



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 07:12 PM UTC

PDB ID : 8IBD / pdb_00008ibd
EMDB ID : EMD-35340
Title : Respiratory complex CI:CIII2, type II, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

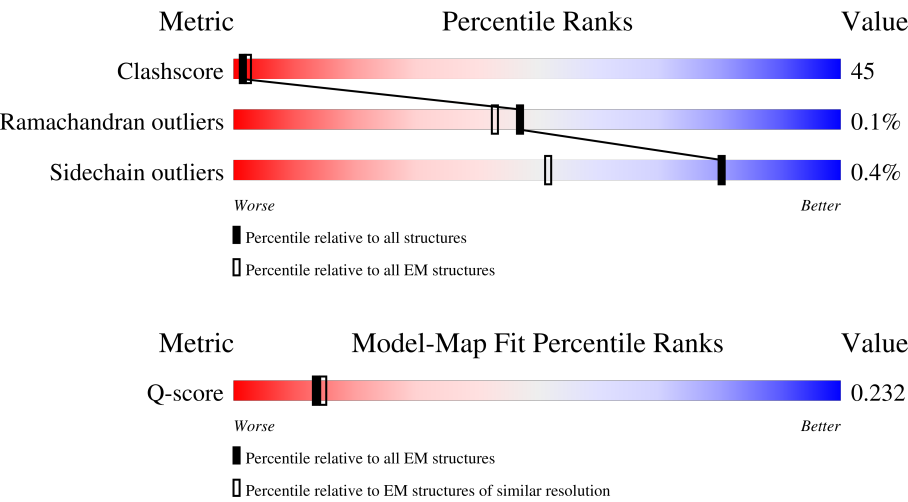
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	217187	24013	-
Ramachandran outliers	211220	23611	-
Sidechain outliers	210688	23127	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	224	
3	C	263	
4	D	463	

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

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	SF4	B	301	-	-	X	-
56	SF4	F	502	-	-	X	-
56	SF4	G	802	-	-	X	-
56	SF4	I	302	-	-	X	-
56	SF4	I	303	-	-	X	-
57	UQ1	B	302	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
63	ADP	O	401	-	-	X	-
71	3PH	Ad	402	-	-	X	-

2 Entry composition

There are 71 unique types of molecules in this entry. The entry contains 96599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			799	552	112	130	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1643	1061	279	300	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	427	Total	C	N	O	S	0	0
			3438	2197	591	626	24		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	172	Total	C	N	O	S	0	0
			1380	869	237	262	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	163	Total	C	N	O	S	0	0
			1229	828	175	211	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	116	LEU	ASN	conflict	UNP P03925
J	117	GLY	LEU	conflict	UNP P03925

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	116	Total	C	N	O	S	0	0
			940	598	161	177	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	89	Total	C	N	O	S	0	0
			718	462	105	146	5		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	138	Total	C	N	O	S	0	0
			1145	736	203	198	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	80	Total	C	N	O	S	0	0
			628	414	99	111	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	105	Total	C	N	O	S	0	0
			877	555	162	152	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	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	95	Total	C	N	O	S	0	0
			802	523	140	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	73	Total	C	N	O	S	0	0
			582	383	102	95	2		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	123	Total	C	N	O	S	0	0
			1025	658	181	182	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	84	Total	C	N	O	S	0	0
			686	435	128	121	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	23	Total	C	N	O	0	0
			193	126	30	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	395	Total	C	N	O	S	0	0
			3077	1918	545	598	16		
45	Aa	394	Total	C	N	O	S	0	0
			3076	1923	545	592	16		

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

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

- Molecule 47 is a protein called Cytochrome b.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	236	Total	C	N	O	S	0	0
			1878	1200	323	341	14		
48	Ad	239	Total	C	N	O	S	0	0
			1903	1215	326	348	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	109	Total	C	N	O	S	0	0
			830	525	152	147	6		
49	AI	28	Total	C	N	O		0	0
			200	129	37	34			

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
49	Ai	28	Total	C	N	O		0	0
			204	130	40	34			

- 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		
50	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
51	Ag	74	Total	C	N	O	S	0	0
			622	404	114	103	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	62	Total	C	N	O	S	0	0
			512	316	93	98	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	21	Total	C	N	O	0	0
			165	109	27	29		
53	Aj	43	Total	C	N	O	0	0
			345	223	59	63		

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

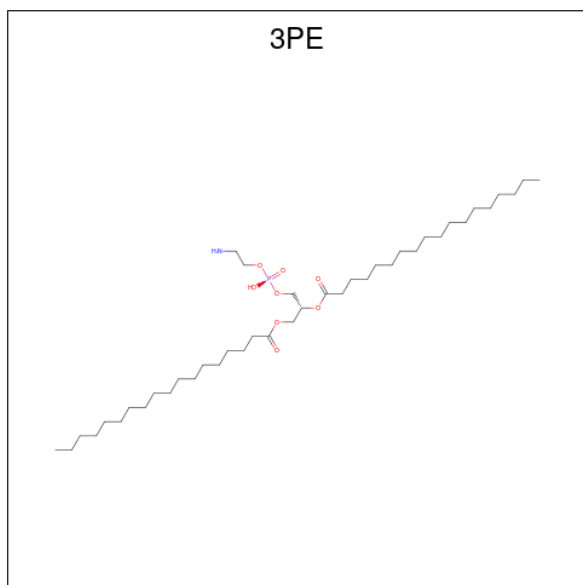
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	17	Total	C	N	O	S	0	0
			118	77	19	21	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	Ak	38	Total	C	N	O	S	0	0
			309	202	58	48	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



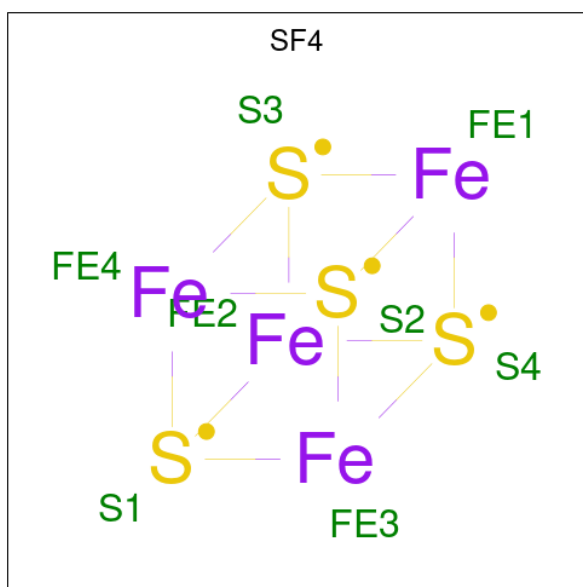
Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
55	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	K	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
55	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
55	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	d	1	Total	C	N	O	P	0
			31	21	1	8	1	
55	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	m	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
55	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



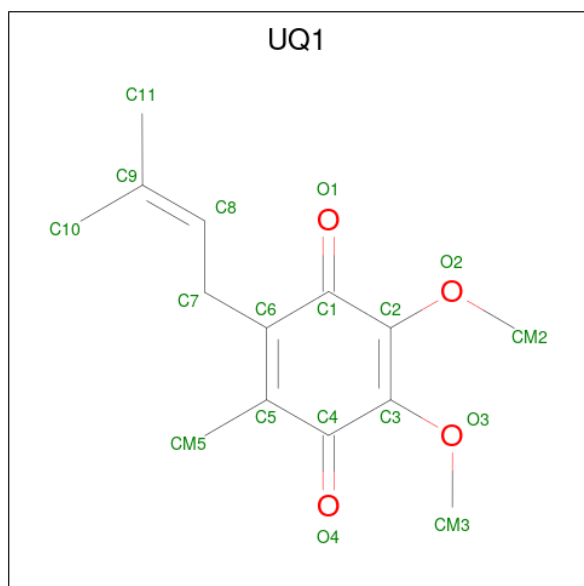
Mol	Chain	Residues	Atoms			AltConf
56	B	1	Total	Fe	S	0
			8	4	4	

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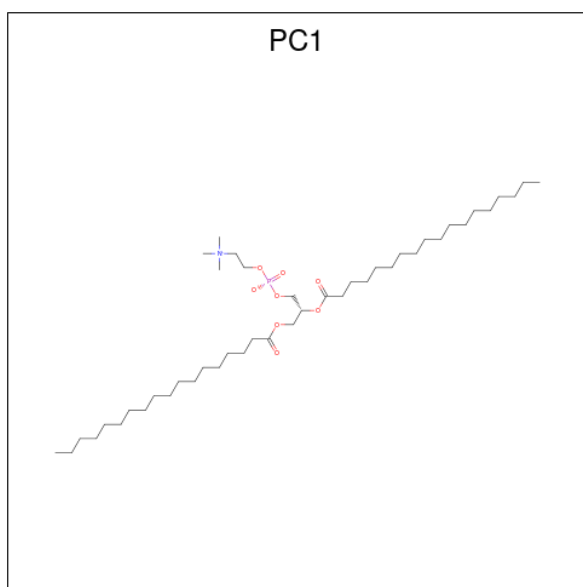
Mol	Chain	Residues	Atoms			AltConf
56	F	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	I	1	Total	Fe	S	0
			8	4	4	
56	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 57 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



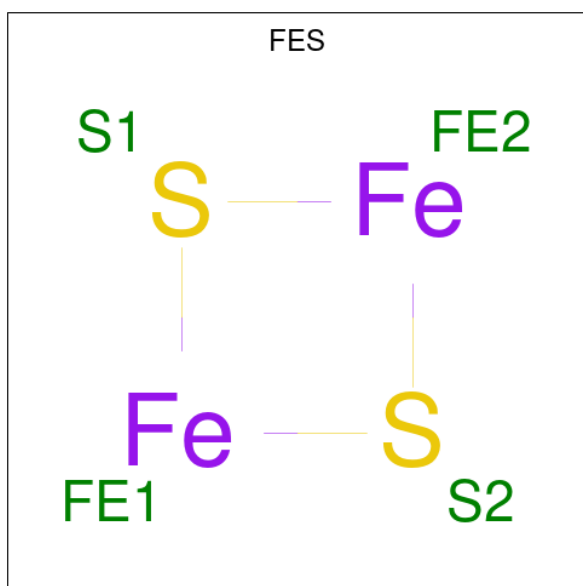
Mol	Chain	Residues	Atoms			AltConf
57	B	1	Total	C	O	0
			18	14	4	

- Molecule 58 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
58	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

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



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

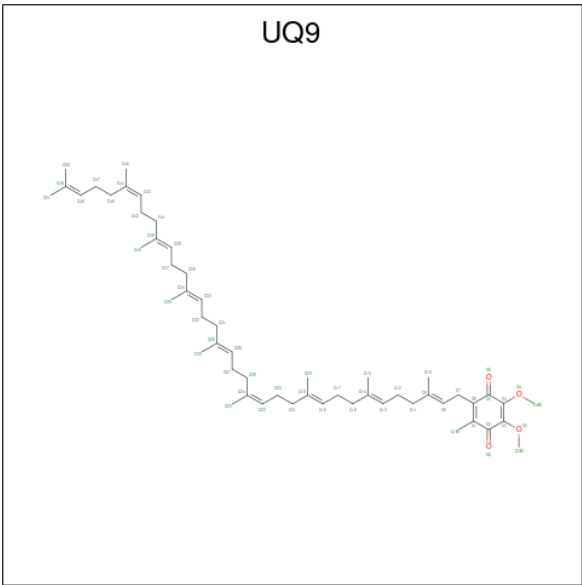
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Mol	Chain	Residues	Atoms			AltConf
59	G	1	Total	Fe	S	0
			4	2	2	

-
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5) and a ribityl chain attached to the N10 position. The ribityl chain is a three-carbon chain (C1', C2', C3') with a phosphate group (O1P, O2P, O3P) attached to the C3' position. The ribityl chain is shown in a chair conformation with stereochemistry indicated by wedges and dashes. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms (O1P, O2P, O3P, and one double-bonded oxygen). The ribityl chain is attached to the N10 position of the isoalloxazine ring system. The ribityl chain is shown in a chair conformation with stereochemistry indicated by wedges and dashes. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms (O1P, O2P, O3P, and one double-bonded oxygen).

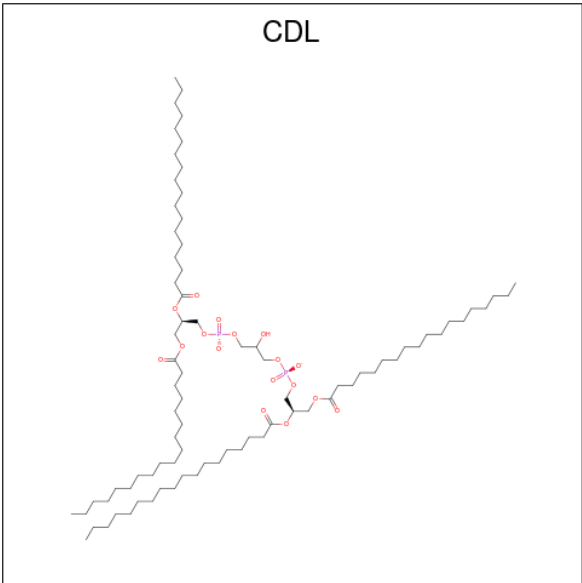
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 



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

- Molecule 62 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



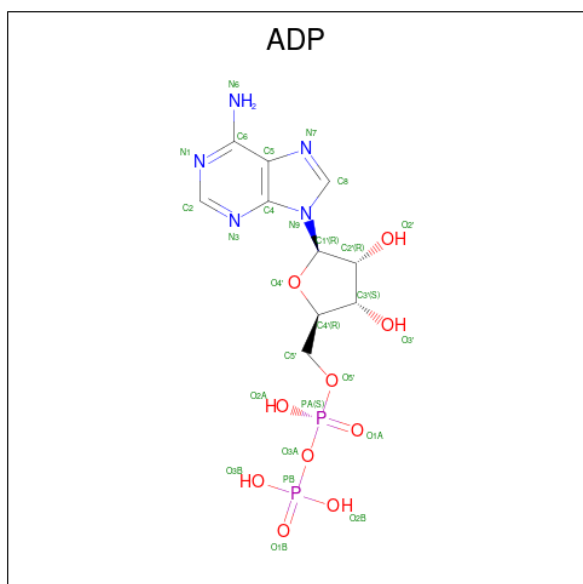
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			78	59	17	2	
62	X	1	Total	C	O	P	0
			67	48	17	2	

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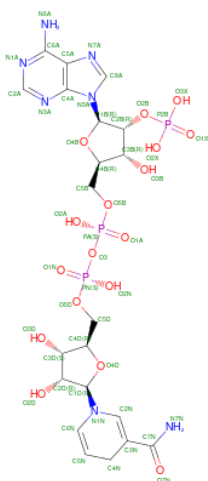
Mol	Chain	Residues	Atoms				AltConf
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	Ag	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

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



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

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



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

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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



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

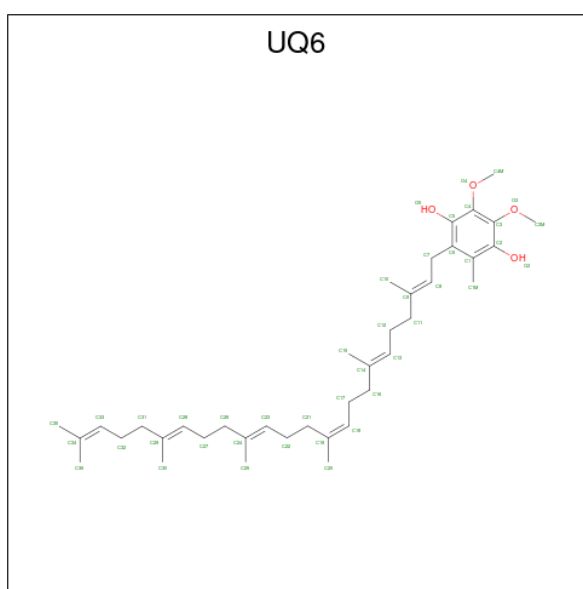


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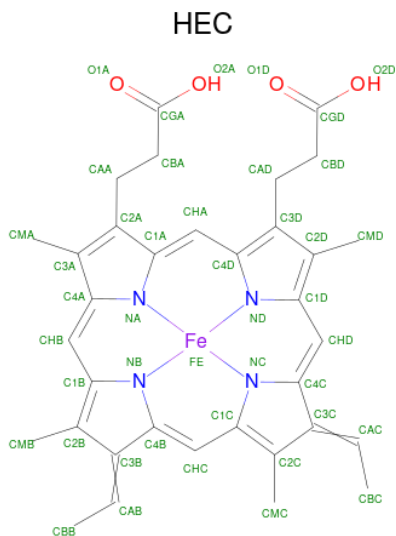
Mol	Chain	Residues	Atoms					AltConf
67	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
67	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 68 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



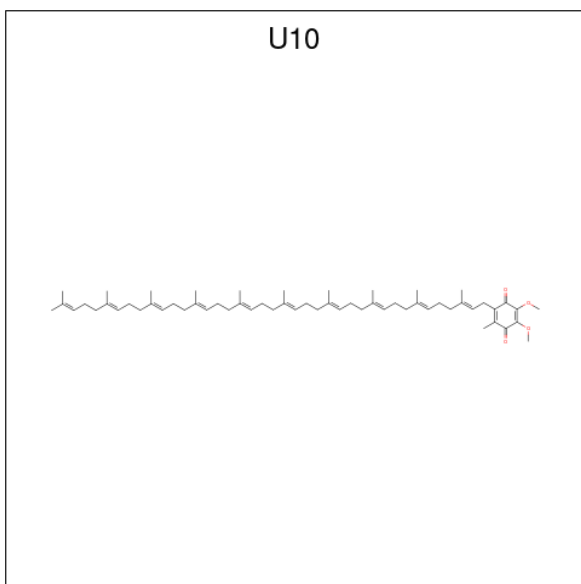
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			28	24	4	
68	Ac	1	Total	C	O	0
			28	24	4	

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



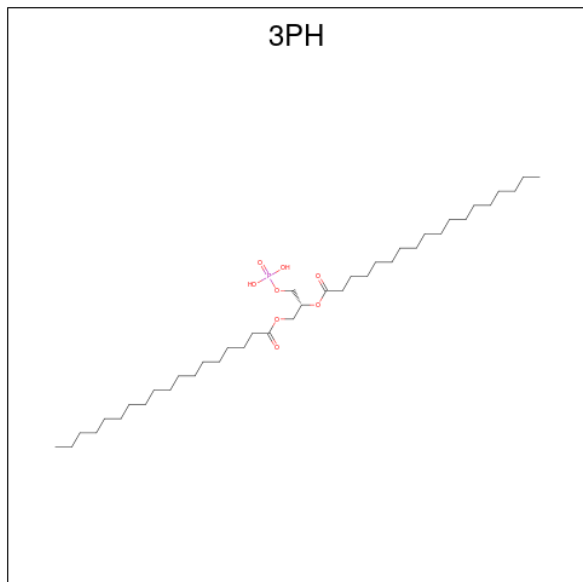
Mol	Chain	Residues	Atoms					AltConf
69	AD	1	Total 43	C 34	Fe 1	N 4	O 4	0
69	Ad	1	Total 43	C 34	Fe 1	N 4	O 4	0

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



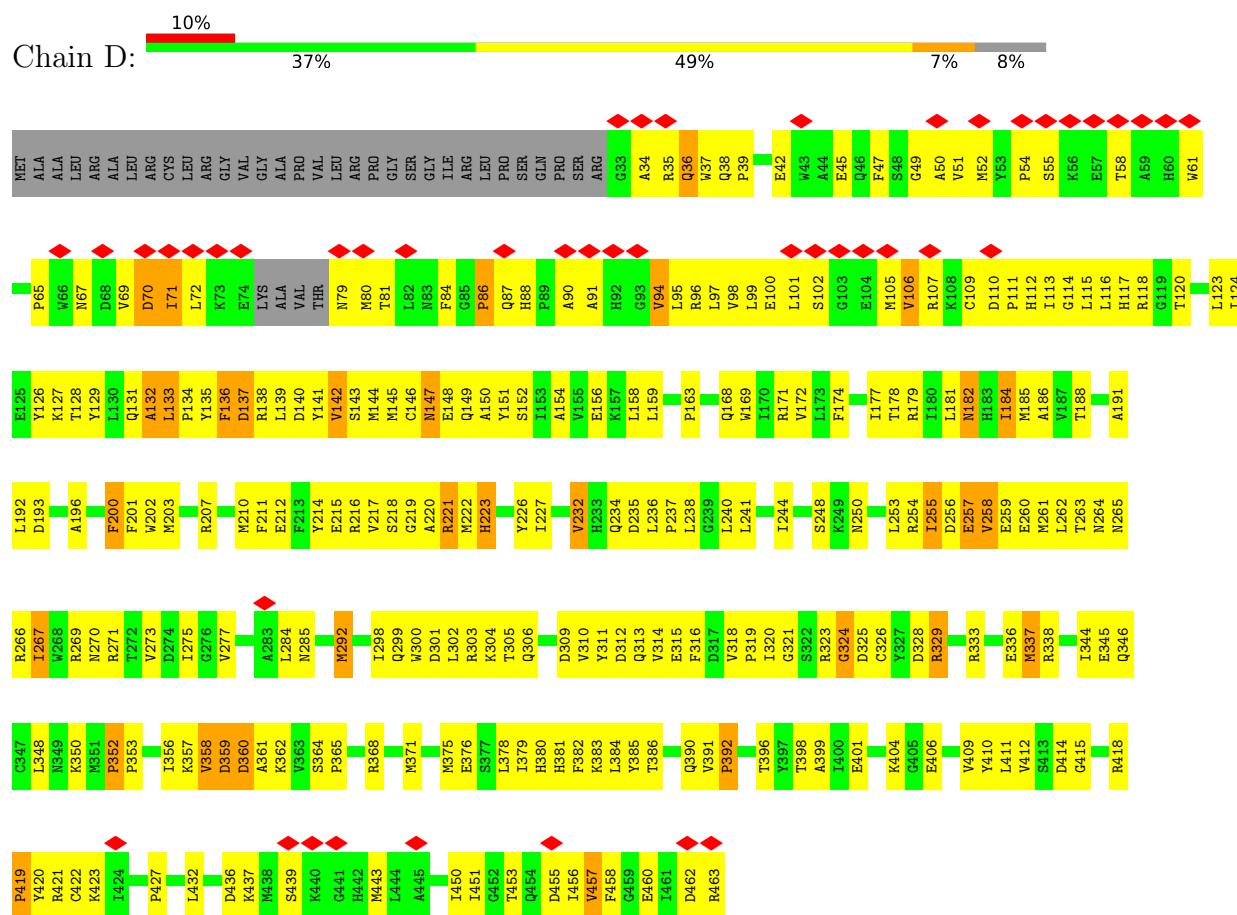
Mol	Chain	Residues	Atoms			AltConf
70	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).

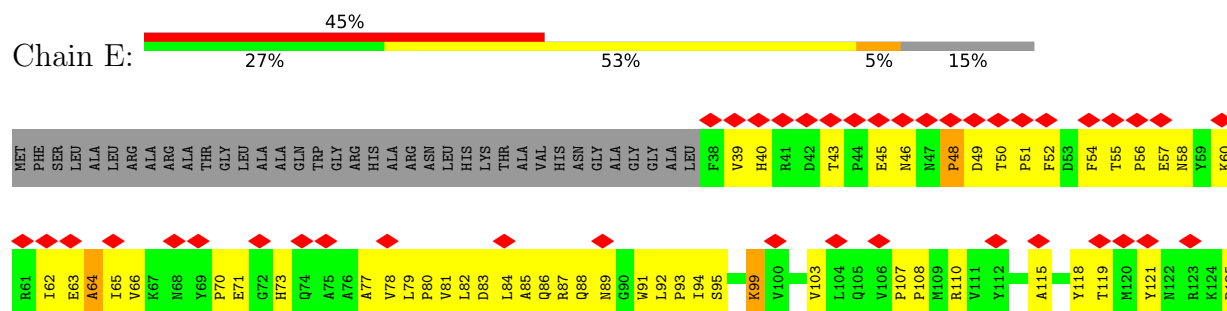


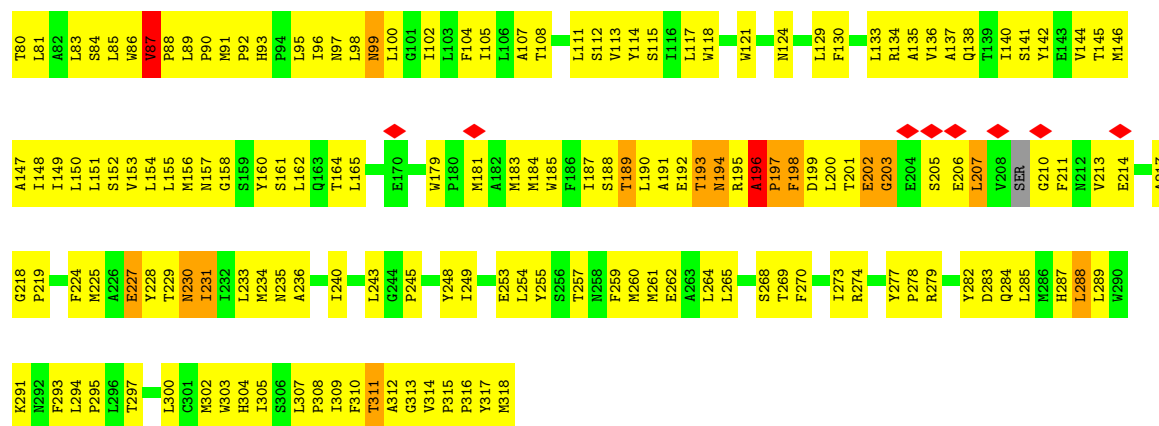
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
71	Ad	1	36	27	8	1	0

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

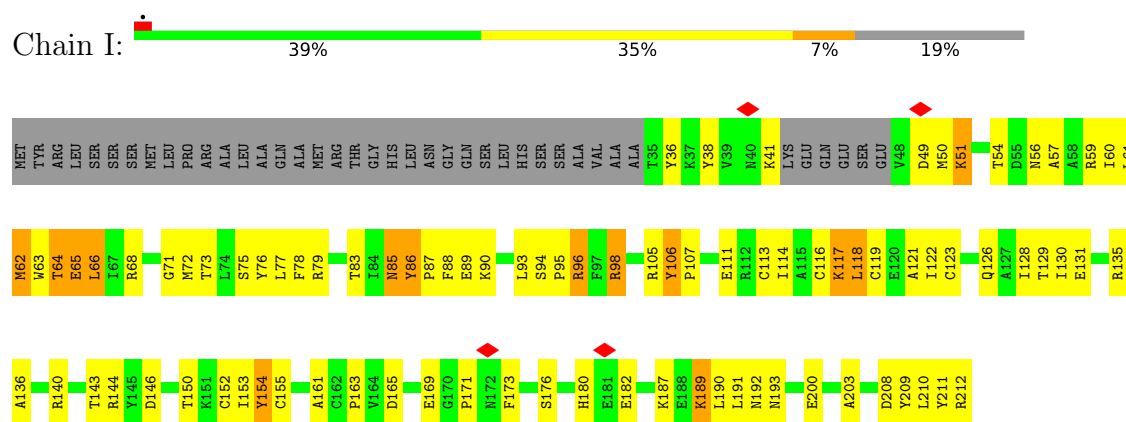


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





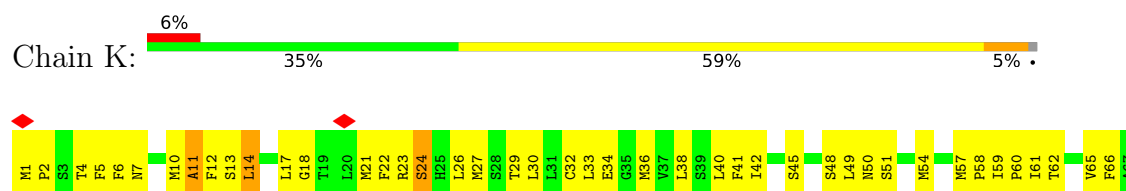
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

