



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 05:59 AM UTC

PDB ID : 8IAO / pdb_00008iao
EMDB ID : EMD-35313
Title : Respiratory complex CI:CIII2, type I, Wild type mouse under thermoneutral temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

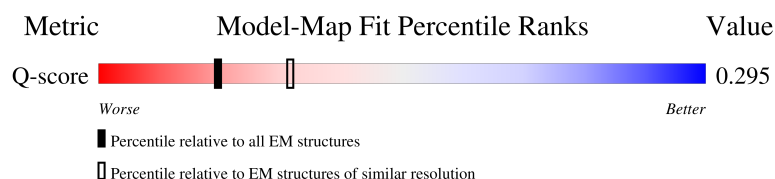
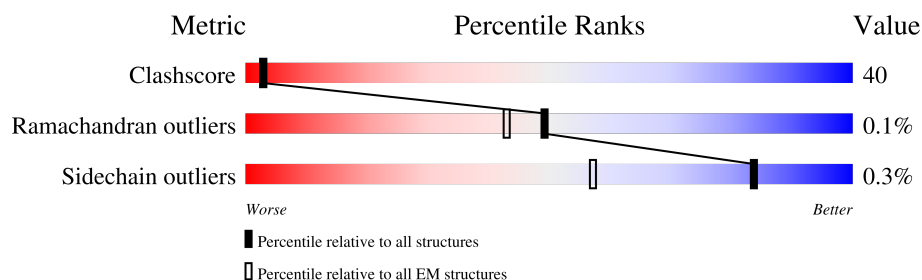
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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.

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1	A	115	
2	B	224	
3	C	263	
4	D	463	

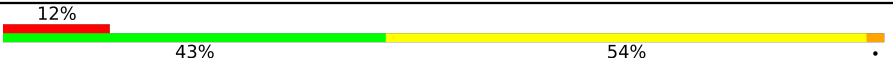
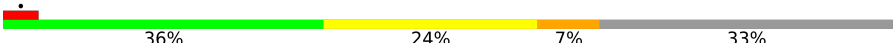
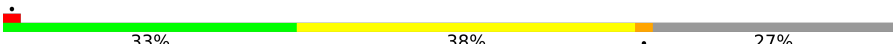
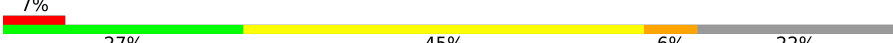
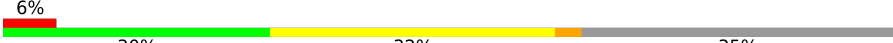
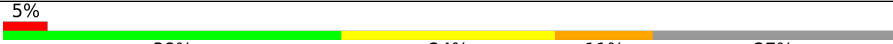
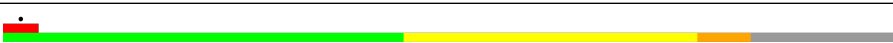
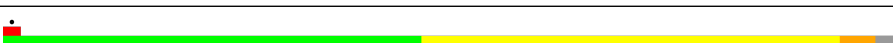
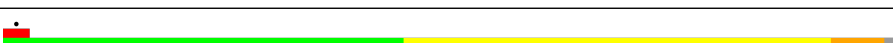
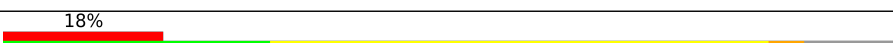
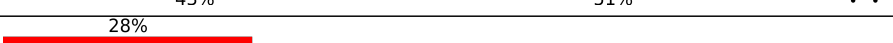
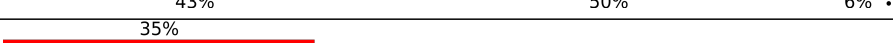
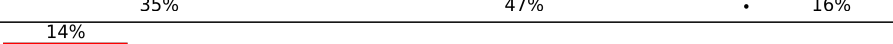
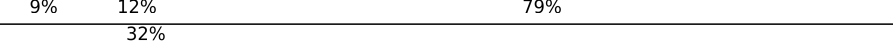
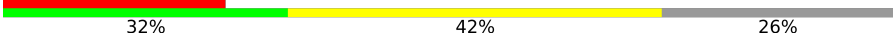
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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	

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Mol	Chain	Length	Quality of chain
49	AI	274	
49	Ae	274	
49	Ai	274	
50	AF	111	
50	Af	111	
51	AG	82	
51	Ag	82	
52	AH	89	
52	Ah	89	
53	AJ	64	
53	Aj	64	
54	AK	56	
54	Ak	56	

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
56	CDL	A	402	-	-	X	-
57	SF4	B	301	-	-	X	-
57	SF4	F	502	-	-	X	-
57	SF4	G	802	-	-	X	-
57	SF4	I	302	-	-	X	-
57	SF4	I	303	-	-	X	-
58	UQ1	D	501	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
68	U10	Ac	404	-	-	X	-
69	UQ6	AC	406	-	-	X	-

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 98999 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	92	Total	C	N	O	S	0	0
			754	523	107	119	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1641	1060	279	299	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	424	Total	C	N	O	S	0	0
			3416	2184	587	621	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1635	1039	275	310	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total	C	N	O	S	0	0
			3288	2073	588	605	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total	C	N	O	S	0	0
			2532	1702	383	425	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1287	866	183	223	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	97	Total	C	N	O	S	0	0
			729	473	111	135	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	52	Total	C	N	O	S	0	0
			447	290	80	75	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	100	Total	C	N	O	S	0	0
			839	546	146	144	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	68	Total	C	N	O	S	0	0
			578	378	96	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	76	Total	C	N	O	S	0	0
			618	410	105	101	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	125	Total	C	N	O		0	0
			1044	673	188	183			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	123	Total	C	N	O	S	0	0
			1050	661	198	182	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	172	Total	C	N	O	S	0	0
			1452	911	260	273	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			764	482	143	136	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	22	Total	C	N	O	0	0
			189	124	29	36		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	403	Total	C	N	O	S	0	0
			3153	1970	560	607	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	412	Total	C	N	O	S	0	0
			3225	2016	569	624	16		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
46	Ab	412	Total	C	N	O	S	0	0
			3094	1945	542	598	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
47	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		
48	Ad	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
49	AI	30	Total	C	N	O		0	0
			217	138	42	37			
49	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
49	Ai	28	Total	C	N	O		0	0
			207	133	40	34			

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AF	98	Total	C	N	O	S	0	0
			864	552	154	155	3		
50	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
51	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	68	Total	C	N	O	S	0	0
			562	343	103	111	5		
52	Ah	68	Total	C	N	O	S	0	0
			562	343	103	111	5		

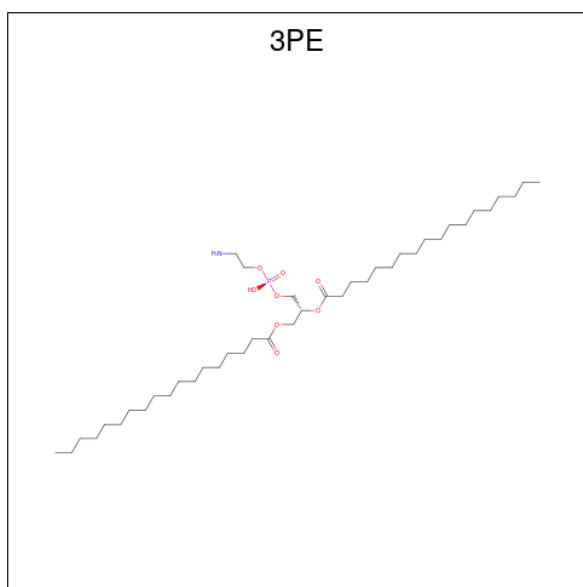
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
53	Aj	48	Total	C	N	O	0	0
			391	257	66	68		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	49	Total	C	N	O	S	0	0
			401	266	71	63	1		
54	Ak	49	Total	C	N	O	S	0	0
			401	266	71	63	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



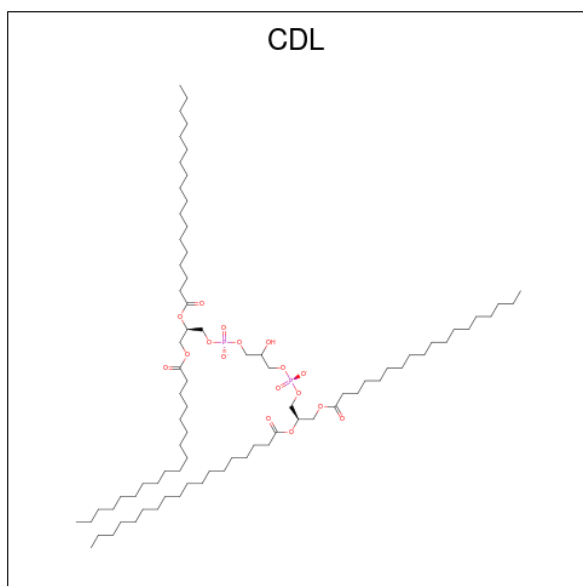
Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
55	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Y	1	Total	C	N	O	P	0
			39	29	1	8	1	
55	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	AC	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
55	AG	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 56 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



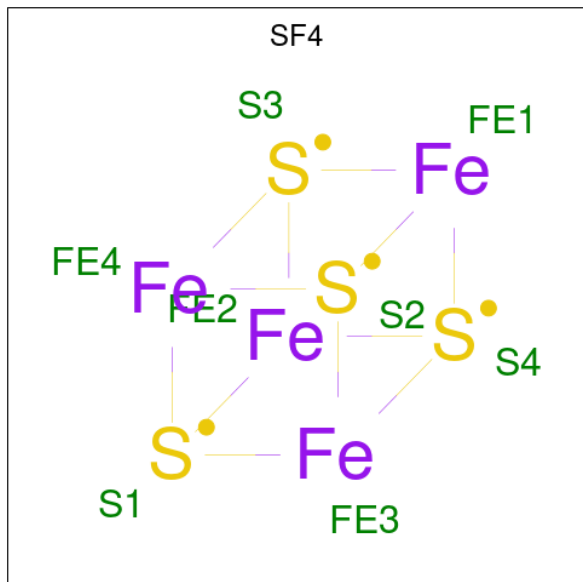
Mol	Chain	Residues	Atoms				AltConf
56	A	1	Total	C	O	P	0
			92	73	17	2	
56	L	1	Total	C	O	P	0
			74	55	17	2	
56	M	1	Total	C	O	P	0
			79	60	17	2	
56	Y	1	Total	C	O	P	0
			81	62	17	2	
56	d	1	Total	C	O	P	0
			84	65	17	2	
56	h	1	Total	C	O	P	0
			93	74	17	2	
56	q	1	Total	C	O	P	0
			57	38	17	2	

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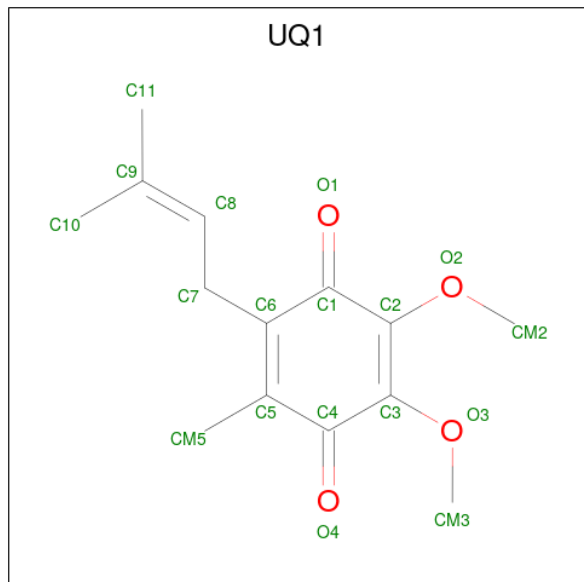
Mol	Chain	Residues	Atoms				AltConf
56	AG	1	Total	C	O	P	0
			42	23	17	2	
56	AG	1	Total	C	O	P	0
			56	37	17	2	
56	Aa	1	Total	C	O	P	0
			46	27	17	2	
56	Ag	1	Total	C	O	P	0
			42	23	17	2	
56	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



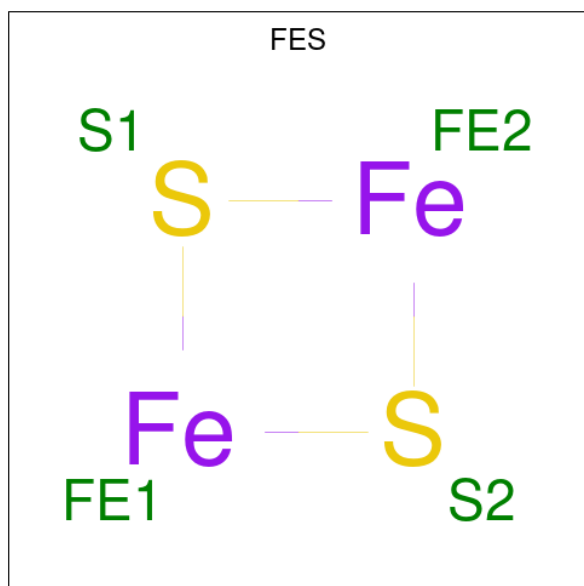
Mol	Chain	Residues	Atoms			AltConf
57	B	1	Total	Fe	S	0
			8	4	4	
57	F	1	Total	Fe	S	0
			8	4	4	
57	G	1	Total	Fe	S	0
			8	4	4	
57	G	1	Total	Fe	S	0
			8	4	4	
57	I	1	Total	Fe	S	0
			8	4	4	
57	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 58 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
58	D	1	Total	C	O	0
			18	14	4	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



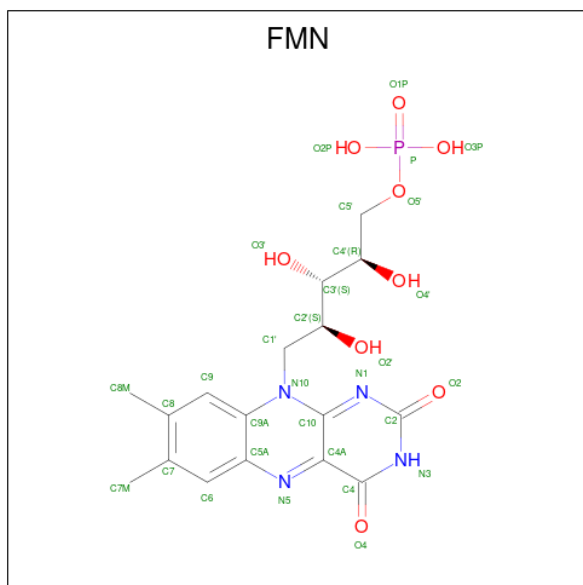
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	

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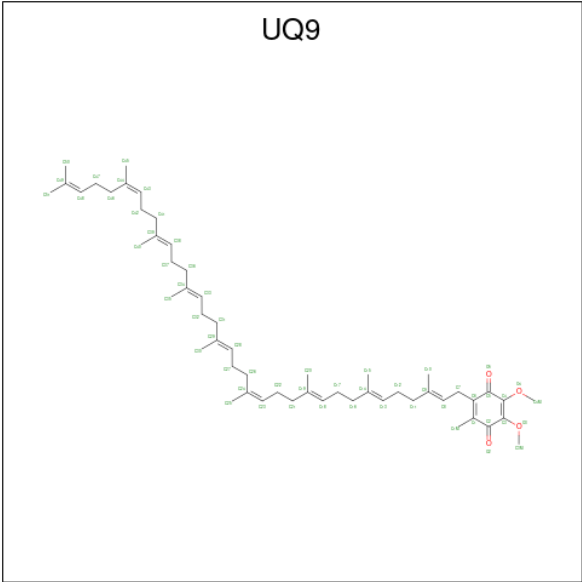
Mol	Chain	Residues	Atoms			AltConf
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



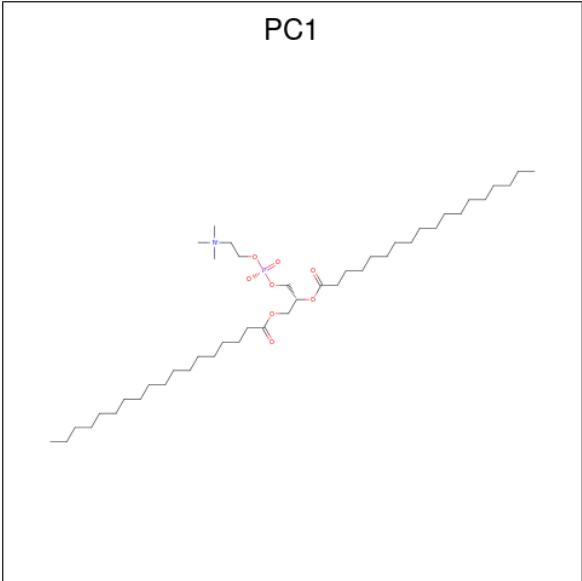
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 61 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 62 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



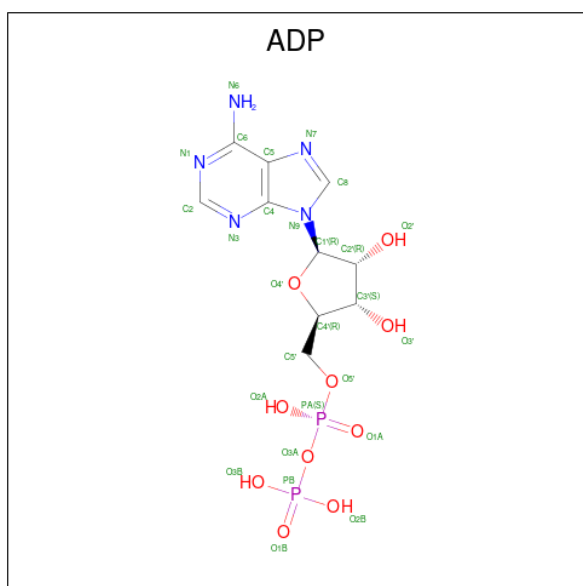
Mol	Chain	Residues	Atoms					AltConf
62	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
62	L	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
62	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
62	q	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	Ae	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 63 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 64 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

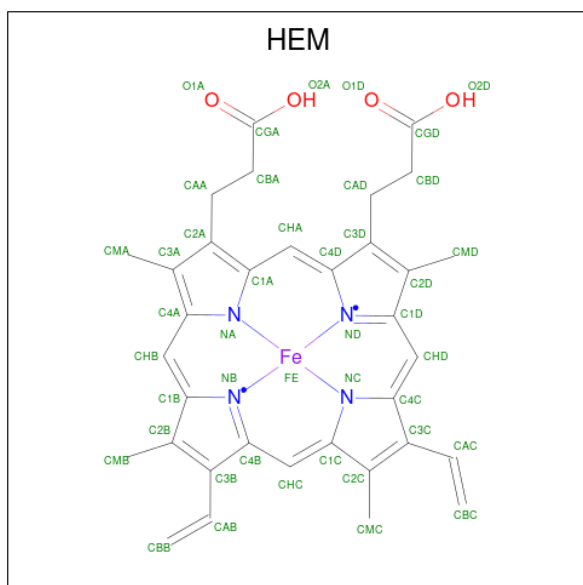
Mol	Chain	Residues	Atoms		AltConf
65	R	1	Total 1	Zn 1	0

- Molecule 66 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).



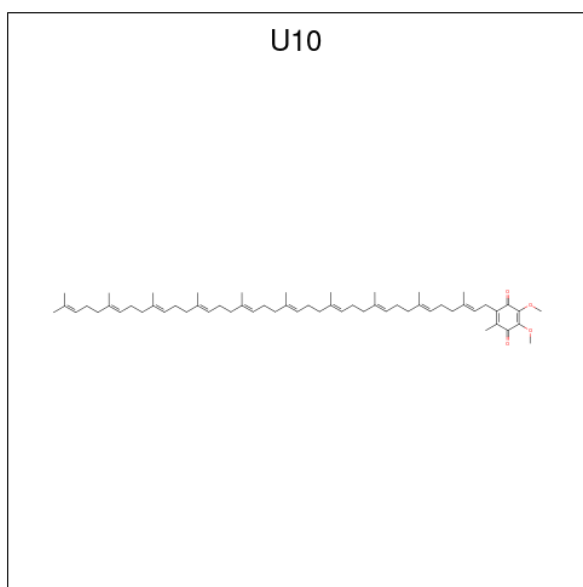
Mol	Chain	Residues	Atoms						AltConf
66	W	1	Total 32	C 19	N 2	O 9	P 1	S 1	0
66	n	1	Total 32	C 19	N 2	O 9	P 1	S 1	0

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



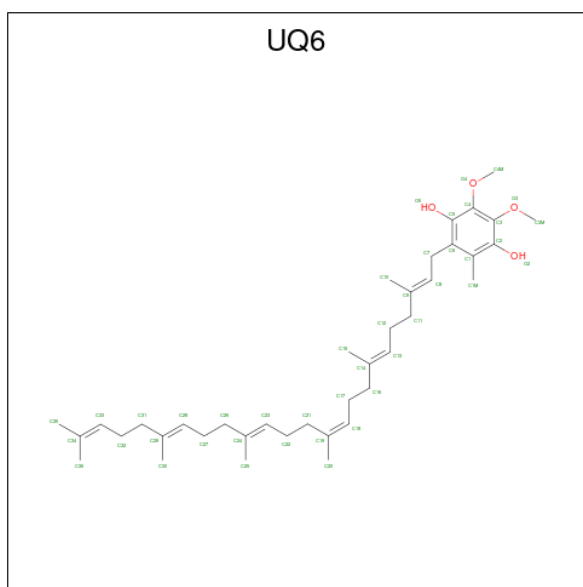
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 68 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			23	19	4	
68	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 69 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



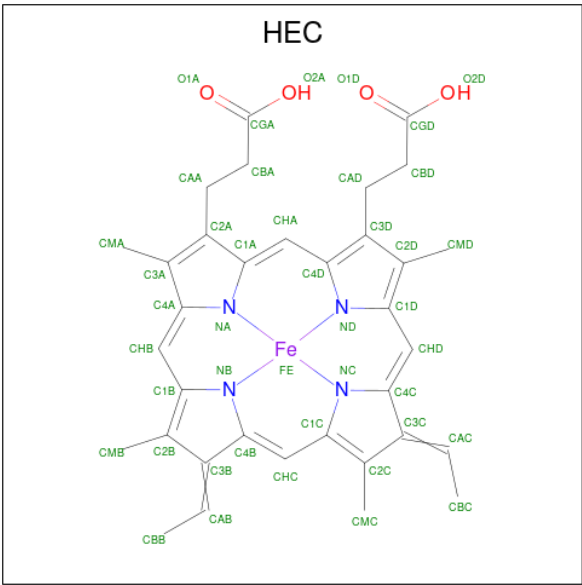
Mol	Chain	Residues	Atoms			AltConf
69	AC	1	Total	C	O	0
			28	24	4	

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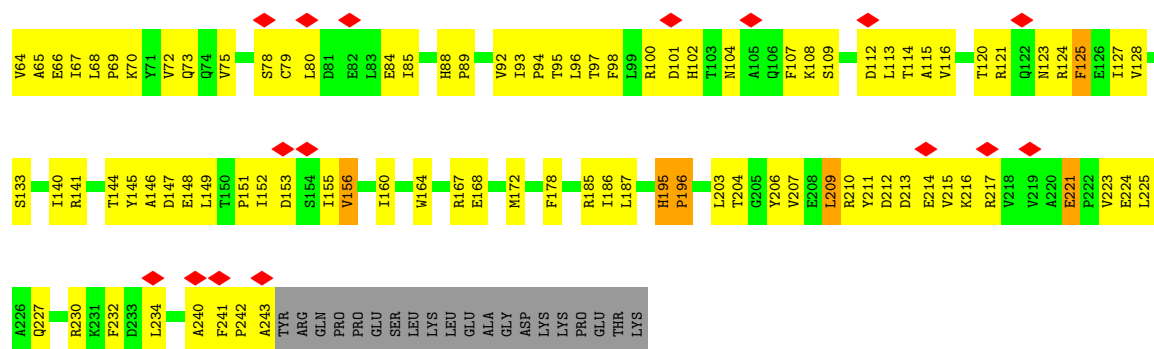
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Mol	Chain	Residues	Atoms			AltConf
69	Ac	1	Total	C	O	0
			28	24	4	

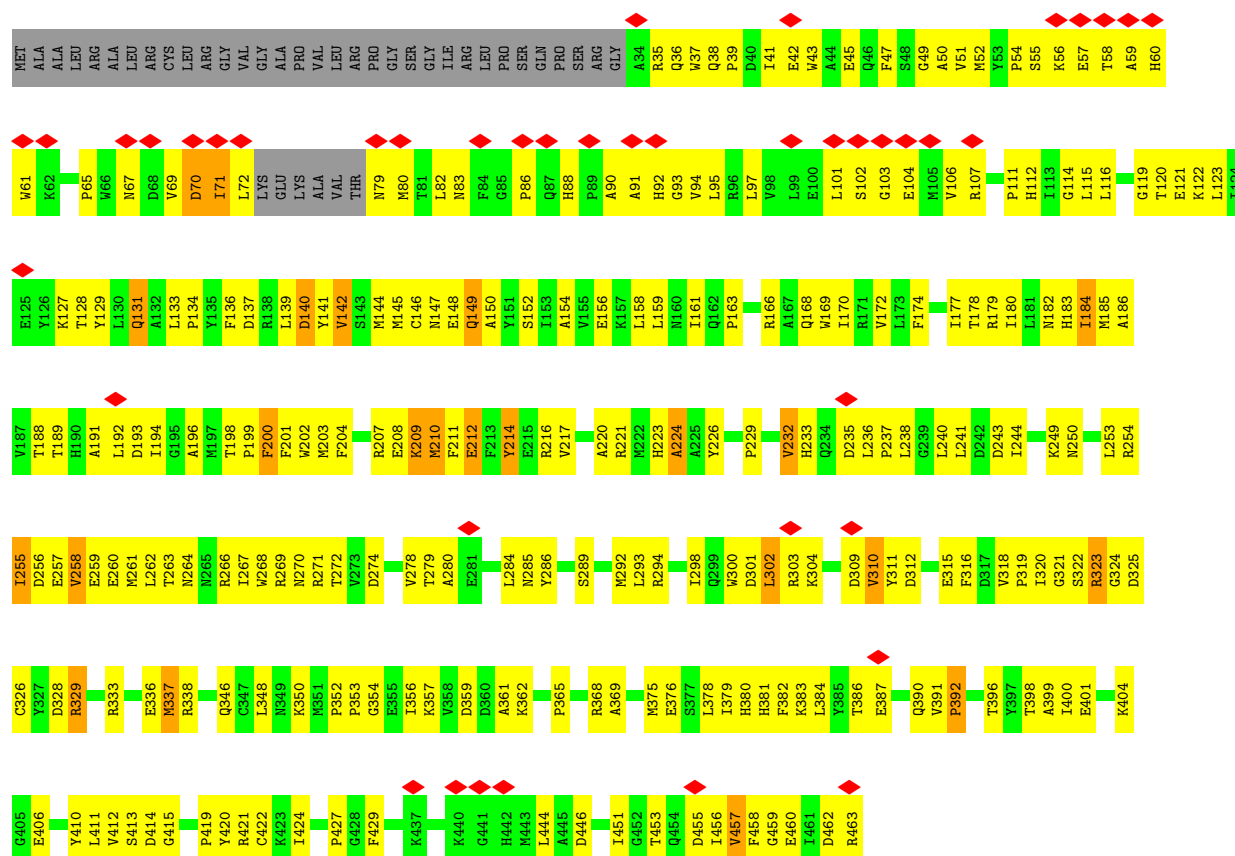
- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



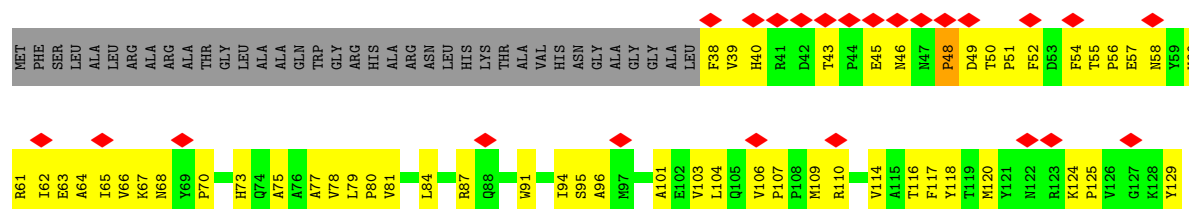
Mol	Chain	Residues	Atoms					AltConf
70	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

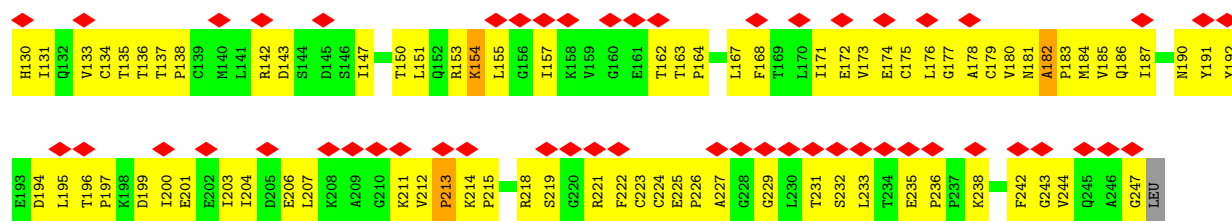


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

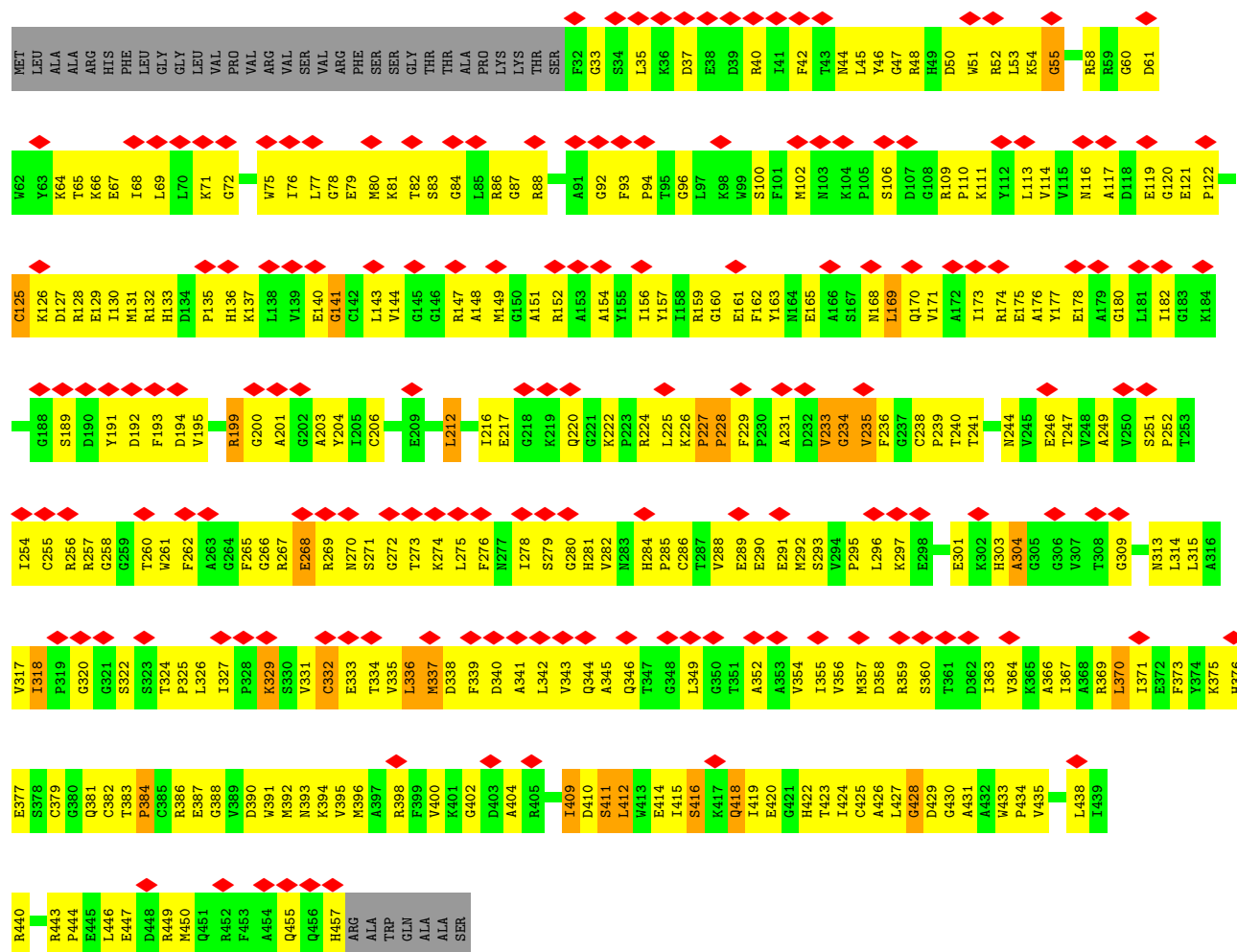


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



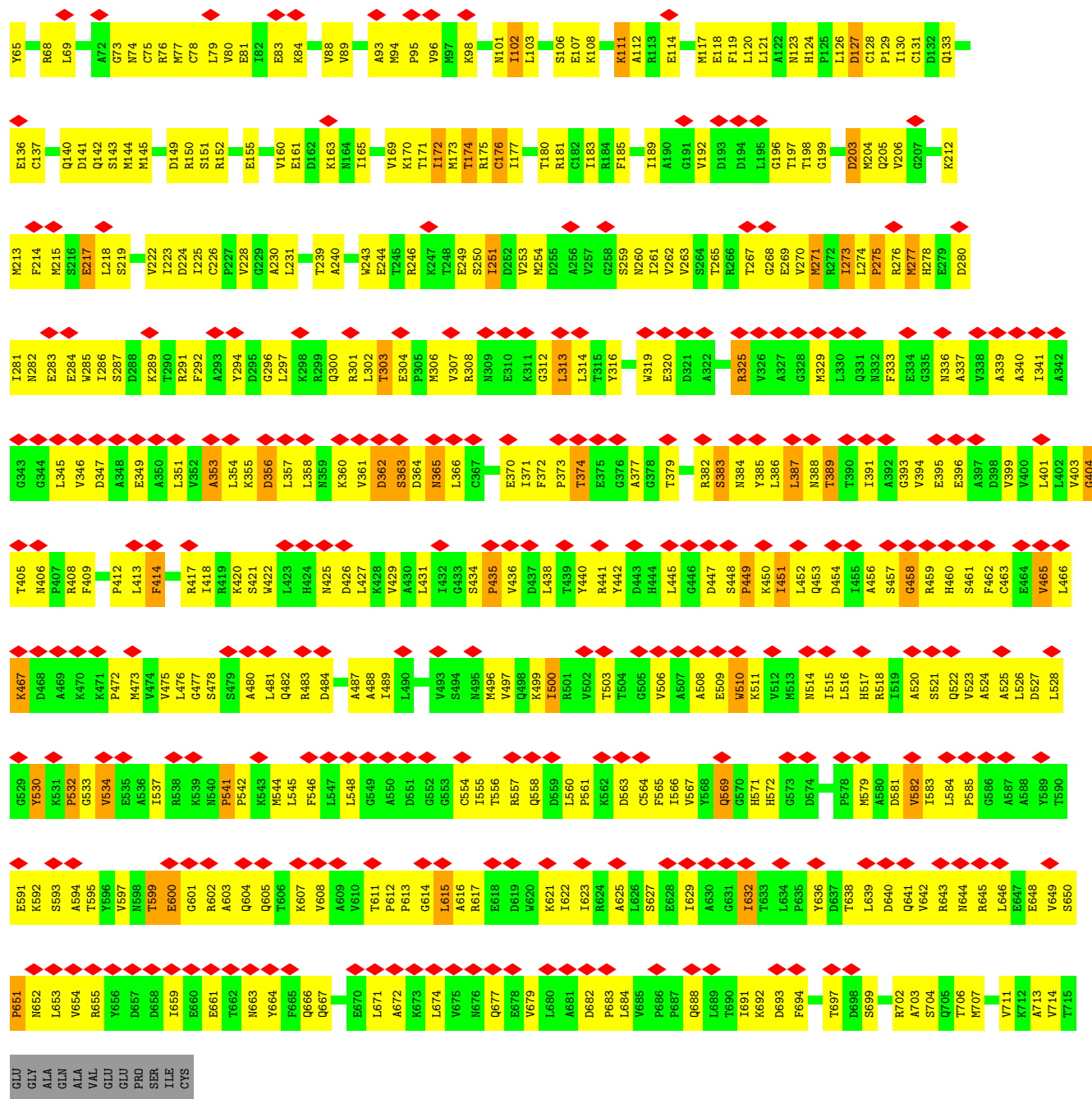


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

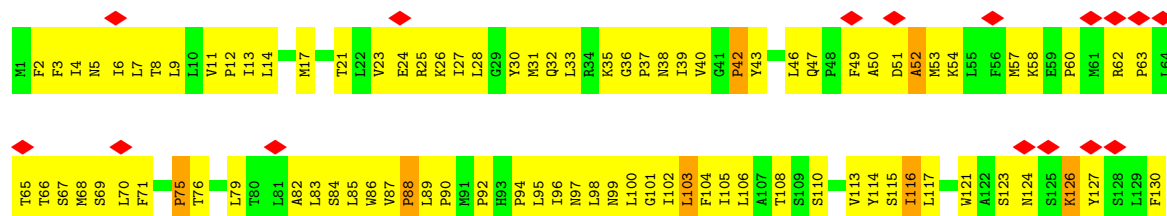


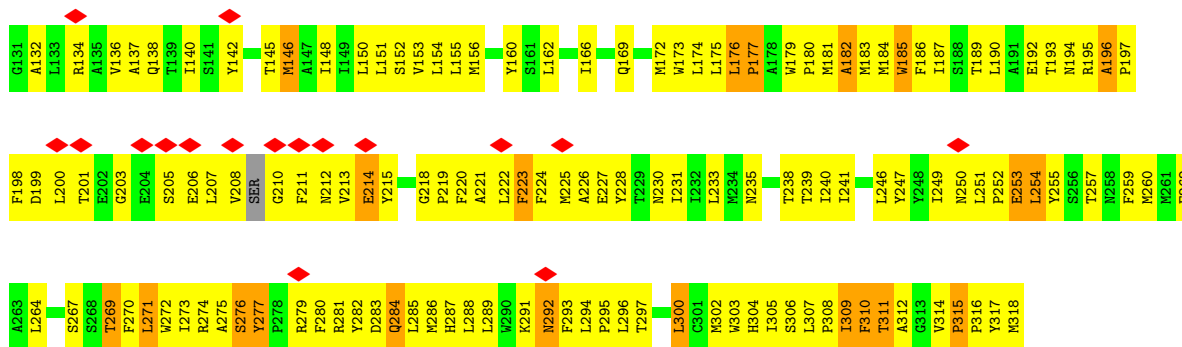
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



