



## wwPDB EM Validation Summary Report ⓘ

Mar 13, 2026 – 11:59 PM UTC

PDB ID : 8IC2 / pdb\_00008ic2  
EMDB ID : EMD-35352  
Title : Respiratory complex CI:CIII2, type I, PERK -/- mouse under cold temperature  
Authors : Shin, Y.-C.; Liao, M.  
Deposited on : 2023-02-10  
Resolution : 6.30 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](mailto: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>.

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

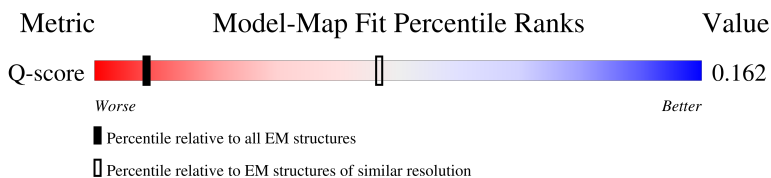
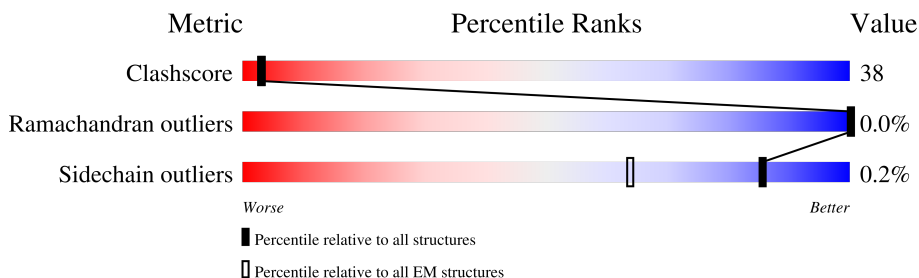
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 6.30 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	550 ( 5.80 - 6.80 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	<p>5% (red), 17% (green), 61% (yellow), 21% (grey)</p>
2	B	224	<p>31% (green), 34% (yellow), 30% (grey)</p>
3	C	263	<p>40% (green), 33% (yellow), 25% (grey)</p>
4	D	463	<p>7% (red), 35% (green), 53% (yellow), 8% (grey)</p>

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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	11% 48% 49%
30	e	106	5% 45% 51%
31	f	57	12% 40% 49% 11%
32	g	151	11% 36% 24% 6% 34%
33	h	189	7% 36% 36% 27%
34	i	128	9% 32% 32% 7% 29%
35	j	105	9% 25% 36% 36%
36	k	104	11% 31% 26% 10% 34%
37	l	186	15% 45% 32% 6% 17%
38	m	129	23% 49% 41% 8%
39	n	179	20% 46% 45% 8%
40	o	137	22% 35% 50% 12%
41	p	176	11% 47% 45% 5%
42	q	145	68% 36% 41% 7% 16%
43	r	113	21% 18% 22% 5% 55%
44	s	104	14% 14% 12% 72%
45	AA	480	81% 51% 32% 16%
45	Aa	480	80% 55% 28% 17%
46	AB	453	90% 60% 30% 9%
46	Ab	453	89% 61% 31% 8%
47	AC	381	96% 69% 28%
47	Ac	381	90% 68% 29%
48	AD	325	73% 36% 36% 27%
48	Ad	325	74% 39% 34% 26%
49	AE	274	65% 22% 43% 34%

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Mol	Chain	Length	Quality of chain
49	AI	274	
49	Ae	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
55	SF4	B	301	-	-	X	-
55	SF4	F	502	-	-	X	-
55	SF4	G	802	-	-	X	-
55	SF4	I	303	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
61	UQ9	H	401	-	-	X	-
62	CDL	q	201	-	-	X	-
67	HEM	AC	402	-	-	X	-
68	UQ6	AC	403	-	-	X	-

## 2 Entry composition [i](#)

There are 70 unique types of molecules in this entry. The entry contains 97017 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	91	737	511	102	118	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	796	223	214	14	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	427	3443	2201	592	626	24	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	424	3273	2062	586	603	22	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	317	2531	1701	383	425	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	173	1389	875	239	263	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	155	1178	797	167	199	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	96	721	468	110	134	9	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	318	2588	1662	426	490	10	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	139	1030	657	174	191	8	0	0

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

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

- 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	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	91	765	500	131	131	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	67	574	376	95	102	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	69	560	370	97	91	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	155	1304	840	218	235	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	m	126	1050	676	189	185	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	177	1534	981	275	267	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	121	1038	654	196	180	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	167	1415	891	254	262	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	122	1020	655	180	181	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	51	418	266	78	73	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	s	29	238	151	39	48	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AA	403	3157	1971	562	608	16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	400	Total	C	N	O	S	0	0
			3131	1957	554	604	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	413	Total	C	N	O	S	0	0
			3097	1949	542	597	9		
46	Ab	417	Total	C	N	O	S	0	0
			3128	1965	550	604	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	369	Total	C	N	O	S	0	0
			2956	1995	457	484	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	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	181	Total	C	N	O	S	0	0
			1397	885	243	263	6		
49	AI	48	Total	C	N	O		0	0
			328	210	61	57			
49	Ae	186	Total	C	N	O	S	0	0
			1436	907	251	271	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AF	97	Total	C	N	O	S	0	0
			855	546	152	154	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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	75	Total	C	N	O	S	0	0
			634	413	115	105	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	64	Total	C	N	O	S	0	0
			527	321	98	103	5		
52	Ah	64	Total	C	N	O	S	0	0
			527	321	98	103	5		

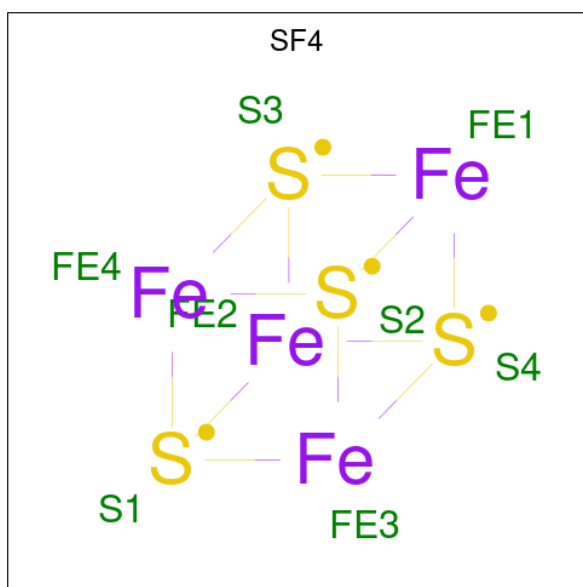
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
53	Aj	41	Total	C	N	O	0	0
			332	216	57	59		

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

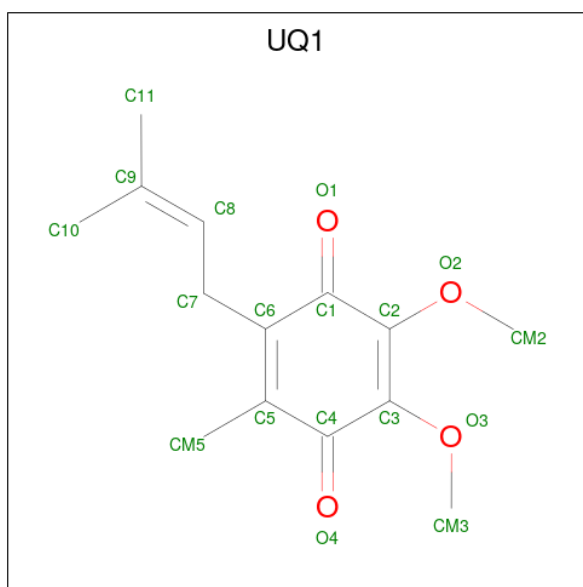
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	43	Total	C	N	O	S	0	0
			355	235	64	55	1		
54	Ak	45	Total	C	N	O	S	0	0
			365	242	64	58	1		

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



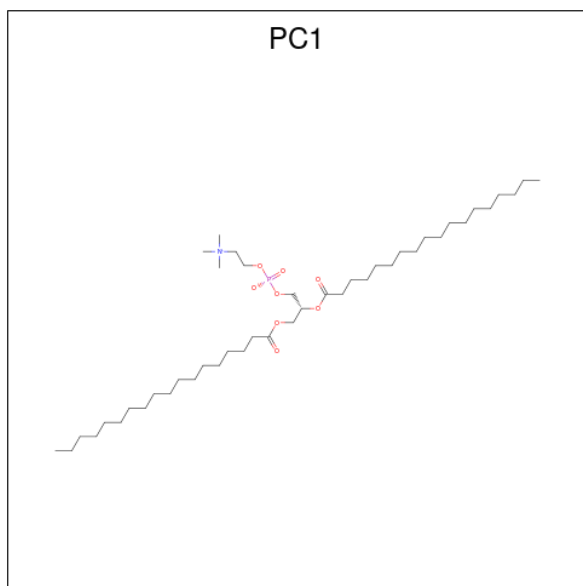
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
55	B	1	8	4	4	0
55	F	1	8	4	4	0
55	G	1	8	4	4	0
55	G	1	8	4	4	0
55	I	1	8	4	4	0
55	I	1	8	4	4	0

- Molecule 56 is UBIQUINONE-1 (CCD ID: UQ1) (formula:  $C_{14}H_{18}O_4$ ) (labeled as "Ligand of Interest" by depositor).



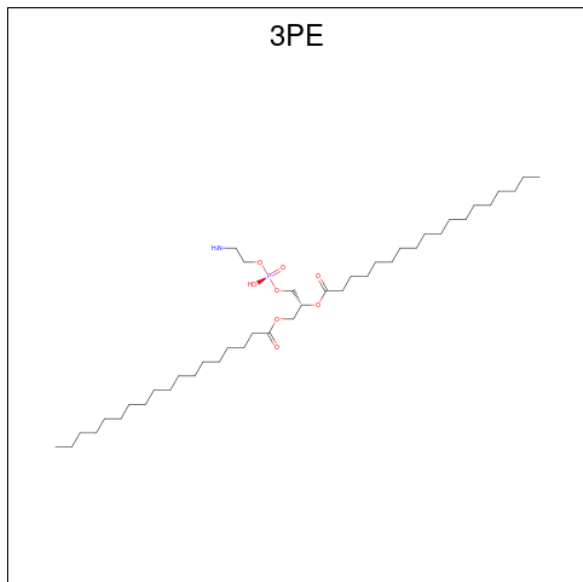
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	B	1	18	14	4	0

- Molecule 57 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	B	1	35	25	1	8	1	0
57	I	1	43	33	1	8	1	0

- Molecule 58 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



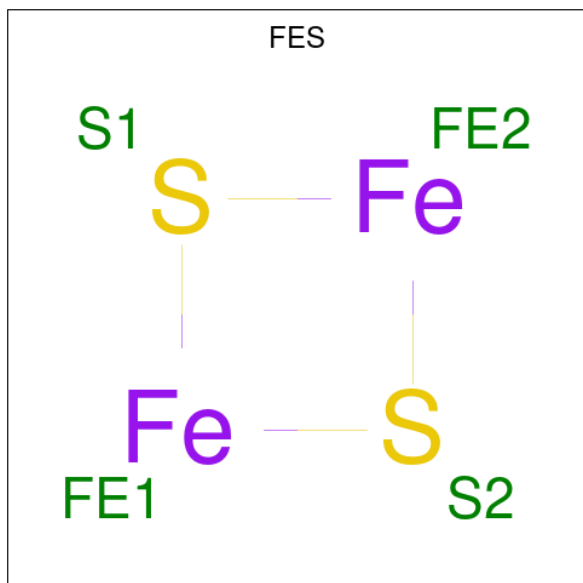
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	D	1	Total 38	28	1	8	1	0
58	H	1	Total 46	36	1	8	1	0
58	H	1	Total 51	41	1	8	1	0
58	J	1	Total 46	36	1	8	1	0
58	L	1	Total 40	30	1	8	1	0
58	L	1	Total 49	39	1	8	1	0
58	L	1	Total 44	34	1	8	1	0
58	M	1	Total 37	27	1	8	1	0
58	M	1	Total 49	39	1	8	1	0
58	i	1	Total 40	30	1	8	1	0
58	m	1	Total 41	31	1	8	1	0
58	Ac	1	Total 23	13	1	8	1	0

*Continued on next page...*

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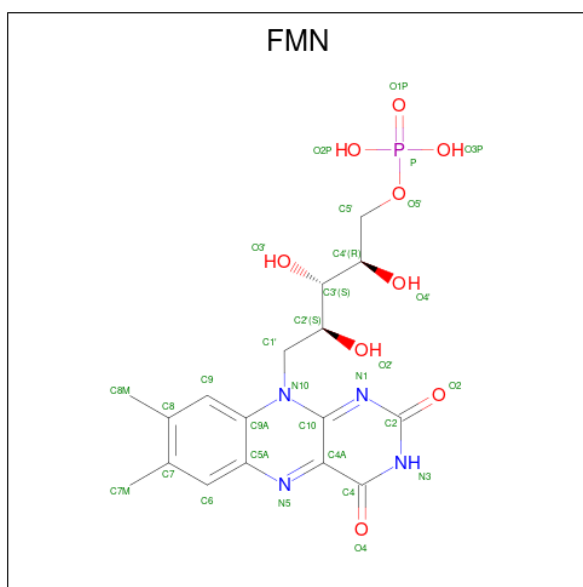
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	Ac	1	Total 35	C 25	N 1	O 8	P 1	0
58	Ag	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



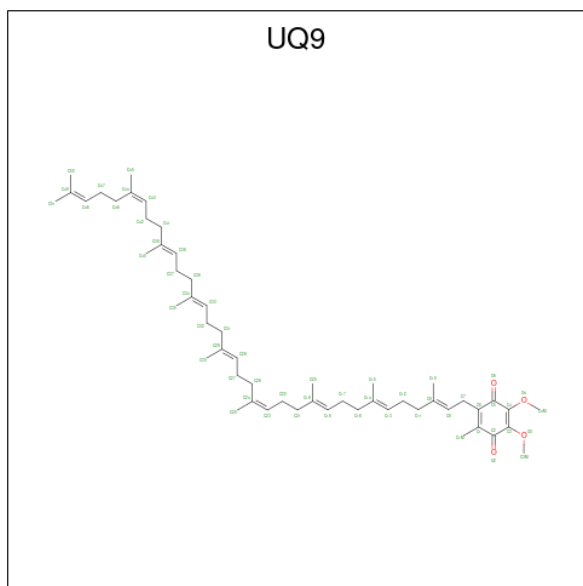
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
59	E	1	Total 4	Fe 2	S 2	0
59	G	1	Total 4	Fe 2	S 2	0

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



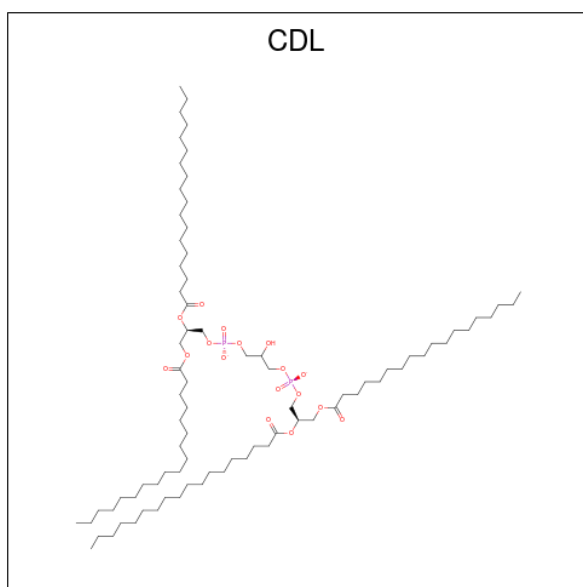
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	F	1	31	17	4	9	1	0

- 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
			Total	C	O	
61	H	1	35	31	4	0

- Molecule 62 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
			Total	C	O	P	
62	L	1	73	54	17	2	0
62	M	1	82	63	17	2	0
62	Y	1	71	52	17	2	0
62	d	1	65	46	17	2	0
62	h	1	68	49	17	2	0
62	q	1	57	38	17	2	0
62	Aa	1	46	27	17	2	0
62	Ag	1	42	23	17	2	0
62	Ag	1	56	37	17	2	0

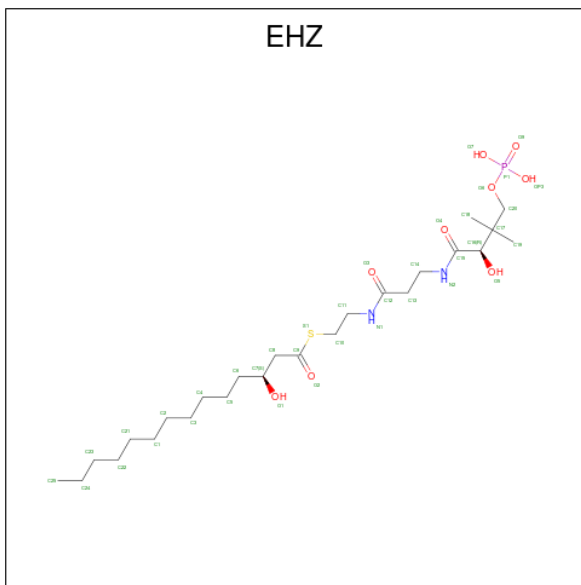
- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
63	L	1	1	1	0
63	R	1	1	1	0



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

- Molecule 66 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS) (labeled as "Ligand of Interest" by depositor).



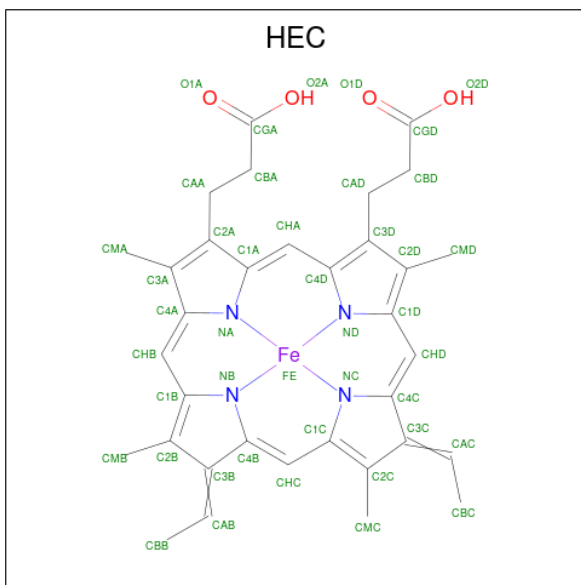
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
66	W	1	32	19	2	9	1	1	0
66	n	1	32	19	2	9	1	1	0

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



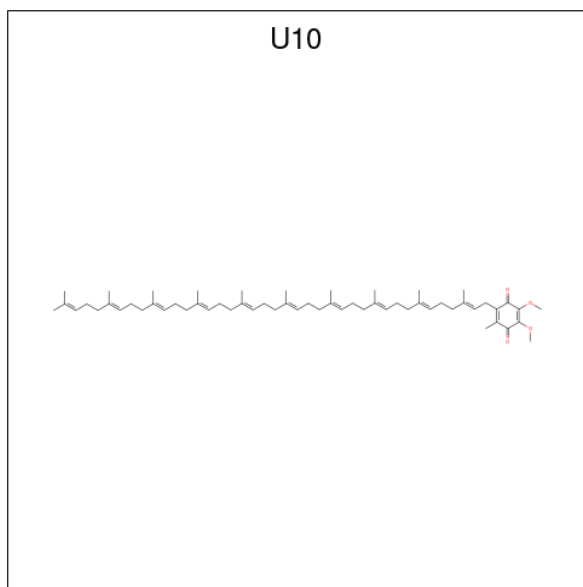
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			28	24	4	
68	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 69 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



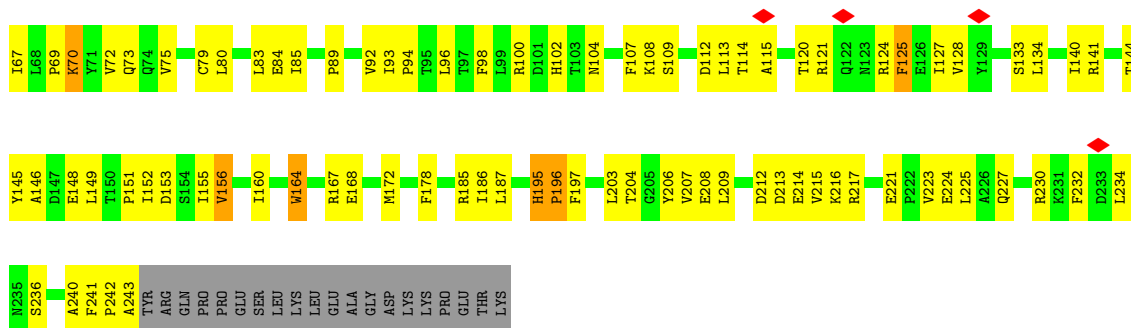
Mol	Chain	Residues	Atoms					AltConf
69	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
69	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 70 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).

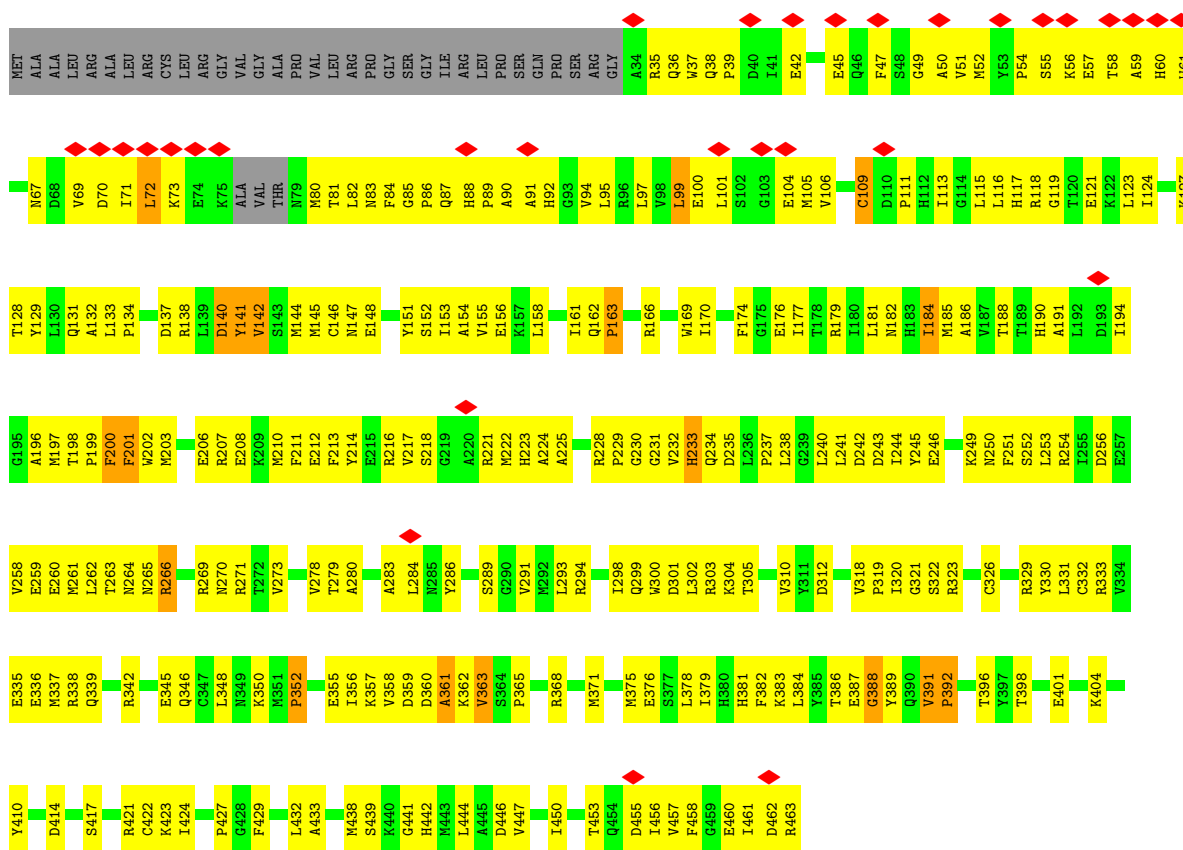


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
70	Ac	1	23	19	4	0

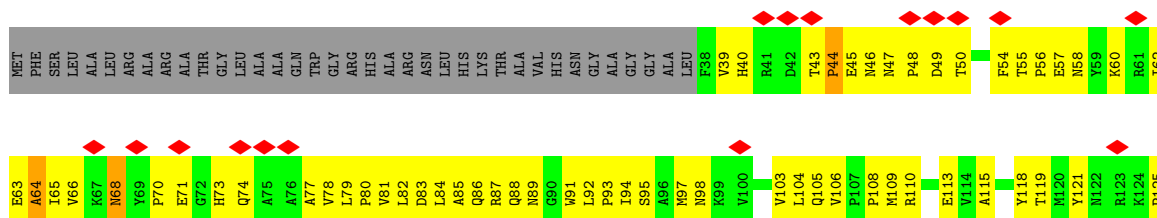




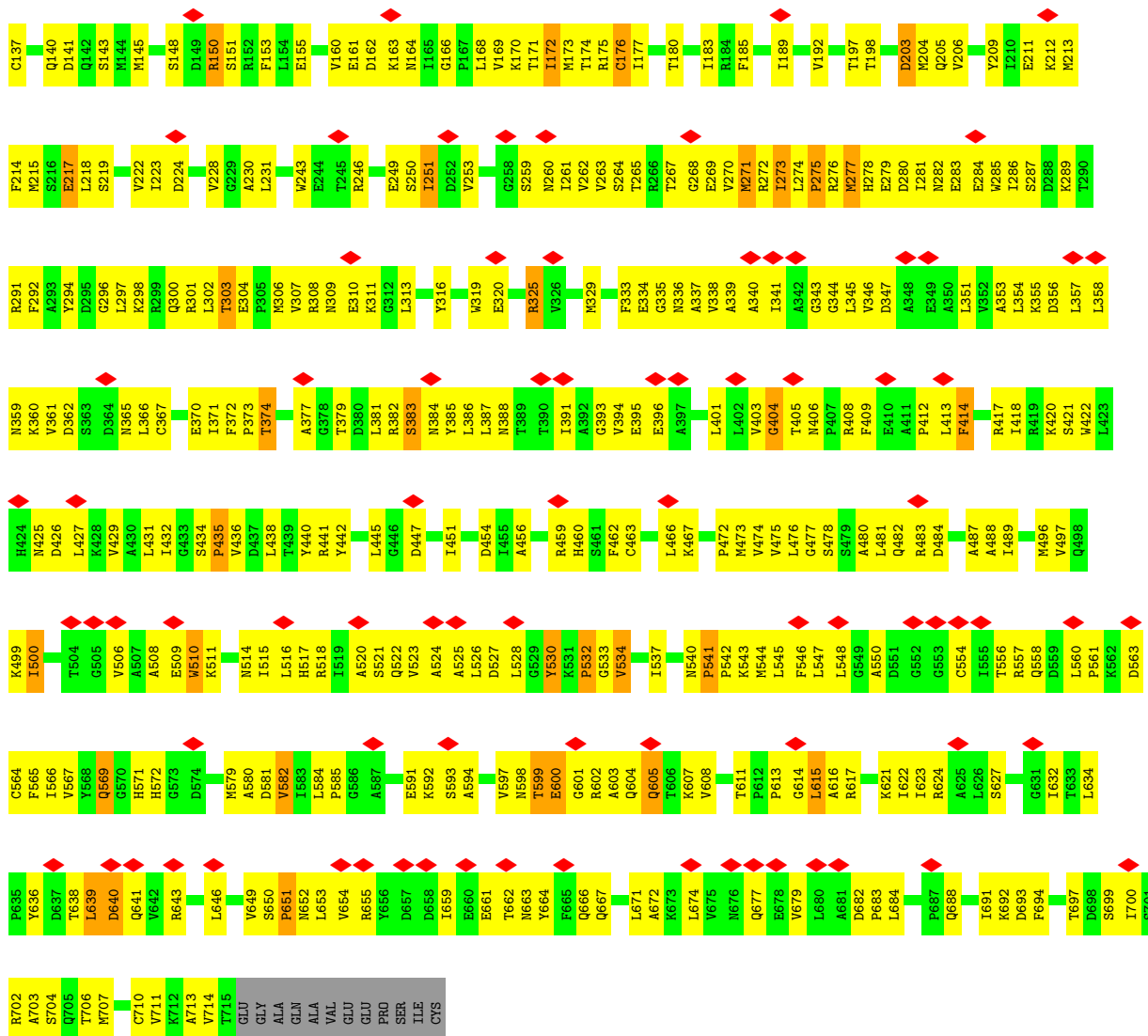
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



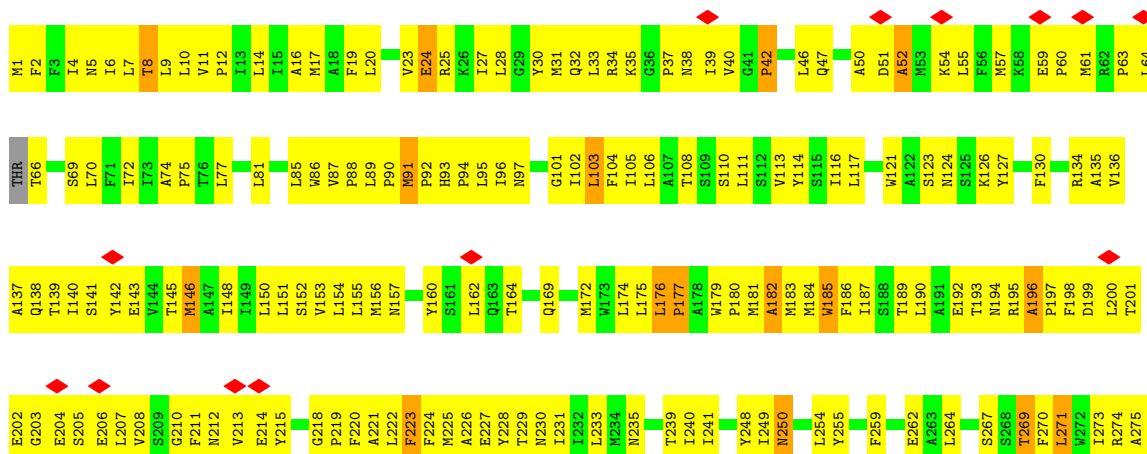
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

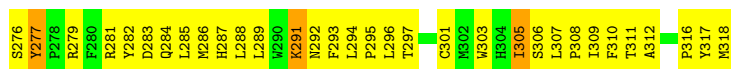




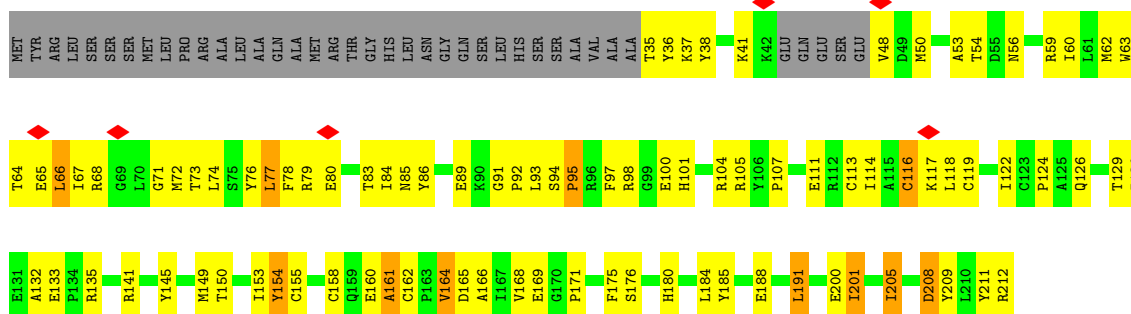


● Molecule 8: NADH-ubiquinone oxidoreductase chain 1

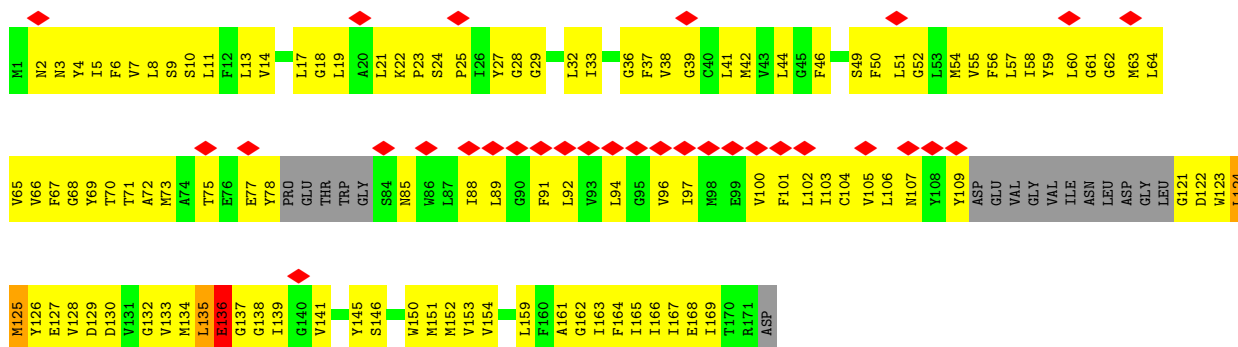




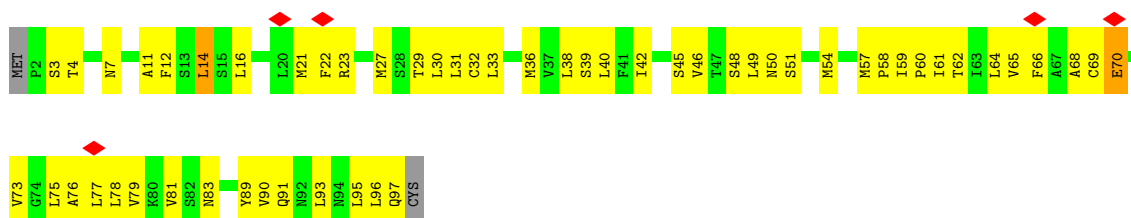
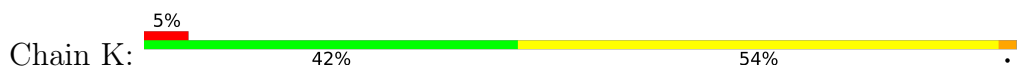
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



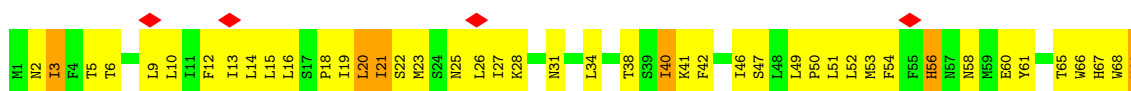
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

