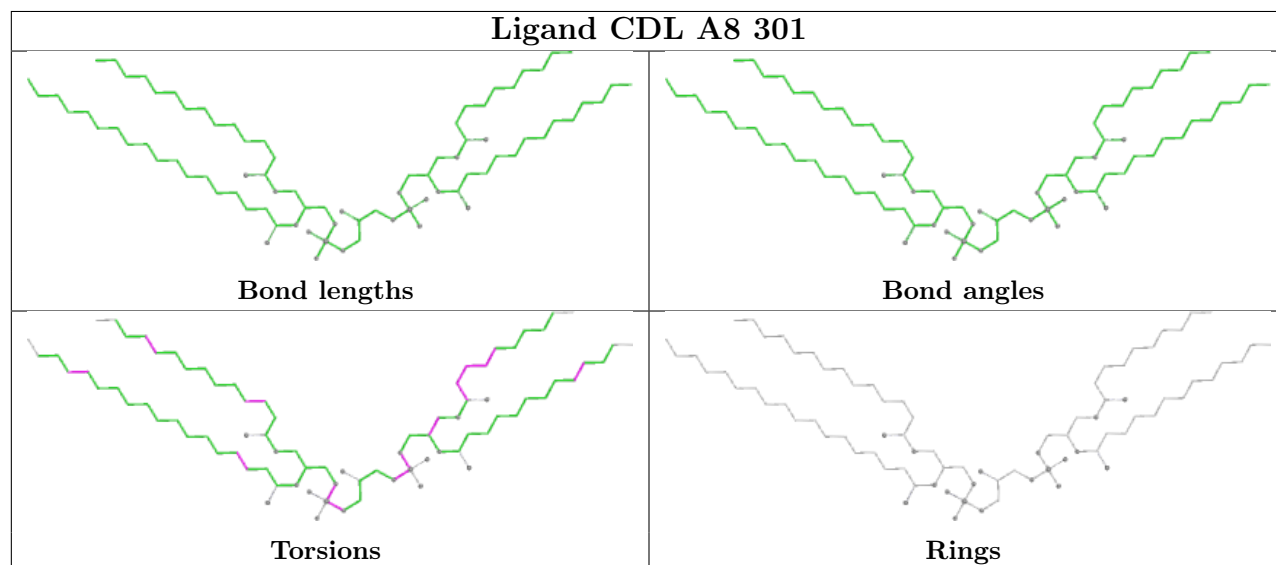
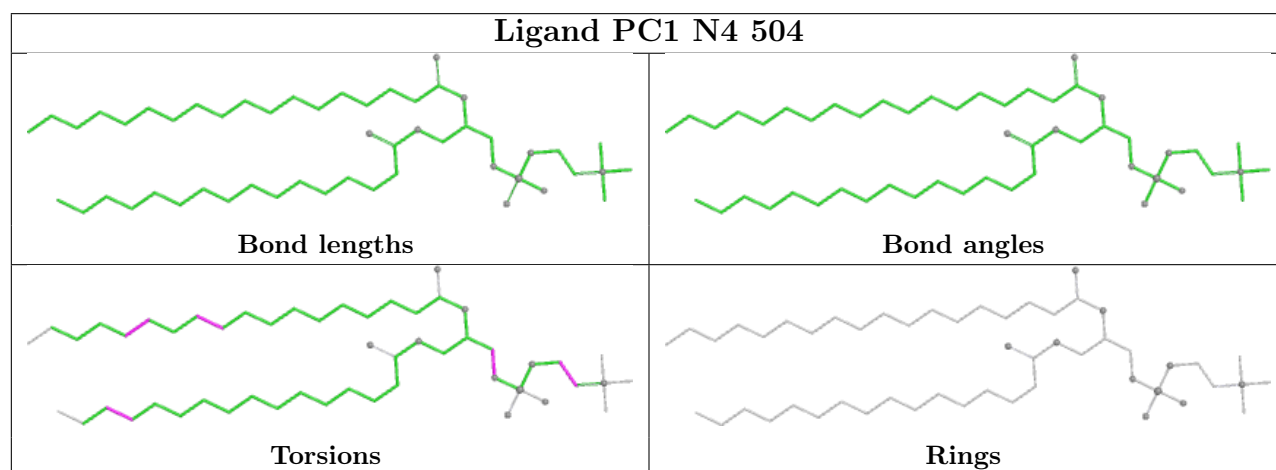
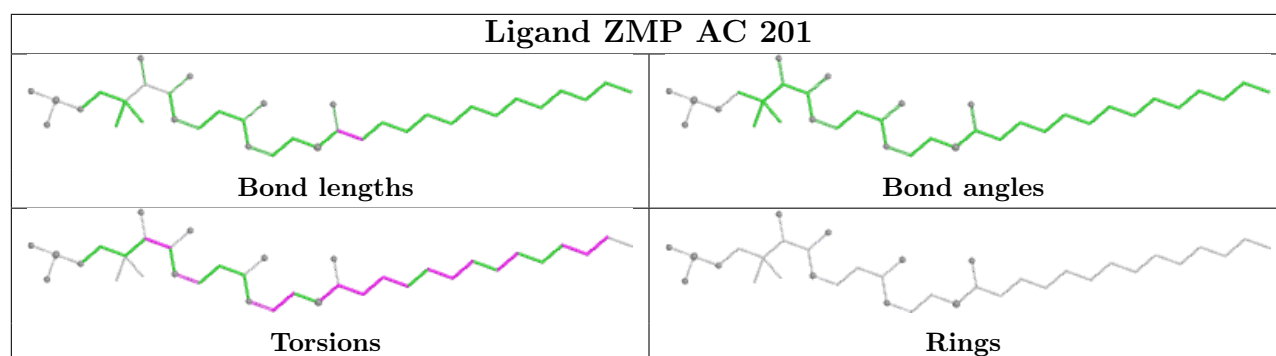
Ligand HEM QC 401

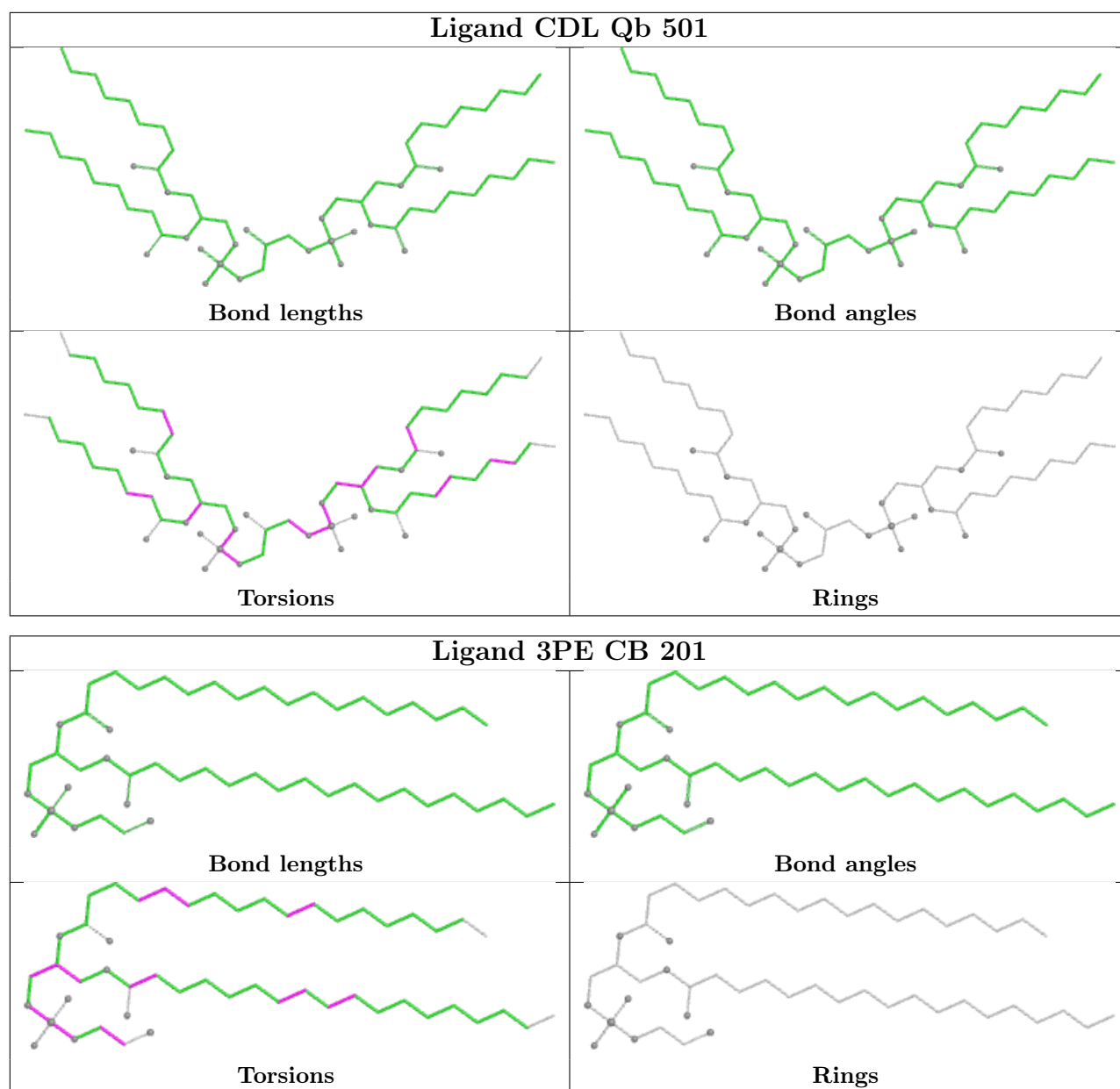


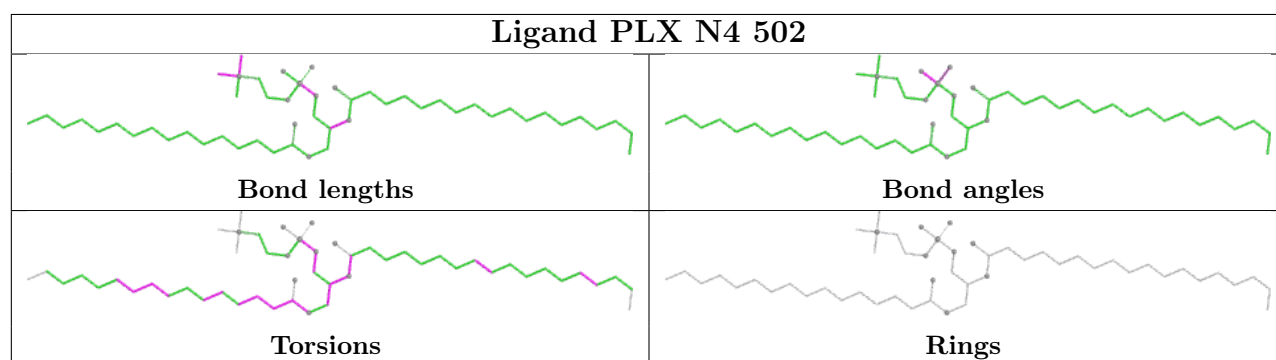
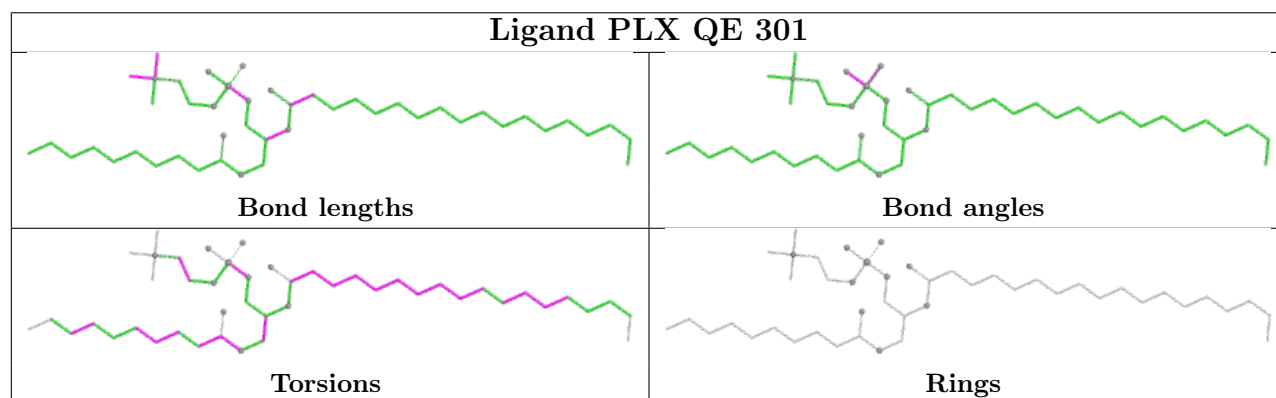
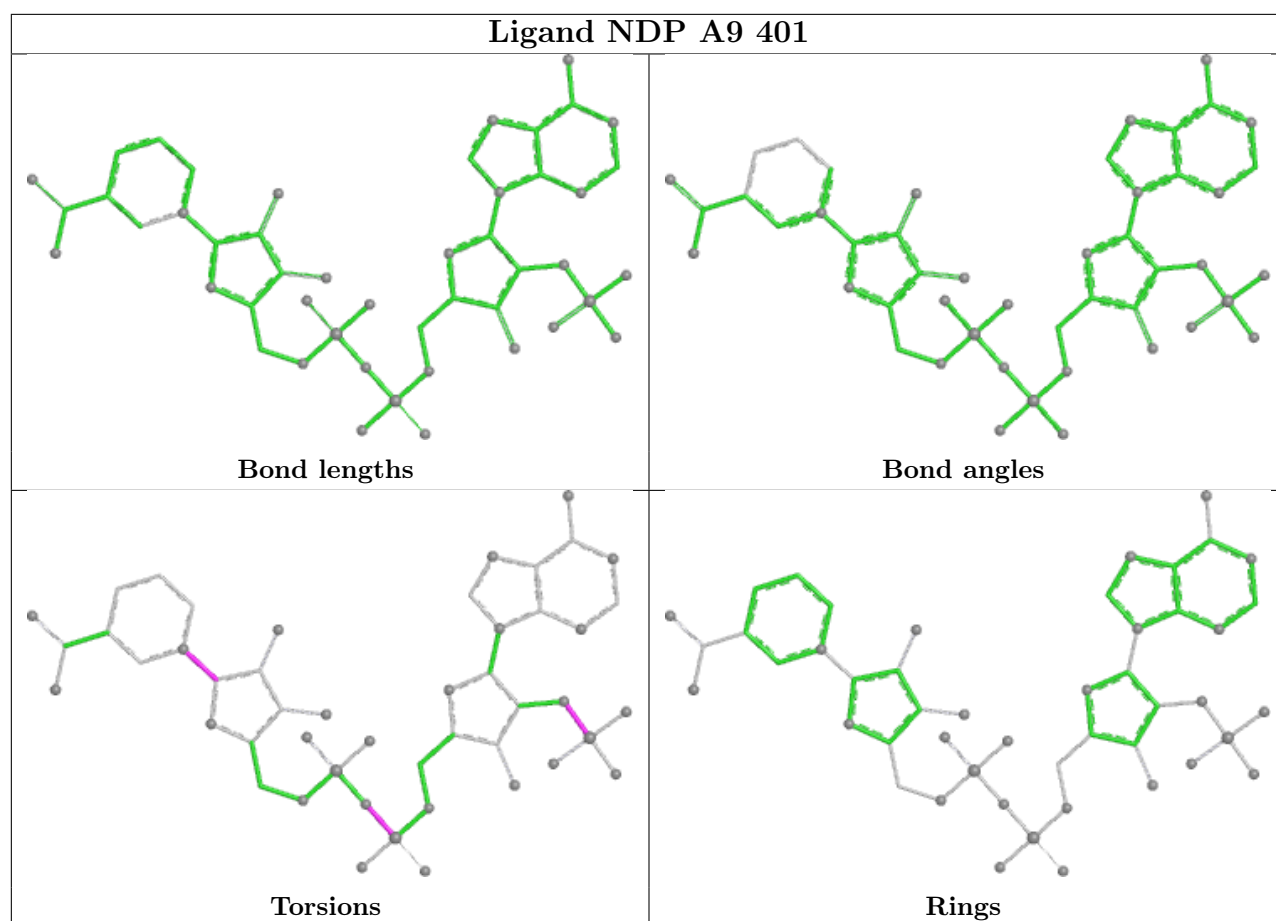
Ligand CDL B4 201