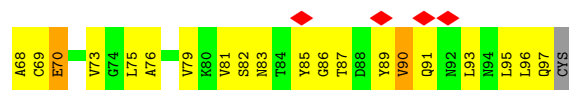


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

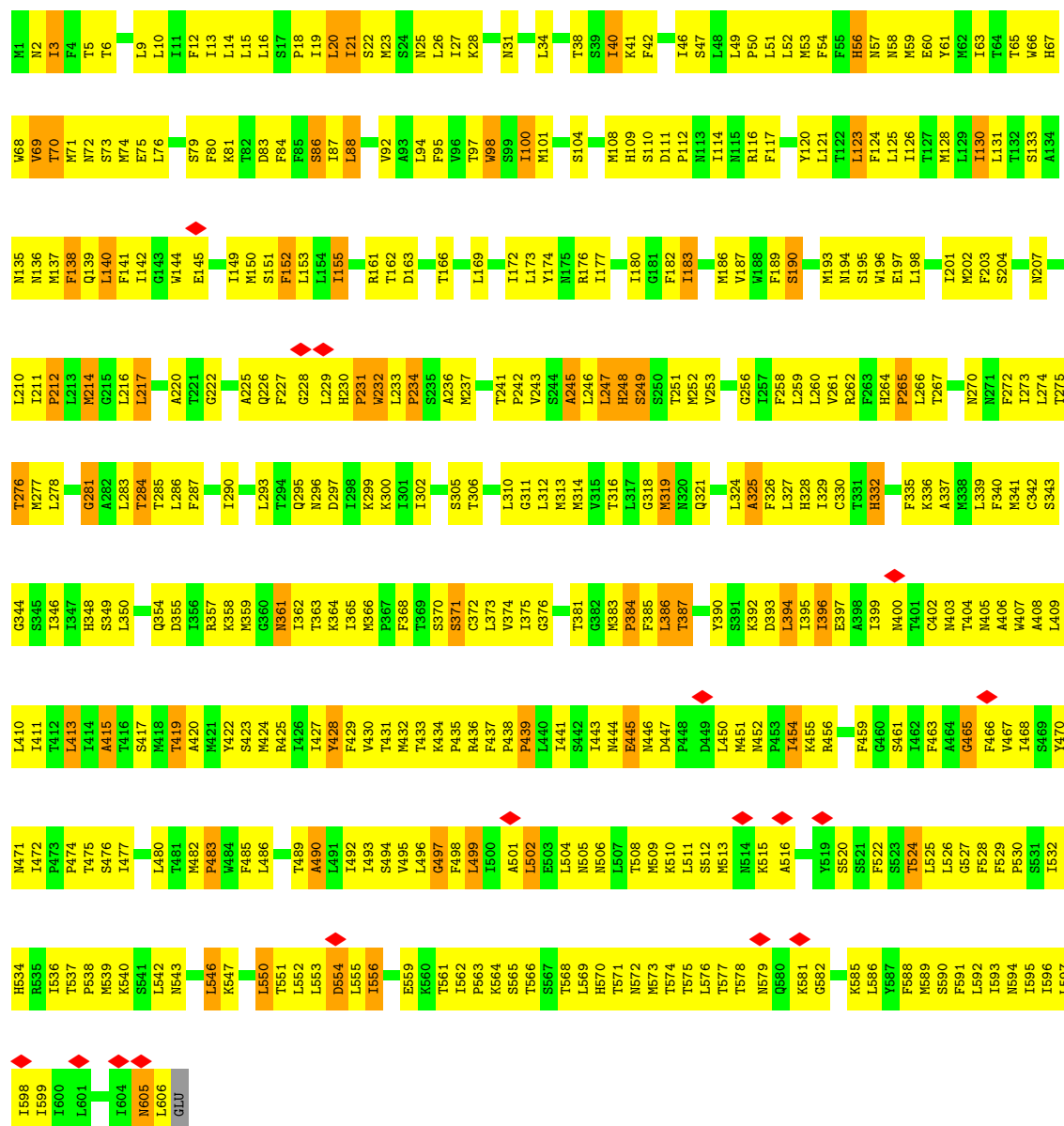
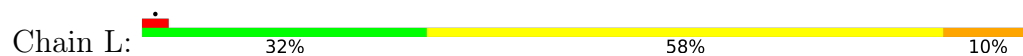


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

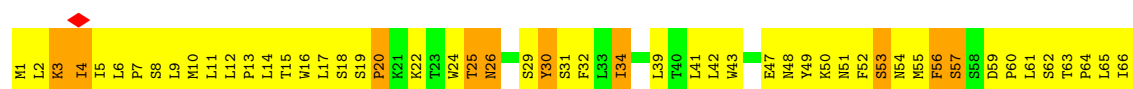


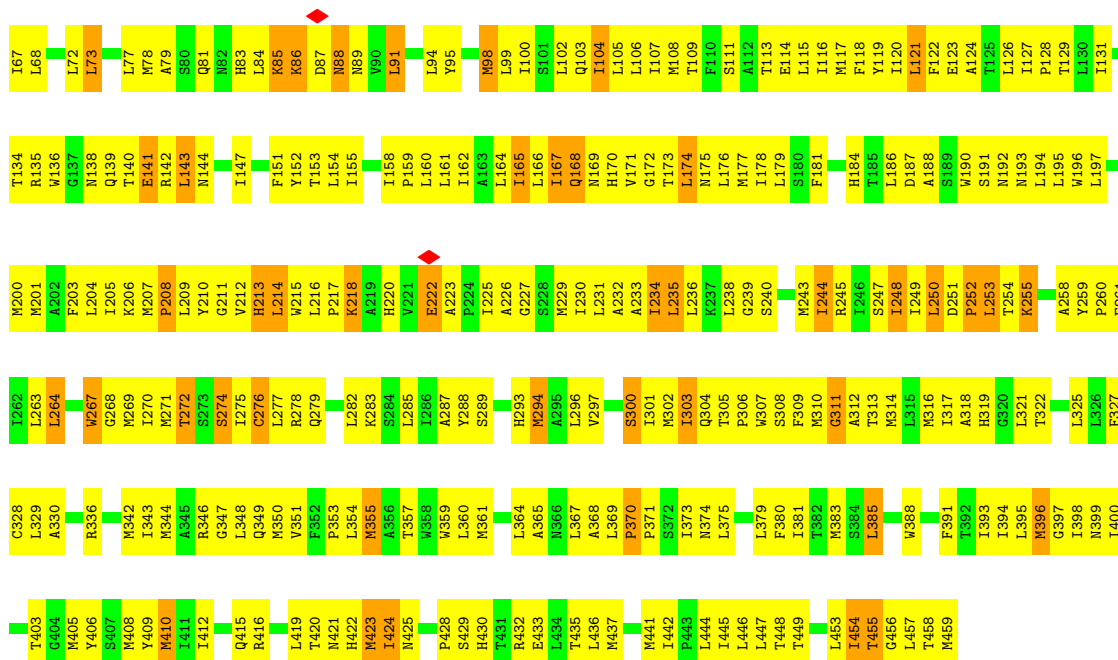


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

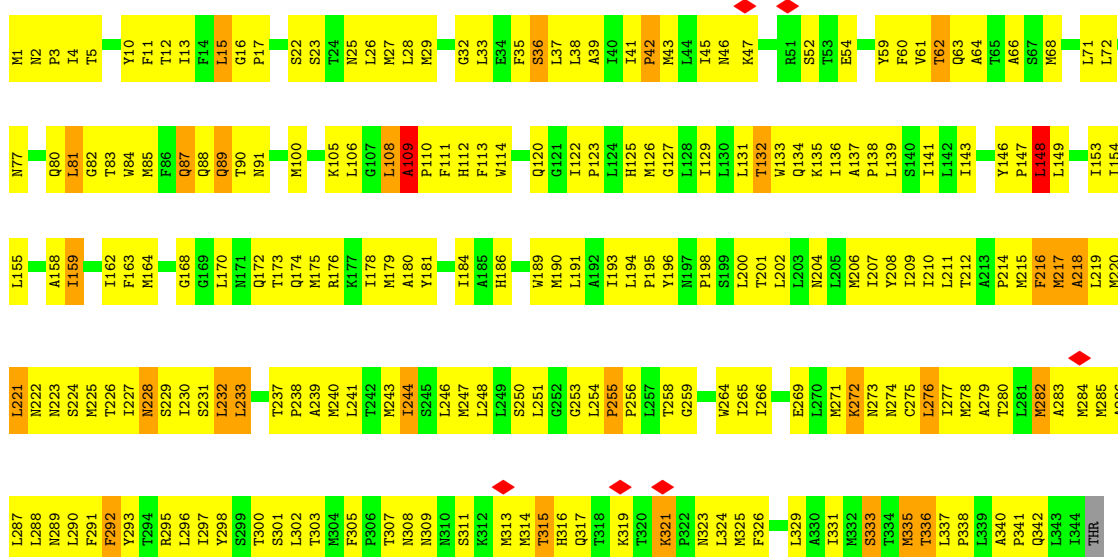


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

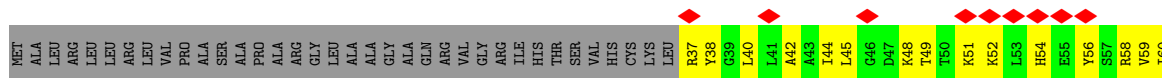


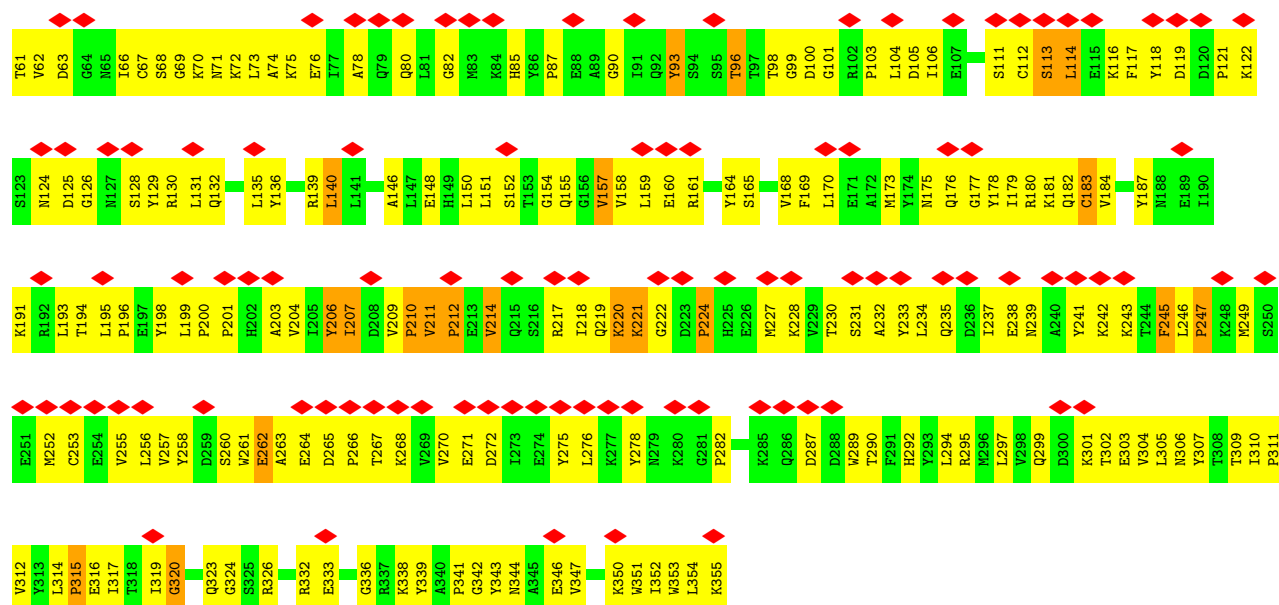


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

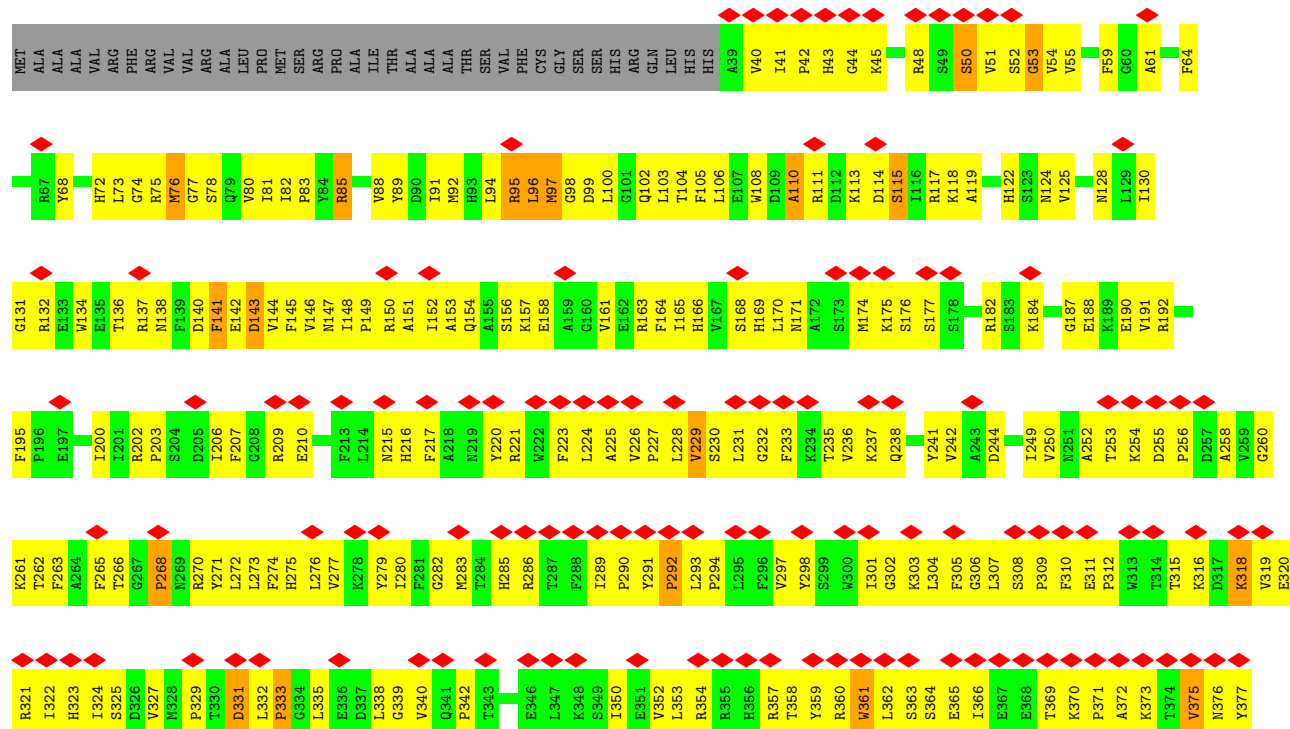


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

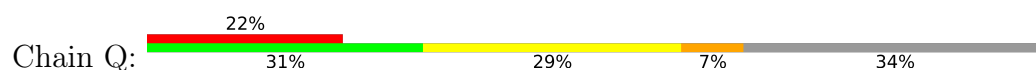




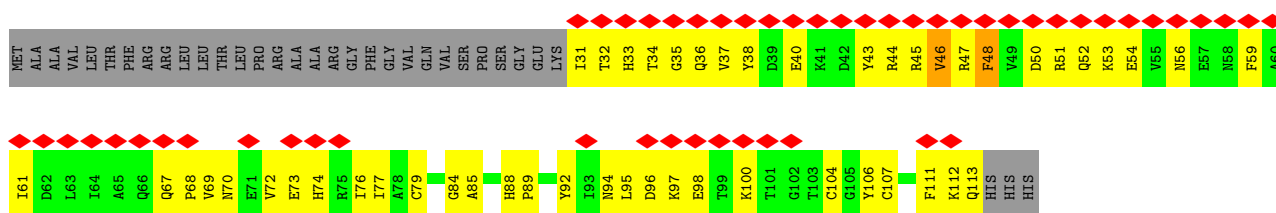
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



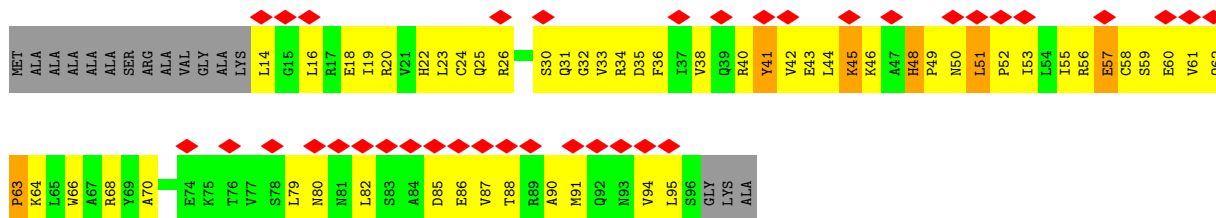
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



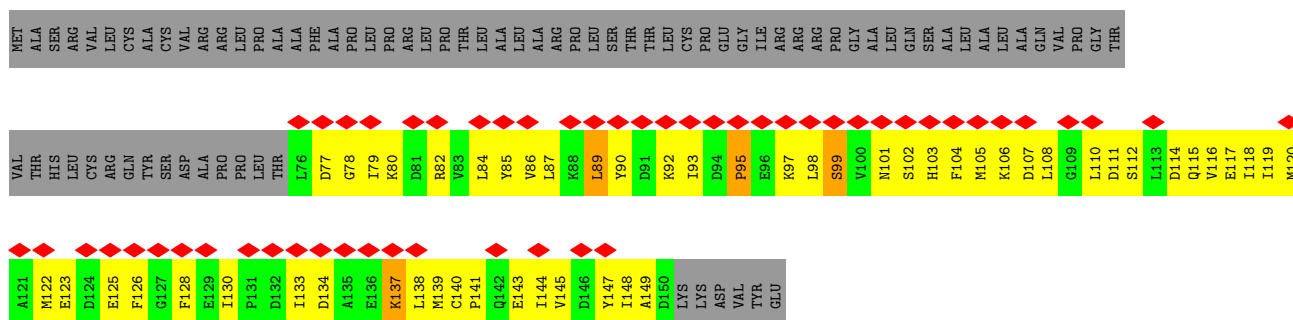
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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

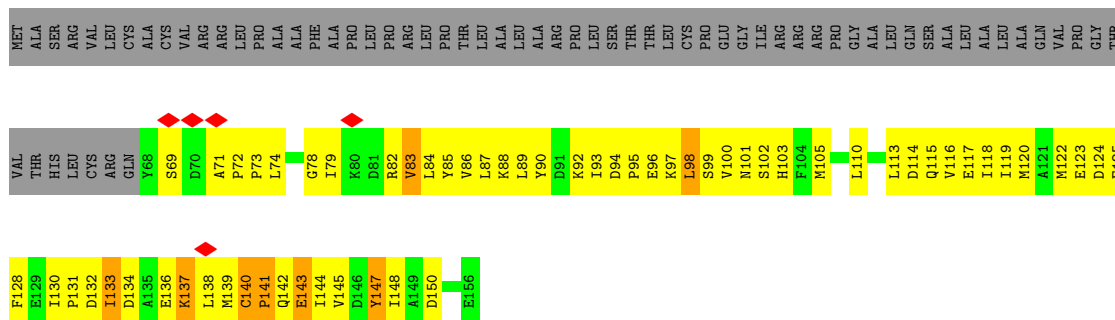


- Molecule 20: Acyl carrier protein, mitochondrial

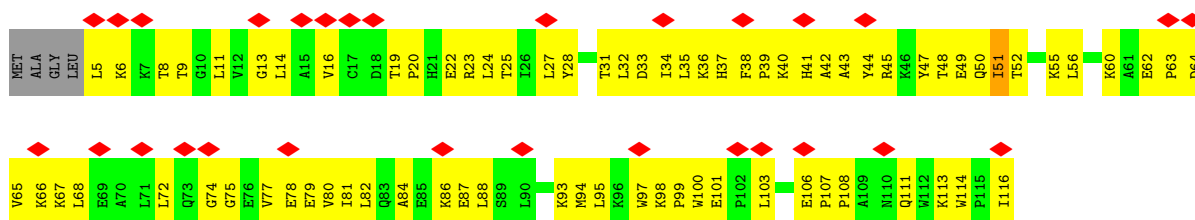


- Molecule 20: Acyl carrier protein, mitochondrial

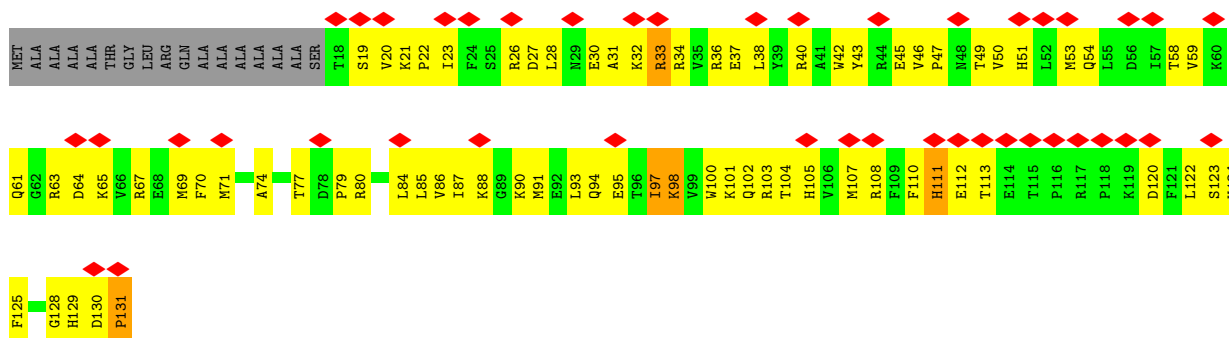




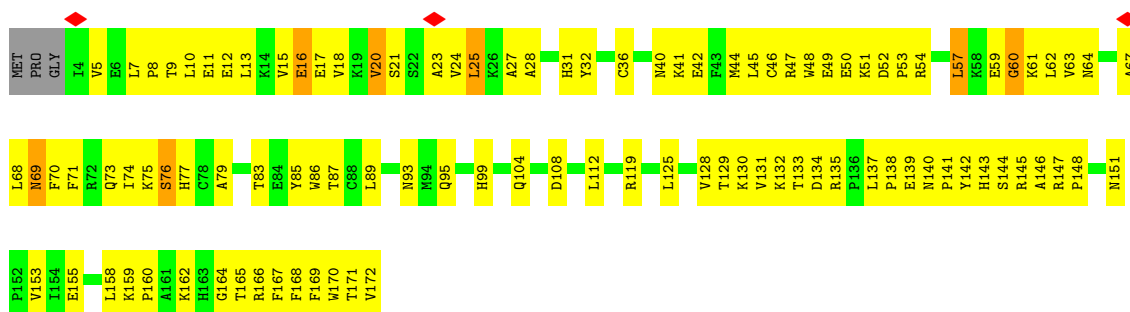
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



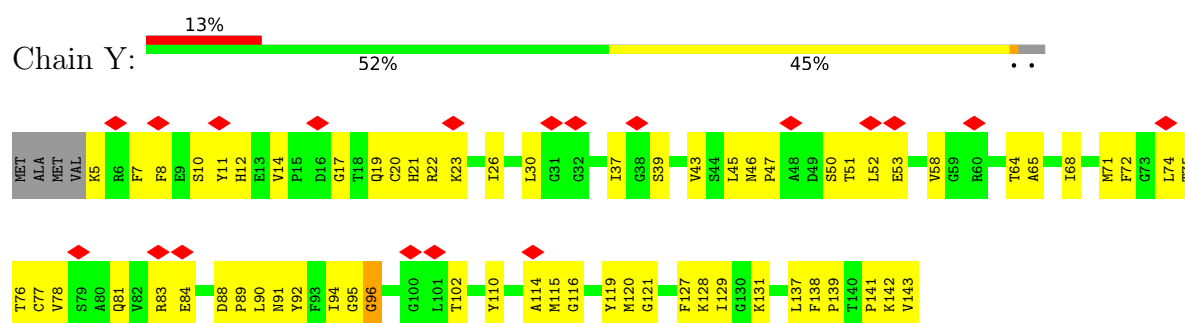
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



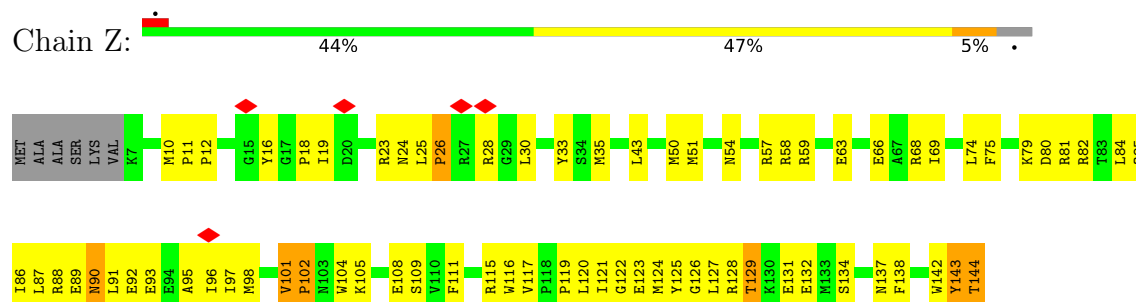
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



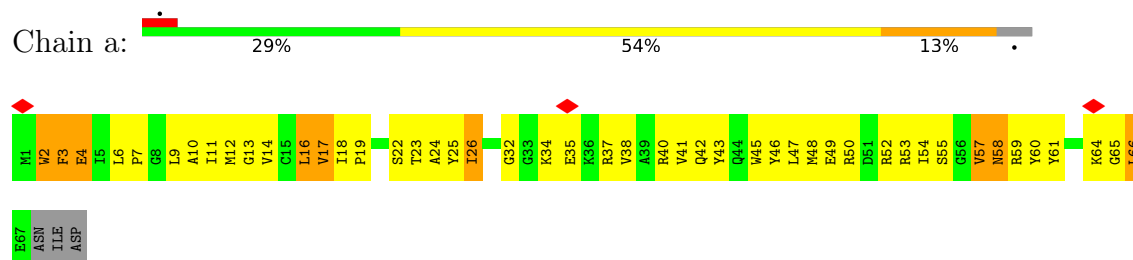
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



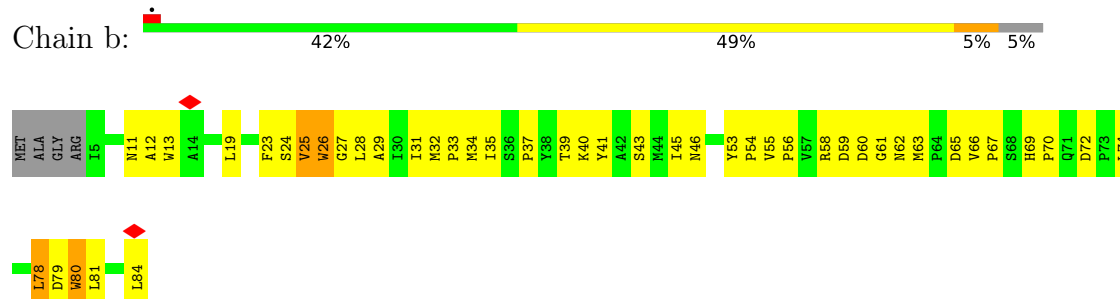
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