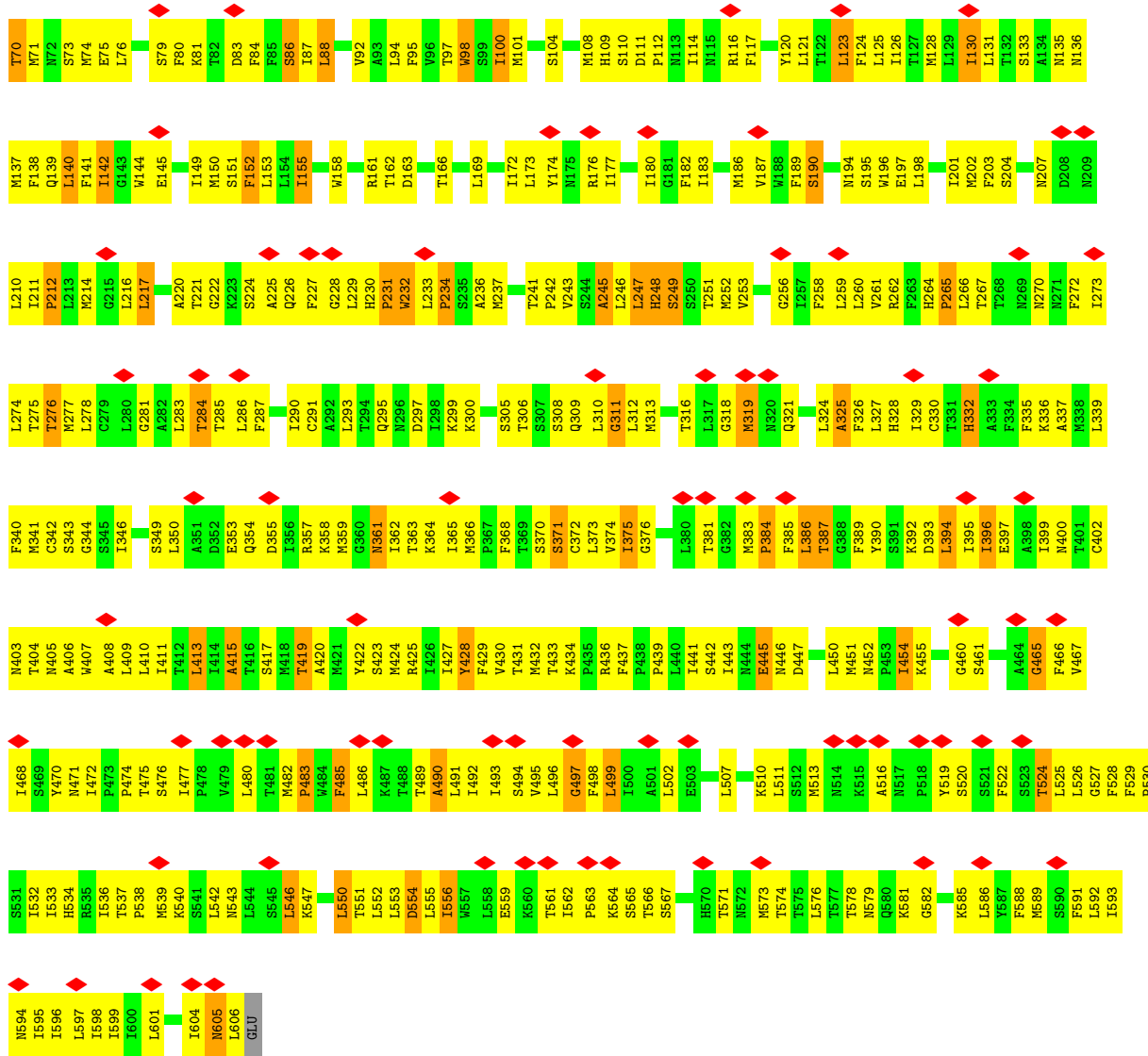


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

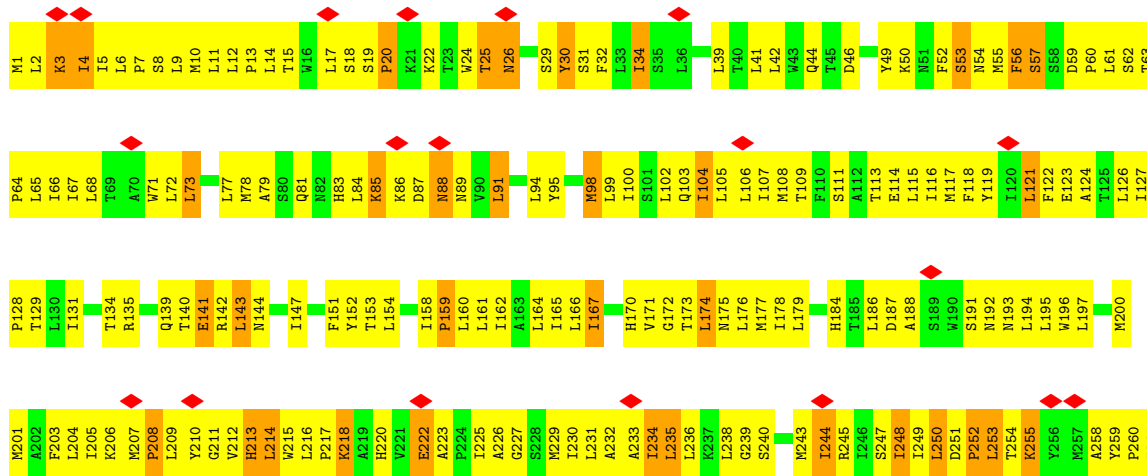


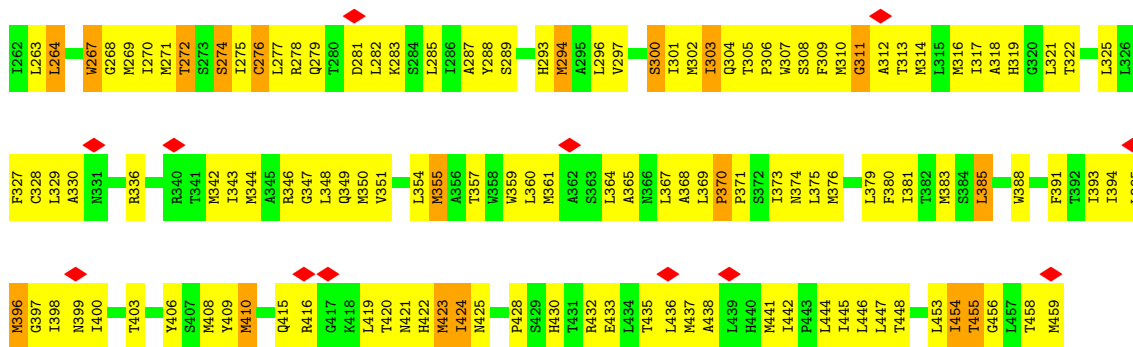
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



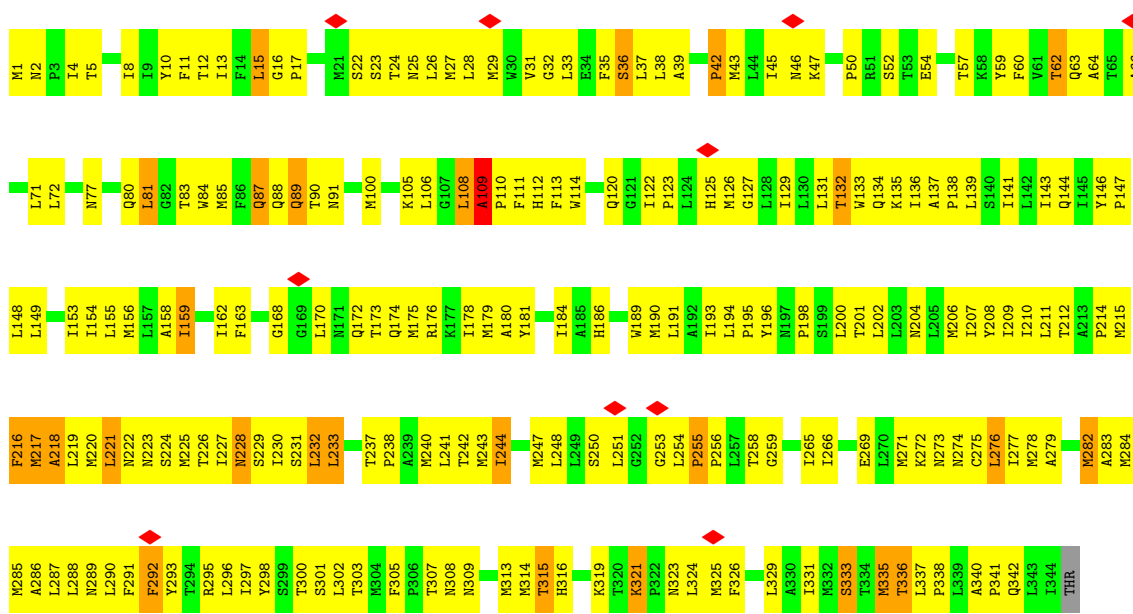
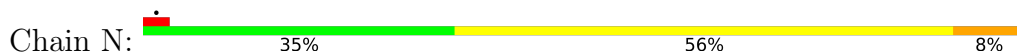


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

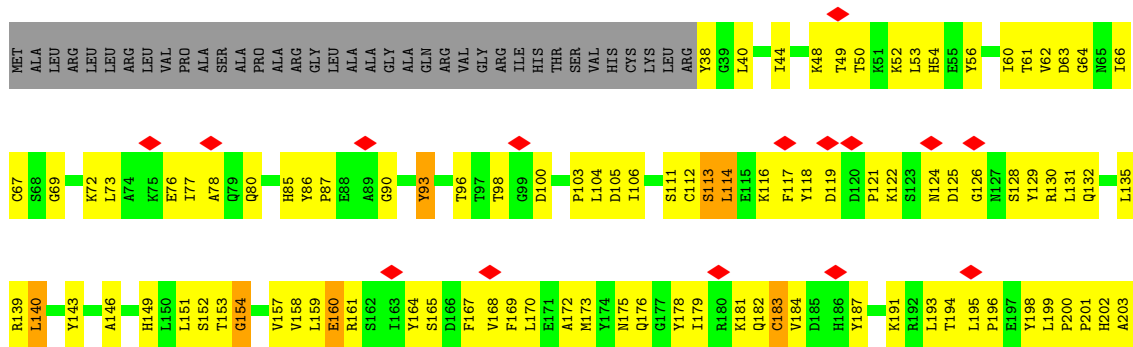


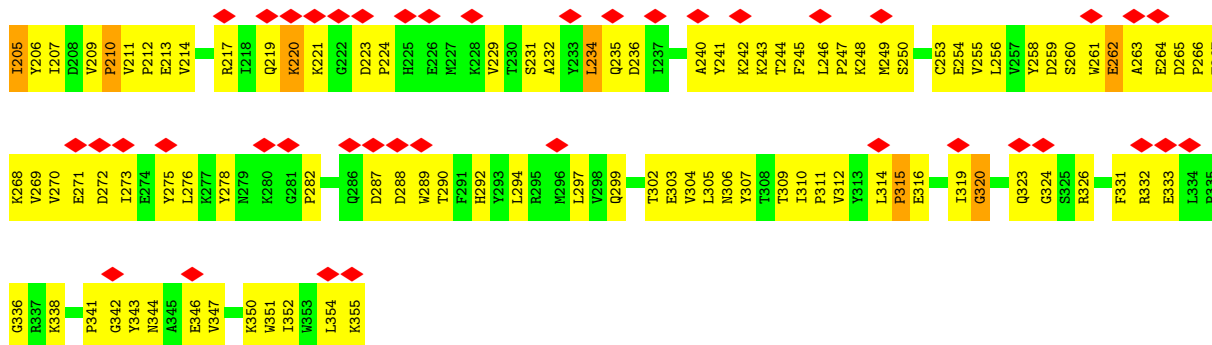


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

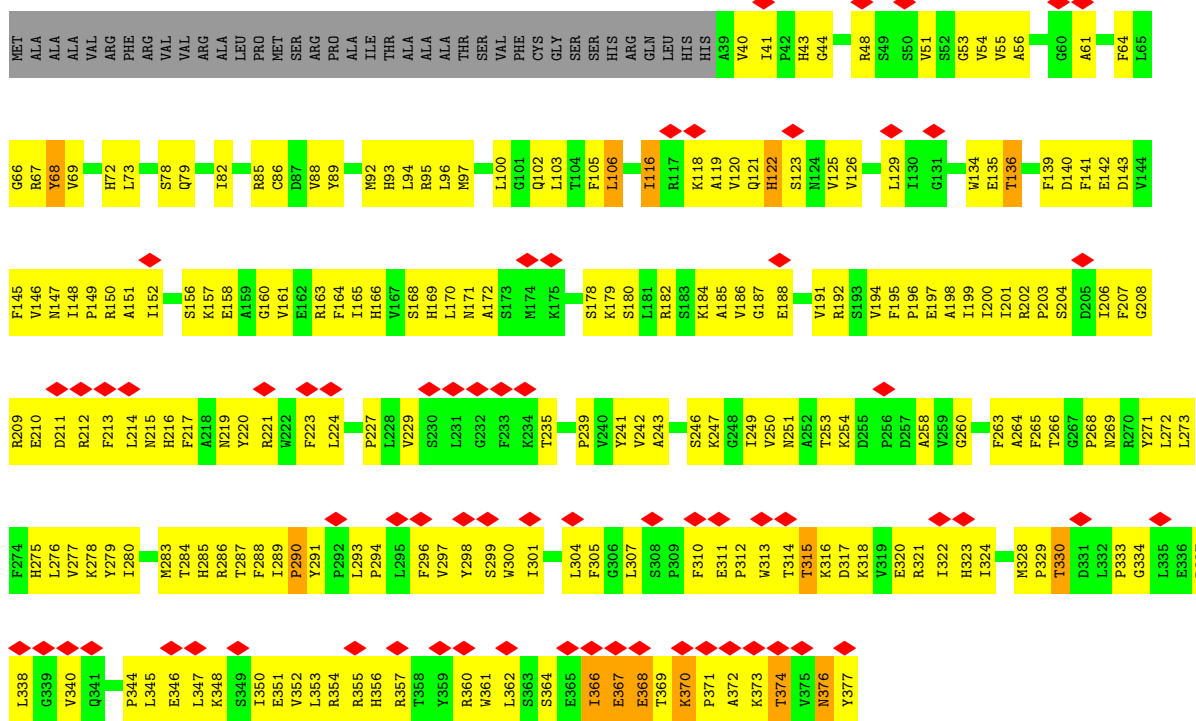


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

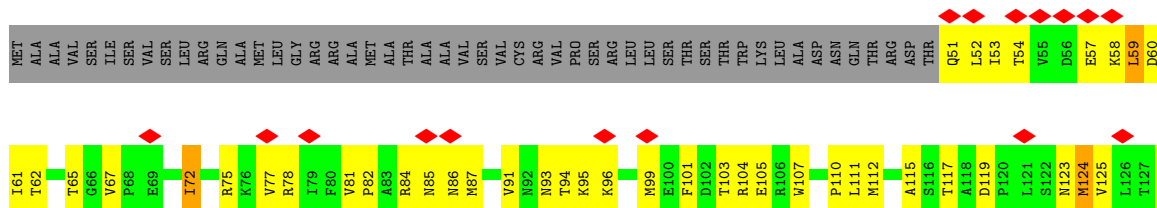


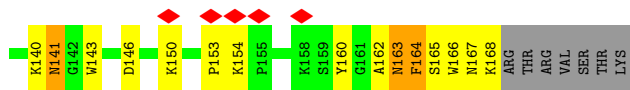


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

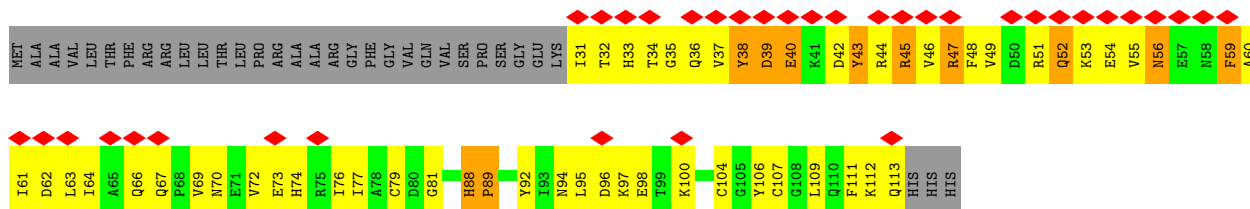
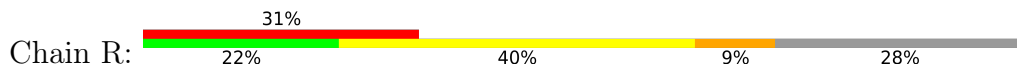


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

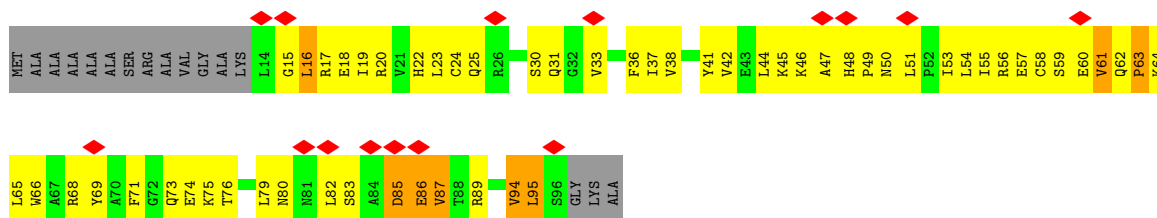




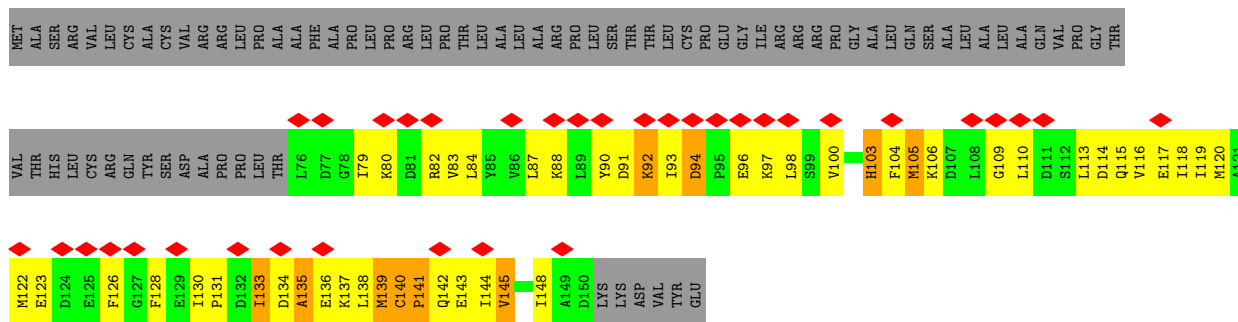
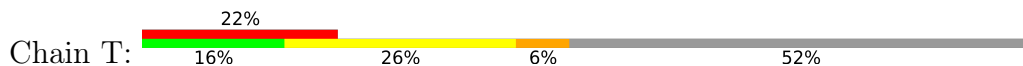
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



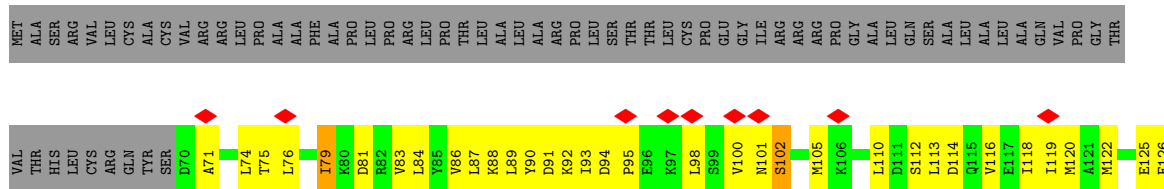
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



• Molecule 20: Acyl carrier protein, mitochondrial

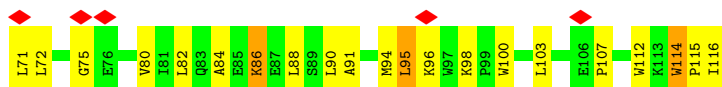


• Molecule 20: Acyl carrier protein, mitochondrial

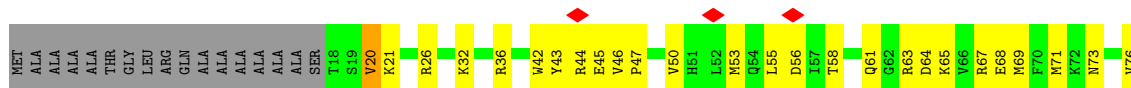




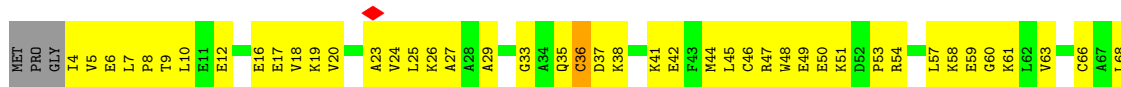
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



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



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

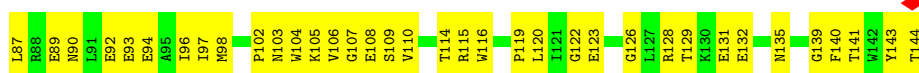


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

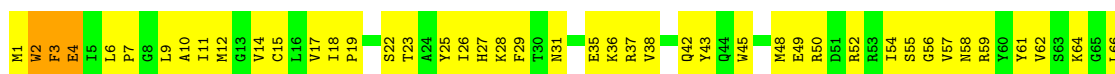




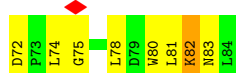
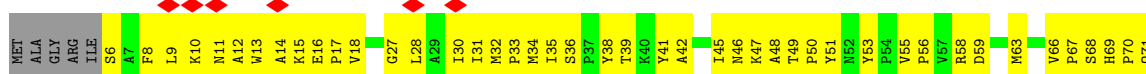
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



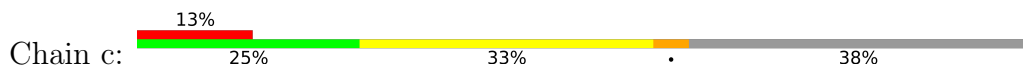
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

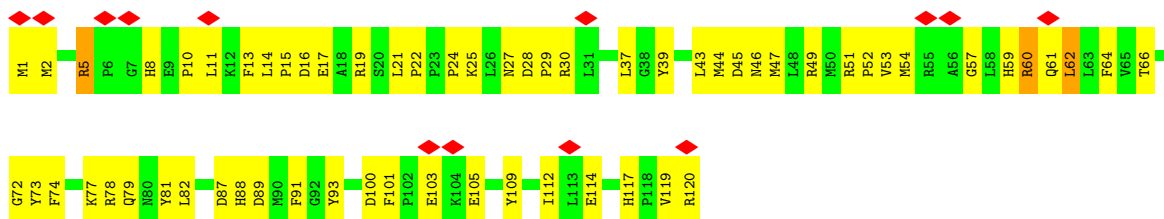


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

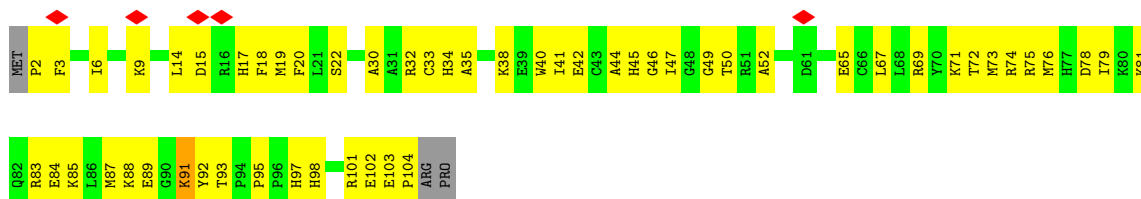


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2





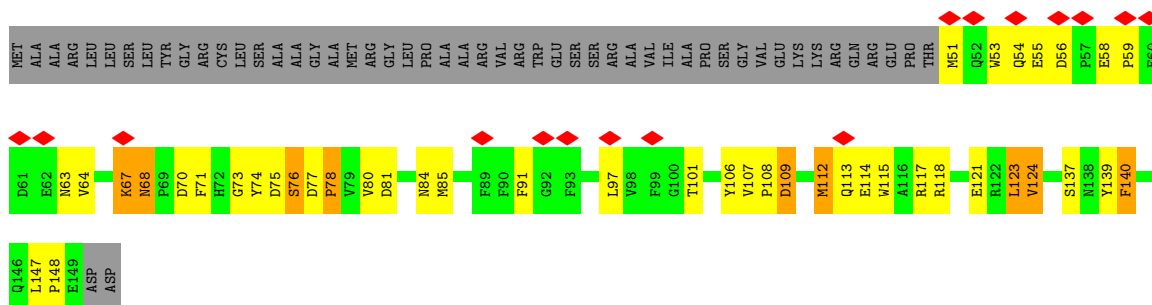
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



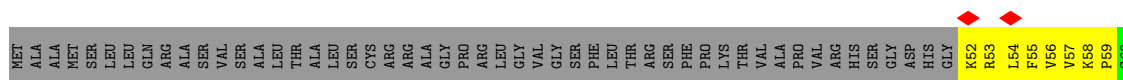
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



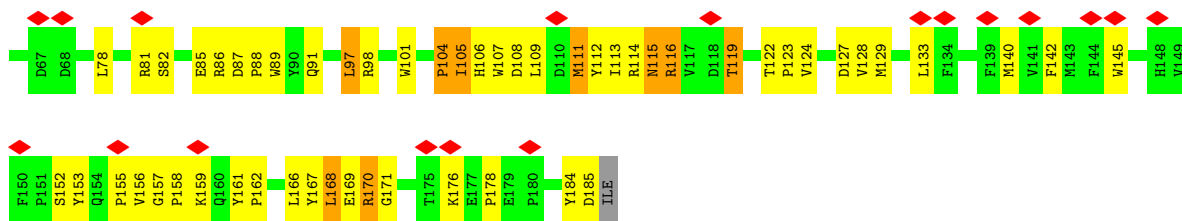
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



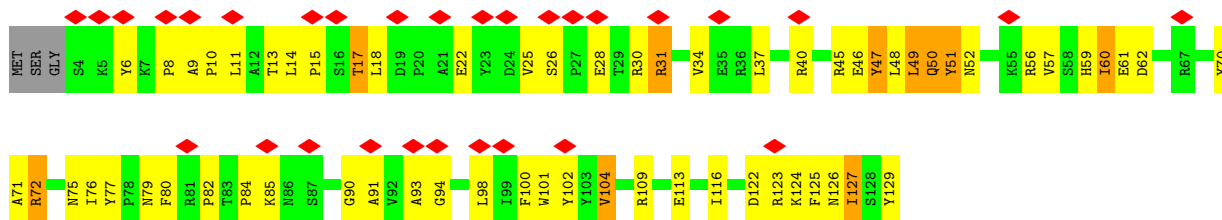
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



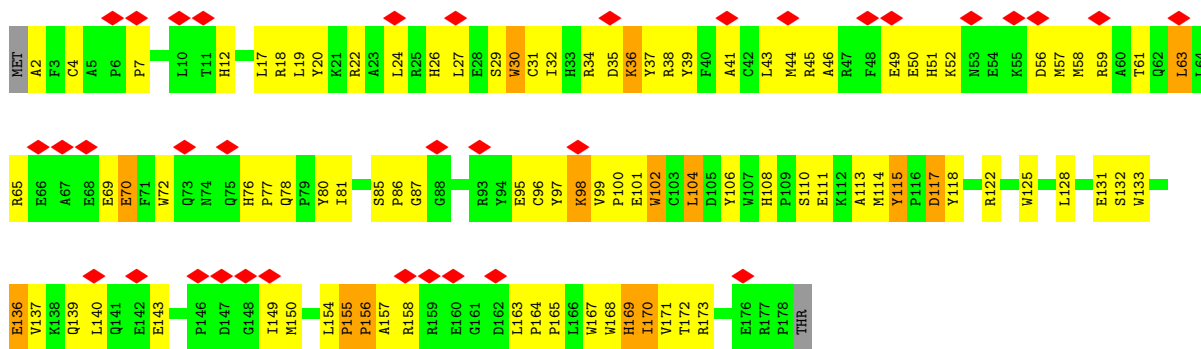




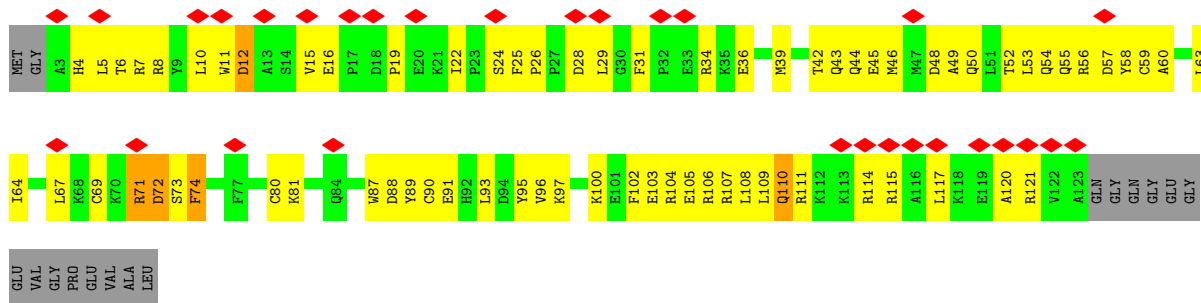
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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

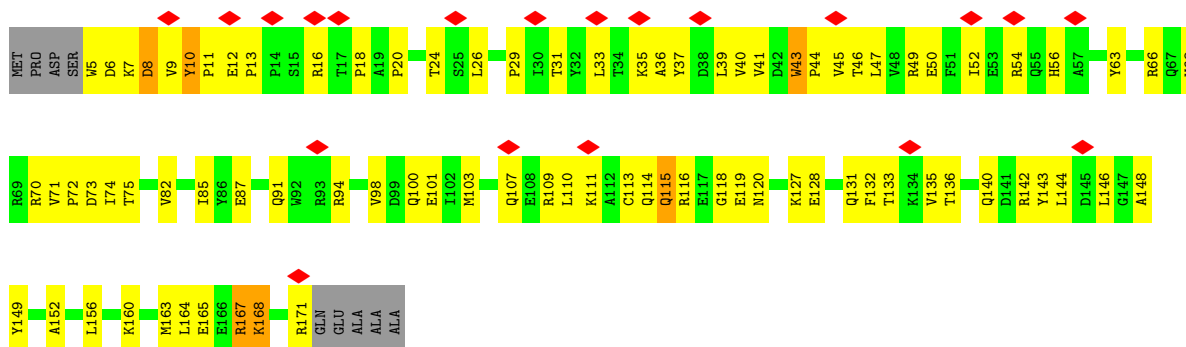


• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

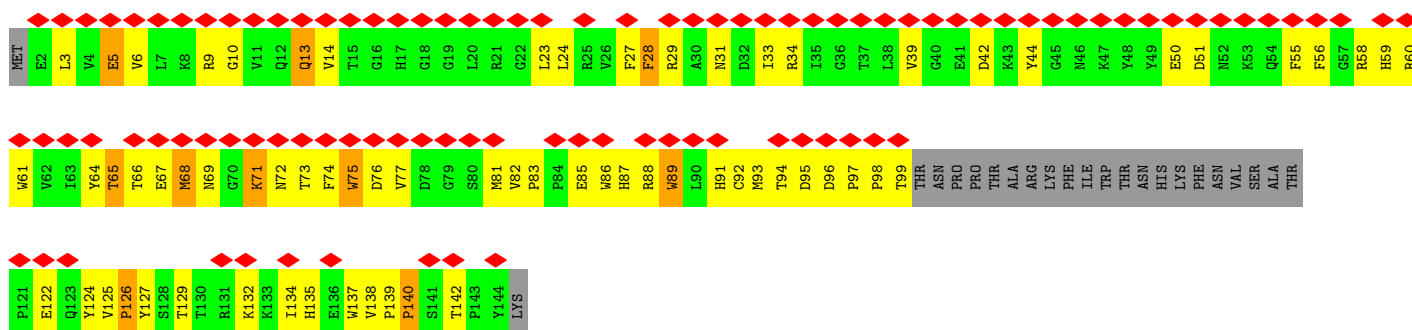


• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

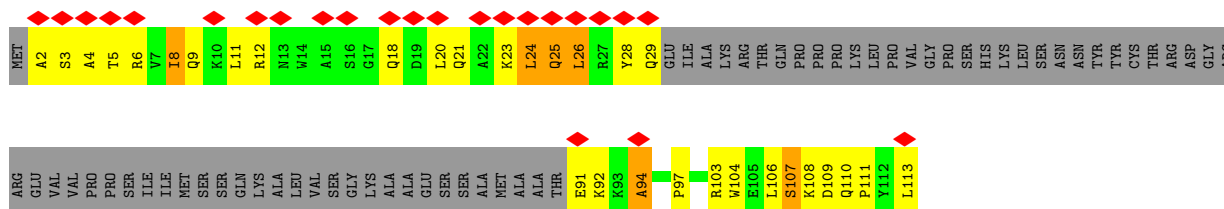
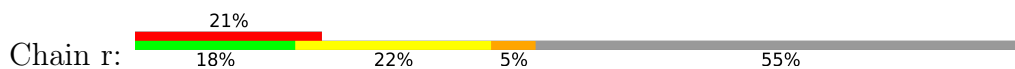




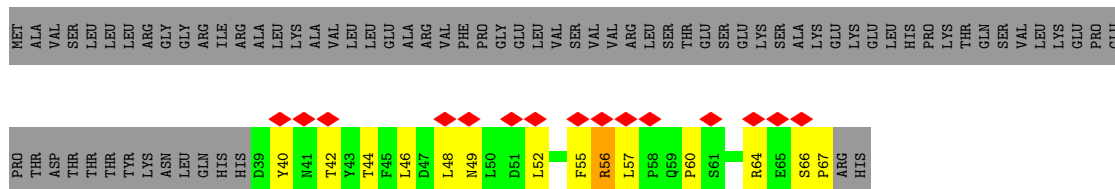
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



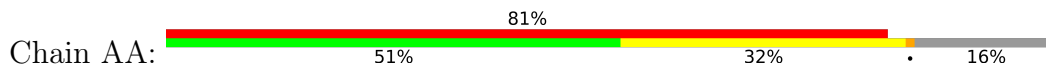
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