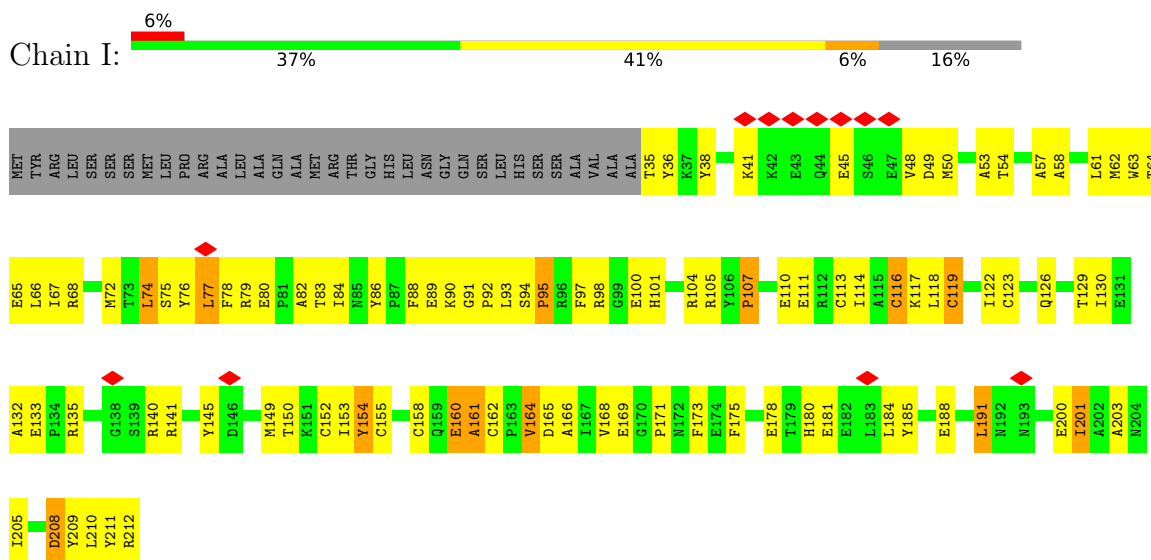


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

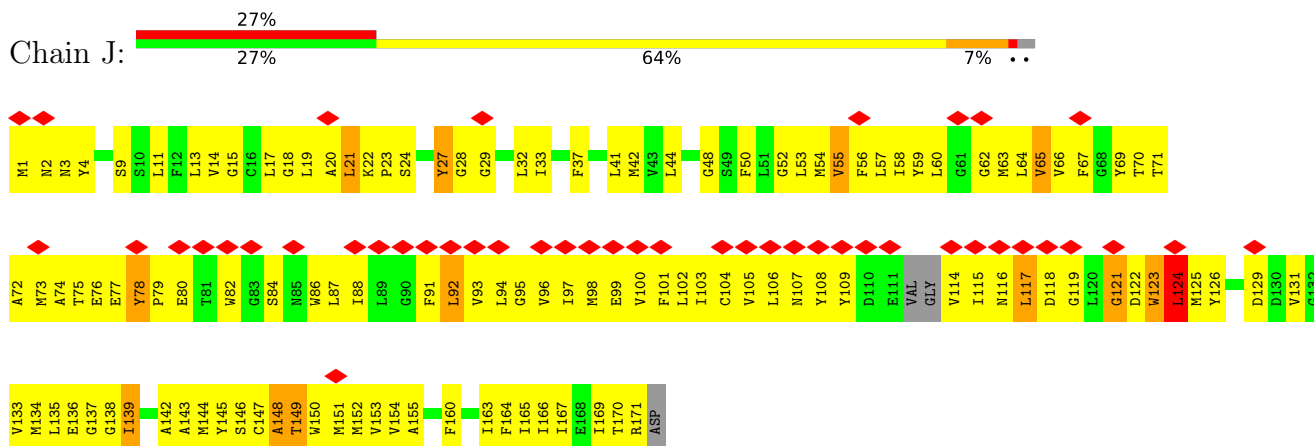




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

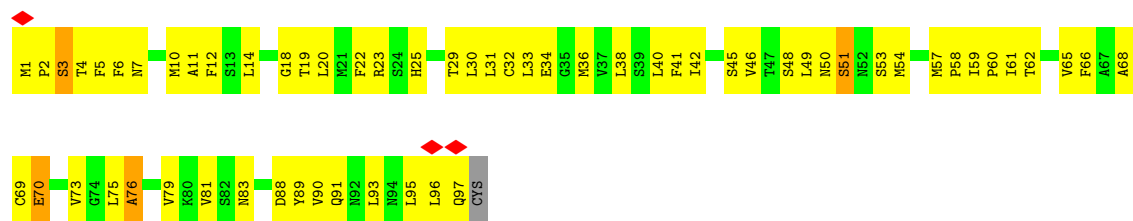


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

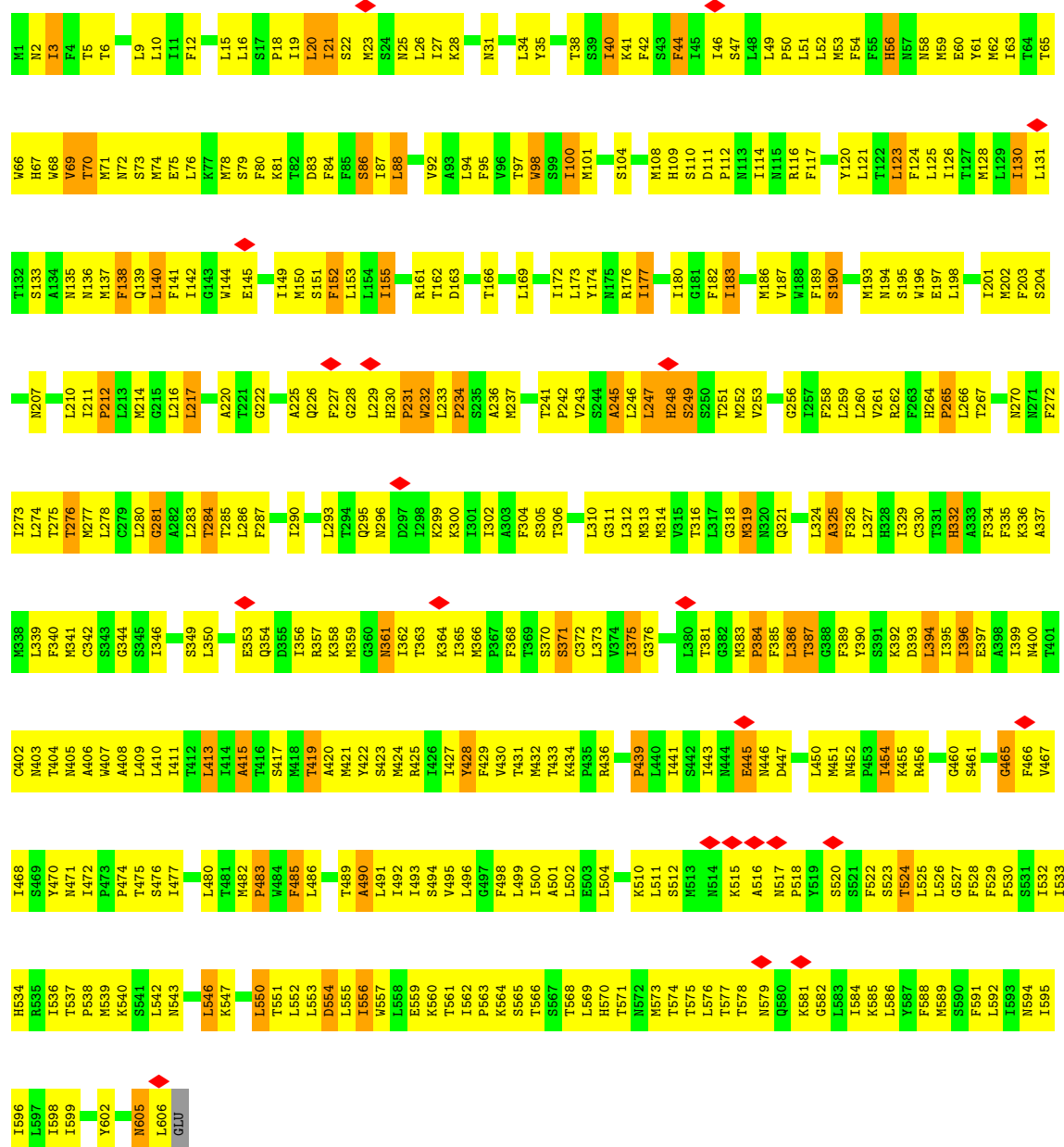


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

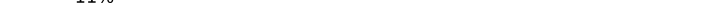


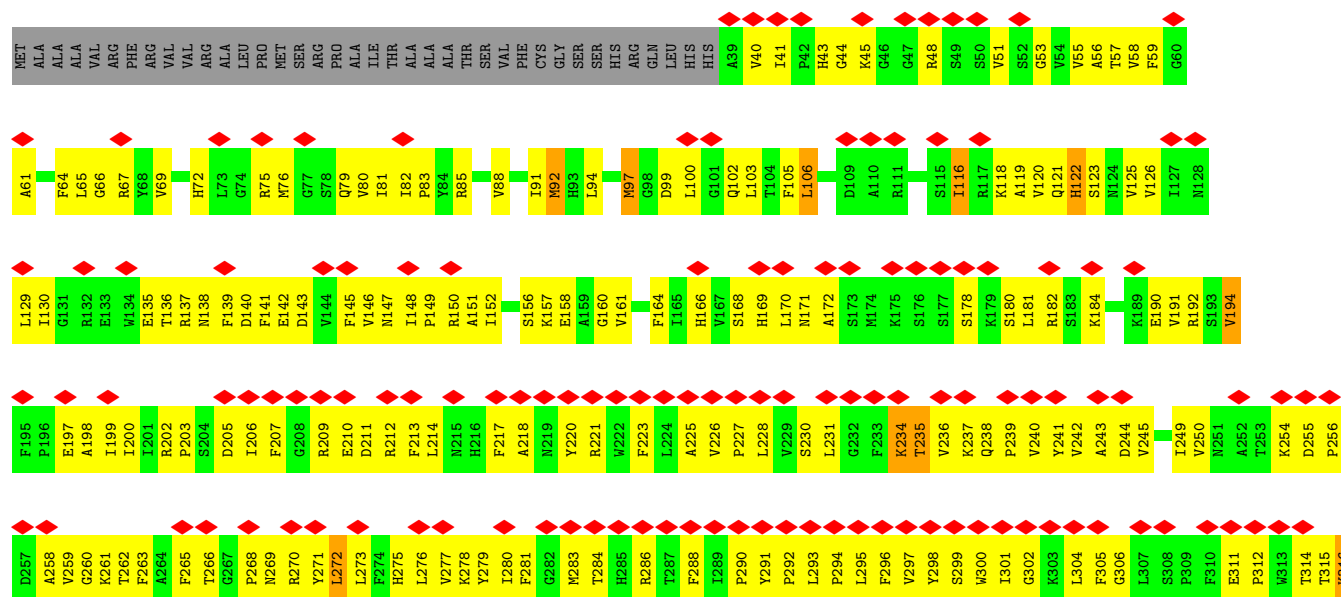
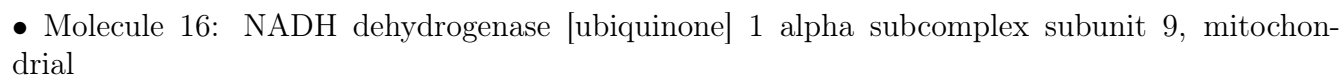


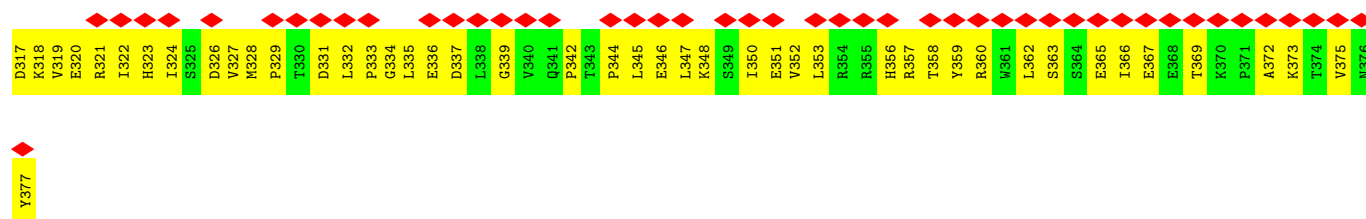
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



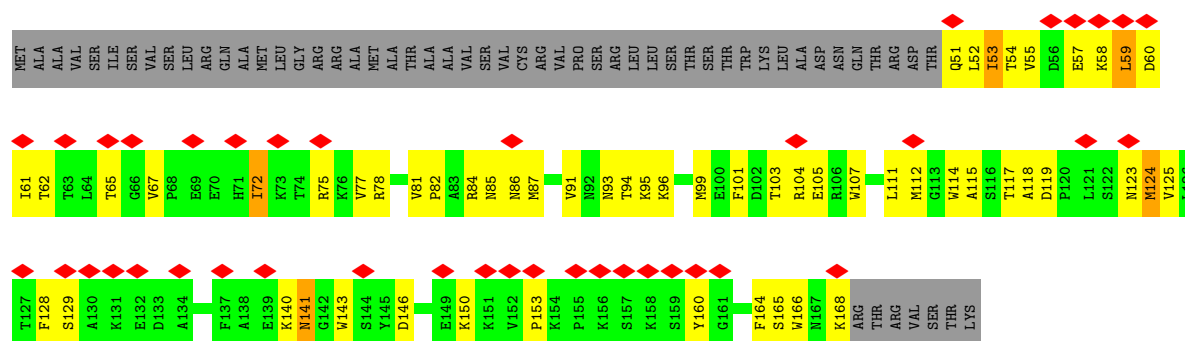
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

- Chain O:  11% 28% 57% 5% 10%

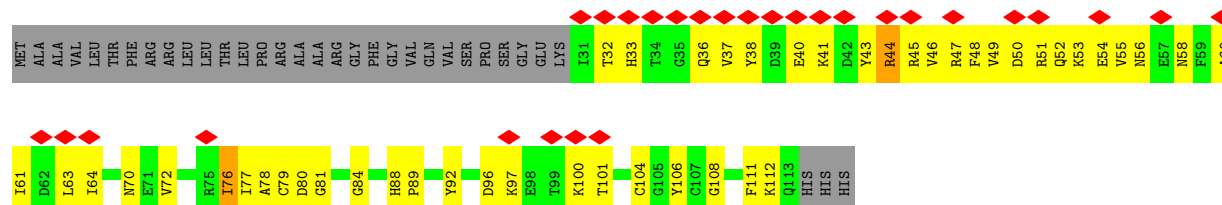




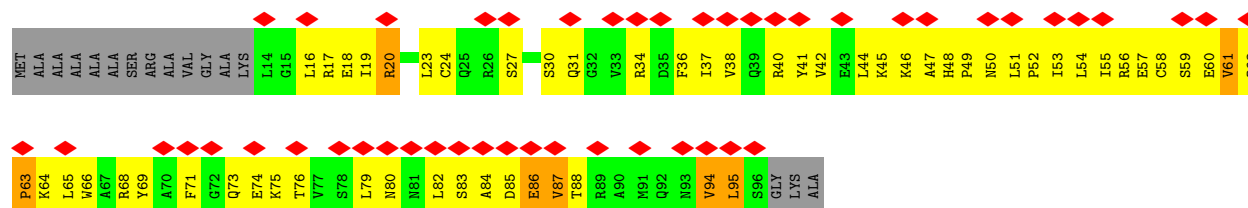
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

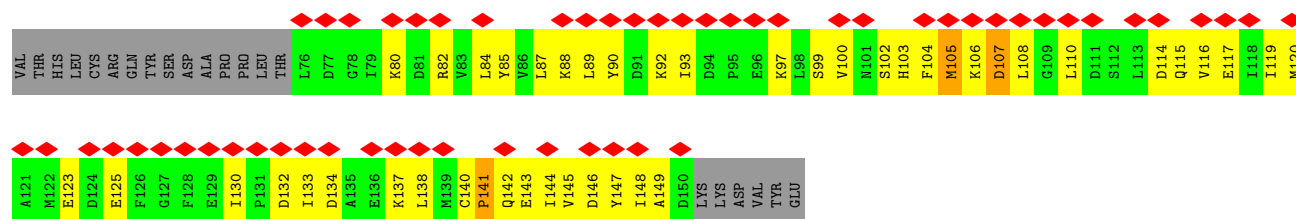


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



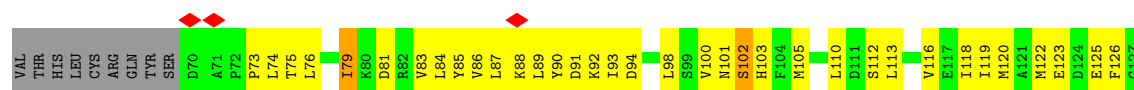
- Molecule 20: Acyl carrier protein, mitochondrial





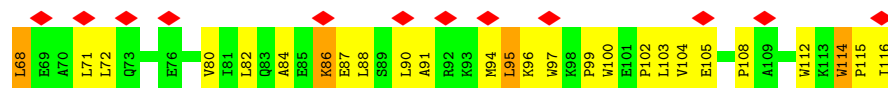
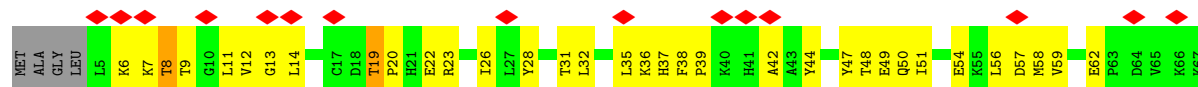
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U: 20% 31% 44%



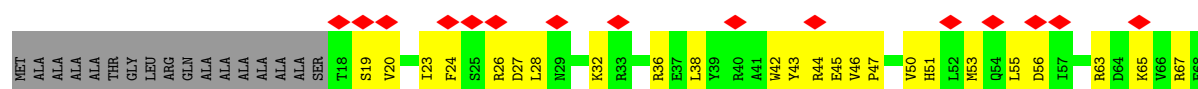
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V: 23% 45% 47% 5%



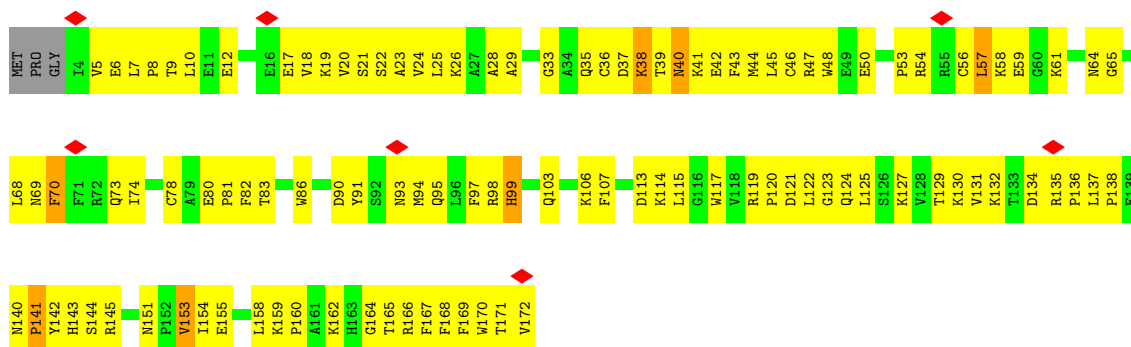
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W: 35% 40% 44% 13%

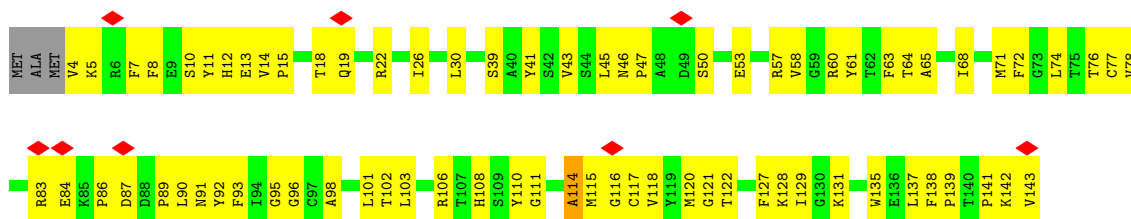


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

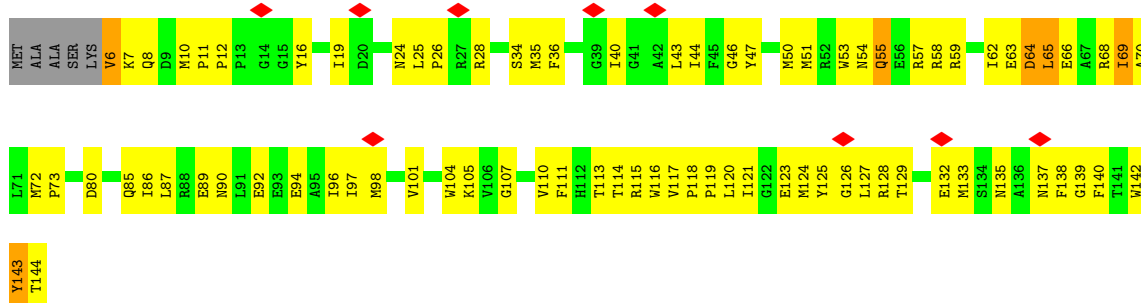
Chain X: 34% 60% 6%



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

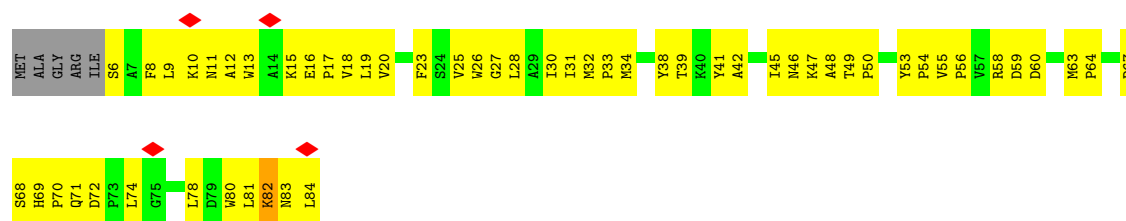


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

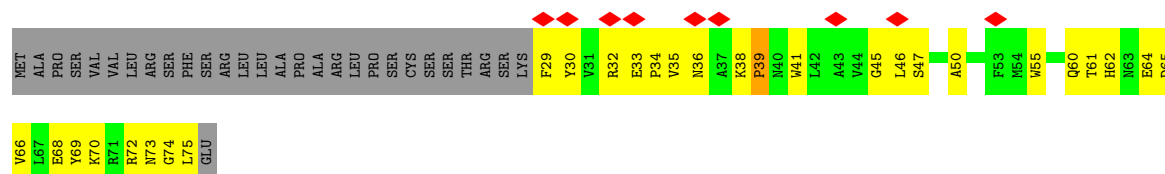
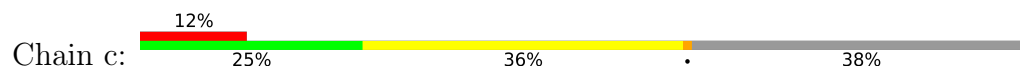


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

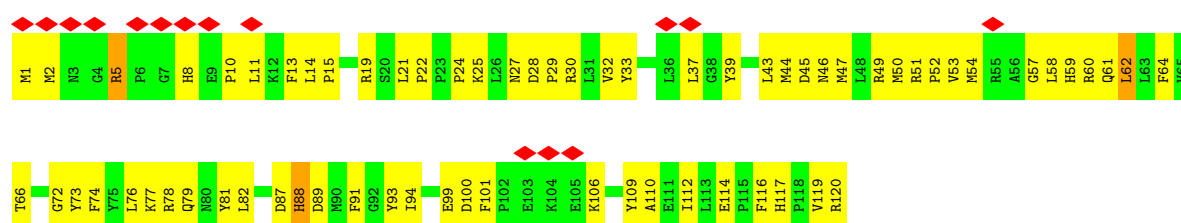
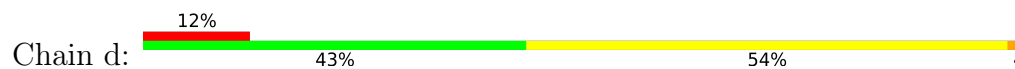




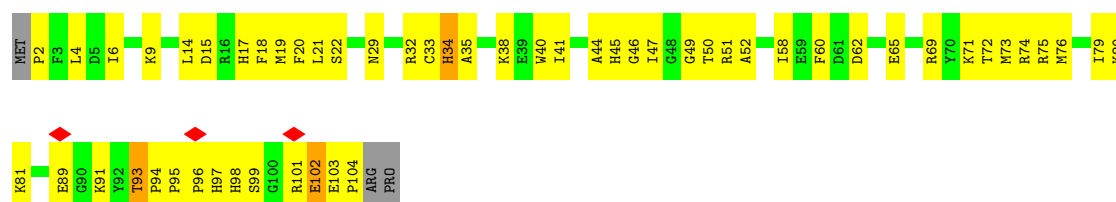
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



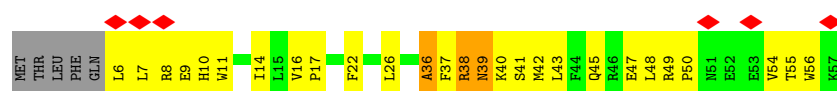
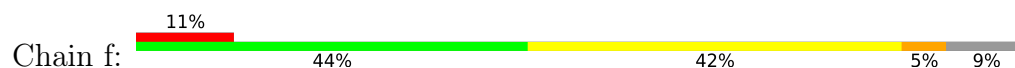
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



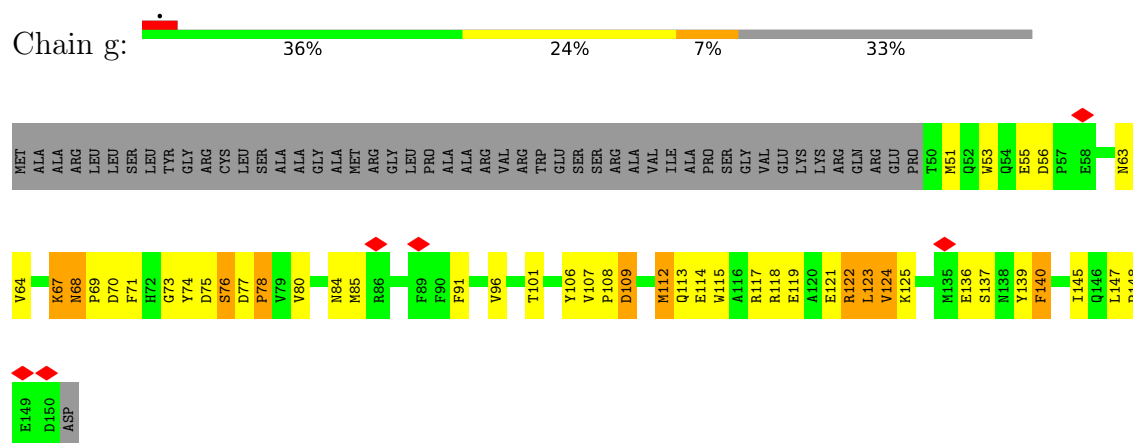
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



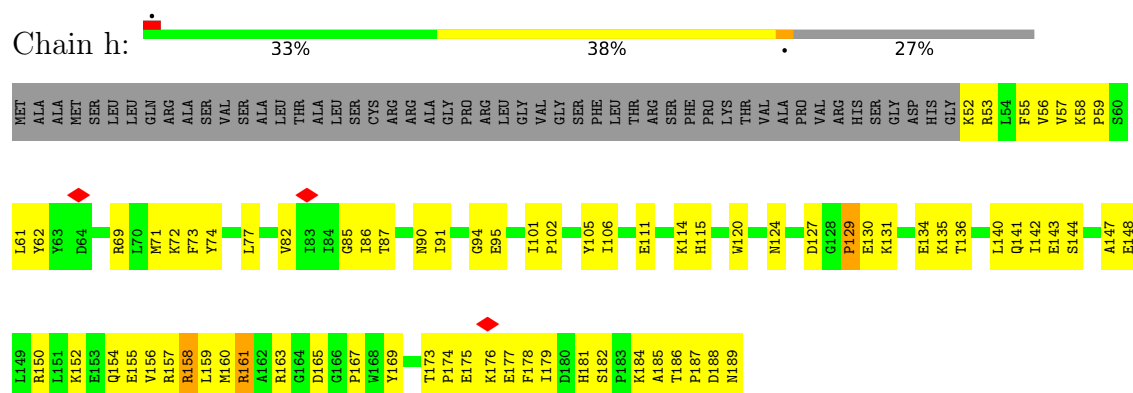
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



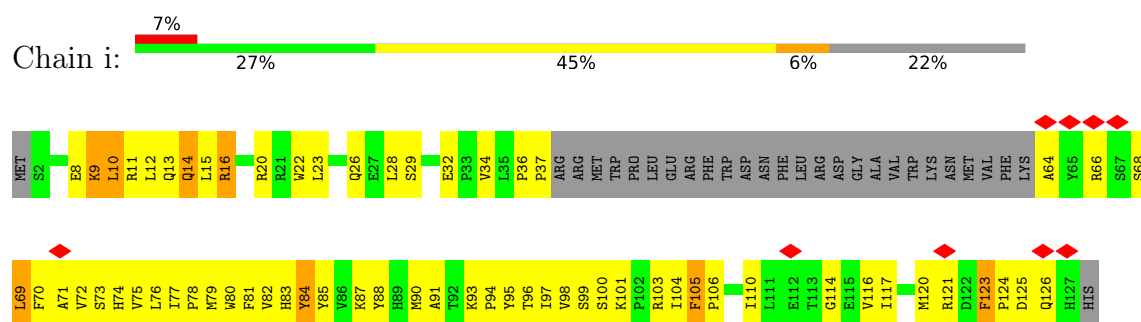
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



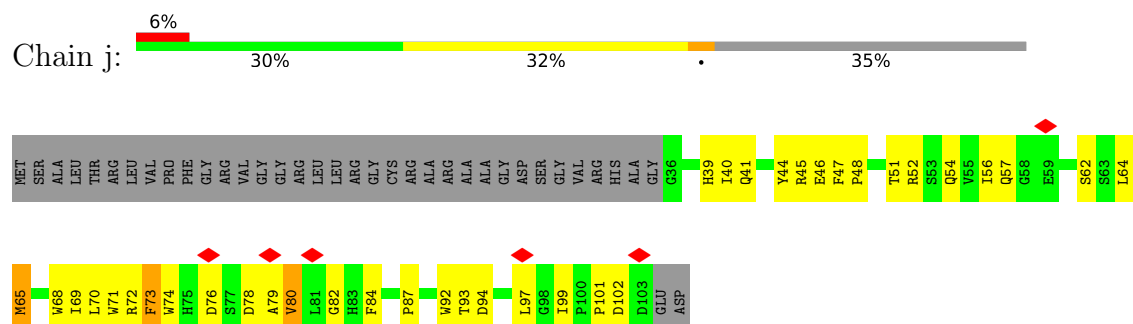
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



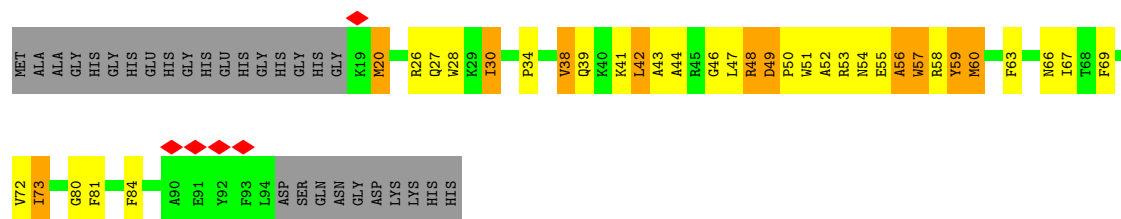
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



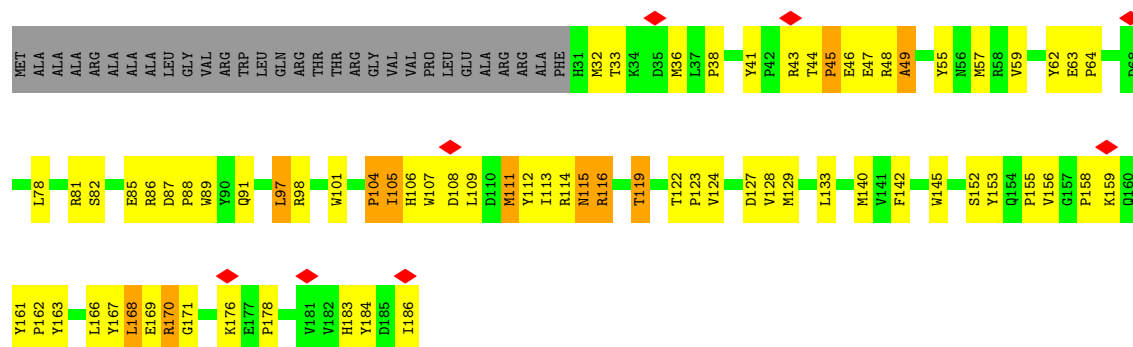
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



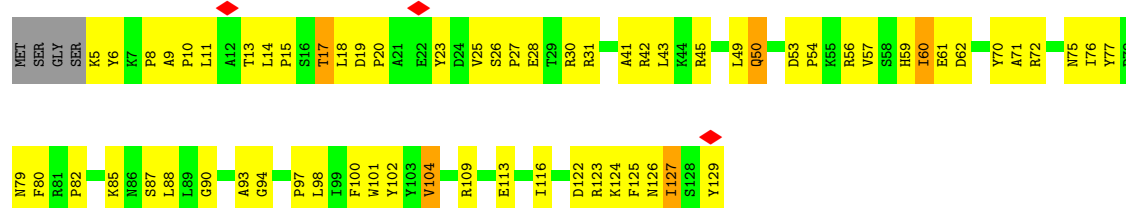
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



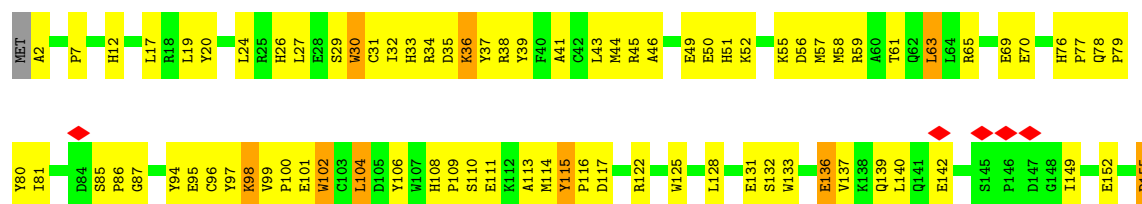
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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

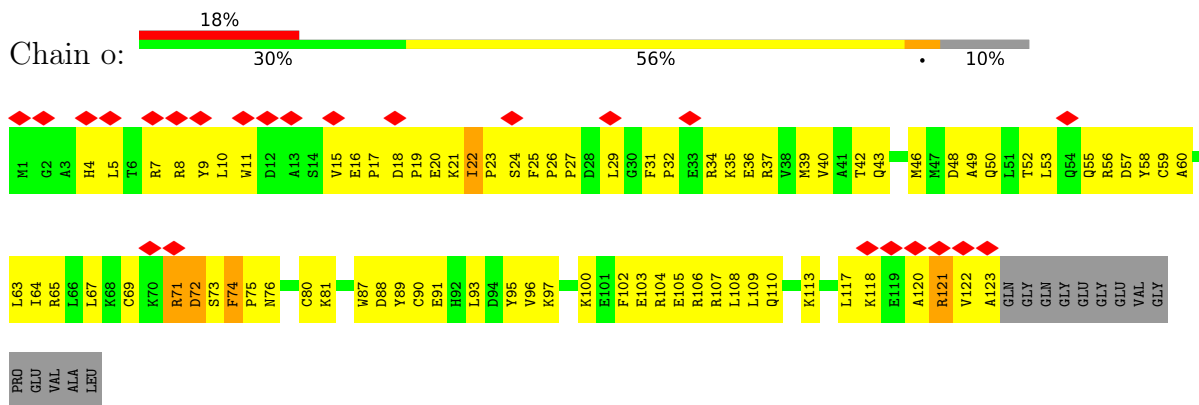


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

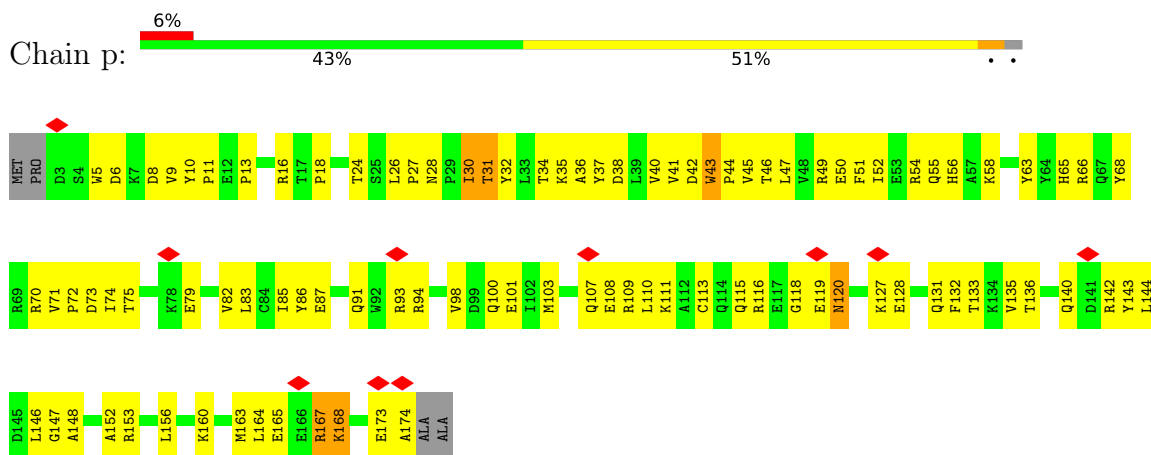




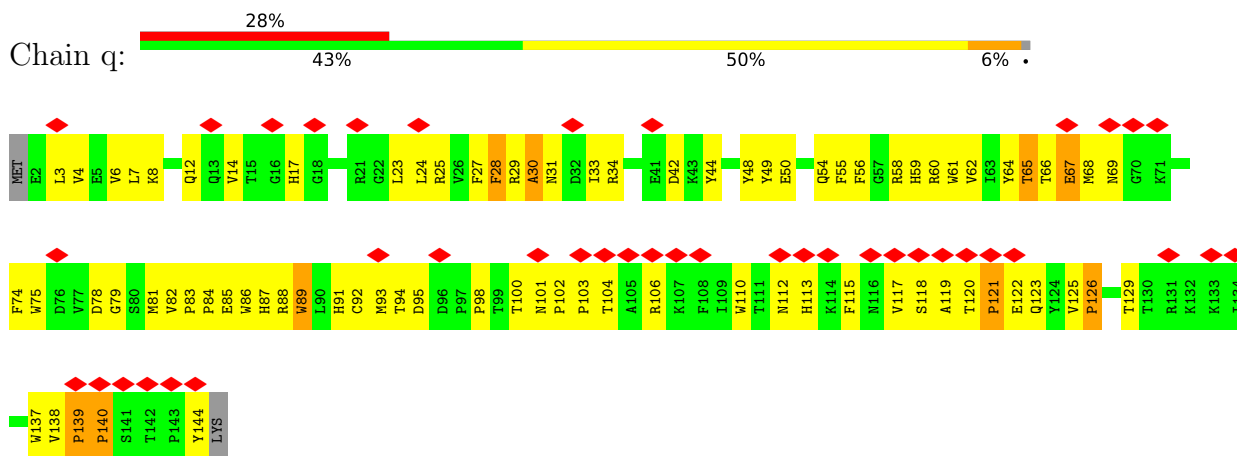
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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

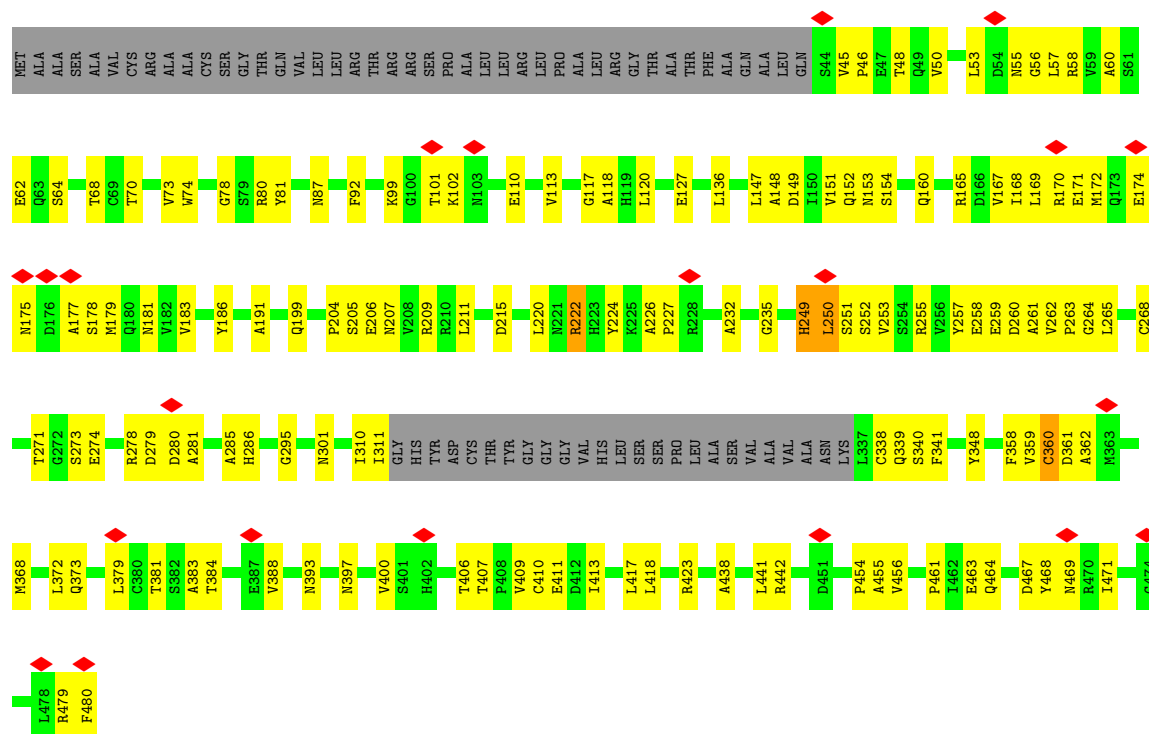


• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

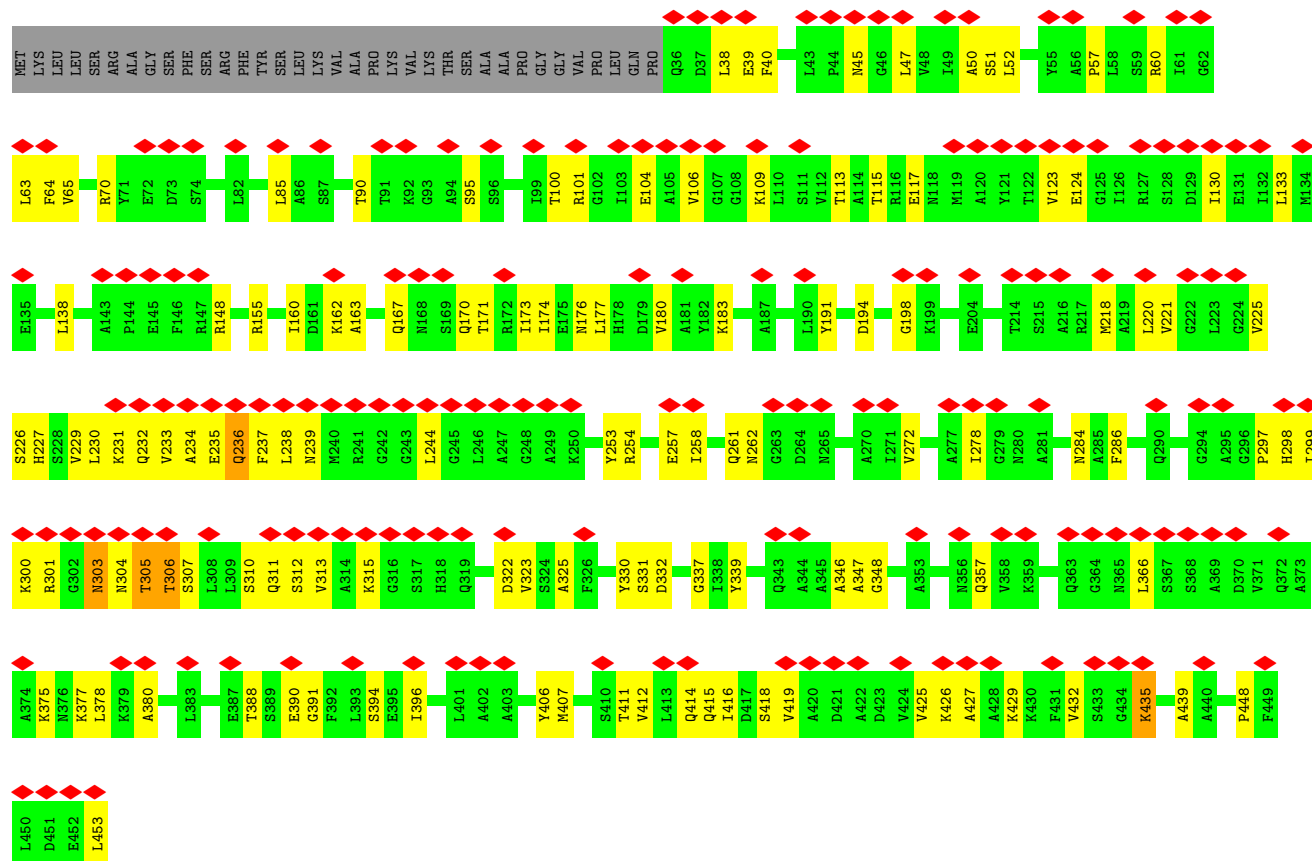
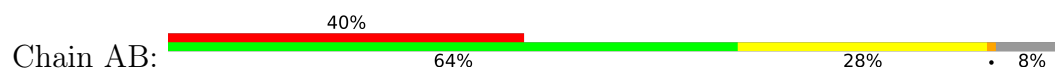