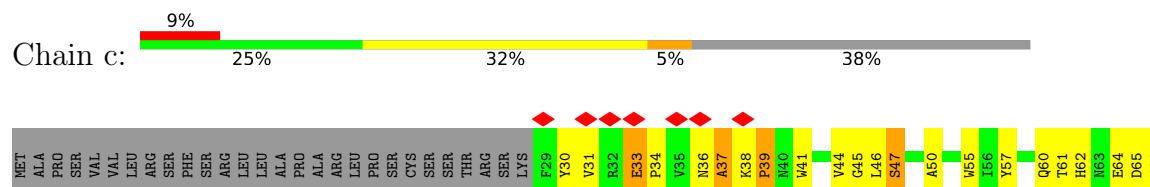
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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

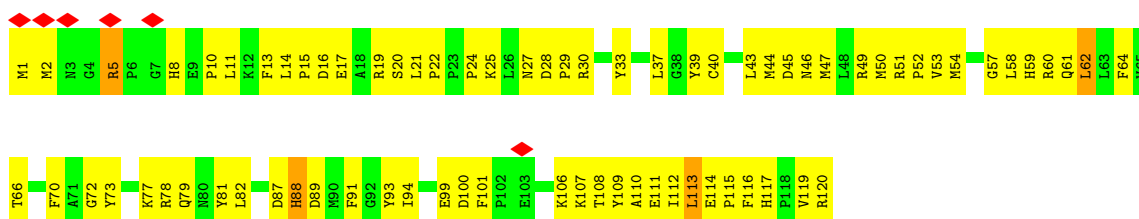


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

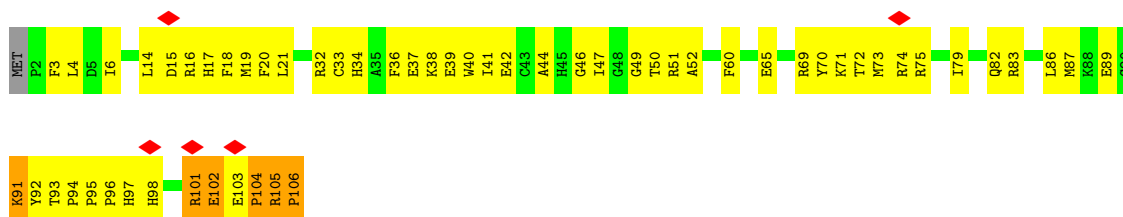
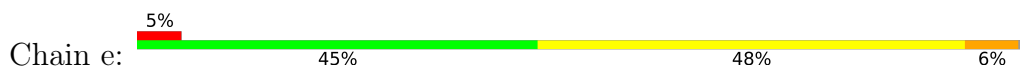




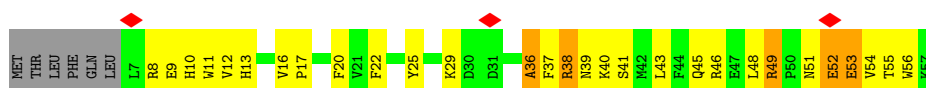
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



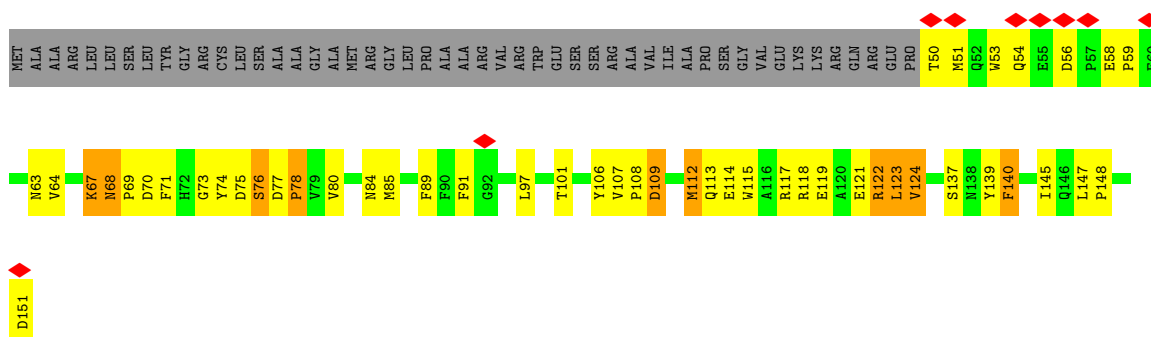
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



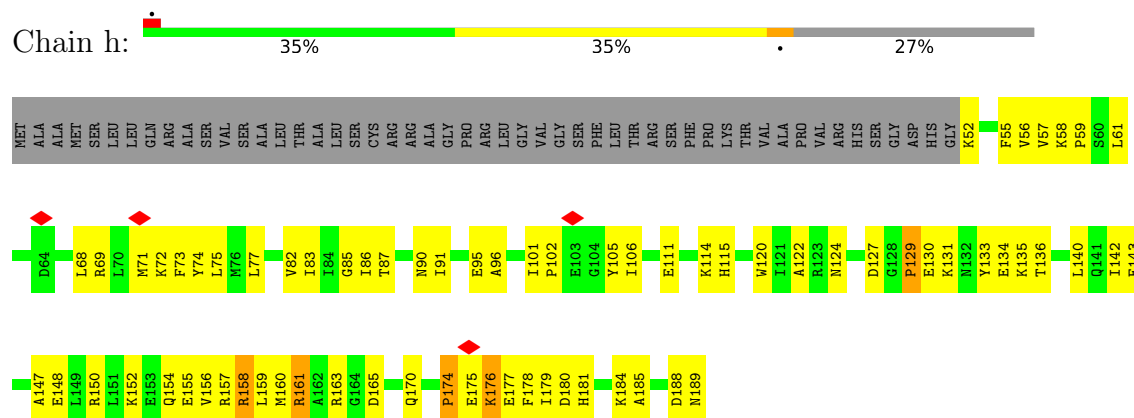
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



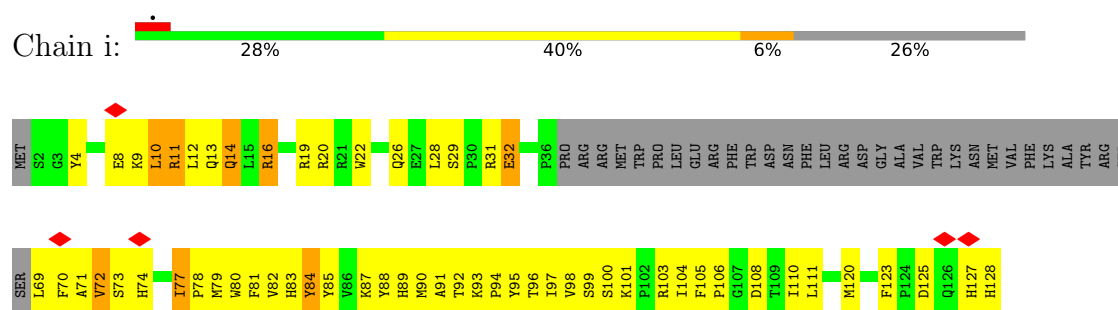
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



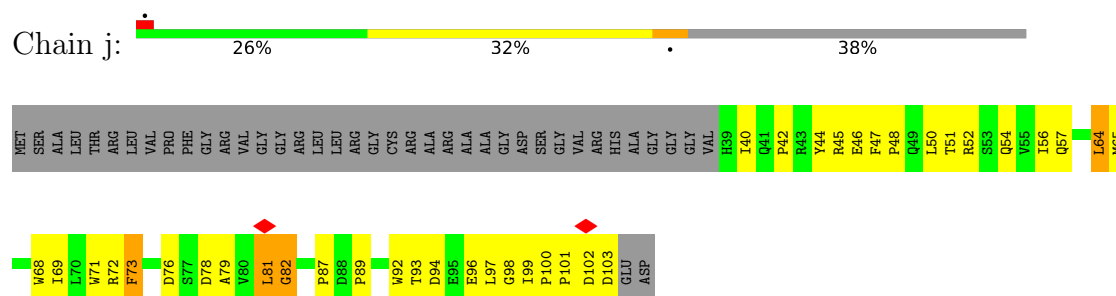
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



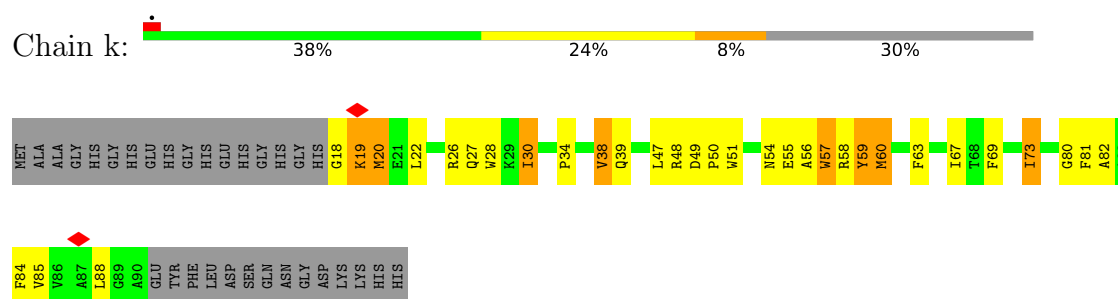
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



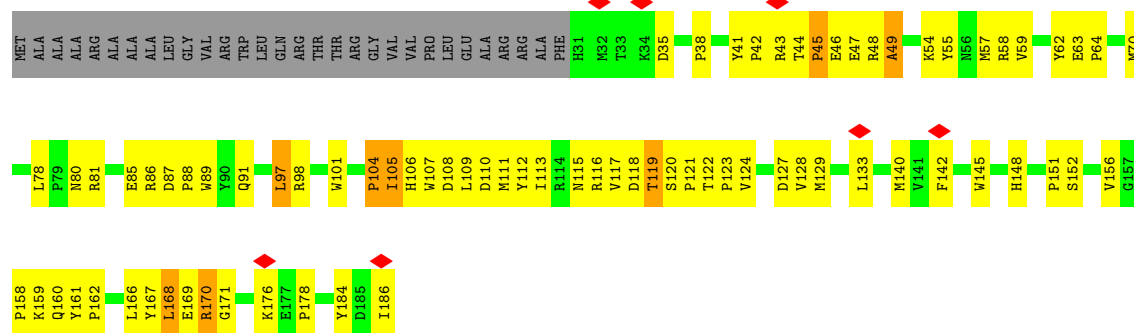
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



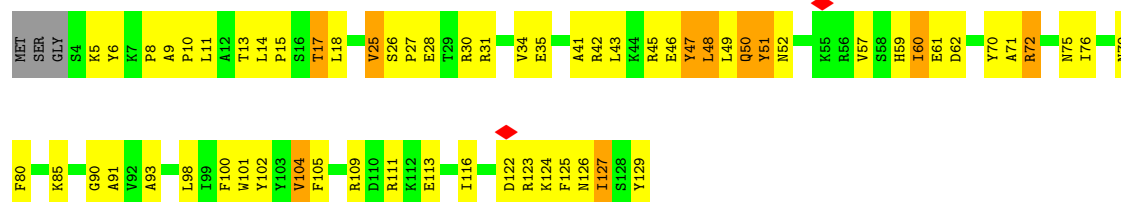
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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



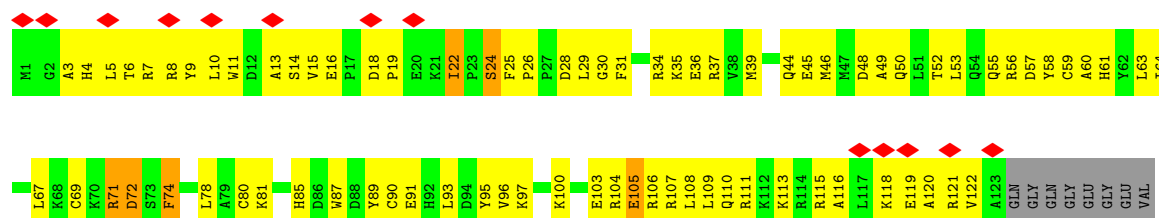
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



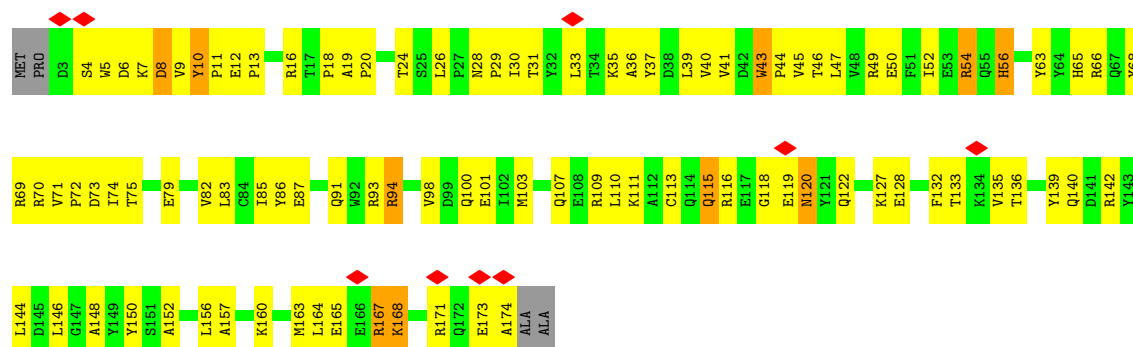
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



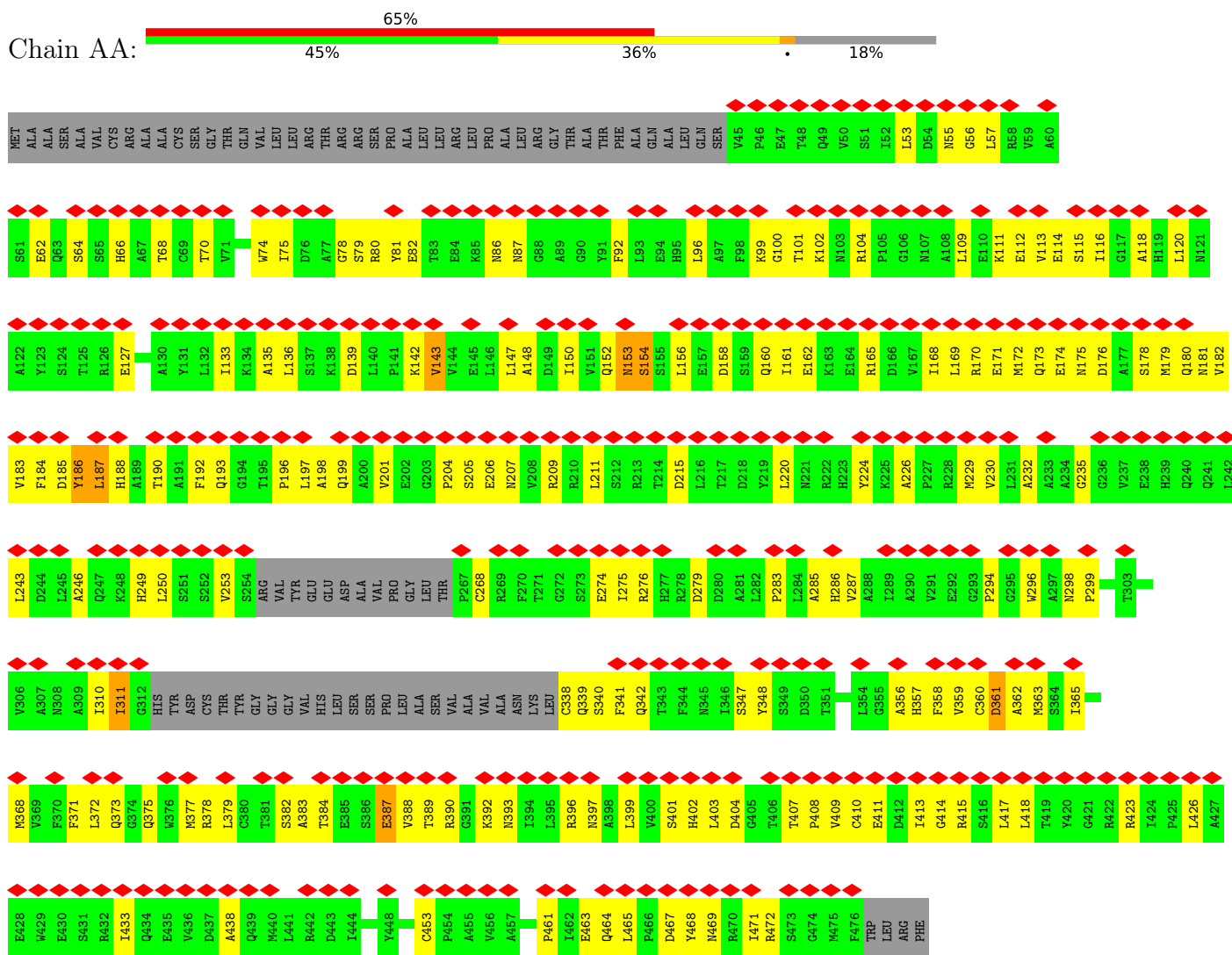
GLY
PRO
GLU
VAL
ALA
LEU

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

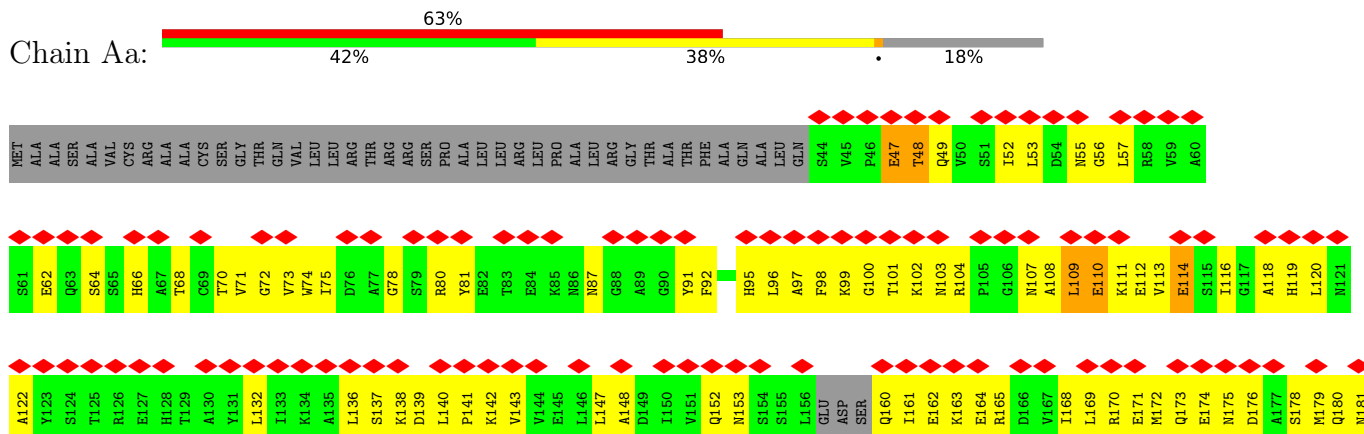
Chain p: 



Chain AA:



Chain Aa:

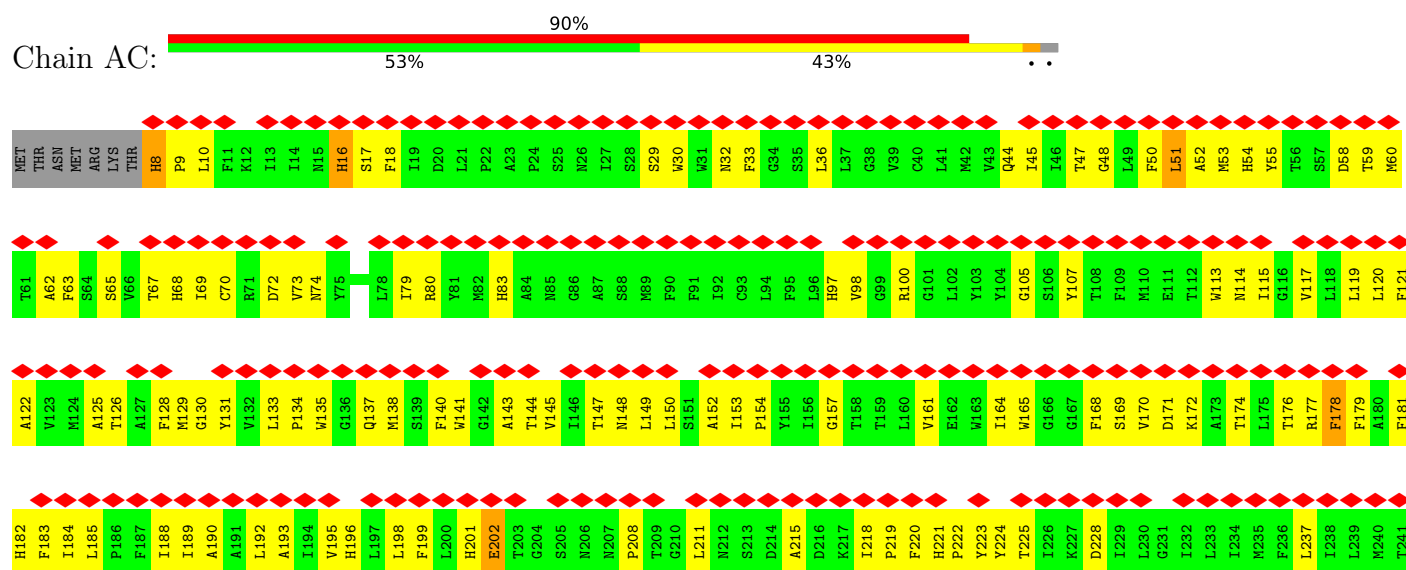




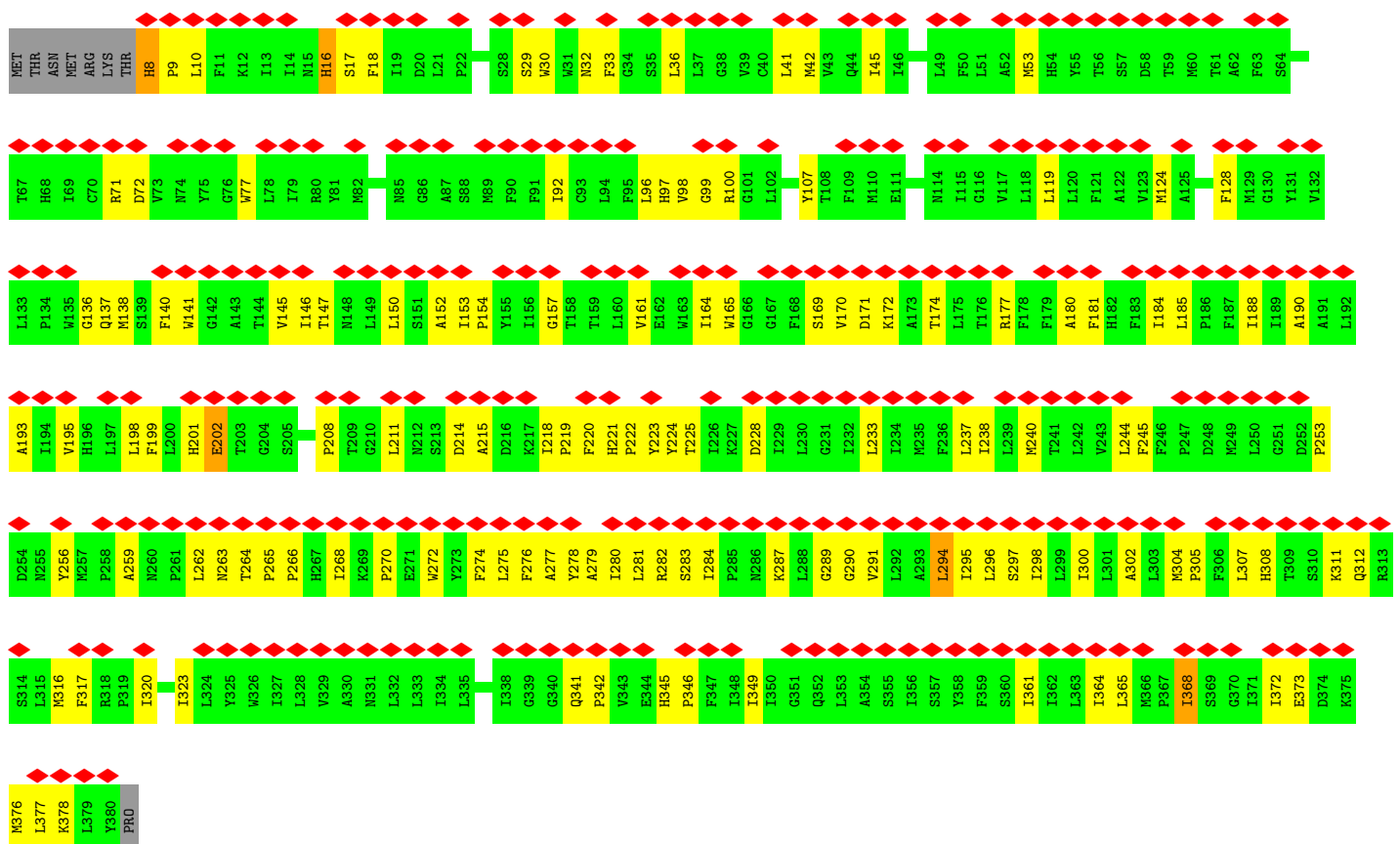
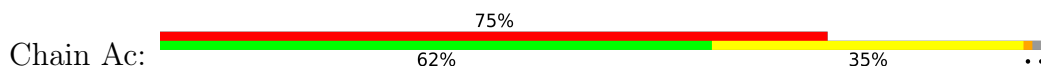
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



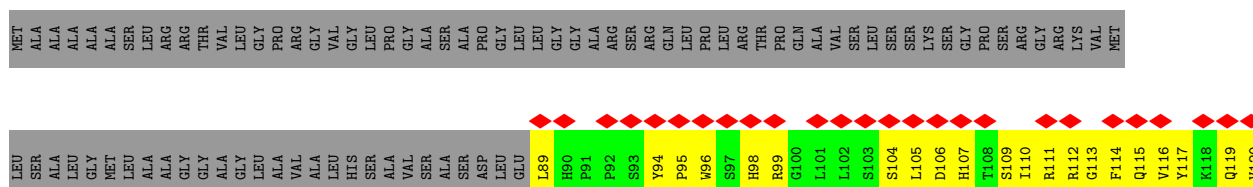
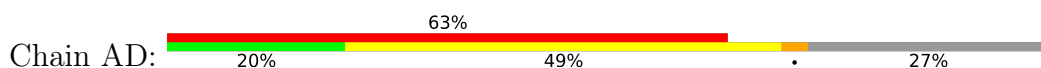
• Molecule 47: Cytochrome b