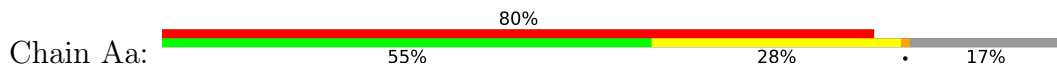


- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

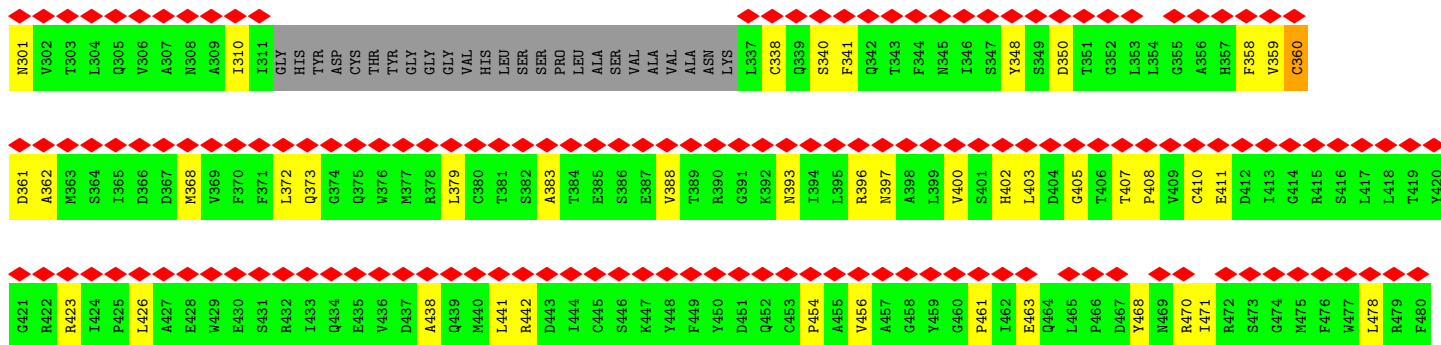


MET	ALA	ALA	SER	ALA	VAL	VAL	ARG	ALA	ALA	CYS	GLY	THR	GLN	VAL	LEU	LEU	ARG	THR	ARG	ARG	PRO	ALA	LEU	LEU	ARG	PRO	PRO	ALA	LEU	ARG	GLY	THR	ALA	THR	PHE	ALA	GLN	ALA	LEU	LEU	GLN	S44	V45	P46	E47	T48	Q49	V50	S51	I52	L53	D54	N55	G56	L57	R58	V59	A60	
S61	E62	Q63	S64	S65	H66	A67	T68	C69	T70	V71	G72	V73	W74	I75	D76	A77	G78	S79	R80	Y81	E82	T83	H84	R85	N86	N87	G88	A89	G90	Y91	F92	L93	E94	H95	L96	A97	F98	K99	G100	T101	K102	N103	R104	P105	G106	N107	A108	L109	E110	K111	E112	V113	E114	S115	G116	G117	A118	H119	L120
M121	A122	Y123	S124	T125	R126	E127	H128	T129	A130	Y131	L132	I133	K134	A135	L136	S137	K138	D139	L140	P141	K142	V143	V144	L146	L147	A148	D149	I150	V151	Q152	M153	S154	S155	L156	E157	D158	S159	Q160	I161	R222	E162	K163	E164	R165	D166	V167	I168	L169	E170	K171	M172	Q173	E174	M175	D176	V177	S178	M179	Q180
M181	V182	V183	F184	D185	Y186	L187	H188	A189	T190	A191	F192	Q193	G194	T195	P196	L197	Q199	A200	V201	E202	G203	P204	S205	E206	N207	V208	R209	R210	L211	S212	R213	T214	D215	L216	T217	D218	Y219	L220	N221	R222	H223	Y224	K225	A226	P227	R228	M229	E292	G293	L231	A232	A233	A234	G235	G236	V237	E238	H239	Q240
Q241	L242	L243	D244	L245	A246	Q247	K248	H249	L250	S251	S252	V253	S254	R255	VAL	TYR	GLU	ASP	ALA	VAL	PRO	GLY	THR	P287	C268	R269	F270	T271	G272	E274	I275	R276	H277	R278	D279	D280	A281	L282	P283	L284	A285	H286	V287	A288	I289	A290	V291	E292	G293	P294	G295	W296	A297	N298	P299	D300			
N301	V302	T303	L304	Q305	V306	A307	N308	A309	I310	I311	G312	H313	Y314	ASP	CYS	THR	TYR	GLY	GLY	VAL	HIS	PRO	LEU	SER	PRO	LEU	ALA	VAL	ASN	LYS	L337	C338	Q339	S340	F341	Q342	T343	F344	N345	I346	S347	Y348	S349	D350	T351	G352	L353	L354	G355	A356	H357	F358	V359	C360					
D361	A362	M363	S364	I365	D366	D367	M368	V369	F370	F371	L372	Q373	G374	Q375	W376	M377	R378	L379	C380	T381	S382	A383	T384	E385	S386	E387	V388	T389	R390	G391	K392	N393	I394	L395	R396	N397	A398	L399	V400	S401	H402	L403	D404	G405	T406	T407	P408	V409	C410	E411	D412	I413	G414	R415	S416	W417	L418	T419	Y420
G421	R422	R423	I424	F425	L426	A427	F428	W429	E430	S431	R432	I433	Q434	E435	W436	D437	A438	Q439	M440	L441	R442	D443	I444	C445	S446	K447	Y448	F449	Y450	D451	A452	C453	P454	A455	V456	A457	G458	Y459	G460	P461	I462	E463	L465	P466	D467	Y468	M469	R470	I471	R472	S473	G474	M475	F476	W477	L478	R479	PHE	

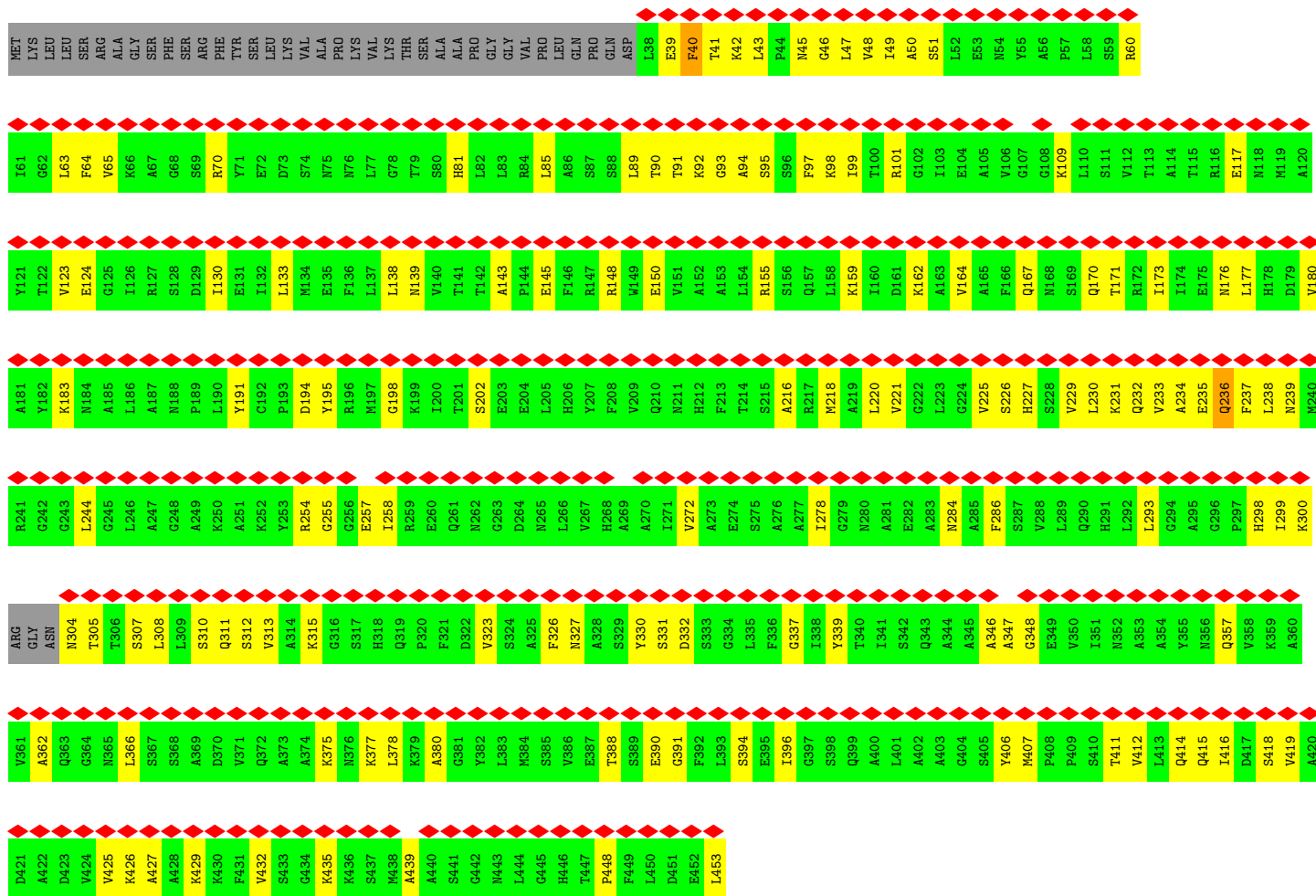
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial



MET	ALA	ALA	SER	ALA	VAL	VAL	ARG	ALA	ALA	CYS	GLY	THR	GLN	VAL	LEU	LEU	ARG	THR	ARG	ARG	PRO	ALA	LEU	LEU	ARG	PRO	PRO	ALA	LEU	ARG	GLY	THR	ALA	THR	PHE	ALA	GLN	ALA	LEU	LEU	GLN	S44	V45	P46	E47	T48	Q49	V50	S51	I52	L53	D54	N55	G56	L57	R58	V59	A60	
S61	E62	Q63	S64	S65	H66	A67	T68	C69	T70	V71	G72	V73	W74	I75	D76	A77	G78	S79	R80	Y81	E82	T83	H84	R85	N86	N87	G88	A89	G90	Y91	F92	L93	E94	H95	L96	A97	F98	K99	G100	T101	K102	N103	R104	P105	G106	N107	A108	L109	E110	K111	E112	V113	E114	S115	G116	G117	A118	H119	L120
M121	A122	Y123	S124	T125	R126	E127	H128	T129	A130	Y131	L132	I133	K134	A135	L136	S137	K138	D139	L140	P141	K142	V143	V144	L146	L147	A148	D149	I150	V151	Q152	M153	S154	S155	L156	E157	D158	S159	Q160	I161	R222	E162	K163	E164	R165	D166	V167	I168	L169	E170	K171	M172	Q173	E174	M175	D176	V177	S178	M179	Q180
M181	V182	V183	F184	D185	Y186	L187	H188	A189	T190	A191	F192	Q193	G194	T195	P196	L197	Q199	A200	V201	E202	G203	P204	S205	E206	N207	V208	R209	R210	L211	S212	R213	T214	D215	L216	T217	D218	Y219	L220	N221	R222	H223	Y224	K225	A226	P227	R228	M229	E292	G293	L231	A232	A233	A234	G235	G236	V237	E238	H239	Q240
Q241	L242	L243	D244	L245	A246	Q247	K248	H249	L250	S251	S252	V253	S254	ARG	VAL	TYR	GLU	ASP	ALA	VAL	PHO	GLY	LEU	THR	P287	C268	R269	F270	T271	G272	E274	I275	R276	H277	R278	D279	D280	A281	L282	P283	L284	A285	H286	V287	A288	I289	A290	V291	E292	G293	P294	G295	W296	A297	N298	P299	D300		



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



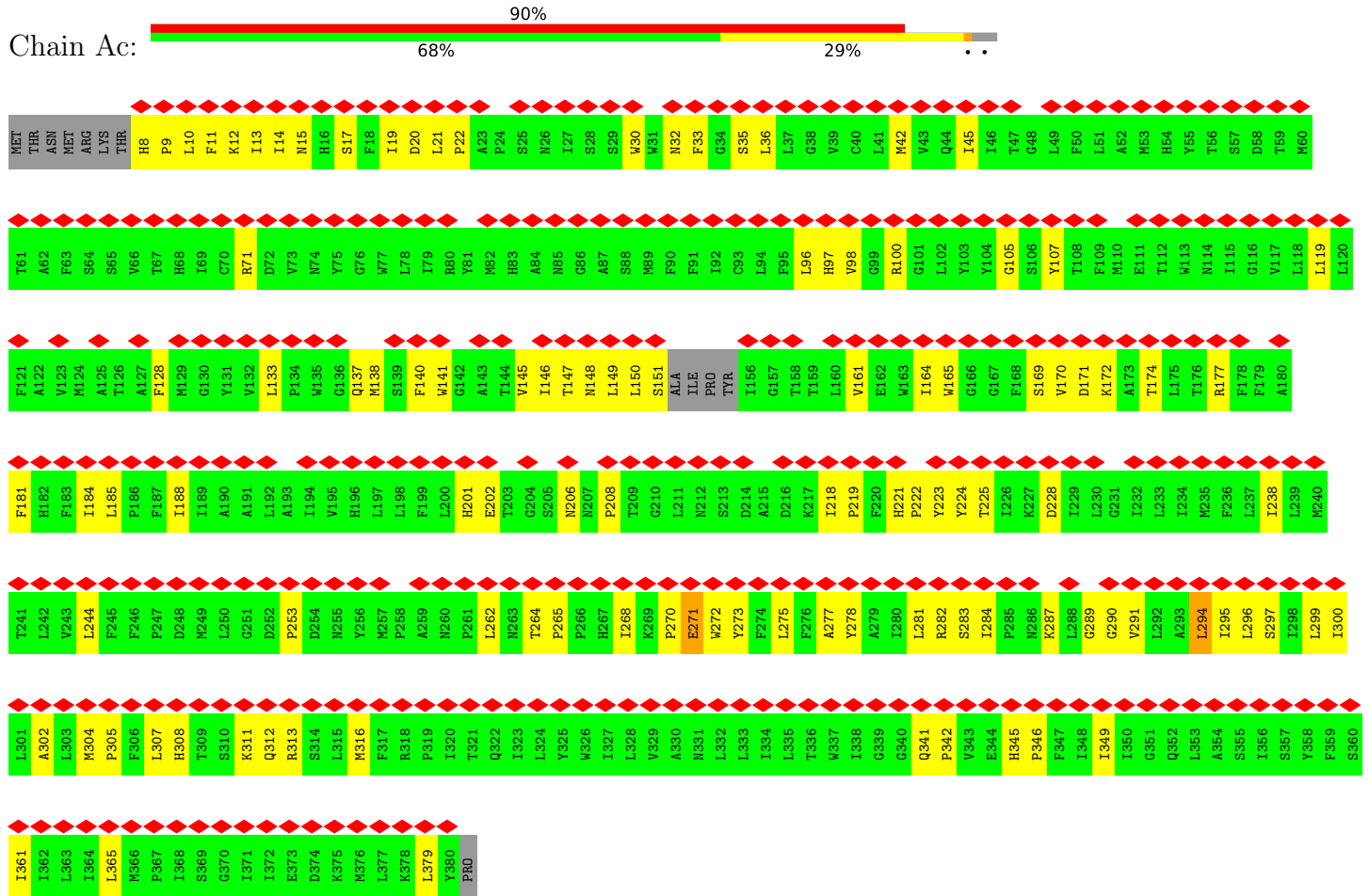
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



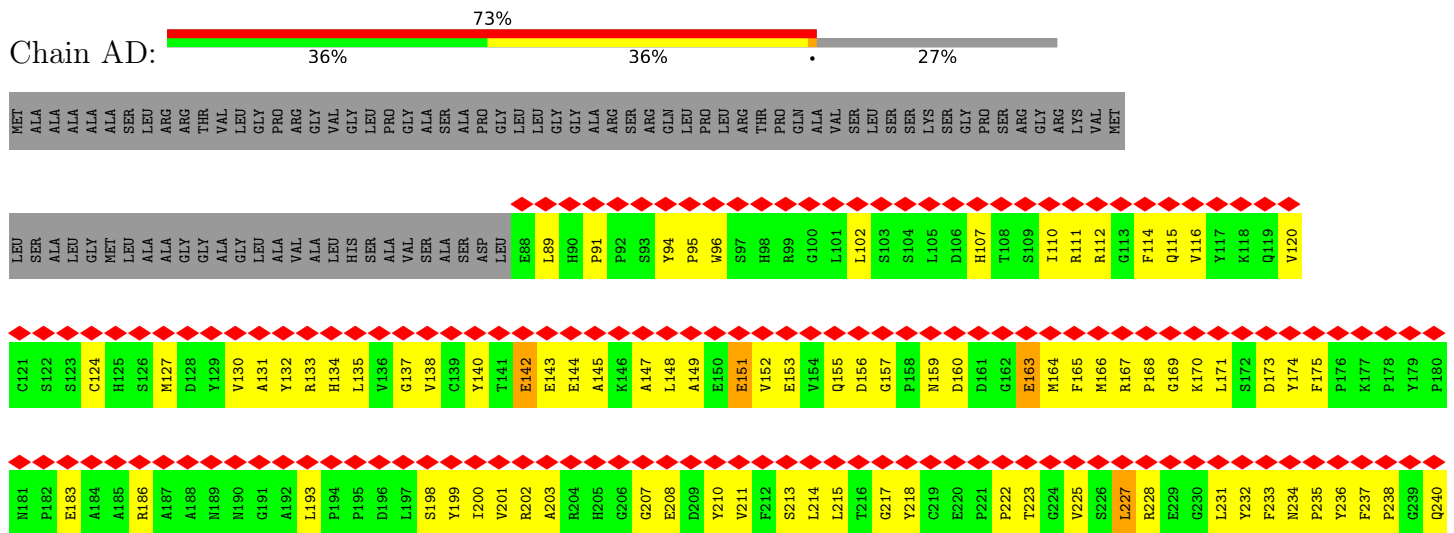




• Molecule 47: Cytochrome b



• Molecule 48: Cytochrome c1, heme protein, mitochondrial

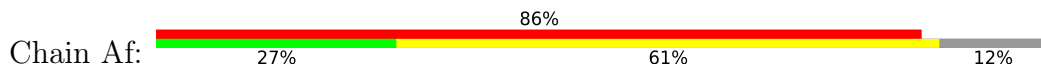




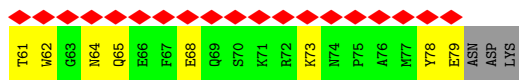
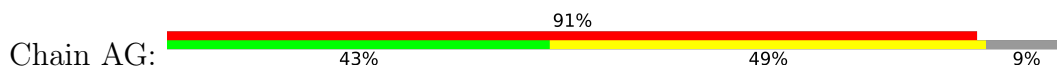




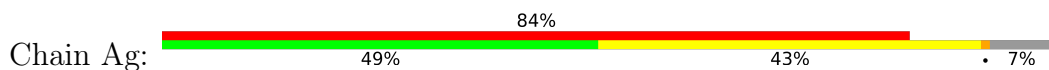
• Molecule 50: Cytochrome b-c1 complex subunit 7



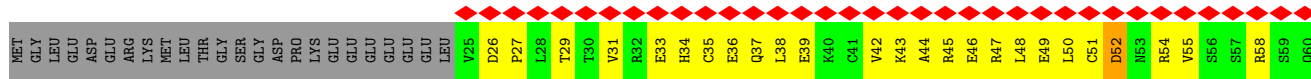
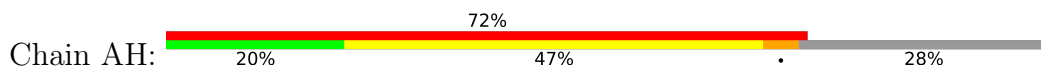
• Molecule 51: Cytochrome b-c1 complex subunit 8



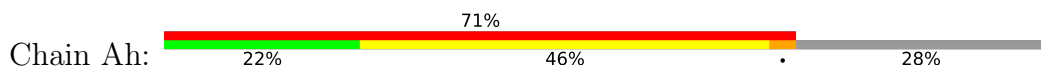
• Molecule 51: Cytochrome b-c1 complex subunit 8

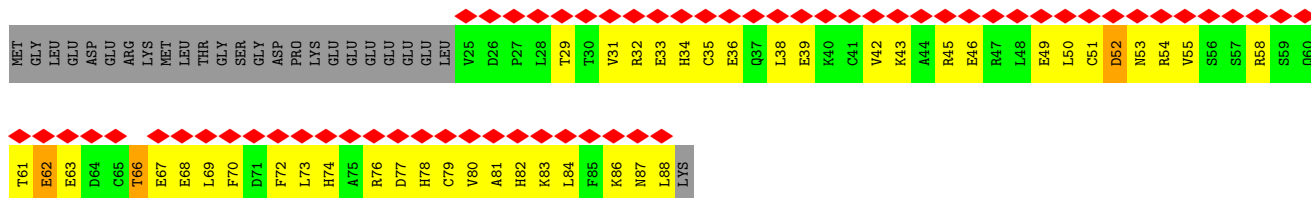


• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

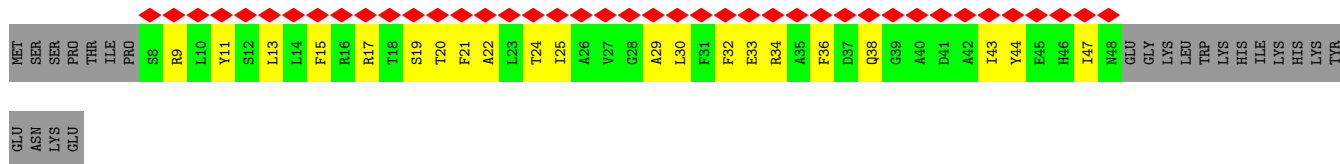


• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

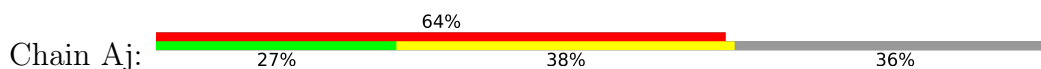




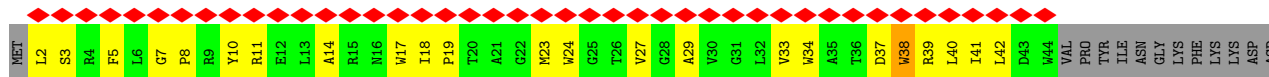
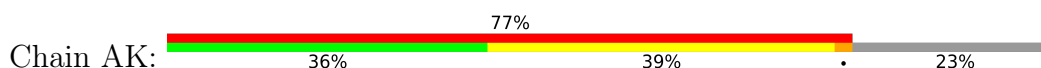
• Molecule 53: Cytochrome b-c1 complex subunit 9



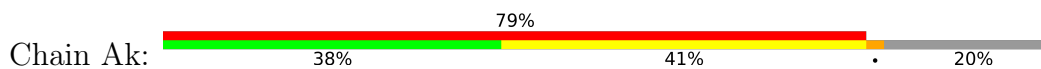
• Molecule 53: Cytochrome b-c1 complex subunit 9



• 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	27478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0082	Depositor
Map size ( $\text{\AA}$ )	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.67	0/755	0.96	3/1029 (0.3%)
2	B	0.96	4/1278 (0.3%)	1.30	11/1730 (0.6%)
3	C	0.88	2/1687 (0.1%)	1.28	13/2297 (0.6%)
4	D	0.91	5/3532 (0.1%)	1.36	33/4782 (0.7%)
5	E	0.82	3/1675 (0.2%)	1.16	18/2282 (0.8%)
6	F	0.82	4/3347 (0.1%)	1.32	41/4522 (0.9%)
7	G	0.88	8/5374 (0.1%)	1.49	86/7281 (1.2%)
8	H	0.83	2/2607 (0.1%)	1.22	30/3561 (0.8%)
9	I	0.90	1/1418 (0.1%)	1.48	18/1915 (0.9%)
10	J	0.55	1/1205 (0.1%)	0.92	6/1633 (0.4%)
11	K	0.85	0/732	1.44	11/994 (1.1%)
12	L	0.97	6/4921 (0.1%)	1.56	108/6696 (1.6%)
13	M	1.01	7/3717 (0.2%)	1.56	85/5062 (1.7%)
14	N	1.00	3/2756 (0.1%)	1.43	50/3751 (1.3%)
15	O	0.86	6/2655 (0.2%)	1.21	27/3601 (0.7%)
16	P	0.79	4/2793 (0.1%)	1.17	23/3787 (0.6%)
17	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
18	R	1.04	4/671 (0.6%)	1.38	13/903 (1.4%)
19	S	0.94	2/678 (0.3%)	1.47	11/915 (1.2%)
20	T	1.03	1/613 (0.2%)	1.56	12/826 (1.5%)
20	U	0.96	1/712 (0.1%)	1.35	12/962 (1.2%)
21	V	0.86	0/937	1.47	14/1270 (1.1%)
22	W	0.73	0/993	0.95	3/1335 (0.2%)
23	X	0.72	0/1422	1.22	15/1921 (0.8%)
24	Y	0.85	0/1054	0.96	3/1429 (0.2%)
25	Z	0.81	1/1183 (0.1%)	1.23	11/1597 (0.7%)
26	a	0.88	0/561	1.38	8/755 (1.1%)
27	b	0.70	0/643	0.94	1/884 (0.1%)
28	c	0.69	0/400	1.24	8/544 (1.5%)
29	d	0.88	1/1028 (0.1%)	1.01	8/1387 (0.6%)
30	e	0.77	1/881 (0.1%)	1.01	4/1173 (0.3%)
31	f	0.59	0/451	0.75	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	g	0.87	3/863 (0.3%)	1.36	18/1175 (1.5%)
33	h	0.76	0/1197	1.22	7/1621 (0.4%)
34	i	0.85	0/790	1.38	16/1074 (1.5%)
35	j	0.75	0/599	1.23	8/820 (1.0%)
36	k	1.05	1/578 (0.2%)	1.56	18/782 (2.3%)
37	l	1.02	4/1359 (0.3%)	1.25	9/1855 (0.5%)
38	m	0.82	1/1079 (0.1%)	1.21	17/1463 (1.2%)
39	n	0.93	1/1589 (0.1%)	1.22	17/2152 (0.8%)
40	o	0.78	0/1063	1.14	7/1427 (0.5%)
41	p	0.72	1/1448 (0.1%)	1.01	13/1957 (0.7%)
42	q	1.04	2/1054 (0.2%)	1.53	19/1431 (1.3%)
43	r	1.16	3/426 (0.7%)	1.71	12/573 (2.1%)
44	s	0.45	0/244	1.10	2/331 (0.6%)
45	AA	0.42	0/3218	0.74	5/4362 (0.1%)
45	Aa	0.38	0/3191	0.69	2/4326 (0.0%)
46	AB	0.39	1/3146 (0.0%)	0.64	5/4252 (0.1%)
46	Ab	0.37	0/3178	0.62	0/4296
47	AC	0.46	1/3089 (0.0%)	0.69	6/4221 (0.1%)
47	Ac	0.47	1/3054 (0.0%)	0.65	1/4170 (0.0%)
48	AD	0.42	0/1955	0.78	6/2655 (0.2%)
48	Ad	0.43	0/1971	0.71	2/2677 (0.1%)
49	AE	0.63	0/1428	1.01	2/1934 (0.1%)
49	AI	0.48	0/331	0.94	0/451
49	Ae	0.62	0/1467	1.00	2/1985 (0.1%)
50	AF	0.38	0/875	0.57	1/1173 (0.1%)
50	Af	0.47	0/884	0.73	1/1184 (0.1%)
51	AG	0.49	0/653	0.89	2/883 (0.2%)
51	Ag	0.47	0/662	0.88	2/895 (0.2%)
52	AH	0.49	0/534	1.04	9/717 (1.3%)
52	Ah	0.57	0/534	1.04	5/717 (0.7%)
53	AJ	0.53	0/339	0.71	0/457
53	Aj	0.53	0/339	0.71	0/457
54	AK	0.49	0/368	0.77	1/504 (0.2%)
54	Ak	0.44	0/379	0.73	1/522 (0.2%)
All	All	0.77	87/97543 (0.1%)	1.17	914/132254 (0.7%)

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	227	ALA	C-O	15.85	1.42	1.24
18	R	89	PRO	N-CD	-15.14	1.26	1.47
12	L	265	PRO	N-CD	13.82	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	AC	271	GLU	C-N	13.68	1.52	1.34
36	k	50	PRO	N-CD	-13.63	1.28	1.47

The worst 5 of 914 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.30	132.46	110.65
4	D	142	VAL	N-CA-C	-19.03	92.53	110.42
7	G	174	THR	N-CA-C	-17.48	89.04	114.39
6	F	332	CYS	N-CA-C	15.59	130.04	111.02
13	M	370	PRO	N-CA-C	14.56	128.46	110.70

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	737	0	800	113	0
2	B	1247	0	1256	144	0
3	C	1641	0	1596	118	0
4	D	3443	0	3389	337	0
5	E	1635	0	1626	171	0
6	F	3273	0	3231	311	0
7	G	5287	0	5323	528	0
8	H	2531	0	2619	350	0
9	I	1389	0	1352	137	0
10	J	1178	0	1204	214	0
11	K	721	0	753	91	0
12	L	4798	0	4986	584	0
13	M	3630	0	3854	500	0
14	N	2694	0	2896	345	0
15	O	2588	0	2539	250	0
16	P	2720	0	2740	227	0
17	Q	957	0	949	84	0
18	R	660	0	639	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	667	0	683	91	0
20	T	604	0	596	87	0
20	U	700	0	691	70	0
21	V	915	0	954	82	0
22	W	970	0	991	67	0
23	X	1385	0	1370	156	0
24	Y	1030	0	1015	80	0
25	Z	1152	0	1148	126	0
26	a	548	0	562	63	0
27	b	620	0	617	83	0
28	c	389	0	385	34	0
29	d	996	0	1001	71	0
30	e	859	0	849	121	0
31	f	439	0	433	35	0
32	g	835	0	772	67	0
33	h	1162	0	1163	121	0
34	i	765	0	769	60	0
35	j	574	0	522	91	0
36	k	560	0	560	47	0
37	l	1304	0	1193	95	0
38	m	1050	0	1061	114	0
39	n	1534	0	1463	135	0
40	o	1038	0	1030	105	0
41	p	1415	0	1385	106	0
42	q	1020	0	976	91	0
43	r	418	0	434	50	0
44	s	238	0	225	24	0
45	AA	3157	0	3075	173	0
45	Aa	3131	0	3052	136	0
46	AB	3097	0	3108	127	0
46	Ab	3128	0	3135	141	0
47	AC	2988	0	3045	146	0
47	Ac	2956	0	3012	123	0
48	AD	1896	0	1845	151	0
48	Ad	1912	0	1860	149	0
49	AE	1397	0	1376	192	0
49	AI	328	0	346	46	0
49	Ae	1436	0	1414	183	0
50	AF	855	0	841	39	0
50	Af	864	0	854	78	0
51	AG	634	0	637	53	0
51	Ag	643	0	643	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AH	527	0	507	66	0
52	Ah	527	0	505	58	0
53	AJ	332	0	324	26	0
53	Aj	332	0	324	31	0
54	AK	355	0	351	23	0
54	Ak	365	0	358	32	0
55	B	8	0	0	3	0
55	F	8	0	0	6	0
55	G	16	0	0	2	0
55	I	16	0	0	5	0
56	B	18	0	18	3	0
57	B	35	0	44	6	0
57	I	43	0	60	8	0
58	Ac	58	0	64	3	0
58	Ag	51	0	82	0	0
58	D	38	0	50	6	0
58	H	97	0	151	18	0
58	J	46	0	66	1	0
58	L	133	0	194	18	0
58	M	86	0	123	15	0
58	i	40	0	54	11	0
58	m	41	0	56	9	0
59	E	4	0	0	4	0
59	G	4	0	0	5	0
60	F	31	0	19	0	0
61	H	35	0	43	28	0
62	Aa	46	0	36	1	0
62	Ag	98	0	84	3	0
62	L	73	0	90	12	0
62	M	82	0	114	12	0
62	Y	71	0	86	5	0
62	d	65	0	74	8	0
62	h	68	0	83	13	0
62	q	57	0	58	22	0
63	L	1	0	0	0	0
63	R	1	0	0	0	0
64	O	27	0	12	3	0
65	P	48	0	26	5	0
66	W	32	0	0	4	0
66	n	32	0	0	1	0
67	AC	86	0	60	31	0
67	Ac	86	0	60	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	AC	28	0	31	29	0
68	Ac	23	0	23	10	0
69	AD	43	0	31	13	0
69	Ad	43	0	31	12	0
70	Ac	23	0	23	11	0
All	All	97017	0	97158	7400	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 38.