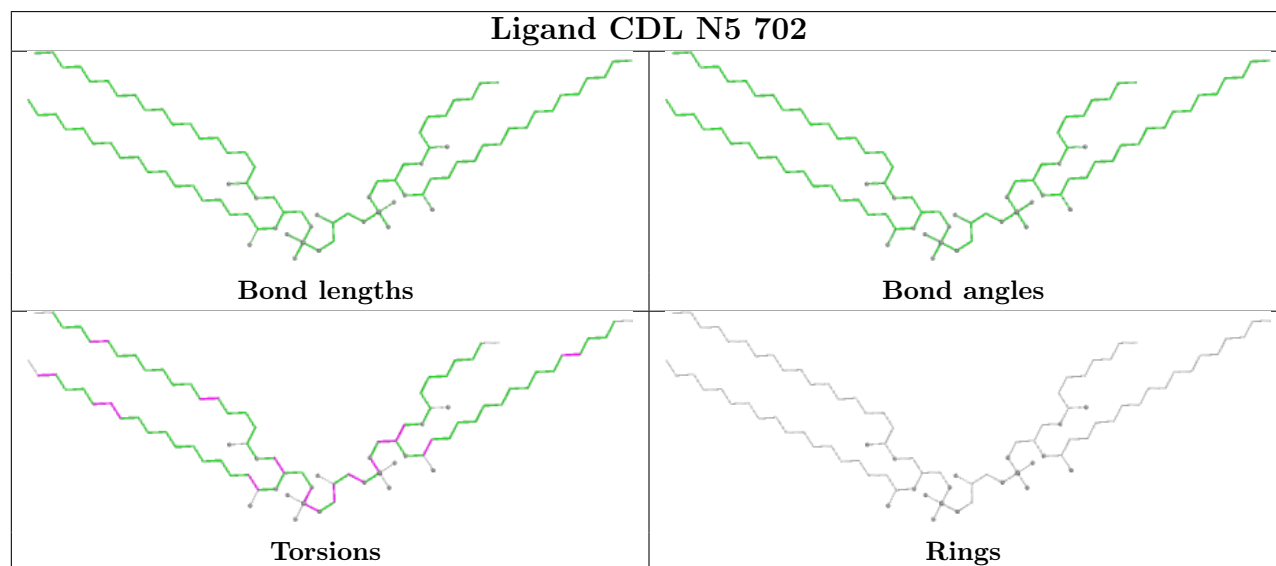
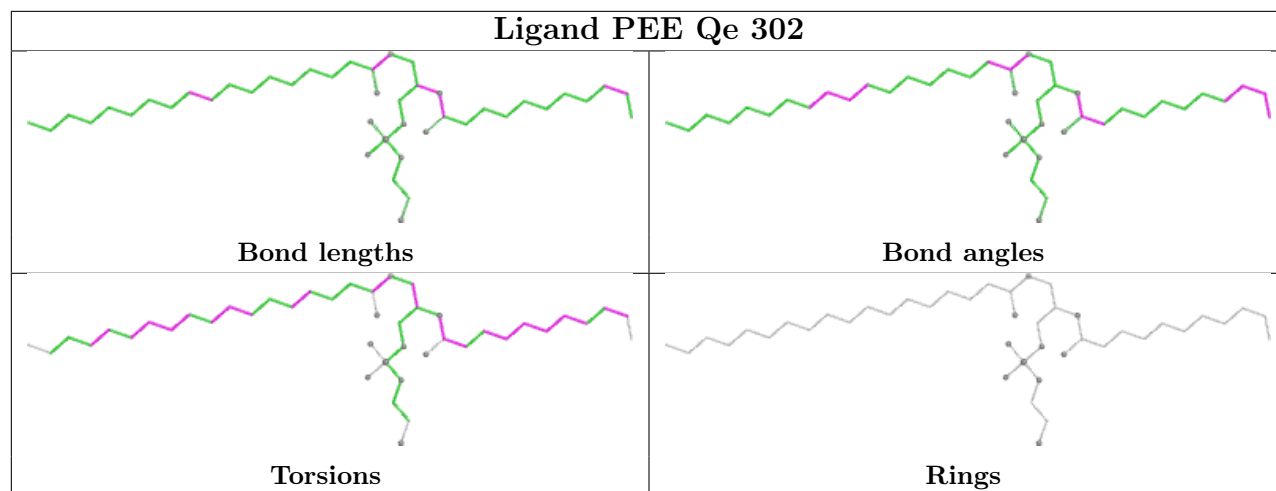