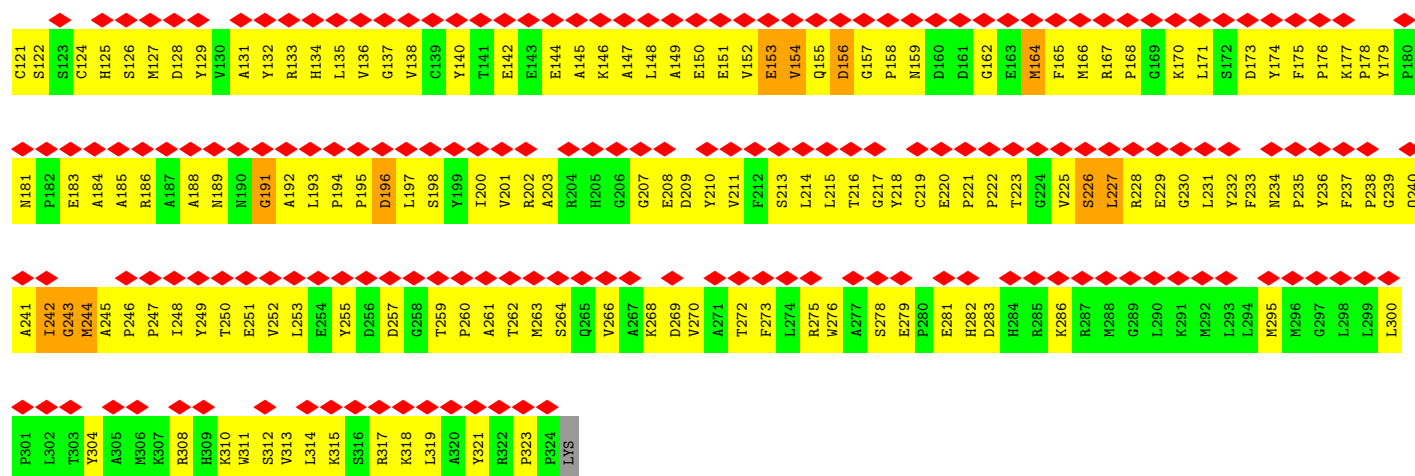


- Molecule 47: Cytochrome b

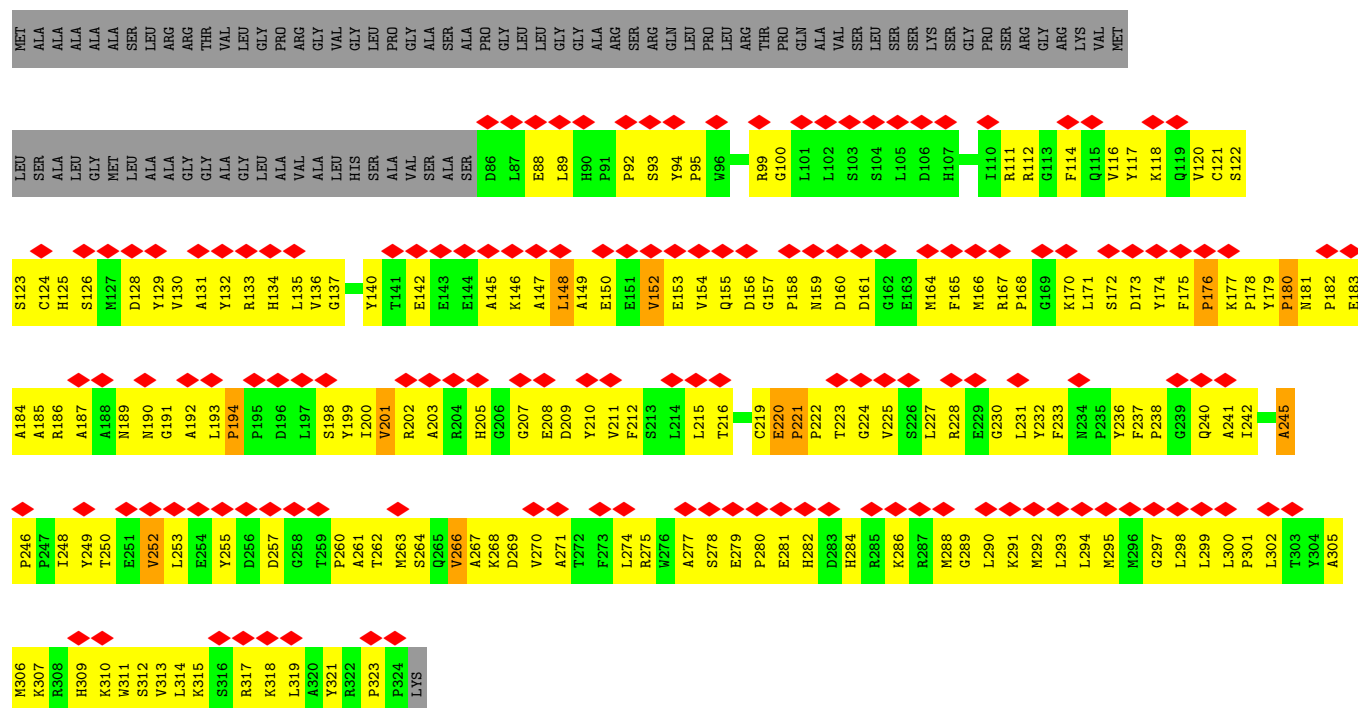


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

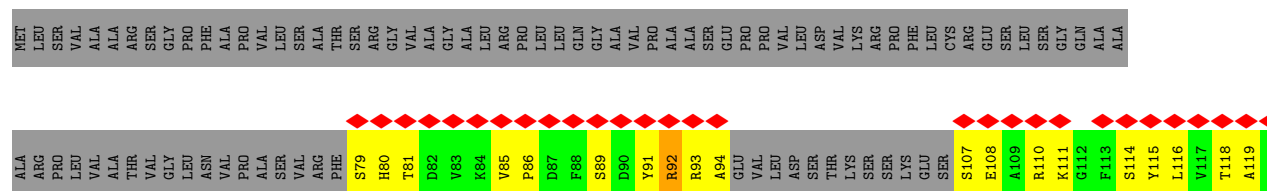


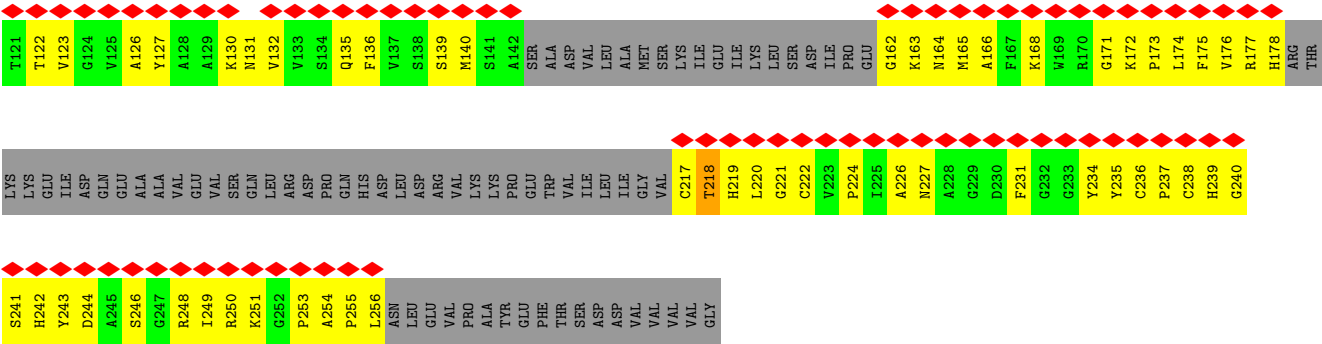


• Molecule 48: Cytochrome c1, heme protein, mitochondrial

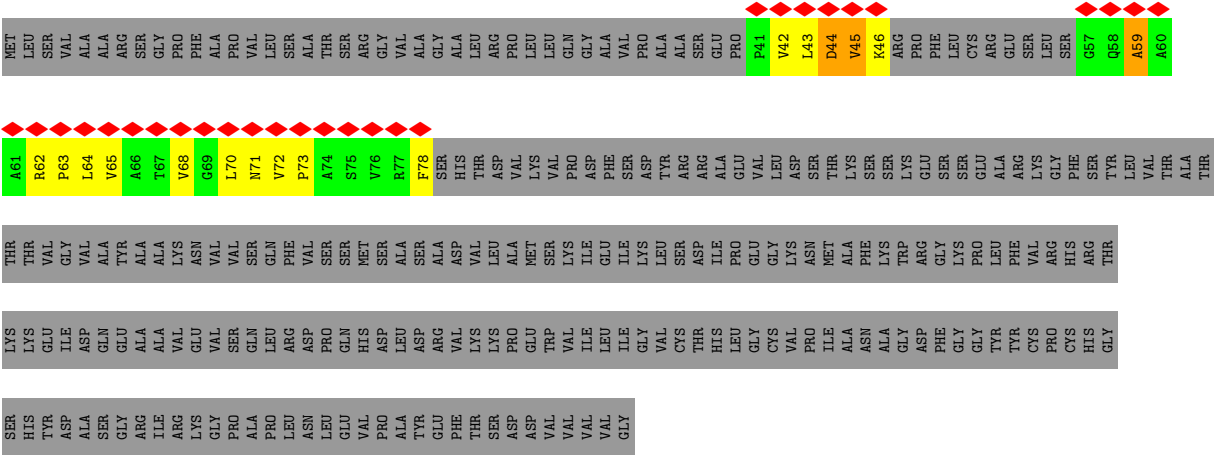


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

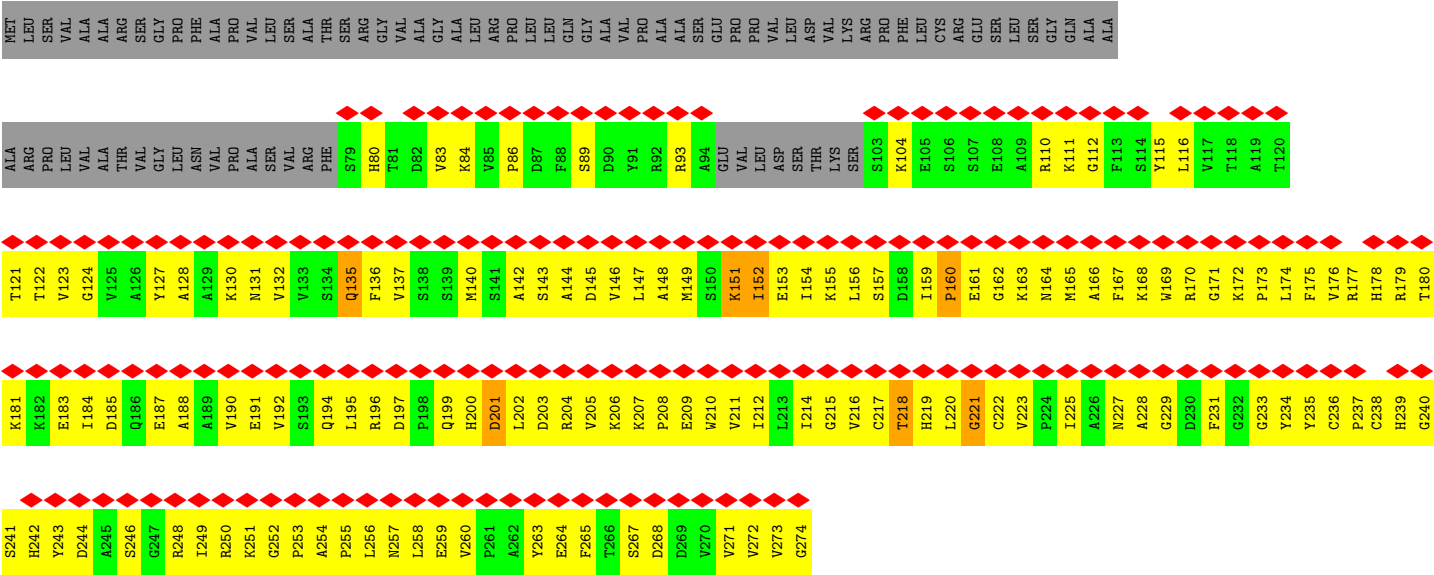
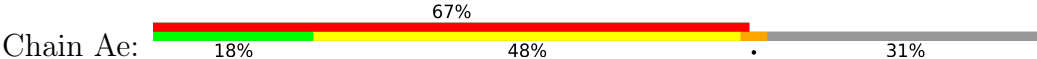


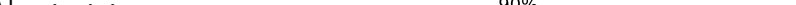


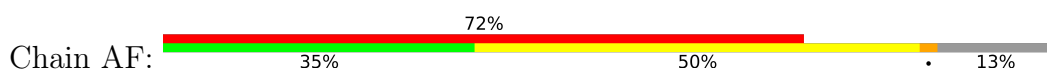
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

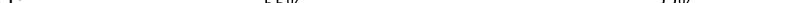


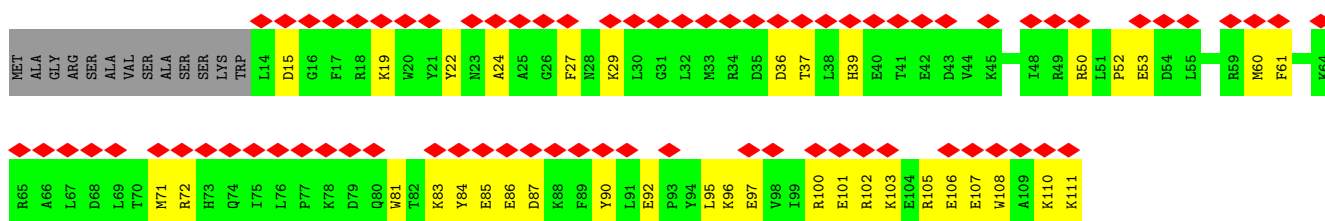
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

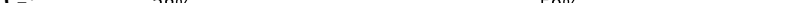


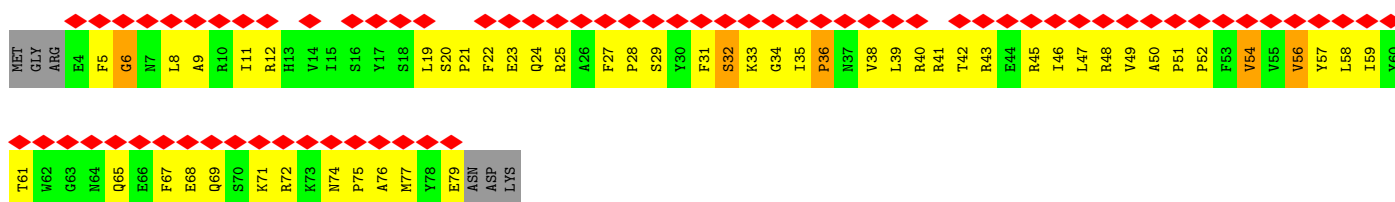
- Chain Ai: 



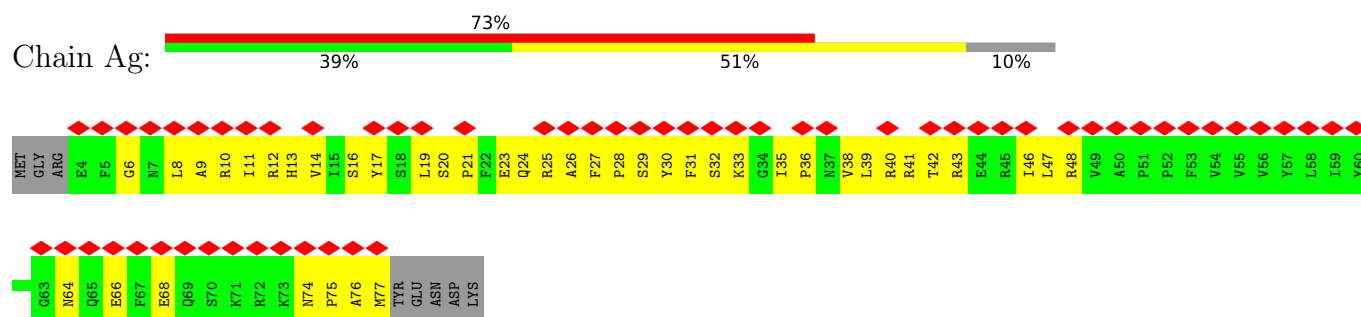
- Chain Af: 



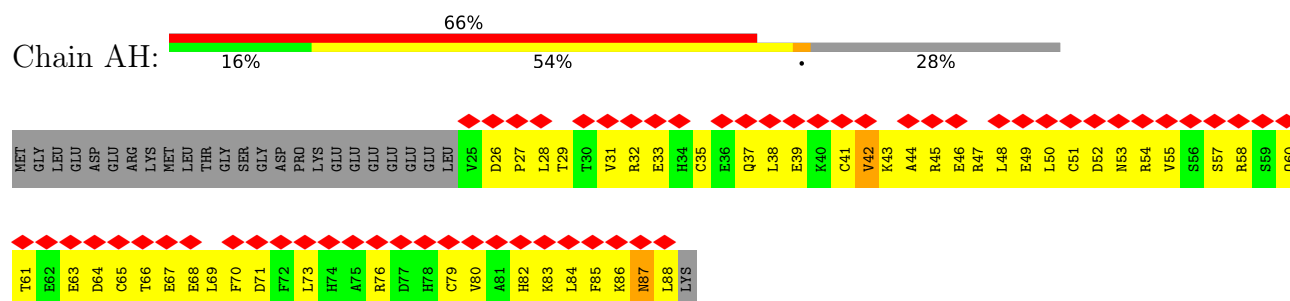
- Chain AG:  28% 87% 59% 6% 7%



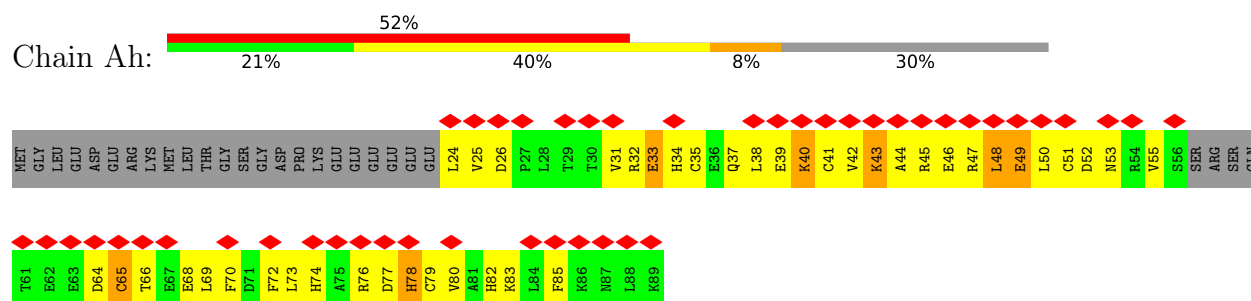
- Molecule 51: Cytochrome b-c1 complex subunit 8



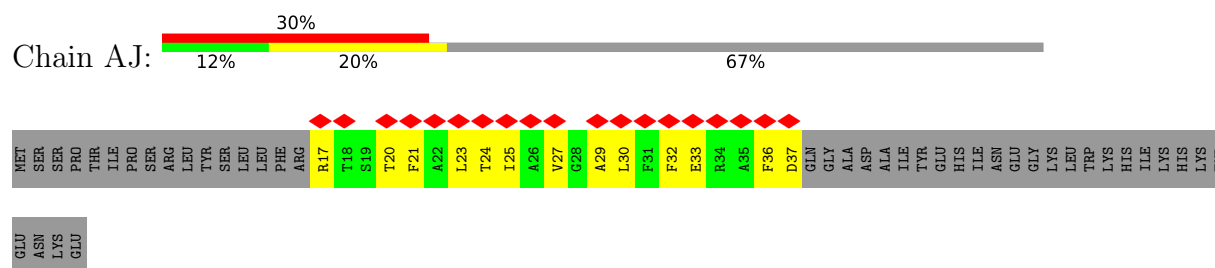
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



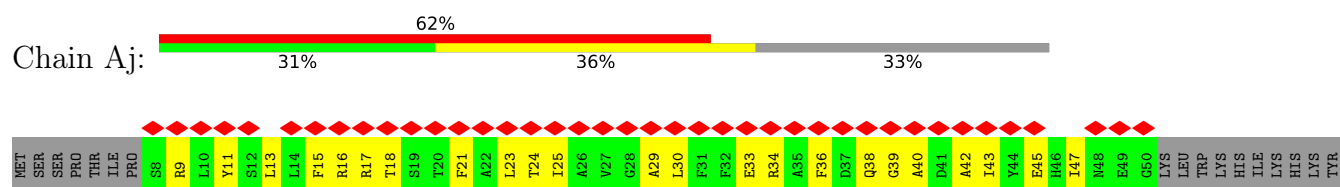
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 53: Cytochrome b-c1 complex subunit 9

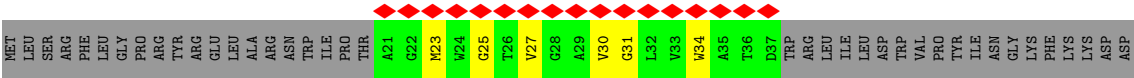


- Molecule 53: Cytochrome b-c1 complex subunit 9

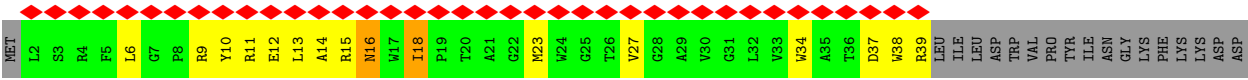


GLU
ASN
LYS
GLU

● 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	62294	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.94	1/820 (0.1%)	1.18	8/1118 (0.7%)
2	B	1.16	6/1272 (0.5%)	1.73	26/1722 (1.5%)
3	C	1.04	1/1689 (0.1%)	1.42	24/2300 (1.0%)
4	D	0.96	3/3527 (0.1%)	1.46	52/4776 (1.1%)
5	E	0.82	2/1675 (0.1%)	1.30	26/2282 (1.1%)
6	F	0.96	6/3363 (0.2%)	1.54	66/4543 (1.5%)
7	G	0.97	13/5374 (0.2%)	1.59	112/7281 (1.5%)
8	H	0.87	2/2608 (0.1%)	1.23	30/3563 (0.8%)
9	I	0.80	3/1409 (0.2%)	1.27	21/1904 (1.1%)
10	J	0.84	1/1257 (0.1%)	1.26	20/1704 (1.2%)
11	K	0.90	0/740	1.54	13/1005 (1.3%)
12	L	0.99	7/4921 (0.1%)	1.57	107/6696 (1.6%)
13	M	1.01	7/3717 (0.2%)	1.57	86/5062 (1.7%)
14	N	1.01	3/2756 (0.1%)	1.44	51/3751 (1.4%)
15	O	1.00	8/2666 (0.3%)	1.40	41/3615 (1.1%)
16	P	0.77	2/2793 (0.1%)	1.19	23/3787 (0.6%)
17	Q	0.97	3/963 (0.3%)	1.40	11/1302 (0.8%)
18	R	0.63	0/671	1.06	4/903 (0.4%)
19	S	0.86	2/678 (0.3%)	1.37	13/915 (1.4%)
20	T	0.75	0/613	1.11	7/826 (0.8%)
20	U	0.98	1/731 (0.1%)	1.30	14/988 (1.4%)
21	V	0.82	0/937	1.24	4/1270 (0.3%)
22	W	0.89	2/993 (0.2%)	0.99	7/1335 (0.5%)
23	X	0.63	0/1422	1.01	8/1921 (0.4%)
24	Y	0.86	0/1054	0.98	2/1429 (0.1%)
25	Z	0.75	2/1176 (0.2%)	1.17	10/1587 (0.6%)
26	a	0.89	0/561	1.60	14/755 (1.9%)
27	b	0.69	0/651	1.11	7/895 (0.8%)
28	c	0.93	1/400 (0.2%)	1.49	12/544 (2.2%)
29	d	1.02	2/1028 (0.2%)	1.16	11/1387 (0.8%)
30	e	0.69	1/900 (0.1%)	1.01	5/1199 (0.4%)
31	f	0.95	1/451 (0.2%)	1.38	12/607 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.89	3/886 (0.3%)	1.35	19/1207 (1.6%)
33	h	0.77	1/1197 (0.1%)	1.26	8/1621 (0.5%)
34	i	0.84	0/829	1.35	14/1127 (1.2%)
35	j	0.80	0/588	1.32	8/805 (1.0%)
36	k	0.98	2/600 (0.3%)	1.44	14/810 (1.7%)
37	l	0.98	3/1367 (0.2%)	1.22	9/1866 (0.5%)
38	m	0.92	2/1079 (0.2%)	1.24	17/1463 (1.2%)
39	n	0.94	2/1596 (0.1%)	1.32	18/2162 (0.8%)
40	o	0.82	1/1075 (0.1%)	1.14	10/1442 (0.7%)
41	p	0.71	1/1485 (0.1%)	1.05	15/2007 (0.7%)
42	q	0.83	5/1059 (0.5%)	1.25	15/1439 (1.0%)
43	r	0.94	2/701 (0.3%)	1.56	12/948 (1.3%)
44	s	1.11	0/198	1.68	5/269 (1.9%)
45	AA	0.62	2/3134 (0.1%)	0.89	11/4248 (0.3%)
45	Aa	0.58	1/3134 (0.0%)	0.89	14/4248 (0.3%)
46	AB	0.44	0/3187	0.65	3/4308 (0.1%)
46	Ab	0.58	1/3187 (0.0%)	0.91	18/4308 (0.4%)
47	AC	0.51	0/3089	0.84	10/4221 (0.2%)
47	Ac	0.45	0/3089	0.73	7/4221 (0.2%)
48	AD	0.54	0/1937	0.97	11/2632 (0.4%)
48	Ad	0.85	3/1962 (0.2%)	1.07	17/2666 (0.6%)
49	AE	0.47	0/851	0.94	3/1146 (0.3%)
49	AI	1.86	2/202 (1.0%)	1.43	4/274 (1.5%)
49	Ae	0.63	0/1483	1.10	7/2007 (0.3%)
49	Ai	1.87	2/205 (1.0%)	1.49	5/277 (1.8%)
50	AF	0.64	0/875	0.90	6/1173 (0.5%)
50	Af	0.38	0/884	0.52	0/1184
51	AG	0.57	1/662 (0.2%)	1.10	5/895 (0.6%)
51	Ag	0.55	0/640	0.93	1/865 (0.1%)
52	AH	0.53	0/534	0.84	2/717 (0.3%)
52	Ah	0.76	0/518	1.14	7/694 (1.0%)
53	AJ	0.41	0/168	0.62	0/226
53	Aj	0.59	0/352	0.78	0/474
54	AK	0.47	0/121	0.84	1/166 (0.6%)
54	Ak	0.52	0/320	1.14	6/437 (1.4%)
All	All	0.83	114/97010 (0.1%)	1.24	1149/131525 (0.9%)

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	AI	44	ASP	C-N	20.17	1.52	1.33
49	Ai	44	ASP	C-N	19.98	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Ad	221	PRO	N-CD	18.51	1.73	1.47
15	O	247	PRO	N-CD	16.66	1.71	1.47
49	Ai	45	VAL	C-N	15.71	1.53	1.33

The worst 5 of 1149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	231	ILE	N-CA-C	-19.19	90.97	113.42
2	B	99	CYS	N-CA-C	-18.00	91.45	113.41
2	B	170	TYR	N-CA-C	-17.69	89.93	111.33
7	G	174	THR	N-CA-C	-16.82	89.07	114.64
2	B	122	ARG	N-CA-CB	-16.68	85.52	110.04

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	799	0	851	162	0
2	B	1241	0	1252	180	0
3	C	1643	0	1598	133	0
4	D	3438	0	3379	391	0
5	E	1635	0	1625	184	0
6	F	3288	0	3243	373	0
7	G	5287	0	5322	585	0
8	H	2532	0	2621	350	0
9	I	1380	0	1339	170	0
10	J	1229	0	1250	230	0
11	K	729	0	764	101	0
12	L	4798	0	4986	608	0
13	M	3630	0	3854	544	0
14	N	2694	0	2896	336	0
15	O	2599	0	2552	306	0
16	P	2720	0	2740	257	0
17	Q	940	0	930	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	660	0	639	69	0
19	S	667	0	685	75	0
20	T	604	0	596	70	0
20	U	718	0	705	89	0
21	V	915	0	954	78	0
22	W	970	0	991	92	0
23	X	1385	0	1366	150	0
24	Y	1030	0	1015	75	0
25	Z	1145	0	1139	171	0
26	a	548	0	562	83	0
27	b	628	0	628	72	0
28	c	389	0	385	48	0
29	d	996	0	1001	93	0
30	e	877	0	869	130	0
31	f	439	0	433	37	0
32	g	858	0	787	75	0
33	h	1162	0	1163	139	0
34	i	802	0	802	84	0
35	j	563	0	510	72	0
36	k	582	0	584	46	0
37	l	1312	0	1204	103	0
38	m	1050	0	1061	109	0
39	n	1541	0	1470	151	0
40	o	1050	0	1045	103	0
41	p	1452	0	1413	140	0
42	q	1025	0	980	80	0
43	r	686	0	710	70	0
44	s	193	0	187	36	0
45	AA	3077	0	2996	199	0
45	Aa	3076	0	3001	230	0
46	AB	3137	0	3143	153	0
46	Ab	3137	0	3143	252	0
47	AC	2988	0	3045	294	0
47	Ac	2988	0	3045	216	0
48	AD	1878	0	1827	294	0
48	Ad	1903	0	1848	279	0
49	AE	830	0	802	136	0
49	AI	200	0	216	32	0
49	Ae	1451	0	1433	264	0
49	Ai	204	0	221	34	0
50	AF	855	0	841	64	0
50	Af	864	0	854	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AG	643	0	643	88	0
51	Ag	622	0	628	54	0
52	AH	527	0	507	76	0
52	Ah	512	0	497	85	0
53	AJ	165	0	162	81	0
53	Aj	345	0	333	37	0
54	AK	118	0	111	39	0
54	Ak	309	0	304	27	0
55	A	42	0	58	8	0
55	Aa	23	0	20	3	0
55	Ac	35	0	44	7	0
55	Ag	38	0	53	9	0
55	H	48	0	73	12	0
55	I	51	0	82	8	0
55	K	46	0	66	9	0
55	L	167	0	233	28	0
55	M	88	0	130	8	0
55	N	51	0	82	11	0
55	Y	41	0	56	8	0
55	d	31	0	36	8	0
55	i	40	0	54	19	0
55	m	139	0	209	23	0
56	B	8	0	0	7	0
56	F	8	0	0	10	0
56	G	16	0	0	10	0
56	I	16	0	0	10	0
57	B	18	0	18	11	0
58	B	78	0	107	23	0
59	E	4	0	0	4	0
59	G	4	0	0	4	0
60	F	31	0	19	3	0
61	H	35	0	43	4	0
62	Ag	98	0	84	9	0
62	L	78	0	100	16	0
62	X	67	0	81	9	0
62	a	57	0	58	12	0
62	h	70	0	87	17	0
63	O	27	0	12	11	0
64	P	48	0	26	7	0
65	R	1	0	0	0	0
66	W	32	0	0	3	0
66	n	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	AC	86	0	60	27	0
67	Ac	86	0	60	11	0
68	AC	28	0	31	11	0
68	Ac	28	0	31	15	0
69	AD	43	0	32	18	0
69	Ad	43	0	32	12	0
70	Ac	23	0	23	20	0
71	Ad	36	0	45	39	0
All	All	96599	0	96831	8626	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 45.