The worst 5 of 7400 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	69:AD:401:HEC:HAC	1.53	1.48
48:Ad:124:CYS:SG	69:Ad:401:HEC:HAC	1.53	1.47
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
67:Ac:403:HEM:CBA	68:Ac:406:UQ6:H4M2	1.64	1.27
10:J:134:MET:HE3	27:b:51:TYR:CD1	1.69	1.27

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	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	11 (7%)	1 (1%)	21	59
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
4	D	423/463 (91%)	392 (93%)	31 (7%)	0	100	100
5	E	208/248 (84%)	193 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	422/464 (91%)	403 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	632 (92%)	53 (8%)	0	100	100
8	H	313/318 (98%)	295 (94%)	18 (6%)	0	100	100
9	I	169/212 (80%)	169 (100%)	0	0	100	100
10	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
11	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
12	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100
13	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	72
15	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
16	P	337/377 (89%)	314 (93%)	23 (7%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	111 (99%)	1 (1%)	0	100	100
23	X	167/172 (97%)	153 (92%)	14 (8%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
25	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
26	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
27	b	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
35	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	21	59
40	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
41	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
42	q	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
44	s	27/104 (26%)	27 (100%)	0	0	100	100
45	AA	397/480 (83%)	385 (97%)	12 (3%)	0	100	100
45	Aa	394/480 (82%)	385 (98%)	9 (2%)	0	100	100
46	AB	409/453 (90%)	397 (97%)	12 (3%)	0	100	100
46	Ab	415/453 (92%)	406 (98%)	9 (2%)	0	100	100
47	AC	371/381 (97%)	365 (98%)	6 (2%)	0	100	100
47	Ac	365/381 (96%)	361 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	238/325 (73%)	229 (96%)	9 (4%)	0	100	100
49	AE	175/274 (64%)	164 (94%)	11 (6%)	0	100	100
49	AI	40/274 (15%)	38 (95%)	2 (5%)	0	100	100
49	Ae	180/274 (66%)	167 (93%)	13 (7%)	0	100	100
50	AF	95/111 (86%)	95 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	73/82 (89%)	73 (100%)	0	0	100	100
51	Ag	74/82 (90%)	74 (100%)	0	0	100	100
52	AH	62/89 (70%)	60 (97%)	2 (3%)	0	100	100
52	Ah	62/89 (70%)	60 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	39/64 (61%)	39 (100%)	0	0	100	100
54	AK	41/56 (73%)	39 (95%)	2 (5%)	0	100	100
54	Ak	43/56 (77%)	40 (93%)	3 (7%)	0	100	100
All	All	11734/14118 (83%)	11218 (96%)	513 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	109	ALA
2	B	195	PRO
39	n	156	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/104 (80%)	83 (100%)	0	100	100
2	B	132/185 (71%)	131 (99%)	1 (1%)	73	80
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	369/395 (93%)	369 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	340/370 (92%)	340 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	87
8	H	279/280 (100%)	278 (100%)	1 (0%)	84	84
9	I	147/178 (83%)	147 (100%)	0	100	100
10	J	124/138 (90%)	123 (99%)	1 (1%)	73	80
11	K	86/88 (98%)	86 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	84
13	M	415/415 (100%)	414 (100%)	1 (0%)	87	87
14	N	307/308 (100%)	306 (100%)	1 (0%)	86	85
15	O	282/309 (91%)	282 (100%)	0	100	100
16	P	296/325 (91%)	296 (100%)	0	100	100
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	78
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	72
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	72
20	T	69/135 (51%)	68 (99%)	1 (1%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	152 (100%)	0	100	100
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	120/123 (98%)	119 (99%)	1 (1%)	73	80
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	47/53 (89%)	47 (100%)	0	100	100
32	g	90/129 (70%)	90 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	86/120 (72%)	86 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	140/161 (87%)	140 (100%)	0	100	100
38	m	112/114 (98%)	111 (99%)	1 (1%)	70	79
39	n	162/164 (99%)	161 (99%)	1 (1%)	78	83
40	o	111/121 (92%)	111 (100%)	0	100	100
41	p	152/158 (96%)	152 (100%)	0	100	100
42	q	110/131 (84%)	110 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	28/95 (30%)	28 (100%)	0	100	100
45	AA	341/398 (86%)	340 (100%)	1 (0%)	86	85
45	Aa	339/398 (85%)	337 (99%)	2 (1%)	78	83
46	AB	324/356 (91%)	324 (100%)	0	100	100
46	Ab	327/356 (92%)	327 (100%)	0	100	100
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	85
47	Ac	322/333 (97%)	321 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	205/260 (79%)	205 (100%)	0	100	100
49	AE	152/224 (68%)	151 (99%)	1 (1%)	76	81
49	AI	33/224 (15%)	33 (100%)	0	100	100
49	Ae	156/224 (70%)	154 (99%)	2 (1%)	61	74
50	AF	89/99 (90%)	89 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	68/74 (92%)	68 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	61/83 (74%)	61 (100%)	0	100	100
52	Ah	61/83 (74%)	61 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	33/55 (60%)	33 (100%)	0	100	100
54	AK	34/46 (74%)	34 (100%)	0	100	100
54	Ak	35/46 (76%)	35 (100%)	0	100	100
All	All	10319/12037 (86%)	10296 (100%)	23 (0%)	85	87

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	n	98	LYS
49	AE	135	GLN
47	AC	294	LEU
45	Aa	249	HIS
13	M	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	51	GLN
48	Ad	155	GLN
35	j	41	GLN
48	Ad	115	GLN
52	AH	60	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 2 are monoatomic - leaving 49 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	SF4	B	301	2	0,12,12	-	-	-		
58	3PE	H	402	-	45,45,50	0.97	2 (4%)	48,50,55	0.98	2 (4%)
68	UQ6	Ac	406	-	23,23,43	2.82	6 (26%)	30,31,55	1.91	5 (16%)
55	SF4	G	801	7	0,12,12	-	-	-		
58	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.15	4 (7%)
61	UQ9	H	401	-	35,35,58	0.79	2 (5%)	43,45,73	0.59	1 (2%)
65	NDP	P	401	-	51,52,52	1.19	5 (9%)	71,80,80	1.57	10 (14%)
67	HEM	Ac	402	47	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
55	SF4	F	502	6	0,12,12	-	-	-		
58	3PE	Ac	404	-	34,34,50	0.33	0	37,39,55	0.41	0
58	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.07	2 (4%)
60	FMN	F	501	-	33,33,33	1.42	4 (12%)	48,50,50	1.23	7 (14%)
62	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.22	6 (9%)
70	U10	Ac	405	-	23,23,63	1.28	3 (13%)	30,31,79	2.05	6 (20%)
62	CDL	Ag	101	-	41,41,99	0.45	0	47,53,111	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.06	3 (7%)
62	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.16	6 (8%)
58	3PE	D	501	-	37,37,50	1.07	2 (5%)	40,42,55	1.09	3 (7%)
68	UQ6	AC	403	-	28,28,43	2.46	6 (21%)	36,37,55	2.02	10 (27%)
62	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.17	7 (9%)
62	CDL	Aa	501	-	45,45,99	0.43	0	51,57,111	0.36	0
58	3PE	L	702	-	48,48,50	0.93	2 (4%)	51,53,55	1.11	3 (5%)
59	FES	E	301	5	0,4,4	-	-	-	-	-
67	HEM	AC	402	47	50,50,50	1.54	8 (16%)	67,82,82	1.80	15 (22%)
69	HEC	AD	401	48	46,50,50	1.83	6 (13%)	58,82,82	1.92	5 (8%)
58	3PE	J	201	-	45,45,50	0.98	2 (4%)	48,50,55	1.07	3 (6%)
67	HEM	AC	401	47	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
62	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.15	6 (7%)
56	UQ1	B	302	-	18,18,18	2.06	2 (11%)	24,25,25	1.29	4 (16%)
66	EHZ	n	201	-	29,31,37	1.82	7 (24%)	37,41,47	1.65	5 (13%)
59	FES	G	803	7	0,4,4	-	-	-	-	-
66	EHZ	W	201	-	29,31,37	1.79	7 (24%)	37,41,47	1.94	12 (32%)
57	PC1	B	303	-	34,34,53	1.16	2 (5%)	40,42,61	1.17	4 (10%)
62	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.15	7 (8%)
58	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.09	3 (6%)
62	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.22	7 (10%)
62	CDL	Ag	102	-	55,55,99	0.38	0	61,67,111	0.33	0
58	3PE	Ac	401	-	22,22,50	0.47	0	25,27,55	0.76	1 (4%)
69	HEC	Ad	401	48	46,50,50	1.83	4 (8%)	58,82,82	1.93	5 (8%)
58	3PE	i	201	-	39,39,50	1.04	2 (5%)	42,44,55	1.15	3 (7%)
57	PC1	I	301	-	42,42,53	1.05	2 (4%)	48,50,61	1.06	3 (6%)
64	ADP	O	401	-	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
67	HEM	Ac	403	47	50,50,50	1.33	5 (10%)	67,82,82	1.57	15 (22%)
58	3PE	H	403	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
58	3PE	m	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.16	3 (6%)
58	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.30	0
55	SF4	G	802	7	0,12,12	-	-	-	-	-
55	SF4	I	302	9	0,12,12	-	-	-	-	-
55	SF4	I	303	9	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
58	3PE	H	402	-	-	13/49/49/54	-
68	UQ6	Ac	406	-	-	2/15/15/39	0/1/1/1
55	SF4	B	301	2	-	-	0/6/5/5
65	NDP	P	401	-	-	6/34/77/77	0/5/5/5
58	3PE	M	502	-	-	14/52/52/54	-
61	UQ9	H	401	-	-	17/30/54/81	0/1/1/1
55	SF4	G	801	7	-	-	0/6/5/5
67	HEM	Ac	402	47	-	9/14/54/54	-
55	SF4	F	502	6	-	-	0/6/5/5
58	3PE	Ac	404	-	-	12/38/38/54	-
60	FMN	F	501	-	-	1/18/18/18	0/3/3/3
58	3PE	L	701	-	-	10/43/43/54	-
62	CDL	q	201	-	-	19/67/67/110	-
70	U10	Ac	405	-	-	6/15/39/87	0/1/1/1
62	CDL	Ag	101	-	-	14/52/52/110	-
58	3PE	M	501	-	-	10/40/40/54	-
62	CDL	h	201	-	-	19/78/78/110	-
58	3PE	D	501	-	-	8/41/41/54	-
68	UQ6	AC	403	-	-	4/21/21/39	0/1/1/1
62	CDL	Y	201	-	-	15/81/81/110	-
62	CDL	Aa	501	-	-	15/56/56/110	-
58	3PE	L	702	-	-	13/52/52/54	-
69	HEC	AD	401	48	-	4/14/54/54	-
67	HEM	AC	402	47	-	8/14/54/54	-
59	FES	E	301	5	-	-	0/1/1/1
58	3PE	J	201	-	-	13/49/49/54	-
67	HEM	AC	401	47	-	9/14/54/54	-
62	CDL	L	703	-	-	20/83/83/110	-
56	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
66	EHZ	n	201	-	-	22/39/39/45	-
59	FES	G	803	7	-	-	0/1/1/1
66	EHZ	W	201	-	-	21/39/39/45	-
57	PC1	B	303	-	-	11/38/38/57	-
62	CDL	M	503	-	-	24/92/92/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	3PE	L	705	-	-	13/47/47/54	-
62	CDL	d	201	-	-	27/75/75/110	-
62	CDL	Ag	102	-	-	12/66/66/110	-
58	3PE	Ac	401	-	-	5/26/26/54	-
69	HEC	Ad	401	48	-	4/14/54/54	-
58	3PE	i	201	-	-	9/43/43/54	-
57	PC1	I	301	-	-	8/46/46/57	-
64	ADP	O	401	-	-	2/16/32/32	0/3/3/3
67	HEM	Ac	403	47	-	8/14/54/54	-
58	3PE	H	403	-	-	12/54/54/54	-
58	3PE	m	201	-	-	10/44/44/54	-
58	3PE	Ag	103	-	-	10/54/54/54	-
55	SF4	G	802	7	-	-	0/6/5/5
55	SF4	I	302	9	-	-	0/6/5/5
55	SF4	I	303	9	-	-	0/6/5/5

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	403	UQ6	C5-C4	8.03	1.52	1.39
56	B	302	UQ1	C6-C5	7.73	1.49	1.35
69	Ad	401	HEC	CAC-C3C	6.11	1.54	1.35
69	AD	401	HEC	CAB-C3B	6.11	1.54	1.35
68	Ac	406	UQ6	C5-C6	6.08	1.49	1.40

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	Ad	401	HEC	CBC-CAC-C3C	-8.59	110.27	127.43
69	AD	401	HEC	CBC-CAC-C3C	-8.58	110.29	127.43
69	Ad	401	HEC	CBB-CAB-C3B	-8.33	110.79	127.43
69	AD	401	HEC	CBB-CAB-C3B	-8.33	110.79	127.43
70	Ac	405	U10	C6-C1-C2	7.75	125.28	119.17

There are no chirality outliers.

5 of 459 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	303	PC1	C1-O11-P-O12

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
57	B	303	PC1	C1-O11-P-O14
57	B	303	PC1	C1-O11-P-O13
57	B	303	PC1	O22-C21-O21-C2
58	D	501	3PE	C1-O11-P-O14

There are no ring outliers.

44 monomers are involved in 338 short contacts:

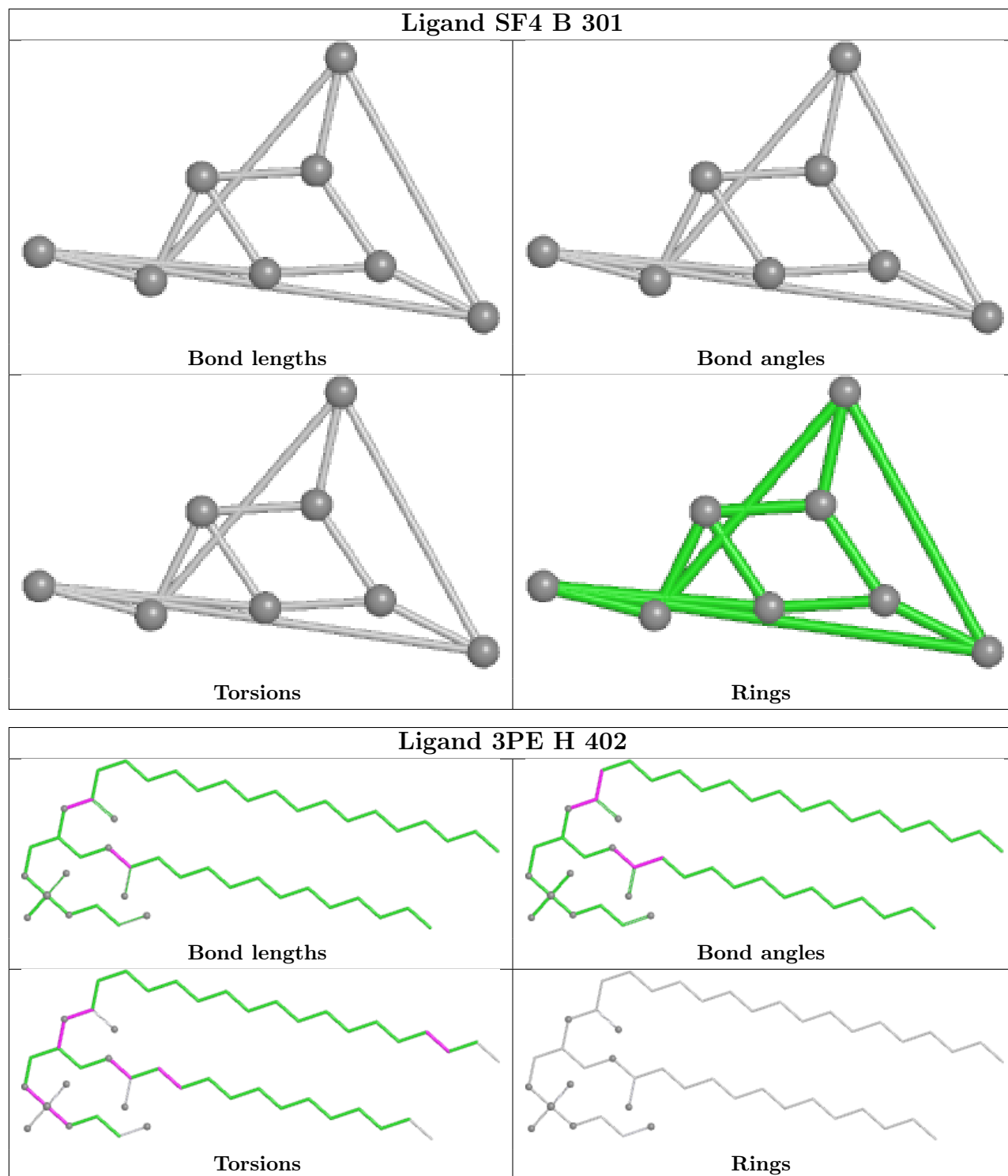
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	B	301	SF4	3	0
58	H	402	3PE	7	0
68	Ac	406	UQ6	10	0
58	M	502	3PE	5	0
61	H	401	UQ9	28	0
65	P	401	NDP	5	0
67	Ac	402	HEM	1	0
55	F	502	SF4	6	0
58	Ac	404	3PE	1	0
58	L	701	3PE	5	0
62	q	201	CDL	22	0
70	Ac	405	U10	11	0
58	M	501	3PE	10	0
62	h	201	CDL	13	0
58	D	501	3PE	6	0
68	AC	403	UQ6	29	0
62	Y	201	CDL	5	0
62	Aa	501	CDL	1	0
58	L	702	3PE	9	0
59	E	301	FES	4	0
67	AC	402	HEM	30	0
69	AD	401	HEC	13	0
58	J	201	3PE	1	0
67	AC	401	HEM	1	0
62	L	703	CDL	12	0
56	B	302	UQ1	3	0
66	n	201	EHZ	1	0
59	G	803	FES	5	0
66	W	201	EHZ	4	0
57	B	303	PC1	6	0
62	M	503	CDL	12	0
58	L	705	3PE	4	0
62	d	201	CDL	8	0

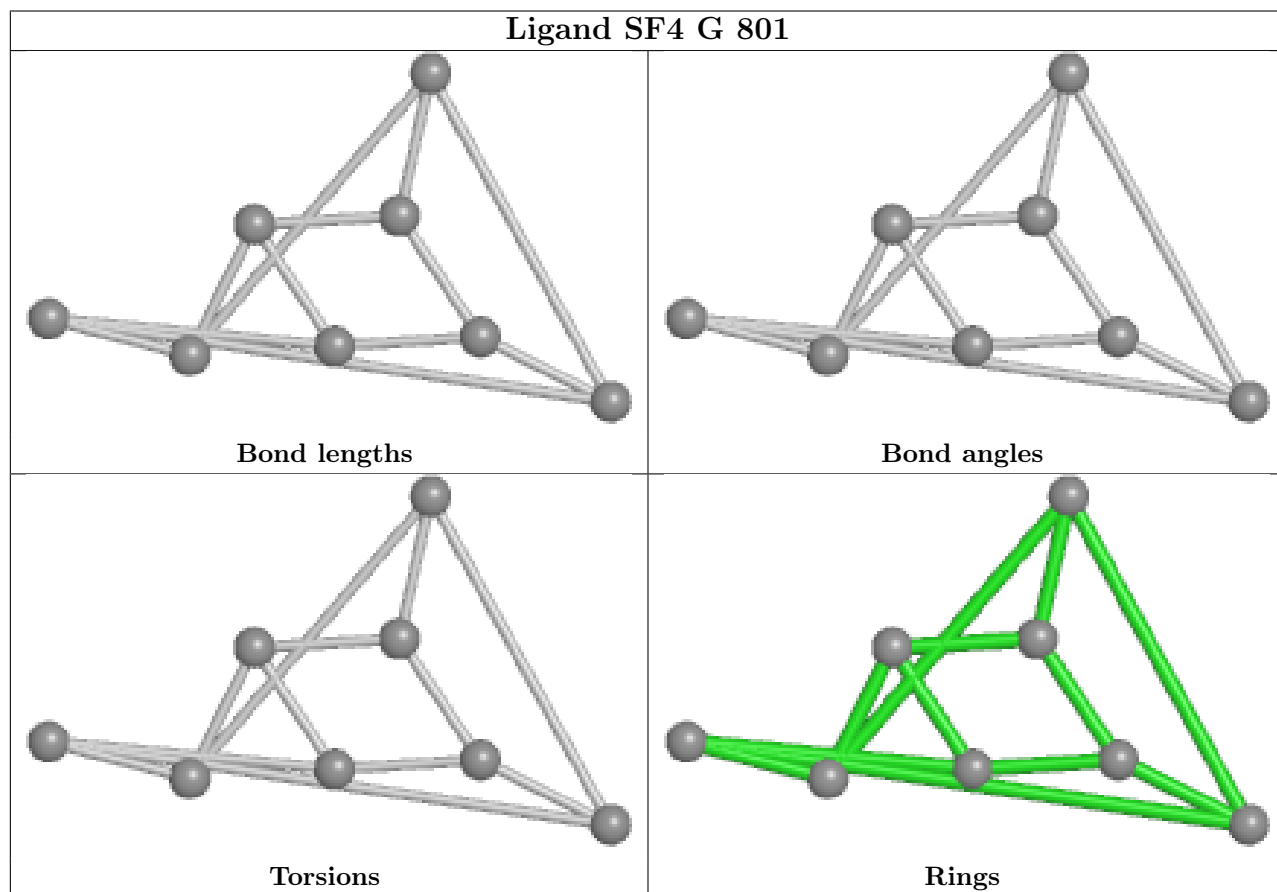
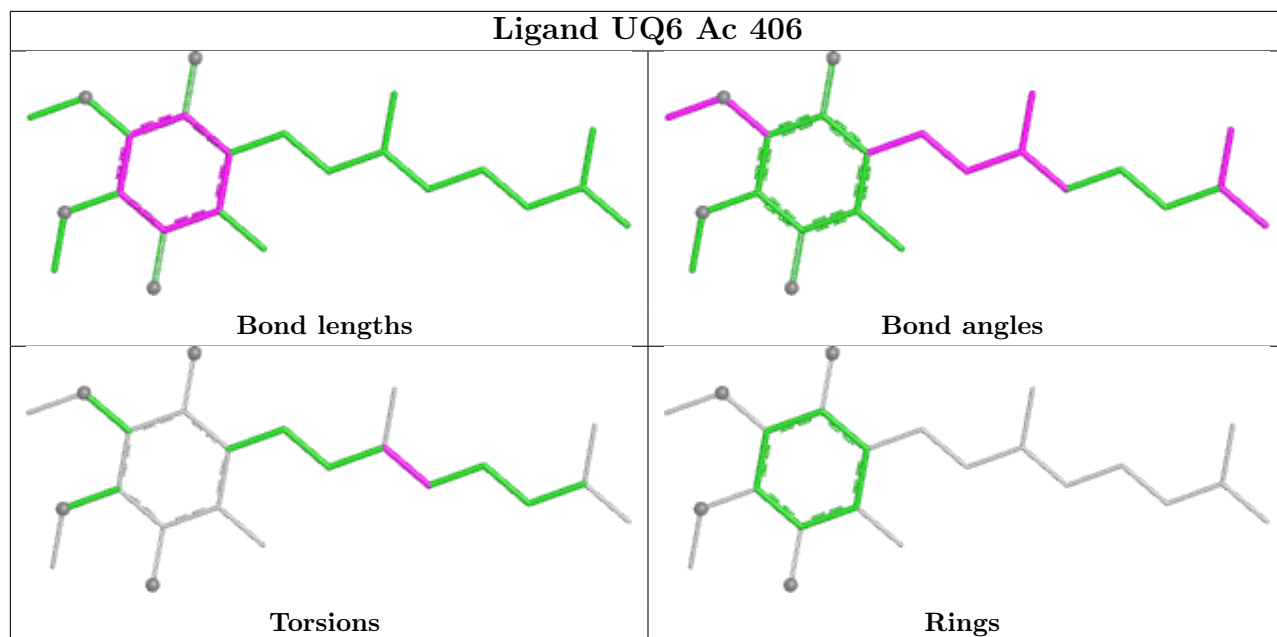
*Continued on next page...*

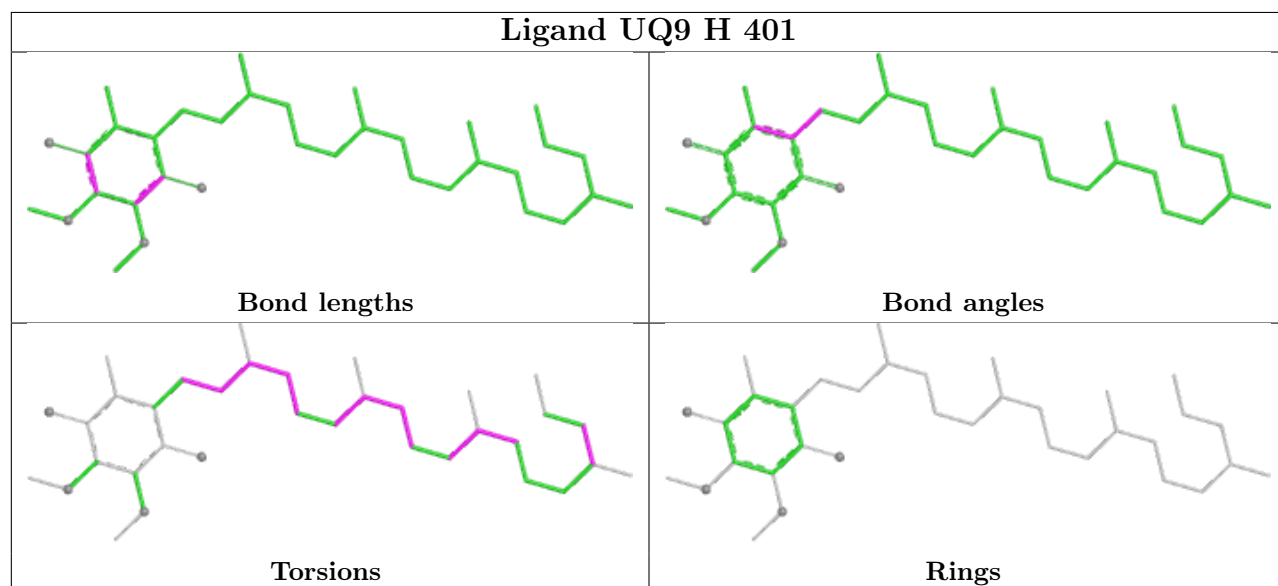
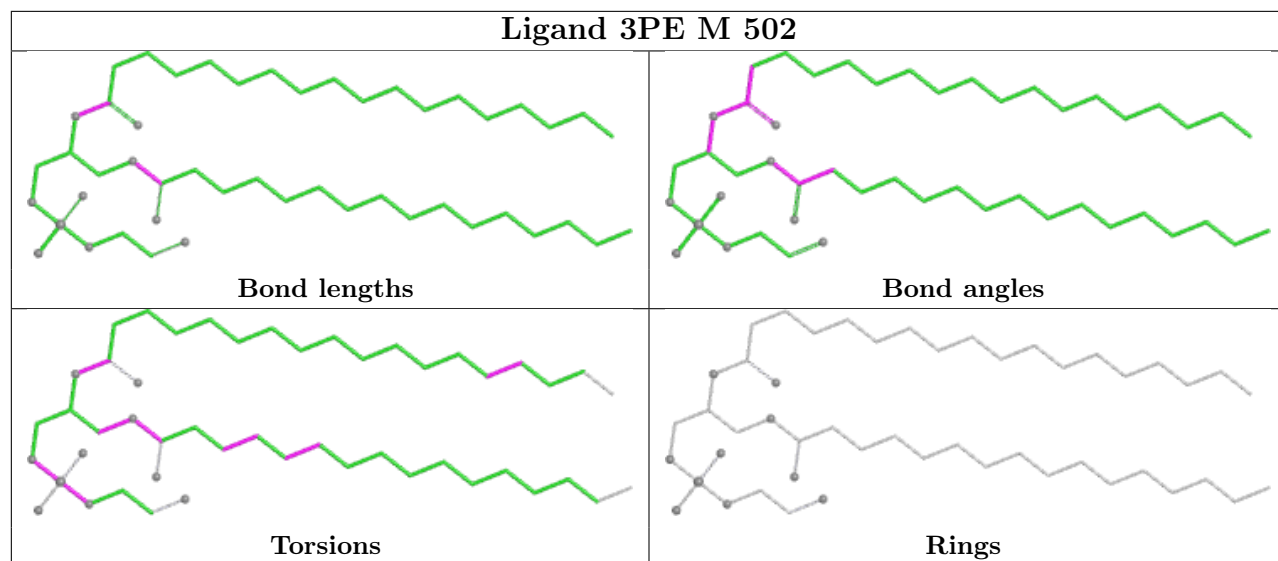
*Continued from previous page...*

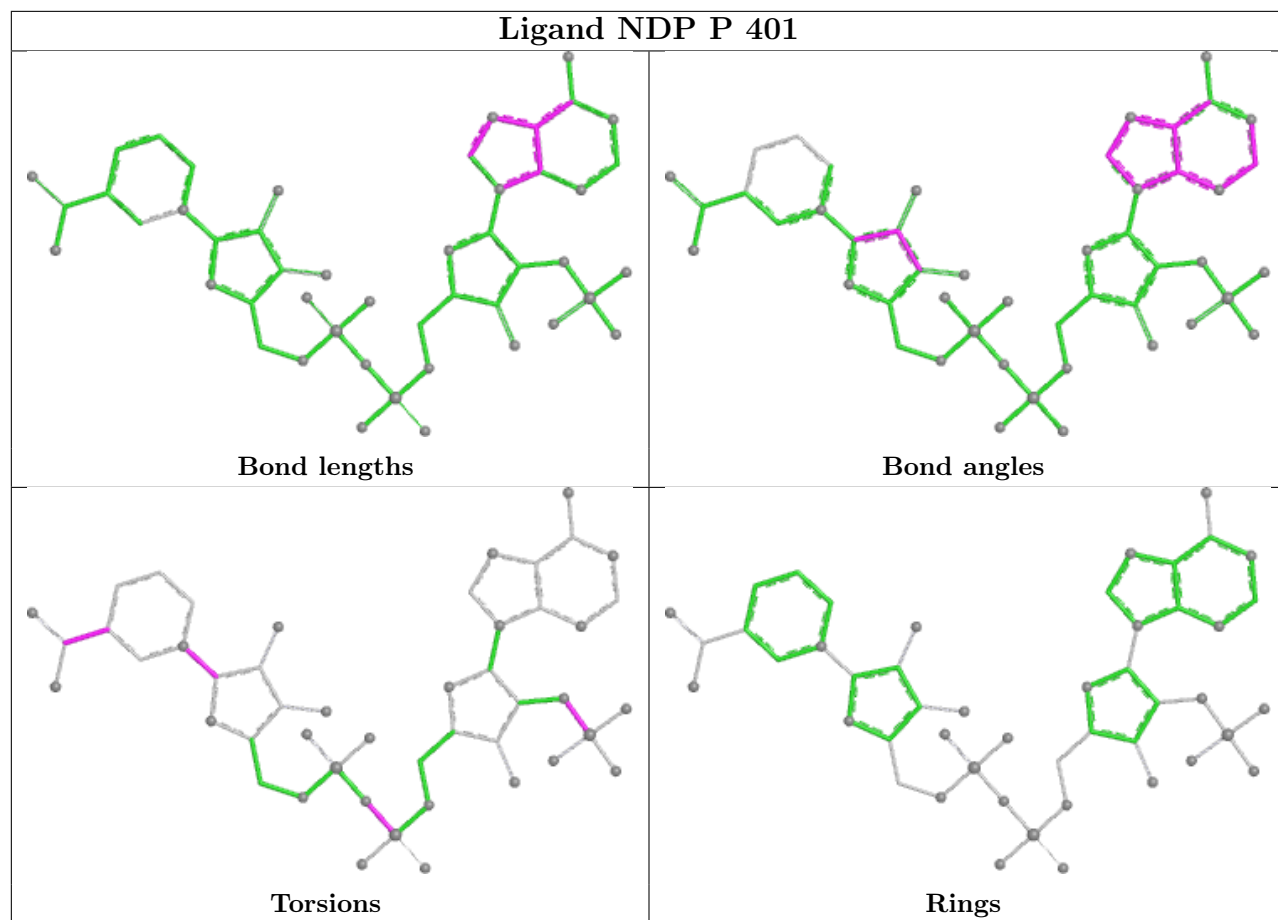
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	Ag	102	CDL	3	0
58	Ac	401	3PE	2	0
69	Ad	401	HEC	12	0
58	i	201	3PE	11	0
57	I	301	PC1	8	0
64	O	401	ADP	3	0
67	Ac	403	HEM	8	0
58	H	403	3PE	11	0
58	m	201	3PE	9	0
55	G	802	SF4	2	0
55	I	303	SF4	5	0

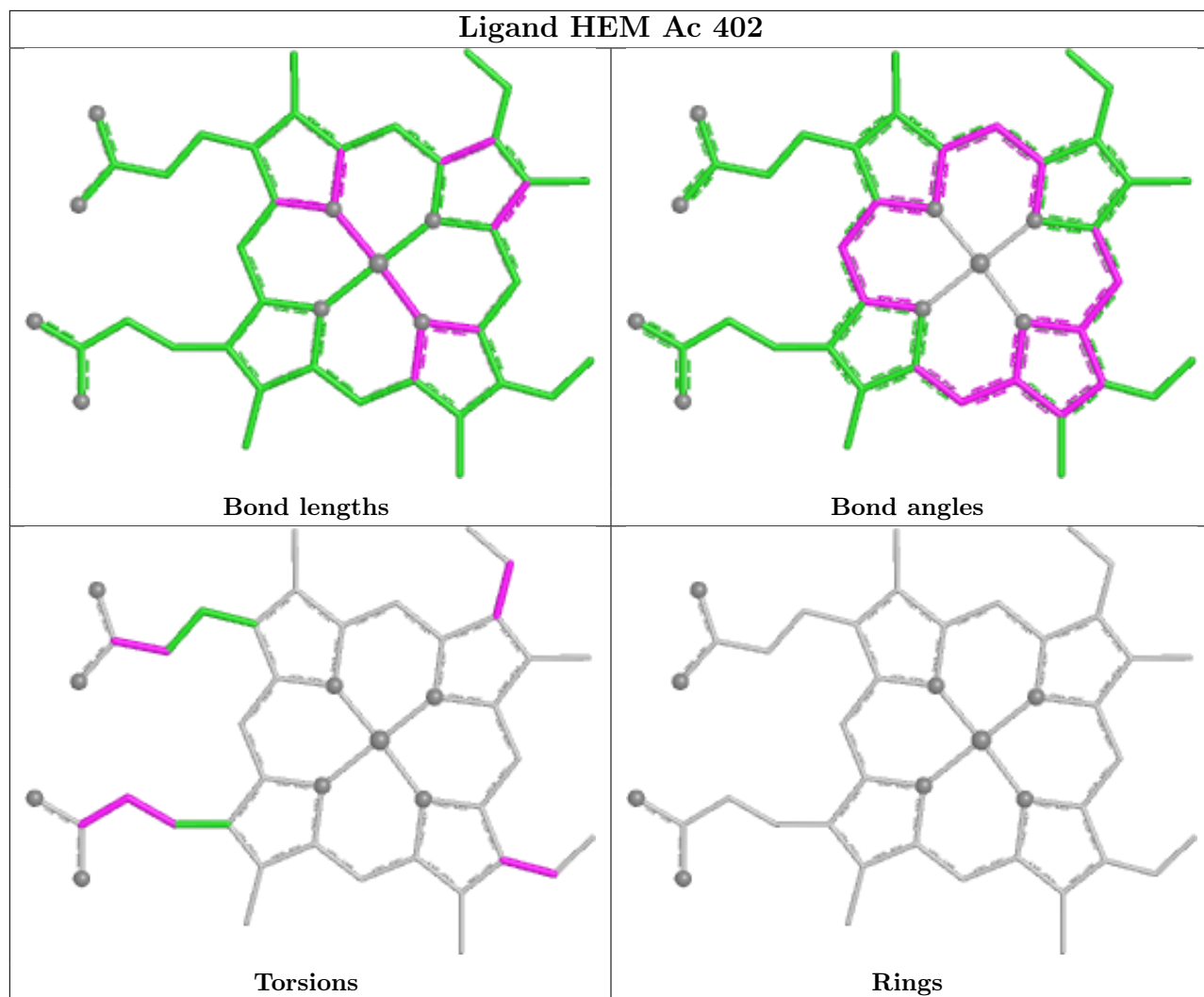
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