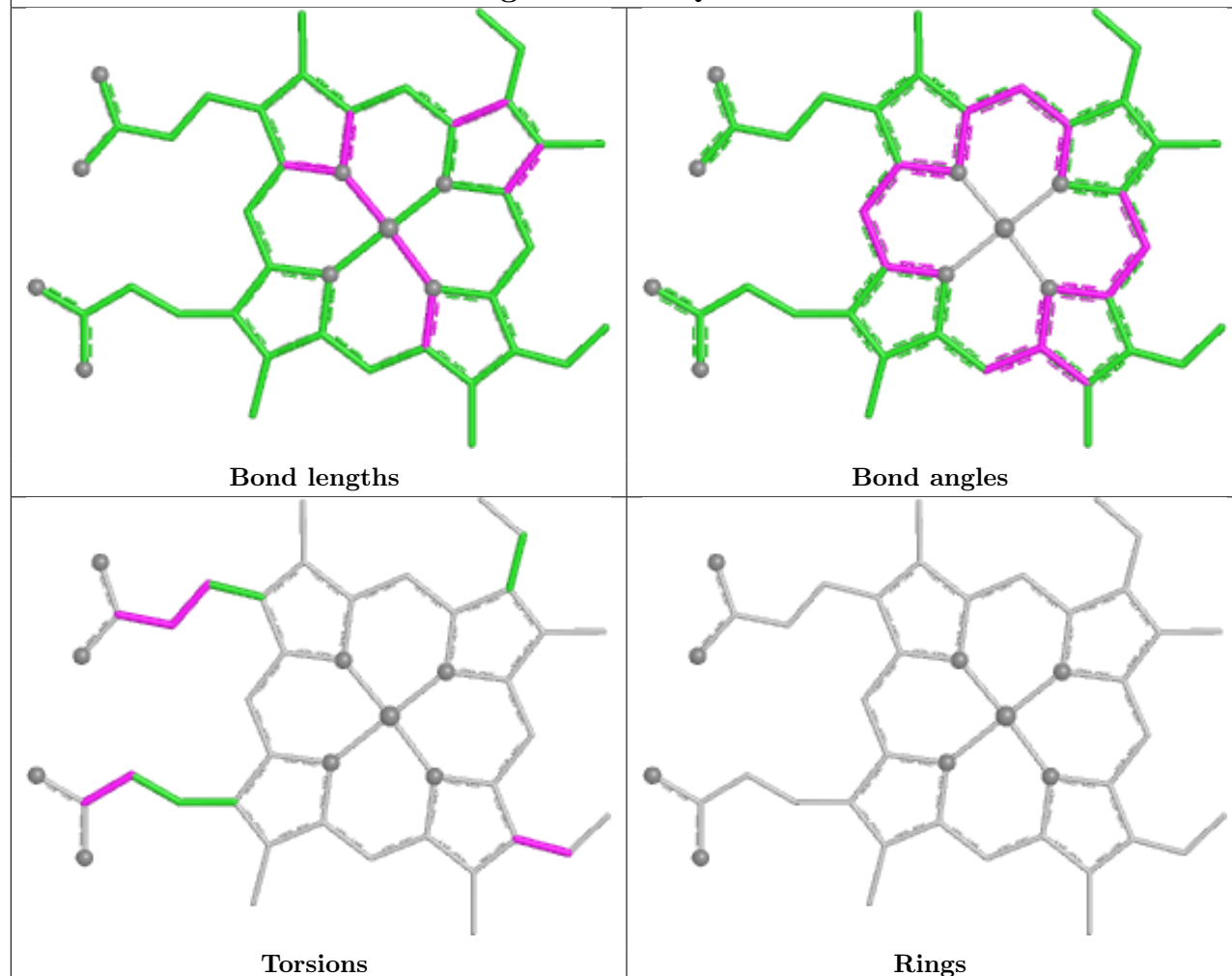




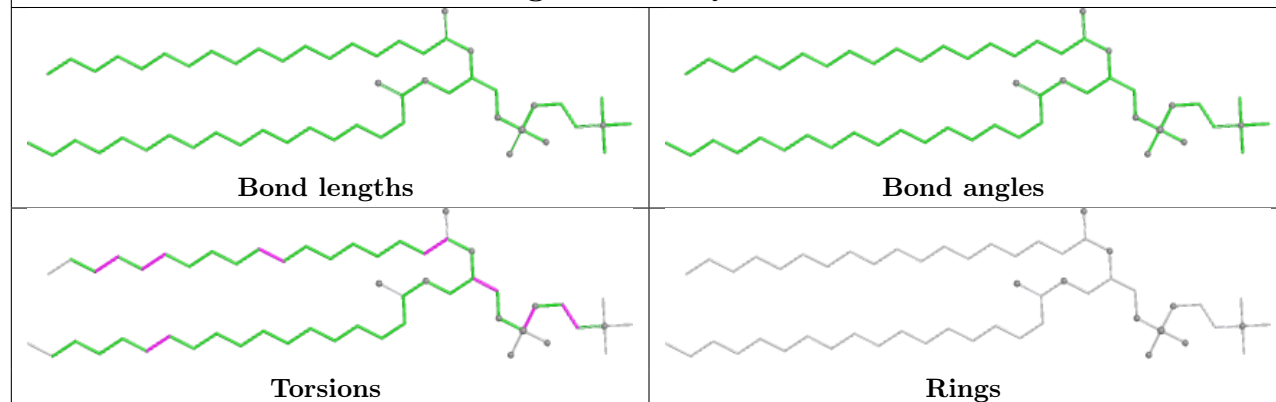


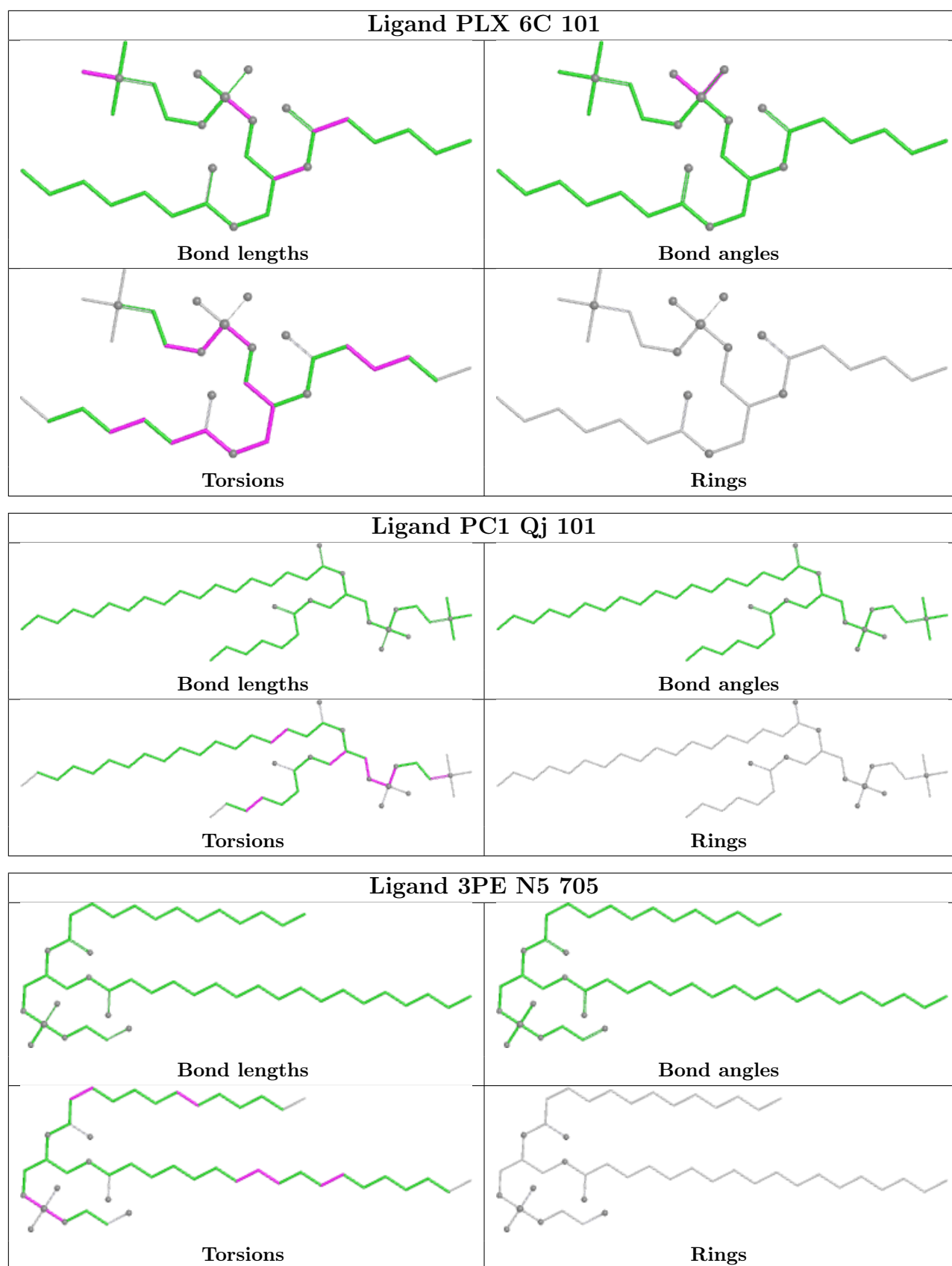


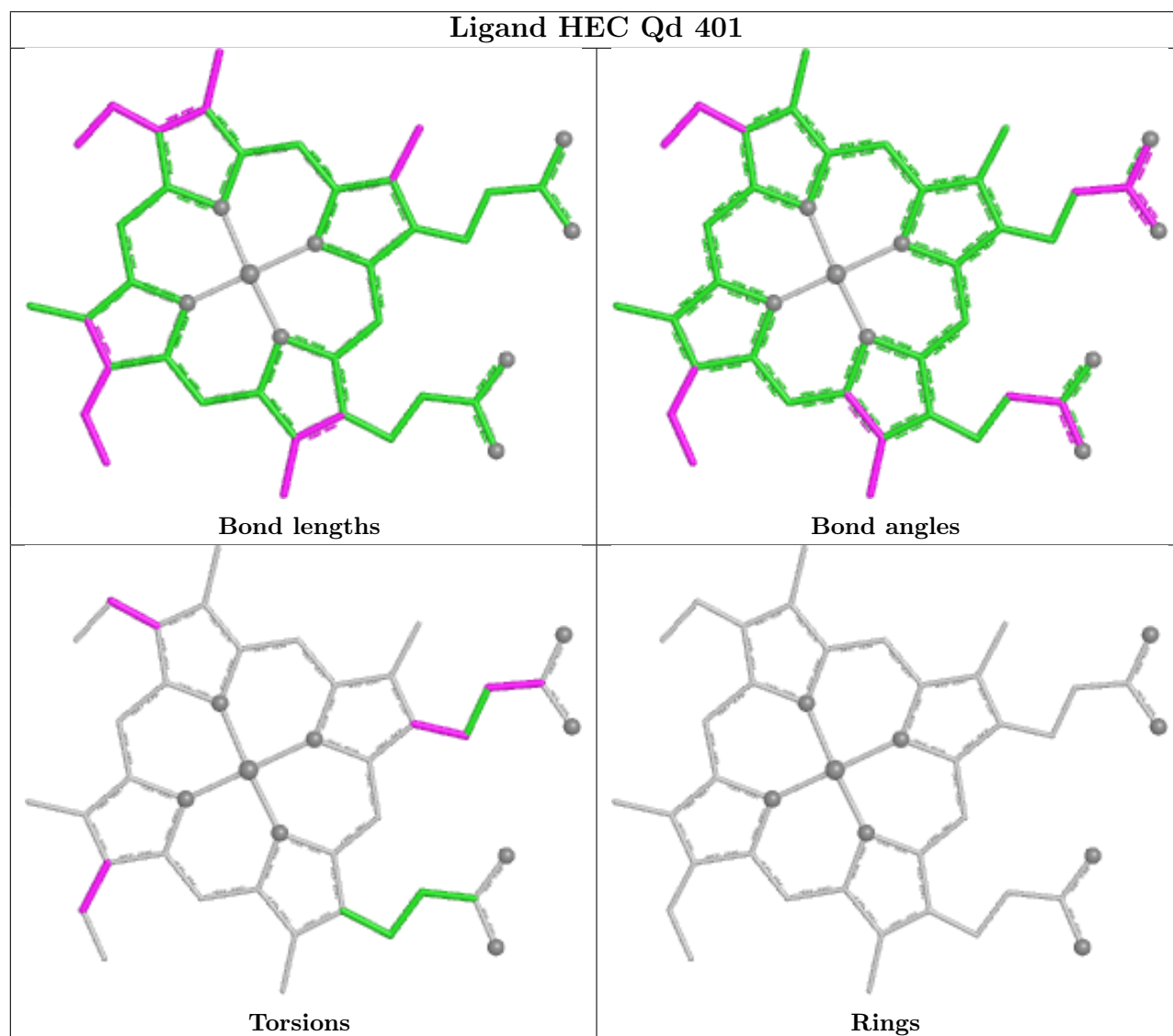
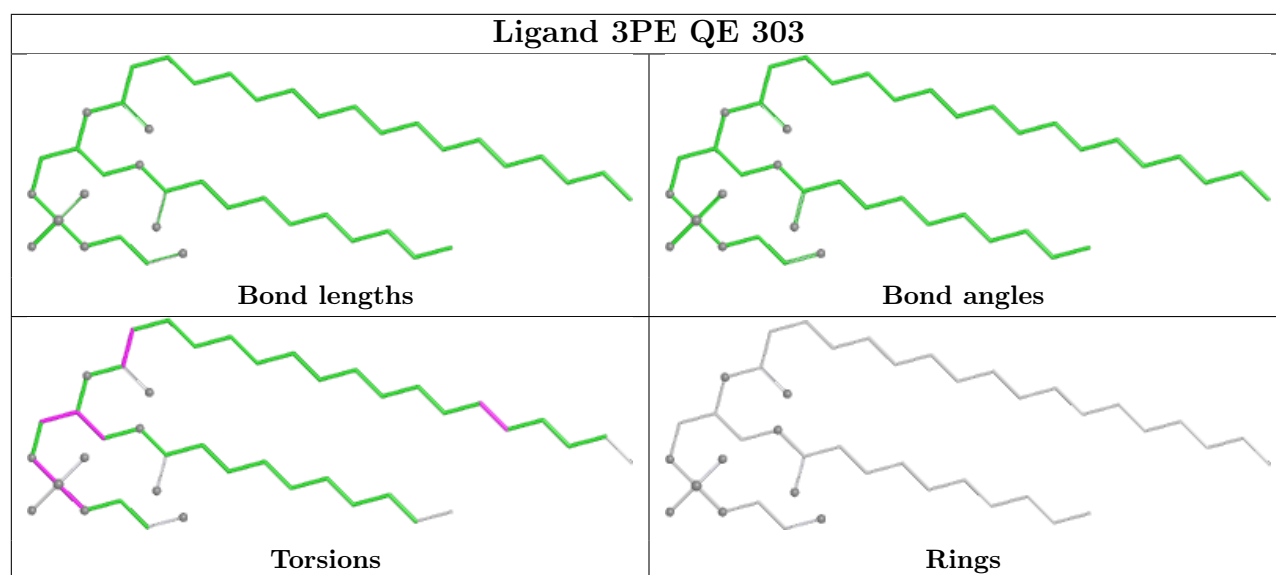
Ligand HEM Qc 402

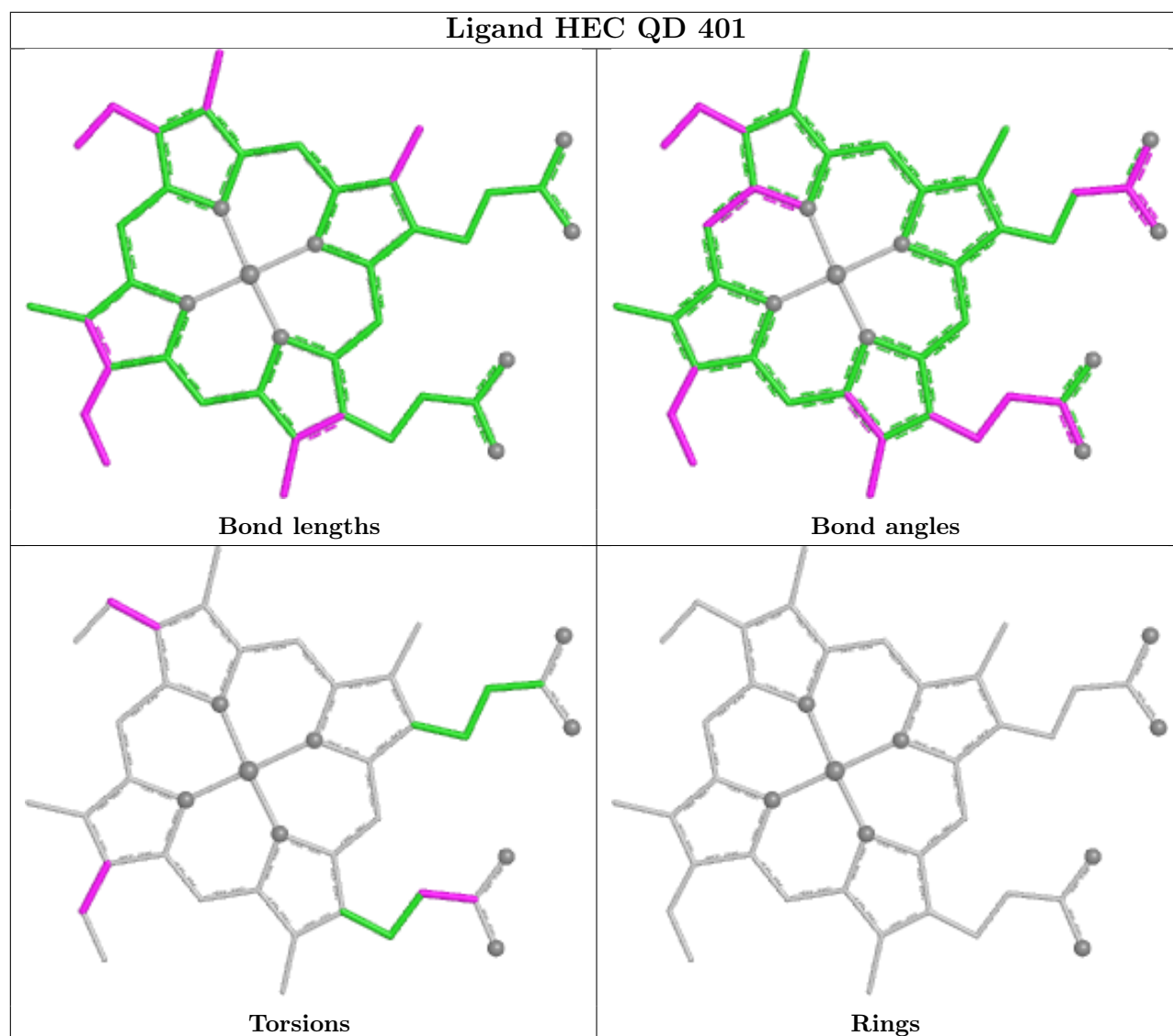
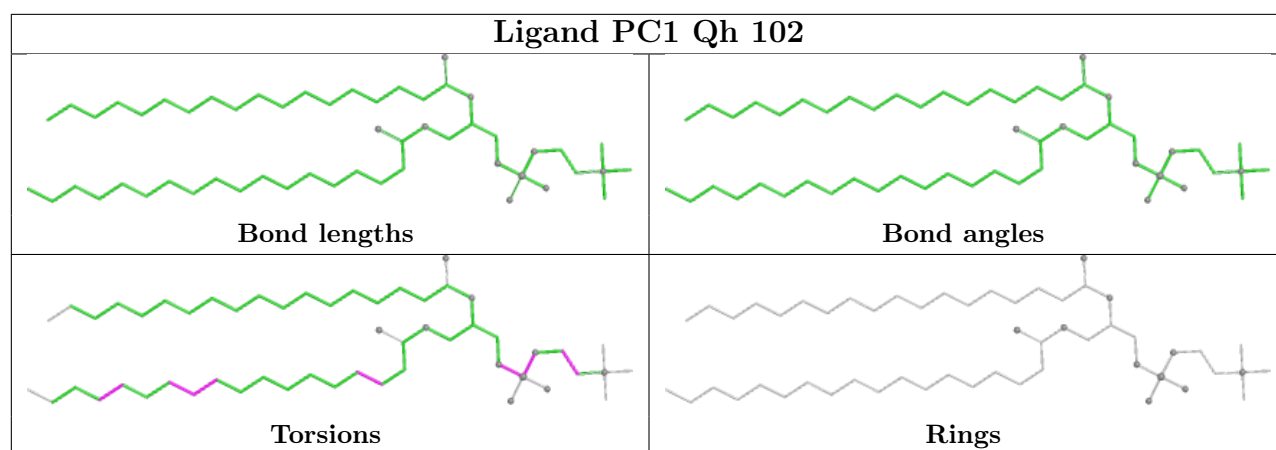