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



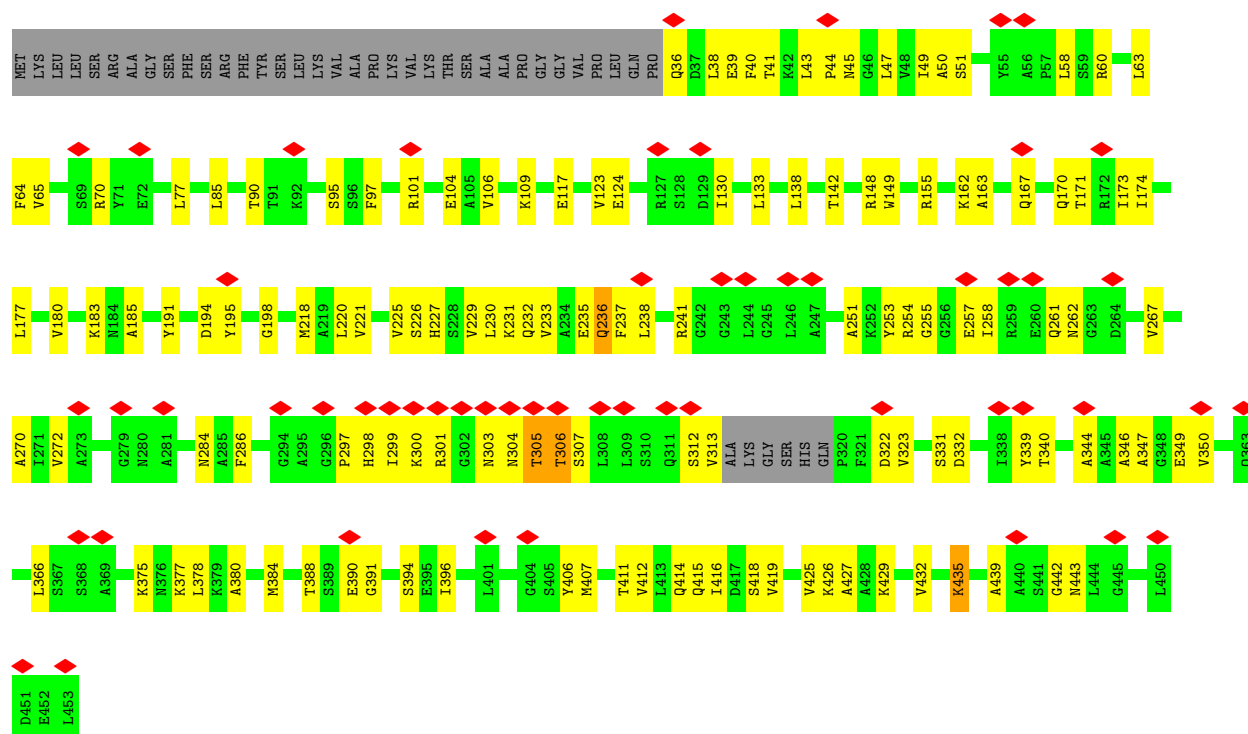


• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



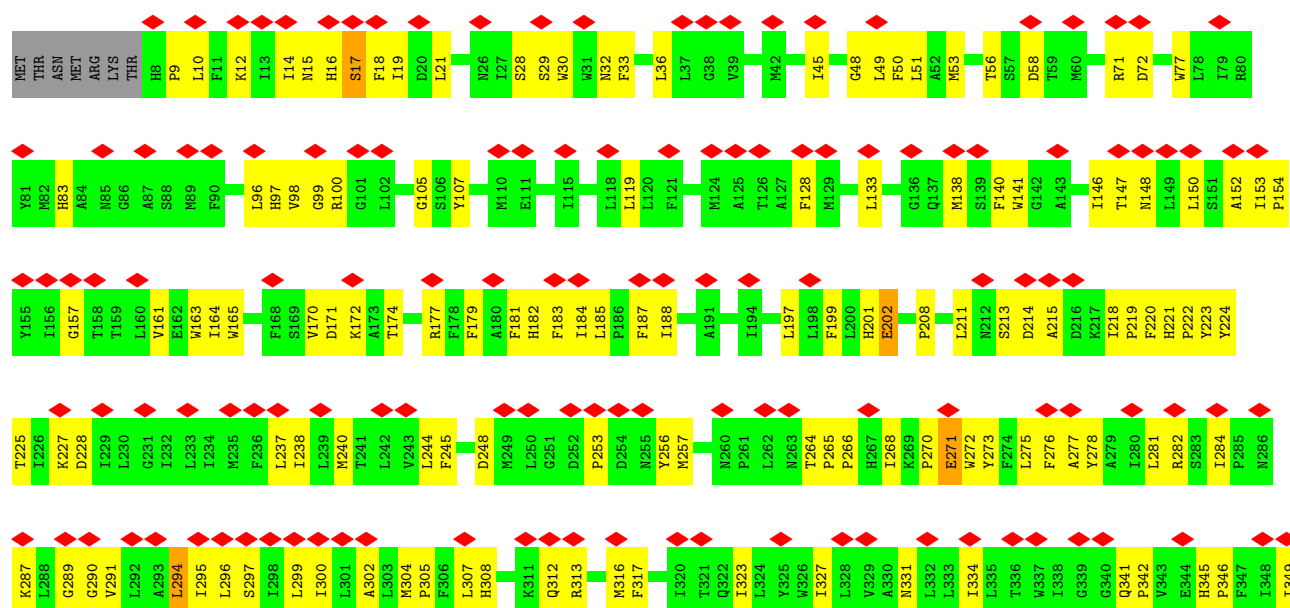
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

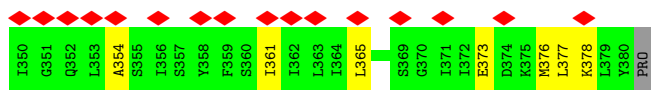
Chain Ab: 12% 62% 28% 9%



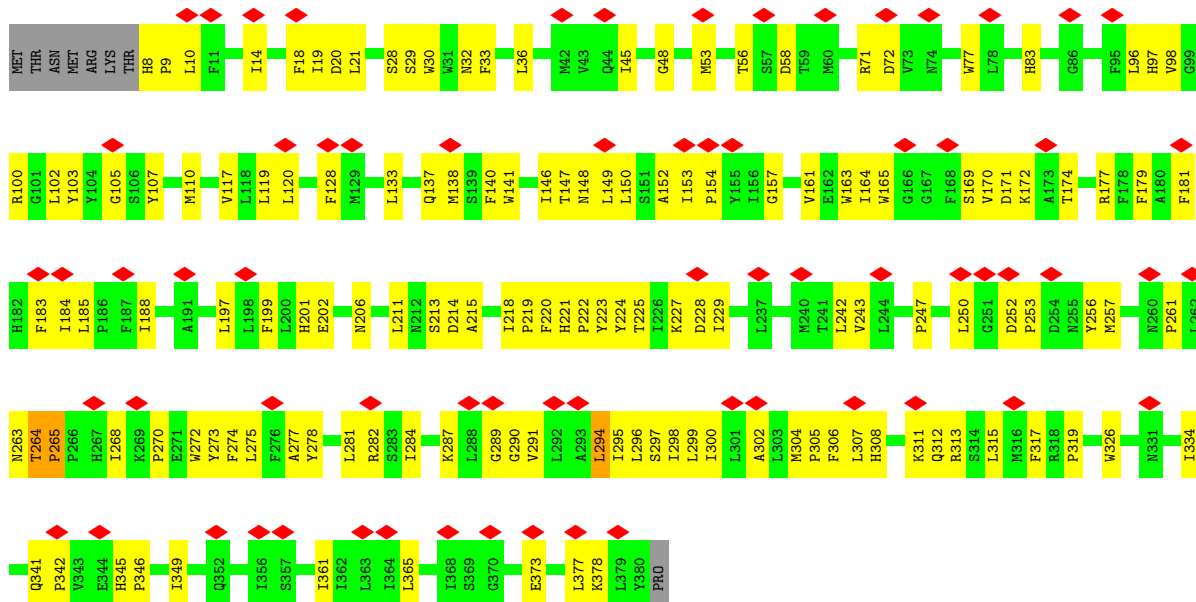
• Molecule 47: Cytochrome b

Chain AC: 39% 60% 37% ..

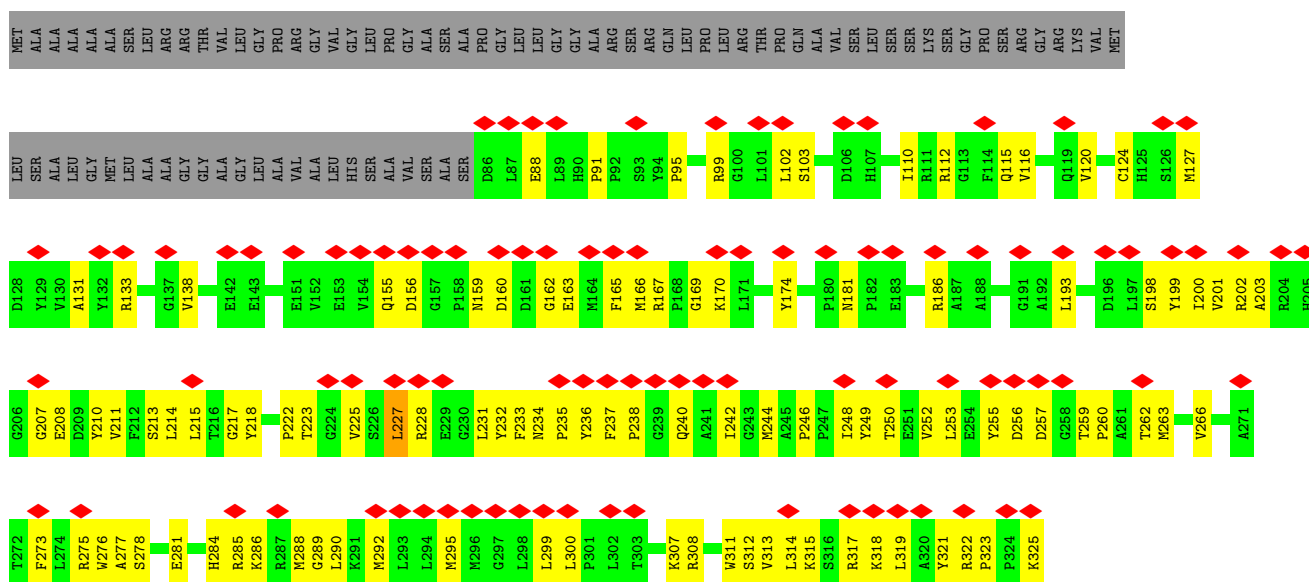
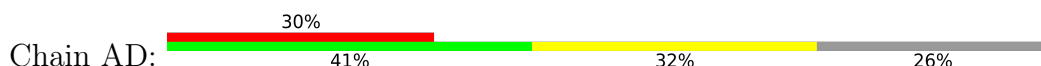




• Molecule 47: Cytochrome b



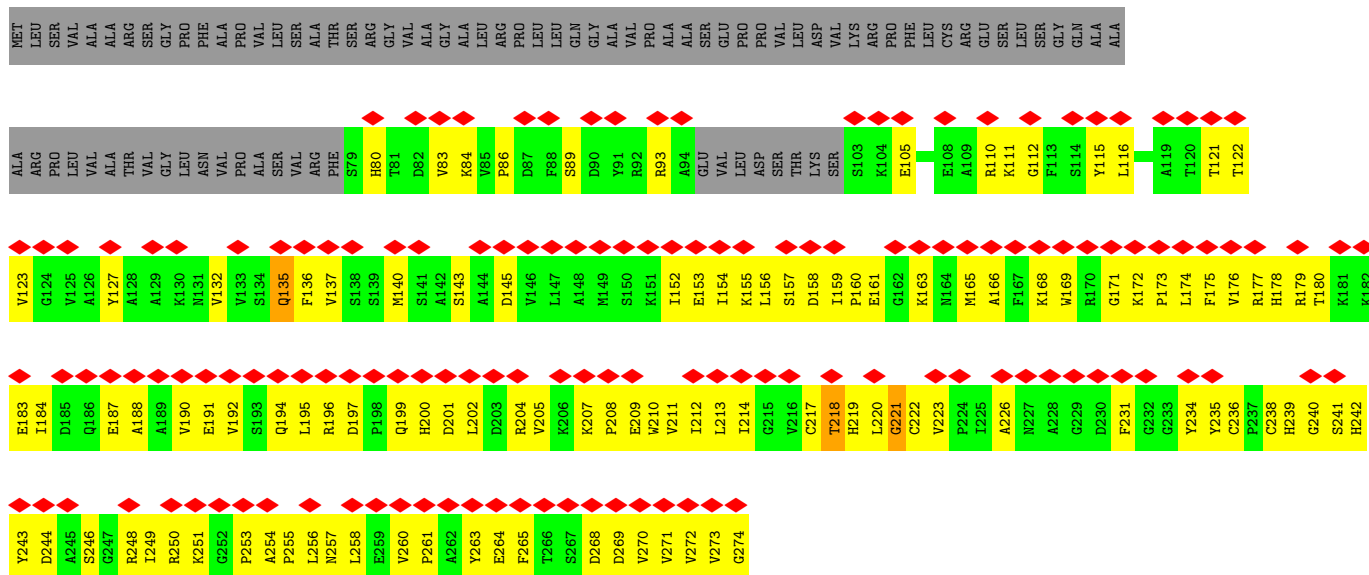
• Molecule 48: Cytochrome c1, heme protein, mitochondrial



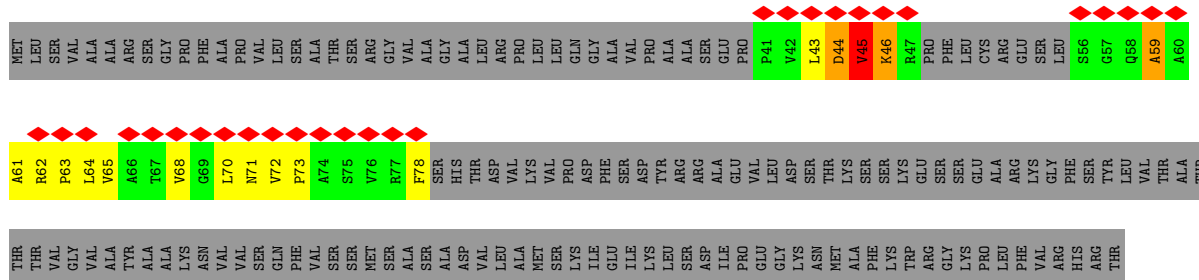
• Molecule 48: Cytochrome c1, heme protein, mitochondrial

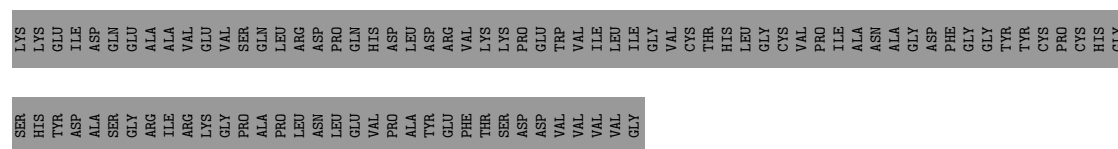


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

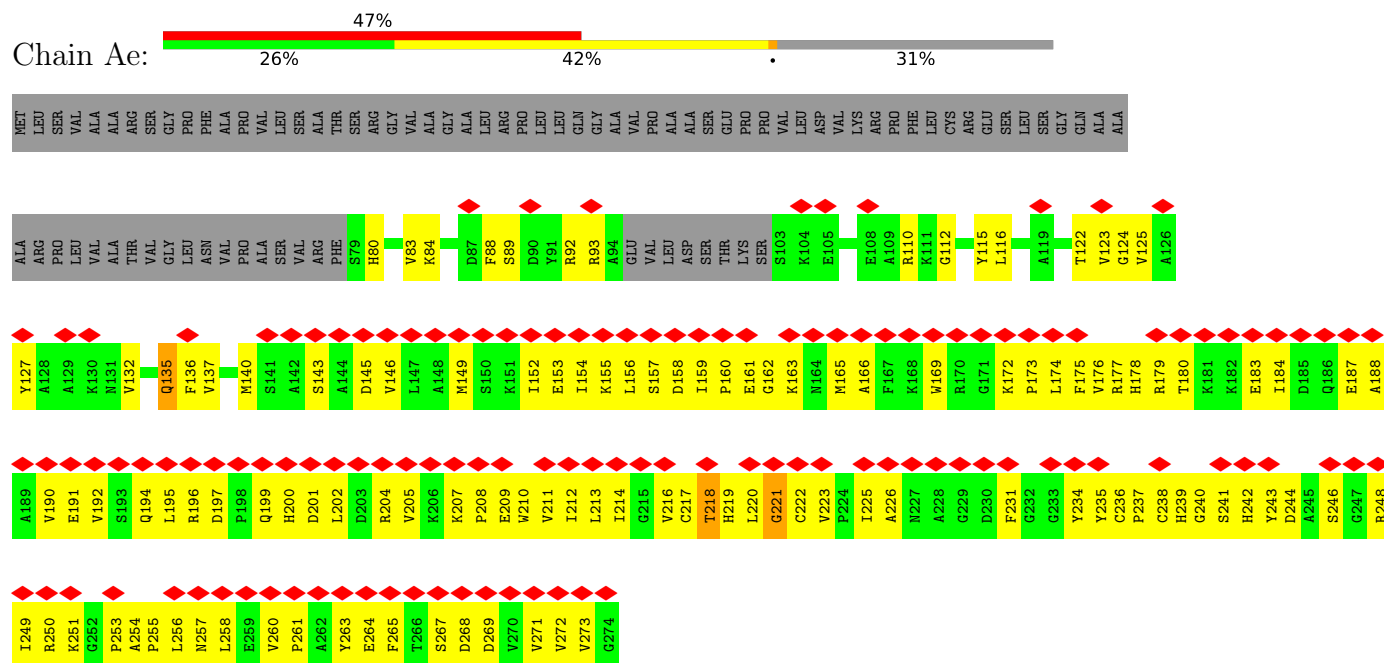


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

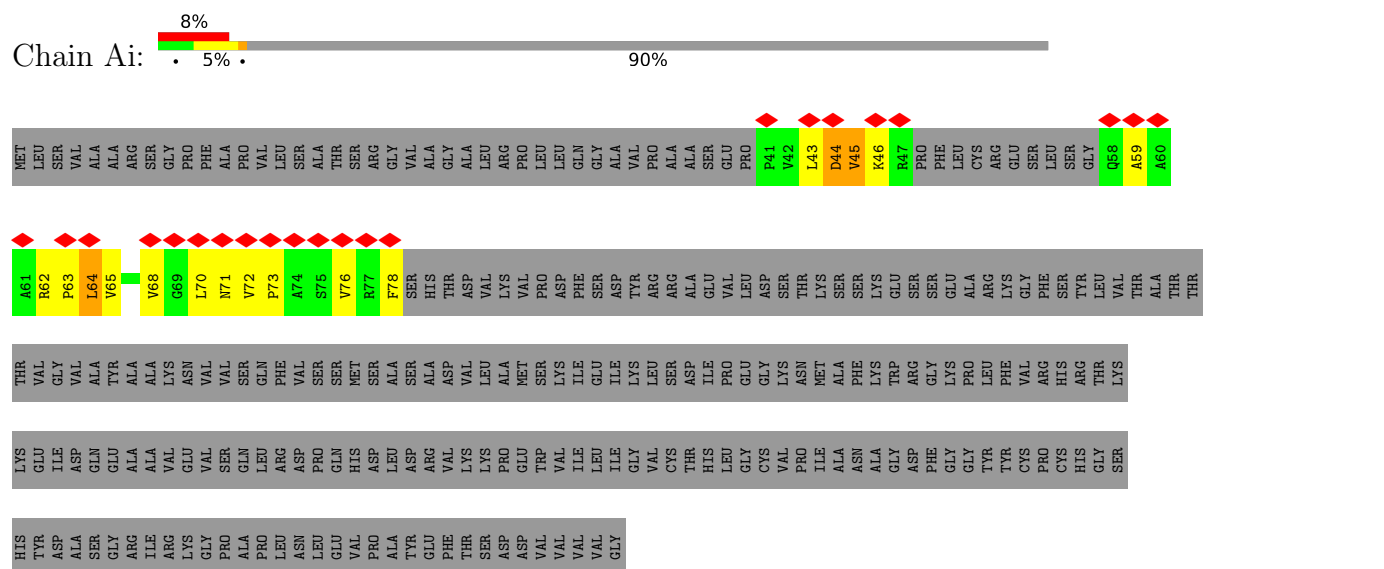




• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

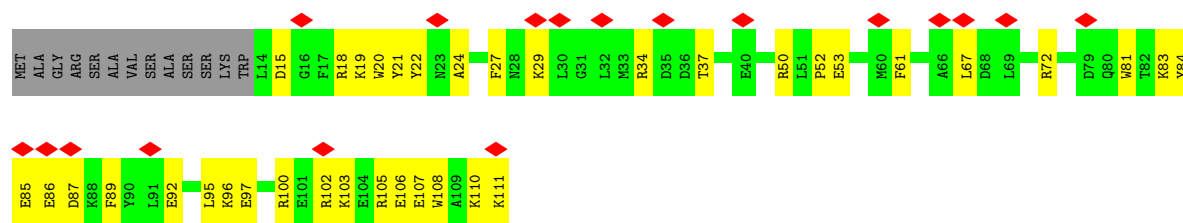


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

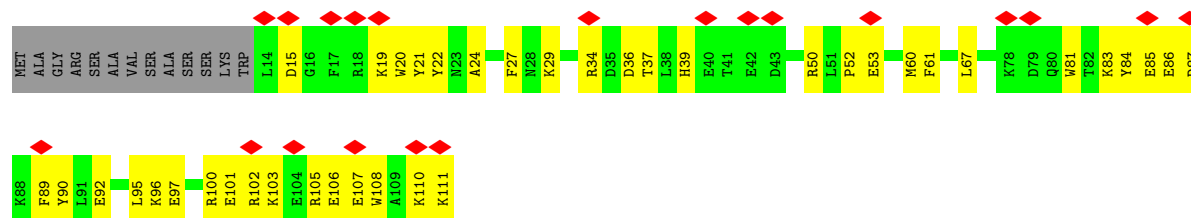


• Molecule 50: Cytochrome b-c1 complex subunit 7

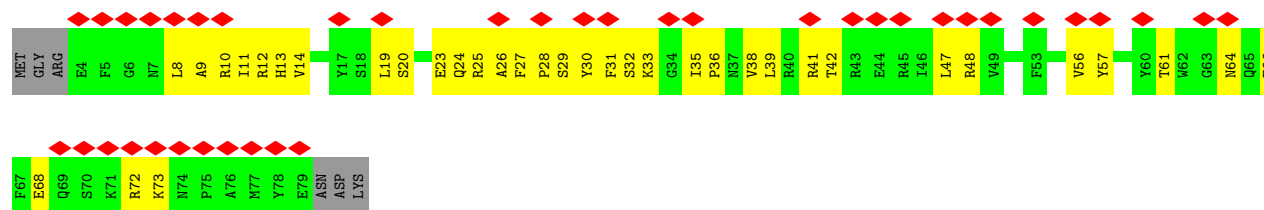




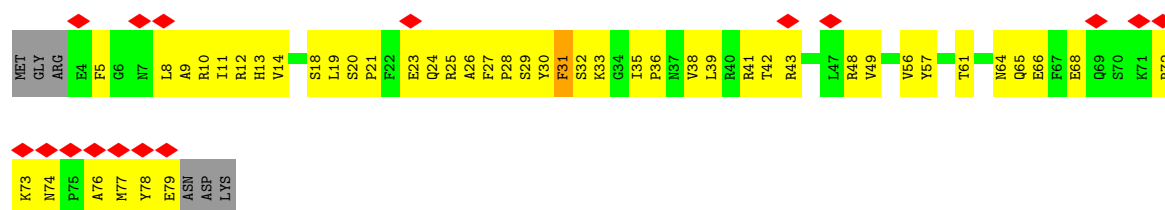
• Molecule 50: Cytochrome b-c1 complex subunit 7



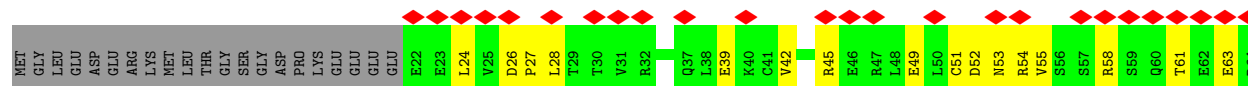
• Molecule 51: Cytochrome b-c1 complex subunit 8



• Molecule 51: Cytochrome b-c1 complex subunit 8

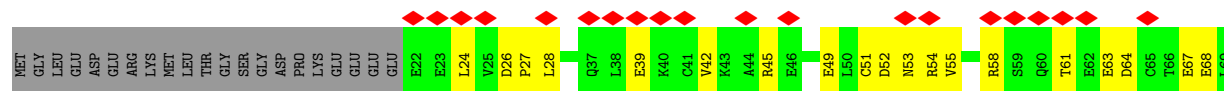


• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

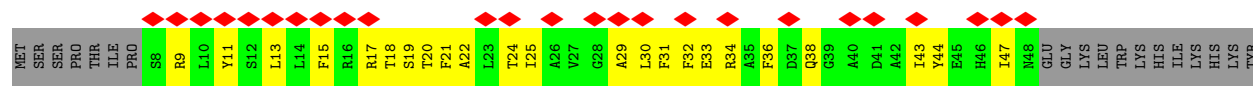
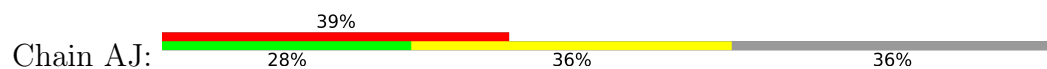




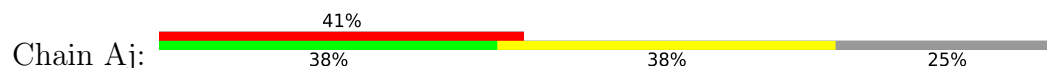
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



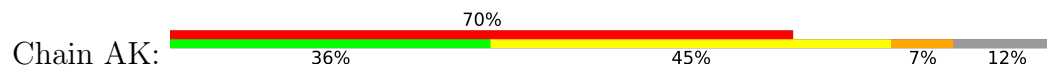
- Molecule 53: Cytochrome b-c1 complex subunit 9



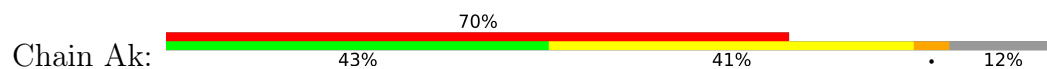
- Molecule 53: Cytochrome b-c1 complex subunit 9



- Molecule 54: Cytochrome b-c1 complex subunit 10



- Molecule 54: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28091	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, U10, EHZ, ADP, FES, HEC, UQ6, ZN, UQ1, FMN, UQ9, PC1, SF4, HEM, NDP, CDL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.79	0/774	1.12	7/1056 (0.7%)
2	B	0.93	1/1289 (0.1%)	1.46	20/1744 (1.1%)
3	C	0.87	0/1687	1.26	11/2297 (0.5%)
4	D	0.93	5/3505 (0.1%)	1.46	40/4748 (0.8%)
5	E	0.72	1/1675 (0.1%)	1.11	13/2282 (0.6%)
6	F	0.90	5/3363 (0.1%)	1.43	54/4543 (1.2%)
7	G	0.93	10/5374 (0.2%)	1.56	101/7281 (1.4%)
8	H	1.00	3/2608 (0.1%)	1.42	48/3563 (1.3%)
9	I	0.92	1/1461 (0.1%)	1.51	20/1974 (1.0%)
10	J	0.90	6/1318 (0.5%)	1.16	13/1791 (0.7%)
11	K	0.90	0/740	1.49	13/1005 (1.3%)
12	L	1.00	9/4921 (0.2%)	1.57	107/6696 (1.6%)
13	M	1.02	7/3717 (0.2%)	1.58	87/5062 (1.7%)
14	N	1.00	4/2756 (0.1%)	1.43	50/3751 (1.3%)
15	O	0.94	8/2666 (0.3%)	1.24	29/3615 (0.8%)
16	P	0.74	1/2793 (0.0%)	1.12	17/3787 (0.4%)
17	Q	0.89	1/980 (0.1%)	1.24	8/1324 (0.6%)
18	R	0.66	0/671	0.92	2/903 (0.2%)
19	S	0.92	2/678 (0.3%)	1.39	10/915 (1.1%)
20	T	0.68	1/613 (0.2%)	0.95	3/826 (0.4%)
20	U	1.01	1/712 (0.1%)	1.46	21/962 (2.2%)
21	V	0.81	0/937	1.38	12/1270 (0.9%)
22	W	0.80	1/993 (0.1%)	1.06	7/1335 (0.5%)
23	X	0.72	0/1422	1.20	14/1921 (0.7%)
24	Y	0.86	0/1061	1.03	4/1439 (0.3%)
25	Z	0.67	1/1183 (0.1%)	1.09	13/1597 (0.8%)
26	a	0.84	0/561	1.11	3/755 (0.4%)
27	b	0.78	1/643 (0.2%)	1.01	3/884 (0.3%)
28	c	0.96	1/400 (0.2%)	1.34	10/544 (1.8%)
29	d	0.89	1/1028 (0.1%)	1.02	8/1387 (0.6%)
30	e	0.88	3/881 (0.3%)	1.07	6/1173 (0.5%)
31	f	0.82	1/459 (0.2%)	0.96	2/618 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.88	3/878 (0.3%)	1.35	18/1196 (1.5%)
33	h	0.75	0/1197	1.21	7/1621 (0.4%)
34	i	0.94	3/867 (0.3%)	1.35	17/1179 (1.4%)
35	j	0.74	0/603	1.21	8/825 (1.0%)
36	k	1.10	2/638 (0.3%)	1.49	19/862 (2.2%)
37	l	1.00	4/1367 (0.3%)	1.26	11/1866 (0.6%)
38	m	0.78	1/1073 (0.1%)	1.10	9/1455 (0.6%)
39	n	0.96	2/1596 (0.1%)	1.28	20/2162 (0.9%)
40	o	0.84	2/1075 (0.2%)	1.12	10/1442 (0.7%)
41	p	0.68	0/1485	0.96	11/2007 (0.5%)
42	q	0.91	4/1234 (0.3%)	1.27	19/1681 (1.1%)
43	r	0.60	0/782	1.04	6/1058 (0.6%)
44	s	0.43	0/194	0.69	0/264
45	AA	0.38	0/3213	0.69	5/4355 (0.1%)
45	Aa	0.50	1/3288 (0.0%)	0.69	3/4462 (0.1%)
46	AB	0.36	0/3187	0.64	5/4308 (0.1%)
46	Ab	0.43	0/3142	0.68	4/4246 (0.1%)
47	AC	0.48	1/3089 (0.0%)	0.68	3/4221 (0.1%)
47	Ac	0.46	1/3089 (0.0%)	0.73	7/4221 (0.2%)
48	AD	0.41	0/1971	0.70	3/2677 (0.1%)
48	Ad	0.54	0/1971	0.81	5/2677 (0.2%)
49	AE	0.63	0/1483	1.03	3/2007 (0.1%)
49	AI	1.83	2/219 (0.9%)	1.48	5/296 (1.7%)
49	Ae	0.63	0/1483	1.03	3/2007 (0.1%)
49	Ai	1.51	1/209 (0.5%)	1.16	1/283 (0.4%)
50	AF	0.38	0/884	0.52	0/1184
50	Af	0.38	0/884	0.52	0/1184
51	AG	0.49	0/662	0.87	1/895 (0.1%)
51	Ag	0.50	0/662	0.89	1/895 (0.1%)
52	AH	0.38	0/569	0.68	0/763
52	Ah	0.38	0/569	0.68	0/763
53	AJ	0.53	0/339	0.71	0/457
53	Aj	0.55	0/401	0.71	0/542
54	AK	0.53	0/416	0.97	5/571 (0.9%)
54	Ak	0.53	0/416	0.81	2/571 (0.4%)
All	All	0.79	102/99004 (0.1%)	1.18	967/134251 (0.7%)

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Ai	44	ASP	C-N	20.05	1.52	1.33
49	AI	44	ASP	C-N	20.05	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Aa	250	LEU	C-N	19.52	1.58	1.33
15	O	247	PRO	N-CD	16.57	1.71	1.47
49	AI	45	VAL	C-N	15.63	1.53	1.33

The worst 5 of 967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-17.48	89.04	114.39
6	F	332	CYS	N-CA-C	15.60	130.05	111.02
13	M	370	PRO	N-CA-C	14.64	128.56	110.70
14	N	255	PRO	N-CA-C	14.43	128.31	110.70
15	O	118	TYR	N-CA-C	13.77	125.80	111.07

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	A	754	0	814	132	0
2	B	1258	0	1269	148	0
3	C	1641	0	1596	159	0
4	D	3416	0	3357	342	0
5	E	1635	0	1624	146	0
6	F	3288	0	3243	383	0
7	G	5287	0	5323	563	0
8	H	2532	0	2621	412	0
9	I	1431	0	1385	176	0
10	J	1287	0	1303	280	0
11	K	729	0	764	128	0
12	L	4798	0	4986	620	0
13	M	3630	0	3854	560	0
14	N	2694	0	2896	376	0
15	O	2599	0	2552	272	0
16	P	2720	0	2740	251	0
17	Q	957	0	949	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	660	0	639	64	0
19	S	667	0	683	70	0
20	T	604	0	596	65	0
20	U	700	0	691	72	0
21	V	915	0	954	97	0
22	W	970	0	991	86	0
23	X	1385	0	1370	149	0
24	Y	1037	0	1022	89	0
25	Z	1152	0	1148	157	0
26	a	548	0	562	46	0
27	b	620	0	617	96	0
28	c	389	0	385	27	0
29	d	996	0	1001	89	0
30	e	859	0	849	107	0
31	f	447	0	444	34	0
32	g	850	0	783	71	0
33	h	1162	0	1163	129	0
34	i	839	0	839	73	0
35	j	578	0	525	66	0
36	k	618	0	616	55	0
37	l	1312	0	1204	100	0
38	m	1044	0	1056	137	0
39	n	1541	0	1470	142	0
40	o	1050	0	1045	110	0
41	p	1452	0	1413	133	0
42	q	1192	0	1145	92	0
43	r	764	0	789	84	0
44	s	189	0	181	18	0
45	AA	3153	0	3077	144	0
45	Aa	3225	0	3141	173	0
46	AB	3137	0	3143	170	0
46	Ab	3094	0	3102	176	0
47	AC	2988	0	3045	214	0
47	Ac	2988	0	3045	188	0
48	AD	1912	0	1860	141	0
48	Ad	1912	0	1860	150	0
49	AE	1451	0	1433	160	0
49	AI	217	0	234	41	0
49	Ae	1451	0	1433	162	0
49	Ai	207	0	226	37	0
50	AF	864	0	854	54	0
50	Af	864	0	854	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AG	643	0	643	50	0
51	Ag	643	0	643	66	0
52	AH	562	0	543	24	0
52	Ah	562	0	543	26	0
53	AJ	332	0	324	31	0
53	Aj	391	0	385	25	0
54	AK	401	0	396	46	0
54	Ak	401	0	396	46	0
55	A	46	0	69	10	0
55	AC	58	0	64	8	0
55	AG	51	0	82	16	0
55	Aa	23	0	20	7	0
55	Ac	35	0	44	4	0
55	Ag	51	0	82	5	0
55	H	46	0	69	16	0
55	J	46	0	66	6	0
55	L	87	0	125	8	0
55	M	88	0	130	11	0
55	Y	39	0	52	4	0
55	b	46	0	69	13	0
55	i	40	0	54	9	0
55	m	92	0	138	25	0
56	A	92	0	134	21	0
56	AG	98	0	84	16	0
56	Aa	46	0	36	4	0
56	Ag	98	0	84	9	0
56	L	74	0	92	11	0
56	M	79	0	105	12	0
56	Y	81	0	106	18	0
56	d	84	0	118	11	0
56	h	93	0	136	11	0
56	q	57	0	58	8	0
57	B	8	0	0	2	0
57	F	8	0	0	9	0
57	G	16	0	0	5	0
57	I	16	0	0	16	0
58	D	18	0	18	14	0
59	E	4	0	0	3	0
59	G	4	0	0	6	0
60	F	31	0	19	2	0
61	H	35	0	43	10	0
62	Ae	35	0	44	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	I	47	0	71	9	0
62	L	48	0	70	12	0
62	l	50	0	74	5	0
62	q	35	0	44	6	0
63	O	27	0	12	8	0
64	P	48	0	26	2	0
65	R	1	0	0	0	0
66	W	32	0	0	0	0
66	n	32	0	0	0	0
67	AC	86	0	60	15	0
67	Ac	86	0	60	12	0
68	AC	23	0	23	19	0
68	Ac	23	0	23	21	0
69	AC	28	0	31	27	0
69	Ac	28	0	31	12	0
70	AD	43	0	31	12	0
70	Ad	43	0	31	11	0
All	All	98999	0	99365	7841	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 40.