The worst 5 of 8626 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)
1:A:52:SER:HB2	1:A:55:PHE:CD2	1.31	1.61
15:O:247:PRO:CD	15:O:247:PRO:N	1.71	1.38
49:Ae:239:HIS:ND1	49:Ae:253:PRO:HG3	1.39	1.37
1:A:52:SER:CB	1:A:55:PHE:CD2	2.10	1.33
1:A:52:SER:CB	1:A:55:PHE:HD2	1.41	1.32

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	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
2	B	153/224 (68%)	141 (92%)	11 (7%)	1 (1%)	18	54
3	C	196/263 (74%)	189 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	423/463 (91%)	398 (94%)	24 (6%)	1 (0%)	43	77
5	E	208/248 (84%)	194 (93%)	14 (7%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	635 (93%)	50 (7%)	0	100	100
8	H	313/318 (98%)	281 (90%)	31 (10%)	1 (0%)	36	71
9	I	168/212 (79%)	152 (90%)	16 (10%)	0	100	100
10	J	157/172 (91%)	148 (94%)	9 (6%)	0	100	100
11	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
12	L	604/607 (100%)	573 (95%)	31 (5%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
16	P	337/377 (89%)	309 (92%)	28 (8%)	0	100	100
17	Q	114/175 (65%)	100 (88%)	14 (12%)	0	100	100
18	R	81/116 (70%)	72 (89%)	9 (11%)	0	100	100
19	S	81/99 (82%)	74 (91%)	7 (9%)	0	100	100
20	T	73/156 (47%)	69 (94%)	4 (6%)	0	100	100
20	U	87/156 (56%)	81 (93%)	6 (7%)	0	100	100
21	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
22	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
23	X	167/172 (97%)	148 (89%)	19 (11%)	0	100	100
24	Y	137/143 (96%)	132 (96%)	5 (4%)	0	100	100
25	Z	136/144 (94%)	129 (95%)	5 (4%)	2 (2%)	8	38
26	a	65/70 (93%)	59 (91%)	6 (9%)	0	100	100
27	b	78/84 (93%)	69 (88%)	9 (12%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	103/106 (97%)	96 (93%)	7 (7%)	0	100	100
31	f	49/57 (86%)	48 (98%)	1 (2%)	0	100	100
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	91/128 (71%)	81 (89%)	10 (11%)	0	100	100
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	71/104 (68%)	68 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	176/179 (98%)	165 (94%)	10 (6%)	1 (1%)	21	58
40	o	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
41	p	170/176 (97%)	153 (90%)	17 (10%)	0	100	100
42	q	119/145 (82%)	110 (92%)	9 (8%)	0	100	100
43	r	78/113 (69%)	75 (96%)	3 (4%)	0	100	100
44	s	21/104 (20%)	20 (95%)	1 (5%)	0	100	100
45	AA	389/480 (81%)	372 (96%)	17 (4%)	0	100	100
45	Aa	386/480 (80%)	369 (96%)	17 (4%)	0	100	100
46	AB	416/453 (92%)	408 (98%)	8 (2%)	0	100	100
46	Ab	416/453 (92%)	396 (95%)	20 (5%)	0	100	100
47	AC	371/381 (97%)	361 (97%)	10 (3%)	0	100	100
47	Ac	371/381 (97%)	366 (99%)	5 (1%)	0	100	100
48	AD	234/325 (72%)	213 (91%)	21 (9%)	0	100	100
48	Ad	237/325 (73%)	224 (94%)	12 (5%)	1 (0%)	30	66
49	AE	101/274 (37%)	95 (94%)	6 (6%)	0	100	100
49	AI	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
49	Ae	184/274 (67%)	168 (91%)	15 (8%)	1 (0%)	24	62
49	Ai	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
50	AF	95/111 (86%)	94 (99%)	1 (1%)	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	70 (95%)	4 (5%)	0	100	100
51	Ag	72/82 (88%)	72 (100%)	0	0	100	100
52	AH	62/89 (70%)	61 (98%)	1 (2%)	0	100	100
52	Ah	58/89 (65%)	55 (95%)	3 (5%)	0	100	100
53	AJ	19/64 (30%)	19 (100%)	0	0	100	100
53	Aj	41/64 (64%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	AK	15/56 (27%)	15 (100%)	0	0	100	100
54	Ak	36/56 (64%)	34 (94%)	2 (6%)	0	100	100
All	All	11672/14392 (81%)	11022 (94%)	641 (6%)	9 (0%)	47	82

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	324	GLY
8	H	196	ALA
14	N	109	ALA
25	Z	129	THR
2	B	195	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/104 (86%)	88 (99%)	1 (1%)	65	73
2	B	131/185 (71%)	129 (98%)	2 (2%)	57	70
3	C	181/227 (80%)	181 (100%)	0	100	100
4	D	368/395 (93%)	366 (100%)	2 (0%)	81	81
5	E	182/206 (88%)	180 (99%)	2 (1%)	65	73
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	84
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	279/280 (100%)	277 (99%)	2 (1%)	76	78
9	I	146/178 (82%)	146 (100%)	0	100	100
10	J	129/137 (94%)	126 (98%)	3 (2%)	44	64
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	415/415 (100%)	414 (100%)	1 (0%)	87	85
14	N	307/308 (100%)	305 (99%)	2 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	296/325 (91%)	295 (100%)	1 (0%)	86	84
17	Q	103/153 (67%)	101 (98%)	2 (2%)	50	66
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	82/135 (61%)	82 (100%)	0	100	100
21	V	100/102 (98%)	98 (98%)	2 (2%)	48	65
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	119/123 (97%)	119 (100%)	0	100	100
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	71/73 (97%)	71 (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	93/94 (99%)	92 (99%)	1 (1%)	65	73
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	90/120 (75%)	89 (99%)	1 (1%)	65	73
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	55/78 (70%)	55 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	162 (99%)	1 (1%)	78	80
40	o	112/121 (93%)	112 (100%)	0	100	100
41	p	156/158 (99%)	156 (100%)	0	100	100
42	q	110/131 (84%)	110 (100%)	0	100	100
43	r	76/96 (79%)	75 (99%)	1 (1%)	61	71
44	s	23/95 (24%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	AA	333/398 (84%)	332 (100%)	1 (0%)	86	84
45	Aa	332/398 (83%)	332 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	327 (100%)	1 (0%)	86	84
47	AC	325/333 (98%)	323 (99%)	2 (1%)	78	80
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	201/260 (77%)	201 (100%)	0	100	100
48	Ad	204/260 (78%)	201 (98%)	3 (2%)	57	70
49	AE	86/224 (38%)	86 (100%)	0	100	100
49	AI	21/224 (9%)	20 (95%)	1 (5%)	23	45
49	Ae	158/224 (70%)	156 (99%)	2 (1%)	61	71
49	Ai	21/224 (9%)	20 (95%)	1 (5%)	23	45
50	AF	89/99 (90%)	89 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	67/74 (90%)	67 (100%)	0	100	100
52	AH	61/83 (74%)	60 (98%)	1 (2%)	55	69
52	Ah	59/83 (71%)	59 (100%)	0	100	100
53	AJ	16/55 (29%)	16 (100%)	0	100	100
53	Aj	34/55 (62%)	34 (100%)	0	100	100
54	AK	10/46 (22%)	10 (100%)	0	100	100
54	Ak	29/46 (63%)	29 (100%)	0	100	100
All	All	10260/12260 (84%)	10218 (100%)	42 (0%)	80	82

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	r	91	GLU
47	Ac	294	LEU
45	AA	387	GLU
52	AH	42	VAL
48	Ad	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 244 such sidechains are listed below:

Mol	Chain	Res	Type
20	U	101	ASN
46	Ab	212	HIS
35	j	83	HIS
45	Aa	402	HIS
49	Ae	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 1 is monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	3PE	H	401	-	47,47,50	0.93	2 (4%)	50,52,55	1.12	3 (6%)
55	3PE	m	202	-	50,50,50	0.91	2 (4%)	53,55,55	1.15	4 (7%)
55	3PE	N	401	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	4 (7%)
58	PC1	B	303	-	34,34,53	1.14	2 (5%)	40,42,61	1.13	3 (7%)
67	HEM	AC	402	47	50,50,50	1.60	9 (18%)	67,82,82	1.75	15 (22%)
55	3PE	m	203	-	40,40,50	1.01	2 (5%)	43,45,55	1.14	3 (6%)
55	3PE	Aa	501	-	22,22,50	1.36	2 (9%)	25,27,55	1.15	3 (12%)
66	EHZ	W	201	-	29,31,37	1.63	5 (17%)	37,41,47	1.62	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	UQ6	Ac	405	-	28,28,43	2.54	6 (21%)	36,37,55	1.49	6 (16%)
55	3PE	A	201	-	41,41,50	1.01	2 (4%)	44,46,55	1.10	2 (4%)
55	3PE	d	201	-	30,30,50	1.15	2 (6%)	33,35,55	1.33	5 (15%)
62	CDL	X	201	-	66,66,99	1.10	4 (6%)	72,78,111	1.29	7 (9%)
62	CDL	h	201	-	69,69,99	1.09	4 (5%)	75,81,111	1.23	7 (9%)
69	HEC	Ad	401	48	46,50,50	1.81	5 (10%)	58,82,82	1.92	5 (8%)
55	3PE	I	301	-	50,50,50	0.91	2 (4%)	53,55,55	1.04	2 (3%)
62	CDL	L	704	-	77,77,99	1.01	4 (5%)	83,89,111	1.14	6 (7%)
55	3PE	M	501	-	36,36,50	1.09	2 (5%)	39,41,55	1.22	4 (10%)
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.22	6 (9%)
64	NDP	P	401	-	51,52,52	1.16	5 (9%)	71,80,80	1.54	11 (15%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	38,40,52	1.29	4 (10%)
55	3PE	L	701	-	39,39,50	1.03	2 (5%)	42,44,55	1.15	3 (7%)
56	SF4	F	502	6	0,12,12	-	-	-	-	-
67	HEM	AC	401	47	50,50,50	1.55	6 (12%)	67,82,82	1.70	11 (16%)
55	3PE	Y	201	-	40,40,50	1.02	2 (5%)	43,45,55	1.19	5 (11%)
63	ADP	O	401	-	28,29,29	1.36	4 (14%)	43,45,45	1.87	10 (23%)
55	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.14	4 (7%)
56	SF4	G	801	7	0,12,12	-	-	-	-	-
55	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.16	3 (8%)
57	UQ1	B	302	-	18,18,18	2.02	2 (11%)	24,25,25	1.39	5 (20%)
55	3PE	K	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.12	4 (8%)
56	SF4	I	303	9	0,12,12	-	-	-	-	-
56	SF4	B	301	2	0,12,12	-	-	-	-	-
56	SF4	G	802	-	0,12,12	-	-	-	-	-
61	UQ9	H	400	-	35,35,58	0.80	2 (5%)	43,45,73	0.60	1 (2%)
70	U10	Ac	404	-	23,23,63	1.29	4 (17%)	30,31,79	2.06	7 (23%)
62	CDL	Ag	102	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	8 (13%)
67	HEM	Ac	401	47	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
58	PC1	B	304	-	42,42,53	1.05	2 (4%)	48,50,61	1.02	3 (6%)
62	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.37	7 (14%)
55	3PE	L	705	-	37,37,50	1.04	2 (5%)	40,42,55	1.14	3 (7%)
68	UQ6	AC	403	-	28,28,43	2.52	6 (21%)	36,37,55	1.61	10 (27%)
69	HEC	AD	401	48	46,50,50	2.53	23 (50%)	58,82,82	2.10	21 (36%)
66	EHZ	n	201	-	29,31,37	1.78	7 (24%)	37,41,47	1.65	7 (18%)
59	FES	E	301	5	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	3PE	i	201	-	39,39,50	1.03	2 (5%)	42,44,55	1.06	2 (4%)
56	SF4	I	302	9	0,12,12	-	-	-		
59	FES	G	803	7	0,4,4	-	-	-		
67	HEM	Ac	402	47	50,50,50	1.61	8 (16%)	67,82,82	1.86	16 (23%)
55	3PE	M	502	-	50,50,50	0.90	2 (4%)	53,55,55	1.16	5 (9%)
55	3PE	m	201	-	46,46,50	0.97	2 (4%)	49,51,55	1.12	3 (6%)
55	3PE	L	703	-	39,39,50	1.02	2 (5%)	42,44,55	1.16	3 (7%)
55	3PE	Ag	103	-	37,37,50	1.06	2 (5%)	40,42,55	1.22	3 (7%)
60	FMN	F	501	-	33,33,33	1.43	5 (15%)	48,50,50	1.19	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	3PE	H	401	-	-	12/51/51/54	-
55	3PE	m	202	-	-	9/54/54/54	-
55	3PE	N	401	-	-	10/54/54/54	-
58	PC1	B	303	-	-	13/38/38/57	-
67	HEM	AC	402	47	-	6/14/54/54	-
55	3PE	m	203	-	-	7/44/44/54	-
55	3PE	Aa	501	-	-	5/26/26/54	-
66	EHZ	W	201	-	-	13/39/39/45	-
68	UQ6	Ac	405	-	-	5/21/21/39	0/1/1/1
55	3PE	A	201	-	-	11/45/45/54	-
55	3PE	d	201	-	-	7/34/34/54	-
62	CDL	X	201	-	-	22/77/77/110	-
62	CDL	h	201	-	-	24/80/80/110	-
69	HEC	Ad	401	48	-	4/14/54/54	-
55	3PE	I	301	-	-	14/54/54/54	-
62	CDL	L	704	-	-	27/88/88/110	-
55	3PE	M	501	-	-	13/40/40/54	-
62	CDL	a	101	-	-	16/67/67/110	-
64	NDP	P	401	-	-	5/34/77/77	0/5/5/5
71	3PH	Ad	402	-	-	9/37/37/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	3PE	L	701	-	-	5/43/43/54	-
56	SF4	F	502	6	-	-	0/6/5/5
67	HEM	AC	401	47	-	9/14/54/54	-
55	3PE	Y	201	-	-	10/44/44/54	-
63	ADP	O	401	-	-	2/16/32/32	0/3/3/3
55	3PE	L	702	-	-	13/52/52/54	-
56	SF4	G	801	7	-	-	0/6/5/5
55	3PE	Ac	403	-	-	2/38/38/54	-
57	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
55	3PE	K	101	-	-	16/49/49/54	-
61	UQ9	H	400	-	-	16/30/54/81	0/1/1/1
56	SF4	B	301	2	-	-	0/6/5/5
70	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
56	SF4	G	802	-	-	-	0/6/5/5
56	SF4	I	303	9	-	-	0/6/5/5
62	CDL	Ag	102	-	-	18/66/66/110	-
67	HEM	Ac	401	47	-	9/14/54/54	-
58	PC1	B	304	-	-	13/46/46/57	-
62	CDL	Ag	101	-	-	11/52/52/110	-
55	3PE	L	705	-	-	14/41/41/54	-
68	UQ6	AC	403	-	-	4/21/21/39	0/1/1/1
69	HEC	AD	401	48	-	3/14/54/54	-
66	EHZ	n	201	-	-	13/39/39/45	-
59	FES	E	301	5	-	-	0/1/1/1
55	3PE	i	201	-	-	15/43/43/54	-
56	SF4	I	302	9	-	-	0/6/5/5
59	FES	G	803	7	-	-	0/1/1/1
67	HEM	Ac	402	47	-	7/14/54/54	-
55	3PE	M	502	-	-	12/54/54/54	-
55	3PE	m	201	-	-	10/50/50/54	-
55	3PE	L	703	-	-	6/43/43/54	-
55	3PE	Ag	103	-	-	8/41/41/54	-
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3

The worst 5 of 175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	302	UQ1	C6-C5	7.48	1.48	1.35
68	Ac	405	UQ6	C5-C6	6.25	1.49	1.40
69	Ad	401	HEC	CAC-C3C	6.07	1.54	1.35
68	AC	403	UQ6	C5-C6	6.06	1.48	1.40
69	Ad	401	HEC	CAB-C3B	6.04	1.54	1.35

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	Ad	401	HEC	CBC-CAC-C3C	-8.55	110.34	127.43
69	Ad	401	HEC	CBB-CAB-C3B	-8.34	110.77	127.43
70	Ac	404	U10	C6-C1-C2	7.81	125.33	119.17
67	Ac	402	HEM	CHC-C4B-NB	6.13	131.03	124.42
66	W	201	EHZ	C8-C9-S1	5.97	121.09	113.56

There are no chirality outliers.

5 of 458 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	201	3PE	C1-O11-P-O14
55	A	201	3PE	C11-O13-P-O11
55	A	201	3PE	C11-O13-P-O14
55	A	201	3PE	C22-C21-O21-C2
55	H	401	3PE	C1-O11-P-O14

There are no ring outliers.

51 monomers are involved in 470 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	H	401	3PE	12	0
55	m	202	3PE	10	0
55	N	401	3PE	11	0
58	B	303	PC1	9	0
67	AC	402	HEM	9	0
55	m	203	3PE	4	0
55	Aa	501	3PE	3	0
66	W	201	EHZ	3	0
68	Ac	405	UQ6	15	0
55	A	201	3PE	8	0
55	d	201	3PE	8	0
62	X	201	CDL	9	0
62	h	201	CDL	17	0

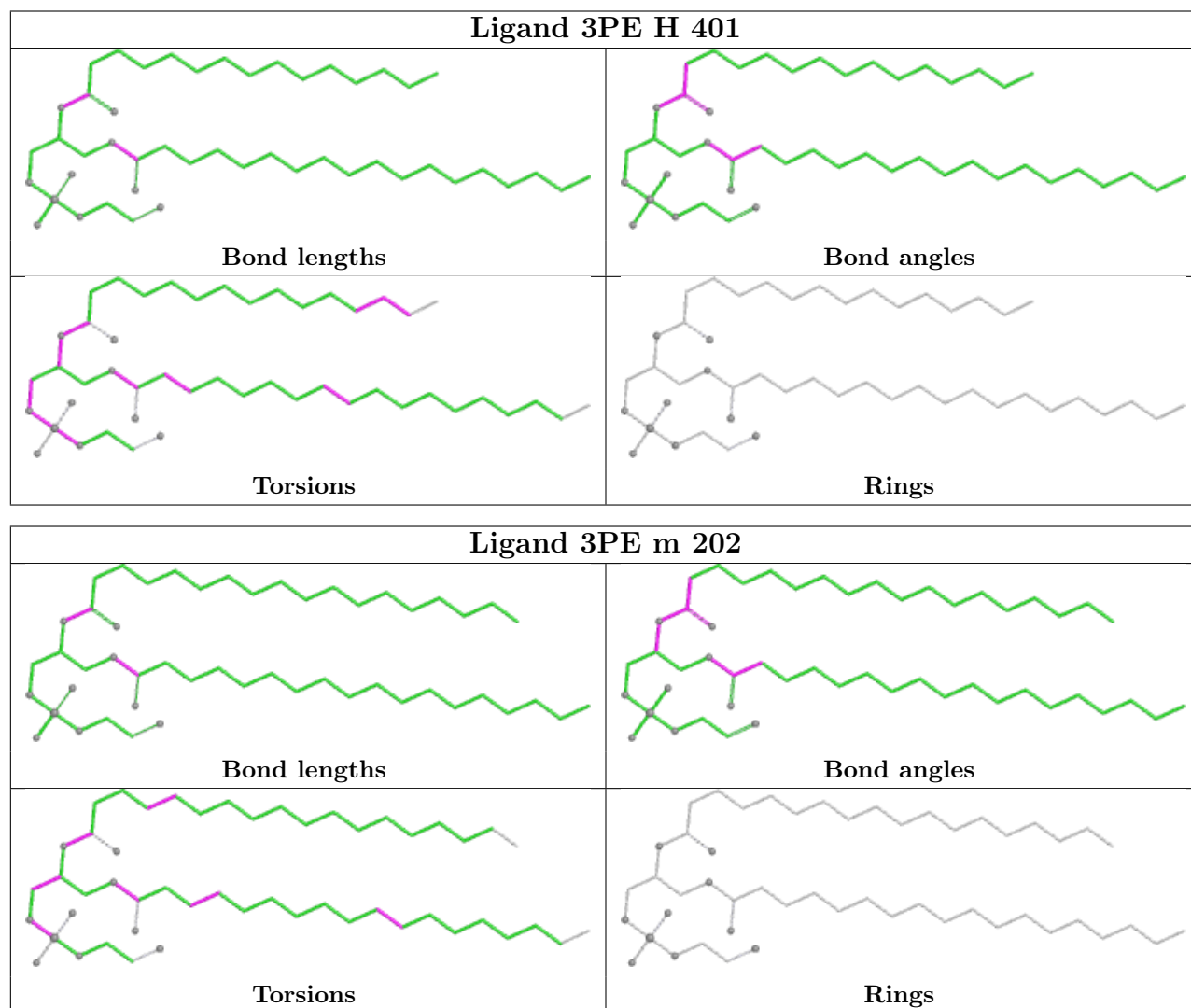
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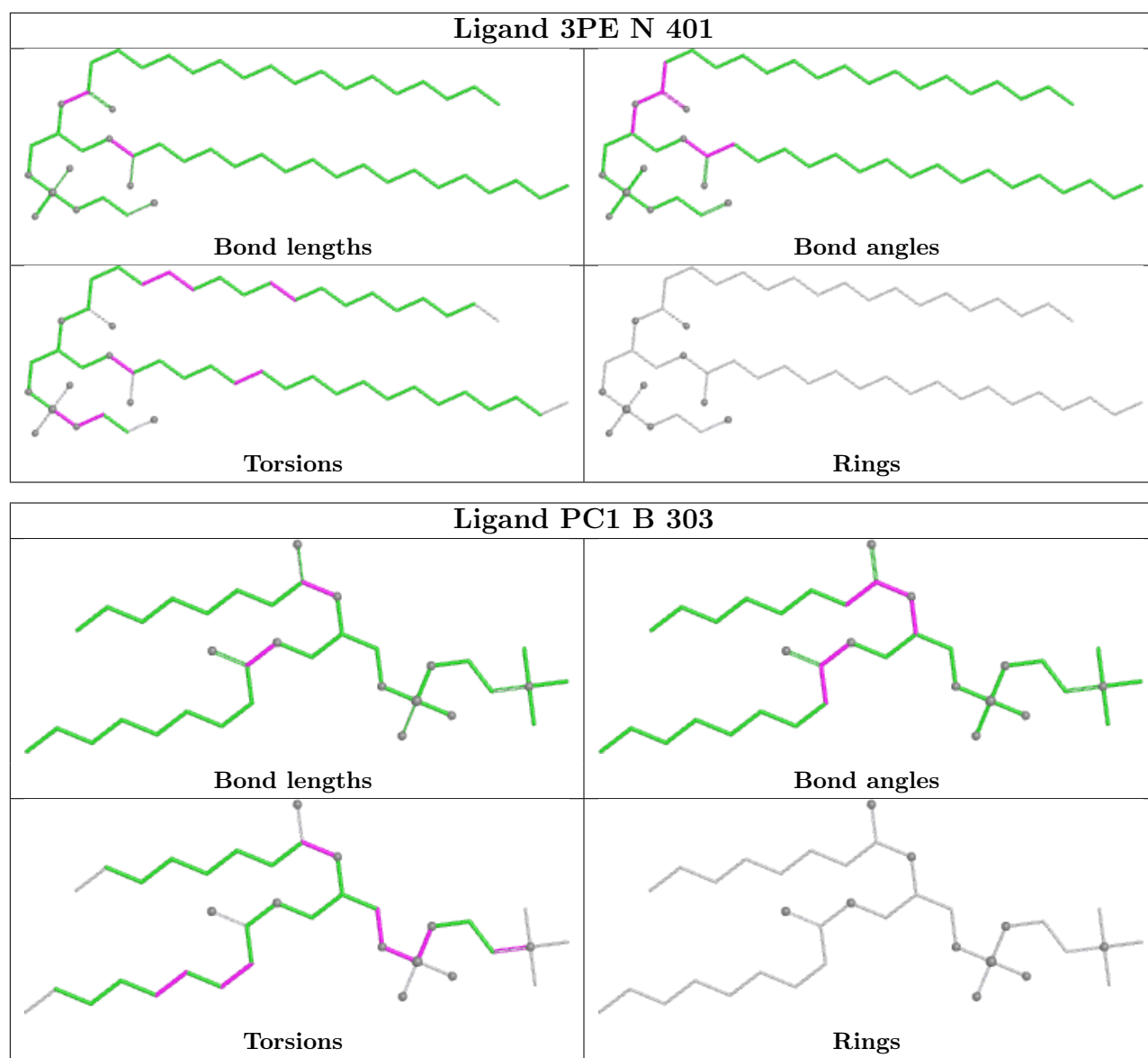
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	Ad	401	HEC	12	0
55	I	301	3PE	8	0
62	L	704	CDL	16	0
55	M	501	3PE	3	0
62	a	101	CDL	12	0
64	P	401	NDP	7	0
71	Ad	402	3PH	39	0
55	L	701	3PE	8	0
56	F	502	SF4	10	0
67	AC	401	HEM	18	0
55	Y	201	3PE	8	0
63	O	401	ADP	11	0
55	L	702	3PE	9	0
55	Ac	403	3PE	7	0
57	B	302	UQ1	11	0
55	K	101	3PE	9	0
56	I	303	SF4	2	0
56	B	301	SF4	7	0
56	G	802	SF4	10	0
61	H	400	UQ9	4	0
70	Ac	404	U10	20	0
62	Ag	102	CDL	4	0
67	Ac	401	HEM	1	0
58	B	304	PC1	14	0
62	Ag	101	CDL	5	0
55	L	705	3PE	5	0
68	AC	403	UQ6	11	0
69	AD	401	HEC	18	0
59	E	301	FES	4	0
55	i	201	3PE	19	0
56	I	302	SF4	8	0
59	G	803	FES	4	0
67	Ac	402	HEM	10	0
55	M	502	3PE	5	0
55	m	201	3PE	12	0
55	L	703	3PE	6	0
55	Ag	103	3PE	9	0
60	F	501	FMN	3	0