Ligand PC1 Qc 404

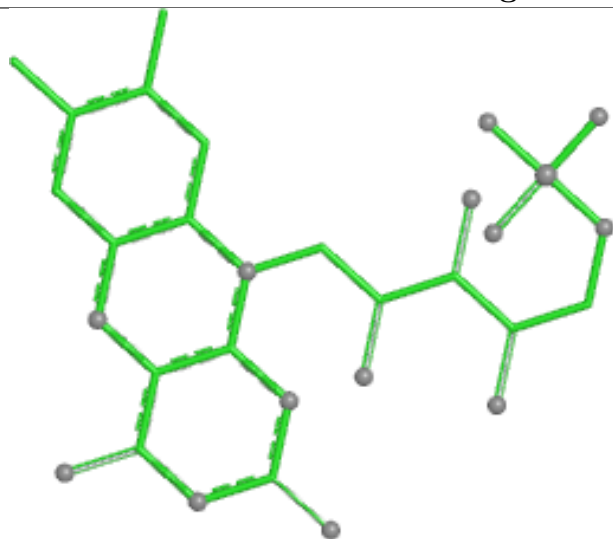




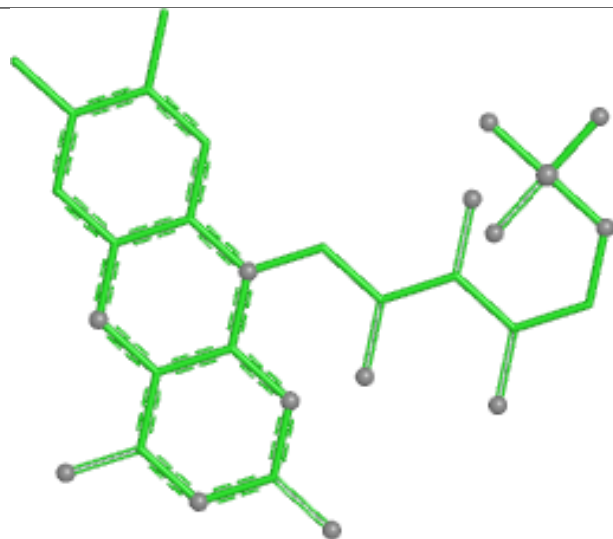




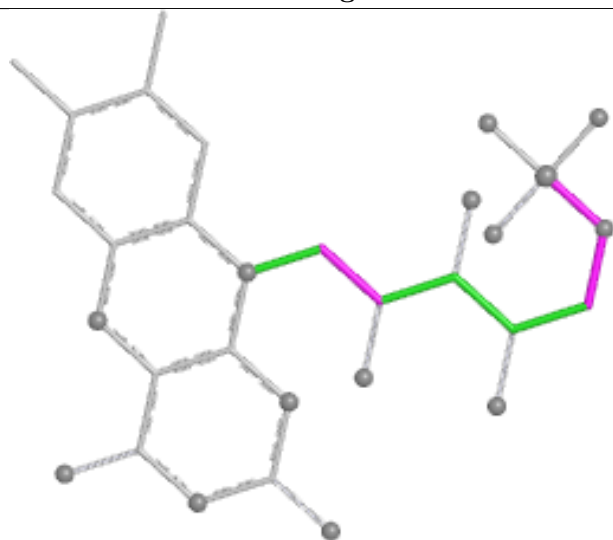
Ligand FMN V1 502



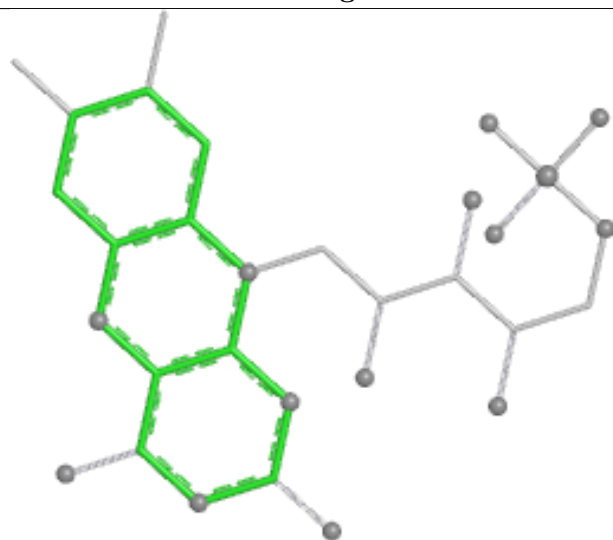
Bond lengths



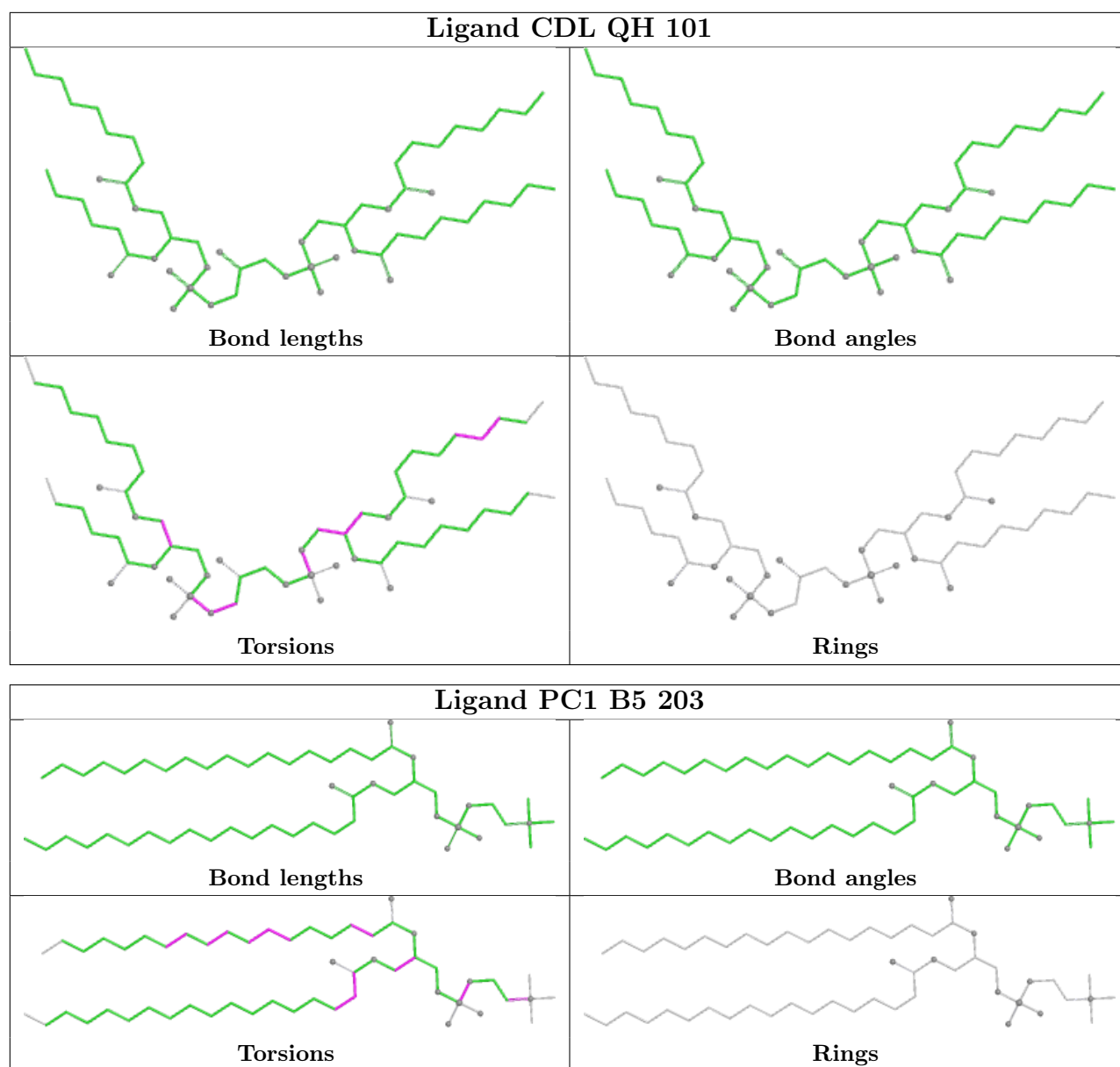
Bond angles

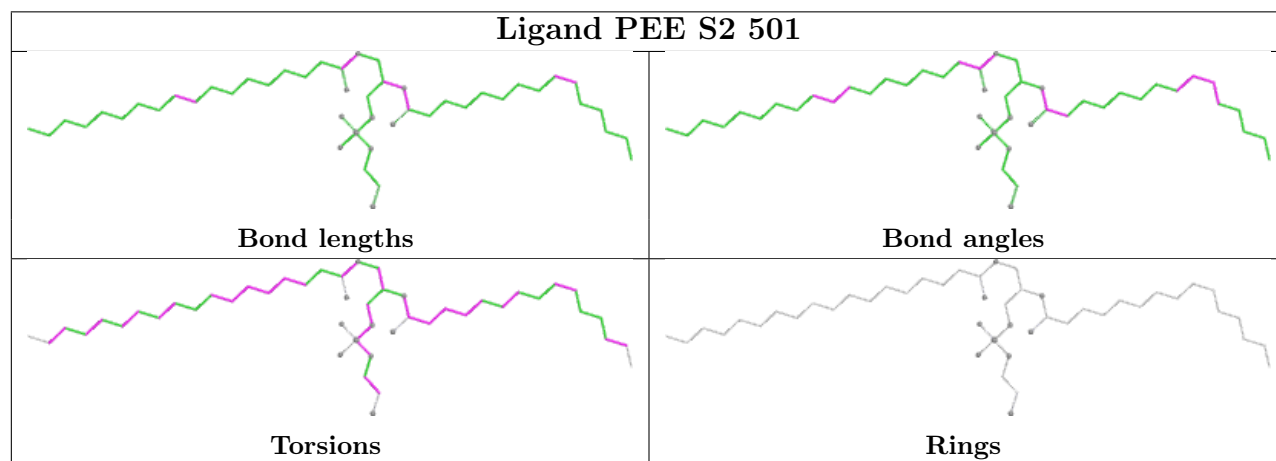
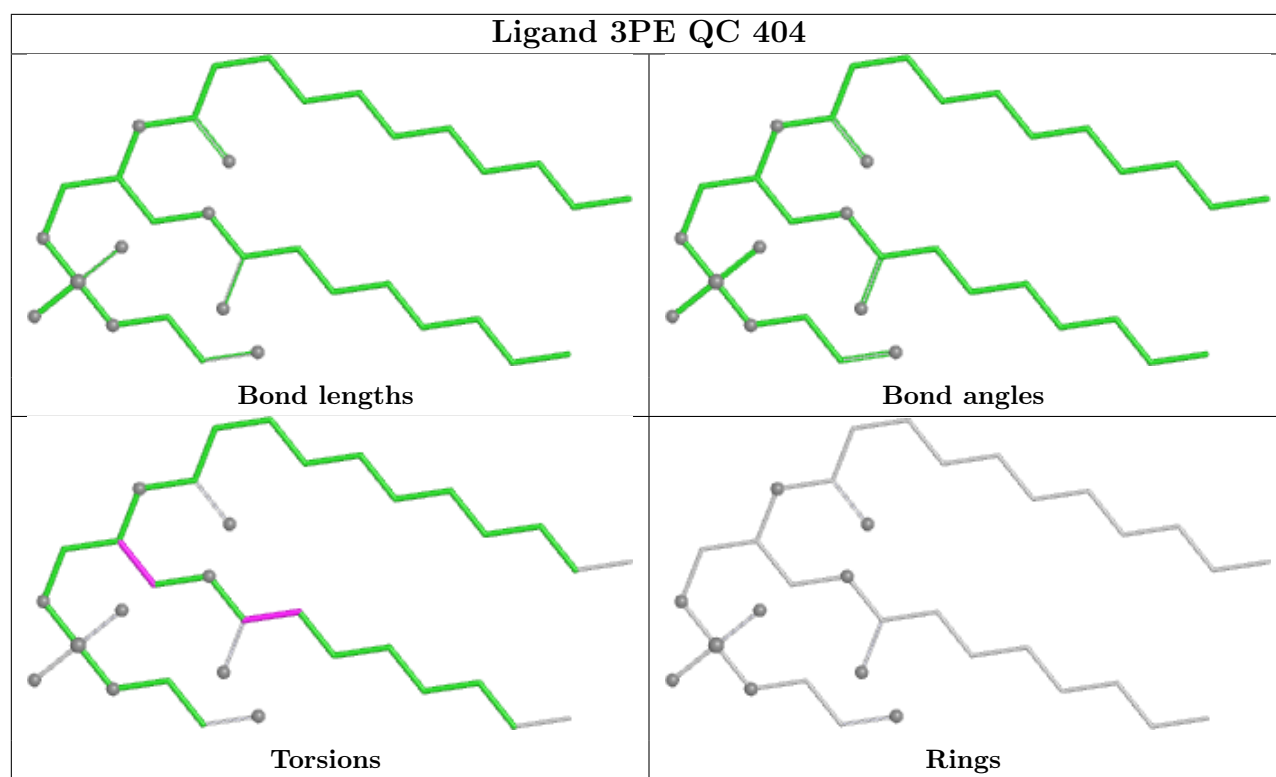