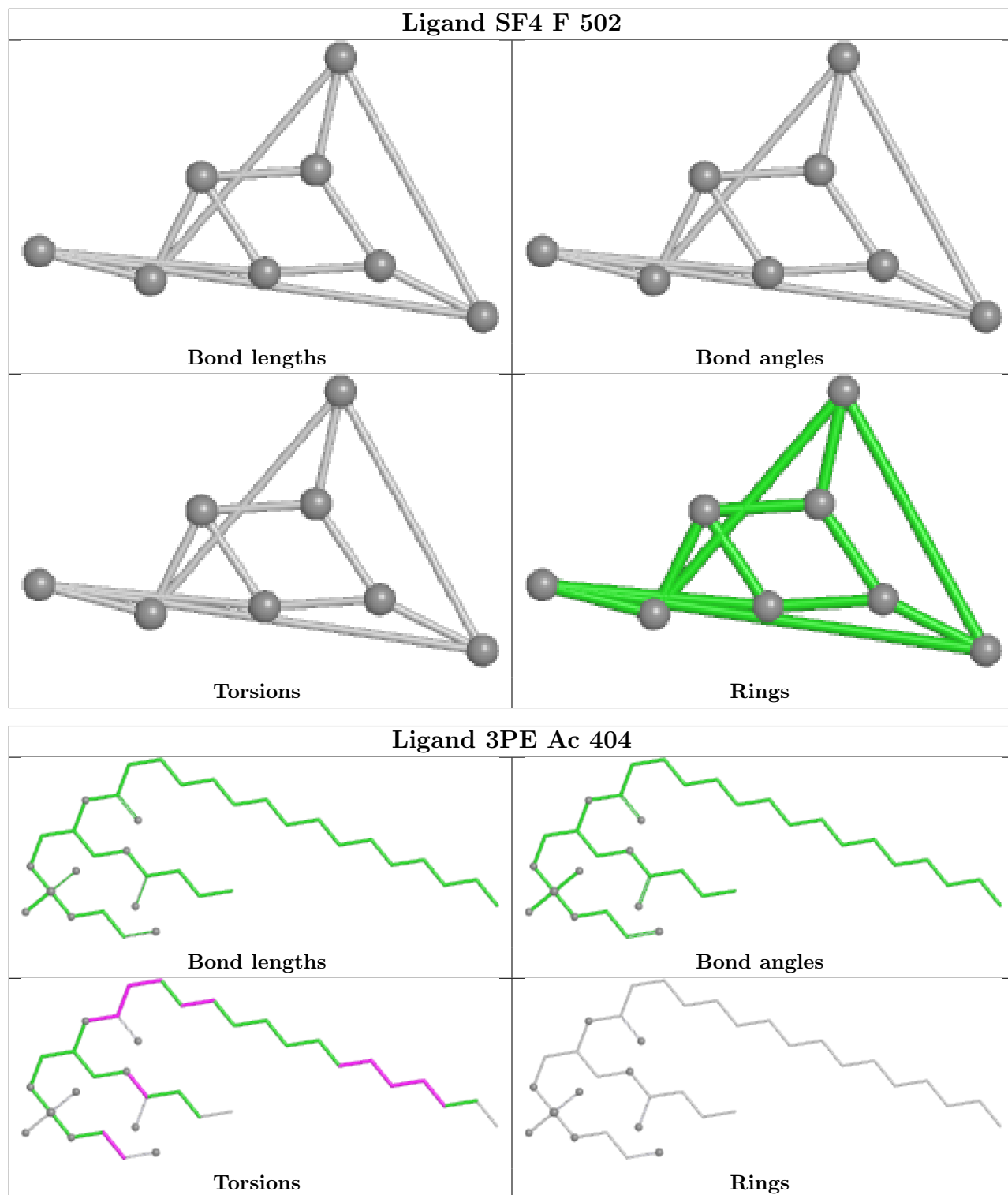


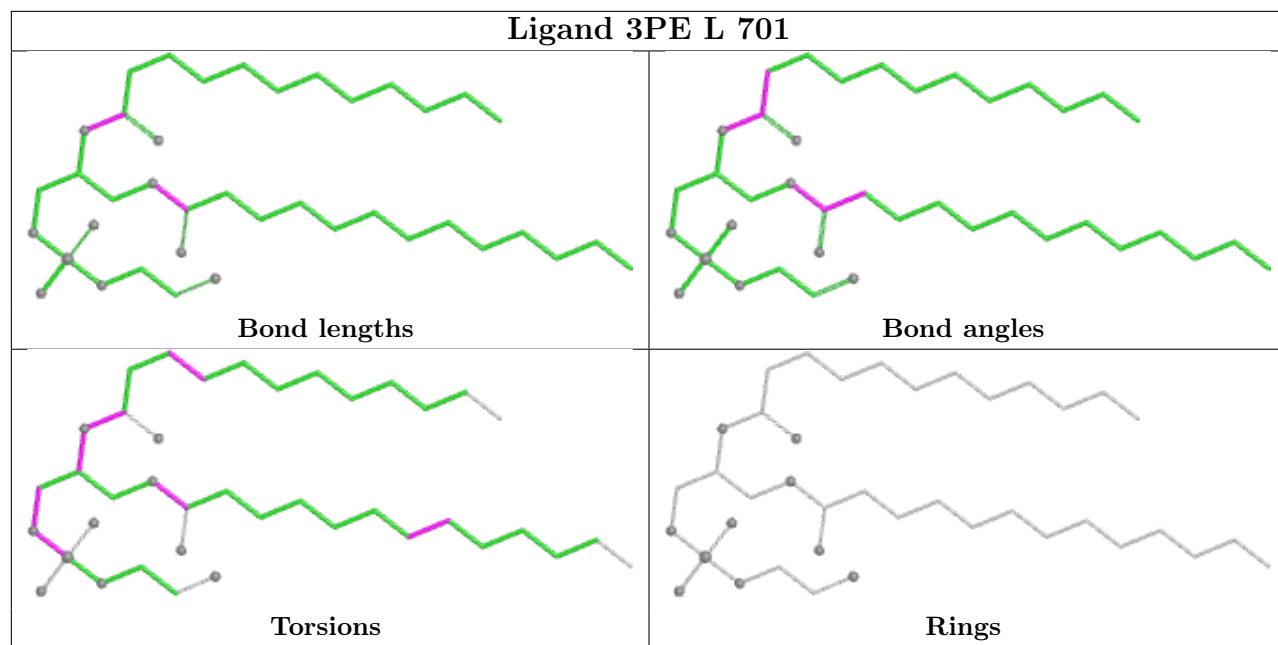


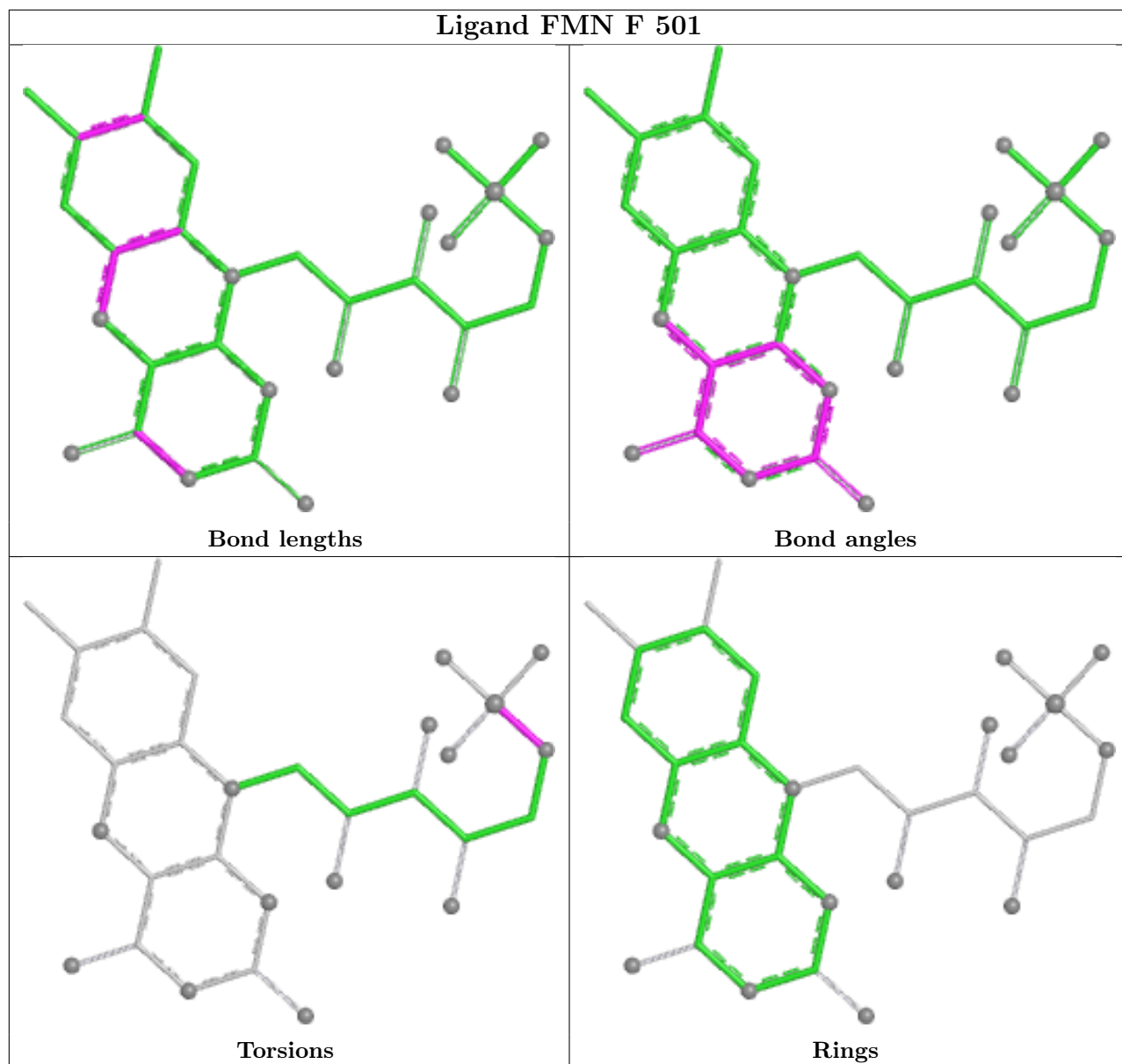


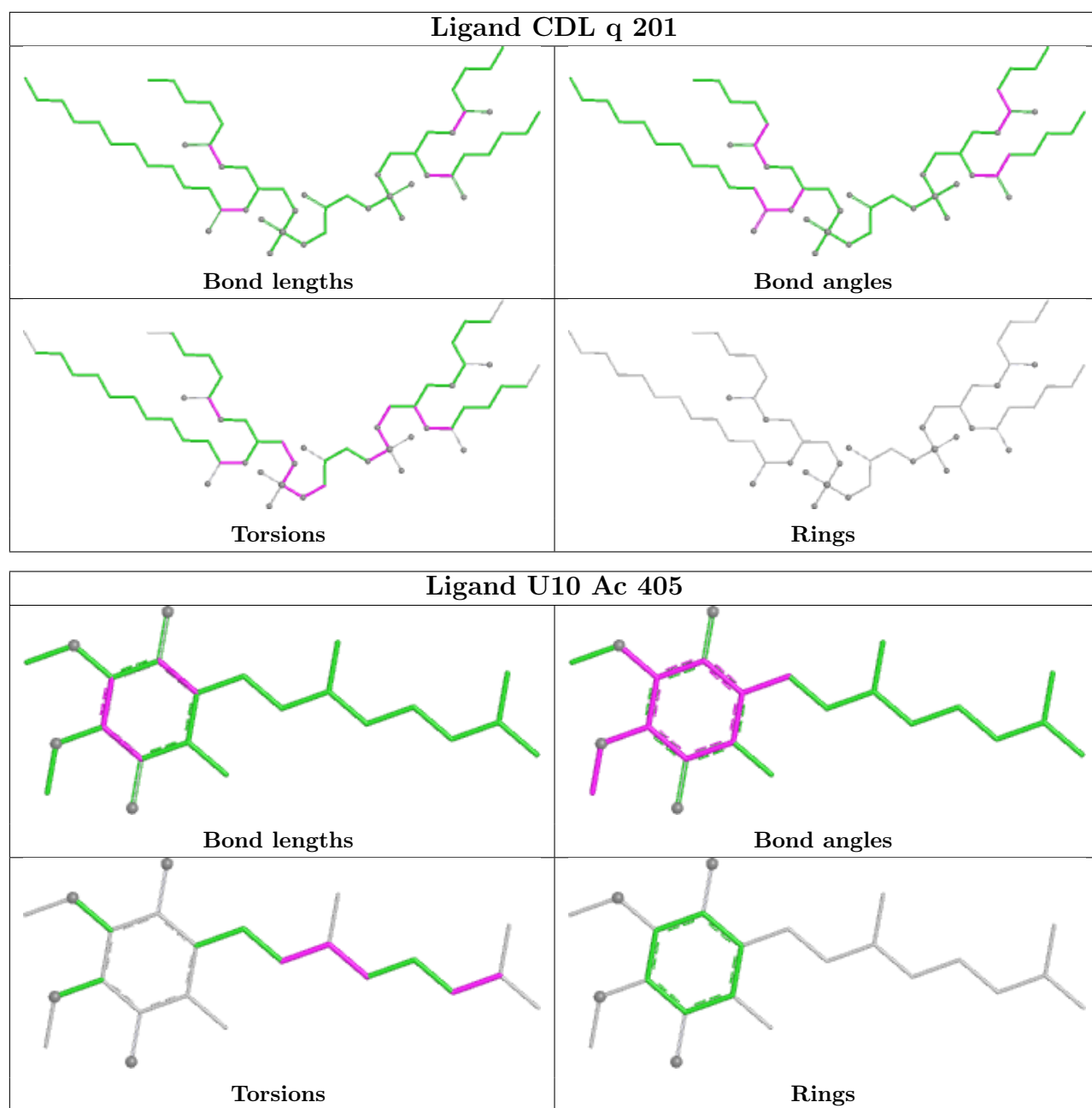


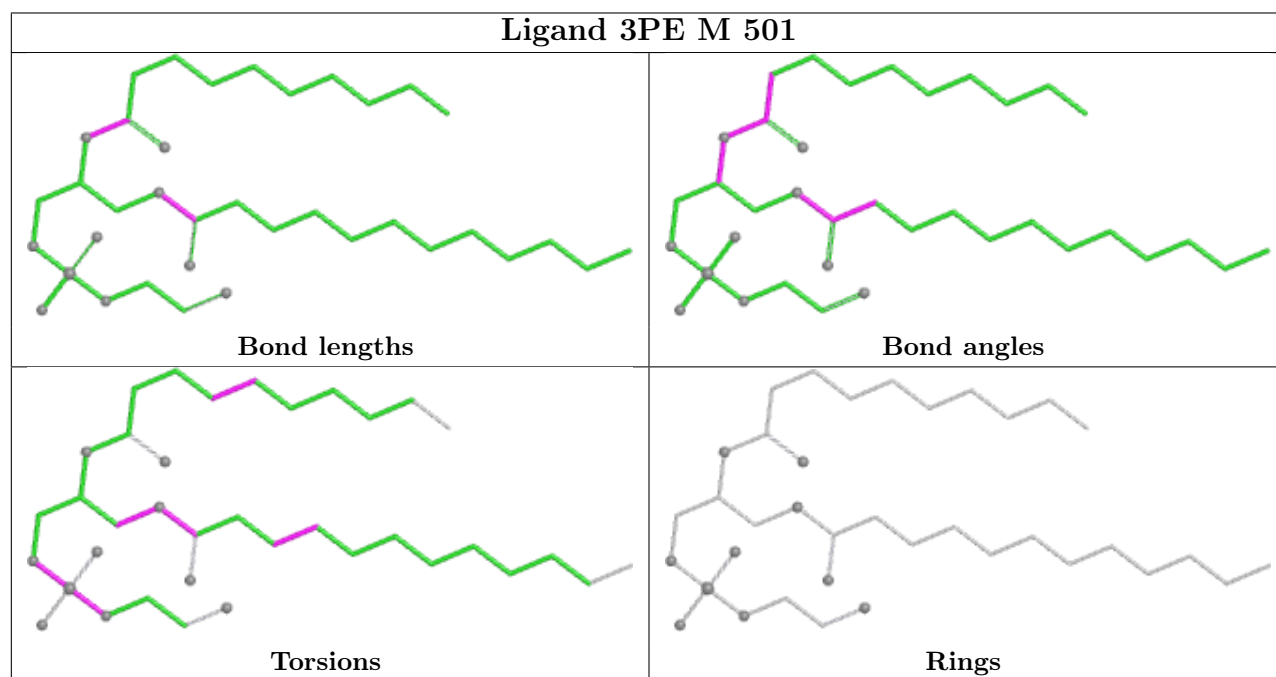
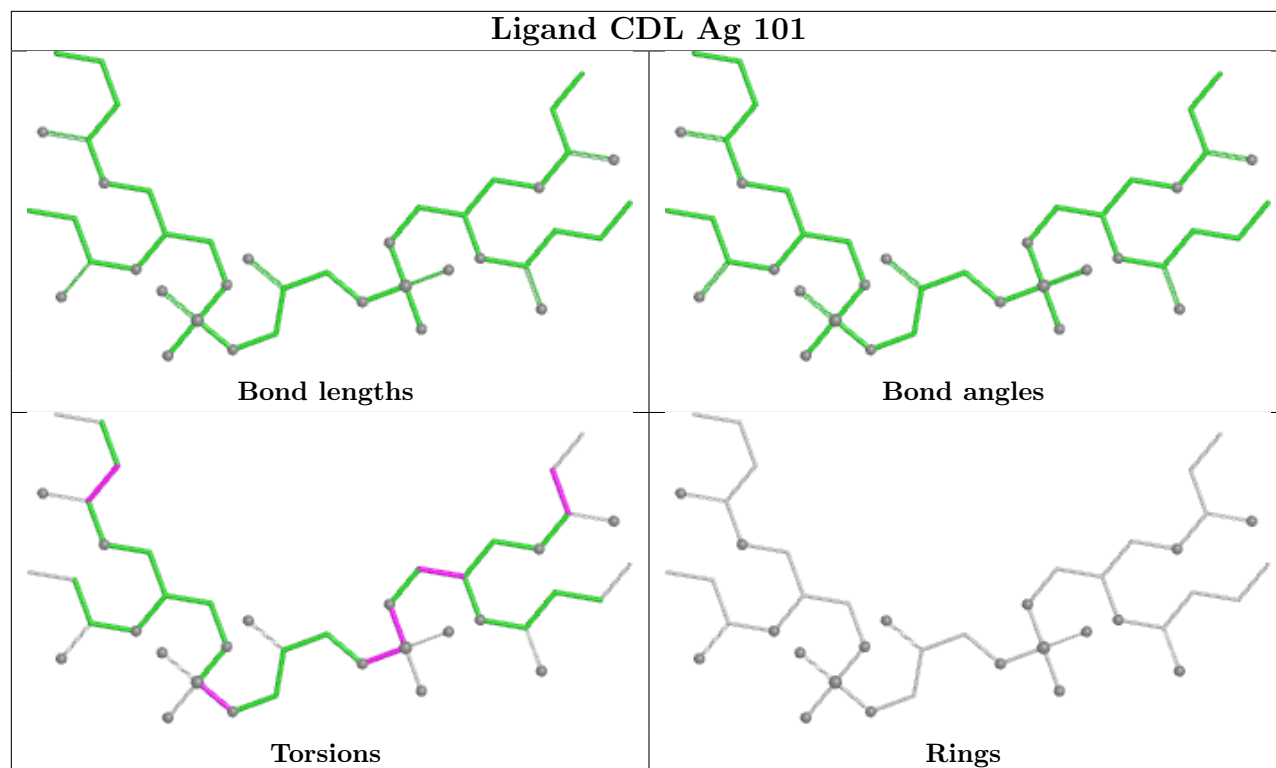


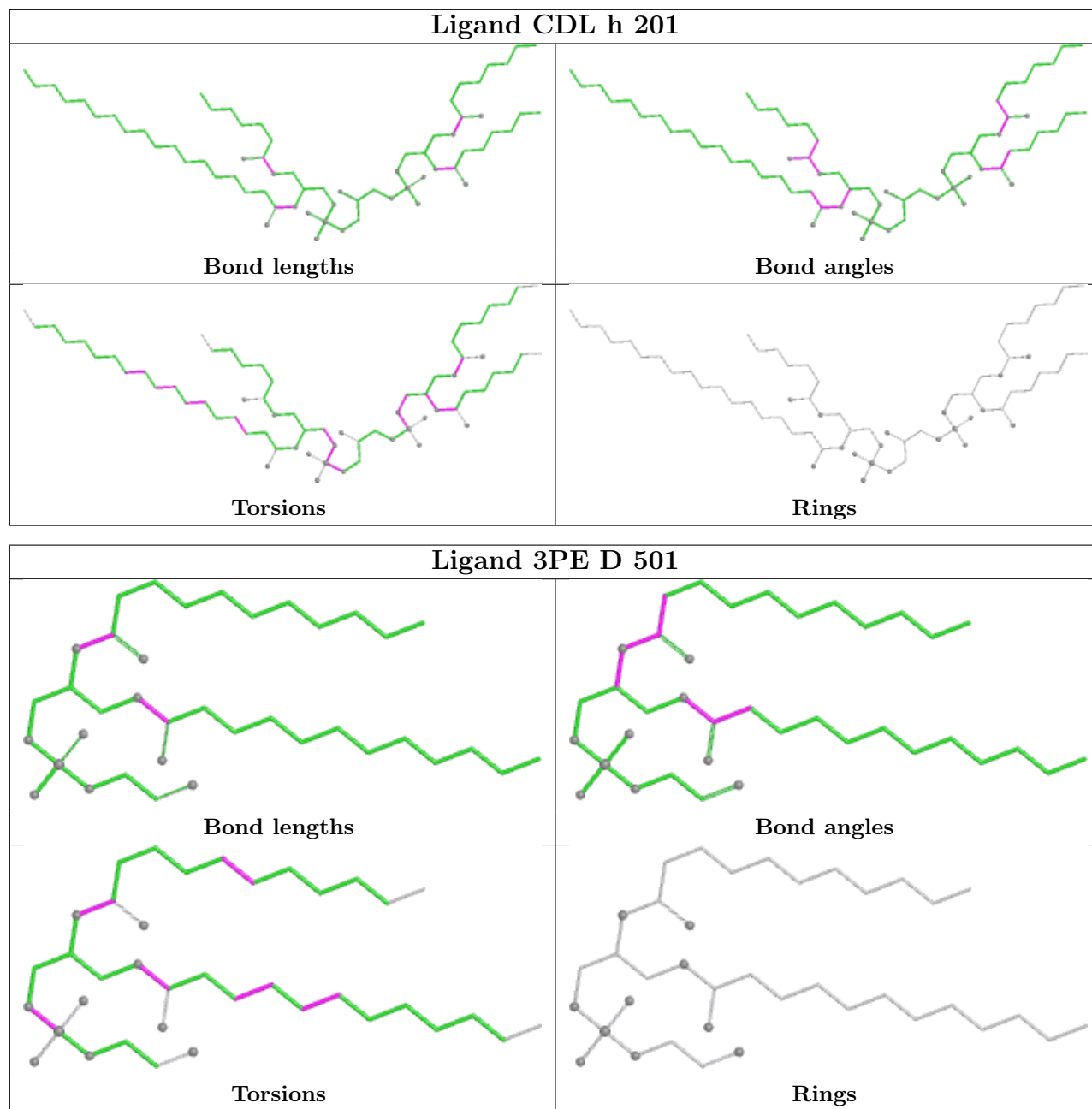


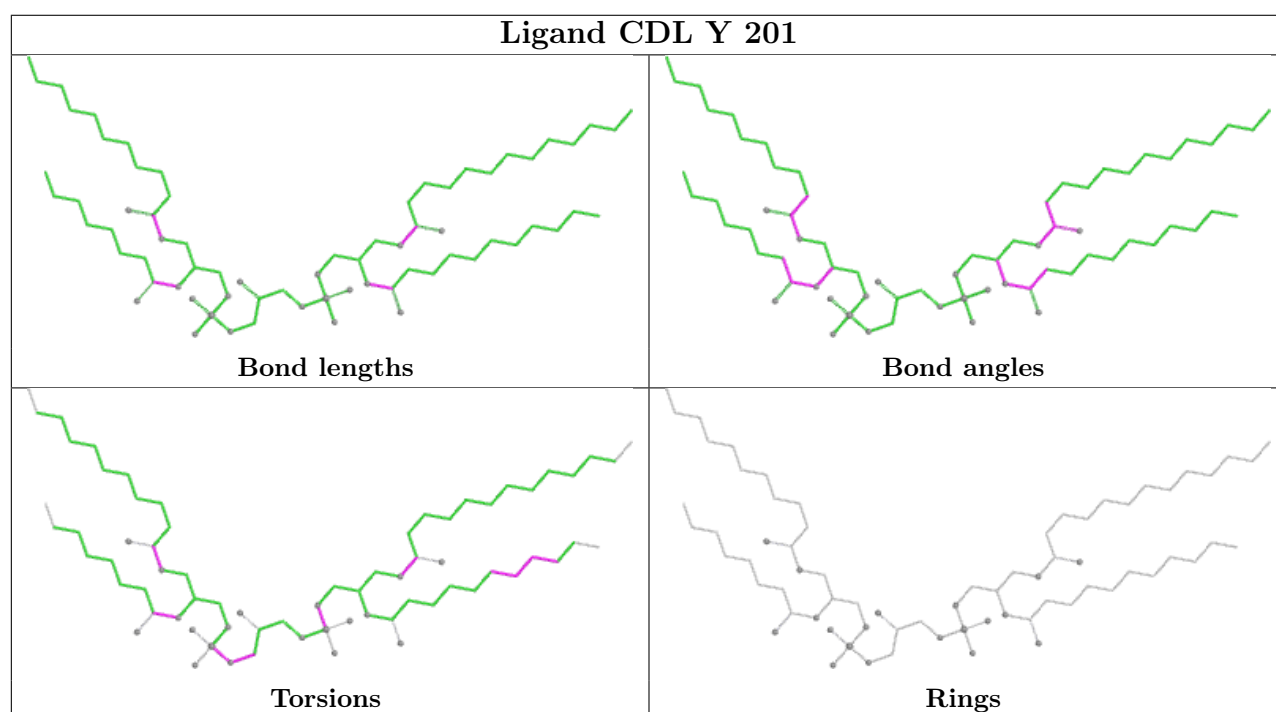
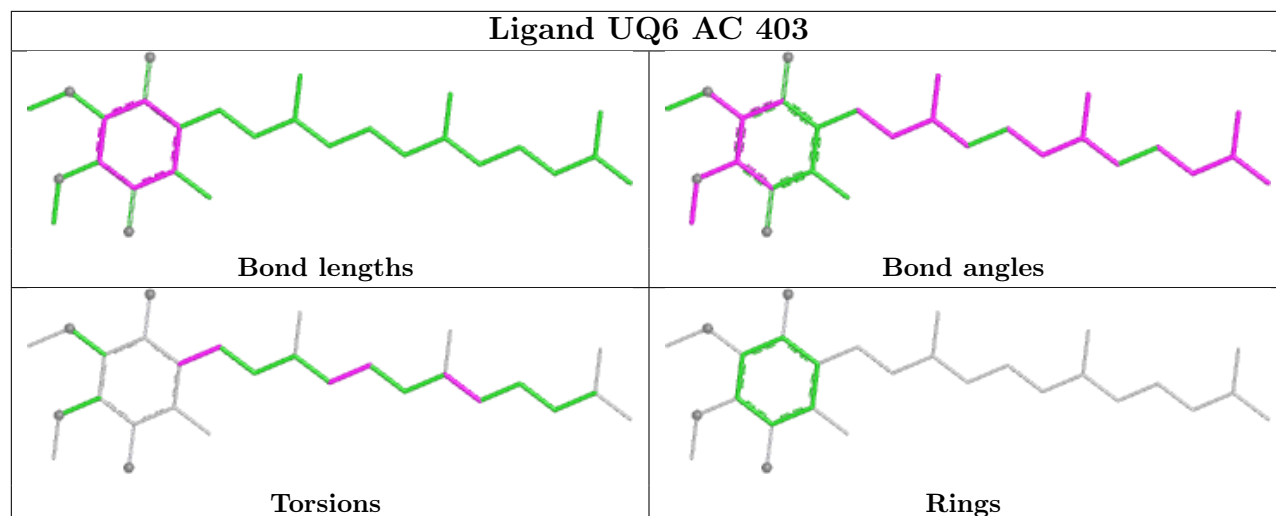