The worst 5 of 7841 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)
48:AD:124:CYS:SG	70:AD:401:HEC:HAC	1.40	1.60
15:O:247:PRO:CD	15:O:247:PRO:N	1.71	1.44
12:L:485:PHE:CE1	12:L:486:LEU:CD1	2.13	1.31
12:L:302:ILE:HG22	12:L:340:PHE:CZ	1.64	1.31
46:AB:297:PRO:CG	46:AB:304:ASN:HD21	1.43	1.29

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	83 (94%)	5 (6%)	0	100	100
2	B	155/224 (69%)	146 (94%)	7 (4%)	2 (1%)	9	41
3	C	196/263 (74%)	186 (95%)	10 (5%)	0	100	100
4	D	420/463 (91%)	401 (96%)	19 (4%)	0	100	100
5	E	208/248 (84%)	203 (98%)	5 (2%)	0	100	100
6	F	424/464 (91%)	409 (96%)	15 (4%)	0	100	100
7	G	685/727 (94%)	633 (92%)	52 (8%)	0	100	100
8	H	313/318 (98%)	298 (95%)	14 (4%)	1 (0%)	36	71
9	I	176/212 (83%)	175 (99%)	1 (1%)	0	100	100
10	J	165/172 (96%)	157 (95%)	8 (5%)	0	100	100
11	K	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
12	L	604/607 (100%)	571 (94%)	33 (6%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
16	P	337/377 (89%)	308 (91%)	28 (8%)	1 (0%)	36	71
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	78 (96%)	3 (4%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
22	W	112/131 (86%)	110 (98%)	2 (2%)	0	100	100
23	X	167/172 (97%)	154 (92%)	13 (8%)	0	100	100
24	Y	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
25	Z	137/144 (95%)	133 (97%)	4 (3%)	0	100	100
26	a	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
27	b	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
28	c	45/76 (59%)	45 (100%)	0	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	e	101/106 (95%)	93 (92%)	8 (8%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	99/151 (66%)	93 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	96/128 (75%)	87 (91%)	9 (9%)	0	100	100
35	j	66/105 (63%)	60 (91%)	6 (9%)	0	100	100
36	k	74/104 (71%)	71 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	m	123/129 (95%)	116 (94%)	7 (6%)	0	100	100
39	n	176/179 (98%)	167 (95%)	8 (4%)	1 (1%)	21	58
40	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
41	p	170/176 (97%)	157 (92%)	13 (8%)	0	100	100
42	q	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
43	r	91/113 (80%)	81 (89%)	9 (10%)	1 (1%)	11	45
44	s	20/104 (19%)	20 (100%)	0	0	100	100
45	AA	397/480 (83%)	388 (98%)	9 (2%)	0	100	100
45	Aa	408/480 (85%)	395 (97%)	13 (3%)	0	100	100
46	AB	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
46	Ab	408/453 (90%)	396 (97%)	12 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	368 (99%)	3 (1%)	0	100	100
48	AD	238/325 (73%)	230 (97%)	8 (3%)	0	100	100
48	Ad	238/325 (73%)	225 (94%)	13 (6%)	0	100	100
49	AE	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
49	AI	26/274 (10%)	23 (88%)	3 (12%)	0	100	100
49	Ae	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
49	Ai	24/274 (9%)	23 (96%)	1 (4%)	0	100	100
50	AF	96/111 (86%)	96 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	74 (100%)	0	0	100	100
51	Ag	74/82 (90%)	74 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	AH	66/89 (74%)	66 (100%)	0	0	100	100
52	Ah	66/89 (74%)	66 (100%)	0	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	46/64 (72%)	46 (100%)	0	0	100	100
54	AK	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
54	Ak	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
All	All	11921/14392 (83%)	11425 (96%)	489 (4%)	7 (0%)	49	82

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	109	ALA
8	H	88	PRO
16	P	329	PRO
2	B	171	TYR
43	r	39	PRO

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	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	77
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	366/395 (93%)	364 (100%)	2 (0%)	81	81
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	81
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	279/280 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/138 (99%)	135 (99%)	1 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	415/415 (100%)	414 (100%)	1 (0%)	87	85
14	N	307/308 (100%)	306 (100%)	1 (0%)	86	84
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	296/325 (91%)	295 (100%)	1 (0%)	86	84
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	70
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	80/135 (59%)	80 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	152/154 (99%)	151 (99%)	1 (1%)	76	78
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	70/73 (96%)	70 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	48/53 (91%)	48 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	94/120 (78%)	94 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	59/78 (76%)	59 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	163/164 (99%)	162 (99%)	1 (1%)	78	80
40	o	112/121 (93%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	p	156/158 (99%)	156 (100%)	0	100	100
42	q	129/131 (98%)	129 (100%)	0	100	100
43	r	85/96 (88%)	84 (99%)	1 (1%)	63	73
44	s	22/95 (23%)	22 (100%)	0	100	100
45	AA	341/398 (86%)	339 (99%)	2 (1%)	78	80
45	Aa	349/398 (88%)	347 (99%)	2 (1%)	78	80
46	AB	328/356 (92%)	327 (100%)	1 (0%)	86	84
46	Ab	324/356 (91%)	323 (100%)	1 (0%)	86	84
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	205/260 (79%)	205 (100%)	0	100	100
48	Ad	205/260 (79%)	205 (100%)	0	100	100
49	AE	158/224 (70%)	157 (99%)	1 (1%)	78	80
49	AI	23/224 (10%)	22 (96%)	1 (4%)	26	48
49	Ae	158/224 (70%)	157 (99%)	1 (1%)	78	80
49	Ai	22/224 (10%)	20 (91%)	2 (9%)	9	29
50	AF	90/99 (91%)	90 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	65/83 (78%)	65 (100%)	0	100	100
52	Ah	65/83 (78%)	65 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100
54	AK	39/46 (85%)	39 (100%)	0	100	100
54	Ak	39/46 (85%)	39 (100%)	0	100	100
All	All	10476/12261 (85%)	10445 (100%)	31 (0%)	84	84

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	X	57	LEU
47	Ac	294	LEU

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Mol	Chain	Res	Type
43	r	92	LYS
49	Ai	45	VAL
45	Aa	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 243 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	216	HIS
45	Aa	207	ASN
31	f	10	HIS
45	Aa	173	GLN
48	Ad	190	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 1 is monoatomic - leaving 60 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	$\# Z > 2$
55	3PE	Y	201	-	38,38,50	1.04	2 (5%)	41,43,55	1.12	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	SF4	I	302	9	0,12,12	-	-	-		
70	HEC	Ad	401	48	46,50,50	1.83	5 (10%)	58,82,82	1.93	5 (8%)
57	SF4	I	303	9	0,12,12	-	-	-		
66	EHZ	n	201	-	29,31,37	1.78	7 (24%)	37,41,47	1.74	10 (27%)
56	CDL	h	201	-	92,92,99	0.94	4 (4%)	98,104,111	1.13	8 (8%)
55	3PE	i	201	-	39,39,50	1.05	2 (5%)	42,44,55	1.04	2 (4%)
62	PC1	I	301	-	46,46,53	0.99	2 (4%)	52,54,61	1.11	5 (9%)
55	3PE	Aa	501	-	22,22,50	1.37	2 (9%)	25,27,55	1.14	2 (8%)
57	SF4	G	802	7	0,12,12	-	-	-		
58	UQ1	D	501	-	18,18,18	1.35	3 (16%)	24,25,25	1.65	6 (25%)
62	PC1	Ae	301	-	34,34,53	1.18	2 (5%)	40,42,61	1.20	4 (10%)
55	3PE	A	401	-	45,45,50	1.13	5 (11%)	48,50,55	1.28	3 (6%)
55	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.09	3 (5%)
55	3PE	b	201	-	45,45,50	0.98	2 (4%)	48,50,55	1.11	3 (6%)
56	CDL	Aa	502	-	45,45,99	1.34	4 (8%)	51,57,111	1.32	6 (11%)
56	CDL	L	703	-	73,73,99	1.06	4 (5%)	79,85,111	1.16	5 (6%)
66	EHZ	W	201	-	29,31,37	1.63	5 (17%)	37,41,47	1.63	7 (18%)
56	CDL	M	503	-	78,78,99	1.02	4 (5%)	84,90,111	1.12	7 (8%)
67	HEM	AC	403	47	50,50,50	1.34	6 (12%)	67,82,82	1.59	15 (22%)
64	NDP	P	401	-	51,52,52	1.17	4 (7%)	71,80,80	1.55	11 (15%)
62	PC1	l	201	-	49,49,53	0.97	2 (4%)	55,57,61	1.02	4 (7%)
55	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.10	4 (7%)
55	3PE	AG	103	-	50,50,50	0.92	2 (4%)	53,55,55	1.07	3 (5%)
60	FMN	F	501	-	33,33,33	1.41	5 (15%)	48,50,50	1.24	8 (16%)
55	3PE	m	201	-	50,50,50	0.91	2 (4%)	53,55,55	1.09	4 (7%)
56	CDL	A	402	-	91,91,99	0.95	4 (4%)	97,103,111	1.10	6 (6%)
56	CDL	AG	102	-	55,55,99	1.20	4 (7%)	61,67,111	1.27	6 (9%)
67	HEM	Ac	401	47	50,50,50	1.31	8 (16%)	67,82,82	1.59	12 (17%)
55	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.30	0
68	U10	AC	405	-	23,23,63	1.28	4 (17%)	30,31,79	2.07	7 (23%)
68	U10	Ac	404	-	23,23,63	1.28	3 (13%)	30,31,79	2.05	6 (20%)
61	UQ9	H	401	-	35,35,58	0.84	3 (8%)	43,45,73	0.74	2 (4%)
57	SF4	F	502	6	0,12,12	-	-	-		
55	3PE	L	704	-	37,37,50	1.05	2 (5%)	40,42,55	1.19	4 (10%)
56	CDL	q	201	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
62	PC1	q	202	-	34,34,53	1.14	2 (5%)	40,42,61	1.22	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	HEM	AC	402	47	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
55	3PE	AC	404	-	34,34,50	1.10	2 (5%)	37,39,55	1.16	3 (8%)
55	3PE	m	202	-	40,40,50	1.02	2 (5%)	43,45,55	1.23	5 (11%)
69	UQ6	Ac	405	-	28,28,43	0.83	2 (7%)	36,37,55	0.81	1 (2%)
55	3PE	H	402	-	45,45,50	0.93	2 (4%)	48,50,55	1.34	5 (10%)
57	SF4	G	801	7	0,12,12	-	-	-	-	-
69	UQ6	AC	406	-	28,28,43	0.83	2 (7%)	36,37,55	0.82	1 (2%)
67	HEM	Ac	402	47	50,50,50	1.33	5 (10%)	67,82,82	1.58	15 (22%)
56	CDL	d	201	-	83,83,99	1.00	4 (4%)	89,95,111	1.11	5 (5%)
56	CDL	Ag	101	-	41,41,99	1.41	4 (9%)	47,53,111	1.31	6 (12%)
55	3PE	Ac	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.23	3 (8%)
56	CDL	AG	101	-	41,41,99	1.41	4 (9%)	47,53,111	1.30	6 (12%)
56	CDL	Y	202	-	80,80,99	1.02	4 (5%)	86,92,111	1.15	7 (8%)
62	PC1	L	701	-	47,47,53	0.99	2 (4%)	53,55,61	1.11	4 (7%)
70	HEC	AD	401	48	46,50,50	1.83	5 (10%)	58,82,82	1.93	5 (8%)
59	FES	E	301	5	0,4,4	-	-	-	-	-
55	3PE	J	201	-	45,45,50	0.96	2 (4%)	48,50,55	1.09	3 (6%)
56	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
59	FES	G	803	7	0,4,4	-	-	-	-	-
63	ADP	O	401	-	28,29,29	1.37	4 (14%)	43,45,45	1.84	9 (20%)
55	3PE	AC	401	-	22,22,50	0.47	0	25,27,55	0.75	1 (4%)
55	3PE	M	501	-	36,36,50	1.07	2 (5%)	39,41,55	1.08	3 (7%)
57	SF4	B	301	2	0,12,12	-	-	-	-	-

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
55	3PE	Y	201	-	-	4/42/42/54	-
57	SF4	I	302	9	-	-	0/6/5/5
70	HEC	Ad	401	48	-	4/14/54/54	-
66	EHZ	n	201	-	-	19/39/39/45	-
57	SF4	I	303	9	-	-	0/6/5/5
56	CDL	h	201	-	-	27/103/103/110	-
55	3PE	i	201	-	-	14/43/43/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	I	301	-	-	11/50/50/57	-
55	3PE	Aa	501	-	-	7/26/26/54	-
58	UQ1	D	501	-	-	5/9/33/33	0/1/1/1
57	SF4	G	802	7	-	-	0/6/5/5
62	PC1	Ae	301	-	-	7/38/38/57	-
55	3PE	A	401	-	-	18/49/49/54	-
55	3PE	M	502	-	-	10/54/54/54	-
55	3PE	b	201	-	-	10/49/49/54	-
56	CDL	Aa	502	-	-	13/56/56/110	-
56	CDL	L	703	-	-	15/84/84/110	-
66	EHZ	W	201	-	-	13/39/39/45	-
56	CDL	M	503	-	-	25/89/89/110	-
67	HEM	AC	403	47	-	8/14/54/54	-
64	NDP	P	401	-	-	2/34/77/77	0/5/5/5
62	PC1	l	201	-	-	7/53/53/57	-
55	3PE	L	702	-	-	14/52/52/54	-
55	3PE	AG	103	-	-	9/54/54/54	-
60	FMN	F	501	-	-	0/18/18/18	0/3/3/3
55	3PE	m	201	-	-	14/54/54/54	-
56	CDL	A	402	-	-	21/102/102/110	-
56	CDL	AG	102	-	-	15/66/66/110	-
67	HEM	Ac	401	47	-	9/14/54/54	-
55	3PE	Ag	103	-	-	11/54/54/54	-
68	U10	AC	405	-	-	6/15/39/87	0/1/1/1
68	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
61	UQ9	H	401	-	-	13/30/54/81	0/1/1/1
57	SF4	F	502	6	-	-	0/6/5/5
55	3PE	L	704	-	-	7/41/41/54	-
56	CDL	q	201	-	-	14/67/67/110	-
62	PC1	q	202	-	-	15/38/38/57	-
67	HEM	AC	402	47	-	9/14/54/54	-
55	3PE	AC	404	-	-	1/38/38/54	-
55	3PE	m	202	-	-	8/44/44/54	-
69	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
55	3PE	H	402	-	-	10/49/49/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	UQ6	AC	406	-	-	13/21/21/39	0/1/1/1
57	SF4	G	801	7	-	-	0/6/5/5
67	HEM	Ac	402	47	-	8/14/54/54	-
56	CDL	d	201	-	-	15/94/94/110	-
56	CDL	Ag	101	-	-	7/52/52/110	-
55	3PE	Ac	403	-	-	3/38/38/54	-
56	CDL	AG	101	-	-	8/52/52/110	-
56	CDL	Y	202	-	-	24/91/91/110	-
62	PC1	L	701	-	-	11/51/51/57	-
70	HEC	AD	401	48	-	4/14/54/54	-
59	FES	E	301	5	-	-	0/1/1/1
55	3PE	J	201	-	-	13/49/49/54	-
56	CDL	Ag	102	-	-	12/66/66/110	-
63	ADP	O	401	-	-	4/16/32/32	0/3/3/3
59	FES	G	803	7	-	-	0/1/1/1
55	3PE	AC	401	-	-	6/26/26/54	-
55	3PE	M	501	-	-	12/40/40/54	-
57	SF4	B	301	2	-	-	0/6/5/5

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	AD	401	HEC	CAC-C3C	6.10	1.54	1.35
70	AD	401	HEC	CAB-C3B	6.08	1.54	1.35
70	Ad	401	HEC	CAC-C3C	6.08	1.54	1.35
70	Ad	401	HEC	CAB-C3B	6.06	1.54	1.35
70	Ad	401	HEC	C3D-C2D	5.75	1.53	1.38

The worst 5 of 275 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	Ad	401	HEC	CBC-CAC-C3C	-8.60	110.25	127.43
70	AD	401	HEC	CBC-CAC-C3C	-8.58	110.28	127.43
70	Ad	401	HEC	CBB-CAB-C3B	-8.36	110.72	127.43
70	AD	401	HEC	CBB-CAB-C3B	-8.34	110.76	127.43
68	AC	405	U10	C6-C1-C2	7.83	125.35	119.17

There are no chirality outliers.

5 of 554 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	401	3PE	O22-C21-O21-C2
55	H	402	3PE	C11-O13-P-O11
55	H	402	3PE	C11-O13-P-O12
55	H	402	3PE	C11-O13-P-O14
55	H	402	3PE	O13-C11-C12-N

There are no ring outliers.

57 monomers are involved in 490 short contacts:

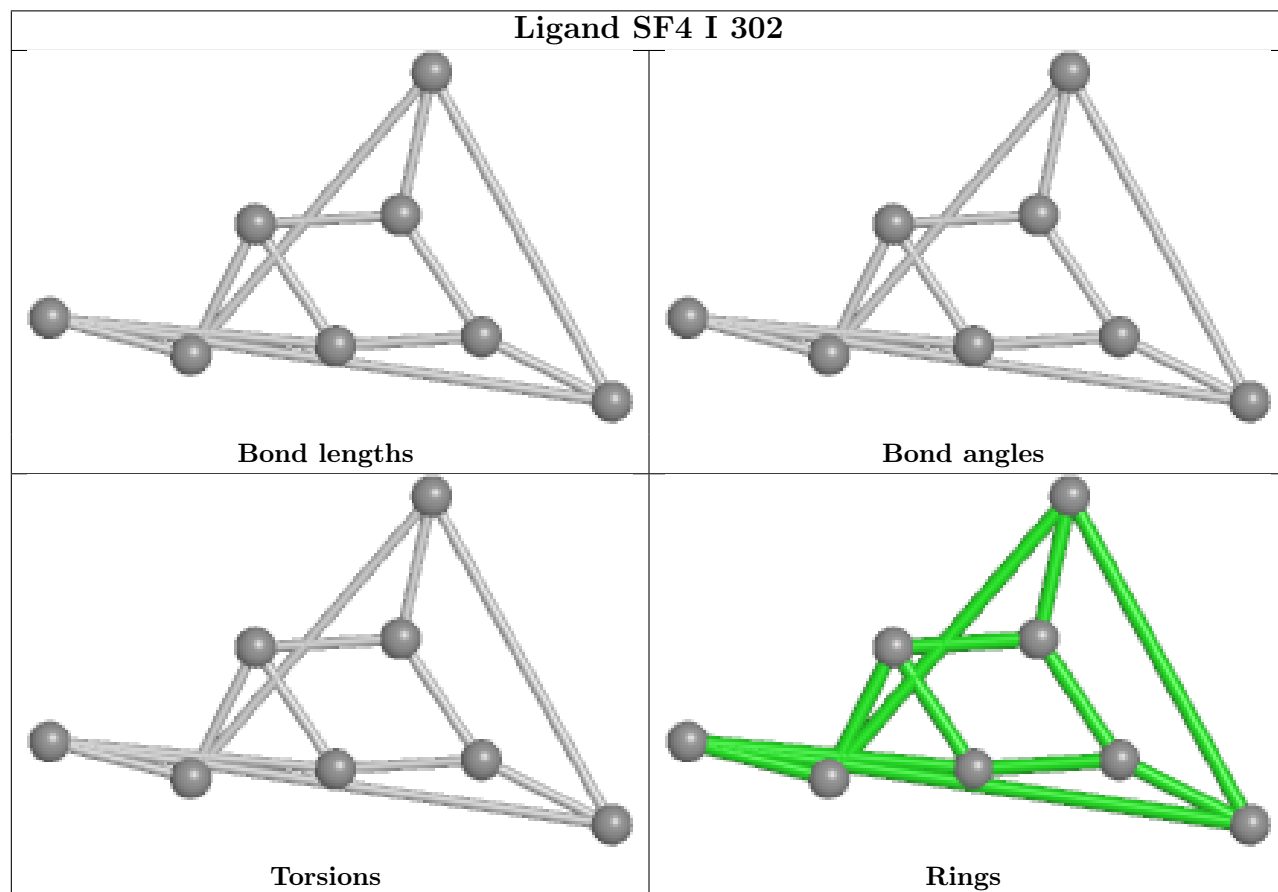
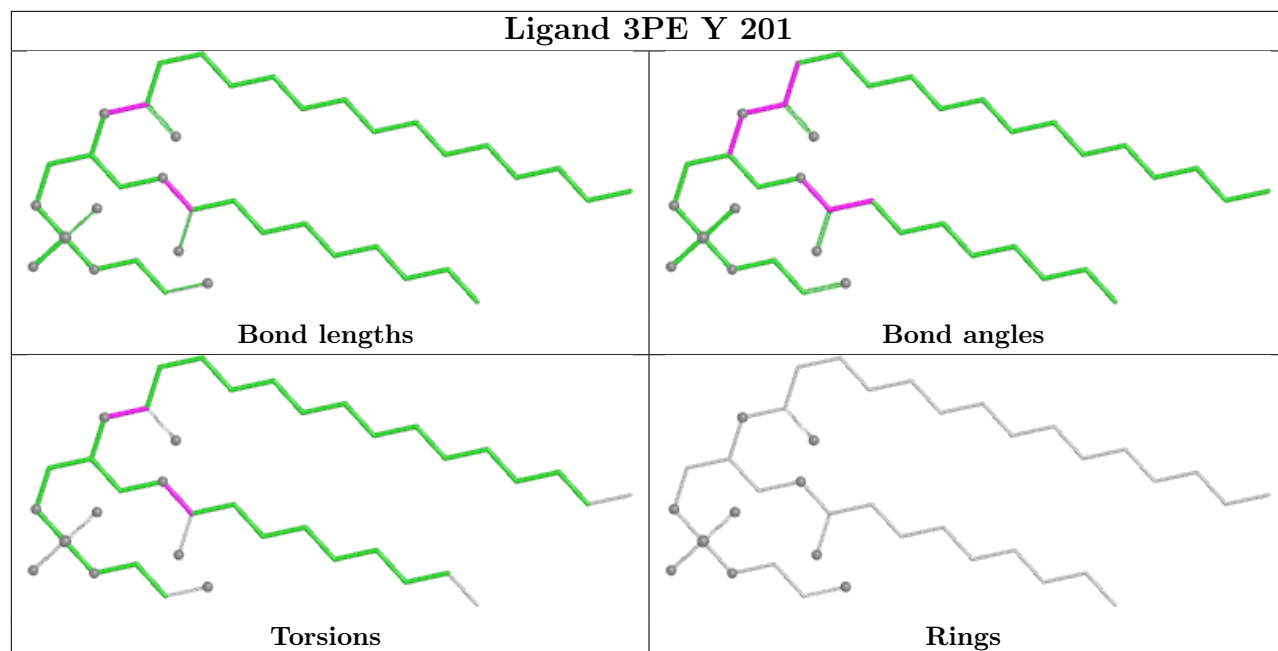
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	Y	201	3PE	4	0
57	I	302	SF4	10	0
70	Ad	401	HEC	11	0
57	I	303	SF4	6	0
56	h	201	CDL	11	0
55	i	201	3PE	9	0
62	I	301	PC1	9	0
55	Aa	501	3PE	7	0
57	G	802	SF4	5	0
58	D	501	UQ1	14	0
62	Ae	301	PC1	6	0
55	A	401	3PE	10	0
55	M	502	3PE	4	0
55	b	201	3PE	13	0
56	Aa	502	CDL	4	0
56	L	703	CDL	11	0
56	M	503	CDL	12	0
67	AC	403	HEM	8	0
64	P	401	NDP	2	0
62	l	201	PC1	5	0
55	L	702	3PE	5	0
55	AG	103	3PE	16	0
60	F	501	FMN	2	0
55	m	201	3PE	17	0
56	A	402	CDL	21	0
56	AG	102	CDL	8	0
67	Ac	401	HEM	3	0
55	Ag	103	3PE	5	0
68	AC	405	U10	19	0
68	Ac	404	U10	21	0
61	H	401	UQ9	10	0
57	F	502	SF4	9	0
55	L	704	3PE	3	0

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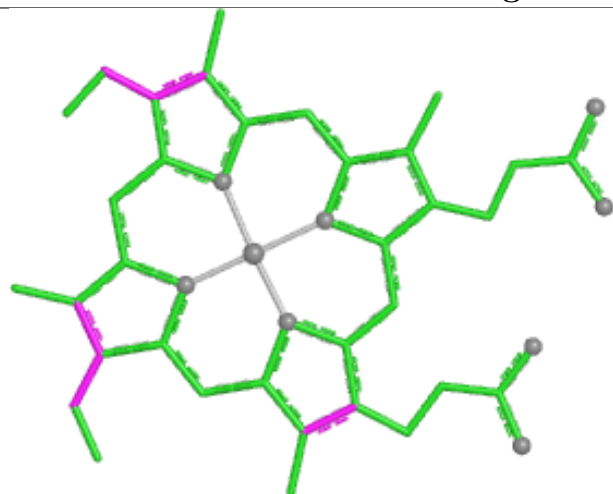
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	q	201	CDL	8	0
62	q	202	PC1	6	0
67	AC	402	HEM	7	0
55	AC	404	3PE	6	0
55	m	202	3PE	8	0
69	Ac	405	UQ6	12	0
55	H	402	3PE	16	0
69	AC	406	UQ6	27	0
67	Ac	402	HEM	9	0
56	d	201	CDL	11	0
56	Ag	101	CDL	4	0
55	Ac	403	3PE	4	0
56	AG	101	CDL	8	0
56	Y	202	CDL	18	0
62	L	701	PC1	12	0
70	AD	401	HEC	12	0
59	E	301	FES	3	0
55	J	201	3PE	6	0
56	Ag	102	CDL	5	0
59	G	803	FES	6	0
63	O	401	ADP	8	0
55	AC	401	3PE	2	0
55	M	501	3PE	7	0
57	B	301	SF4	2	0

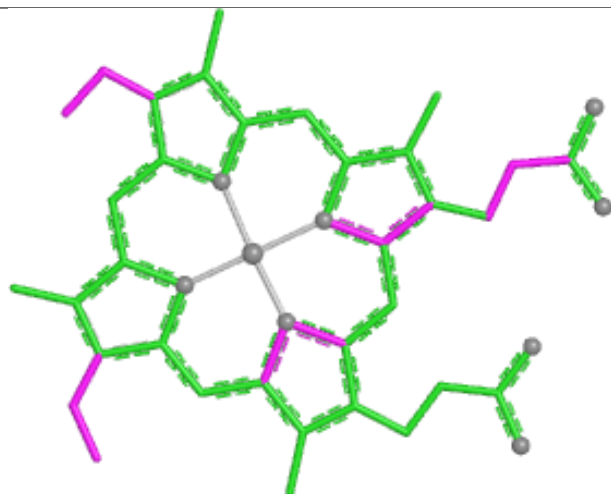
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



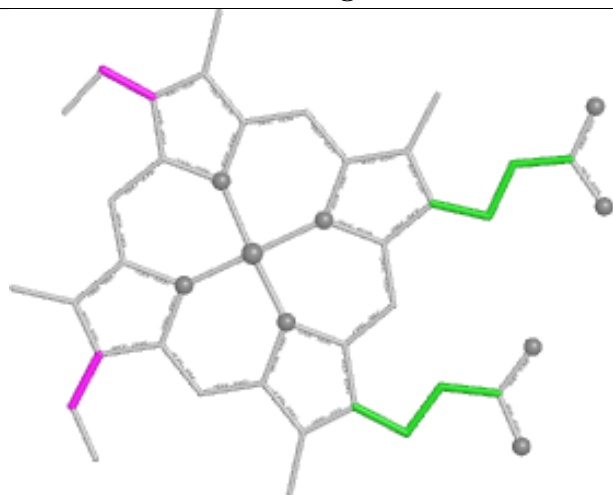
Ligand HEC Ad 401



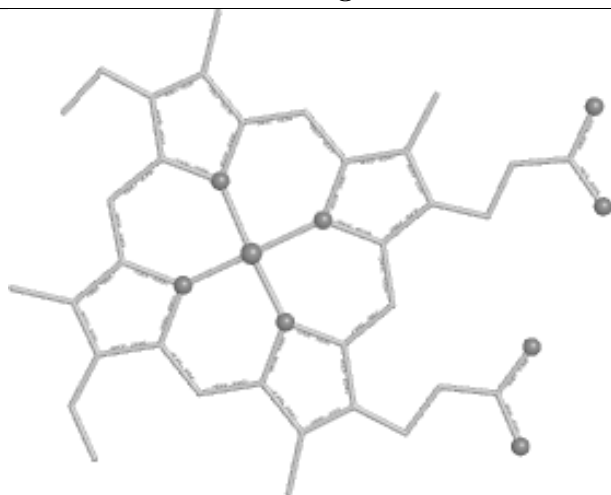
Bond lengths



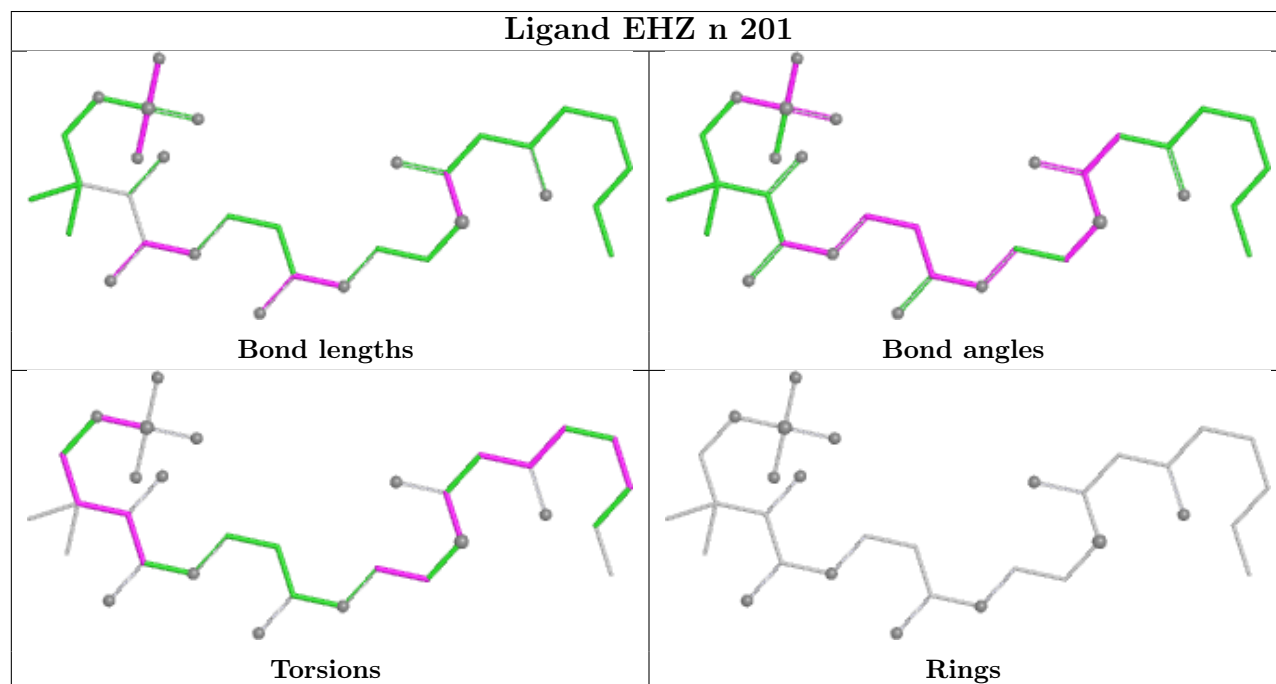
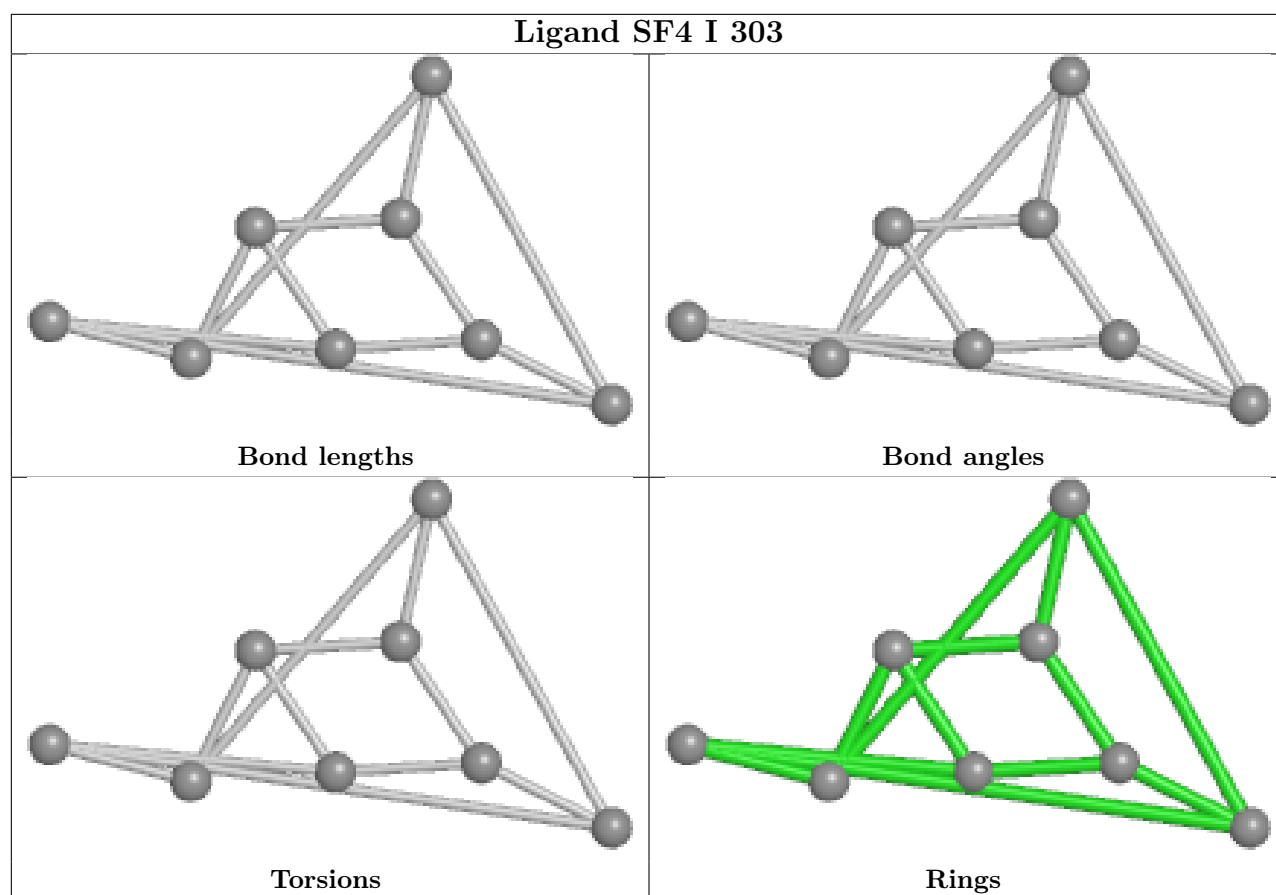
Bond angles