Torsions

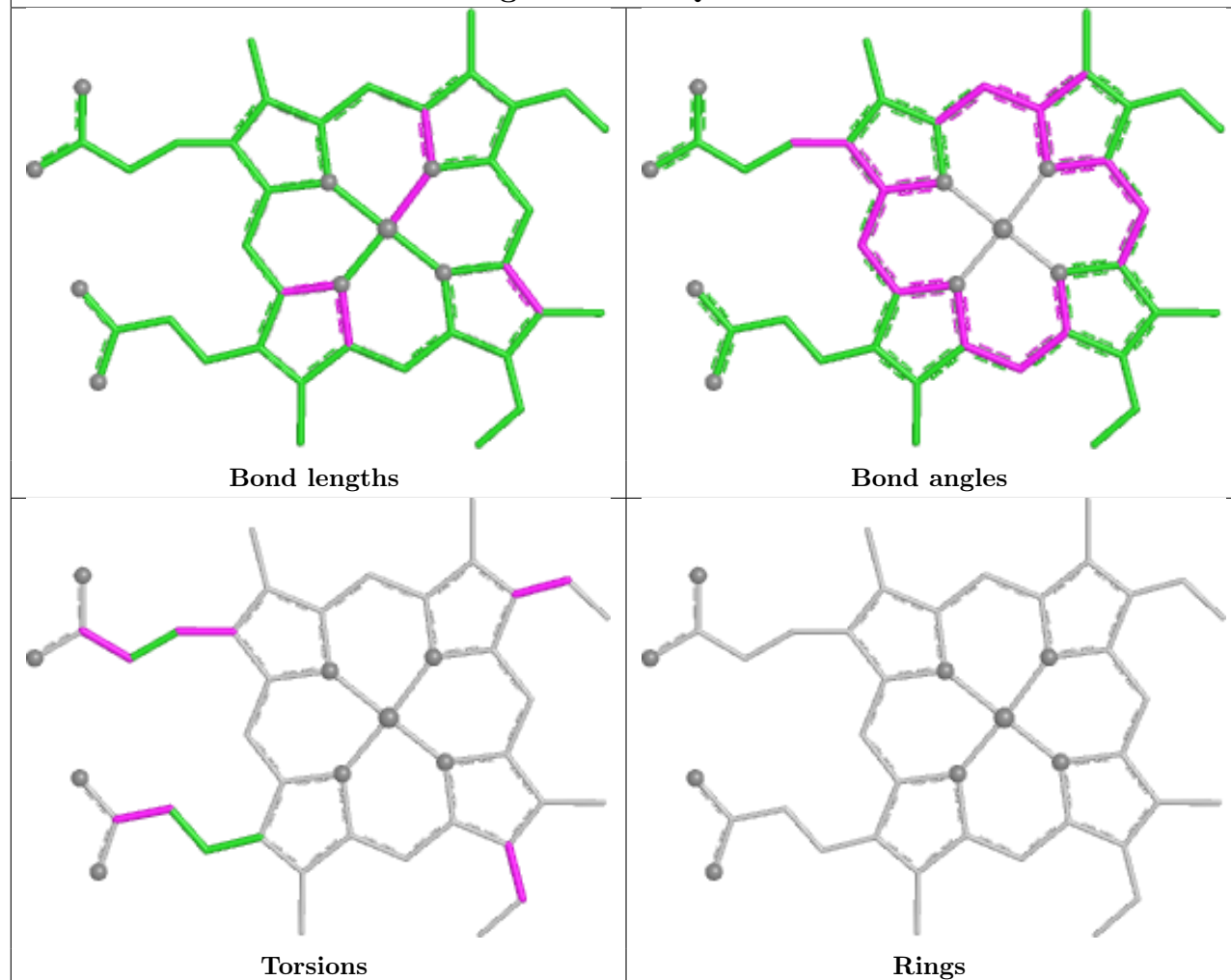


Rings

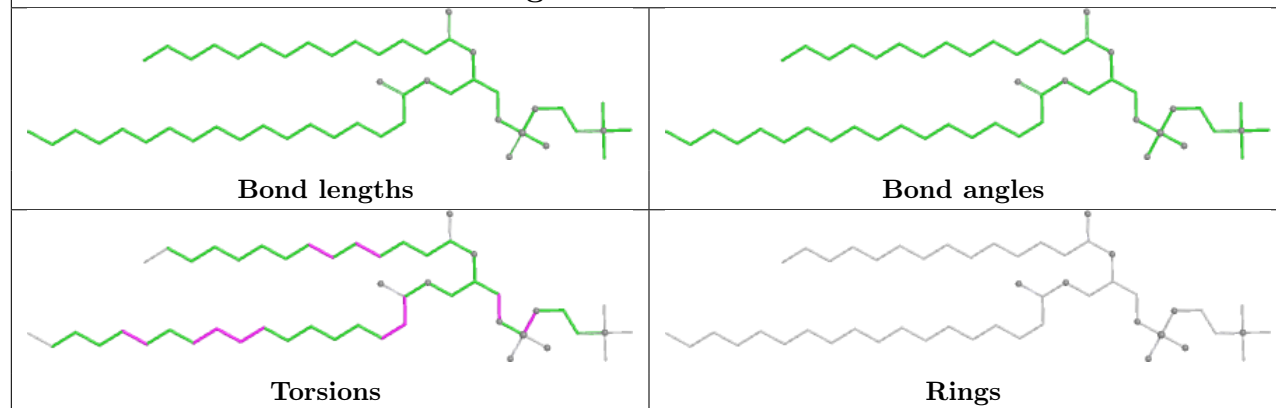




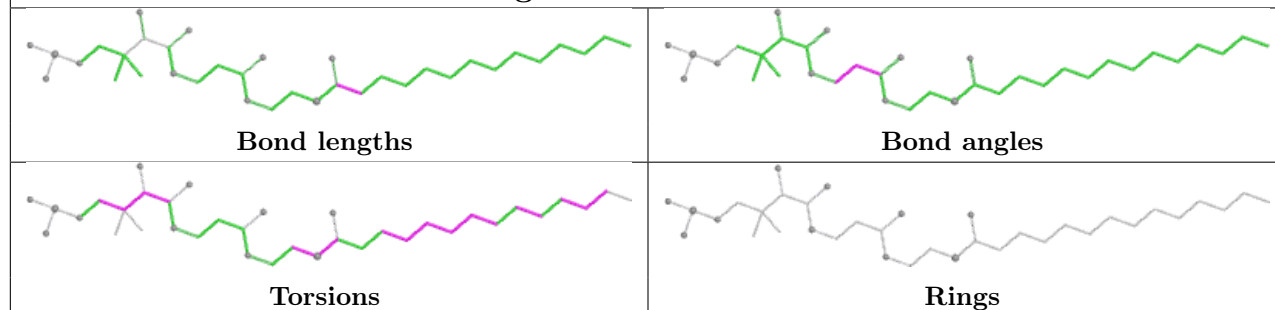
Ligand HEM Qc 403



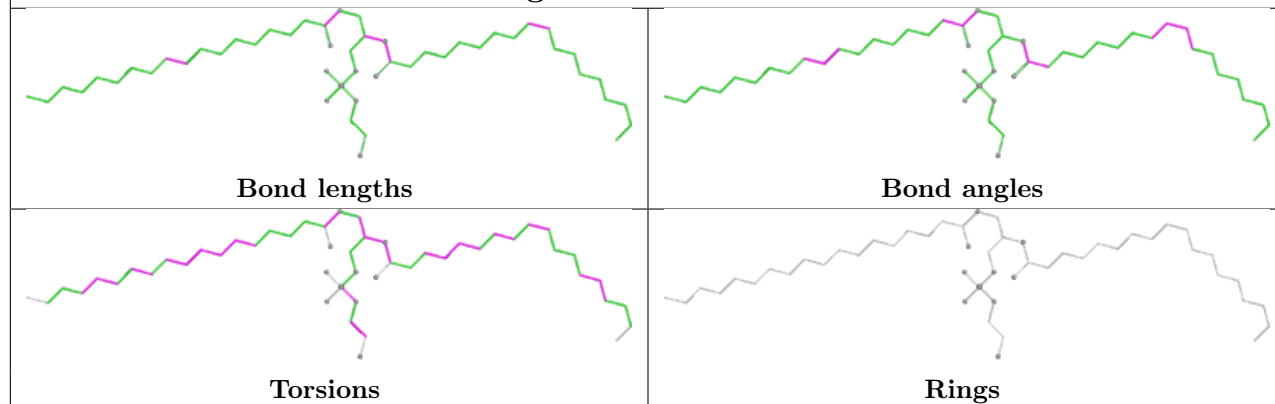
Ligand PC1 C3 302



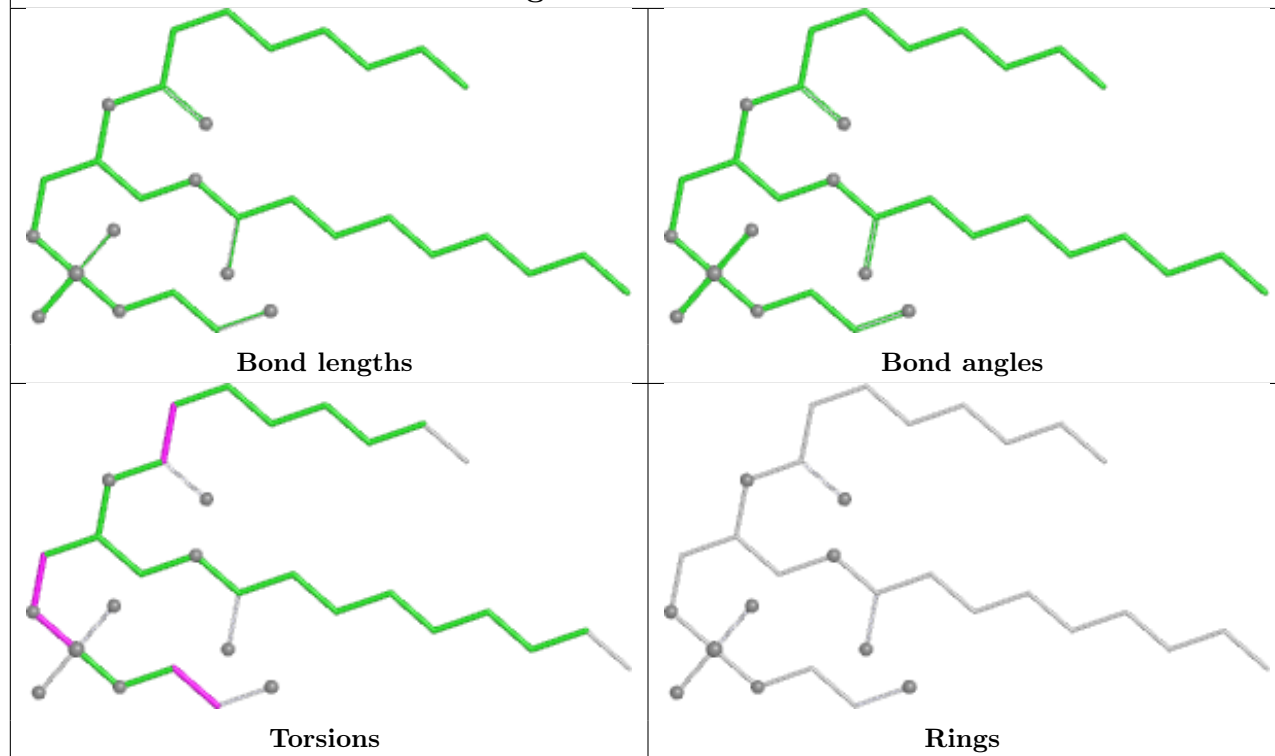
Ligand ZMP AB 201

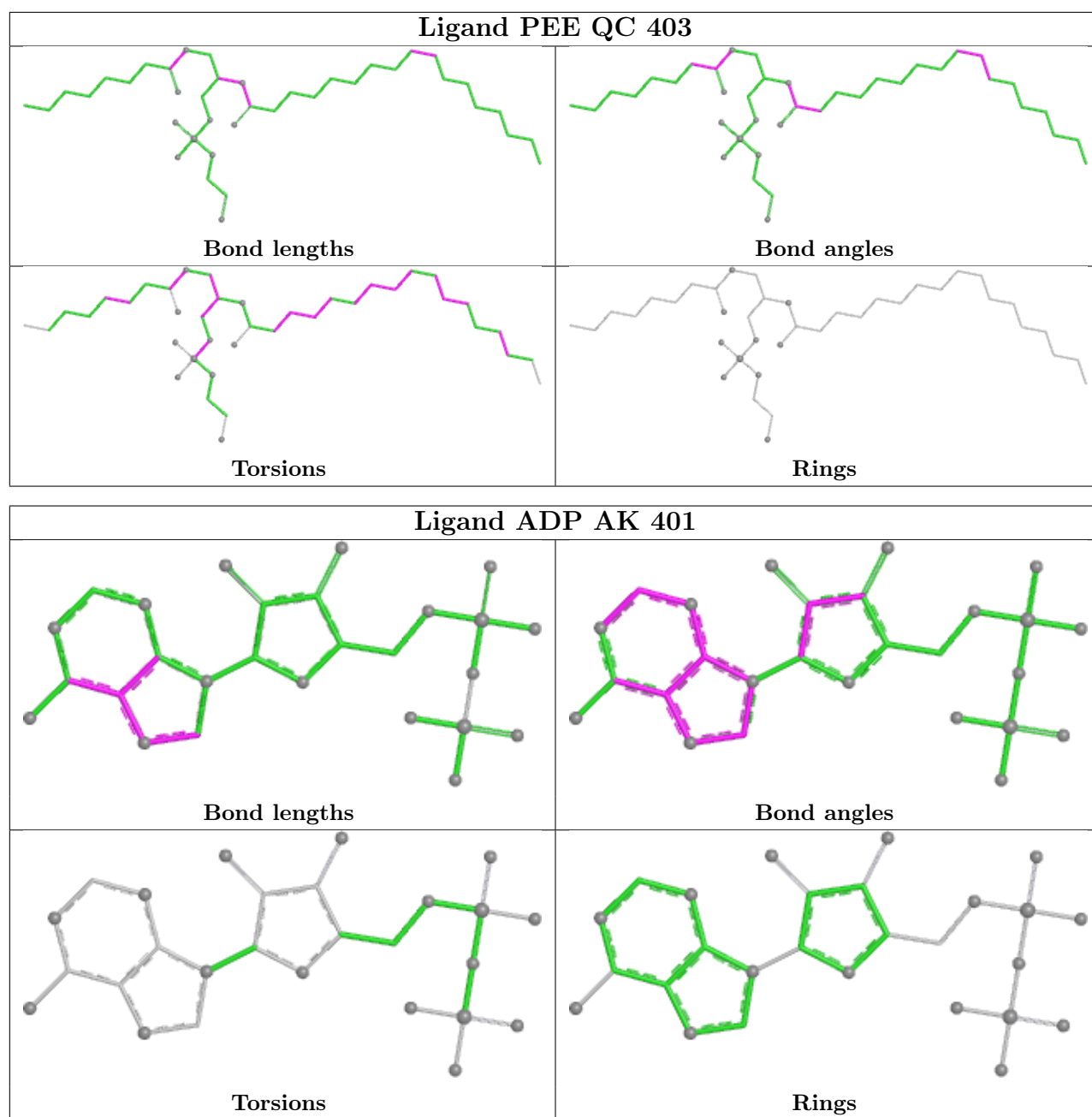


Ligand PEE S8 303



Ligand 3PE B8 201





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.

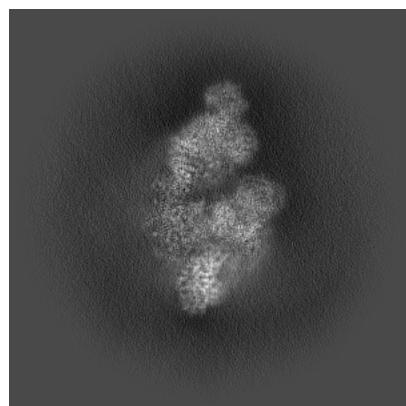
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60422. These allow visual inspection of the internal detail of the map and identification of artifacts.