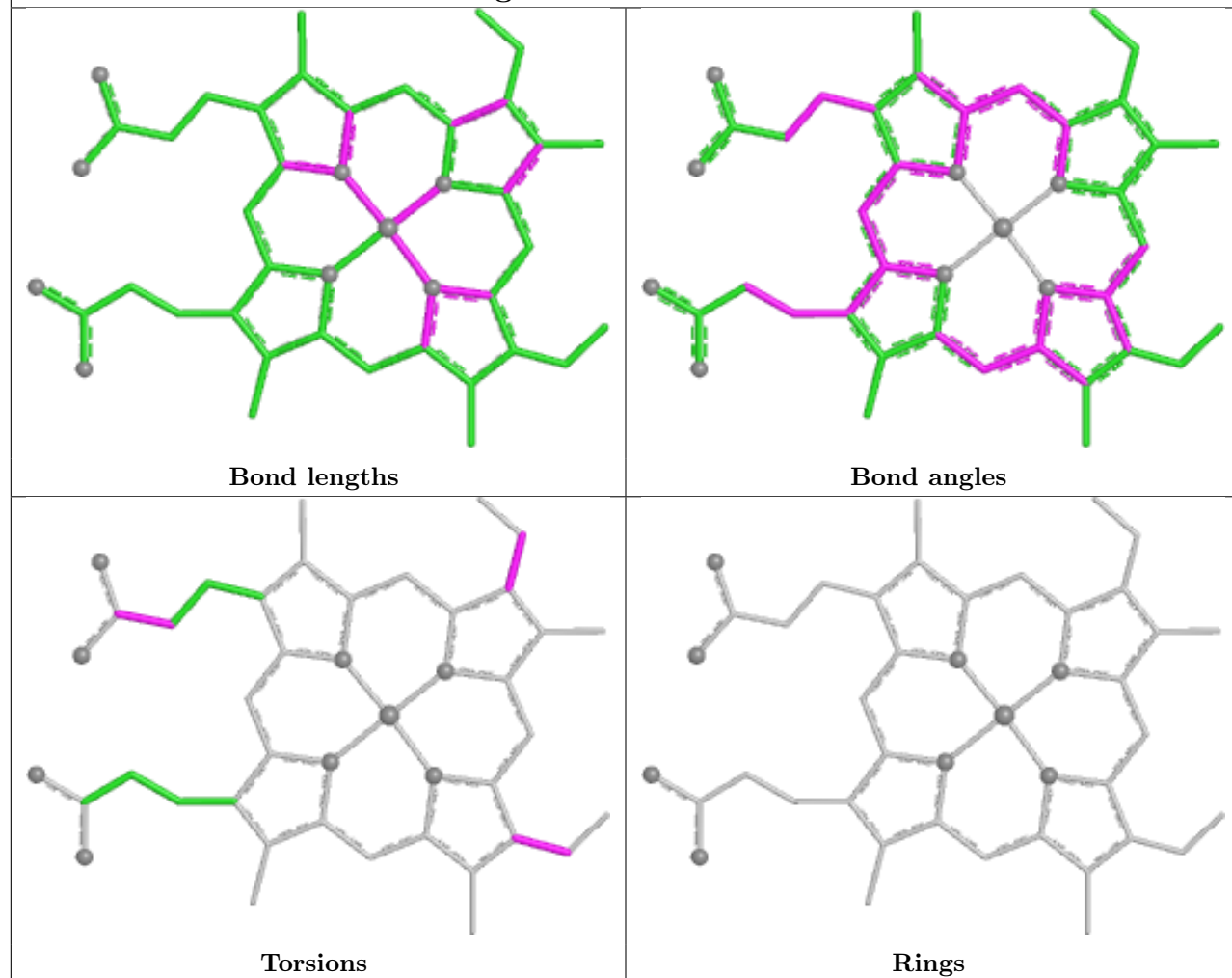
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

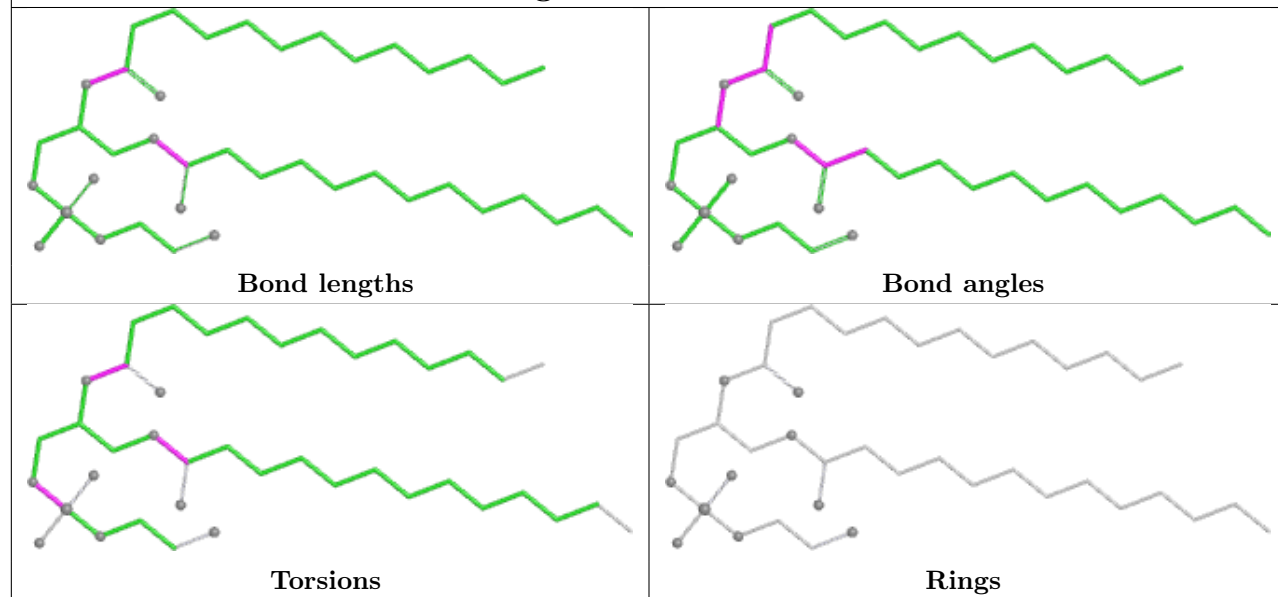


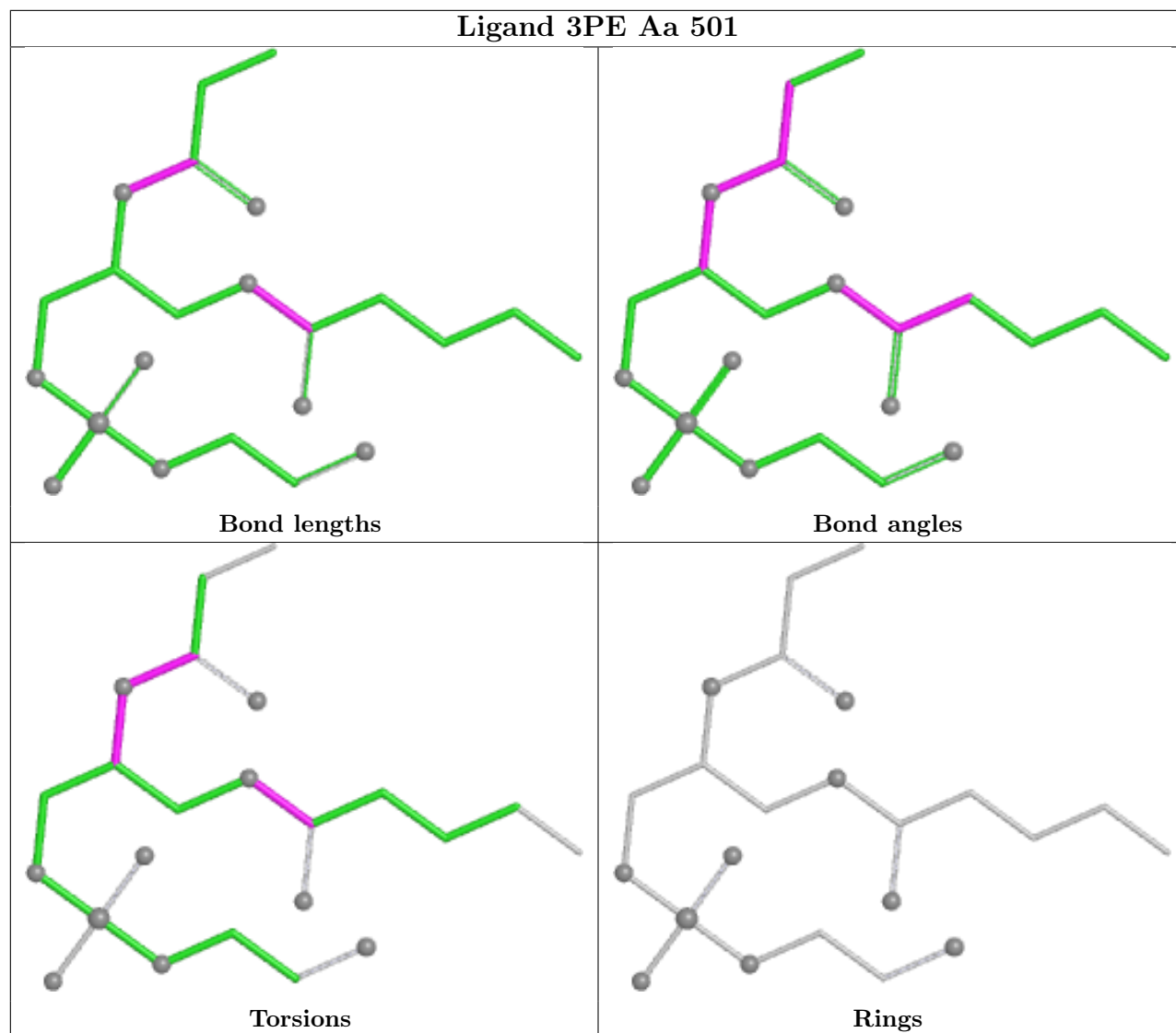


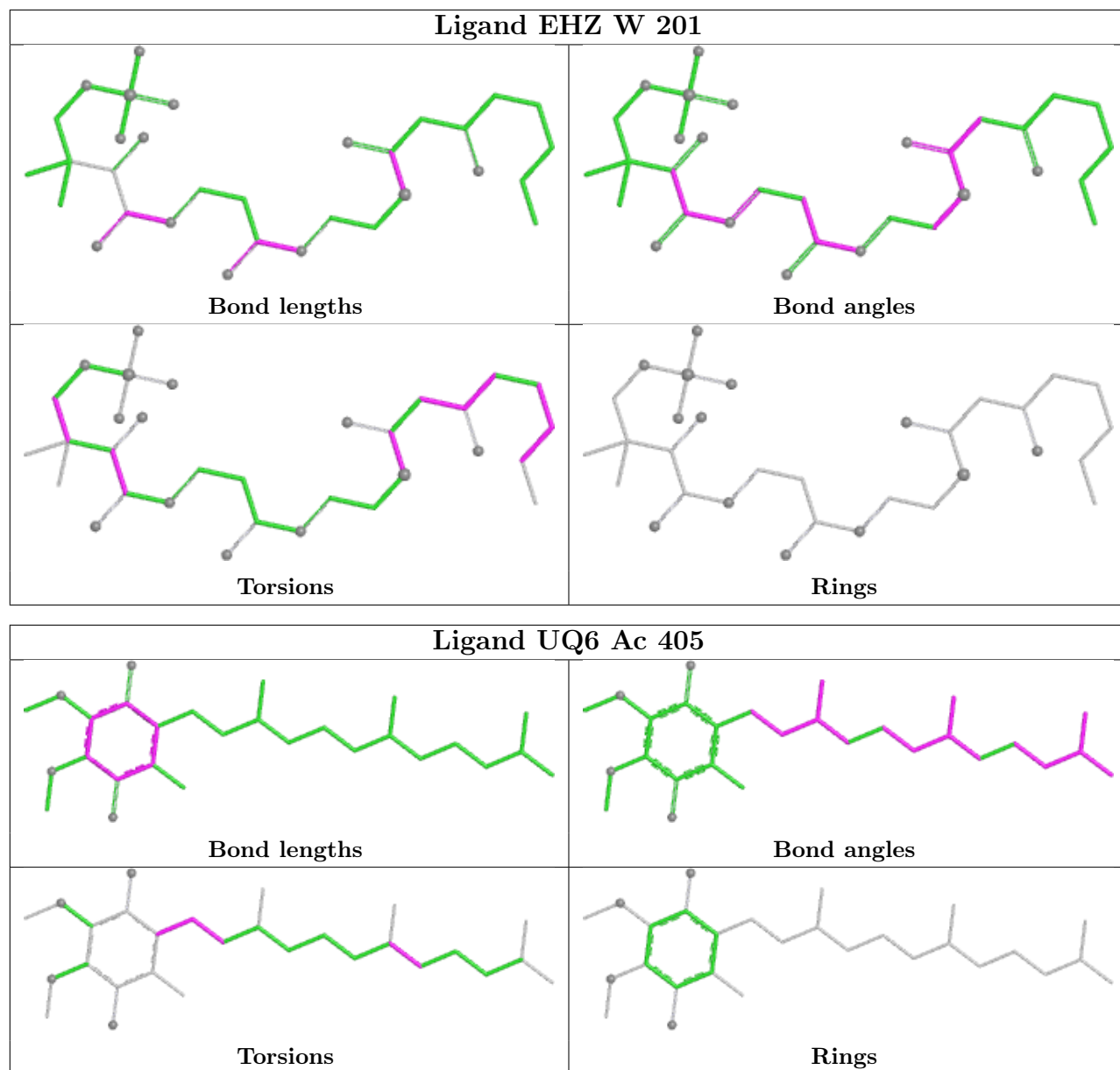
Ligand HEM AC 402

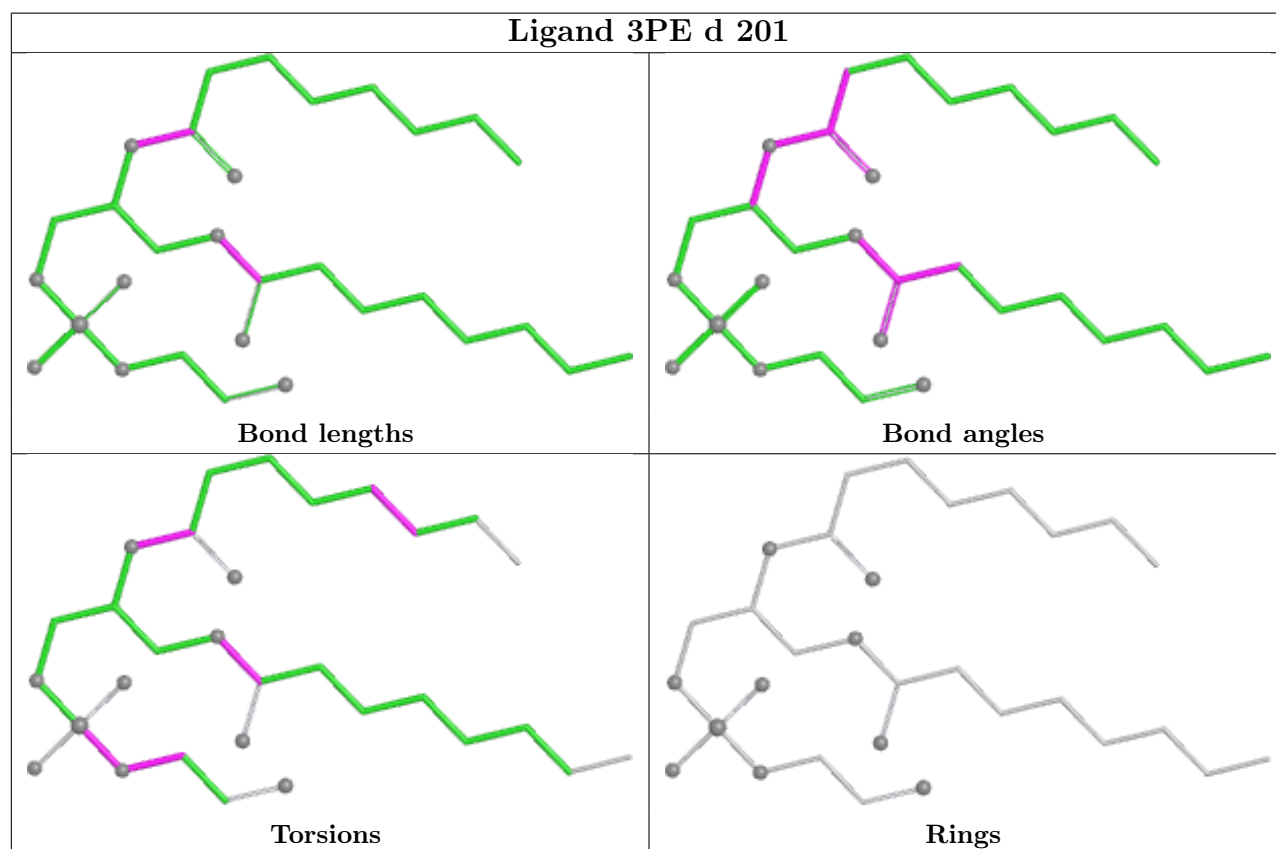
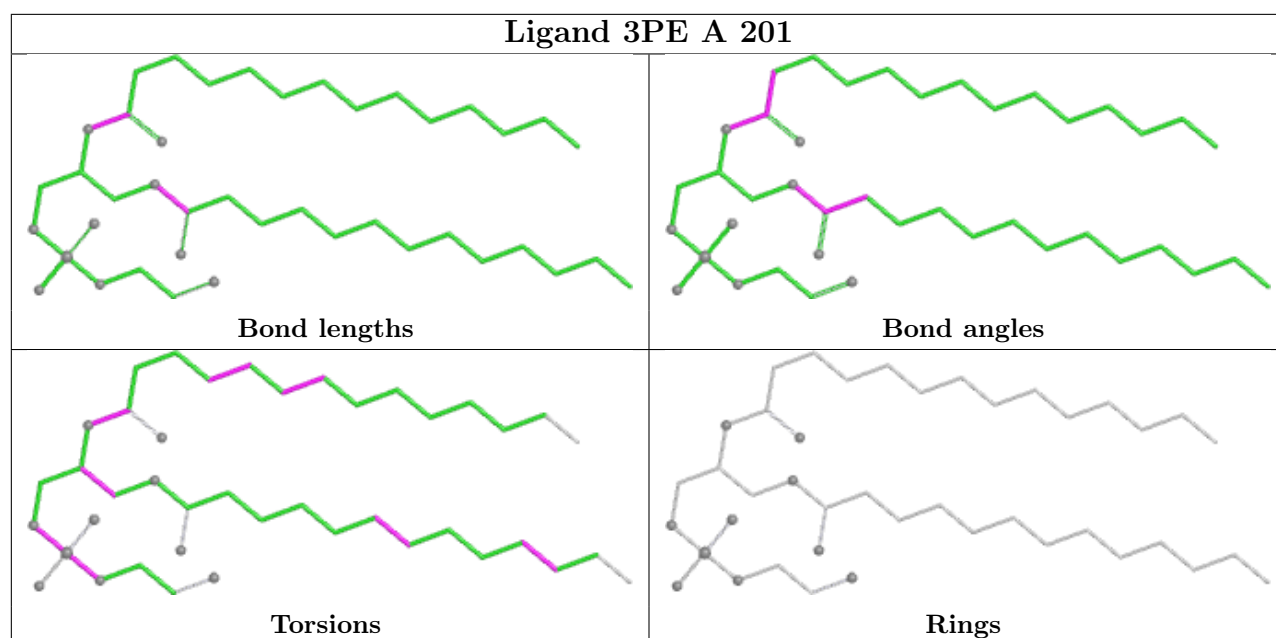