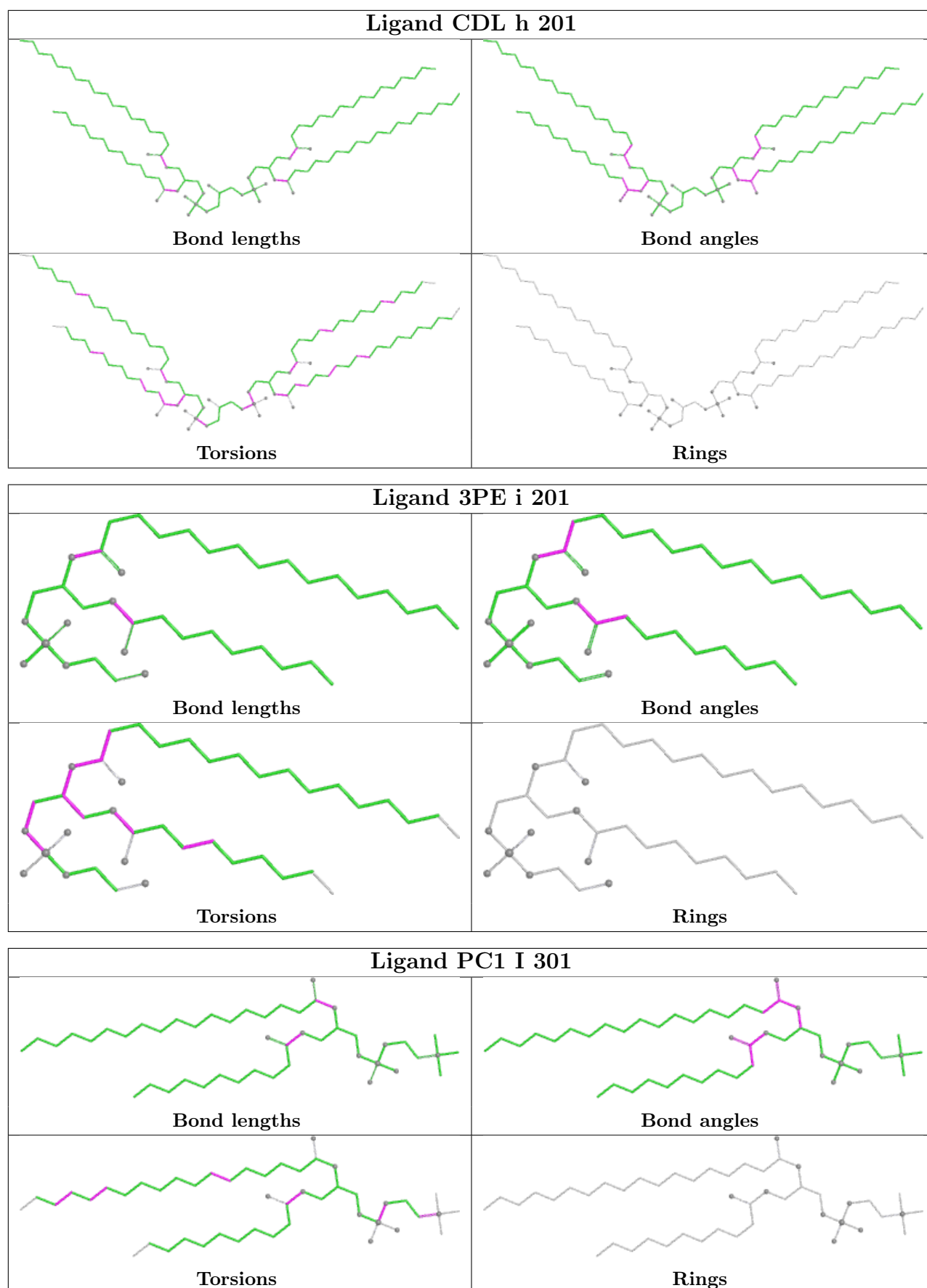


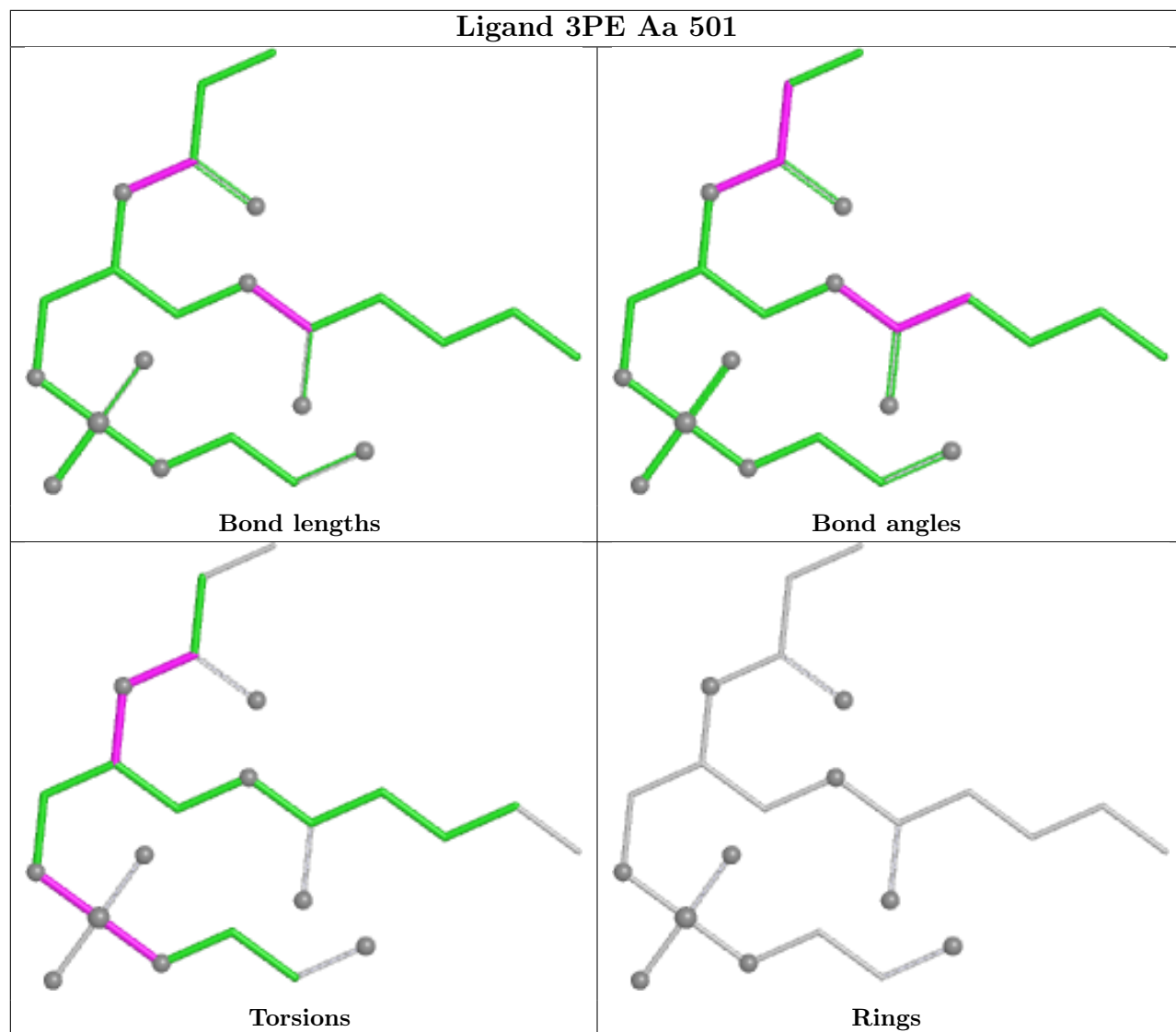
Torsions

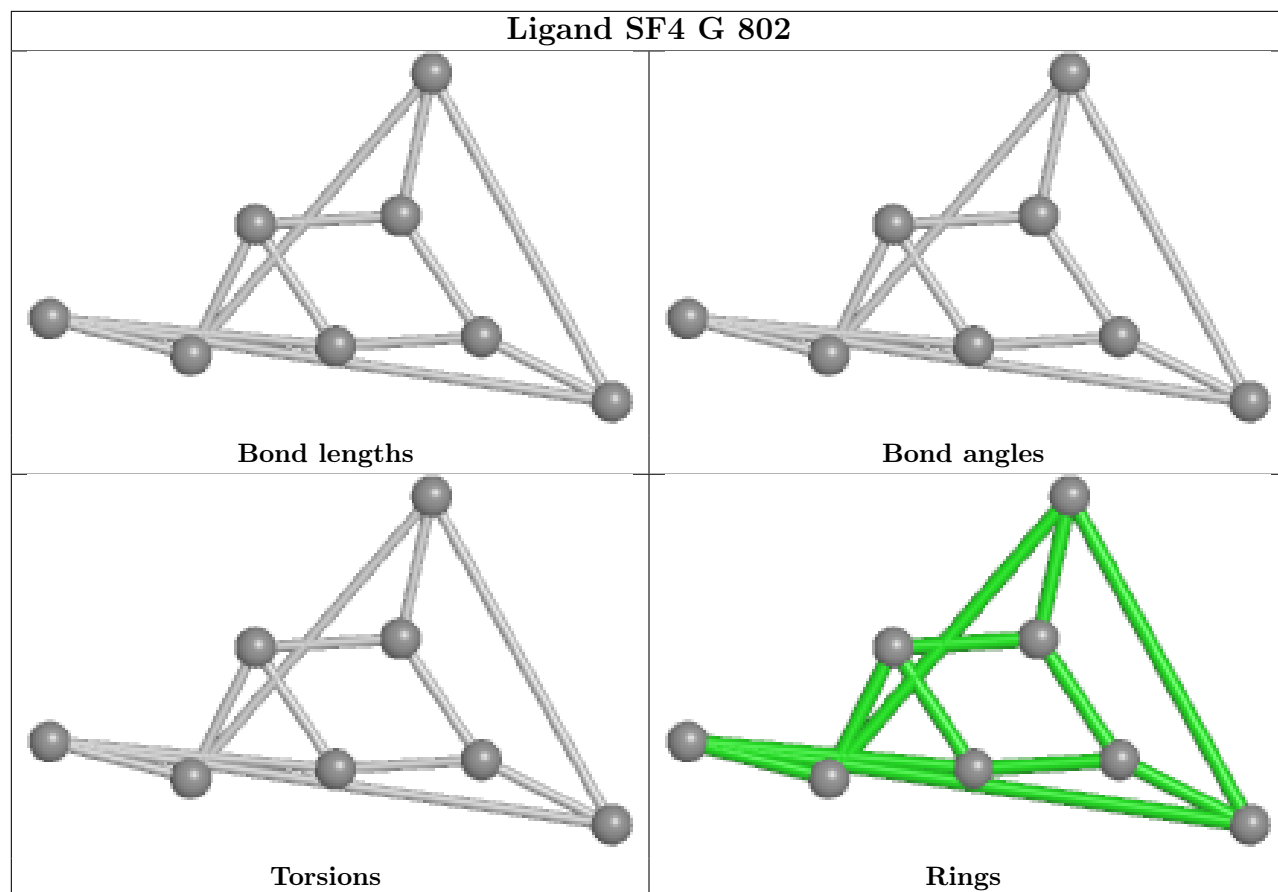


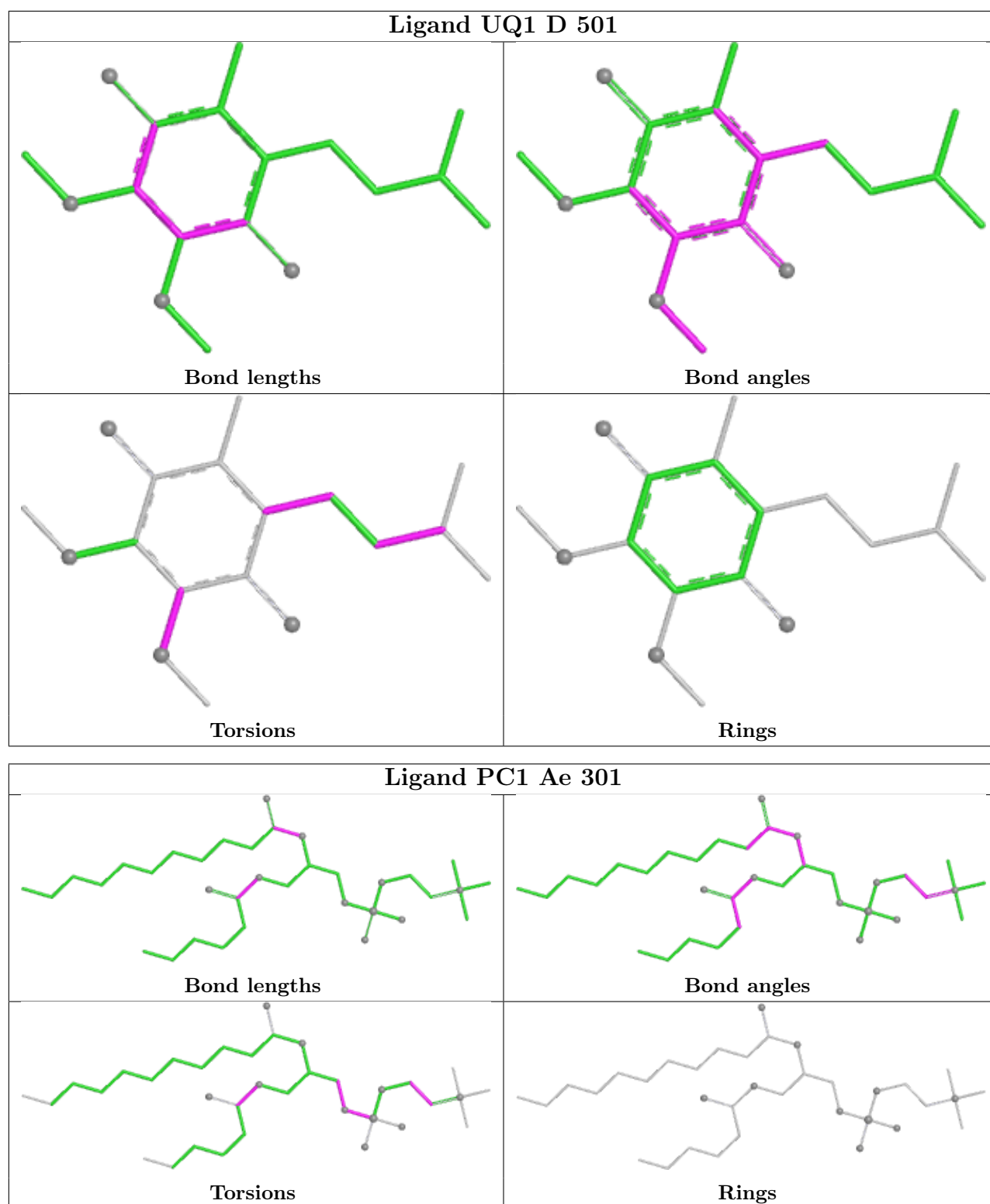
Rings

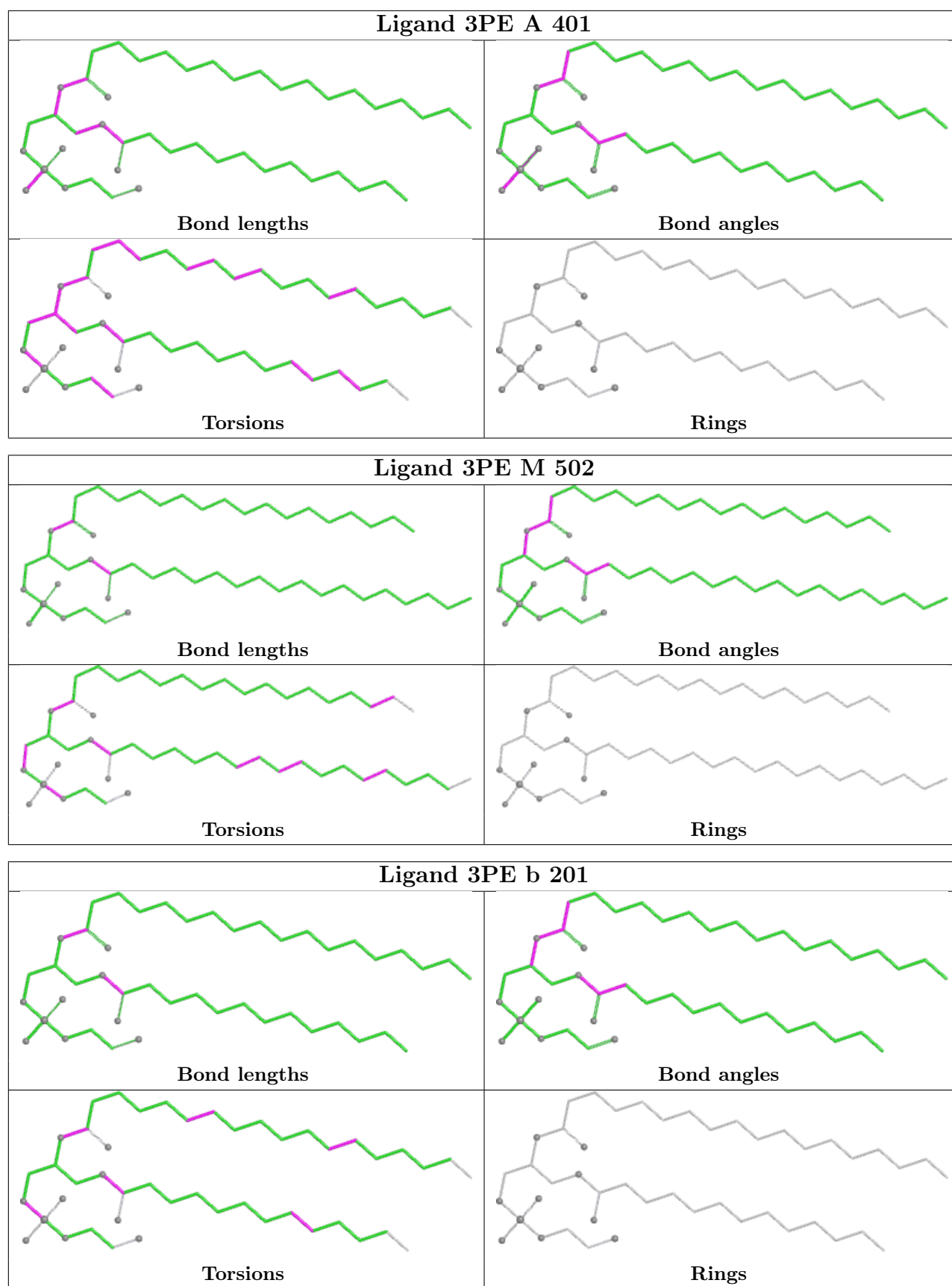


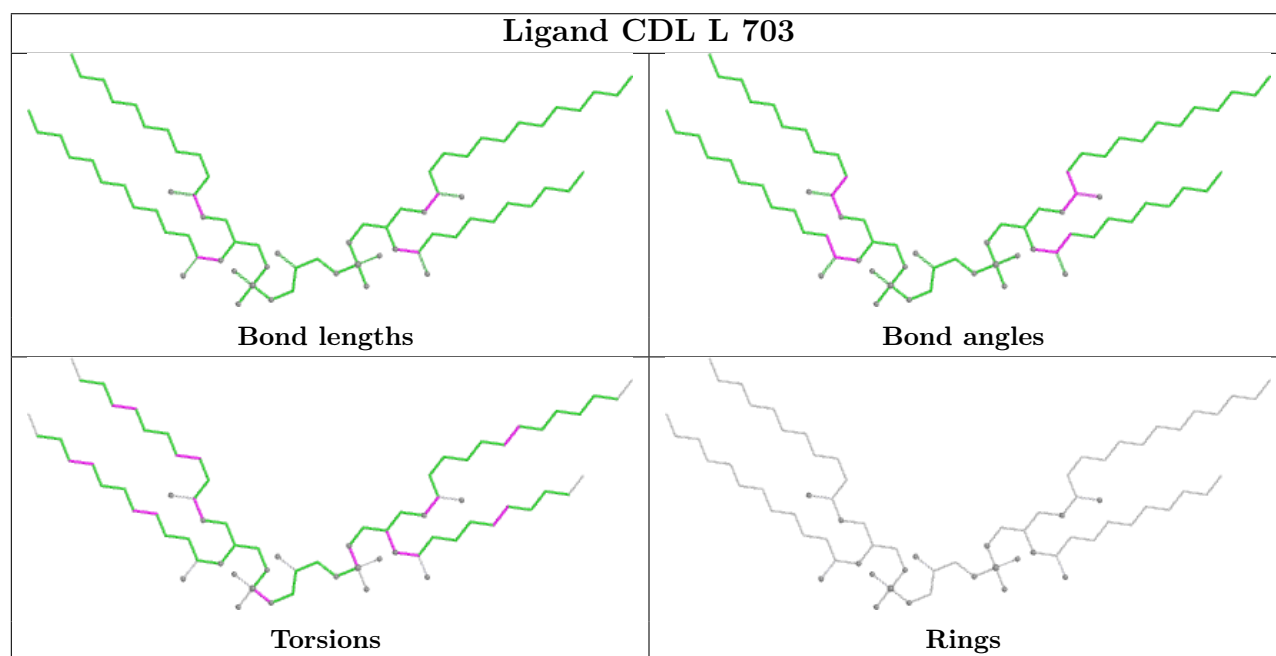
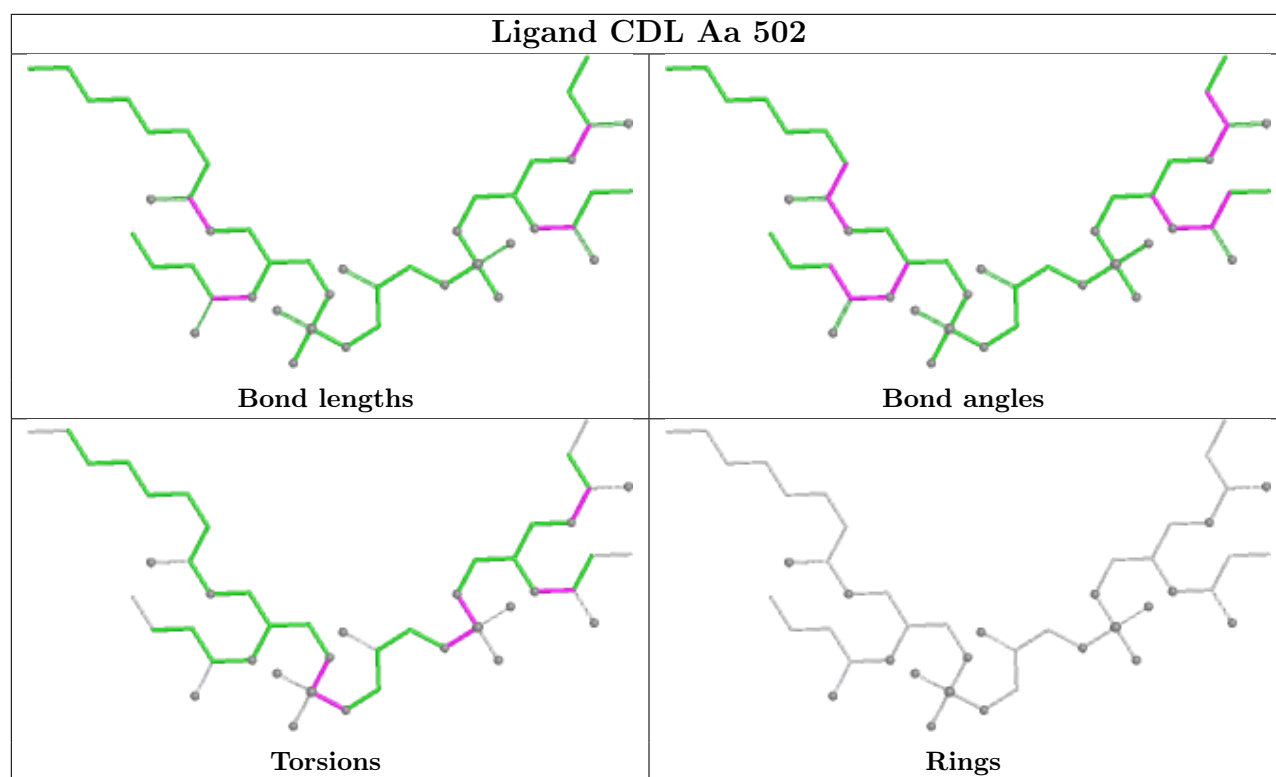


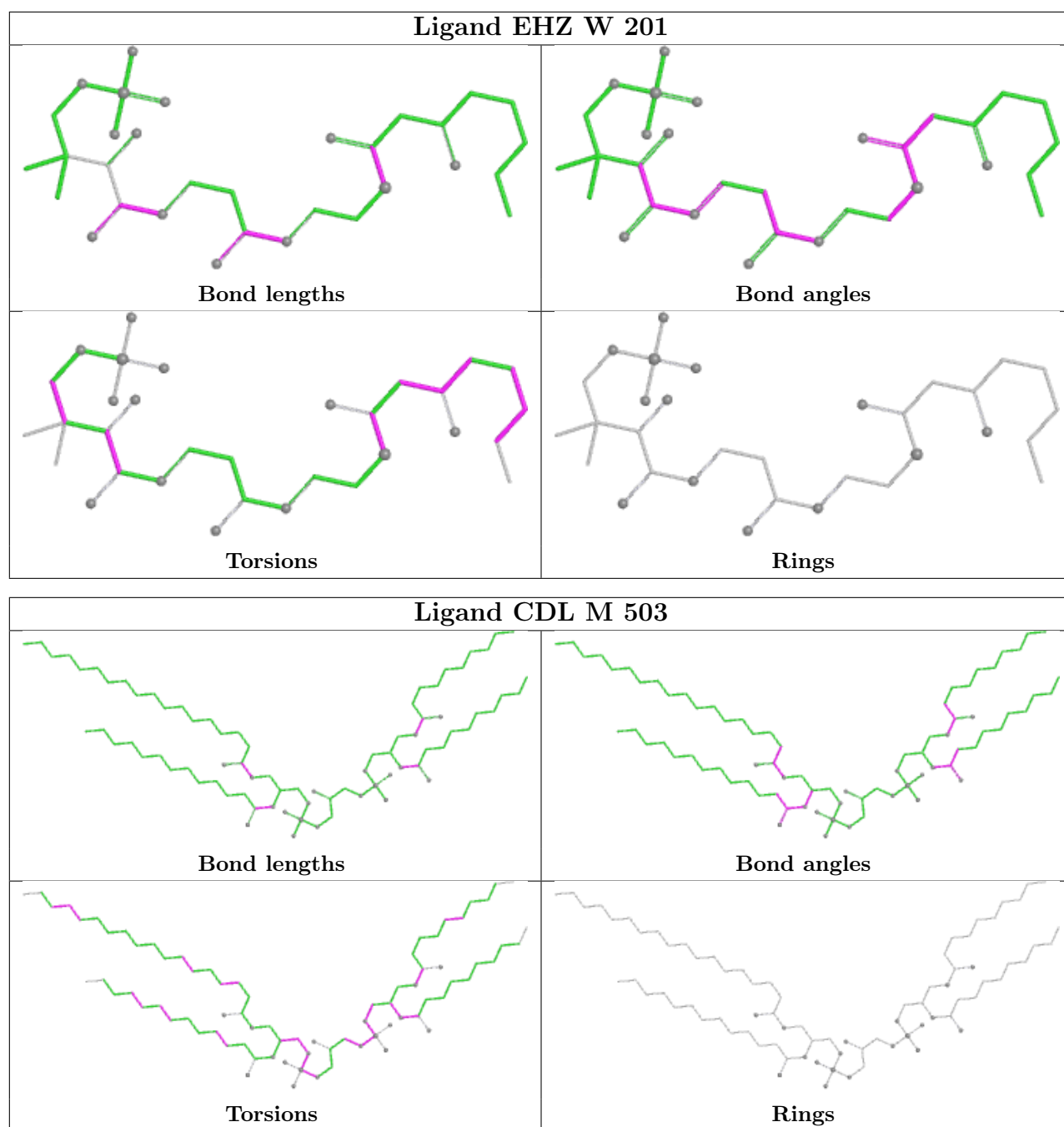




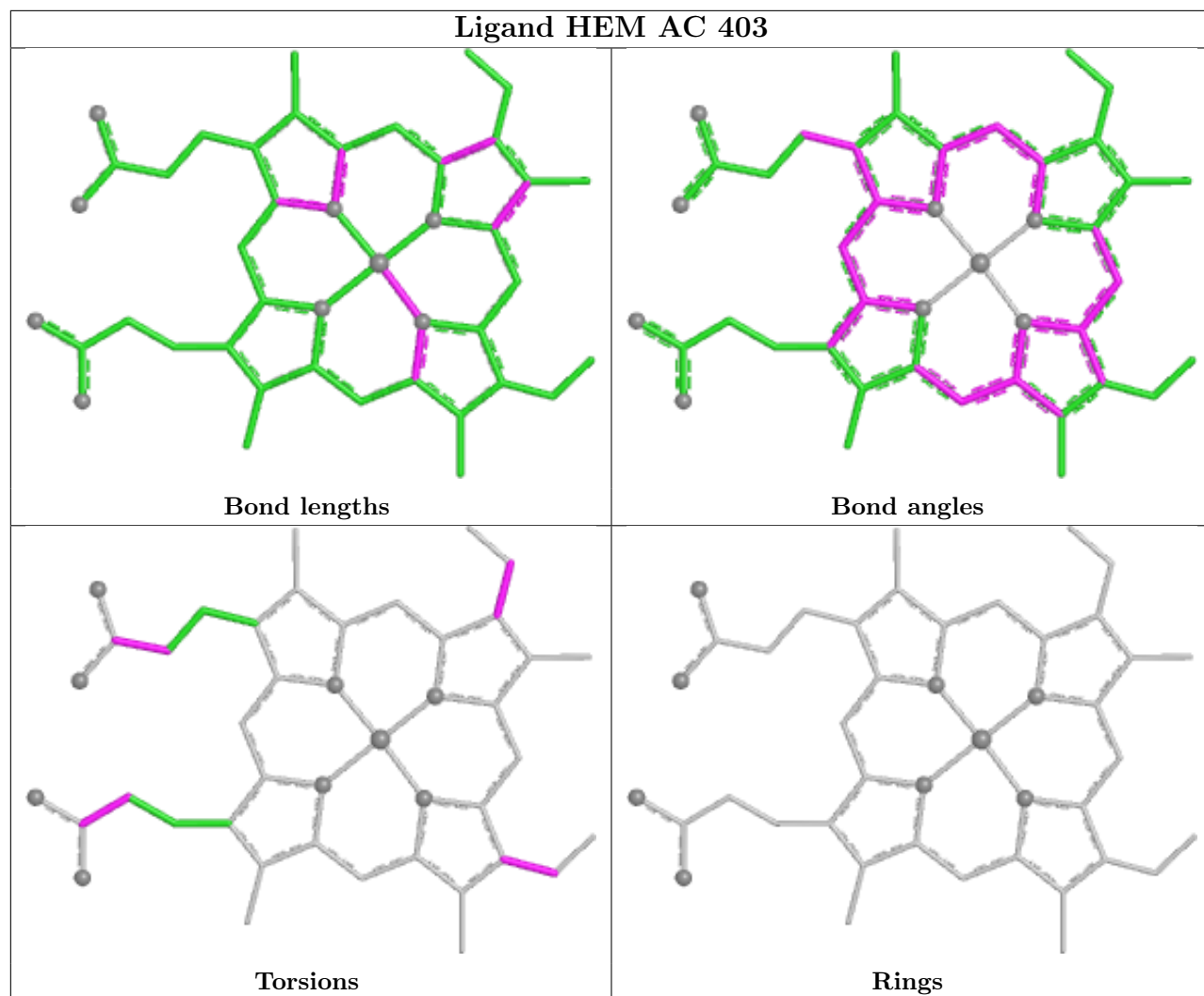


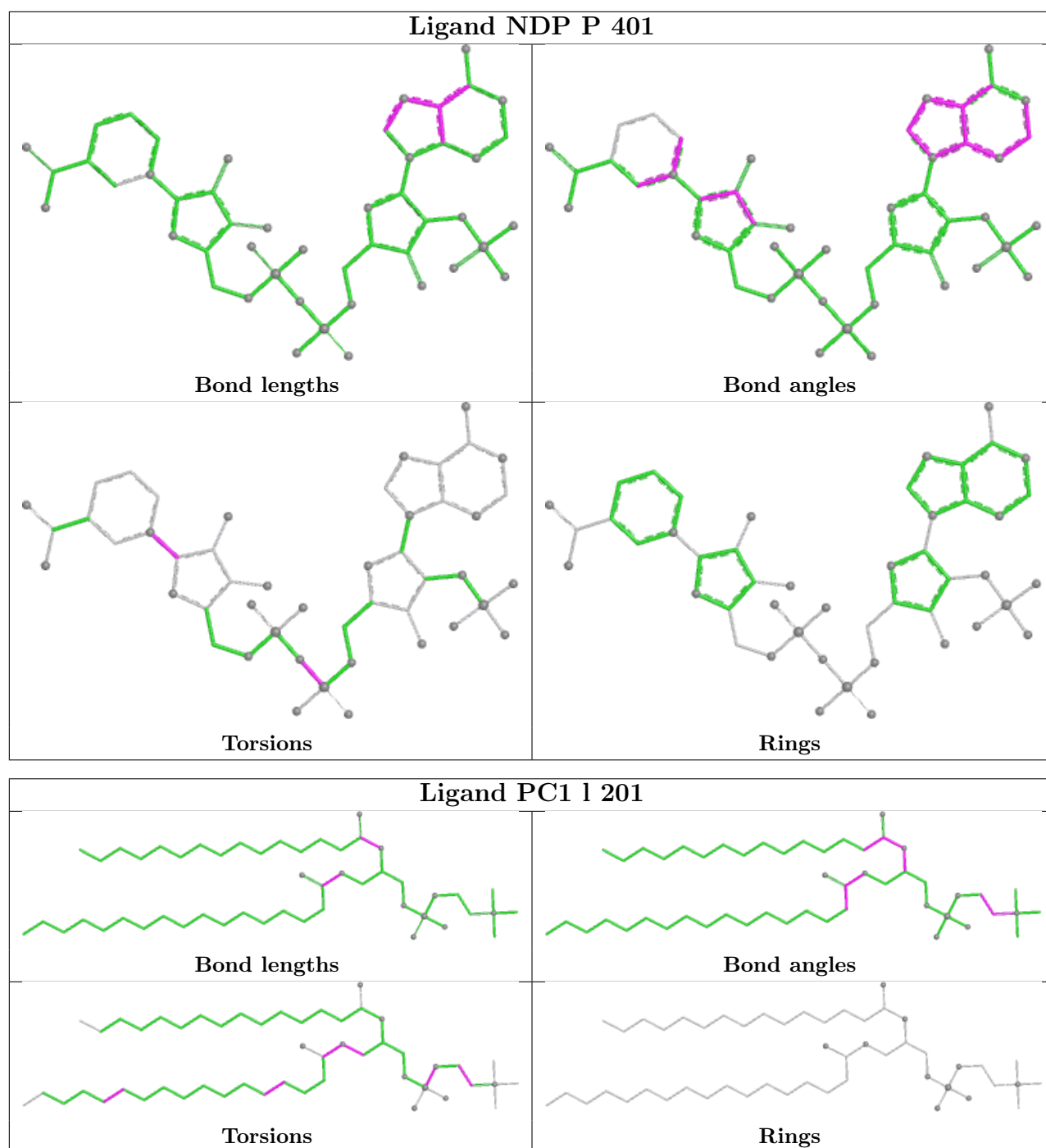


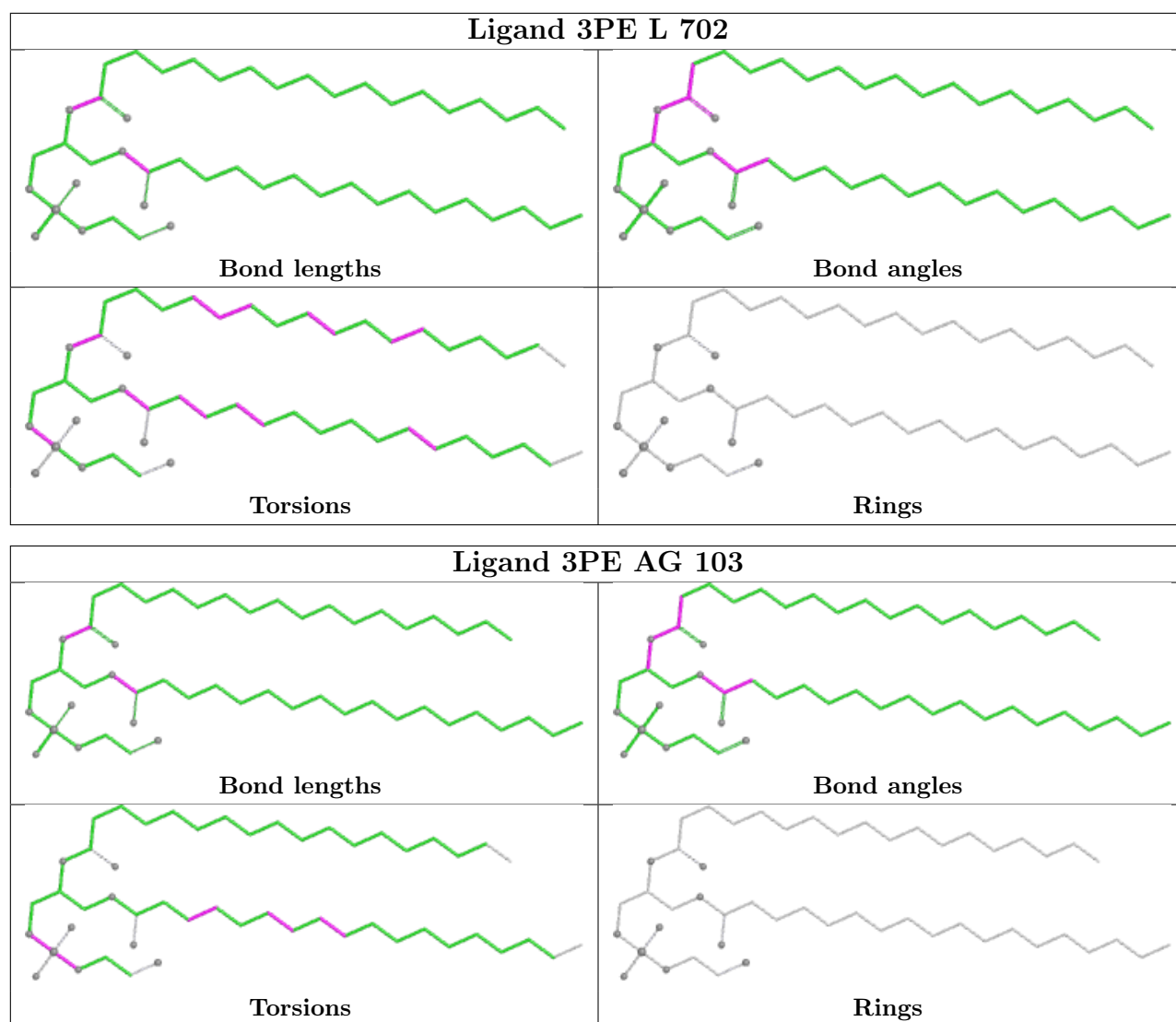


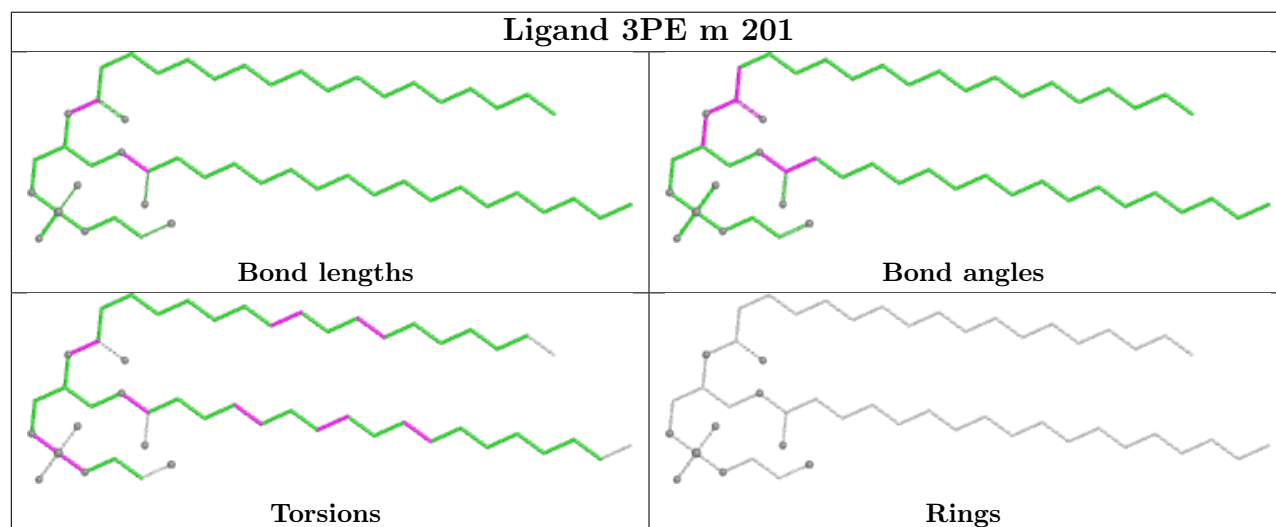
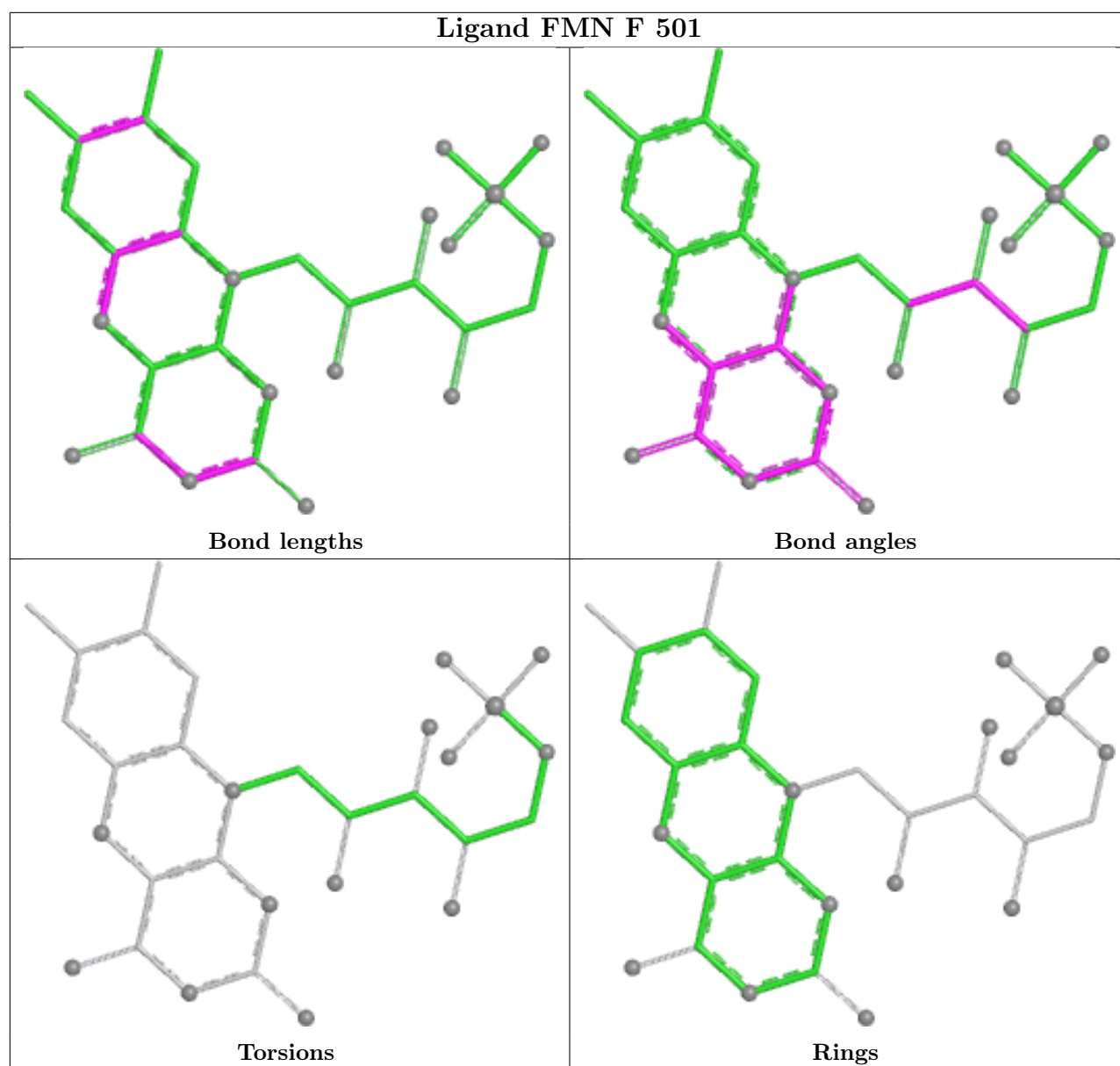


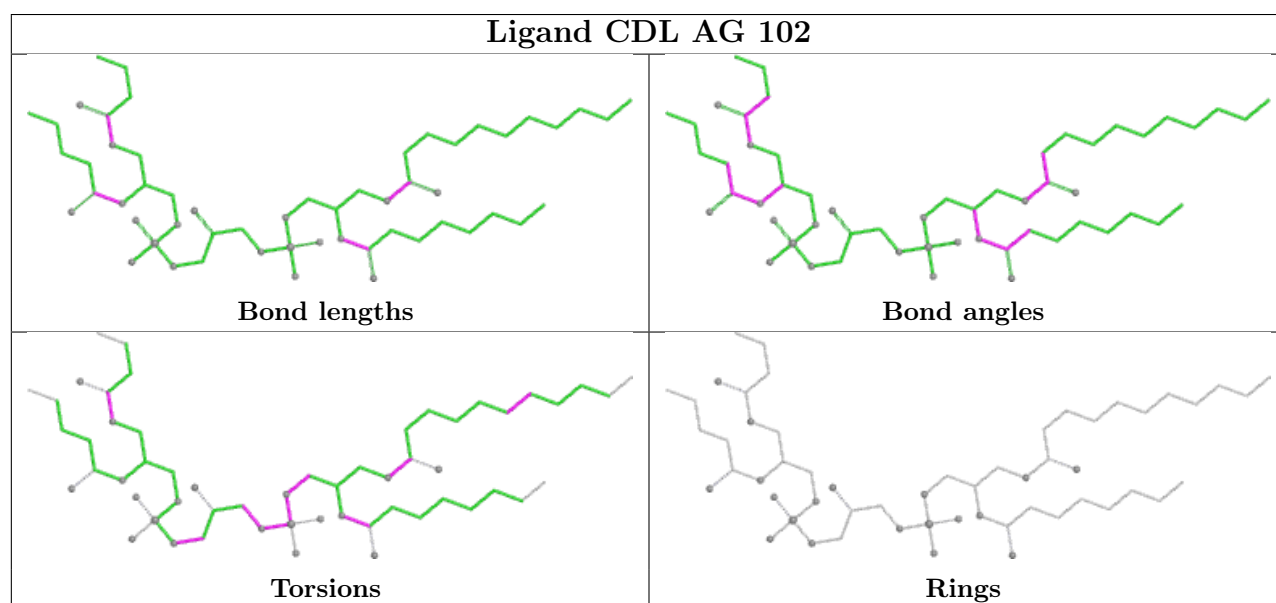
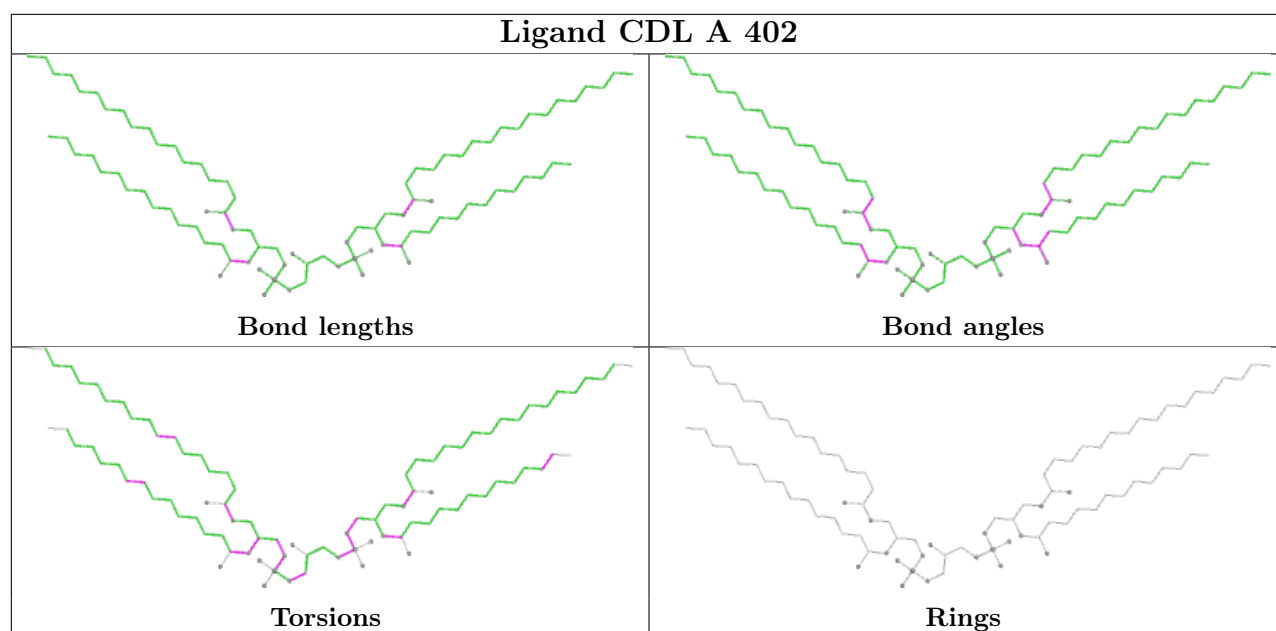
Ligand HEM AC 403



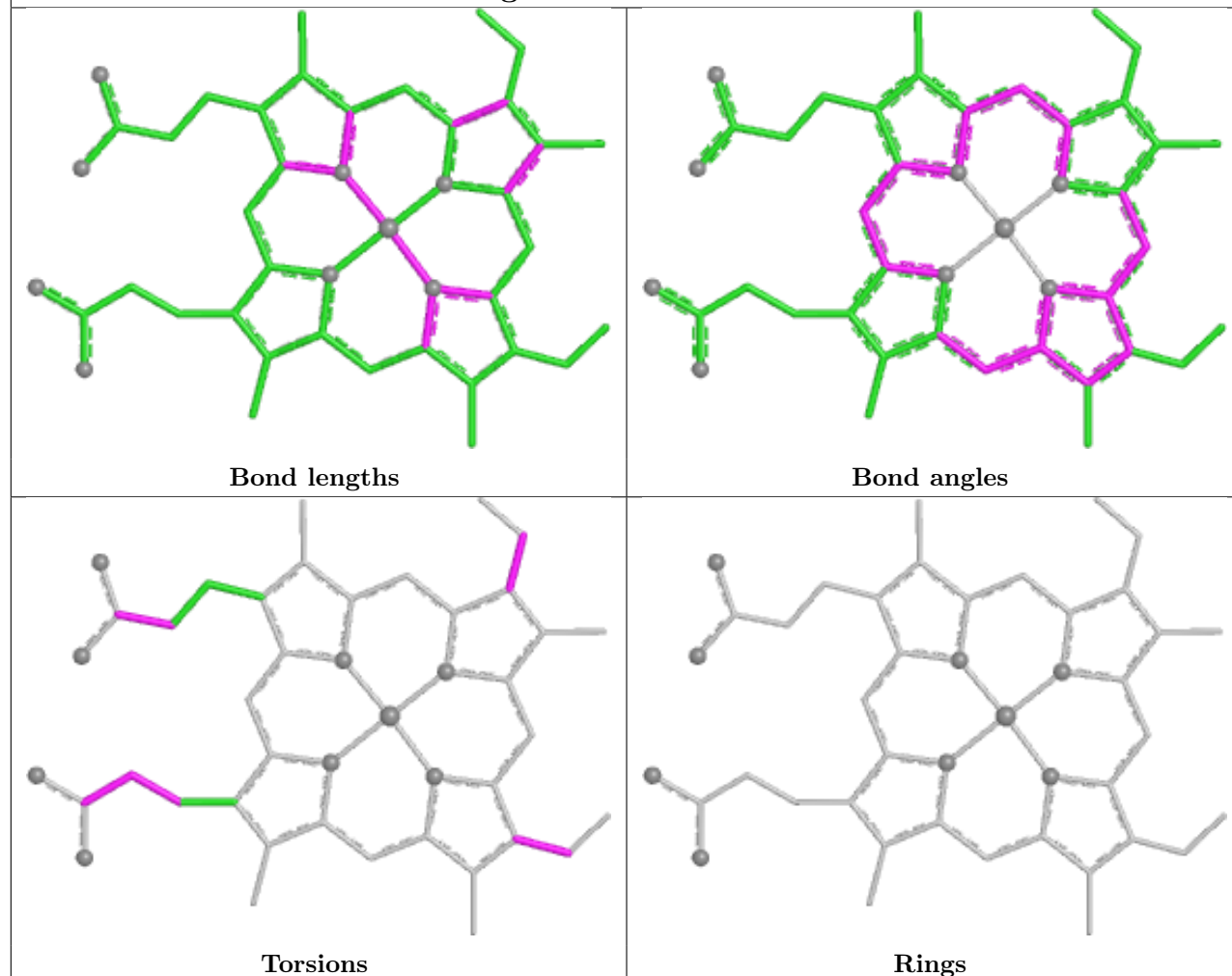




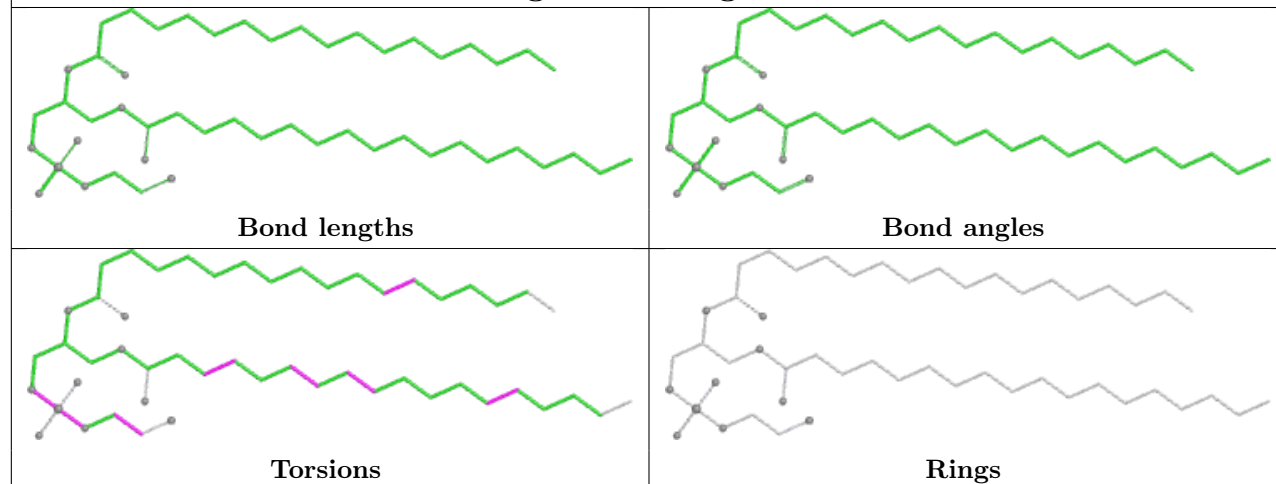


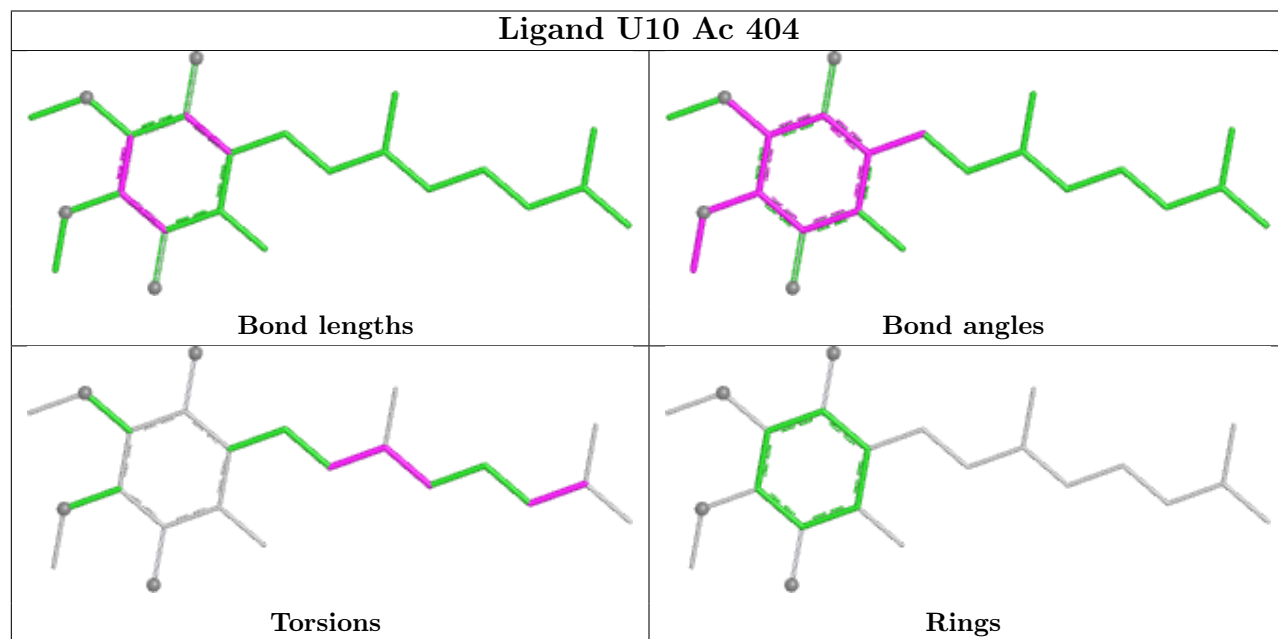
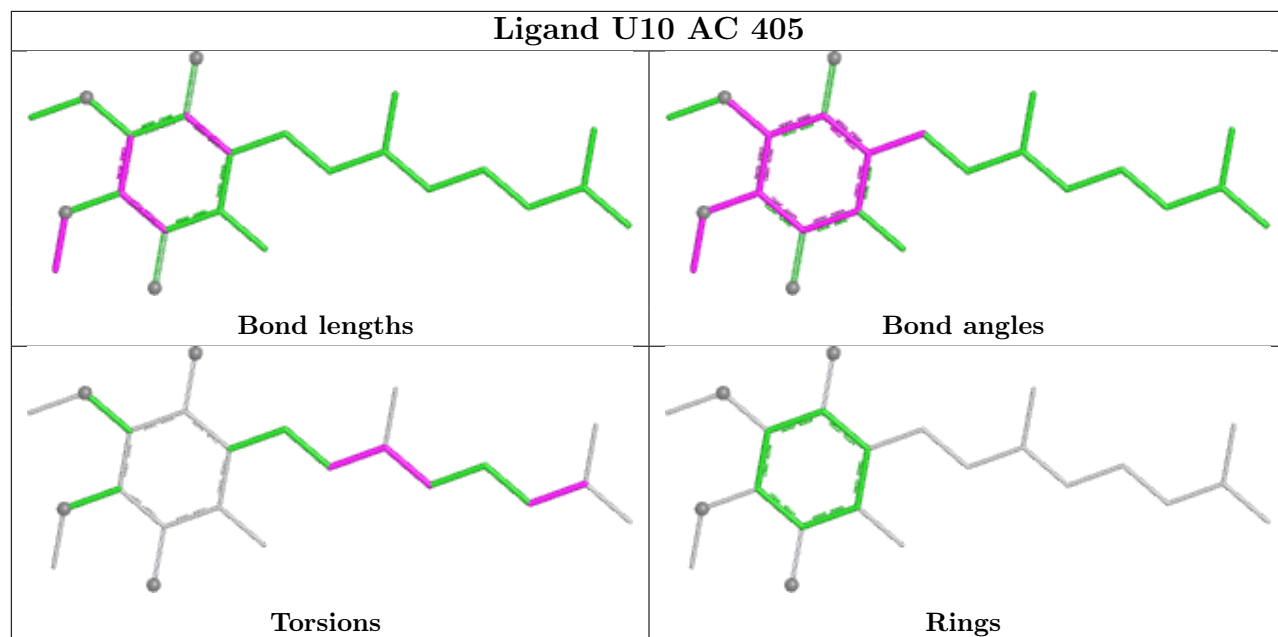