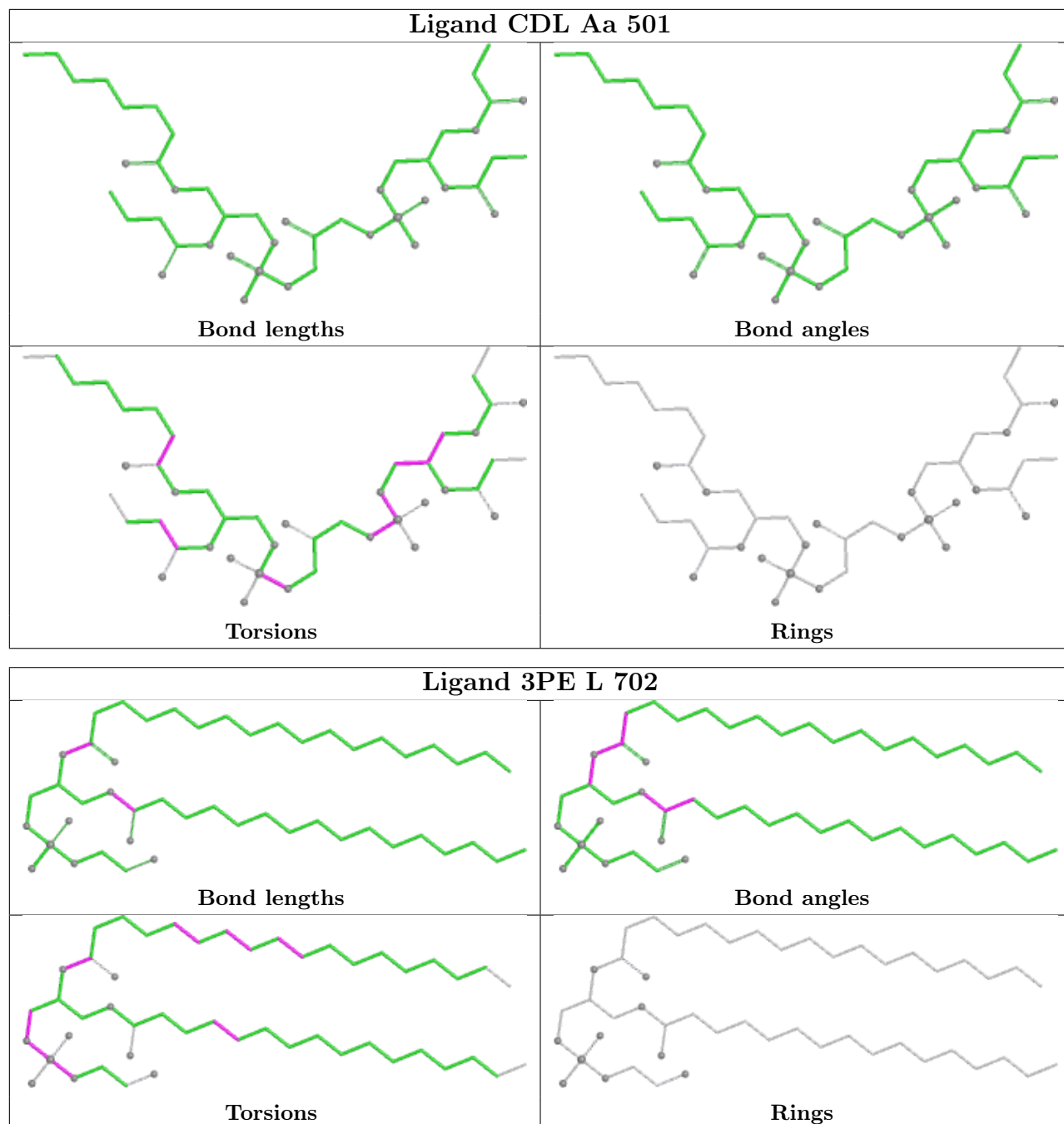


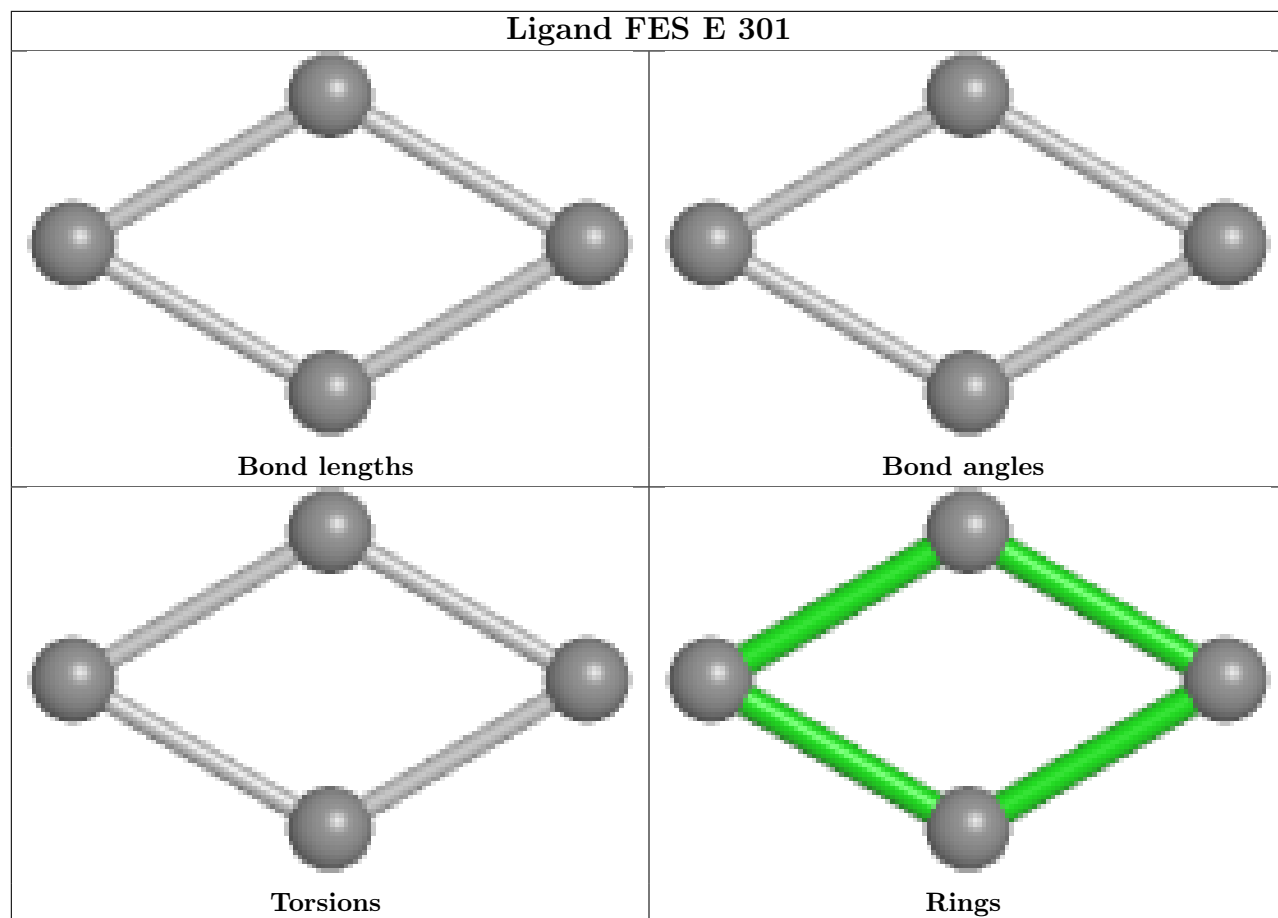


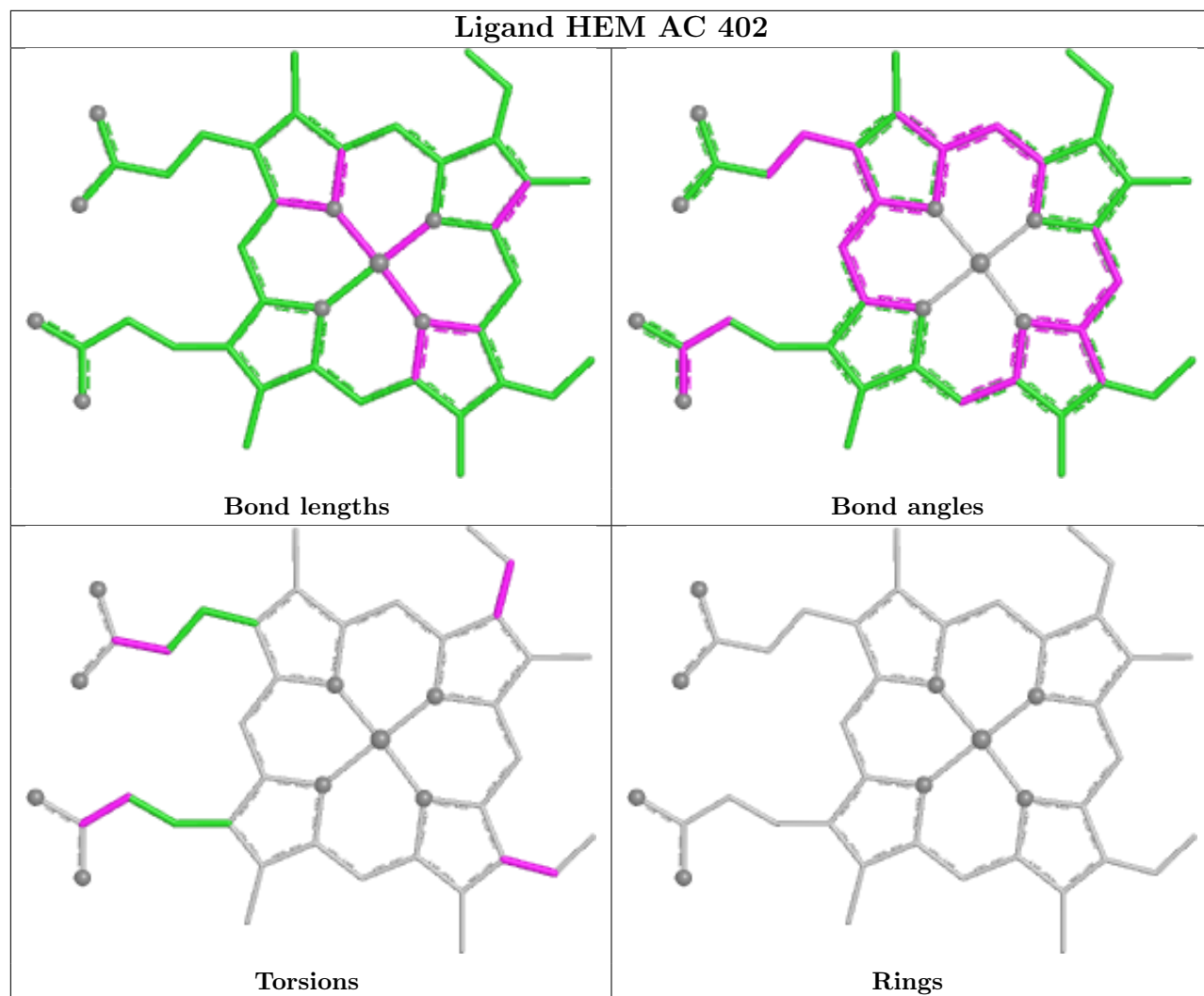


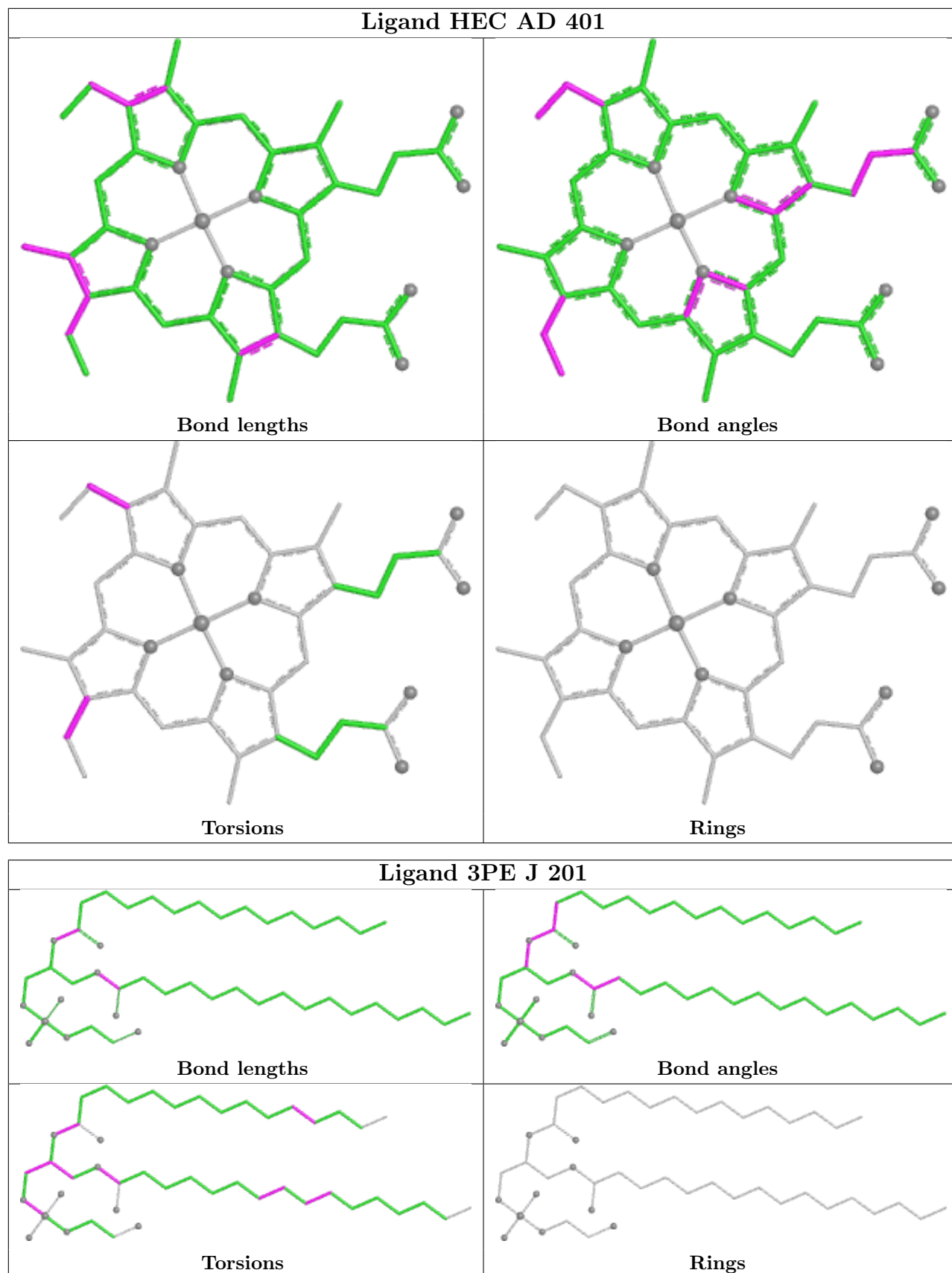


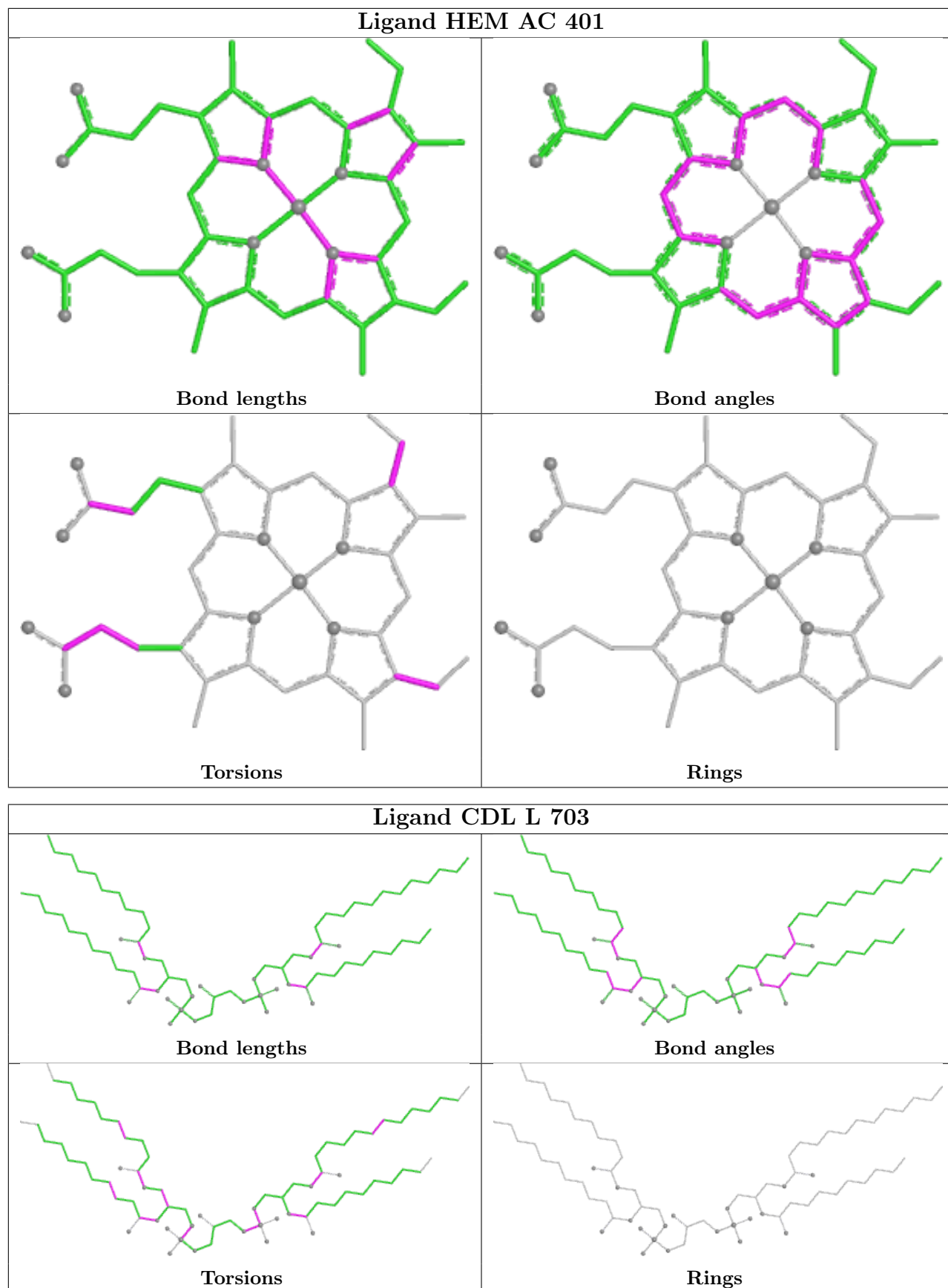


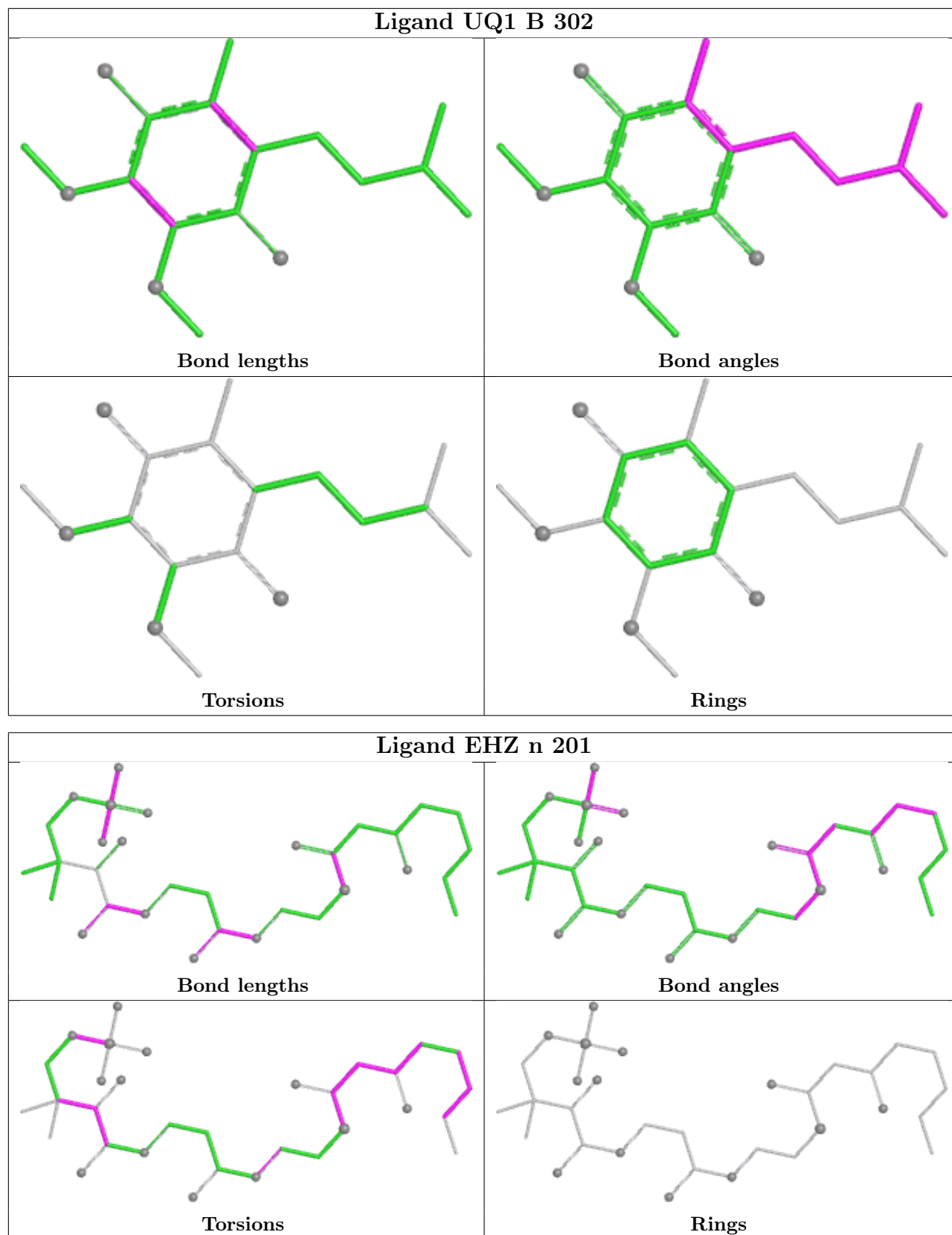


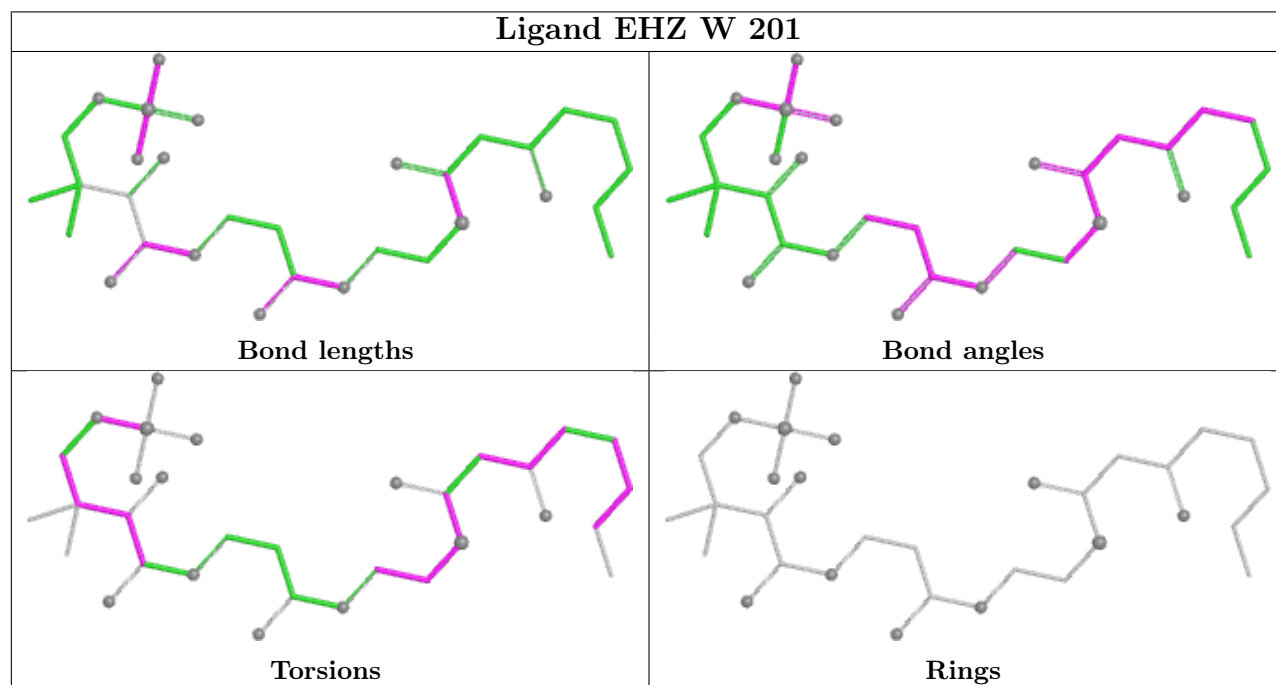
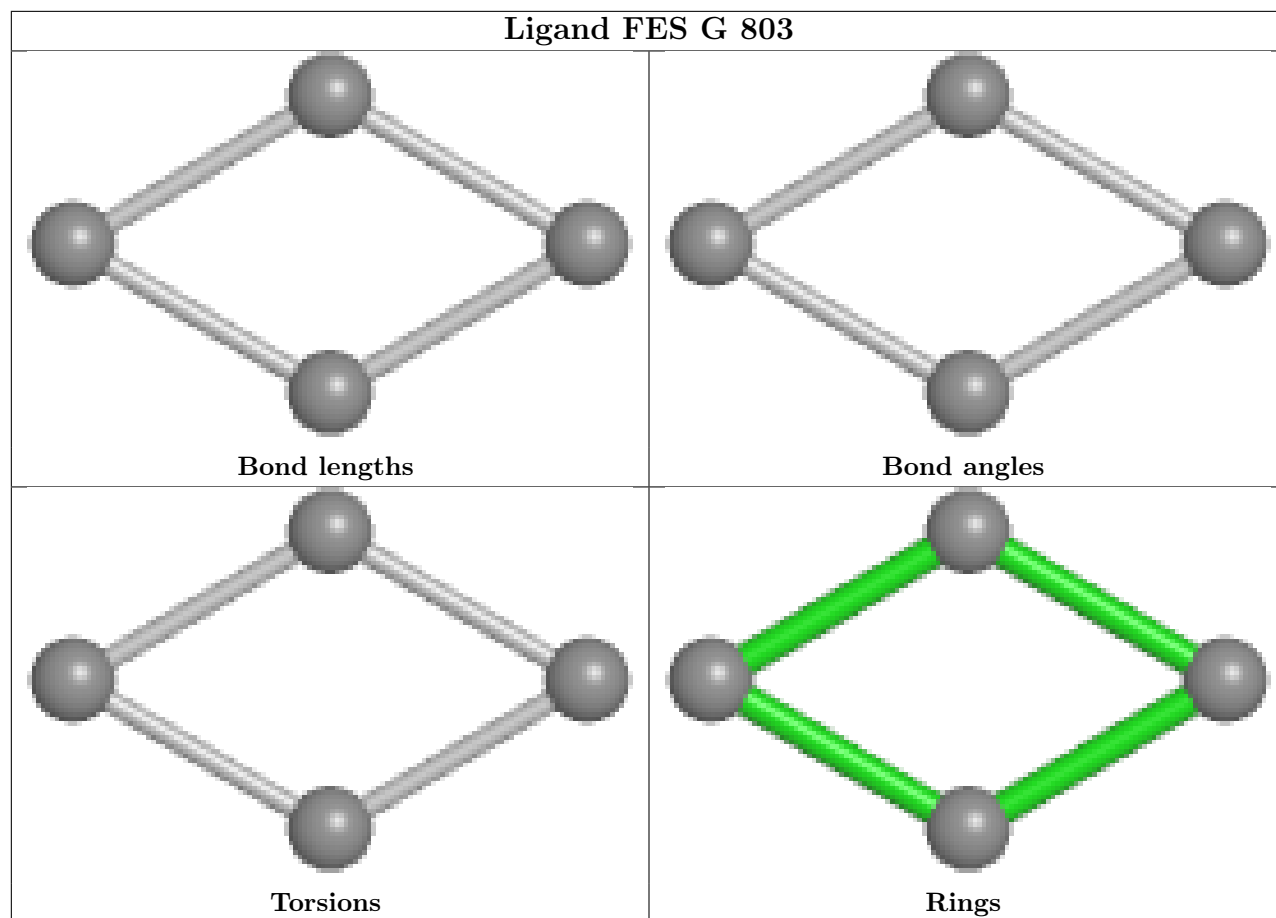