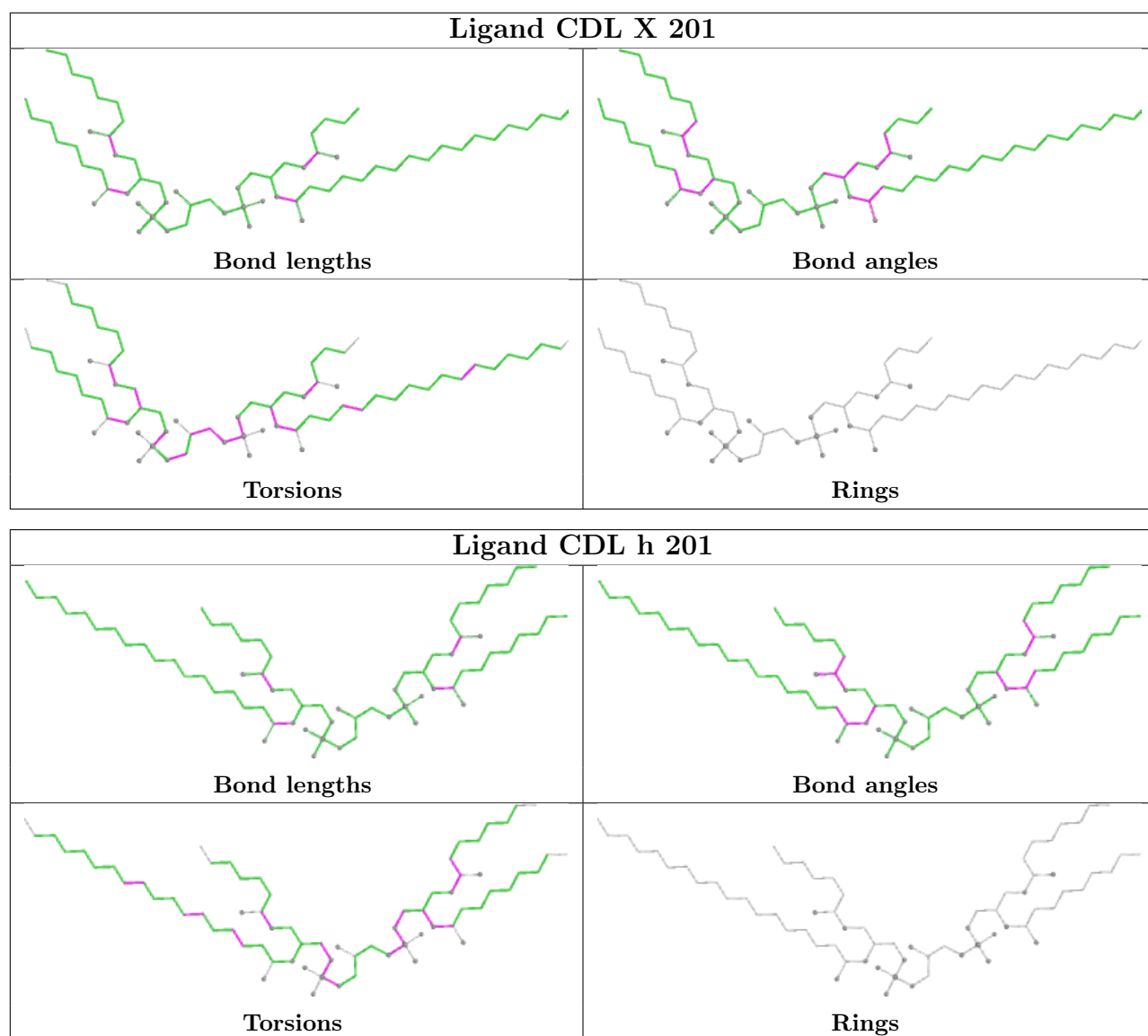
Ligand 3PE m 203



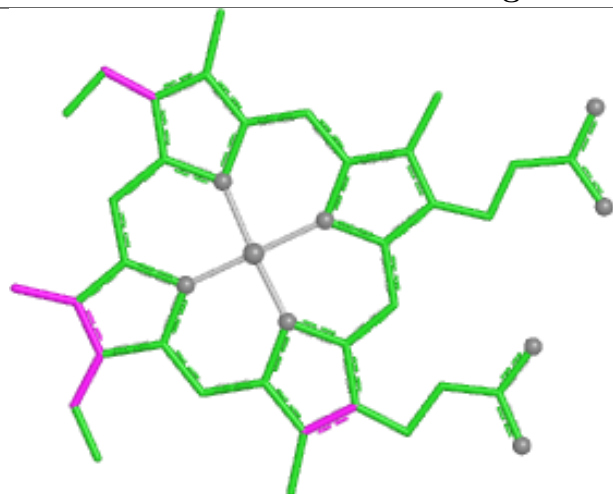




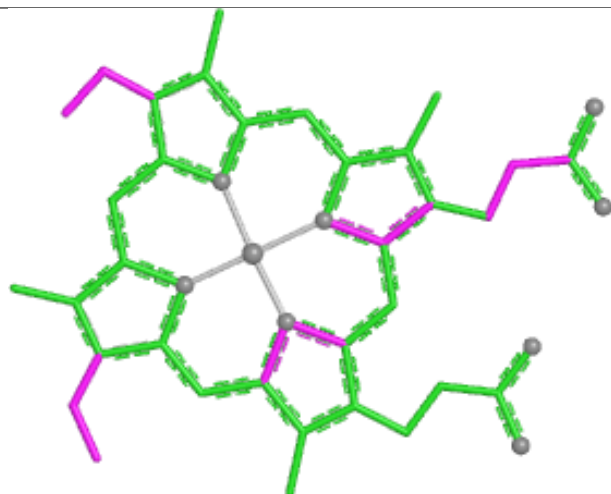




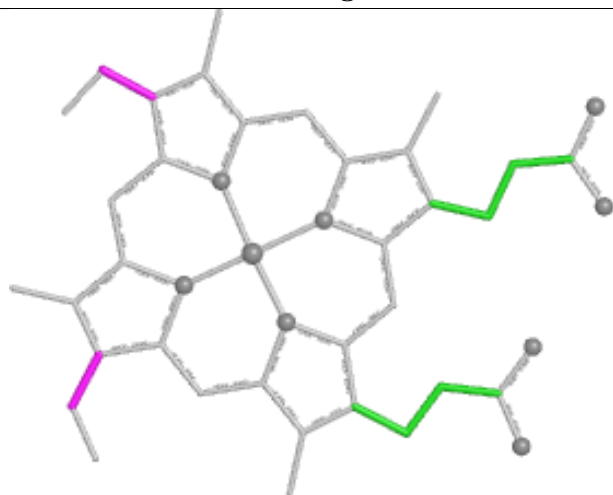
Ligand HEC Ad 401



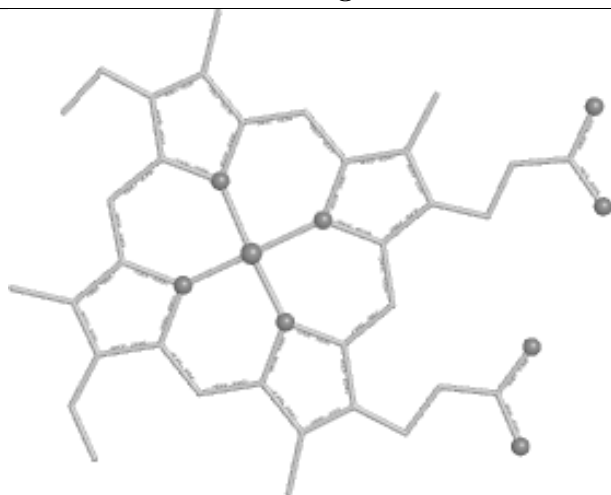
Bond lengths



Bond angles

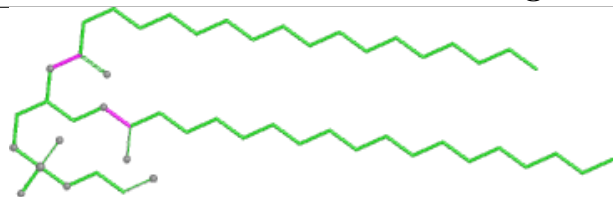


Torsions

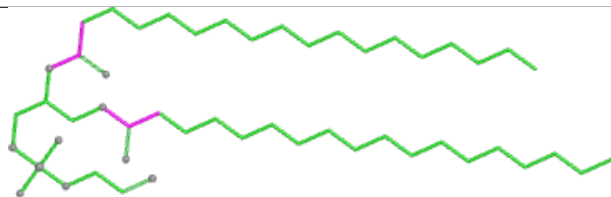


Rings

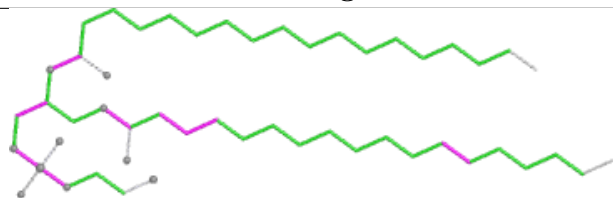
Ligand 3PE I 301



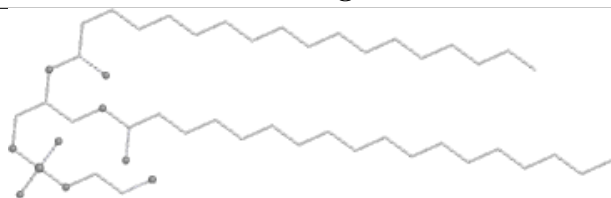
Bond lengths



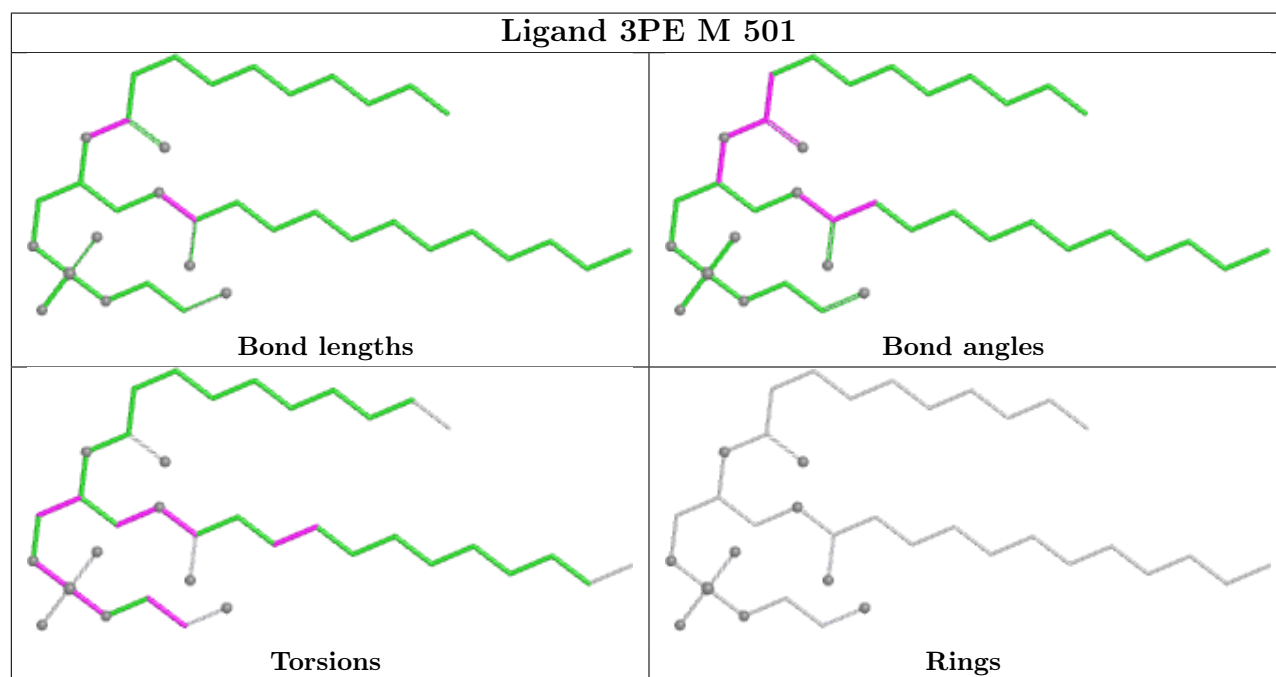
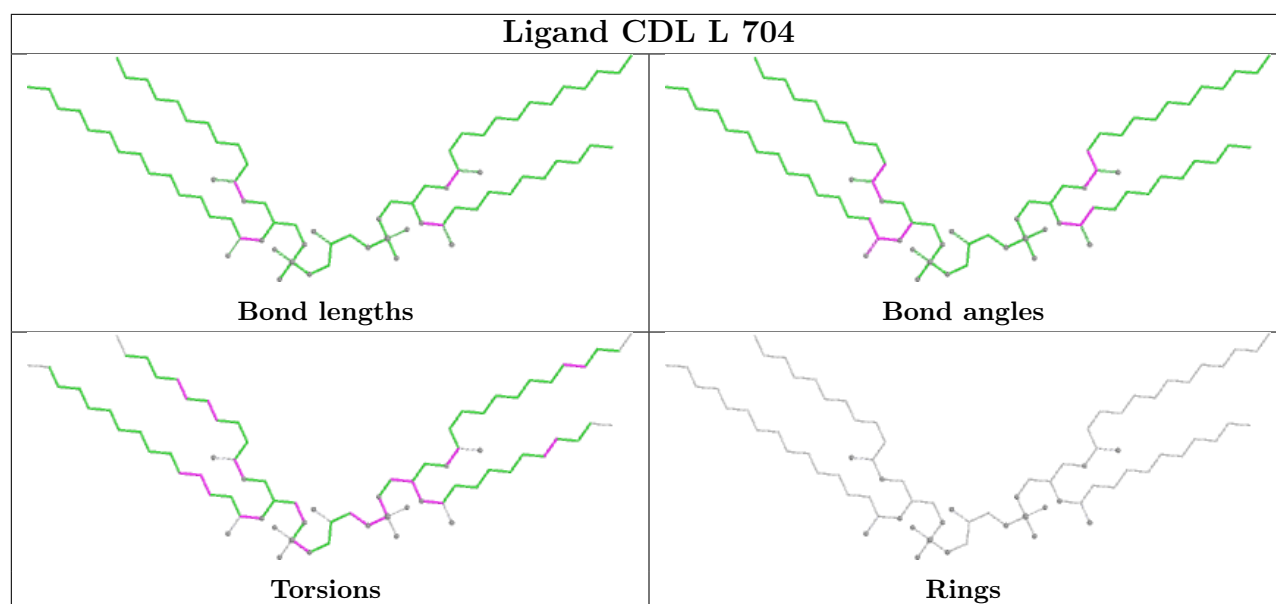
Bond angles

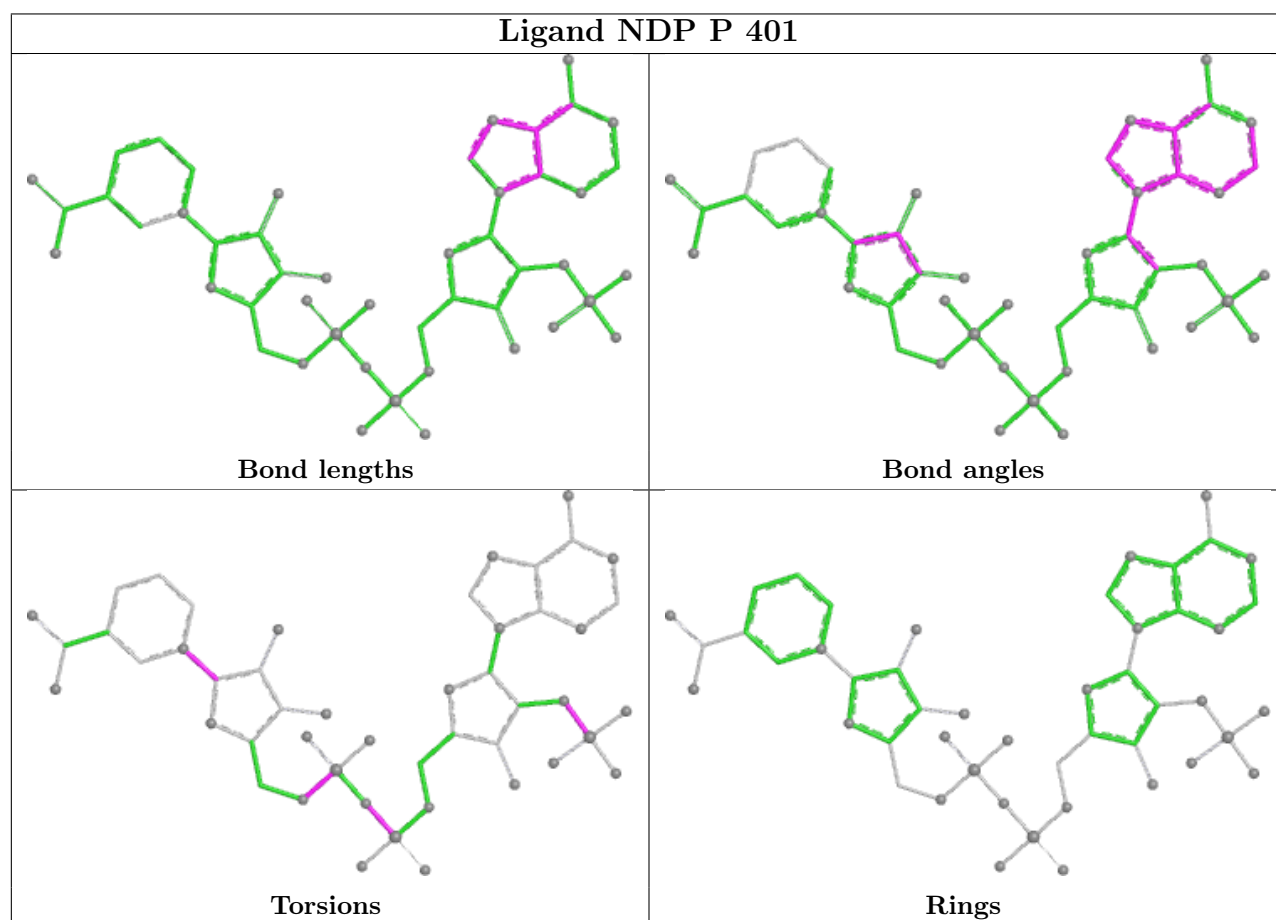
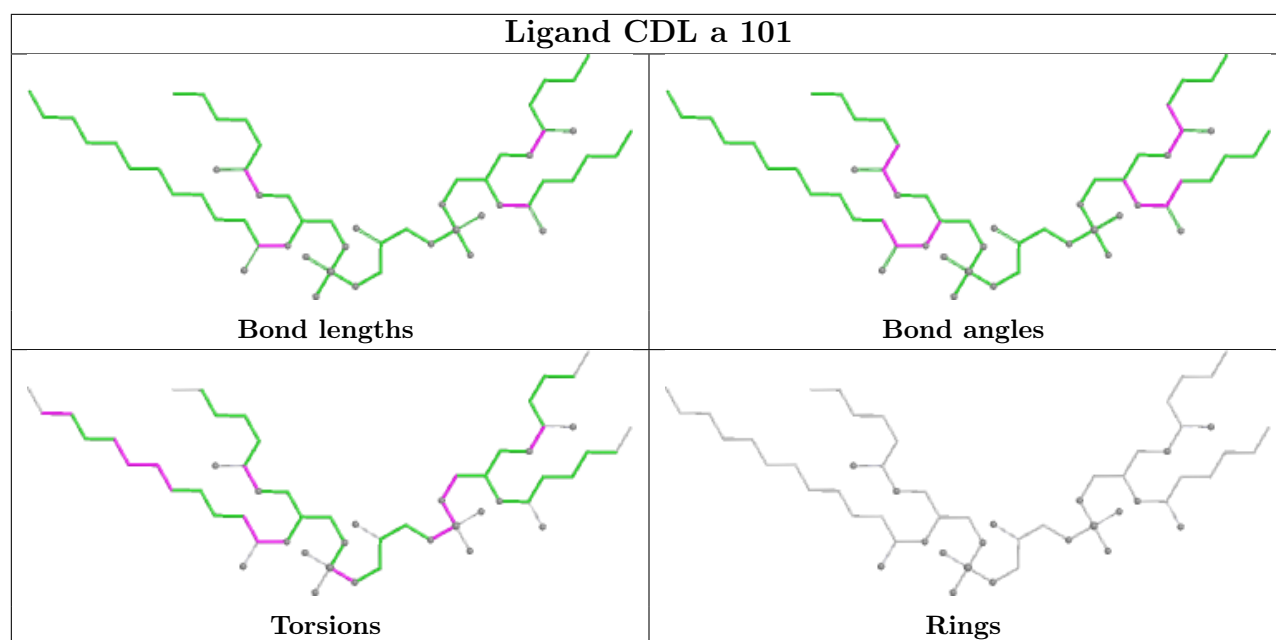