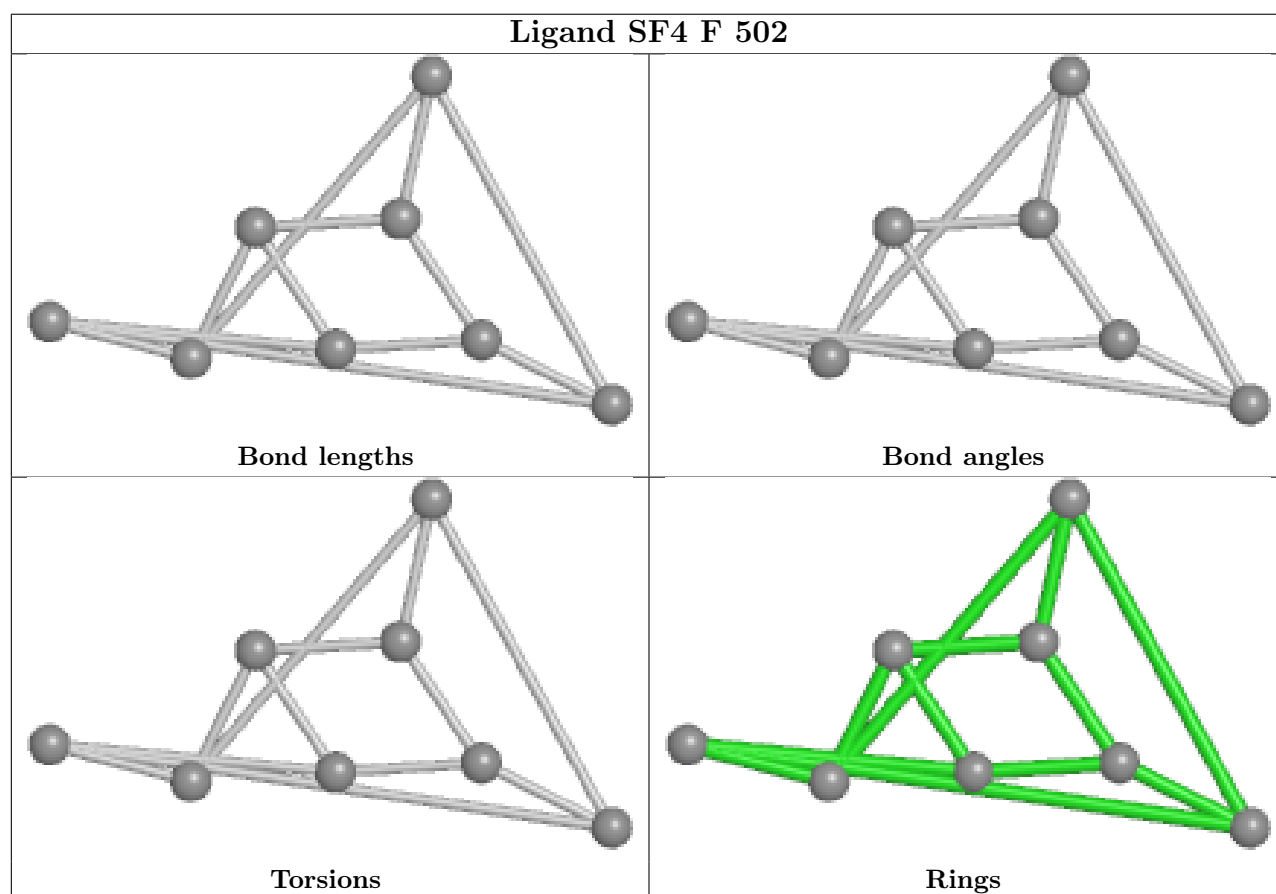
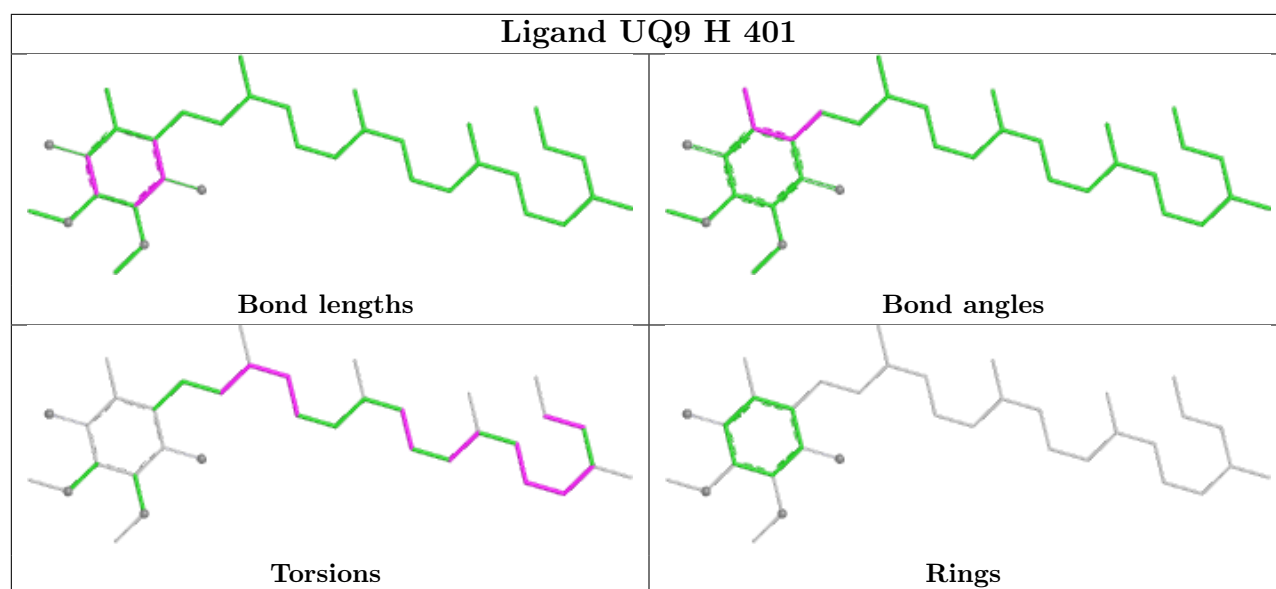
Ligand HEM Ac 401

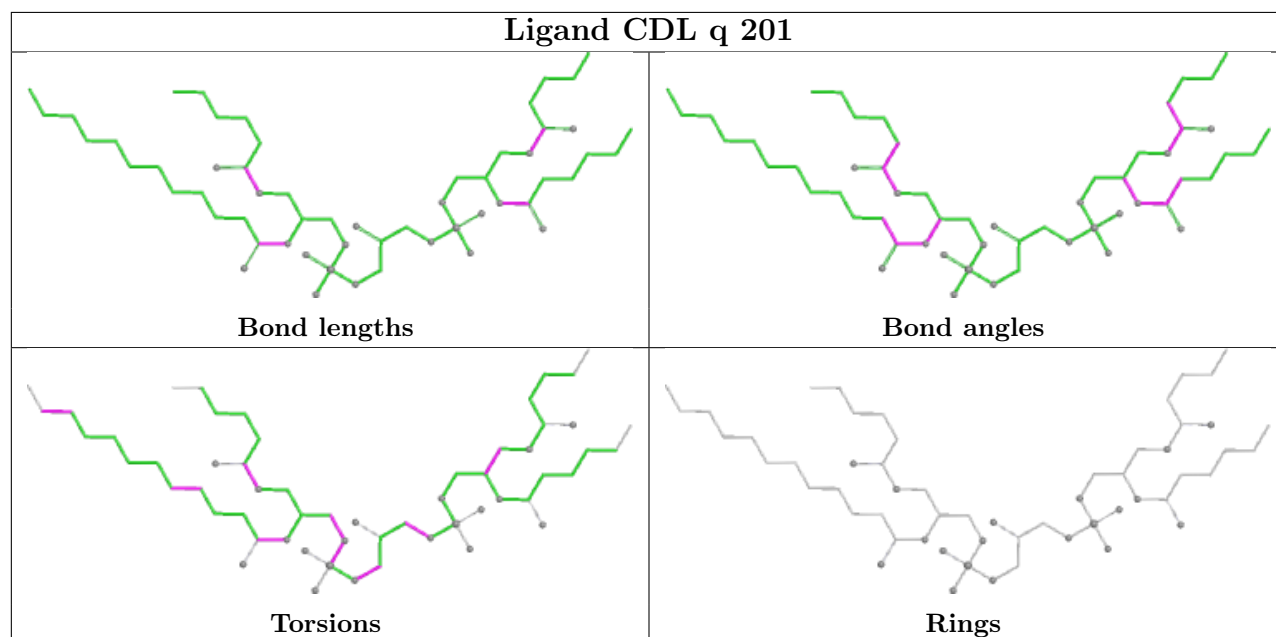
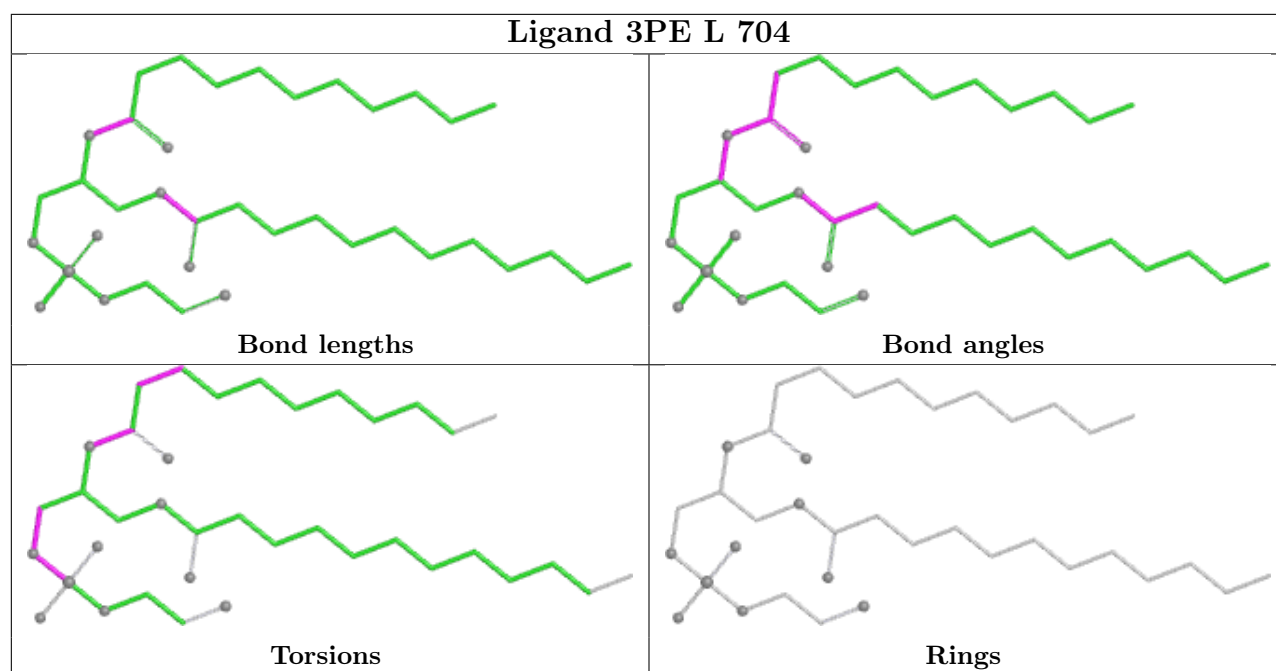


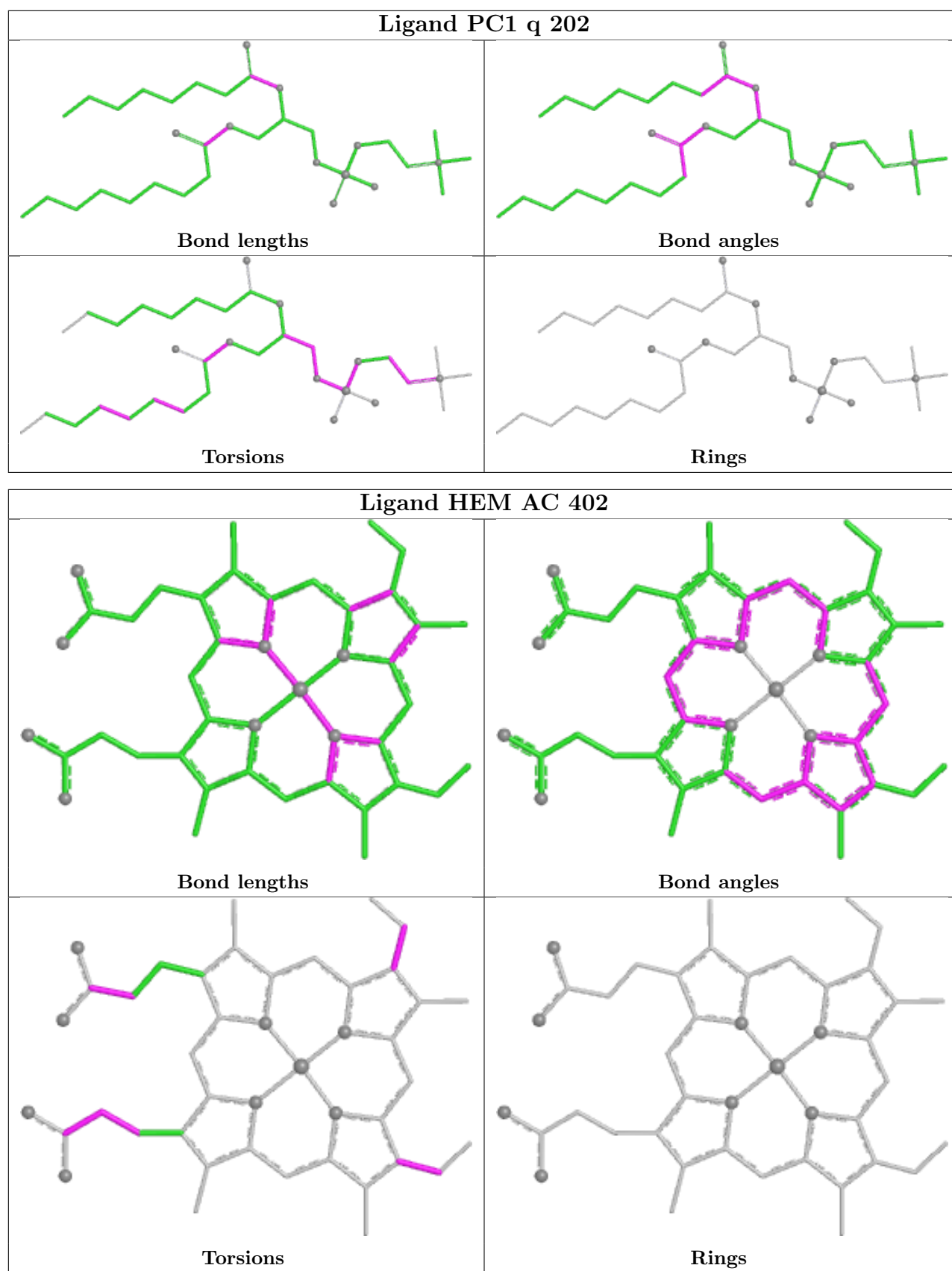
Ligand 3PE Ag 103

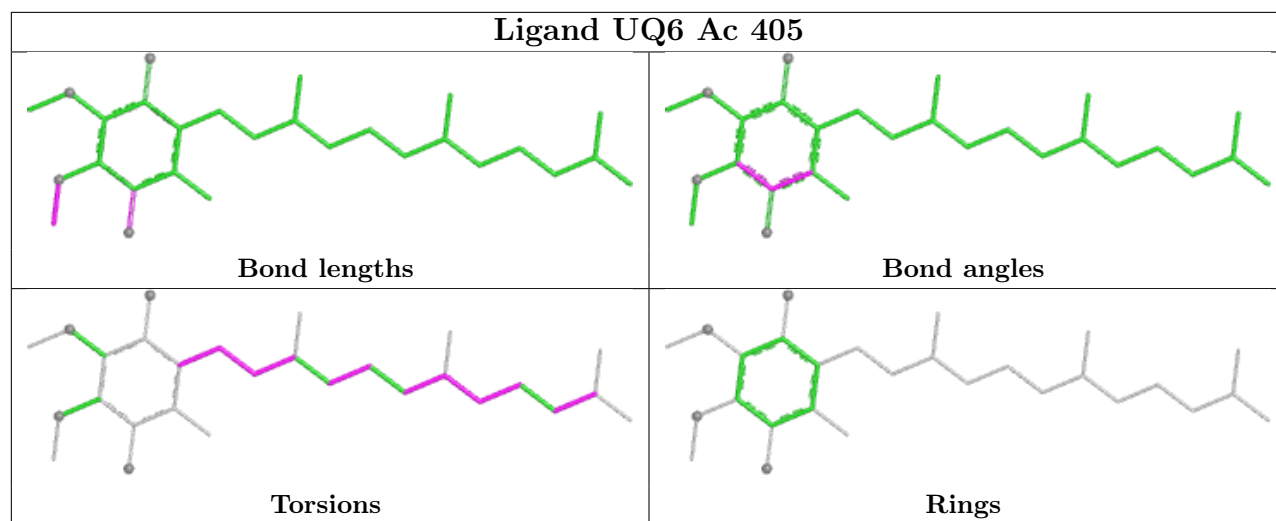
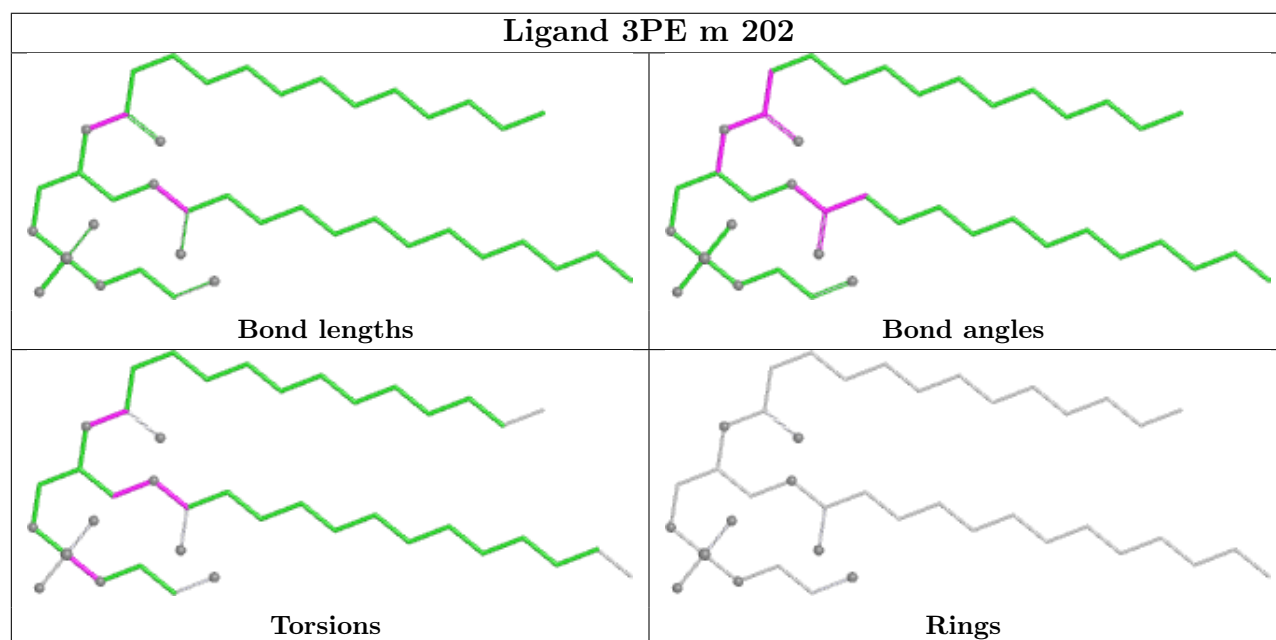
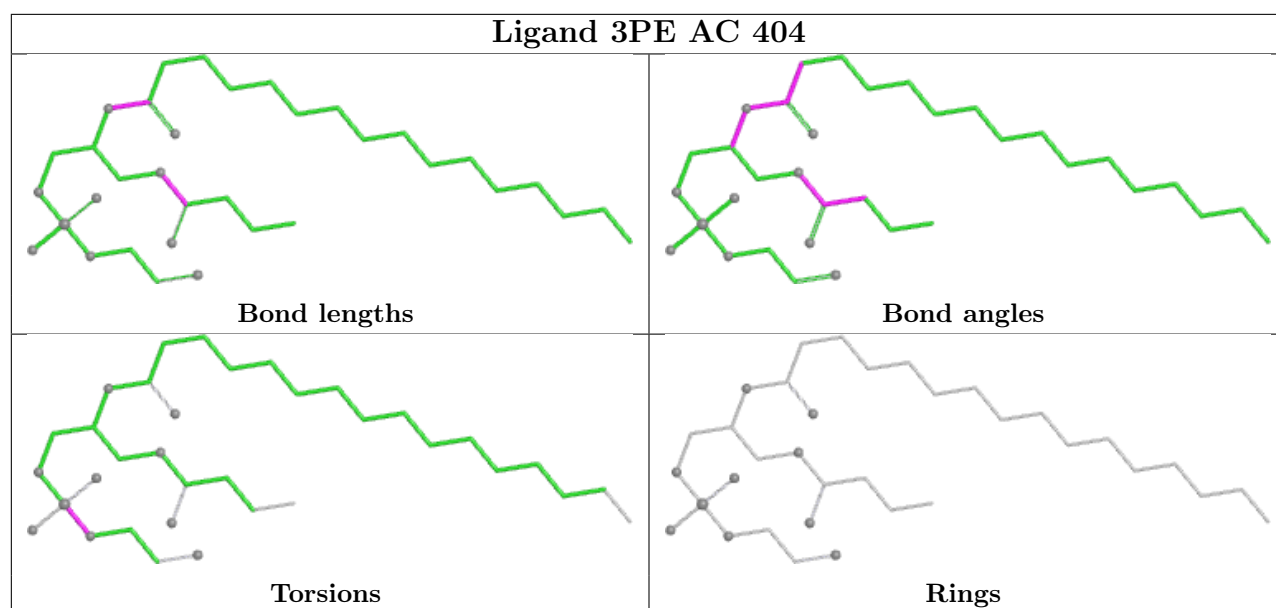


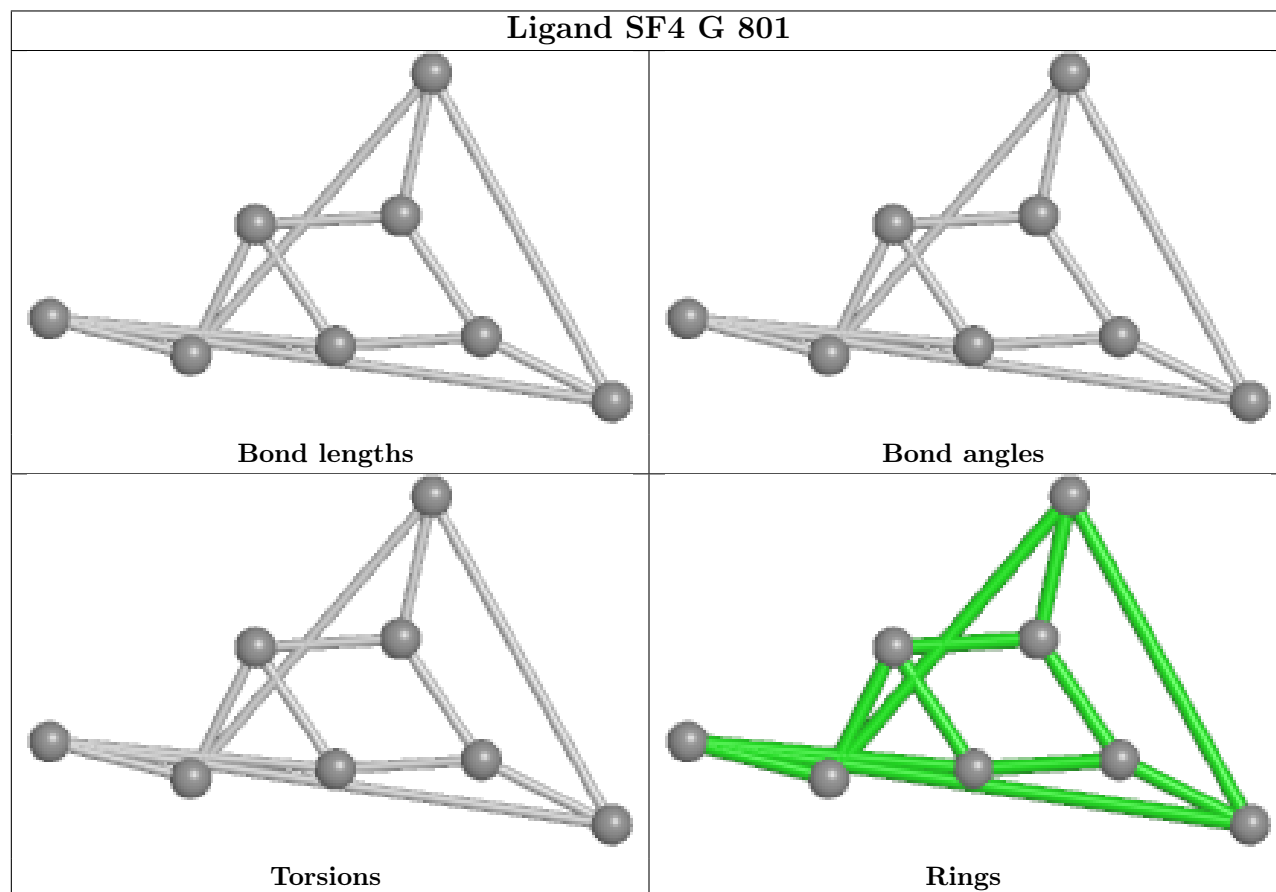
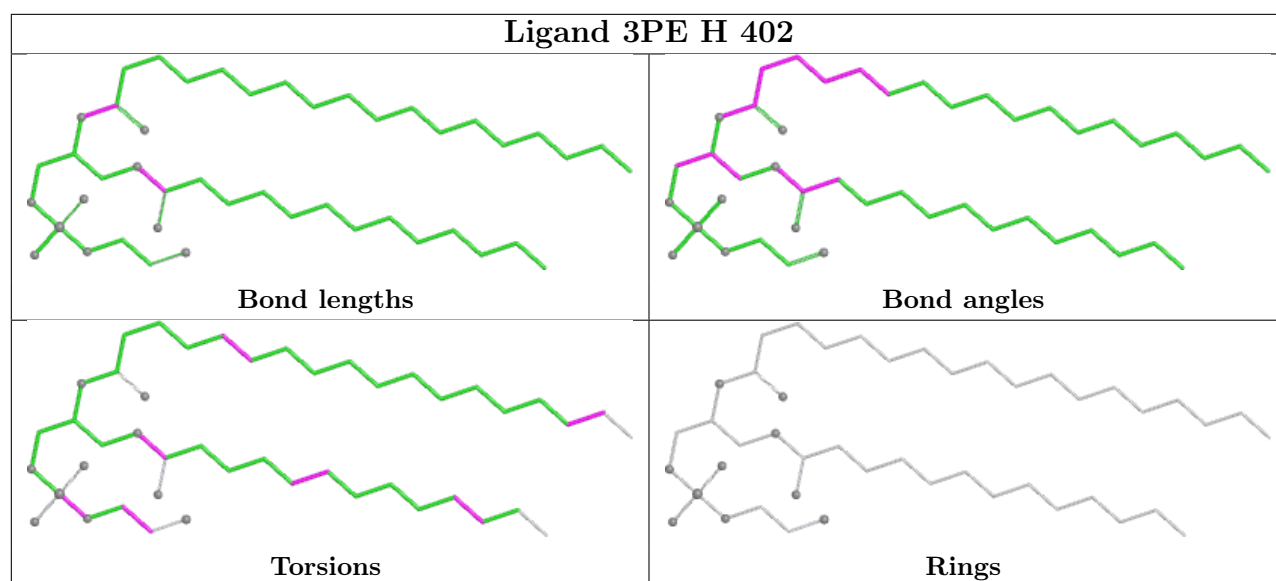


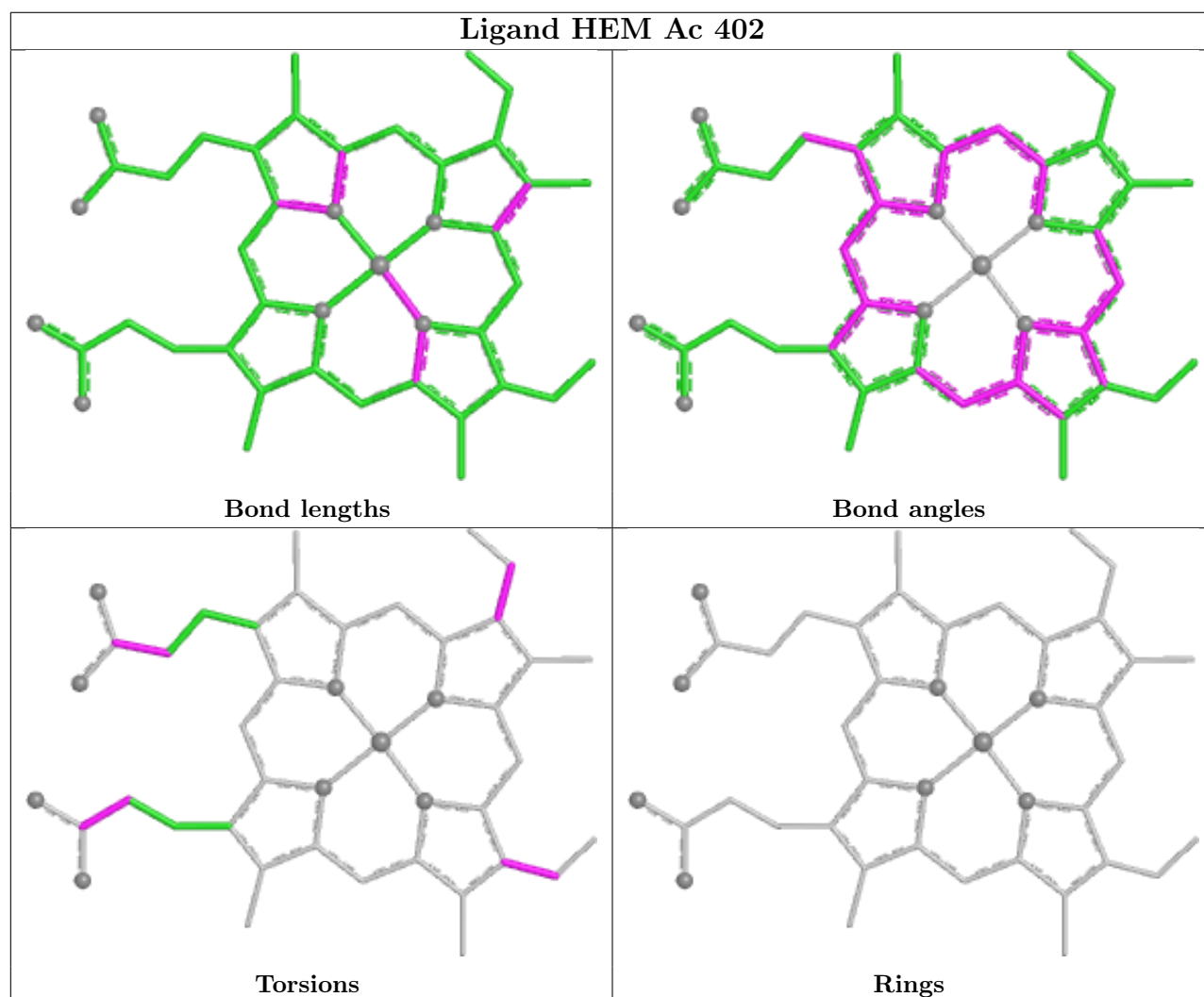
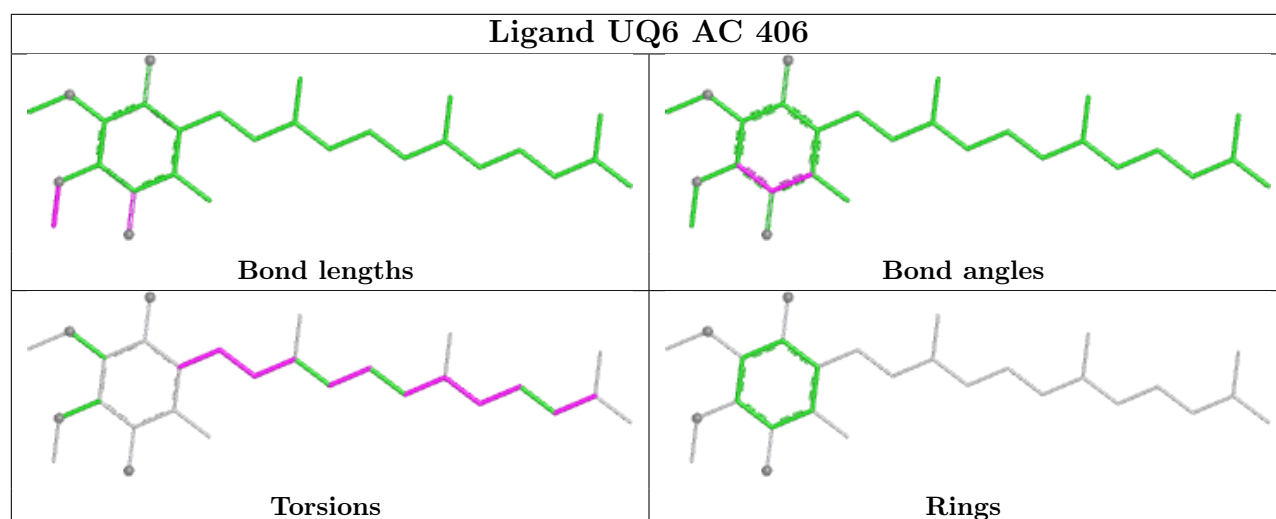


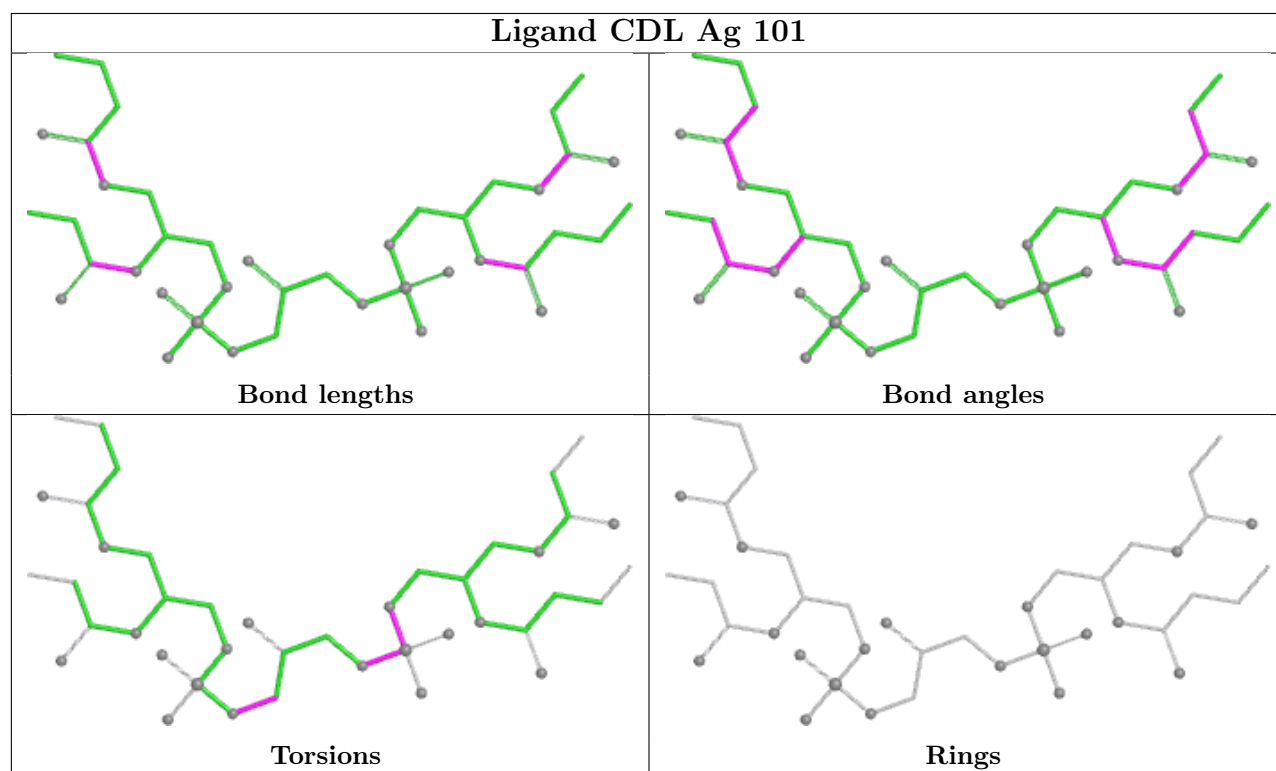
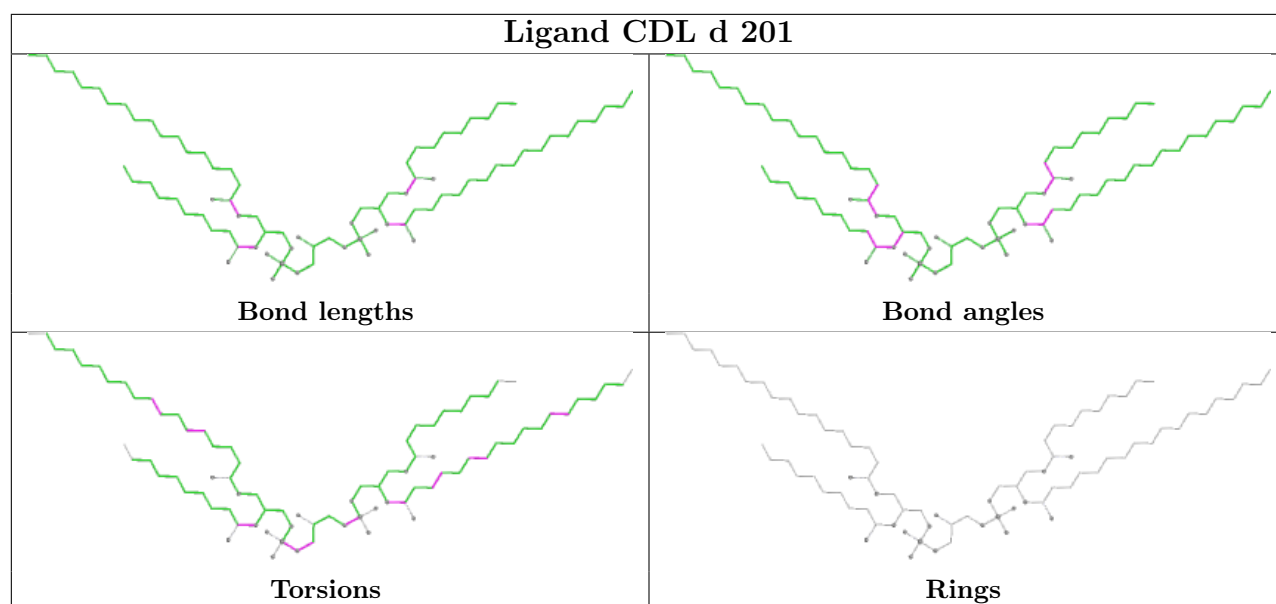