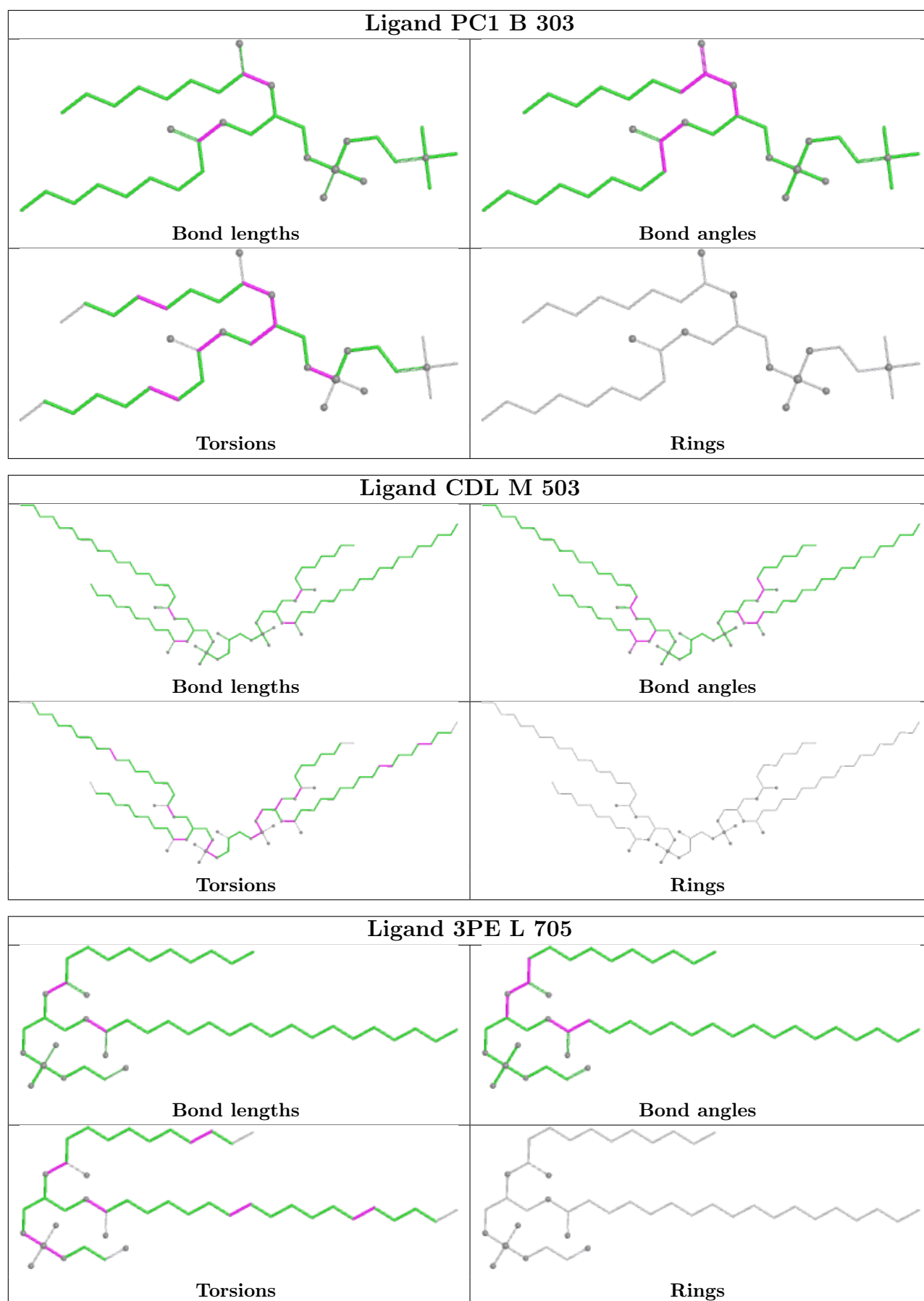


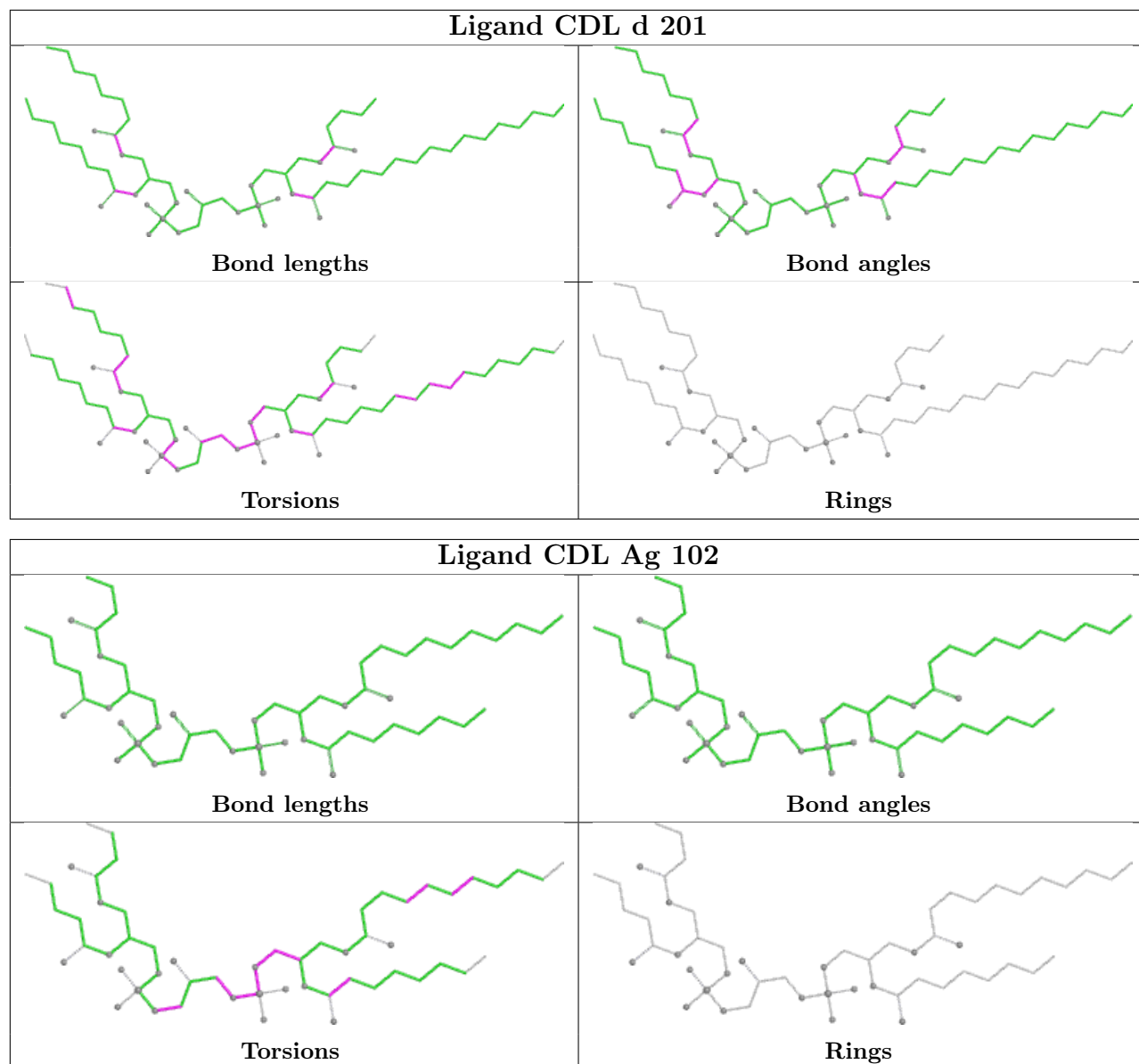


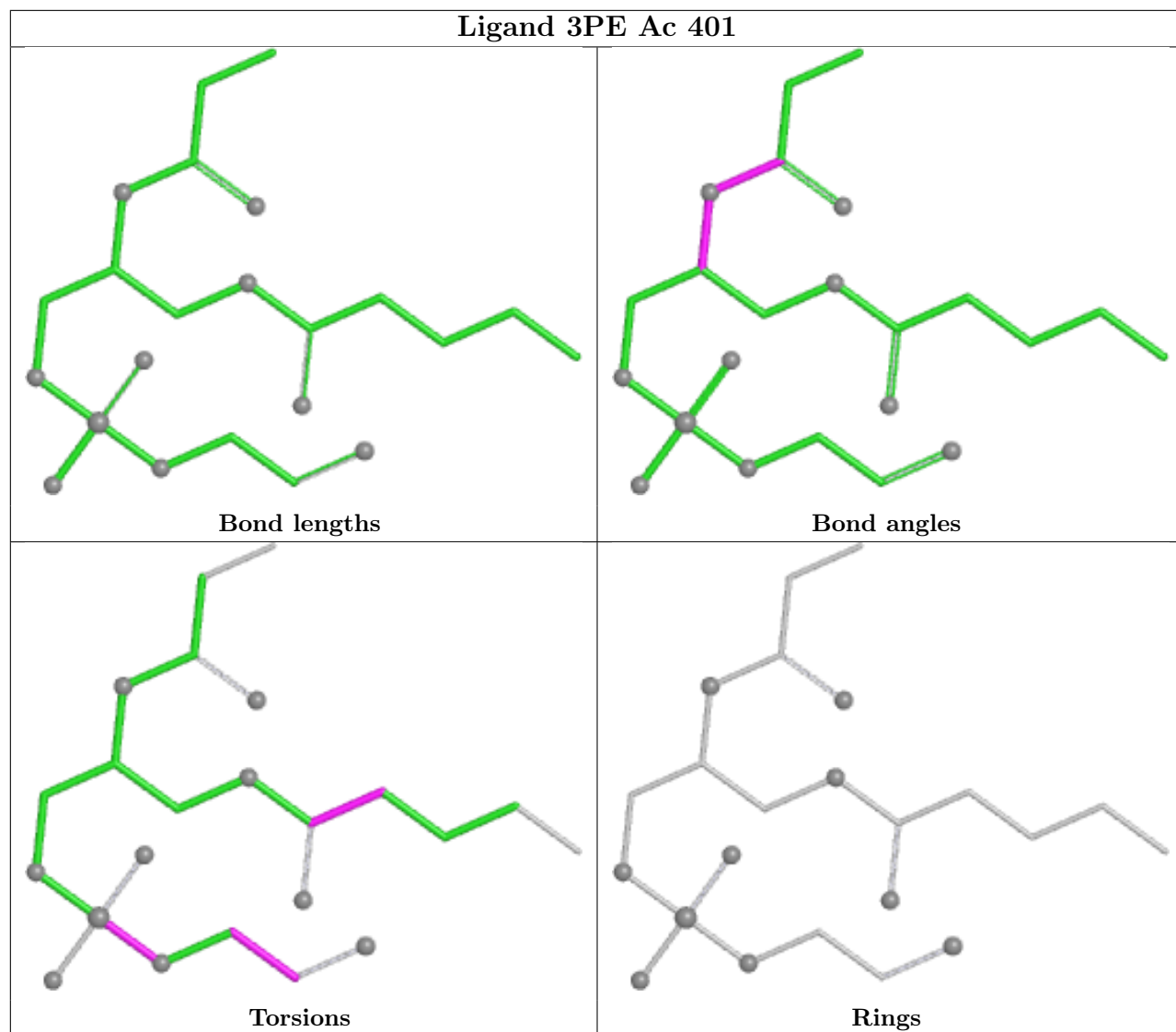


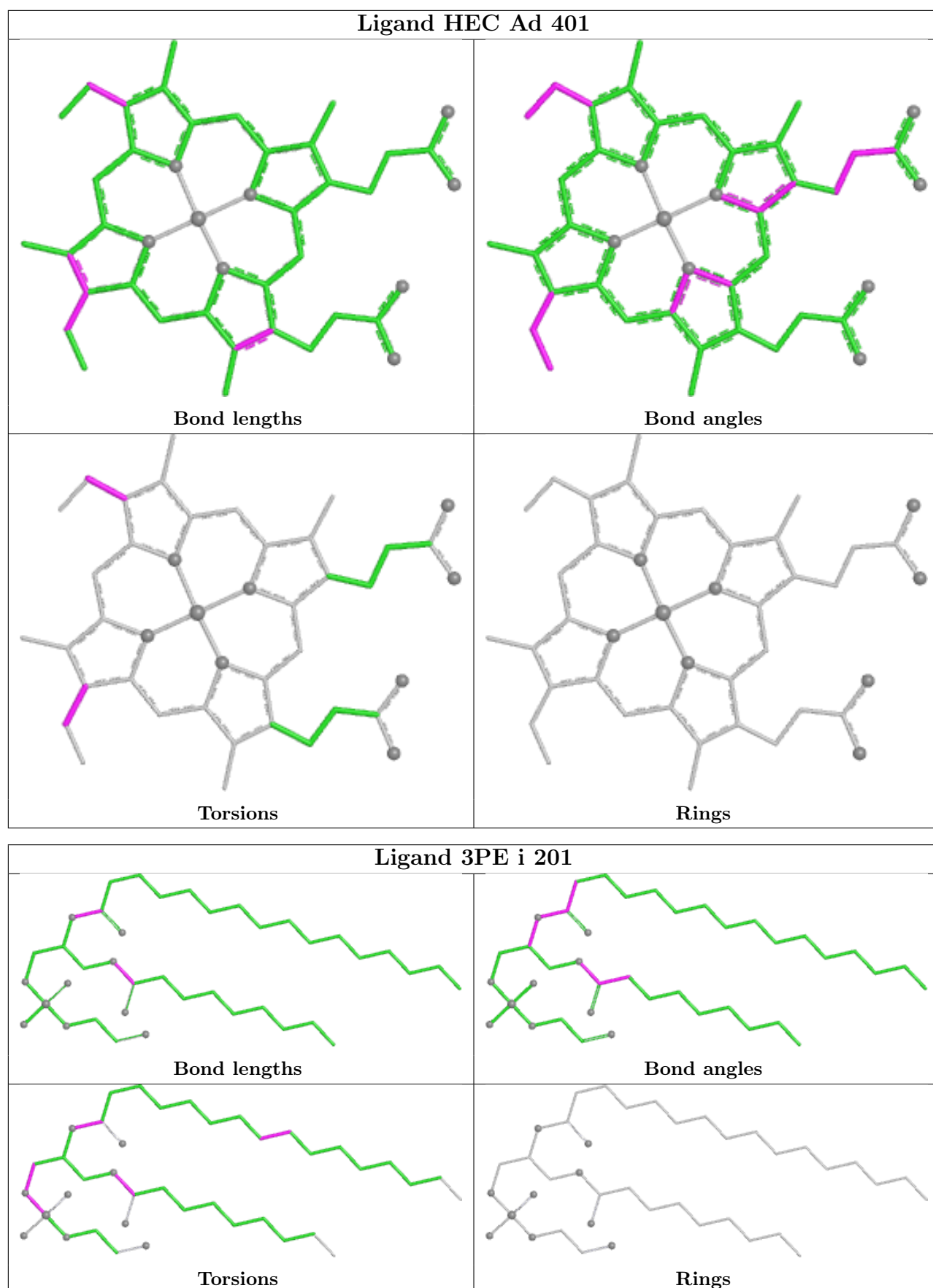


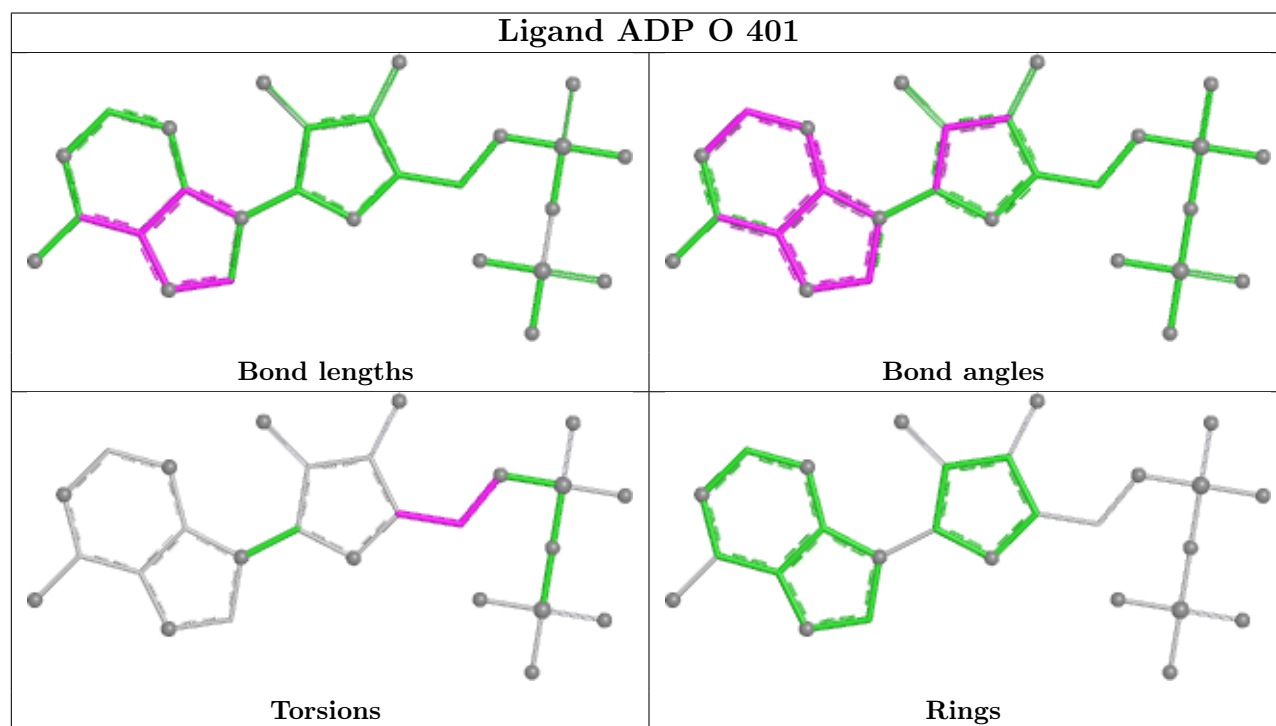
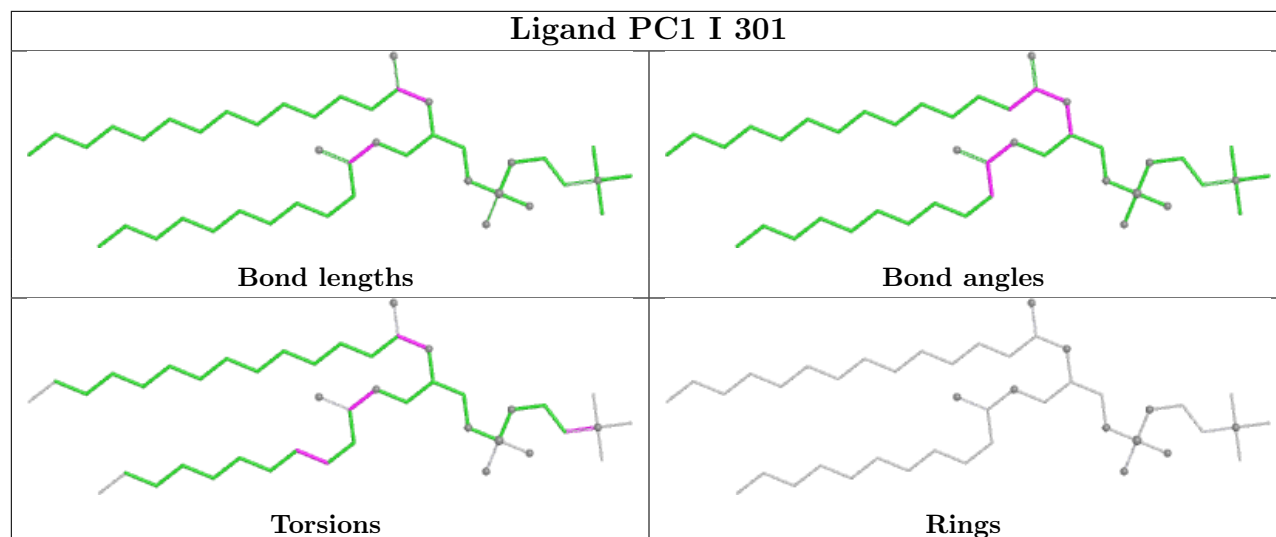


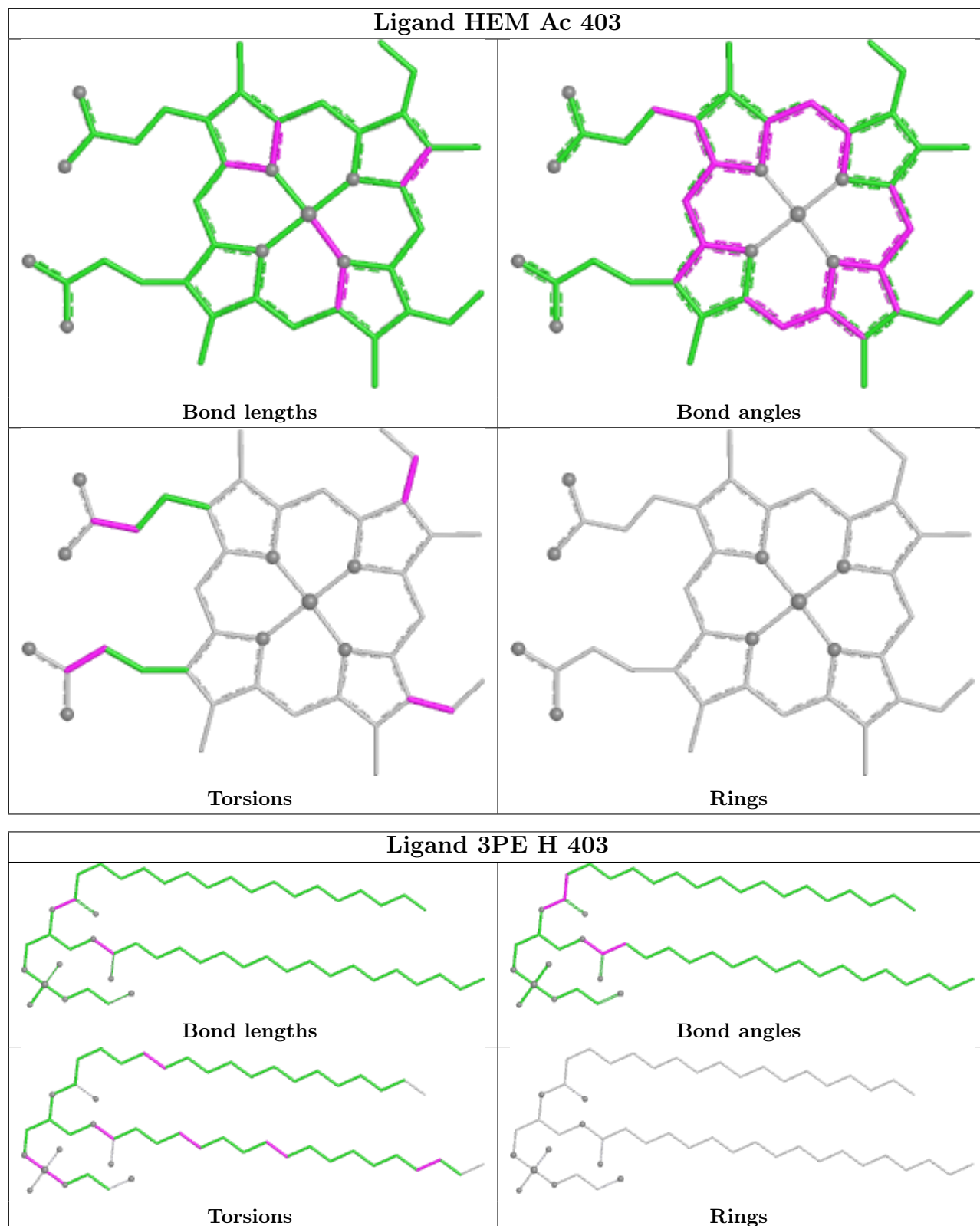


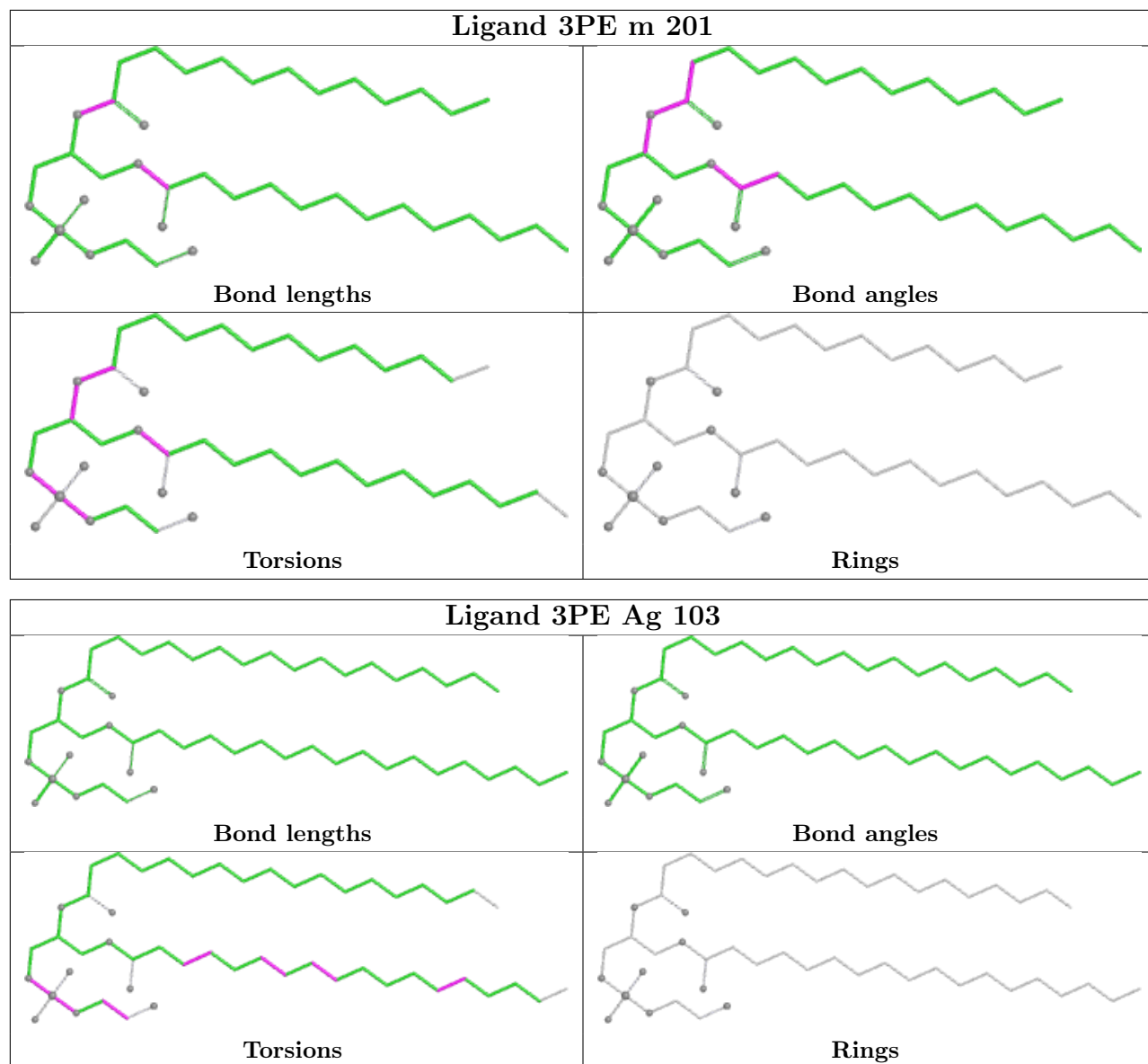


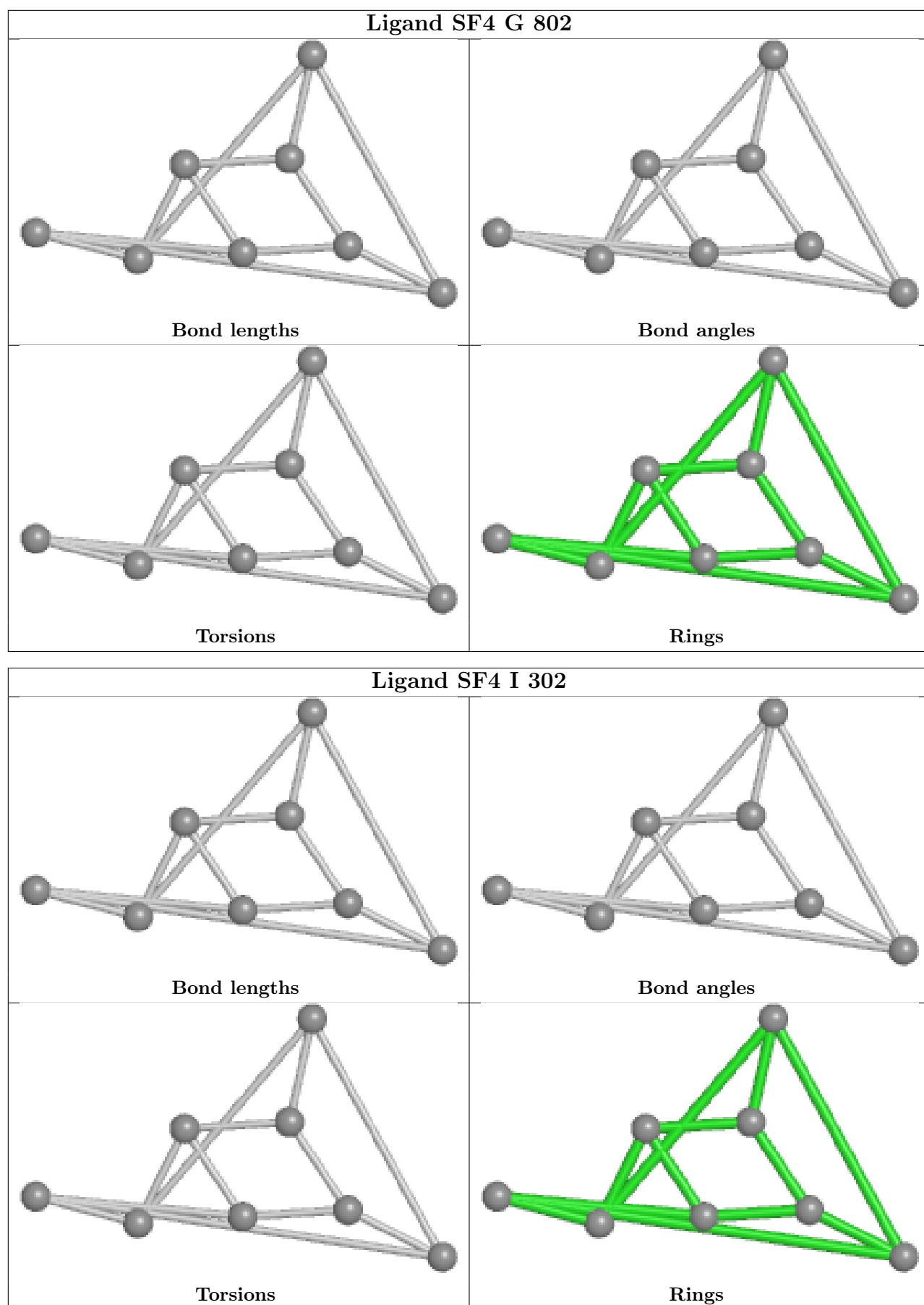


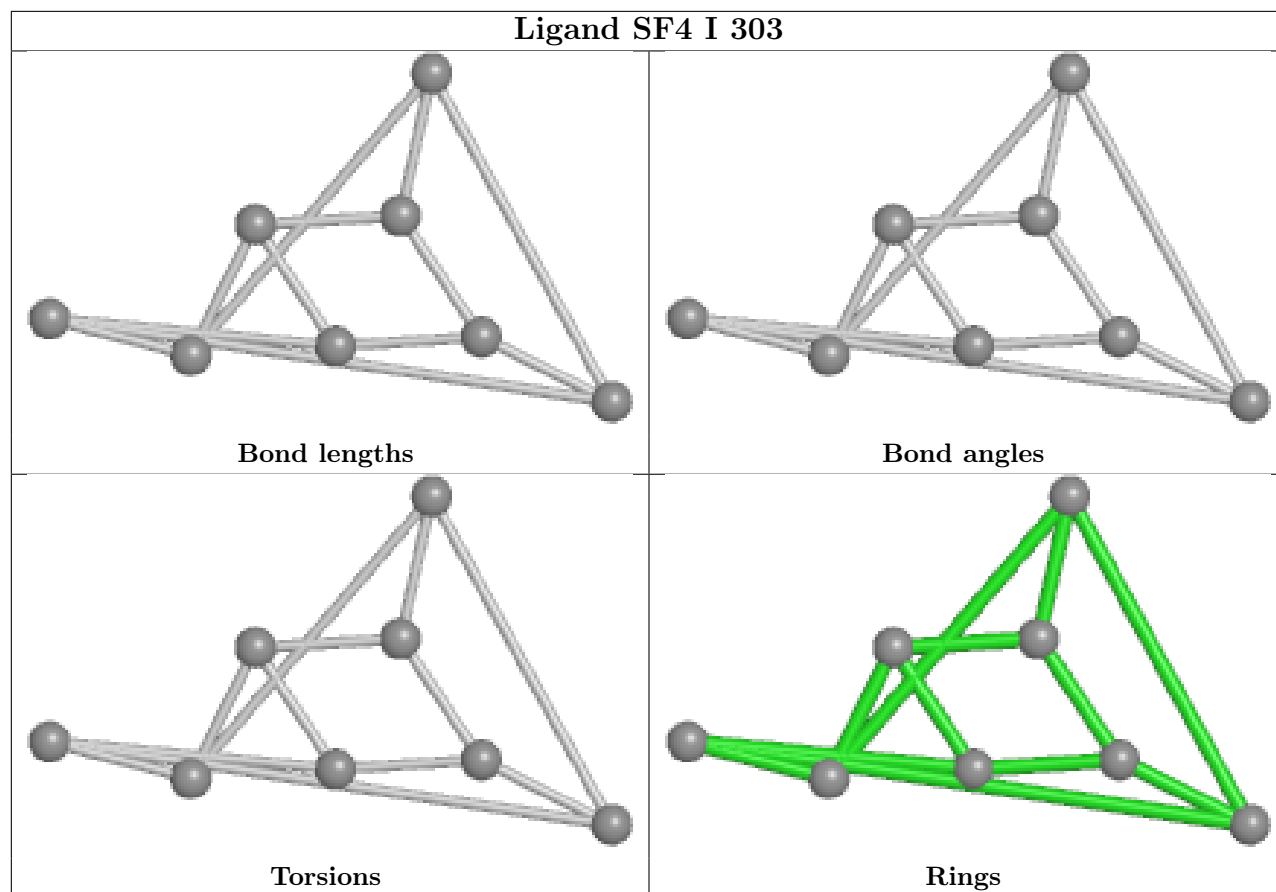












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

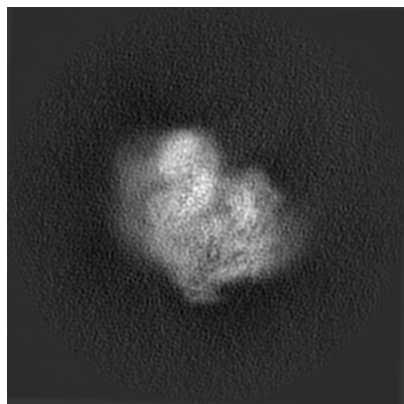
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35352. These allow visual inspection of the internal detail of the map and identification of artifacts.

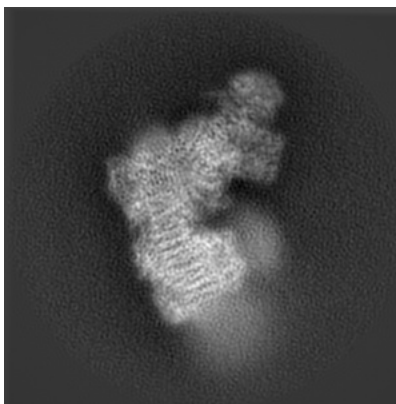
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

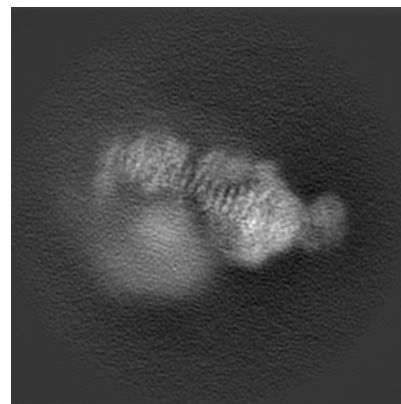
#### 6.1.1 Primary map



X

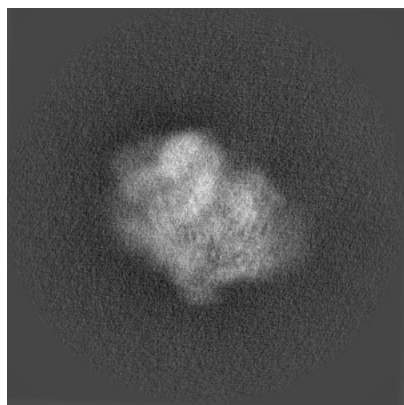


Y

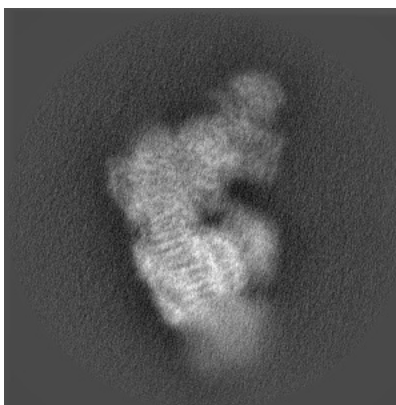


Z

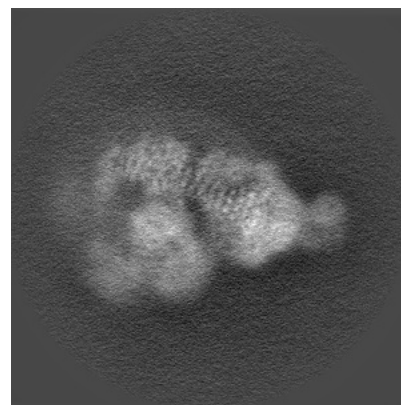
#### 6.1.2 Raw map



X



Y

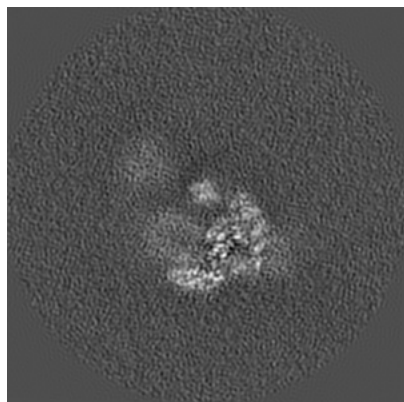


Z

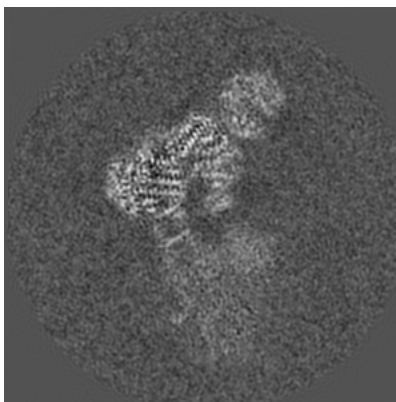
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

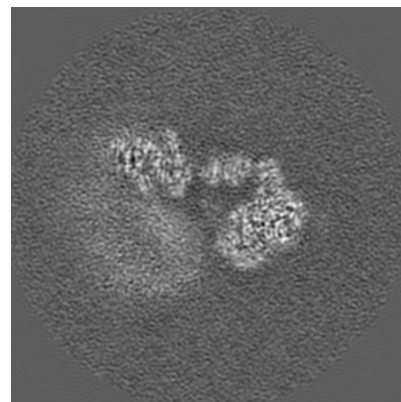
### 6.2.1 Primary map



X Index: 256

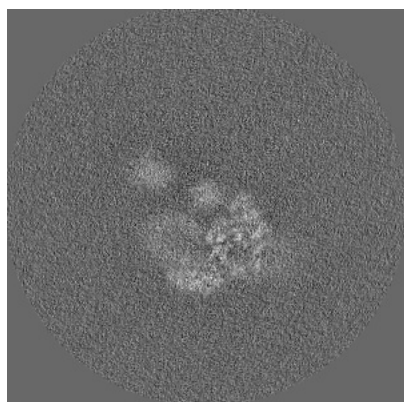


Y Index: 256

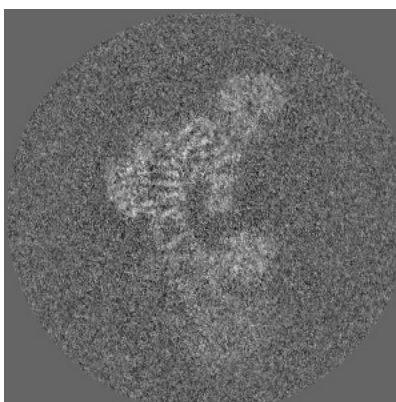


Z Index: 256

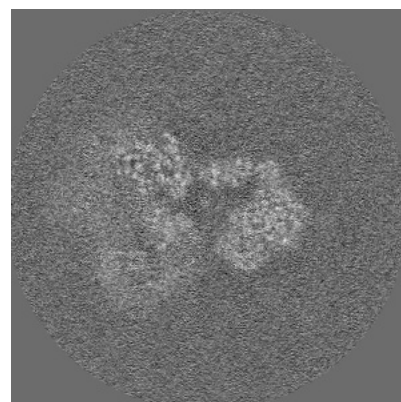
### 6.2.2 Raw map



X Index: 256



Y Index: 256

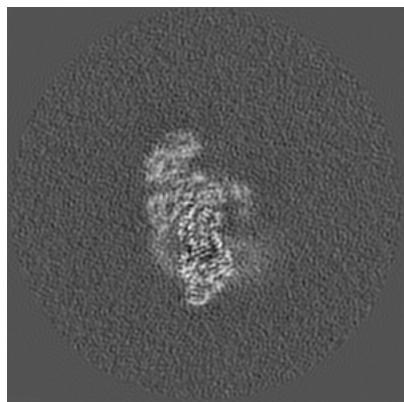


Z Index: 256

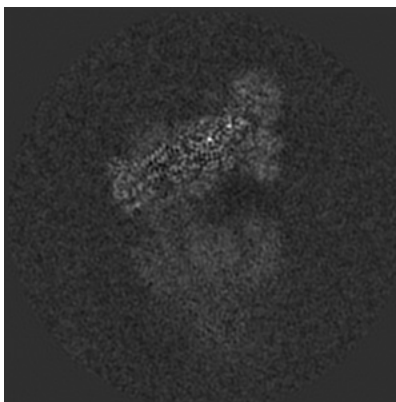
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

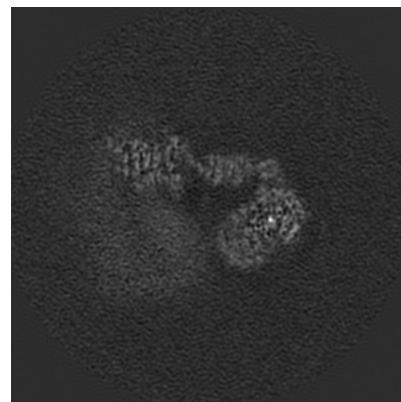
### 6.3.1 Primary map



X Index: 310

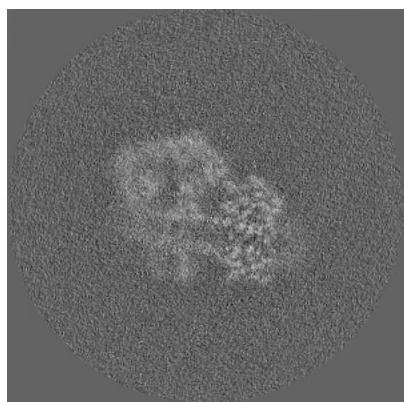


Y Index: 232

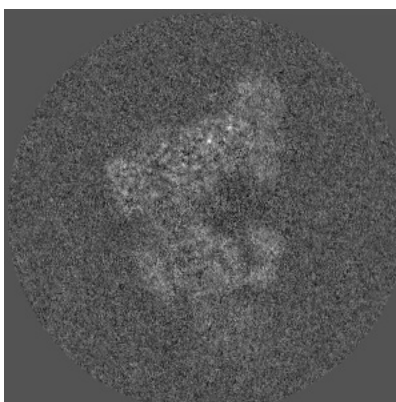


Z Index: 252

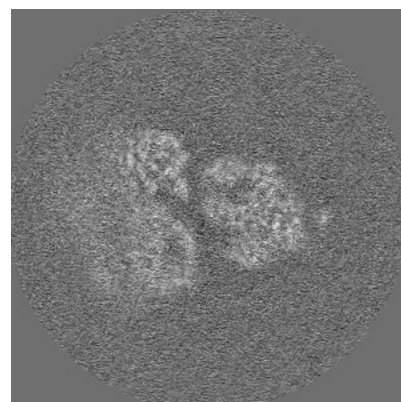
### 6.3.2 Raw map



X Index: 205



Y Index: 234

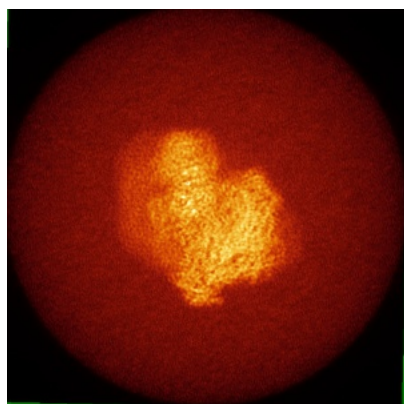


Z Index: 268

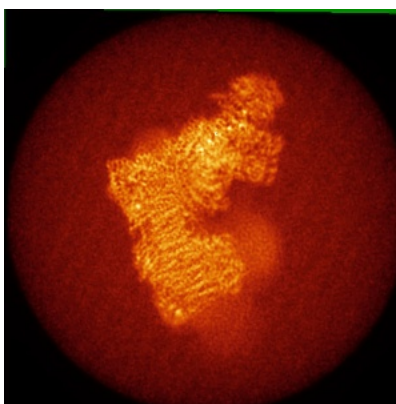
The images above show the largest variance slices of the map in three orthogonal directions.