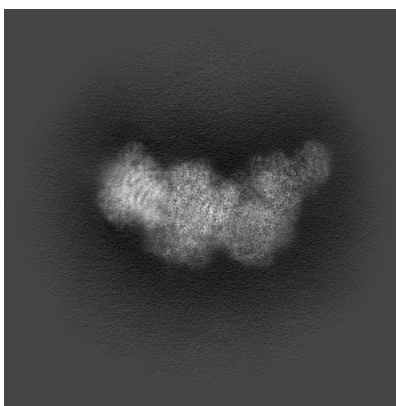
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

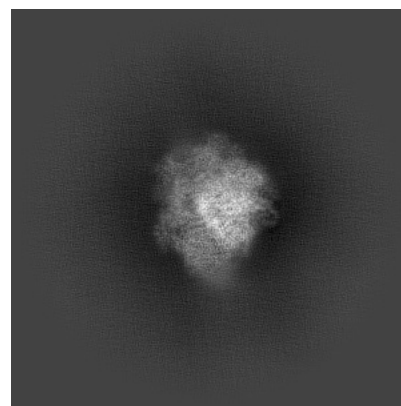
6.1.1 Primary map



X

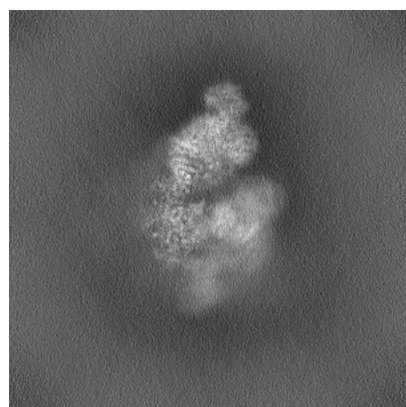


Y

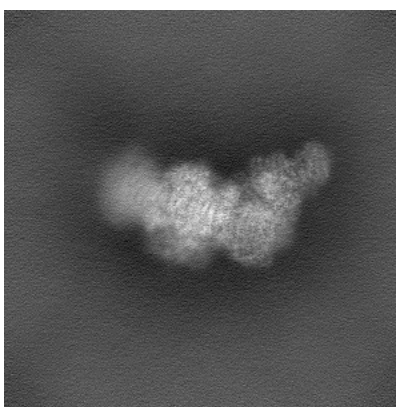


Z

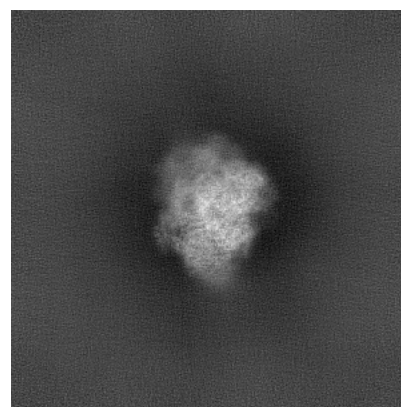
6.1.2 Raw map



X



Y

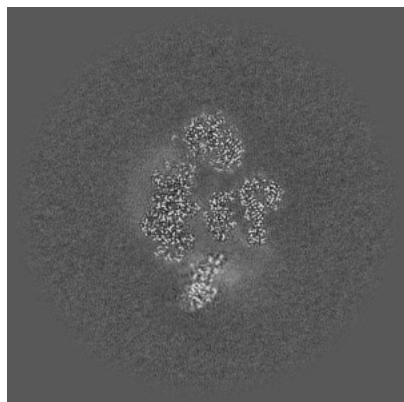


Z

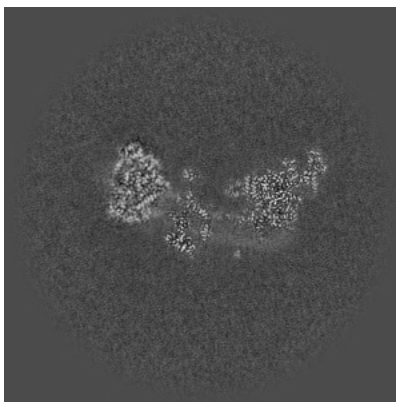
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

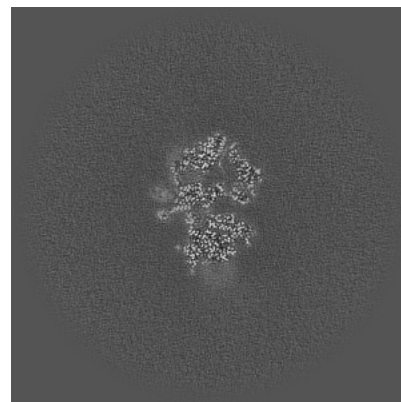
6.2.1 Primary map



X Index: 240

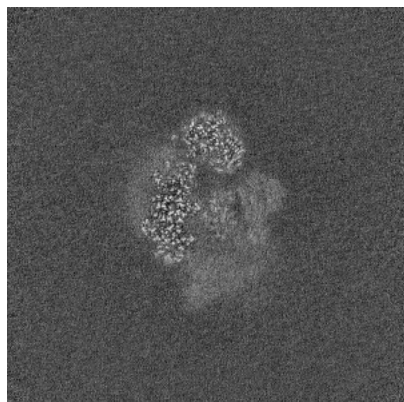


Y Index: 240



Z Index: 240

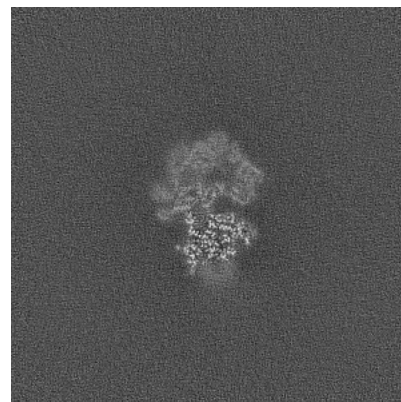
6.2.2 Raw map



X Index: 240



Y Index: 240

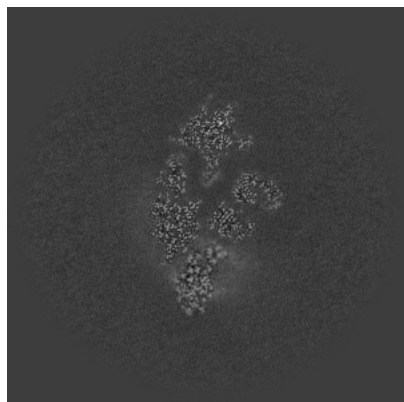


Z Index: 240

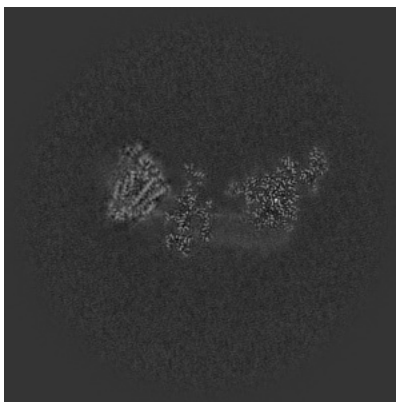
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

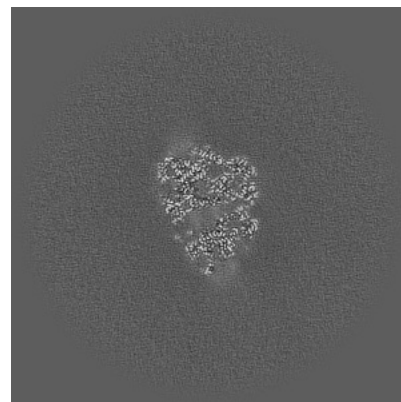
6.3.1 Primary map



X Index: 256

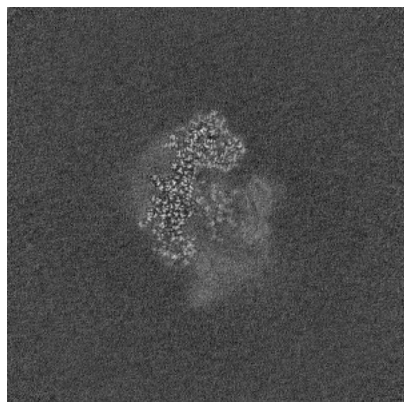


Y Index: 243

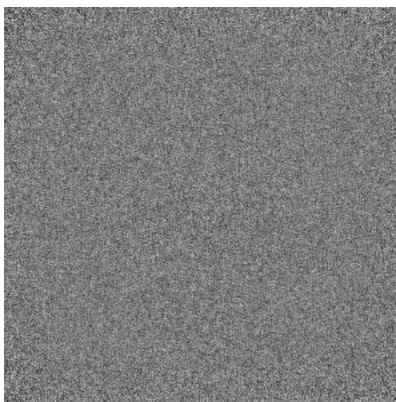


Z Index: 217

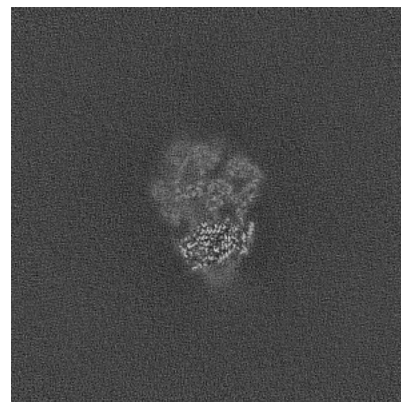
6.3.2 Raw map



X Index: 234



Y Index: 0

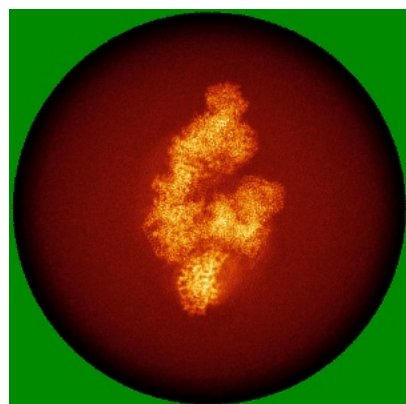


Z Index: 230

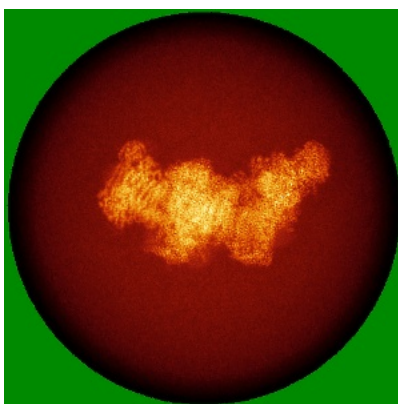
The images above show the largest variance slices of the map in three orthogonal directions.

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

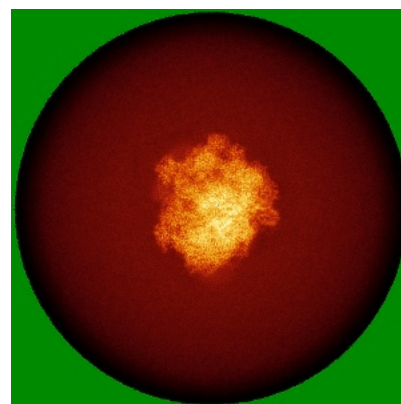
6.4.1 Primary map



X

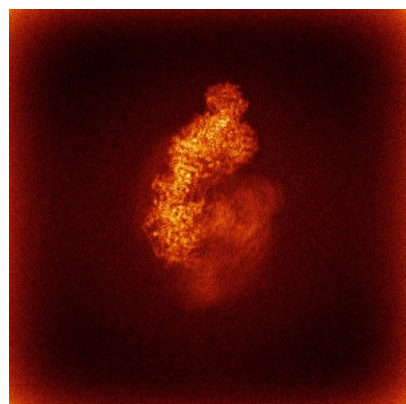


Y

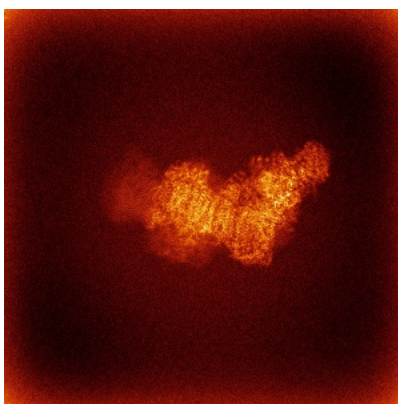


Z

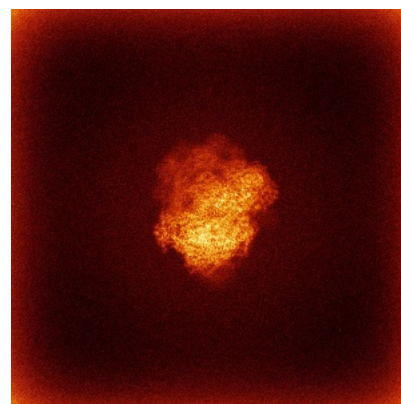
6.4.2 Raw map



X



Y

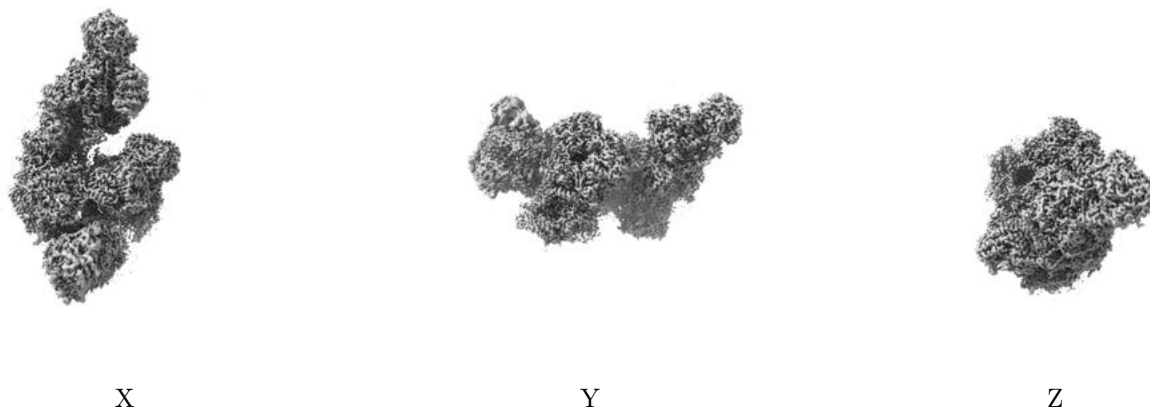


Z

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.