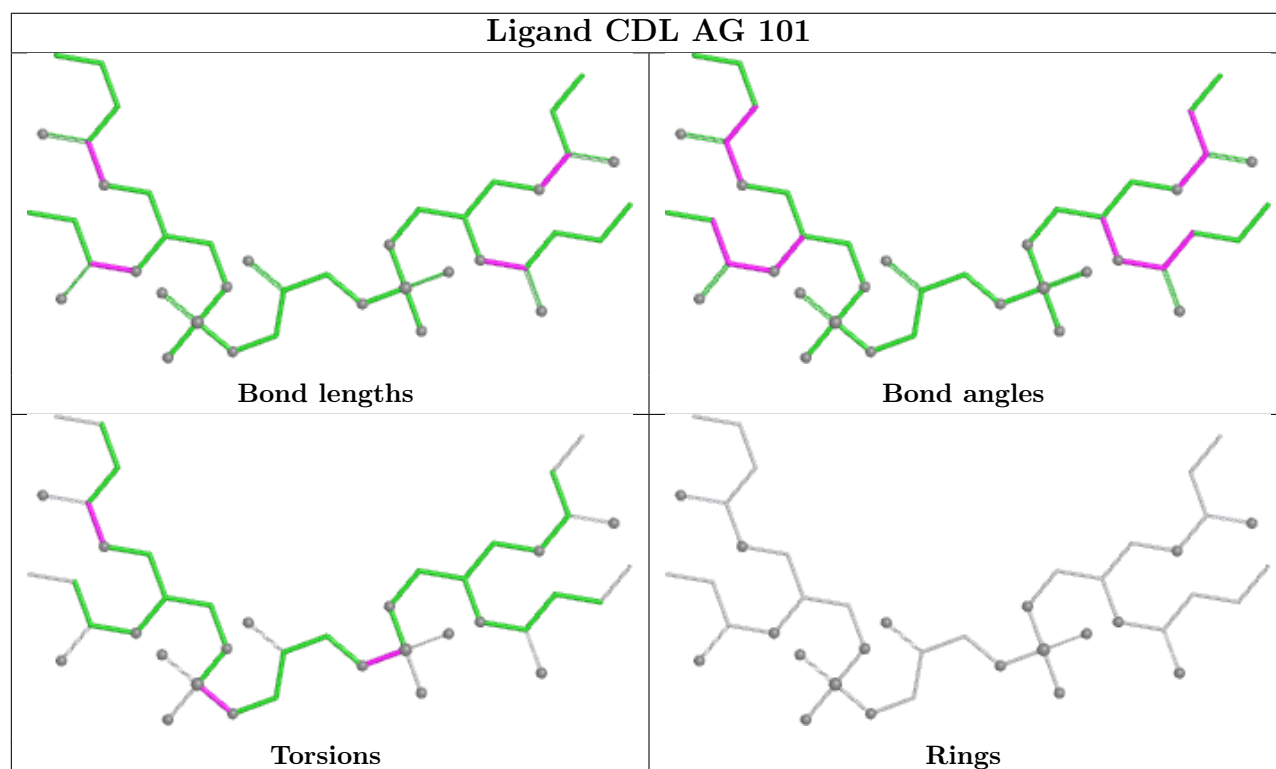
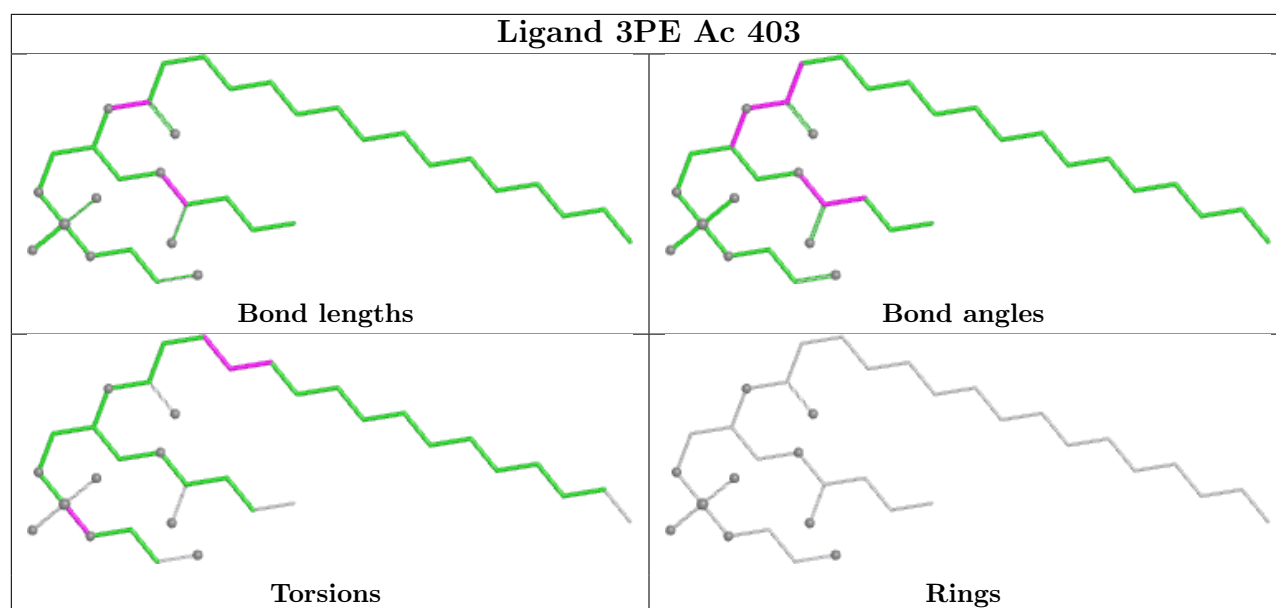


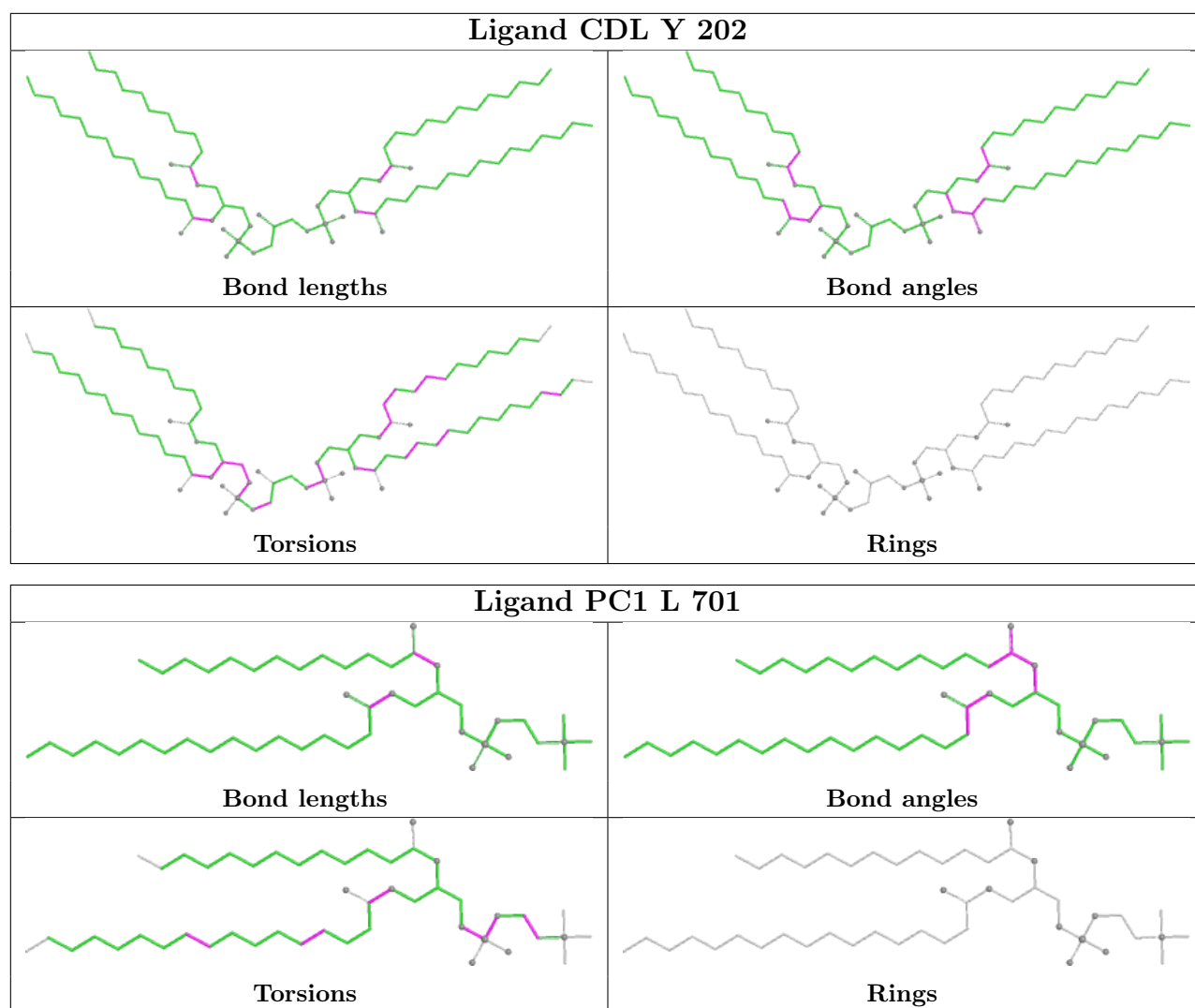




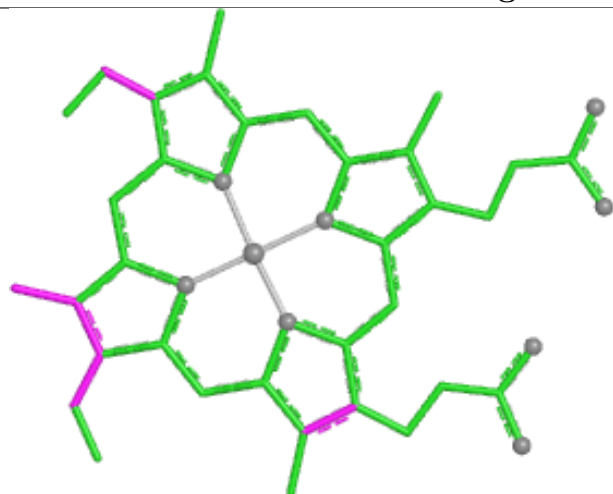




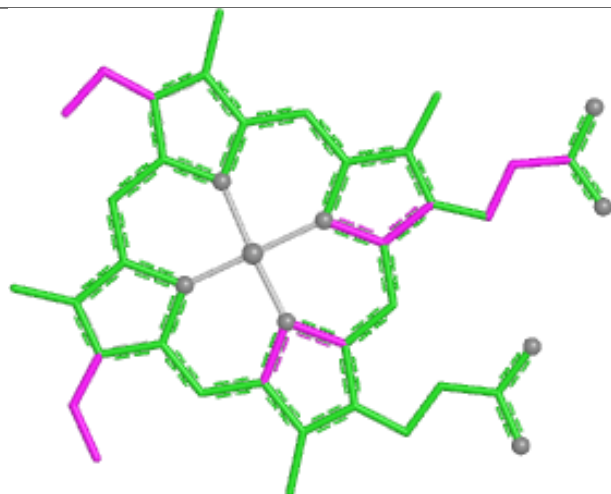




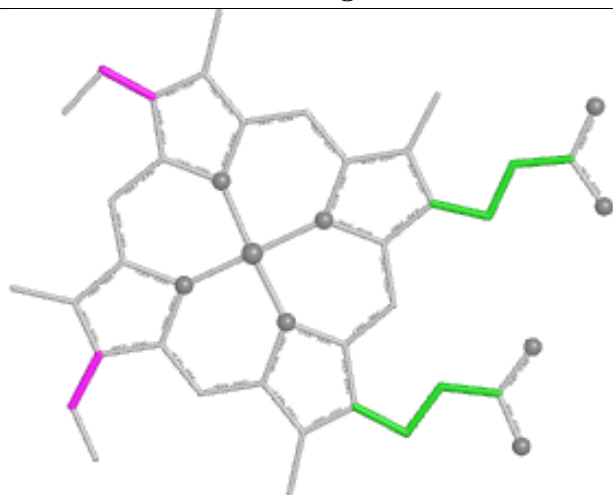
Ligand HEC AD 401



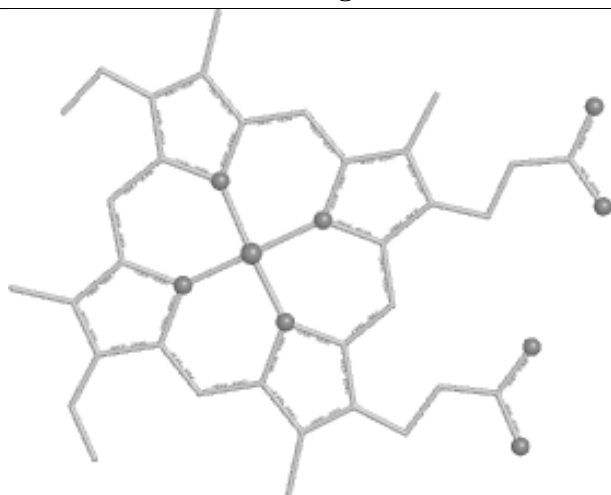
Bond lengths



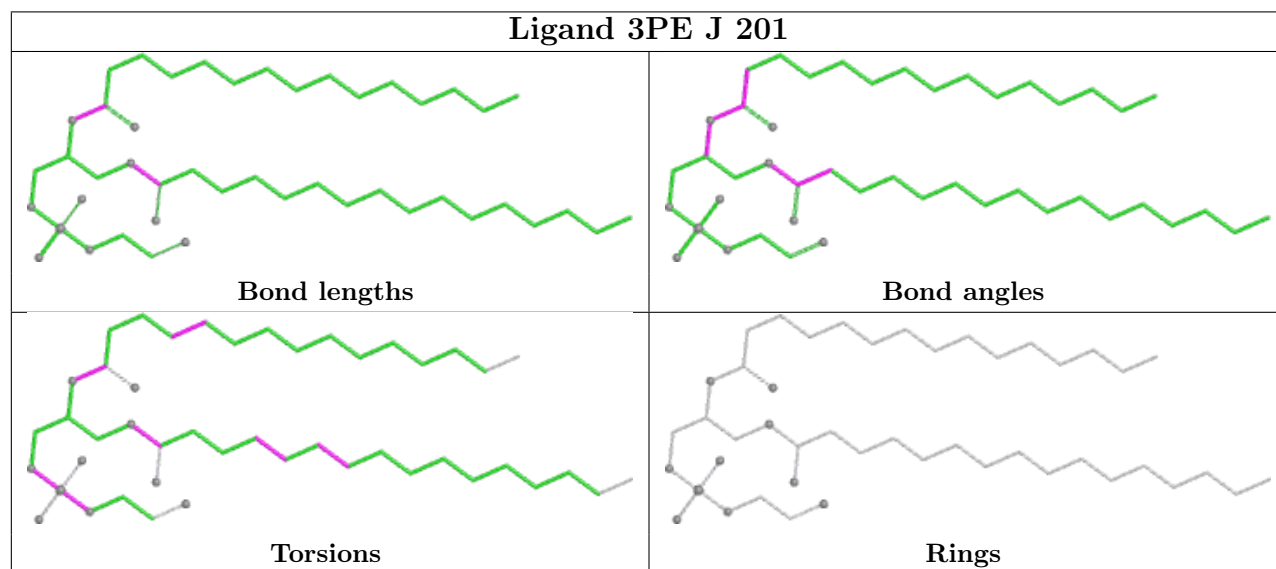
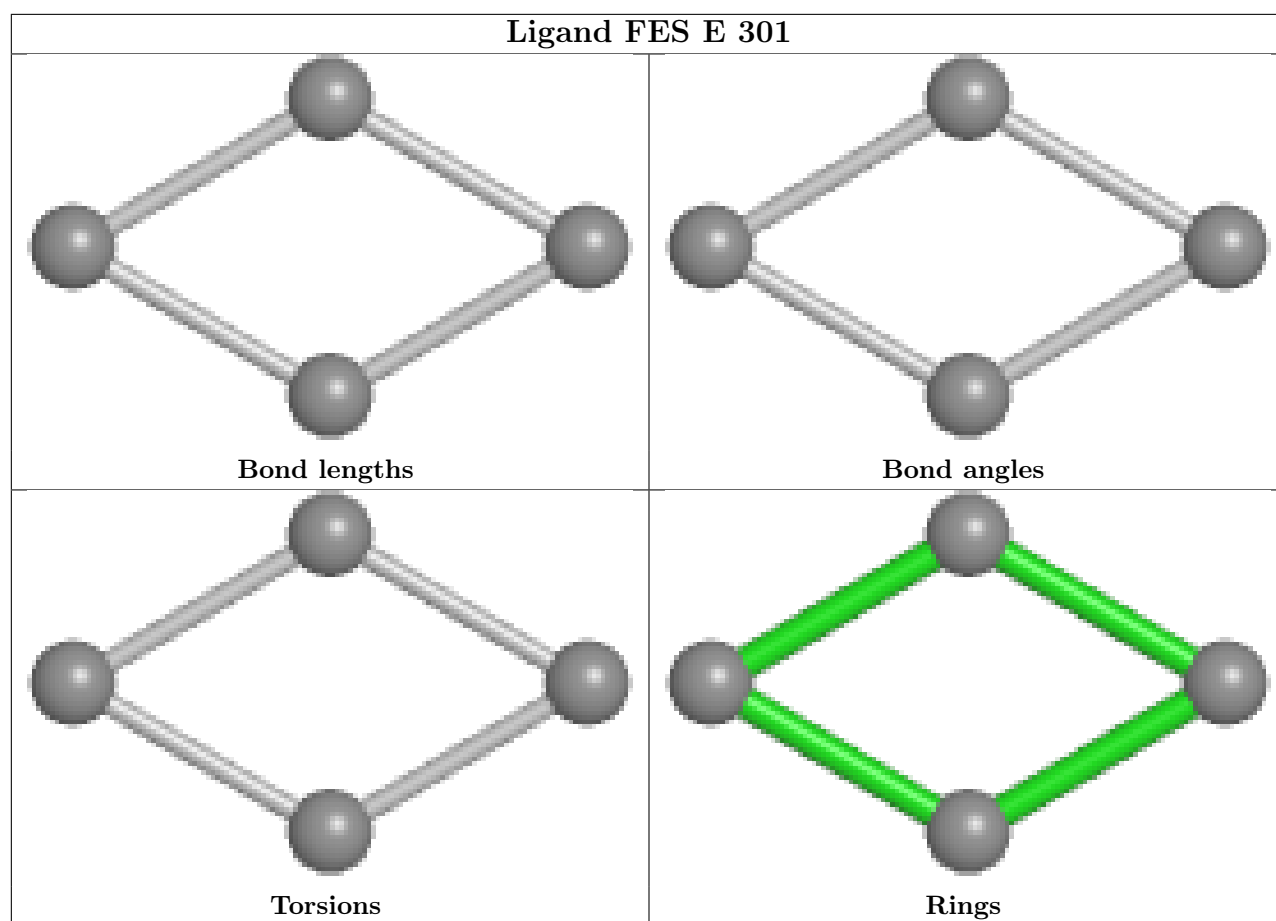
Bond angles

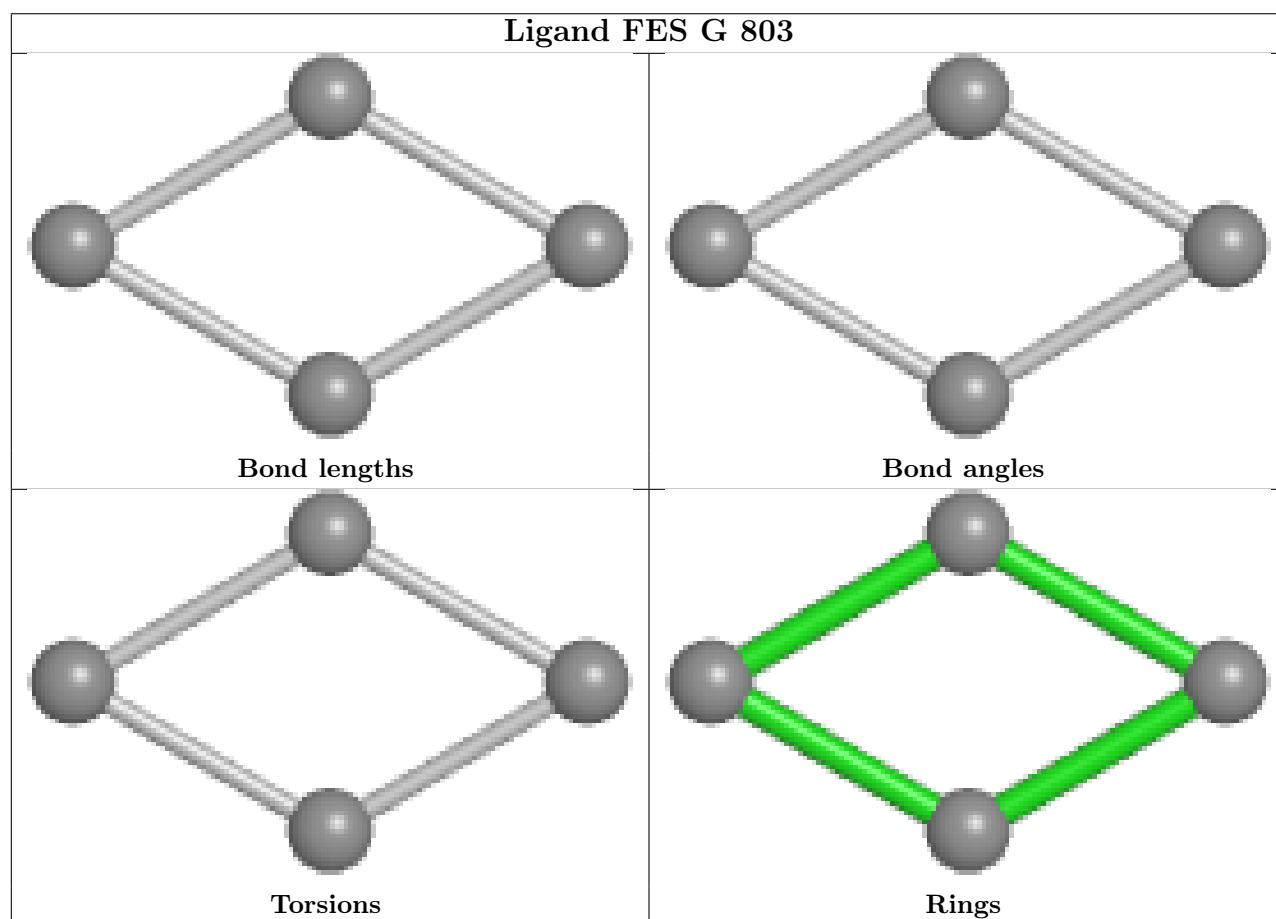
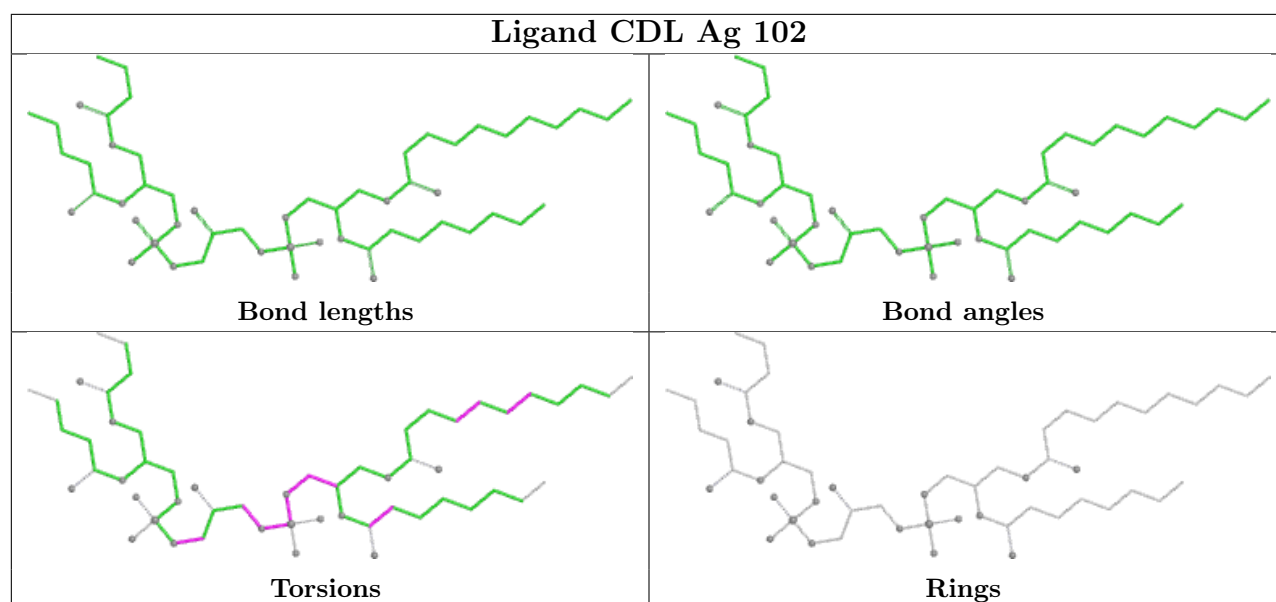


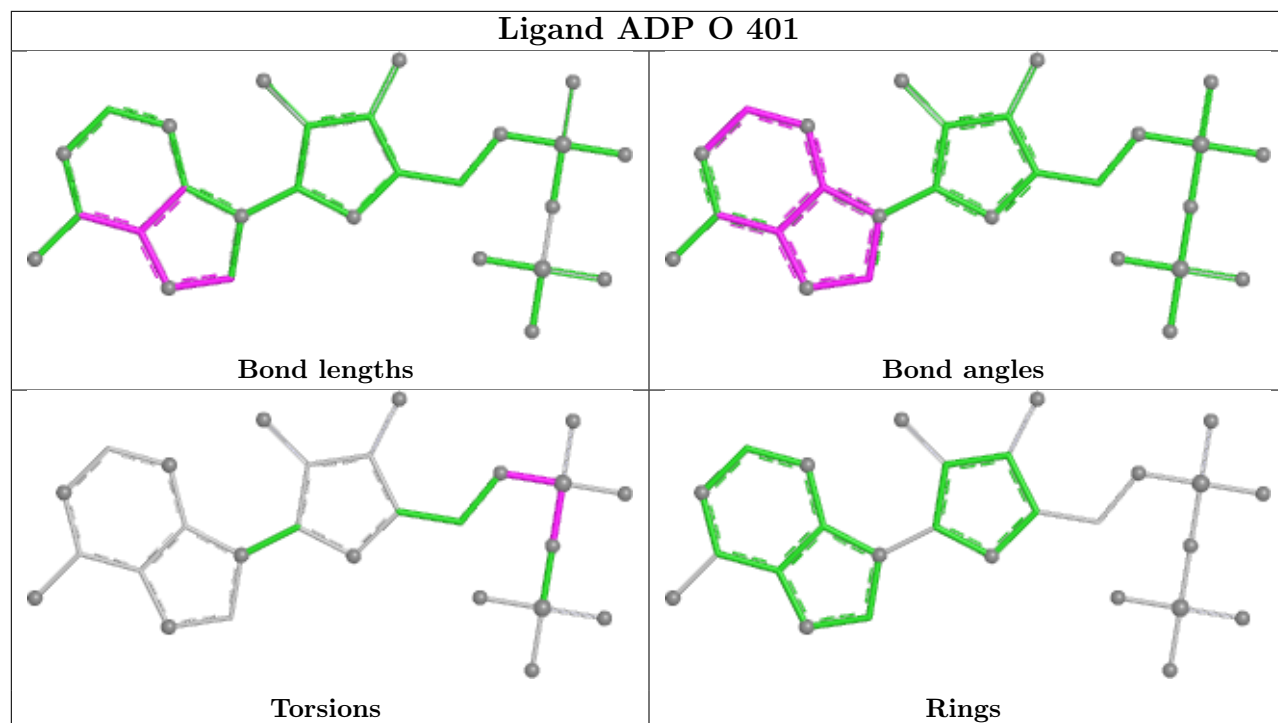
Torsions



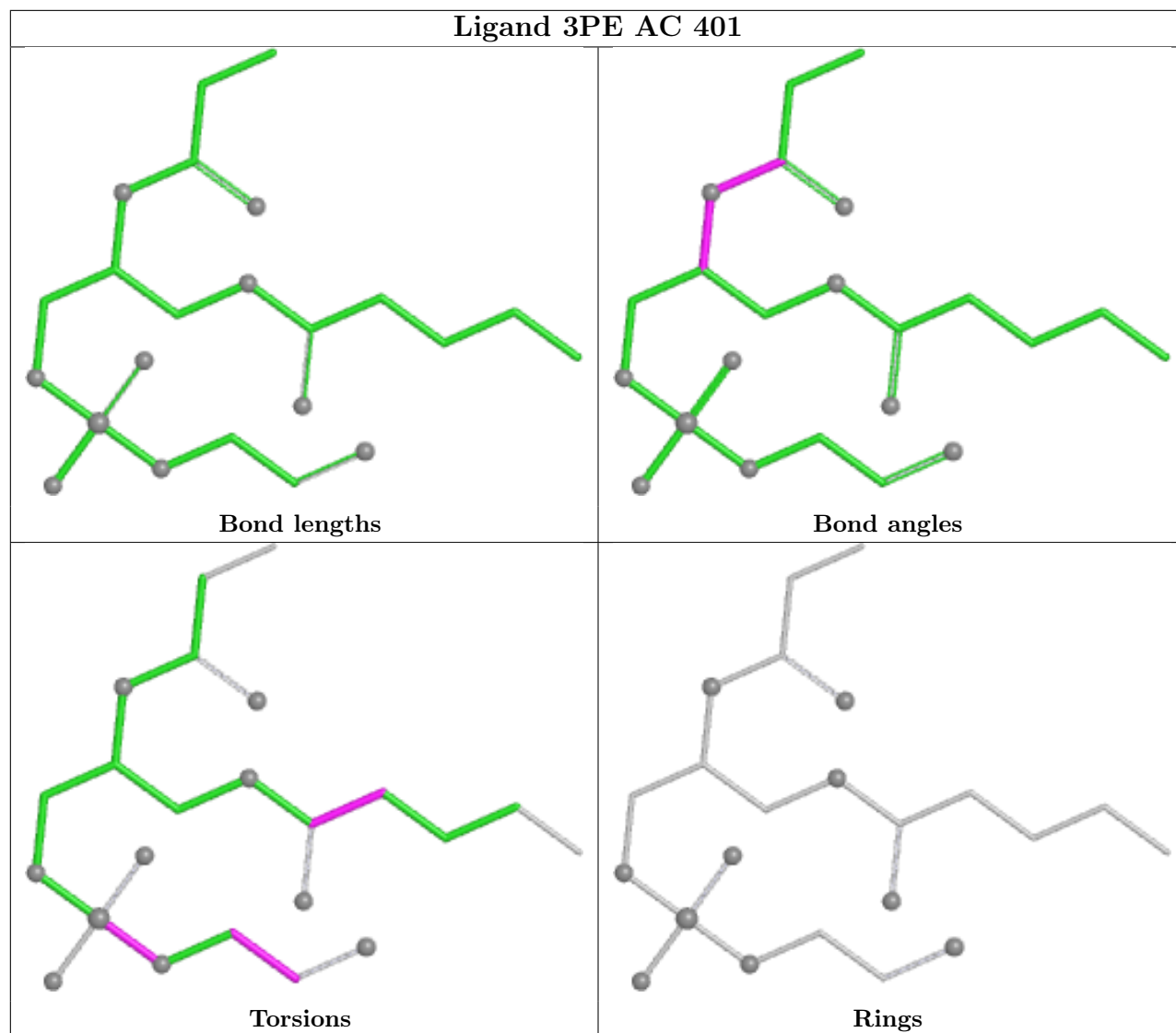
Rings



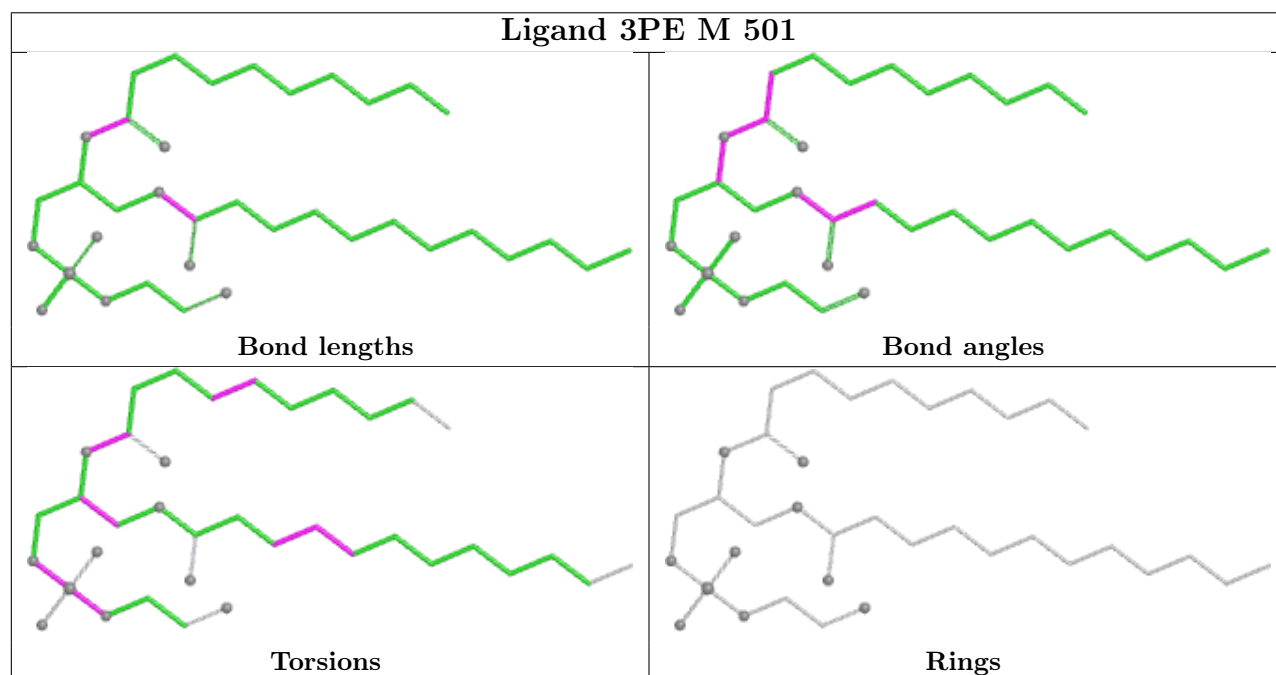


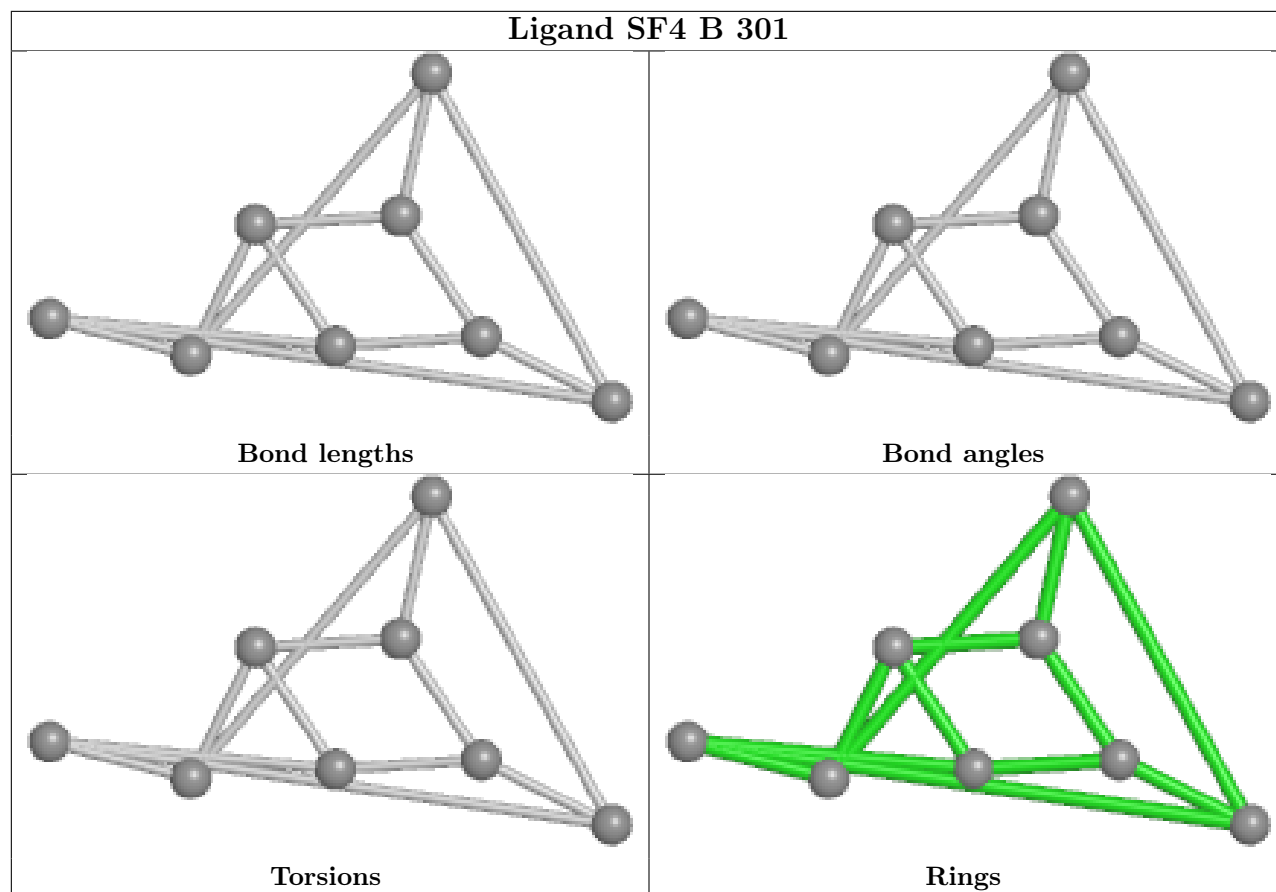


Ligand 3PE AC 401



Ligand 3PE M 501





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.

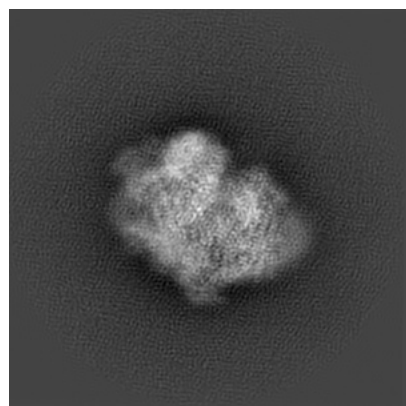
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35313. These allow visual inspection of the internal detail of the map and identification of artifacts.