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

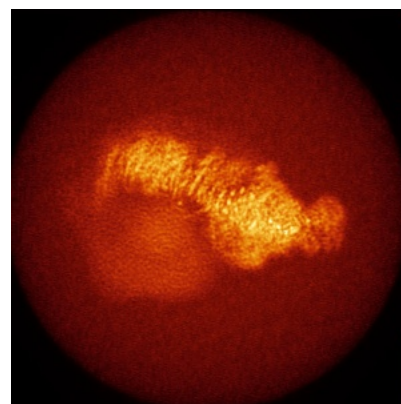
### 6.4.1 Primary map



X

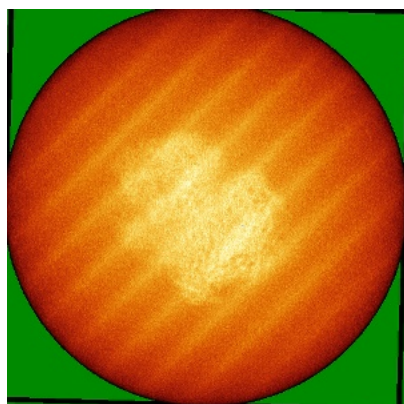


Y

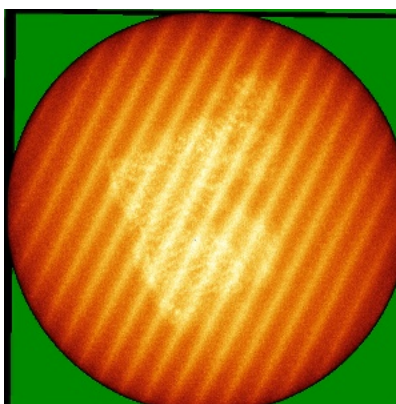


Z

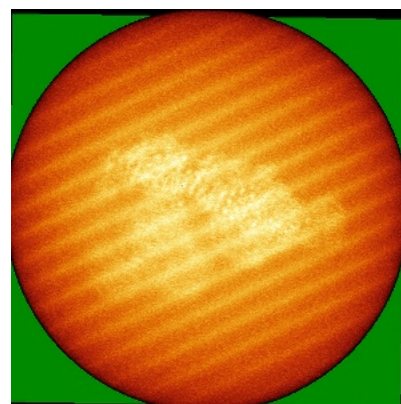
### 6.4.2 Raw map



X



Y

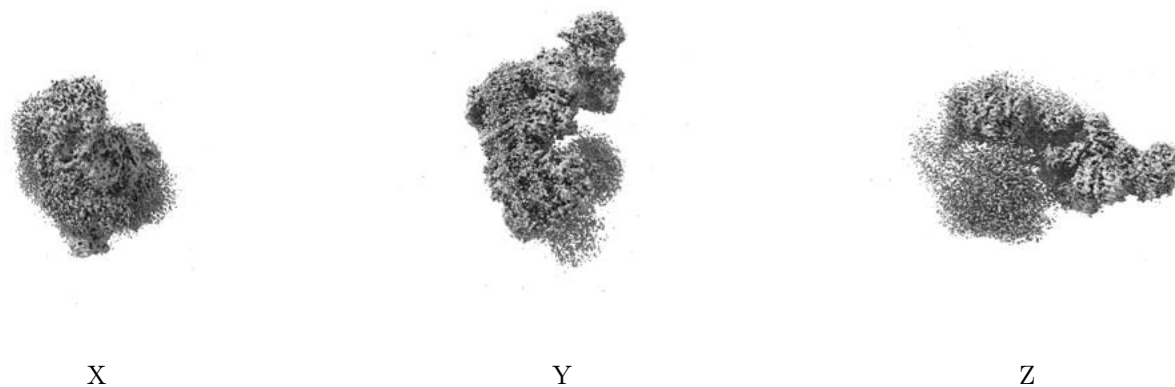


Z

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.

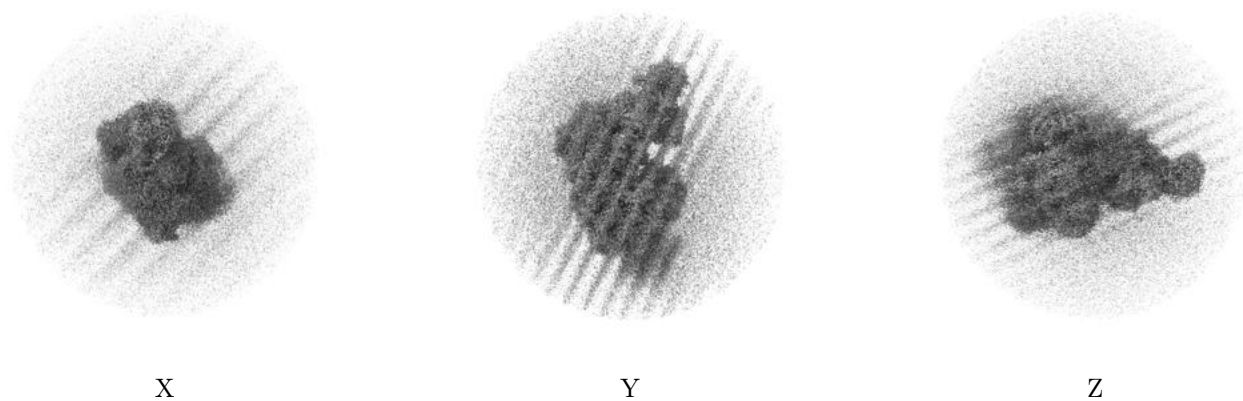
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0082. 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.

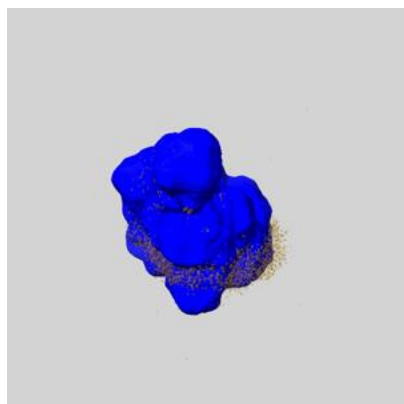
## 6.6 Mask visualisation [i](#)

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

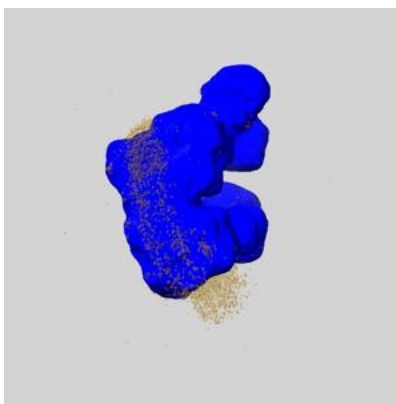
A mask typically either:

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

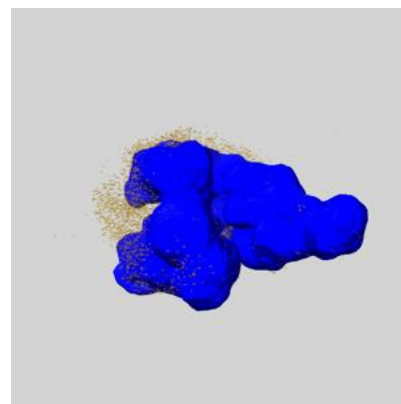
### 6.6.1 emd\_35352\_msk\_1.map [i](#)



X



Y

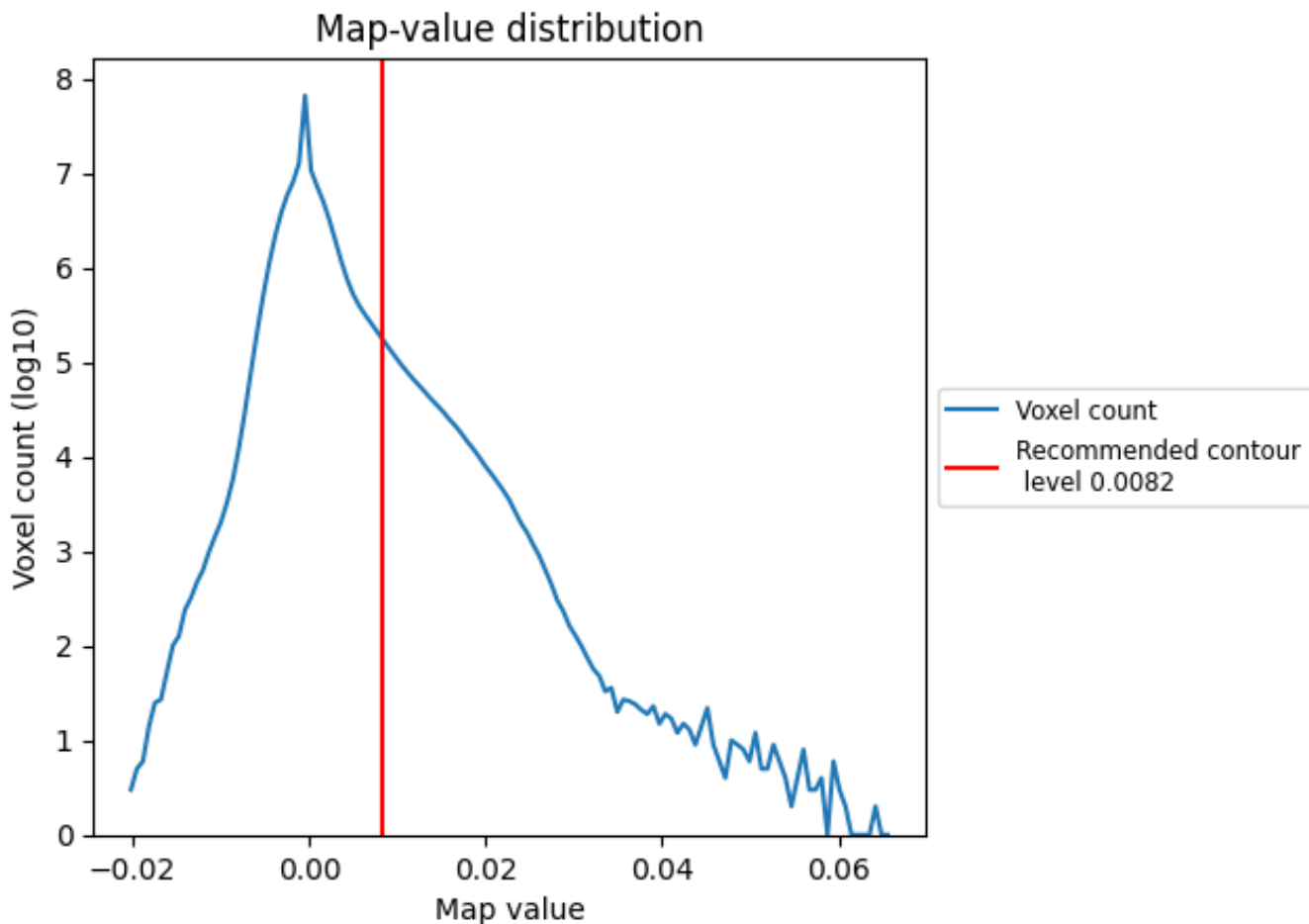


Z

## 7 Map analysis [i](#)

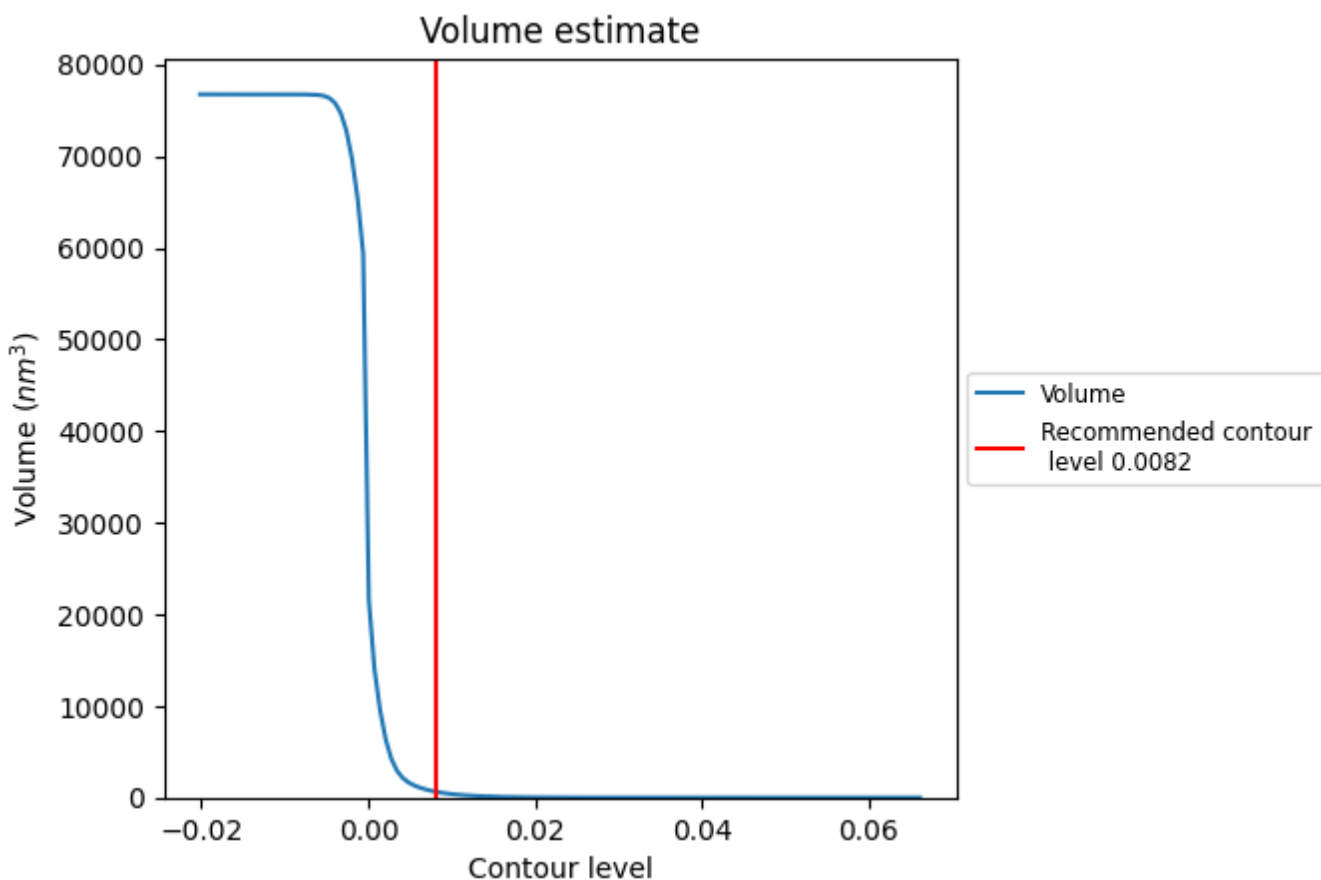
This section contains the results of statistical analysis of the map.

### 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.

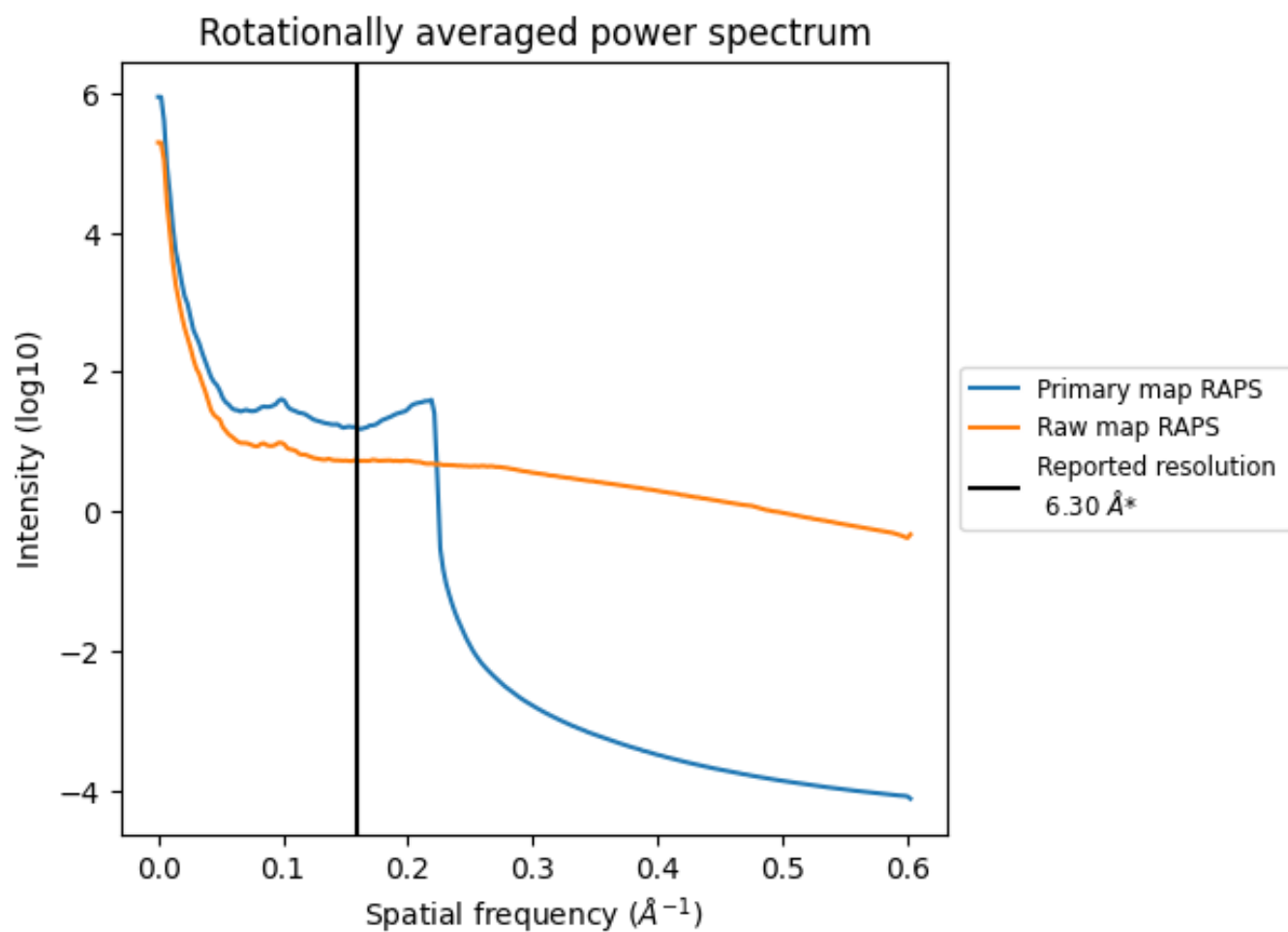
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm<sup>3</sup>; this corresponds to an approximate mass of 557 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

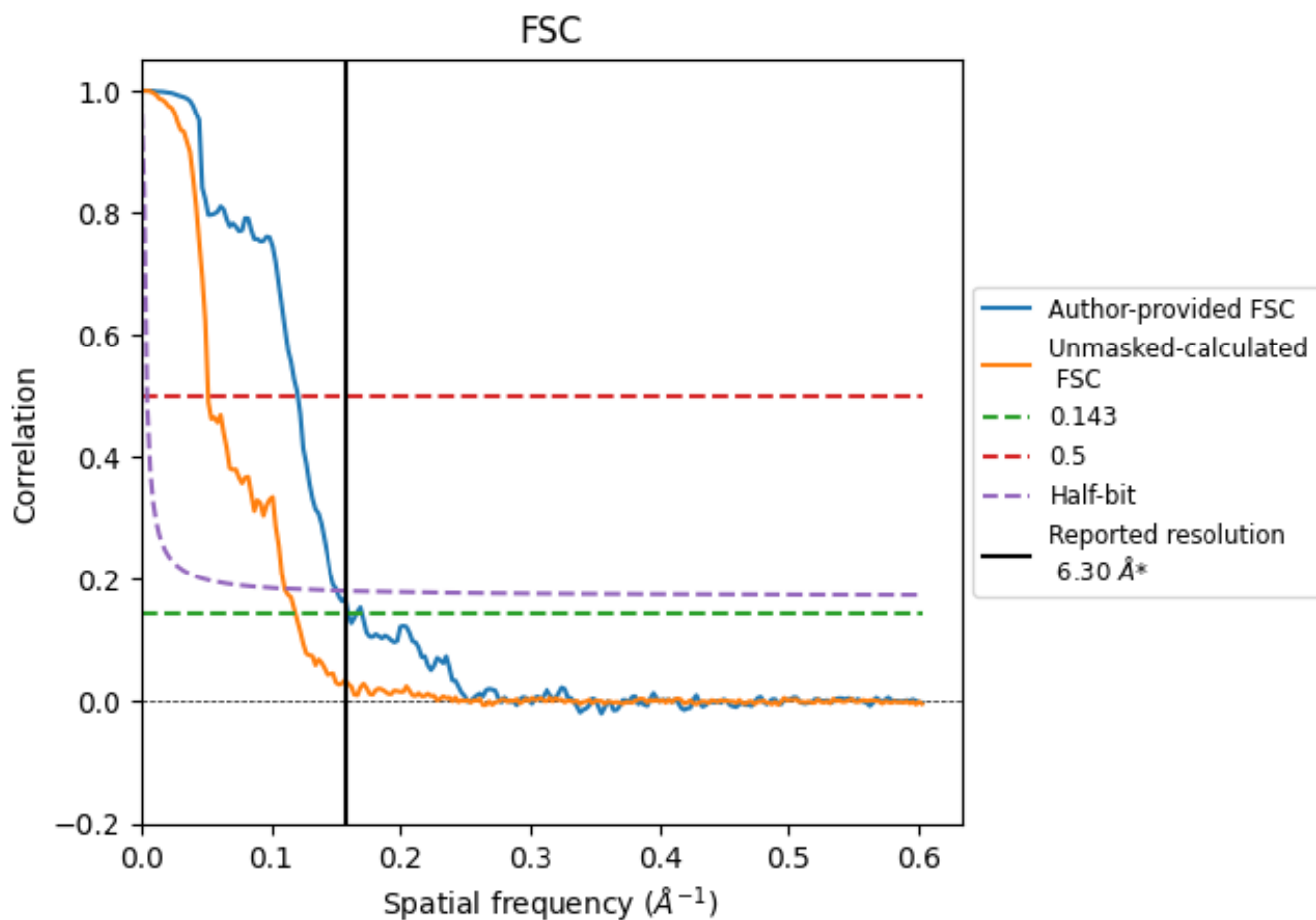


\*Reported resolution corresponds to spatial frequency of 0.159 Å<sup>-1</sup>

## 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 0.159 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

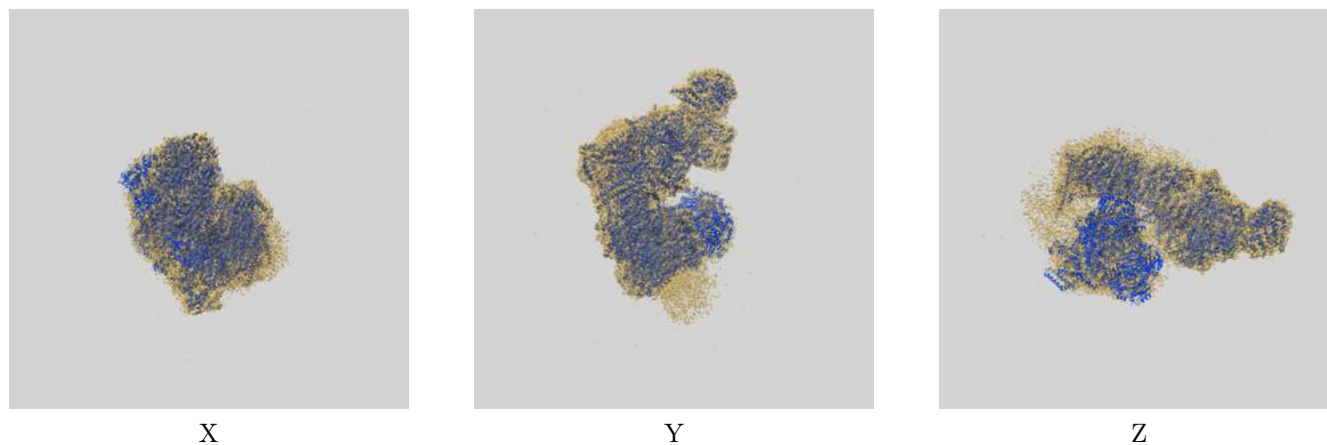
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.25	8.30	6.61
Unmasked-calculated*	8.42	19.38	9.06

\*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 8.42 differs from the reported value 6.3 by more than 10 %

## 9 Map-model fit [i](#)

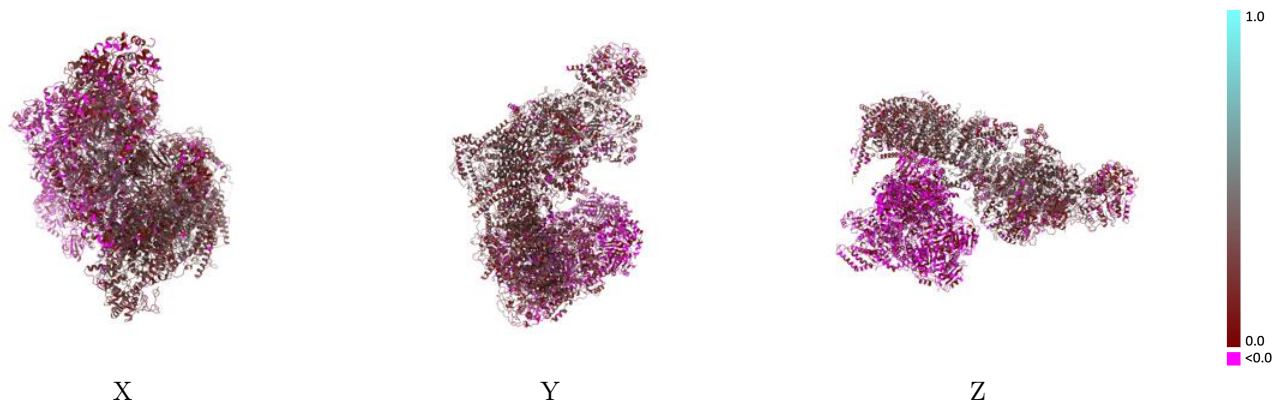
This section contains information regarding the fit between EMDB map EMD-35352 and PDB model 8IC2. Per-residue inclusion information can be found in section 3 on page 26.

### 9.1 Map-model overlay [i](#)



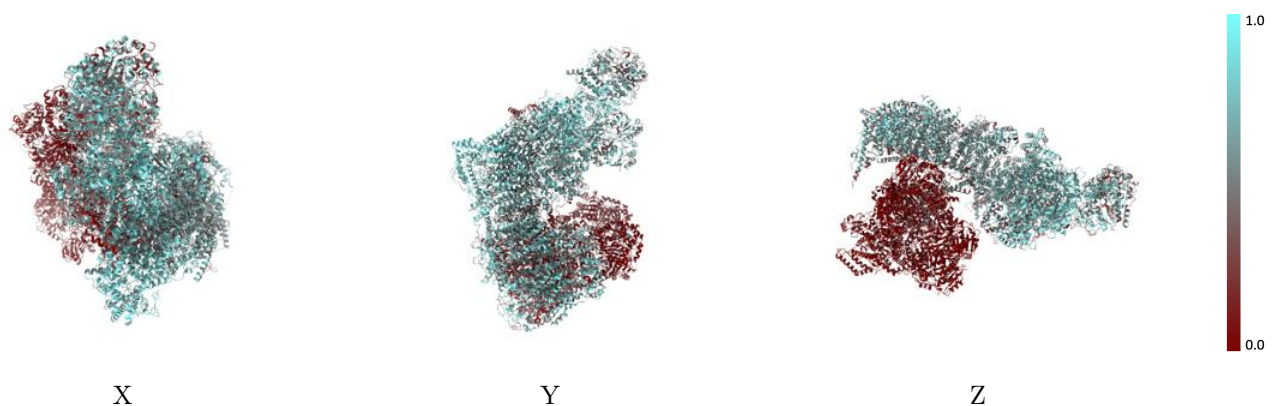
The images above show the 3D surface view of the map at the recommended contour level 0.0082 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



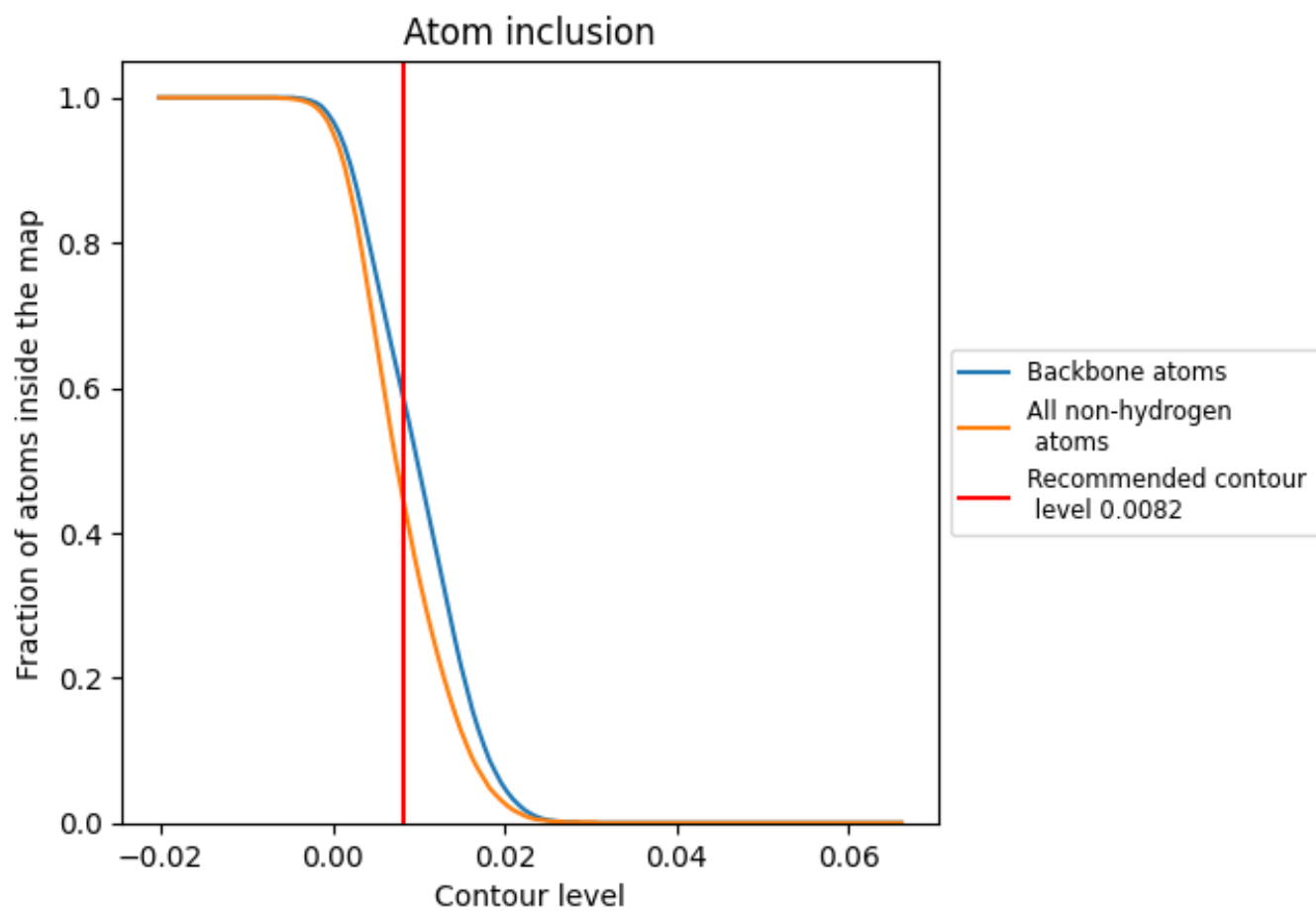
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0082).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 45% 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 (0.0082) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4470	 0.1620
A	 0.6300	 0.2860
AA	 0.0700	 0.0200
AB	 0.0460	 0.0120
AC	 0.0610	 -0.0060
AD	 0.0420	 -0.0050
AE	 0.0500	 -0.0000
AF	 0.0580	 0.0020
AG	 0.0440	 -0.0140
AH	 0.0140	 0.0180
AI	 0.0780	 -0.0240
AJ	 0.0650	 -0.0270
AK	 0.0500	 -0.0080
Aa	 0.0790	 0.0060
Ab	 0.0970	 0.0020
Ac	 0.1120	 0.0070
Ad	 0.0490	 -0.0020
Ae	 0.0270	 0.0020
Af	 0.0760	 0.0280
Ag	 0.1020	 0.0200
Ah	 0.0230	 0.0210
Aj	 0.0370	 -0.0150
Ak	 0.0460	 -0.0170
B	 0.7370	 0.2950
C	 0.7190	 0.2680
D	 0.7110	 0.3040
E	 0.5840	 0.1820
F	 0.5730	 0.1700
G	 0.6660	 0.2170
H	 0.6640	 0.2950
I	 0.7580	 0.3010
J	 0.5800	 0.2550
K	 0.6600	 0.2980
L	 0.6060	 0.2500
M	 0.6240	 0.2910



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Chain	Atom inclusion	Q-score
N	 0.6810	 0.3080
O	 0.6070	 0.2140
P	 0.6080	 0.1960
Q	 0.6230	 0.2630
R	 0.4540	 0.1950
S	 0.6130	 0.1520
T	 0.4760	 0.1260
U	 0.6600	 0.2200
V	 0.6430	 0.1750
W	 0.6640	 0.2260
X	 0.7620	 0.2650
Y	 0.4750	 0.2170
Z	 0.7340	 0.2500
a	 0.7750	 0.2800
b	 0.7270	 0.2540
c	 0.5820	 0.2290
d	 0.6170	 0.2230
e	 0.7340	 0.2790
f	 0.6200	 0.2590
g	 0.6070	 0.2300
h	 0.6340	 0.2510
i	 0.6070	 0.2300
j	 0.6300	 0.1610
k	 0.6270	 0.2090
l	 0.6080	 0.2260
m	 0.5370	 0.2100
n	 0.6180	 0.2200
o	 0.5820	 0.1390
p	 0.6770	 0.2430
q	 0.2250	 0.1500
r	 0.4090	 0.1190
s	 0.3530	 0.0670