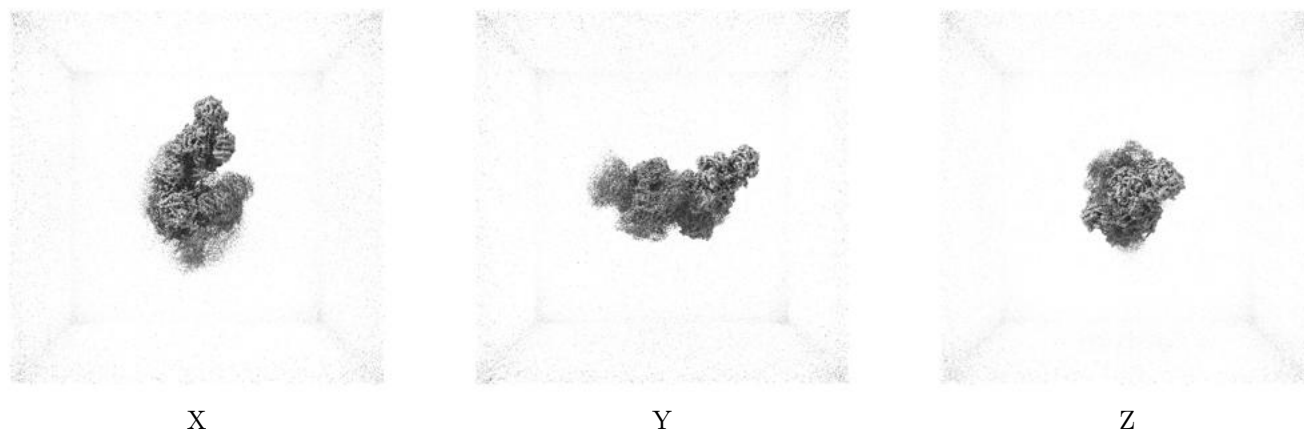
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

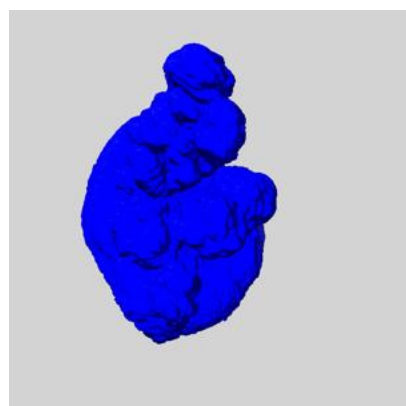
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

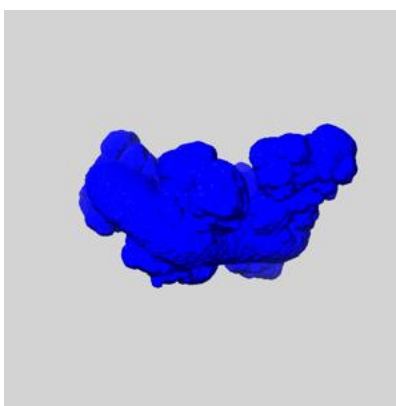
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

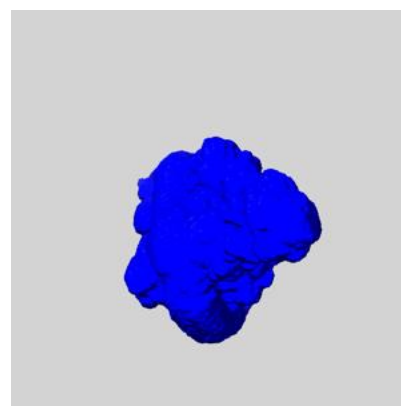
6.6.1 emd_60422_msk_1.map [i](#)



X



Y

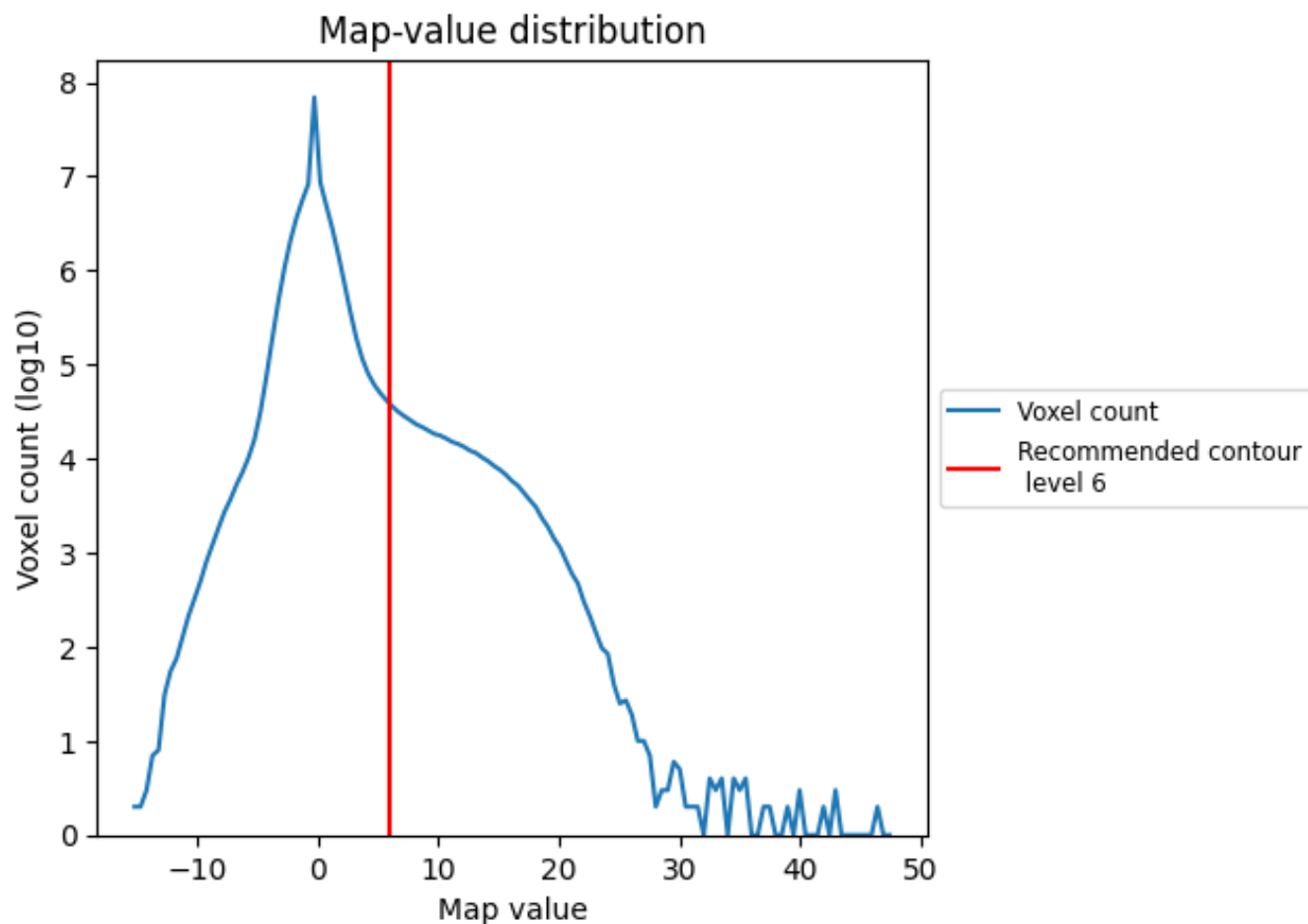


Z

7 Map analysis [i](#)

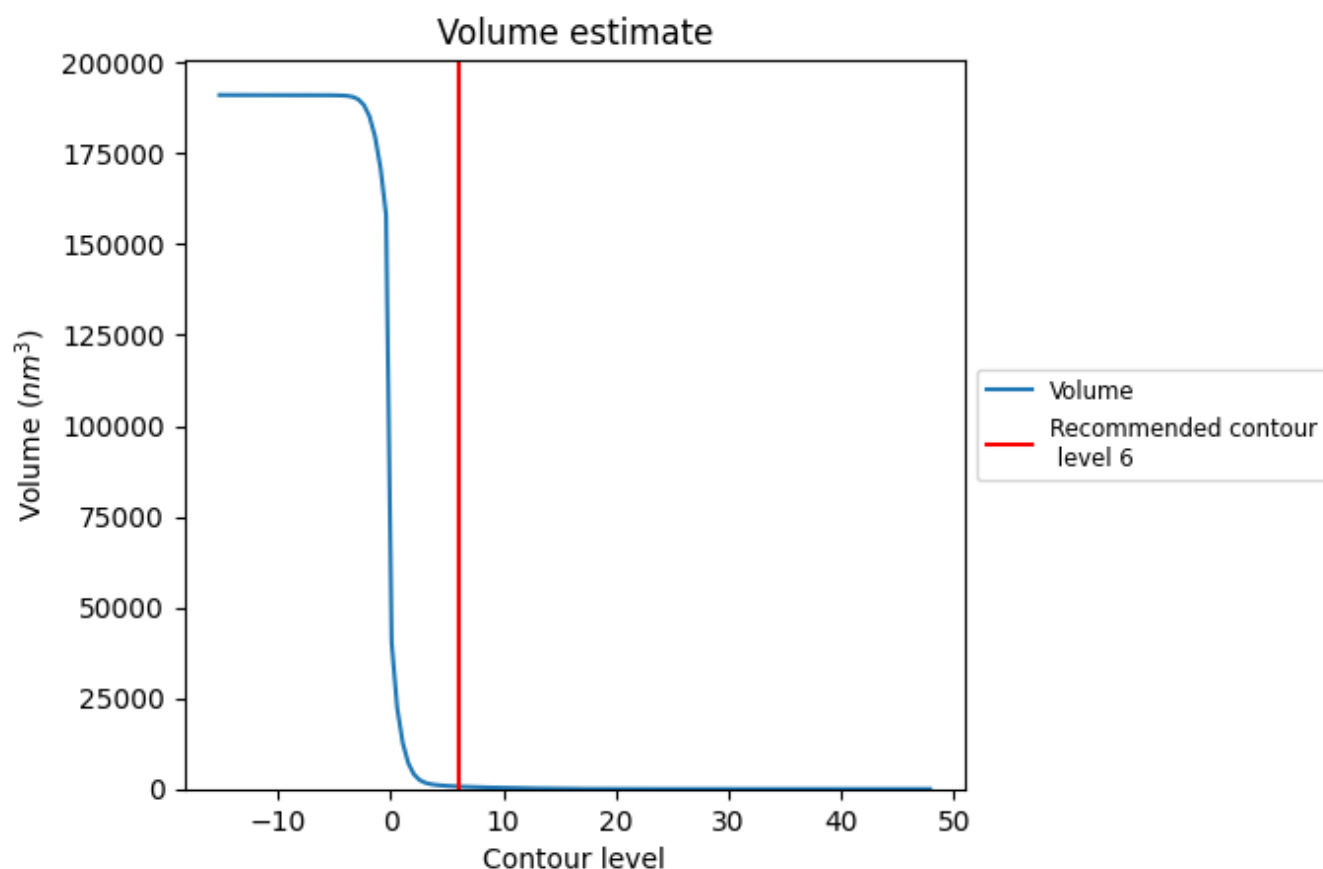
This section contains the results of statistical analysis of the map.

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.

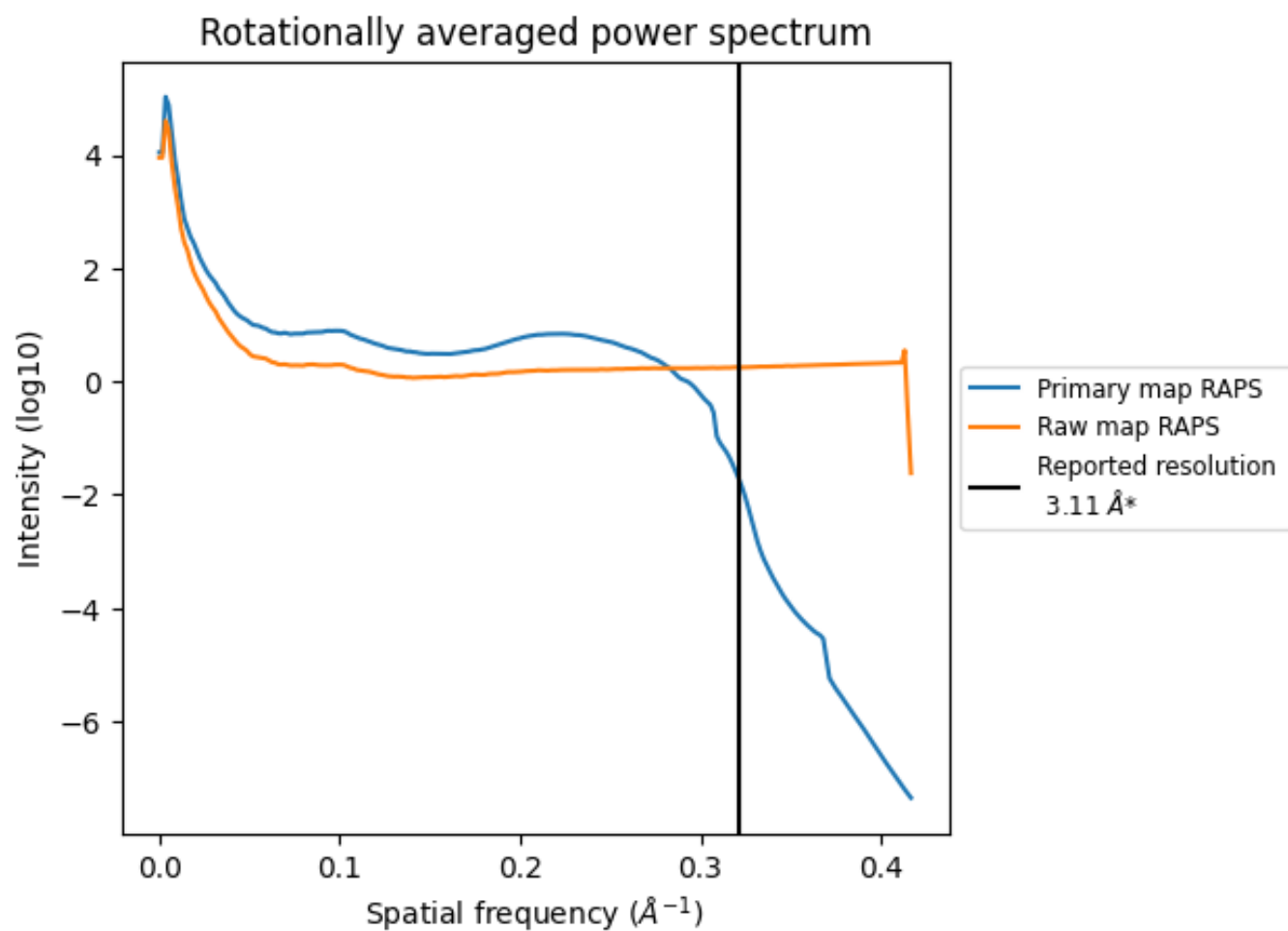
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 677 nm^3 ; this corresponds to an approximate mass of 611 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 ⓘ