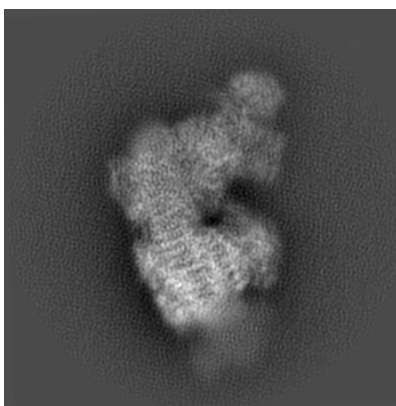
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

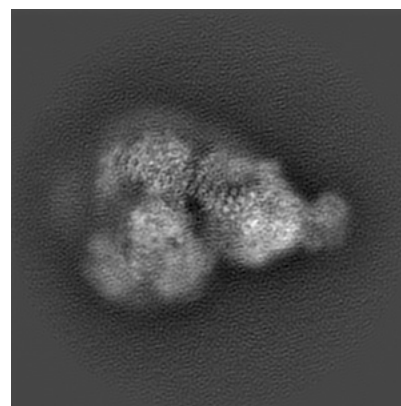
6.1.1 Primary map



X

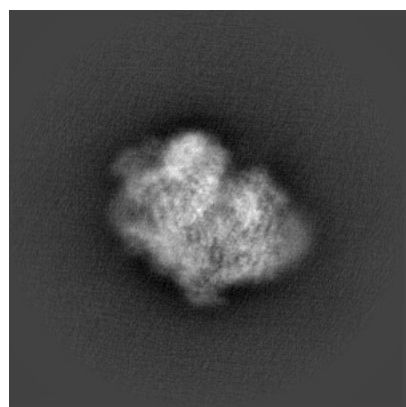


Y

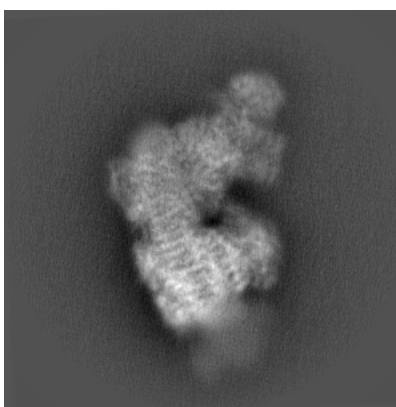


Z

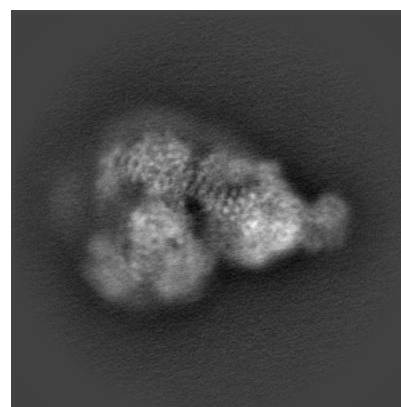
6.1.2 Raw map



X



Y

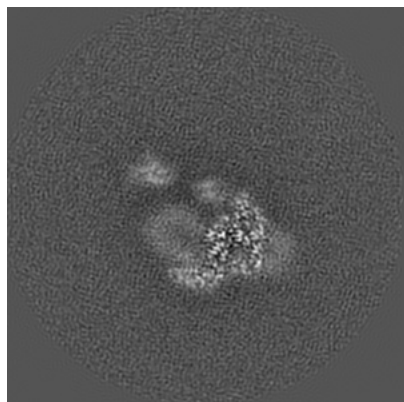


Z

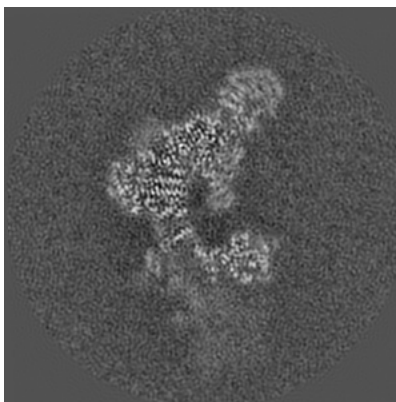
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

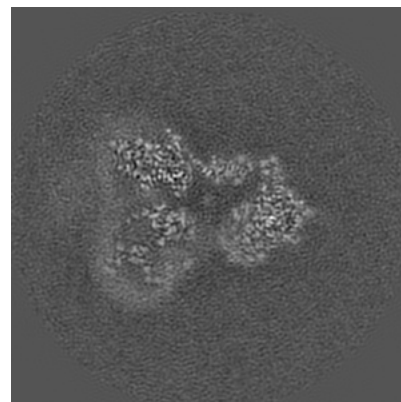
6.2.1 Primary map



X Index: 192

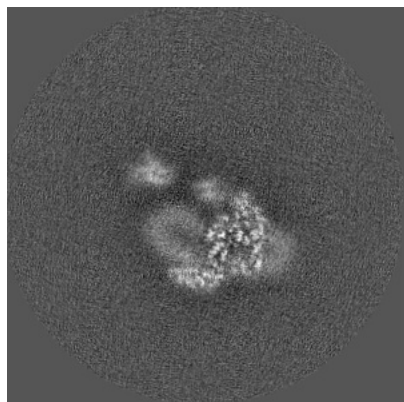


Y Index: 192

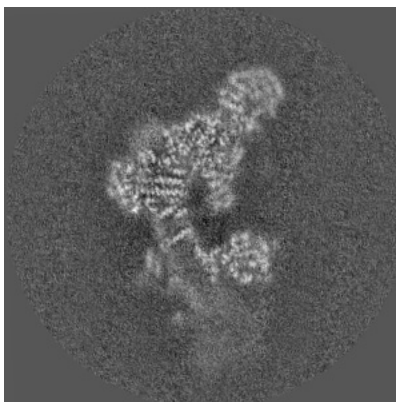


Z Index: 192

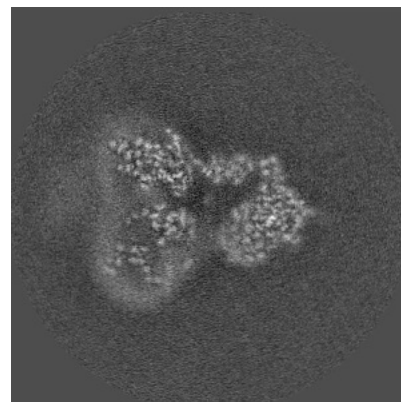
6.2.2 Raw map



X Index: 192



Y Index: 192

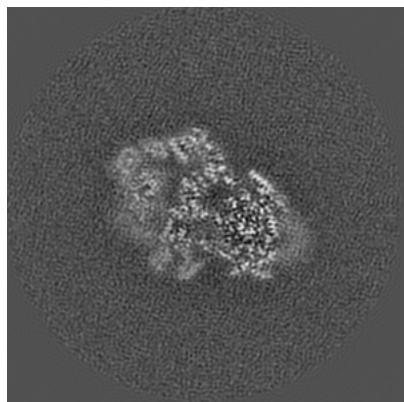


Z Index: 192

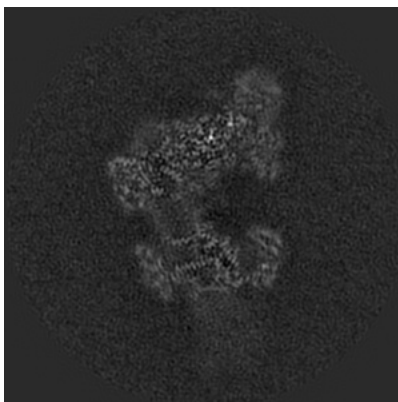
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

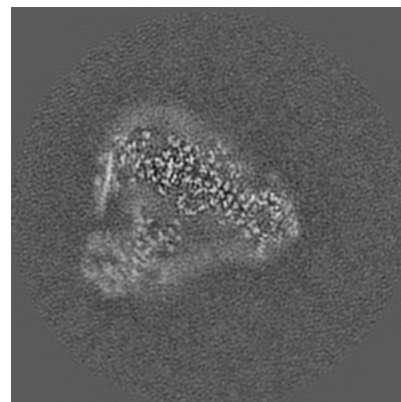
6.3.1 Primary map



X Index: 153

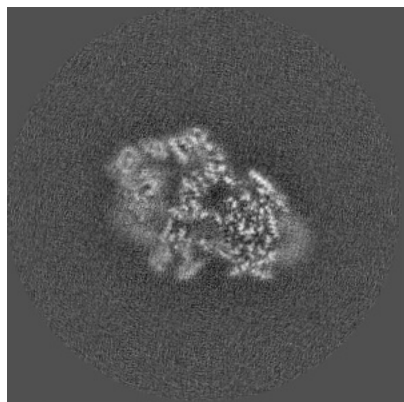


Y Index: 177

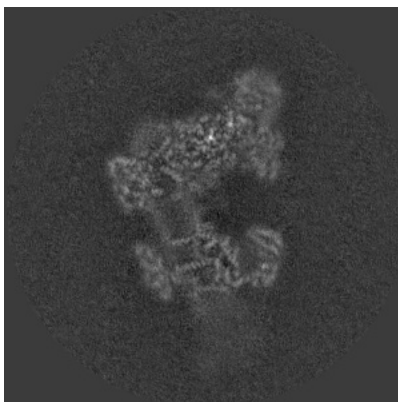


Z Index: 167

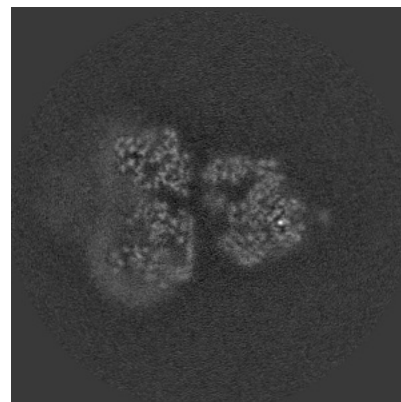
6.3.2 Raw map



X Index: 153



Y Index: 177

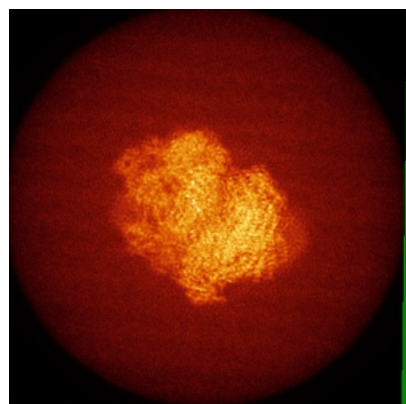


Z Index: 198

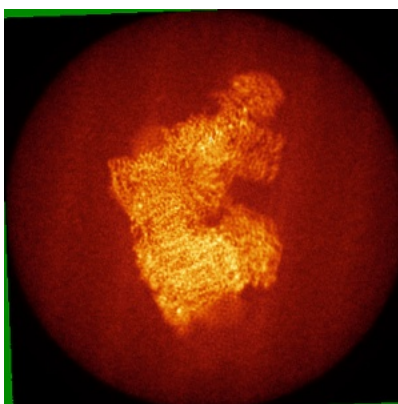
The images above show the largest variance slices of the map in three orthogonal directions.

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

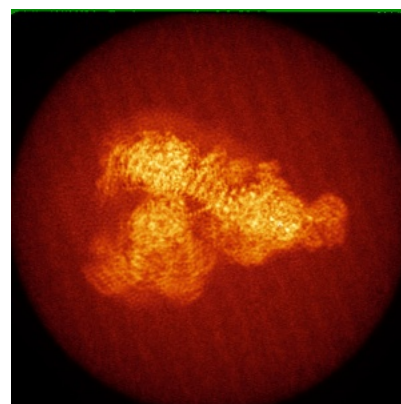
6.4.1 Primary map



X

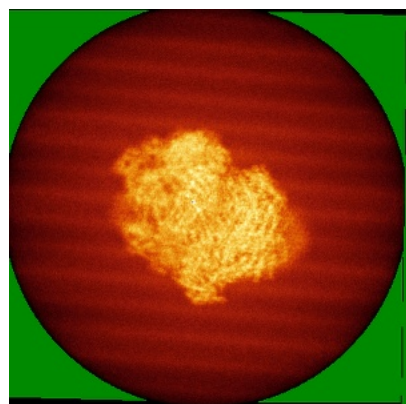


Y

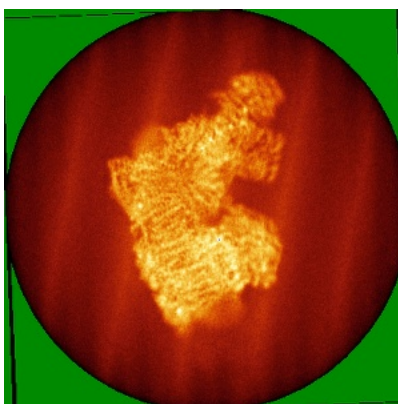


Z

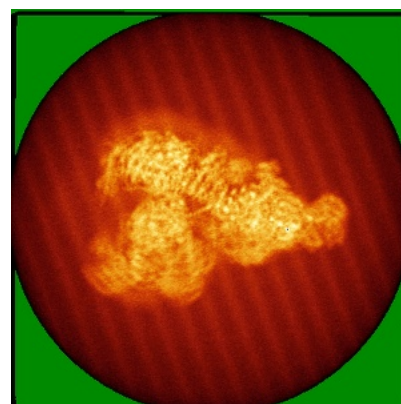
6.4.2 Raw map



X



Y

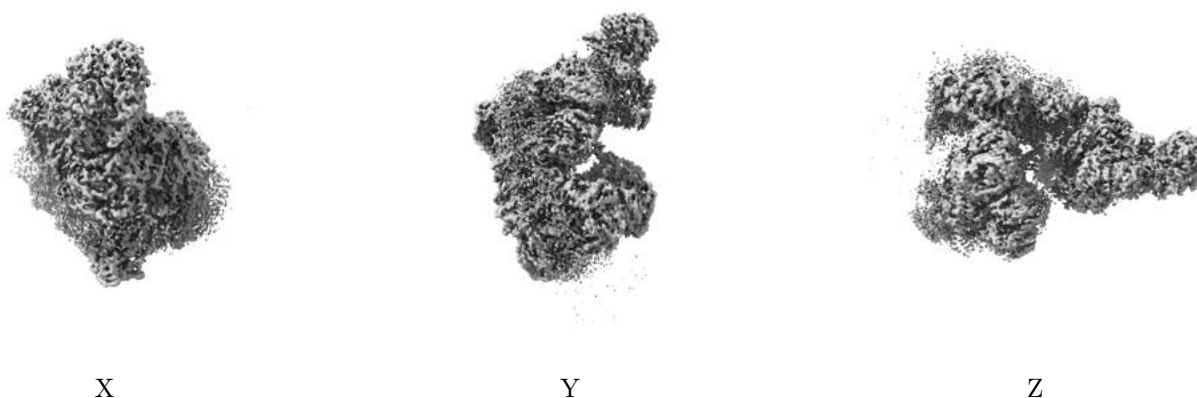


Z

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.

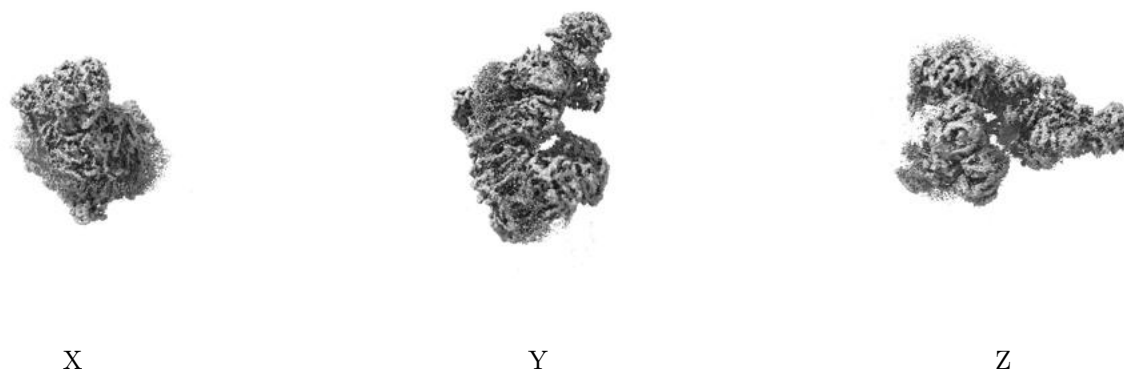
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

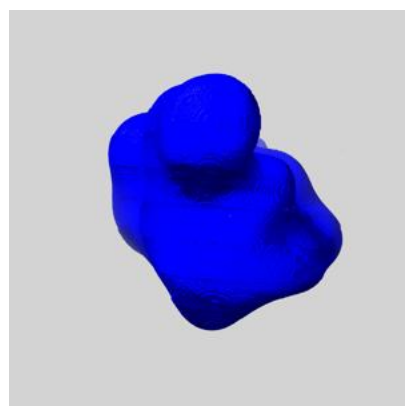
6.6 Mask visualisation [i](#)

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

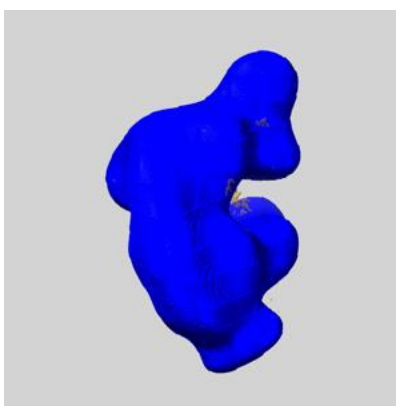
A mask typically either:

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

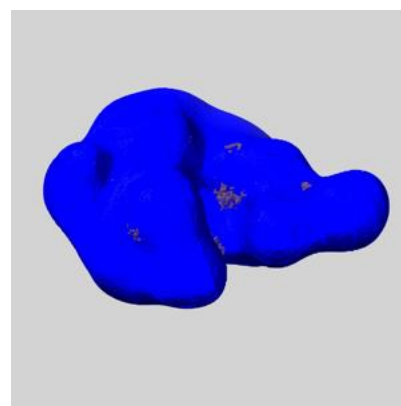
6.6.1 emd_35313_msk_1.map [i](#)



X



Y

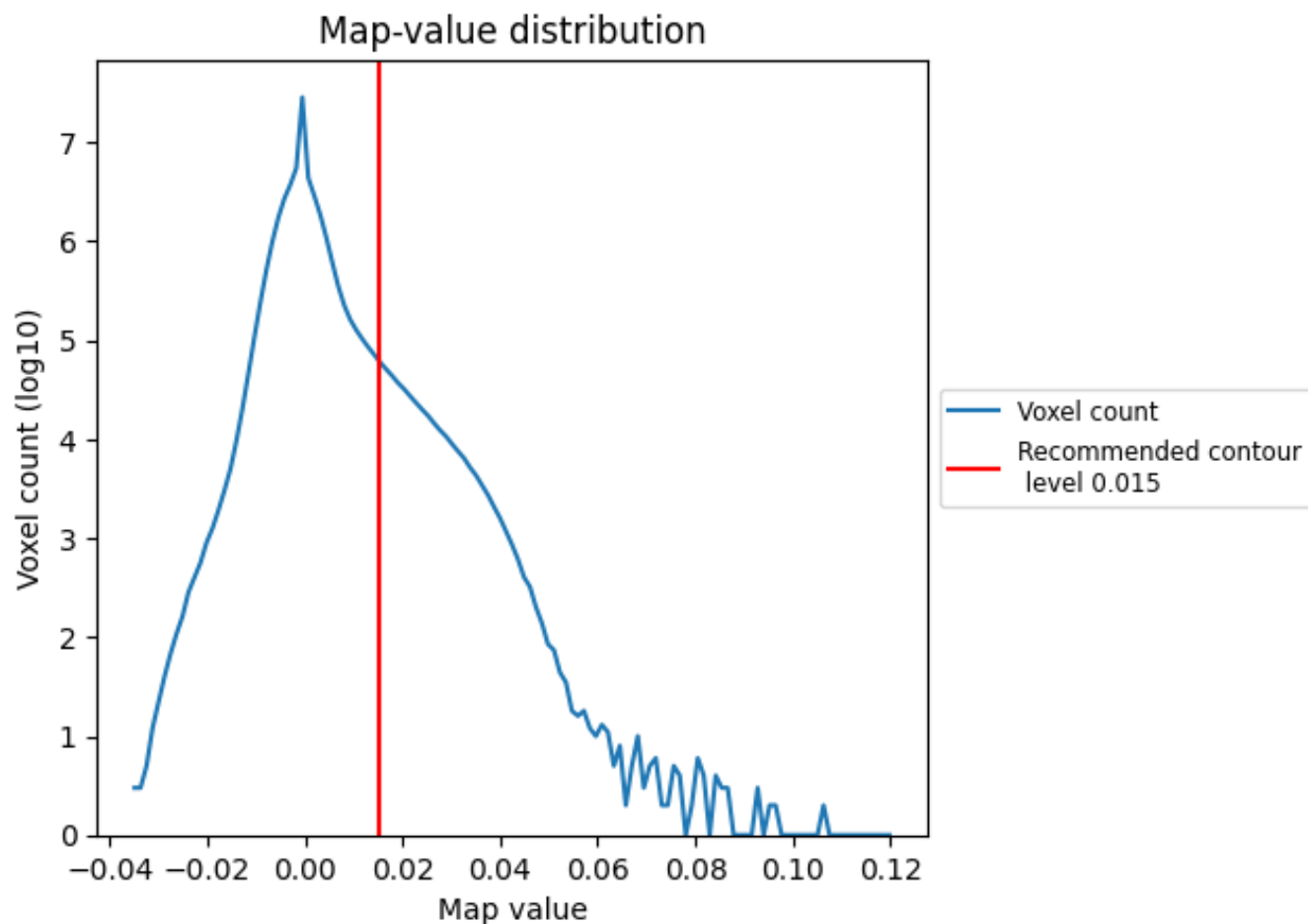


Z

7 Map analysis [i](#)

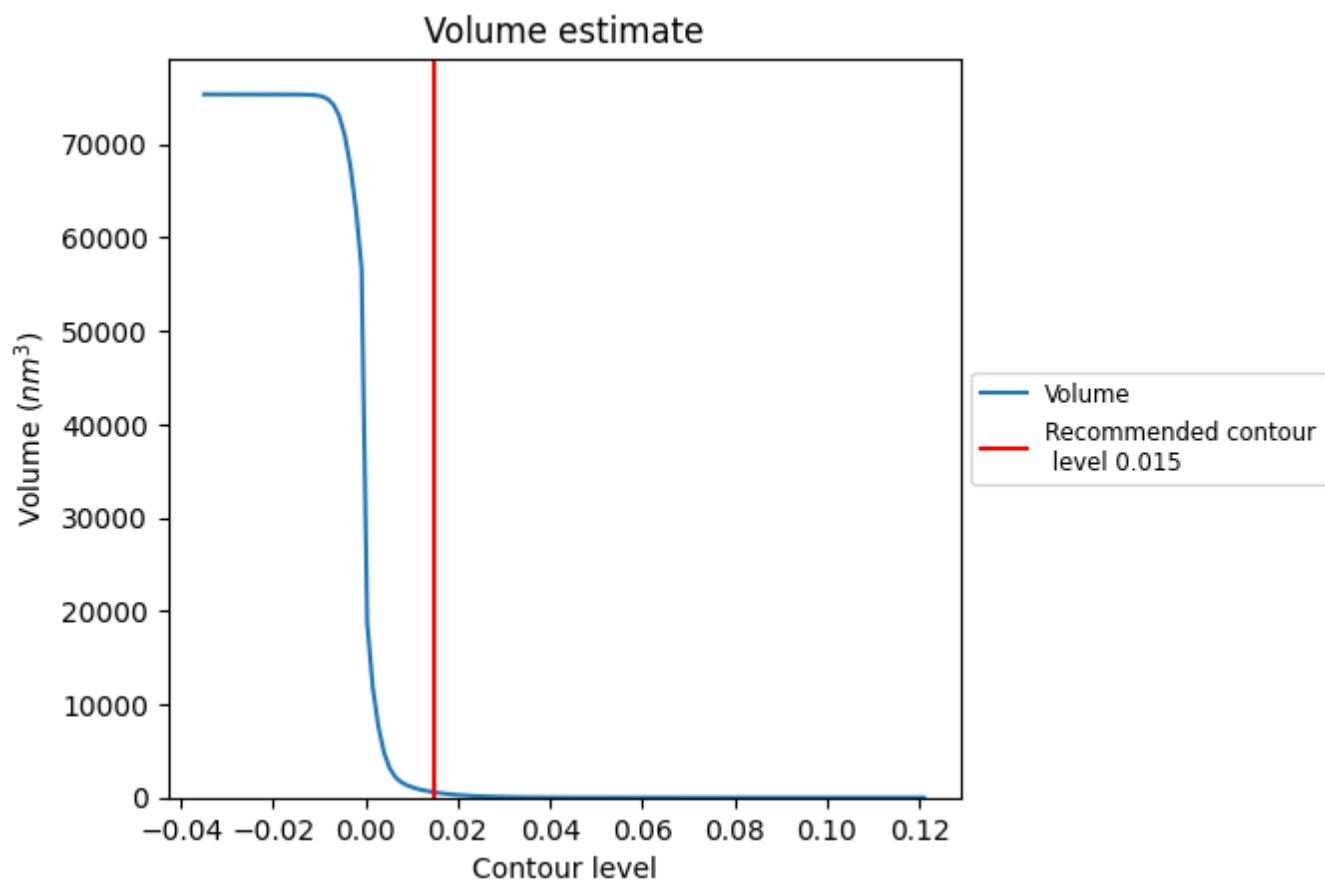
This section contains the results of statistical analysis of the map.

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.

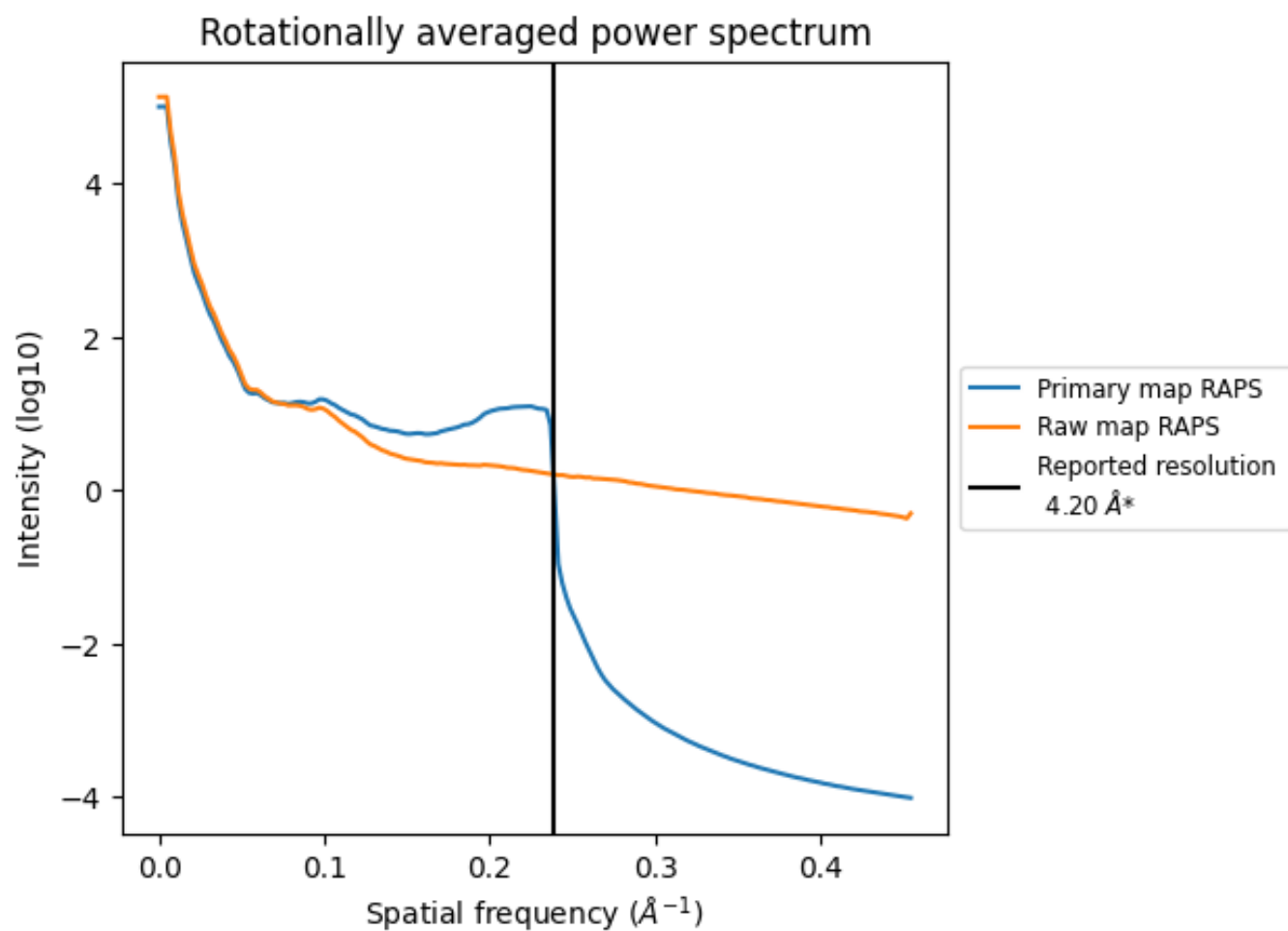
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 556 nm³; this corresponds to an approximate mass of 502 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 ⓘ

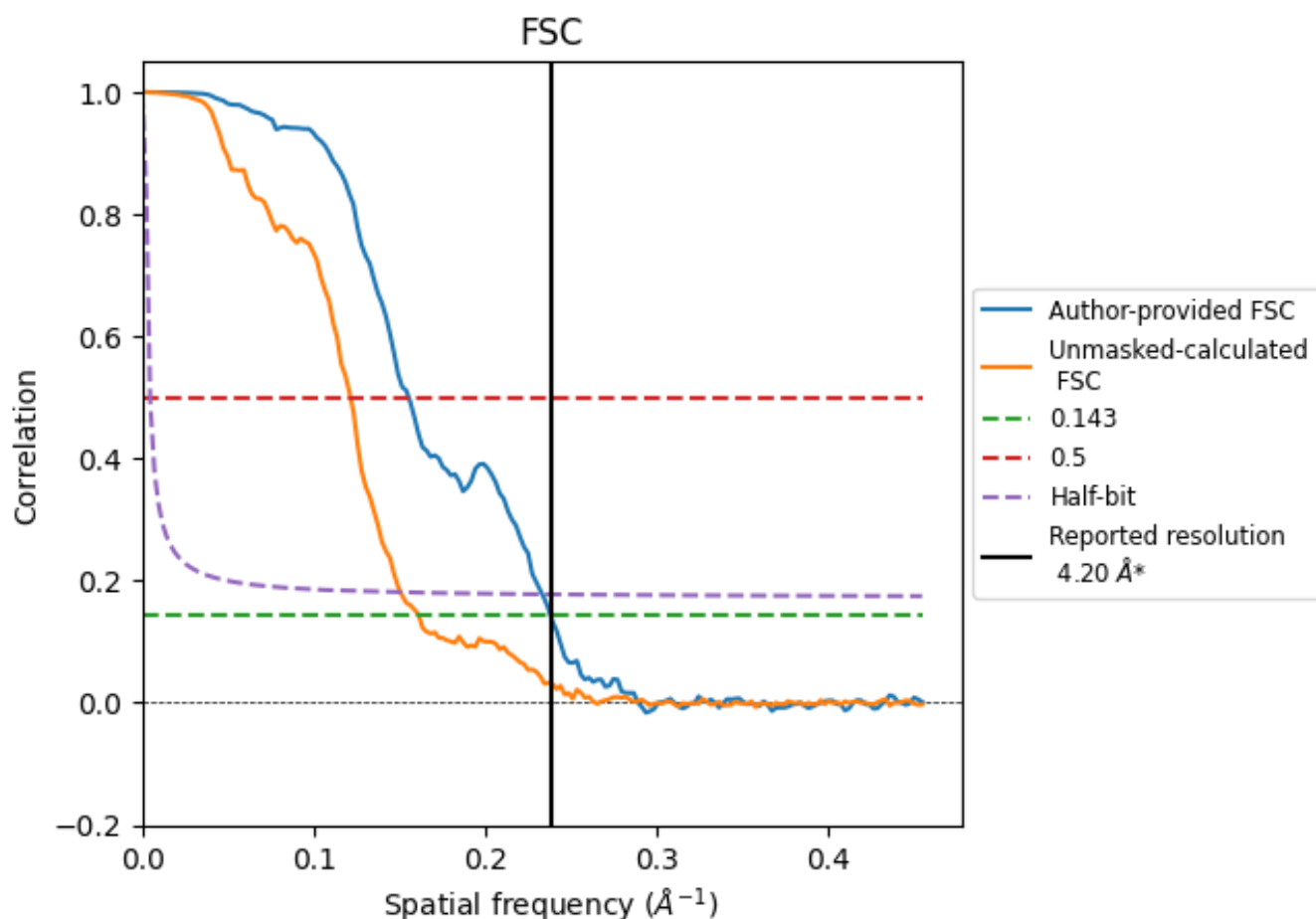


*Reported resolution corresponds to spatial frequency of $0.238 \text{ \AA}^{-1}$

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

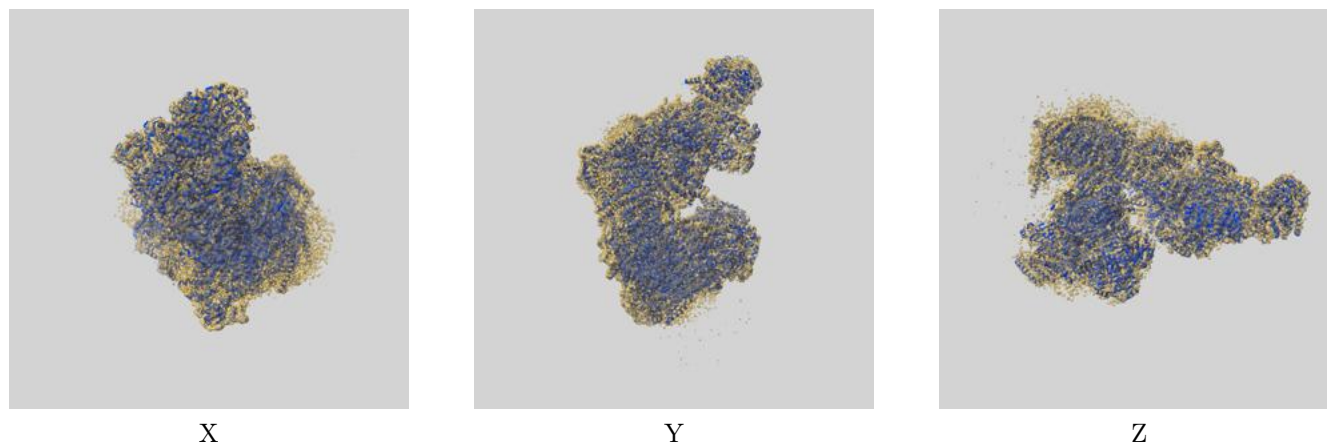
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.44	4.29
Unmasked-calculated*	6.21	8.24	6.64

*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 6.21 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

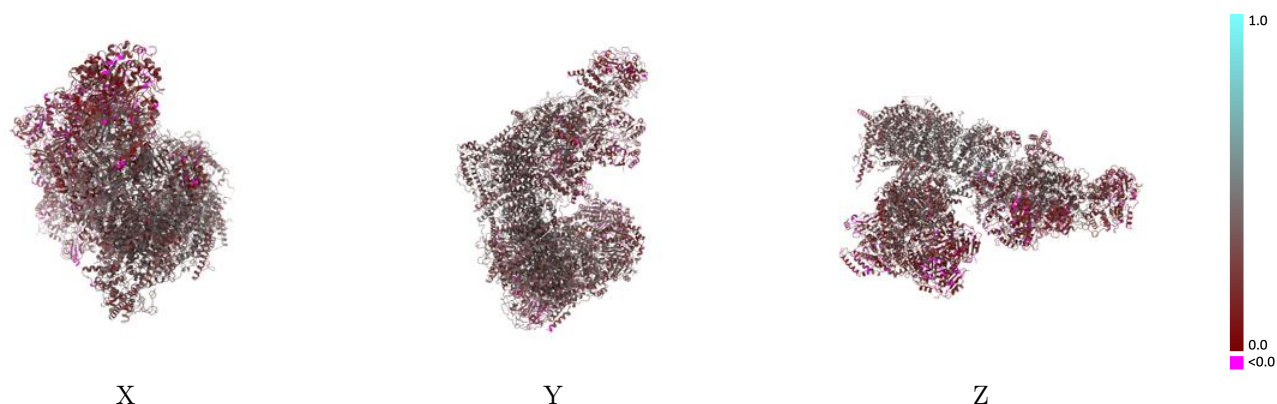
This section contains information regarding the fit between EMDB map EMD-35313 and PDB model 8IAO. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



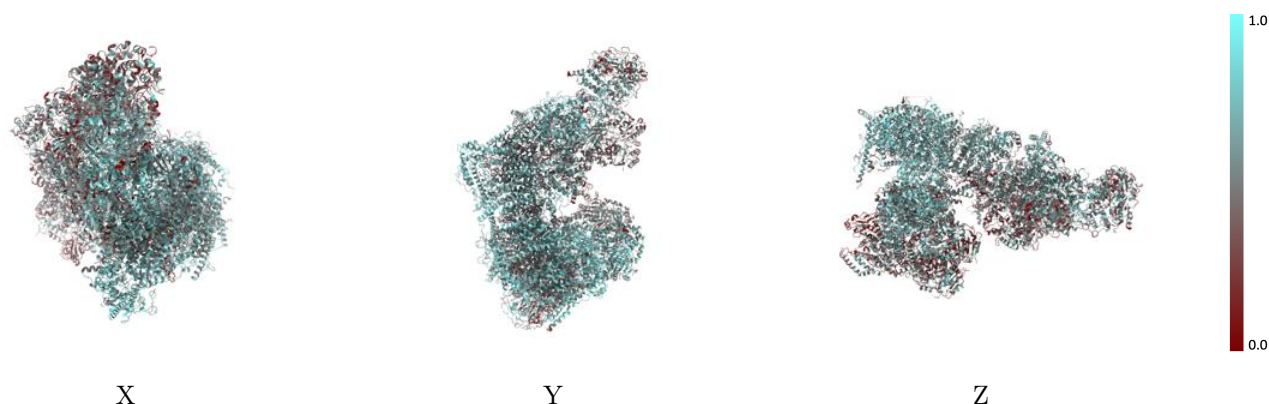
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



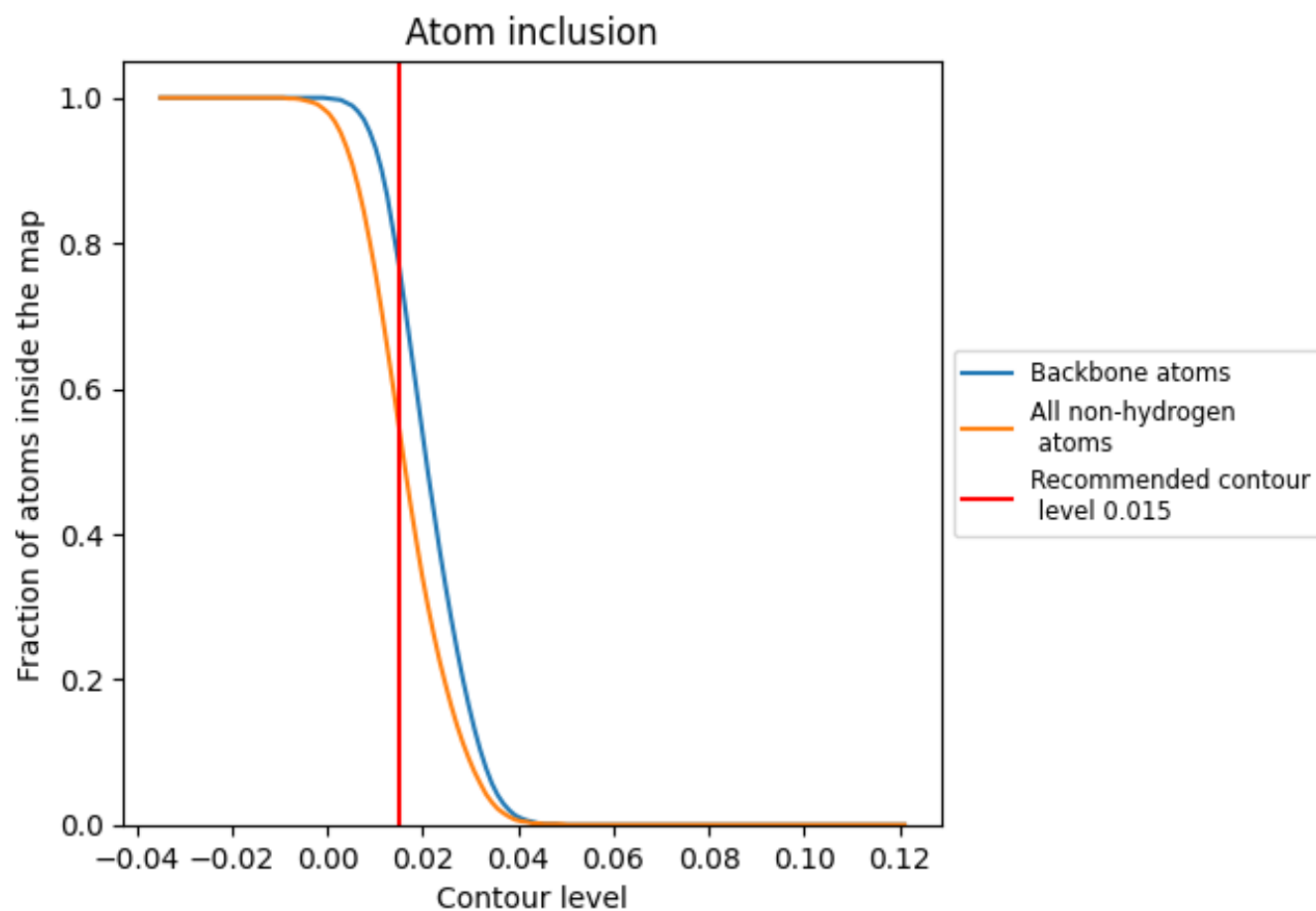
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5480	 0.2950
A	 0.4860	 0.3410
AA	 0.4790	 0.1900
AB	 0.4570	 0.2030
AC	 0.4580	 0.2680
AD	 0.4900	 0.2020
AE	 0.2500	 0.1680
AF	 0.5790	 0.2560
AG	 0.3290	 0.1880
AH	 0.4340	 0.1150
AI	 0.1140	 0.1520
AJ	 0.3730	 0.2090
AK	 0.2270	 0.1820
Aa	 0.6570	 0.3410
Ab	 0.6130	 0.2800
Ac	 0.5380	 0.3210
Ad	 0.5200	 0.2490
Ae	 0.2530	 0.1840
Af	 0.5570	 0.2980
Ag	 0.4900	 0.3220
Ah	 0.4380	 0.1750
Ai	 0.2340	 0.2550
Aj	 0.3740	 0.2260
Ak	 0.2810	 0.2340
B	 0.6520	 0.3650
C	 0.6110	 0.3230
D	 0.6340	 0.3640
E	 0.4710	 0.2200
F	 0.4780	 0.2120
G	 0.4680	 0.2300
H	 0.5830	 0.3630
I	 0.6470	 0.3510
J	 0.4890	 0.3360
K	 0.6140	 0.3890
L	 0.6360	 0.3700



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Chain	Atom inclusion	Q-score
M	 0.6520	 0.4030
N	 0.6470	 0.3960
O	 0.6120	 0.3250
P	 0.3820	 0.1950
Q	 0.4740	 0.2750
R	 0.4820	 0.2780
S	 0.3800	 0.1320
T	 0.2640	 0.1360
U	 0.6950	 0.3650
V	 0.5510	 0.2390
W	 0.4310	 0.2360
X	 0.6940	 0.3350
Y	 0.5540	 0.3560
Z	 0.6820	 0.3230
a	 0.6990	 0.3640
b	 0.6520	 0.3380
c	 0.5850	 0.2880
d	 0.6340	 0.3740
e	 0.6710	 0.3650
f	 0.6220	 0.3180
g	 0.6470	 0.3470
h	 0.6460	 0.3530
i	 0.6530	 0.3580
j	 0.6570	 0.3130
k	 0.7120	 0.3440
l	 0.6680	 0.3680
m	 0.6300	 0.3620
n	 0.7200	 0.3760
o	 0.5940	 0.2710
p	 0.6840	 0.3510
q	 0.5190	 0.3170
r	 0.4450	 0.2750
s	 0.3350	 0.1910