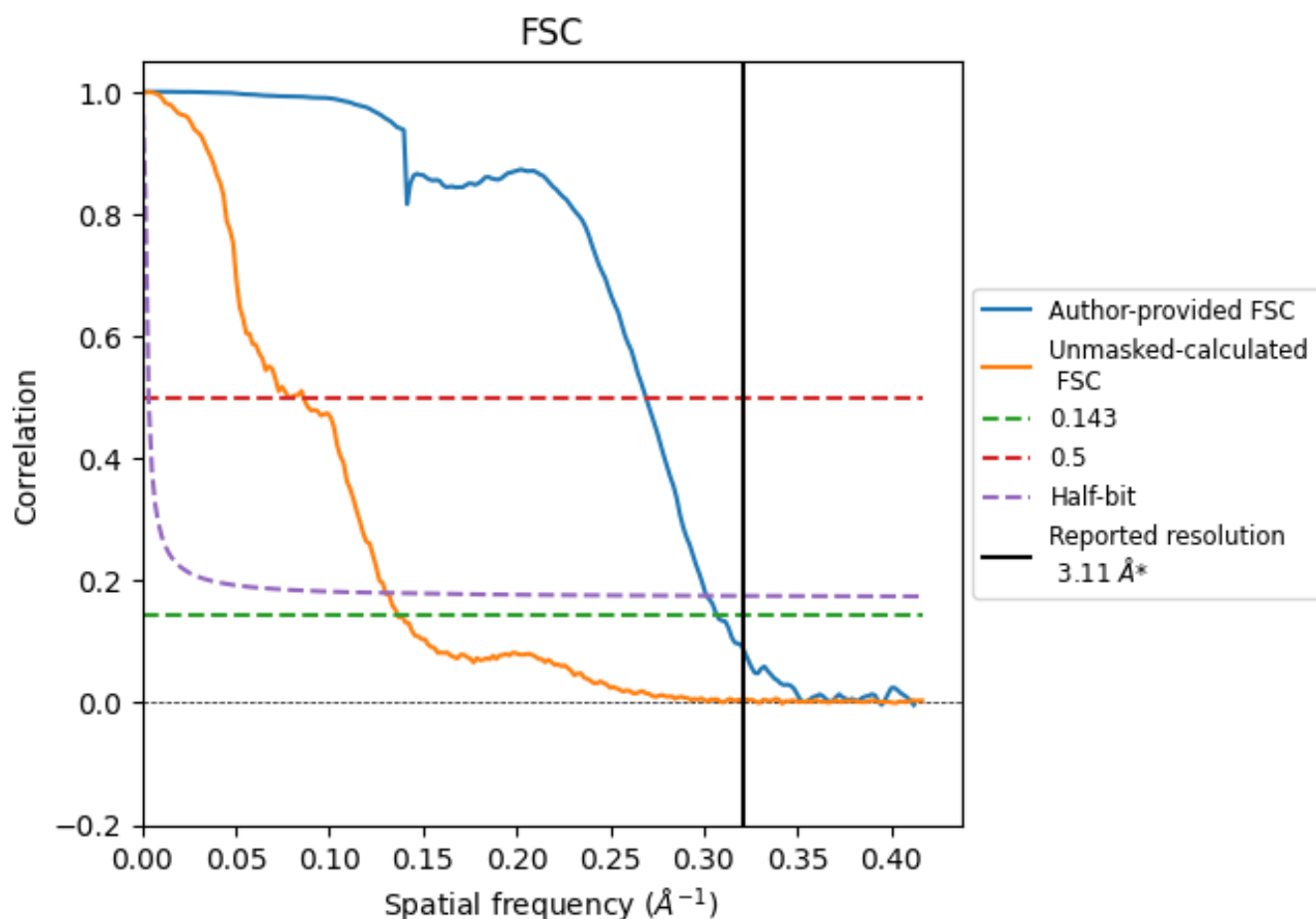


*Reported resolution corresponds to spatial frequency of 0.322 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

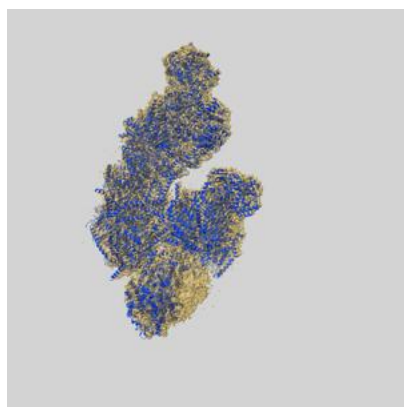
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.26	3.72	3.32
Unmasked-calculated*	7.32	12.82	7.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.32 differs from the reported value 3.11 by more than 10 %

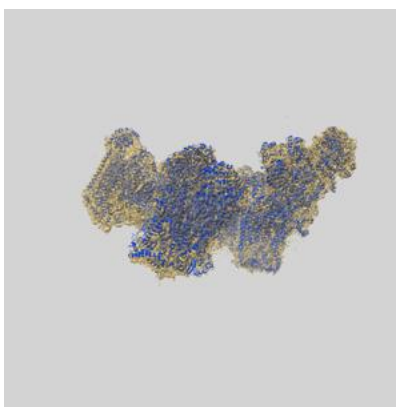
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60422 and PDB model 8ZSO. Per-residue inclusion information can be found in section [3](#) on page [30](#).

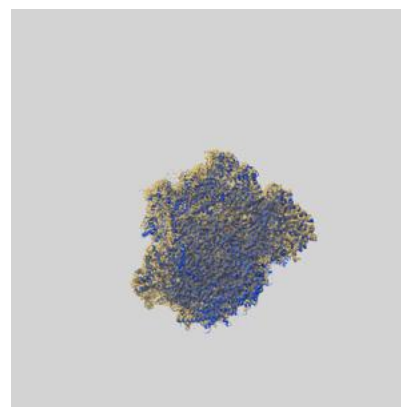
9.1 Map-model overlay [i](#)



X



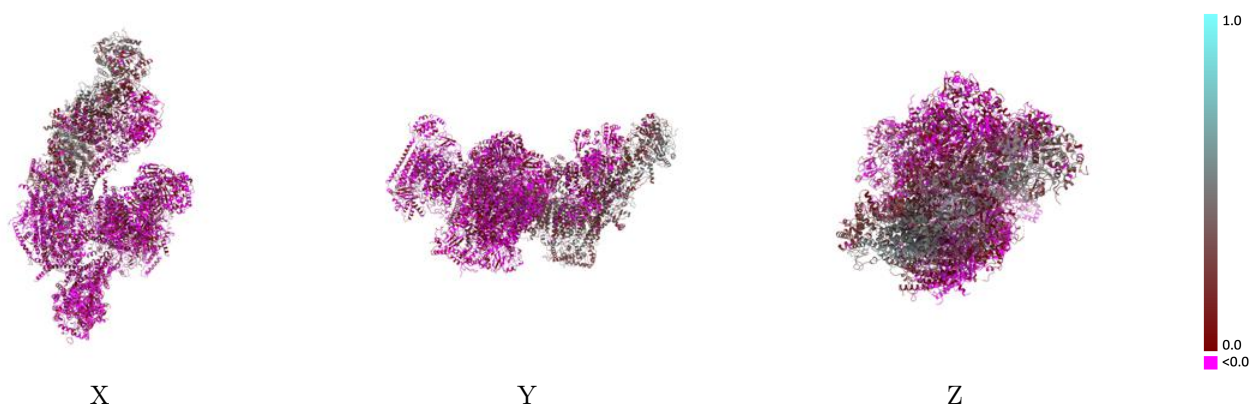
Y



Z

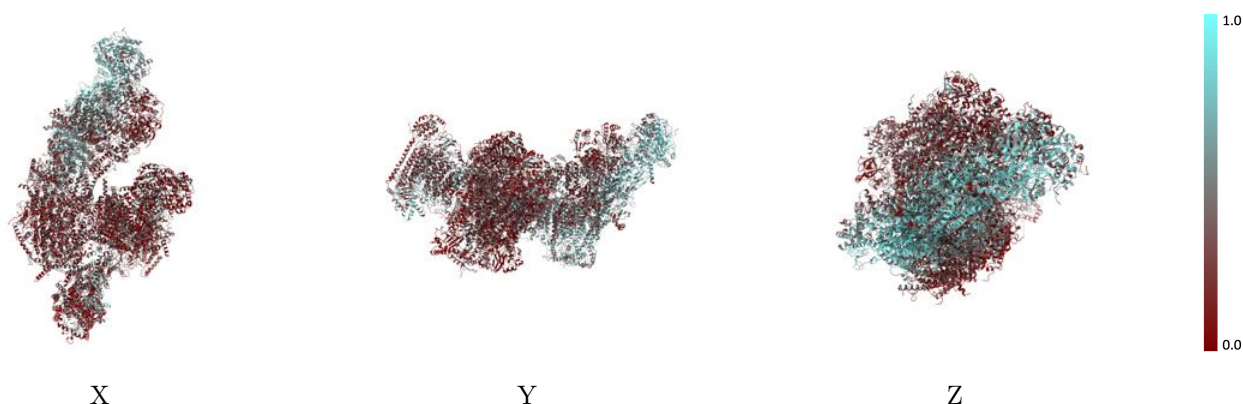
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



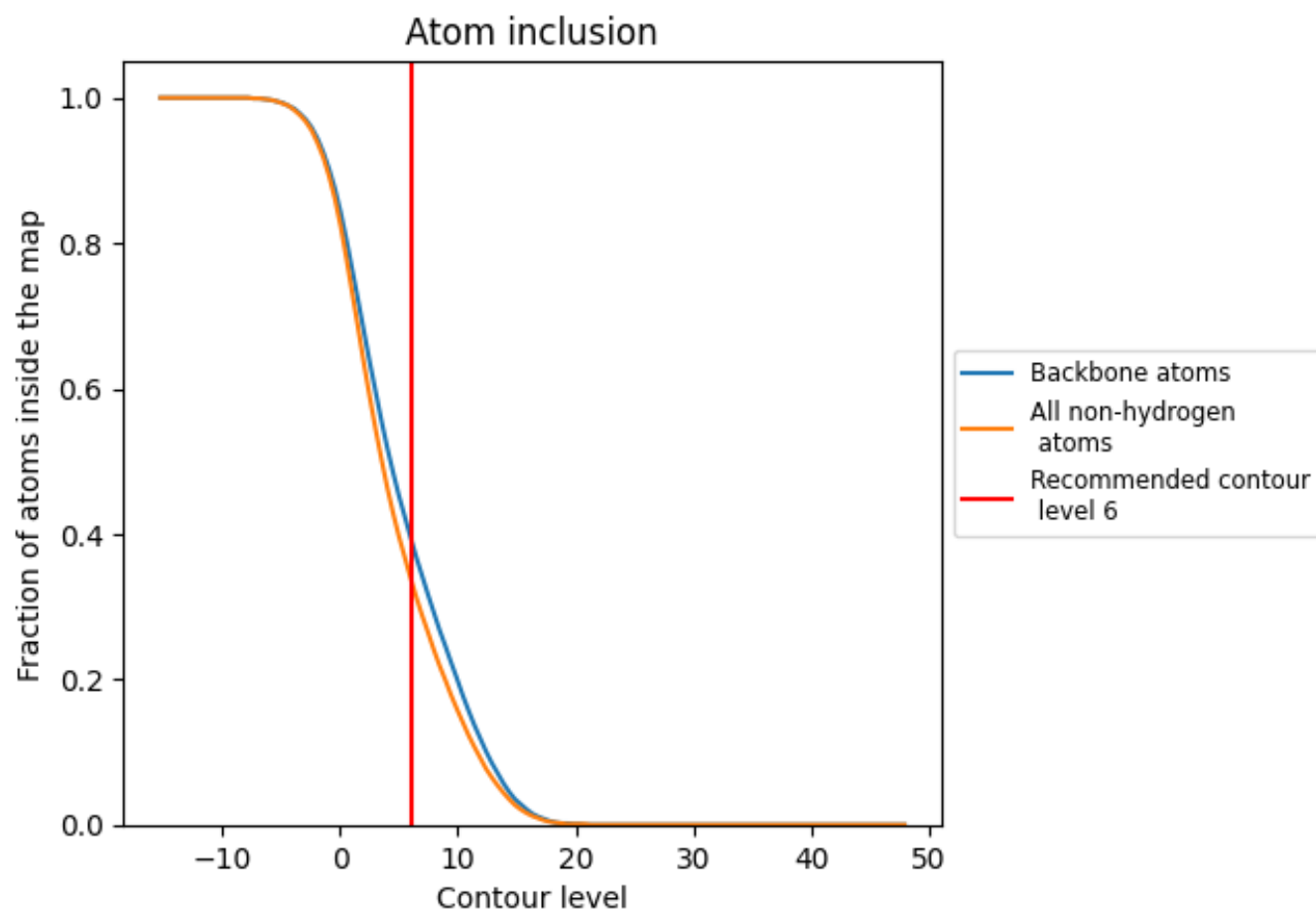
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion ⓘ



At the recommended contour level, 40% of all backbone atoms, 34% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3390	 0.0830
4L	 0.6310	 0.3660
5A	 0.2190	 -0.0300
5B	 0.3280	 -0.0290
6A	 0.3900	 -0.0110
6B	 0.5320	 0.0310
6C	 0.1700	 -0.0220
7A	 0.2190	 -0.0060
7B	 0.0550	 -0.0010
7C	 0.3450	 0.0400
8B	 0.1480	 -0.0470
A1	 0.6060	 0.3150
A2	 0.2410	 0.0140
A3	 0.7220	 0.4490
A5	 0.3120	 0.0990
A6	 0.2700	 0.0320
A7	 0.5030	 0.3660
A8	 0.5770	 0.3130
A9	 0.2600	 -0.0080
AB	 0.1740	 0.0290
AC	 0.2310	 0.0260
AK	 0.3940	 0.1700
AL	 0.2720	 0.0240
AM	 0.4170	 0.2530
AN	 0.6460	 0.3810
B1	 0.2310	 -0.0230
B2	 0.1930	 0.0190
B3	 0.1790	 0.0240
B4	 0.1930	 -0.0690
B5	 0.3180	 0.0340
B6	 0.1900	 -0.0050
B7	 0.2870	 0.0240
B8	 0.2060	 -0.0550
B9	 0.2000	 -0.0040
BK	 0.2100	 -0.0470



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Chain	Atom inclusion	Q-score
BL	 0.2040	 -0.0380
C1	 0.3640	 -0.0380
C2	 0.3820	 0.0080
C3	 0.3810	 -0.0010
C4	 0.1980	 -0.0110
CA	 0.3420	 0.0850
CB	 0.3950	 0.1270
N1	 0.6410	 0.3750
N2	 0.5170	 0.2280
N3	 0.5890	 0.3610
N4	 0.2410	 -0.0760
N5	 0.2270	 -0.0300
N6	 0.5070	 0.3170
QA	 0.2370	 0.0180
QB	 0.2310	 0.0190
QC	 0.2550	 -0.0330
QD	 0.2360	 -0.0190
QE	 0.1260	 0.0380
QF	 0.1480	 -0.0090
QG	 0.2140	 -0.0070
QH	 0.1870	 -0.0020
QI	 0.2230	 -0.0280
QJ	 0.1780	 0.0020
QK	 0.1230	 -0.0020
Qa	 0.2190	 0.0060
Qb	 0.2360	 -0.0040
Qc	 0.2200	 0.0080
Qd	 0.2190	 0.0020
Qe	 0.0950	 -0.0240
Qf	 0.1940	 -0.0450
Qg	 0.2370	 -0.0080
Qh	 0.1940	 -0.0330
Qi	 0.2020	 0.0360
Qj	 0.2110	 0.0490
S1	 0.3490	 0.0710
S2	 0.6190	 0.3260
S3	 0.3940	 0.1080
S4	 0.3290	 0.0790
S5	 0.6050	 0.3740
S6	 0.4560	 0.1940
S7	 0.5750	 0.2630
S8	 0.6830	 0.3730

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Chain	Atom inclusion	Q-score
V1	 0.6430	 0.3620
V2	 0.6090	 0.3610
V3	 0.5260	 0.3240