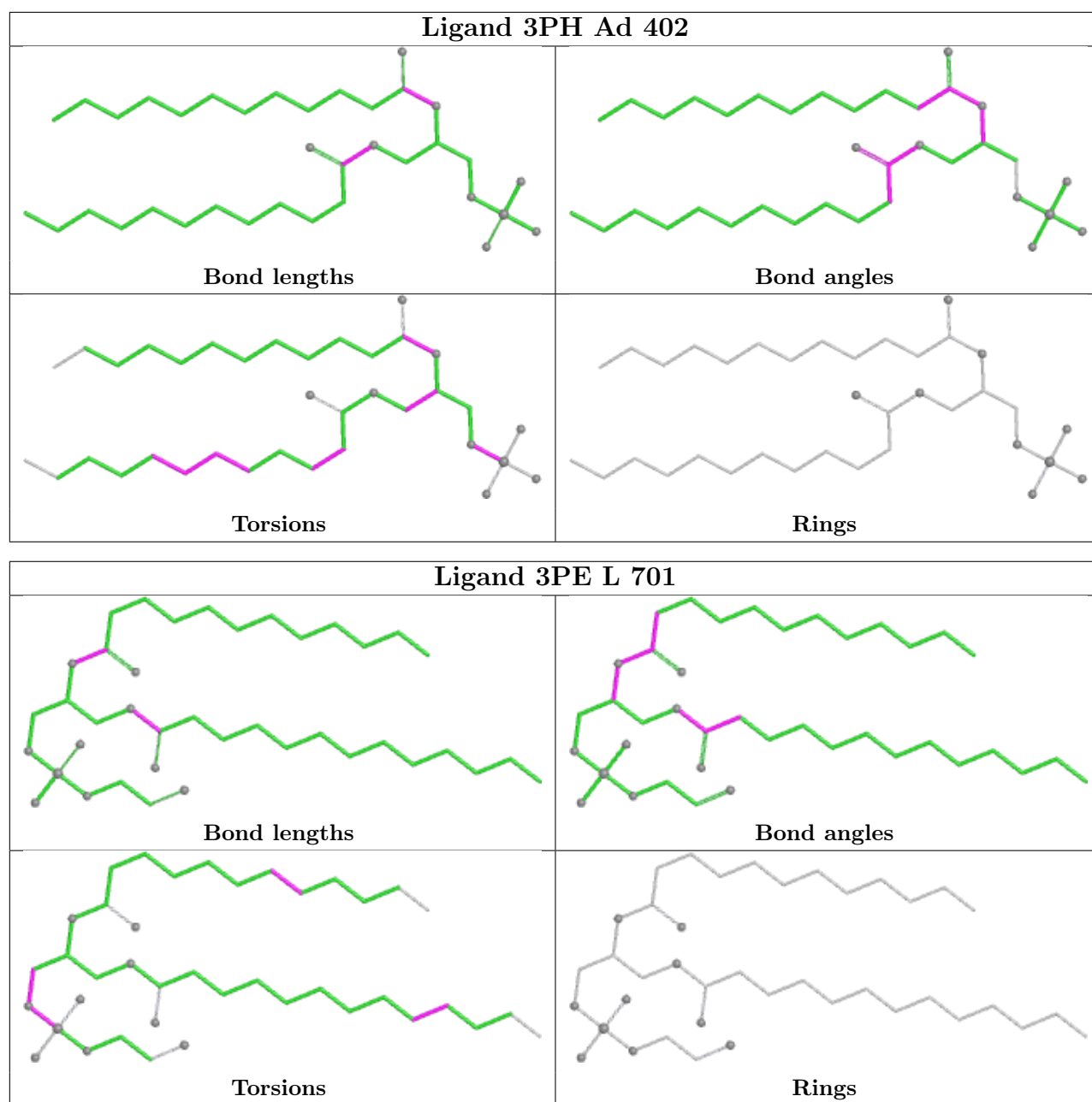
Torsions

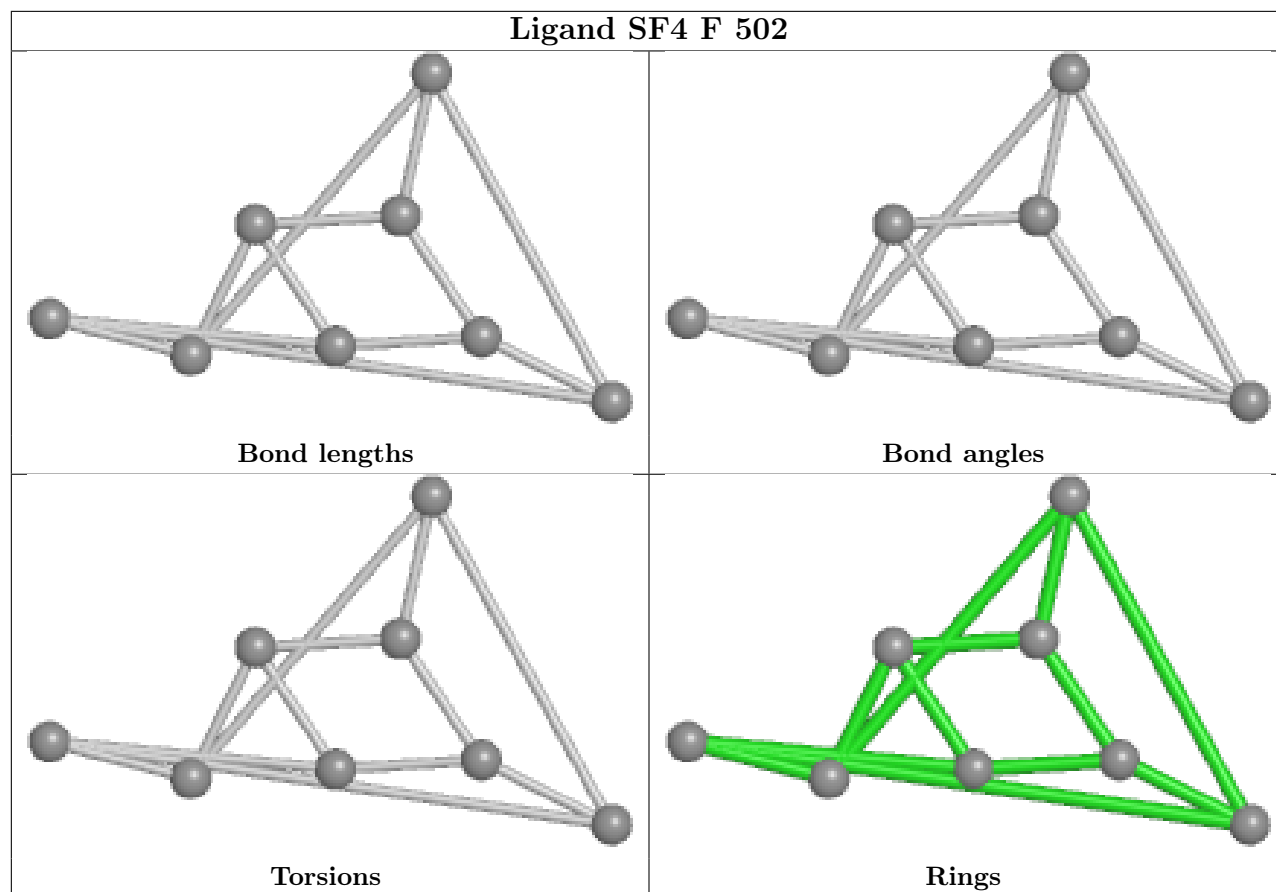


Rings

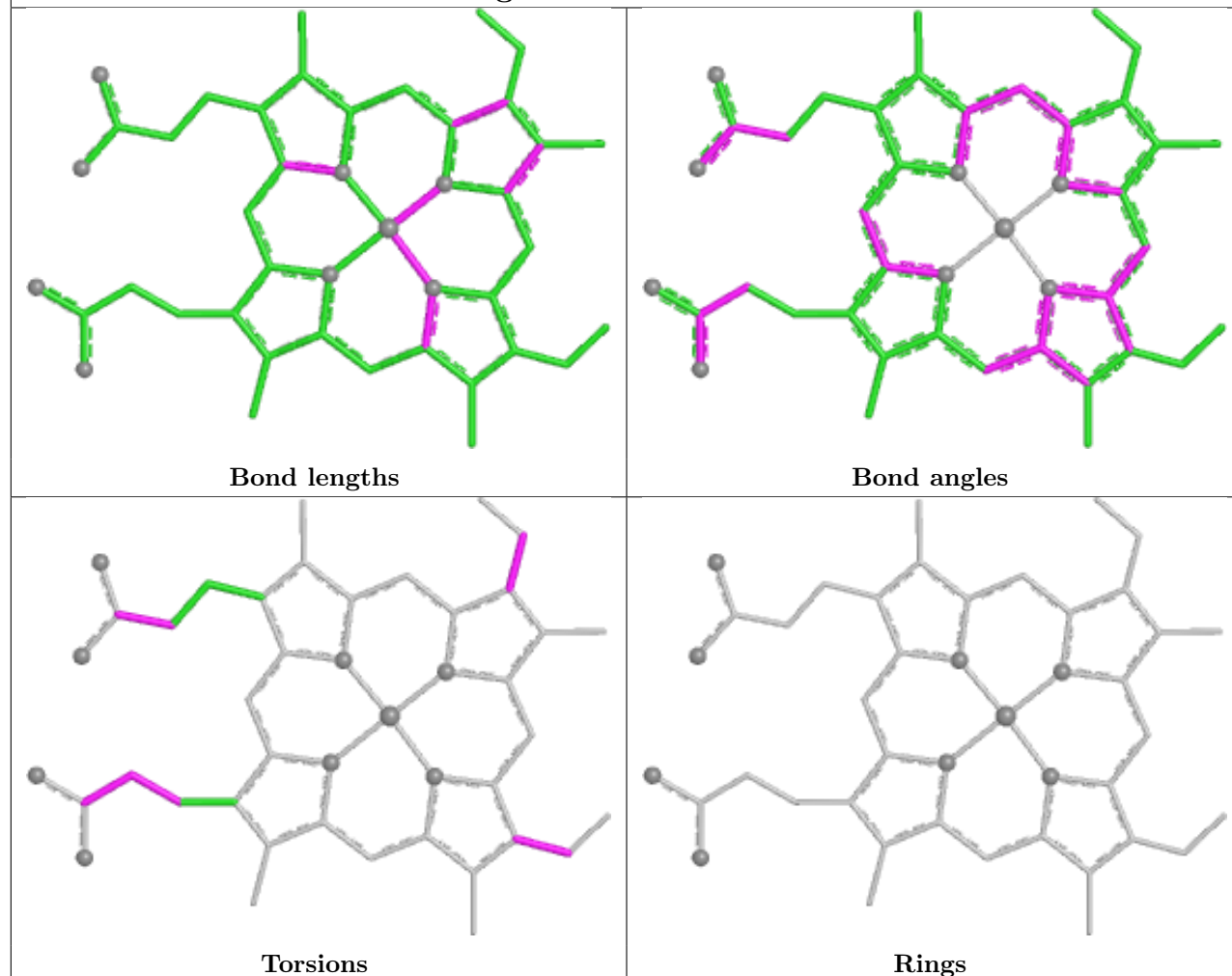




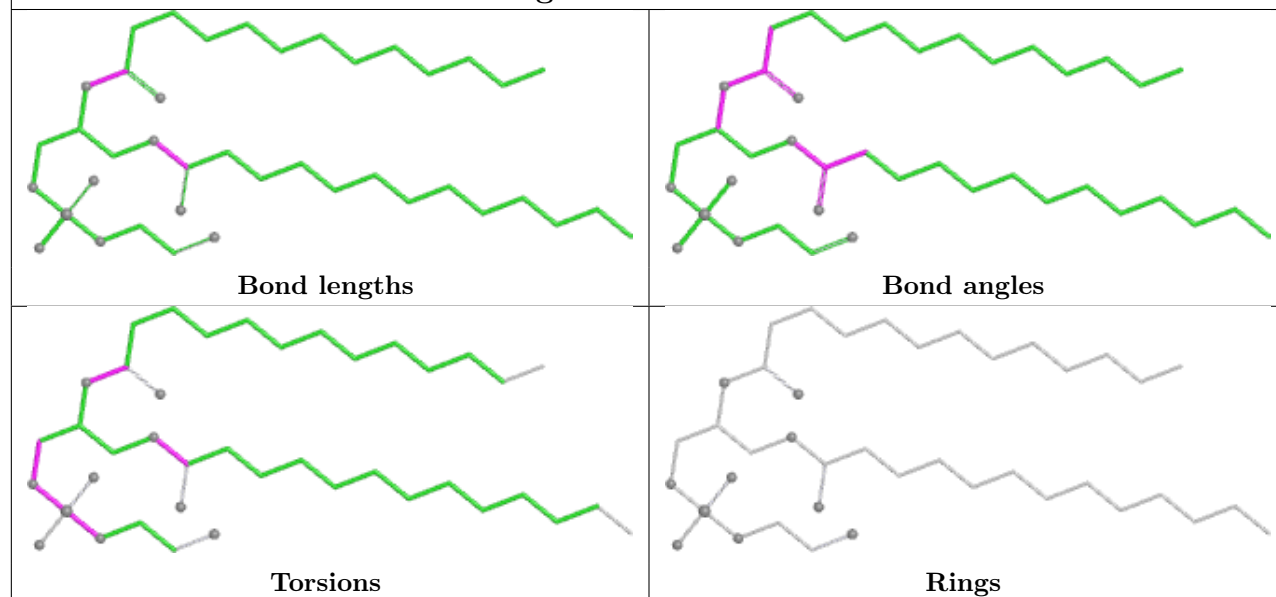


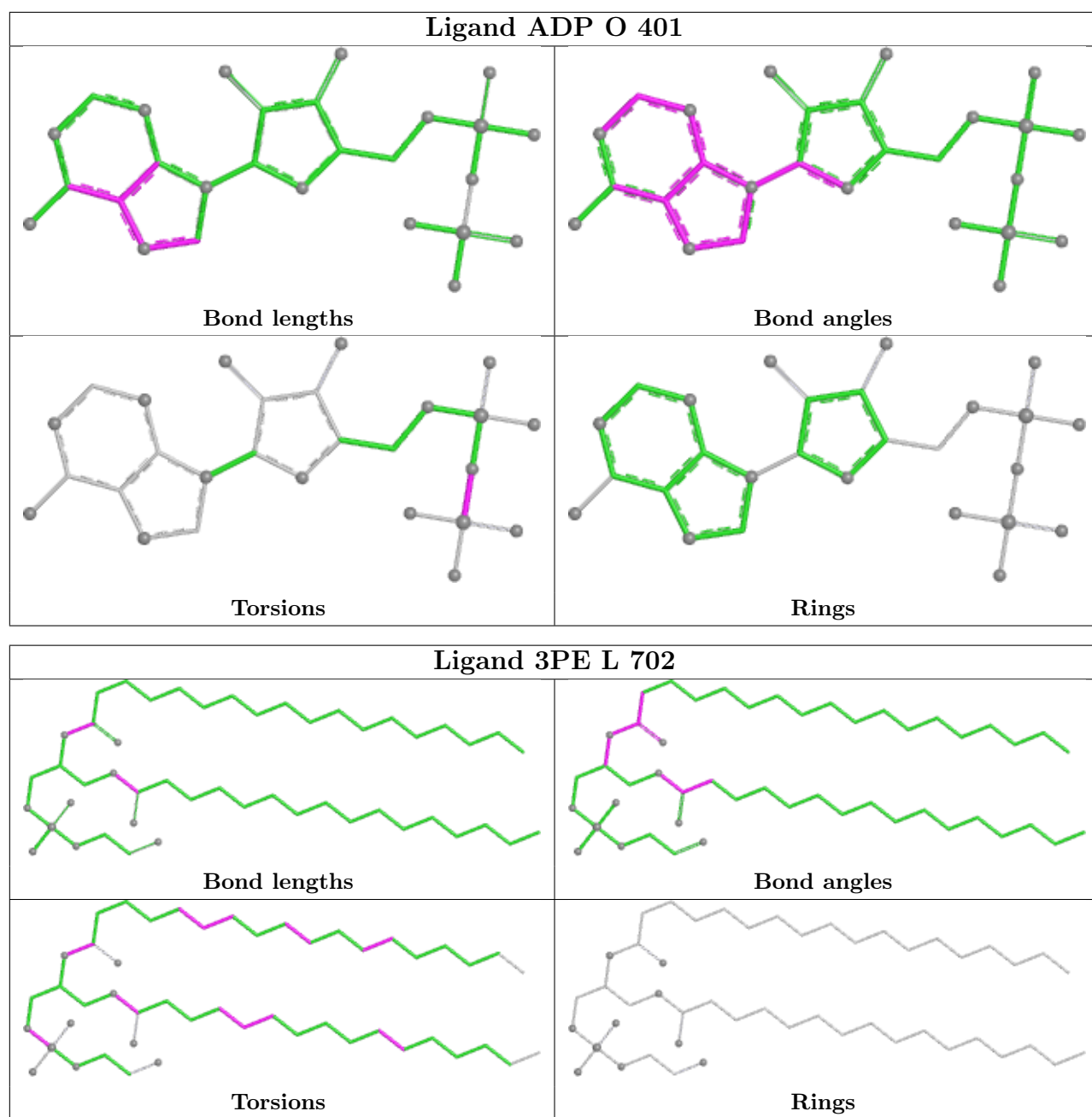


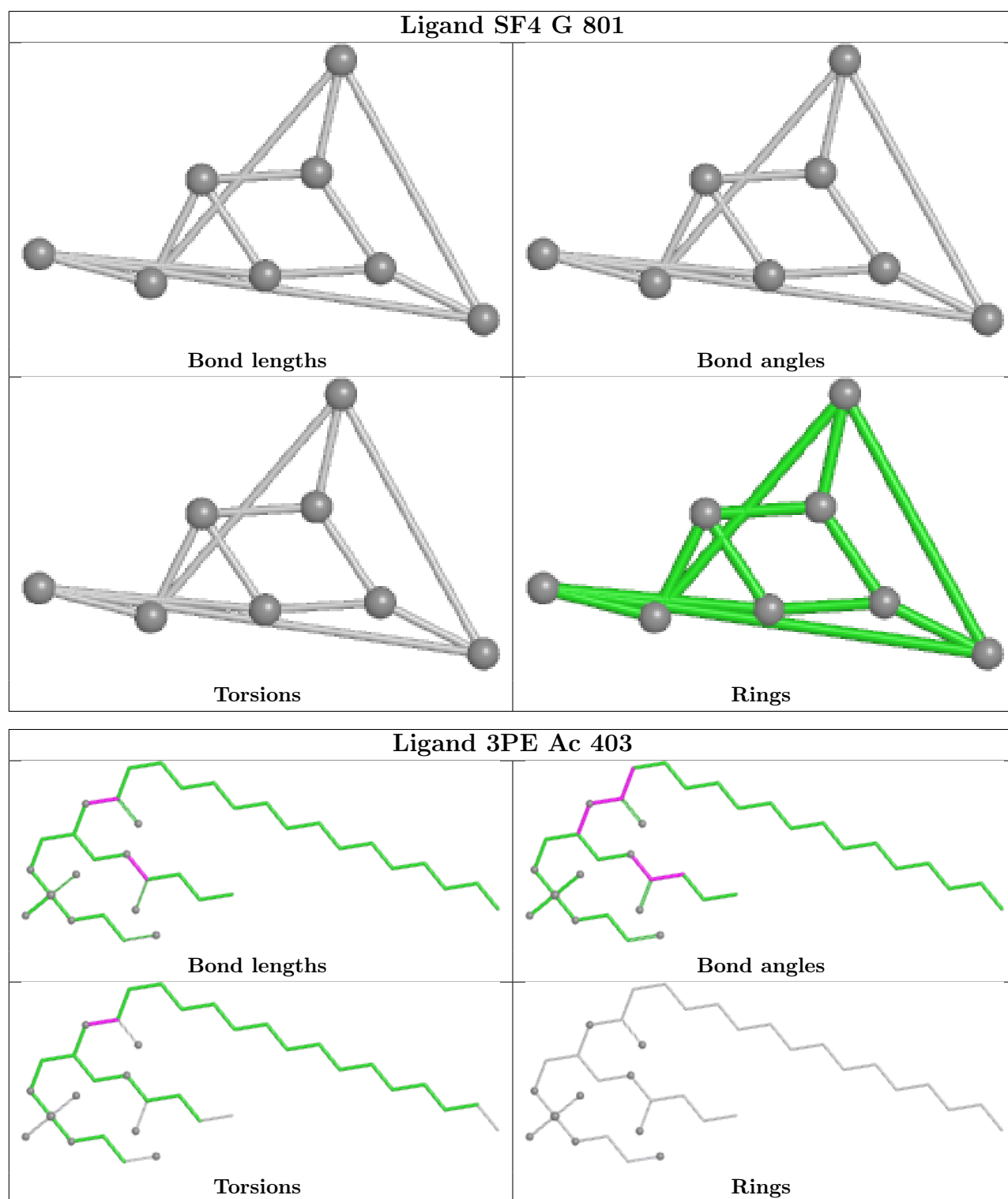
Ligand HEM AC 401

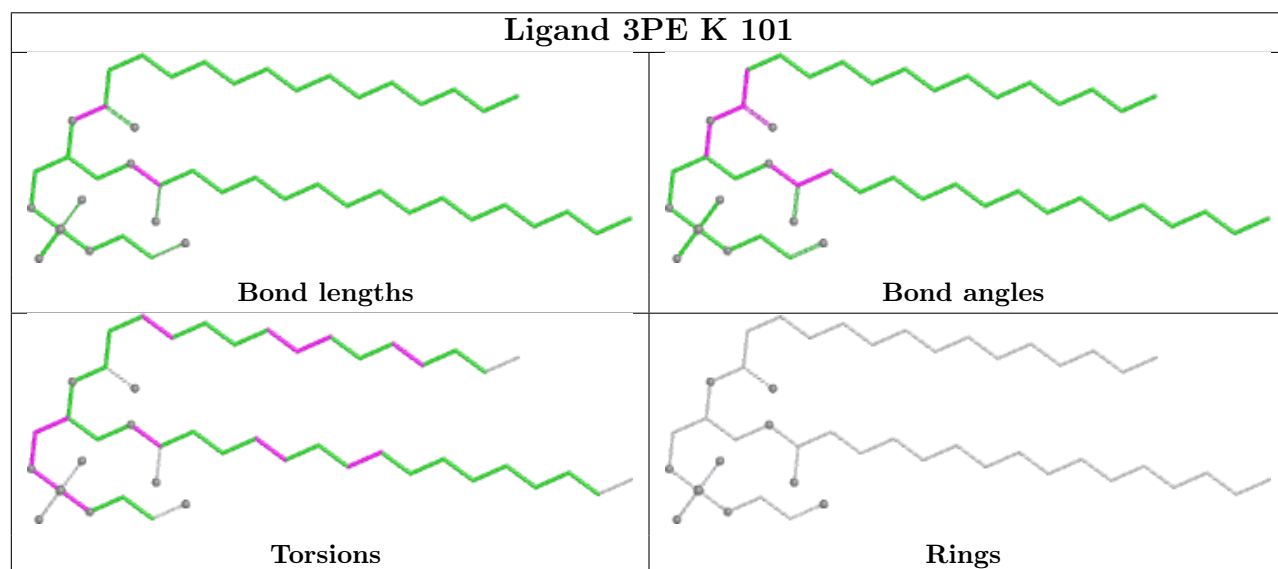
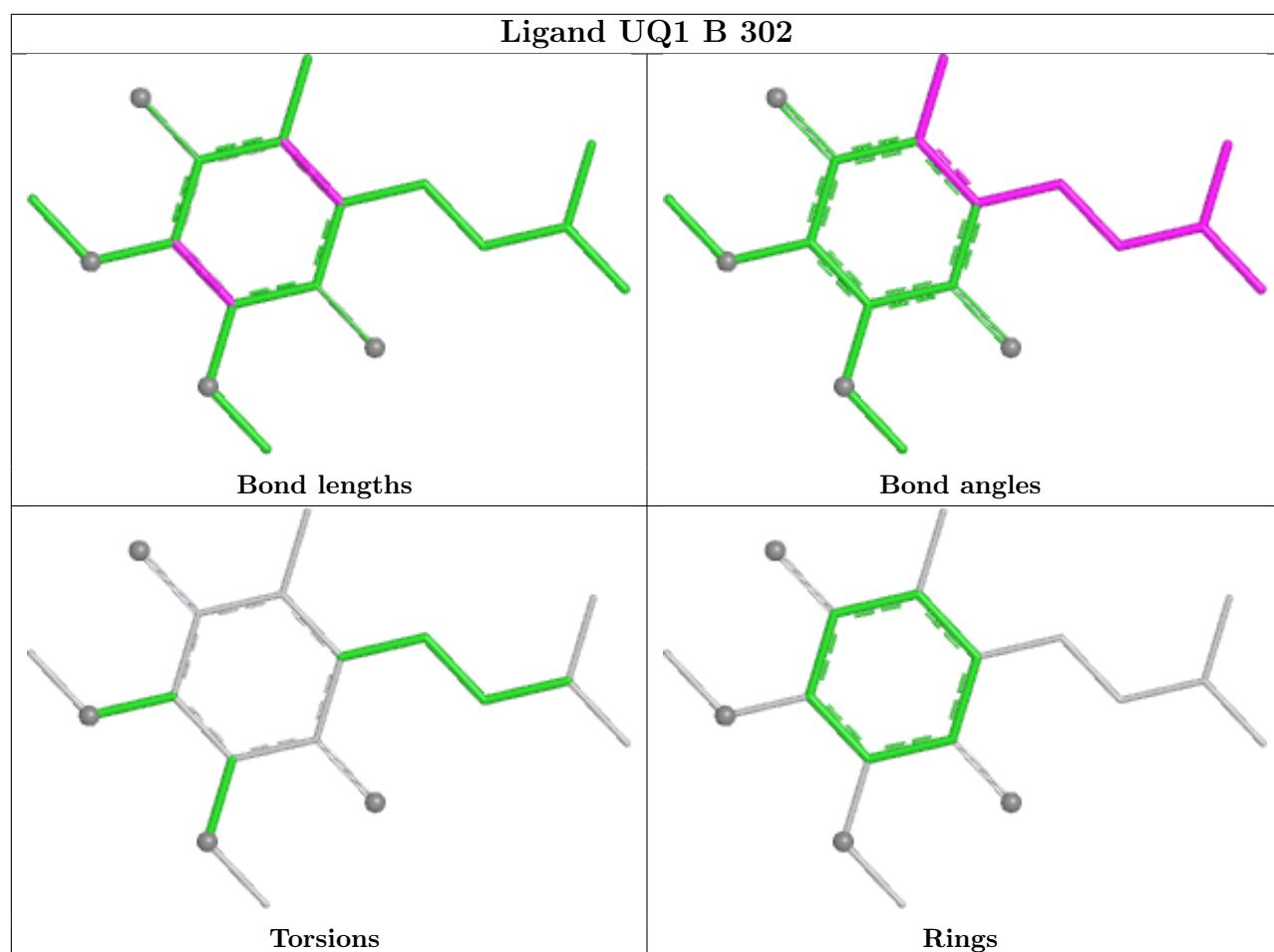


Ligand 3PE Y 201

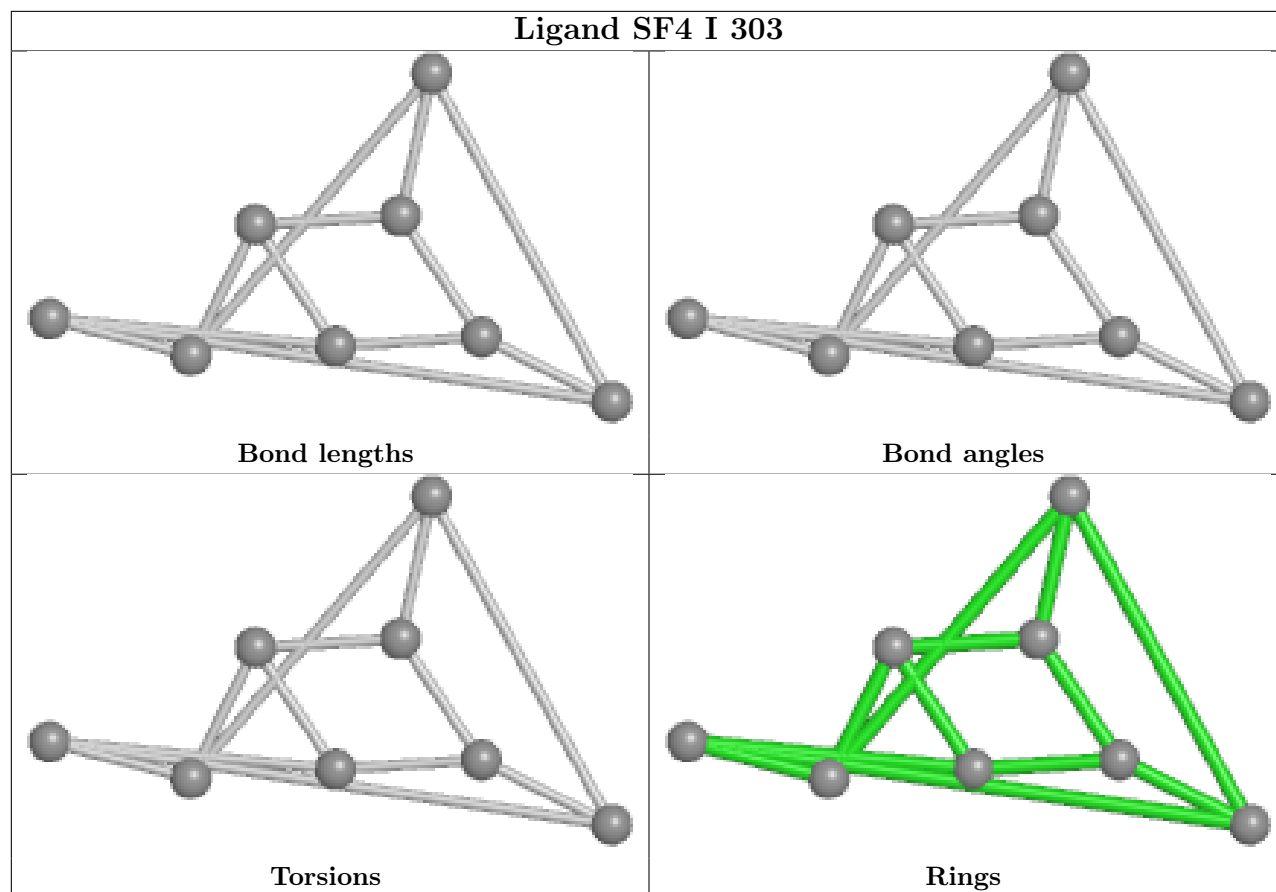




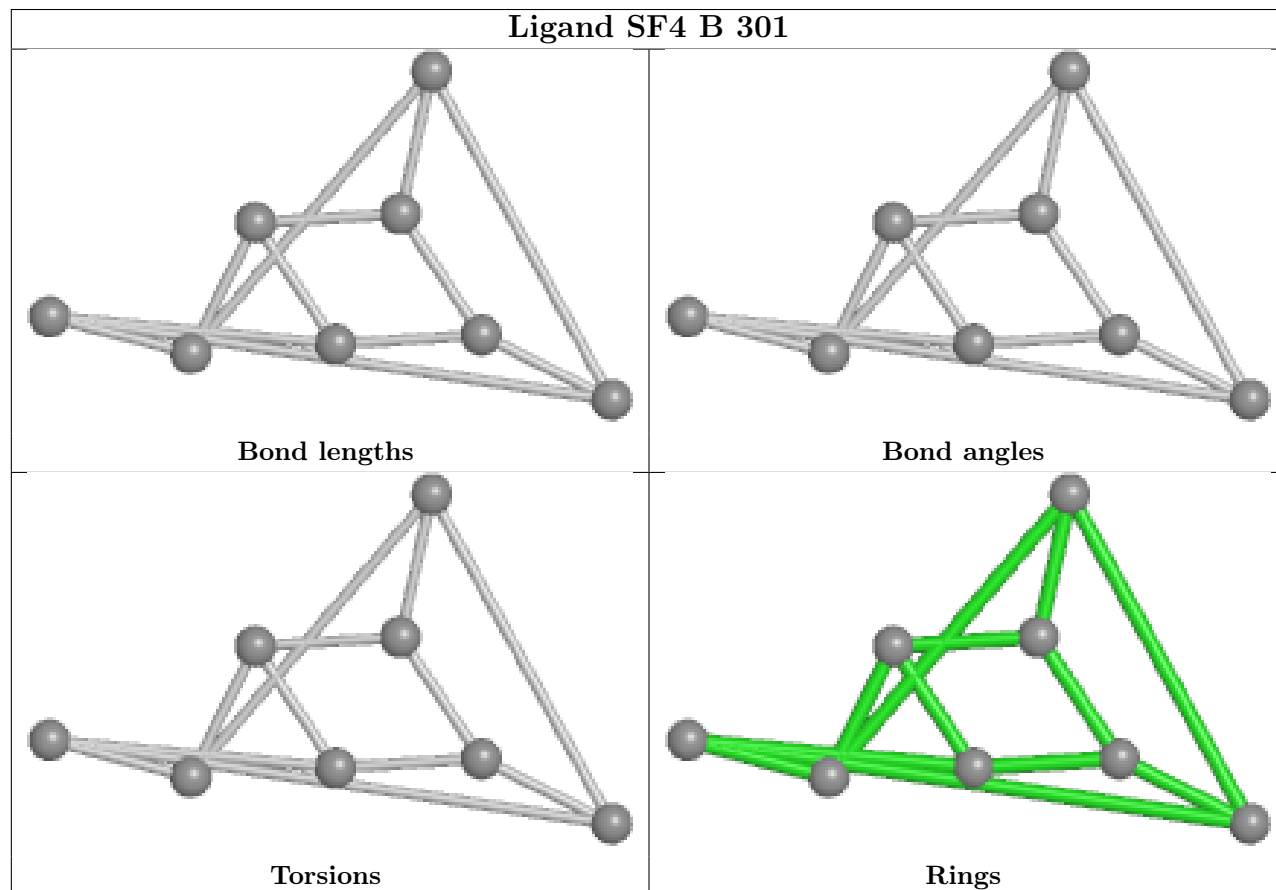


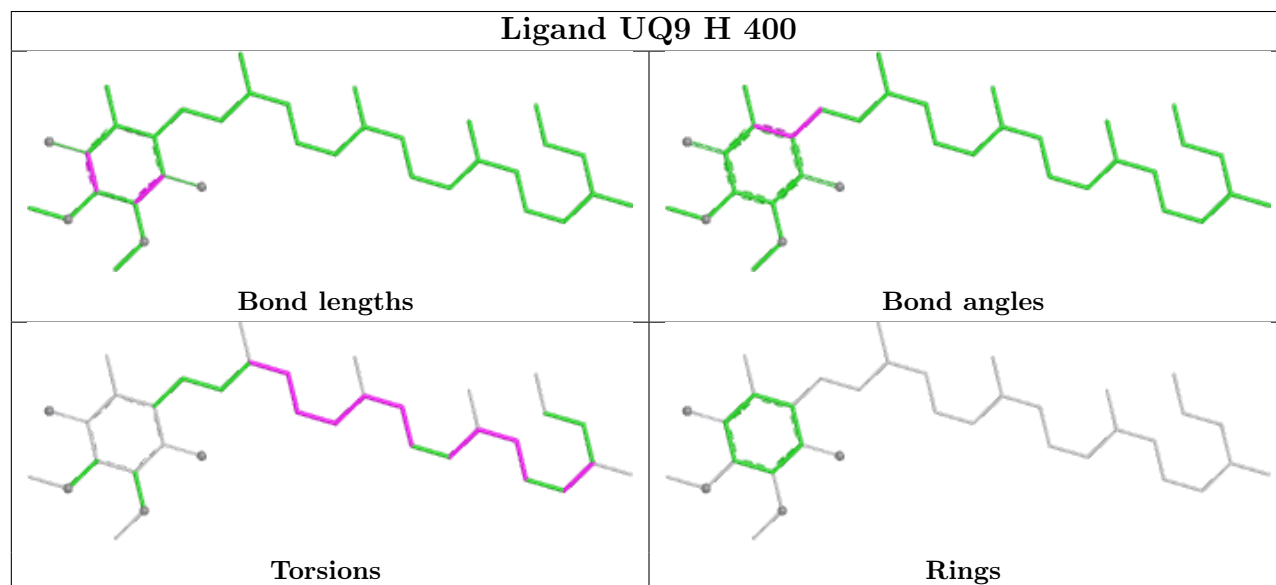
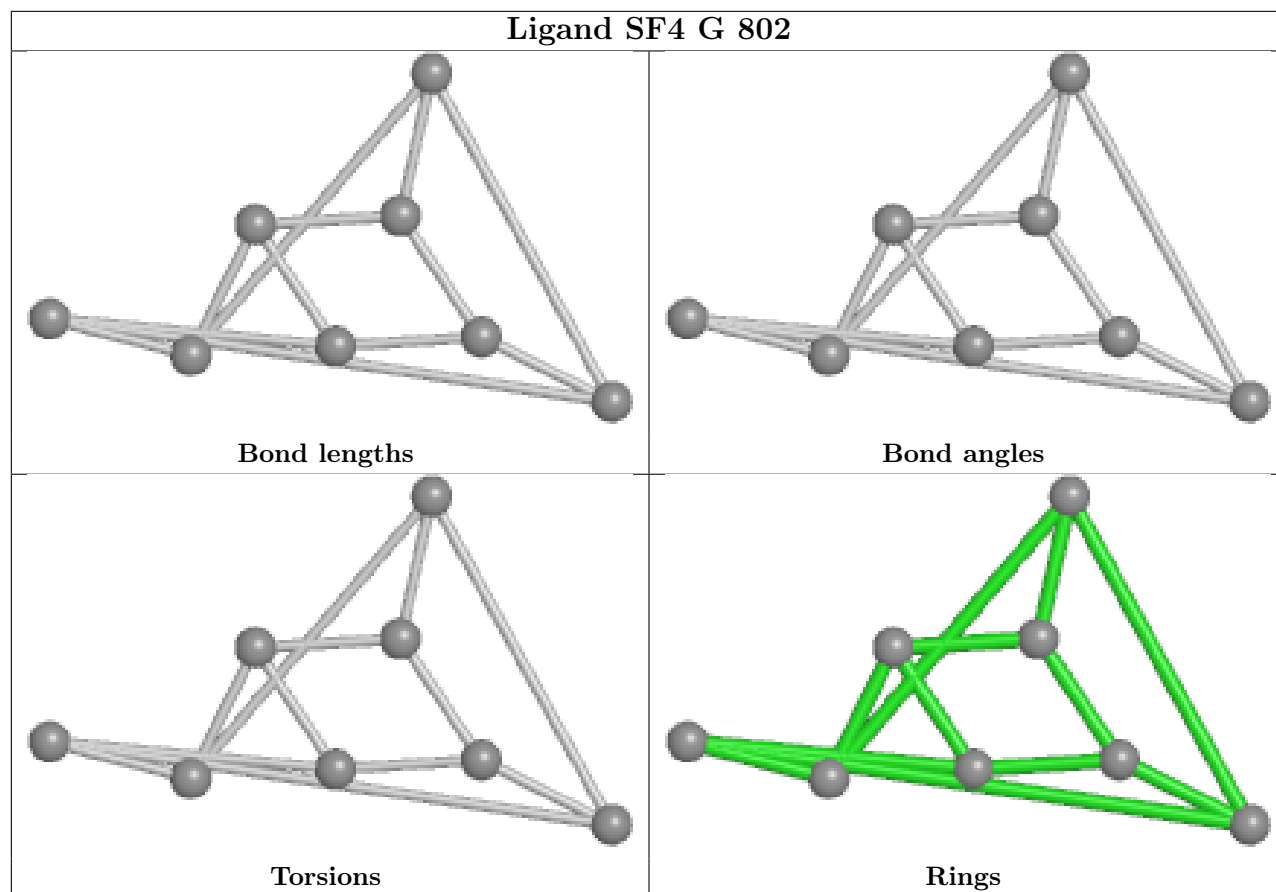


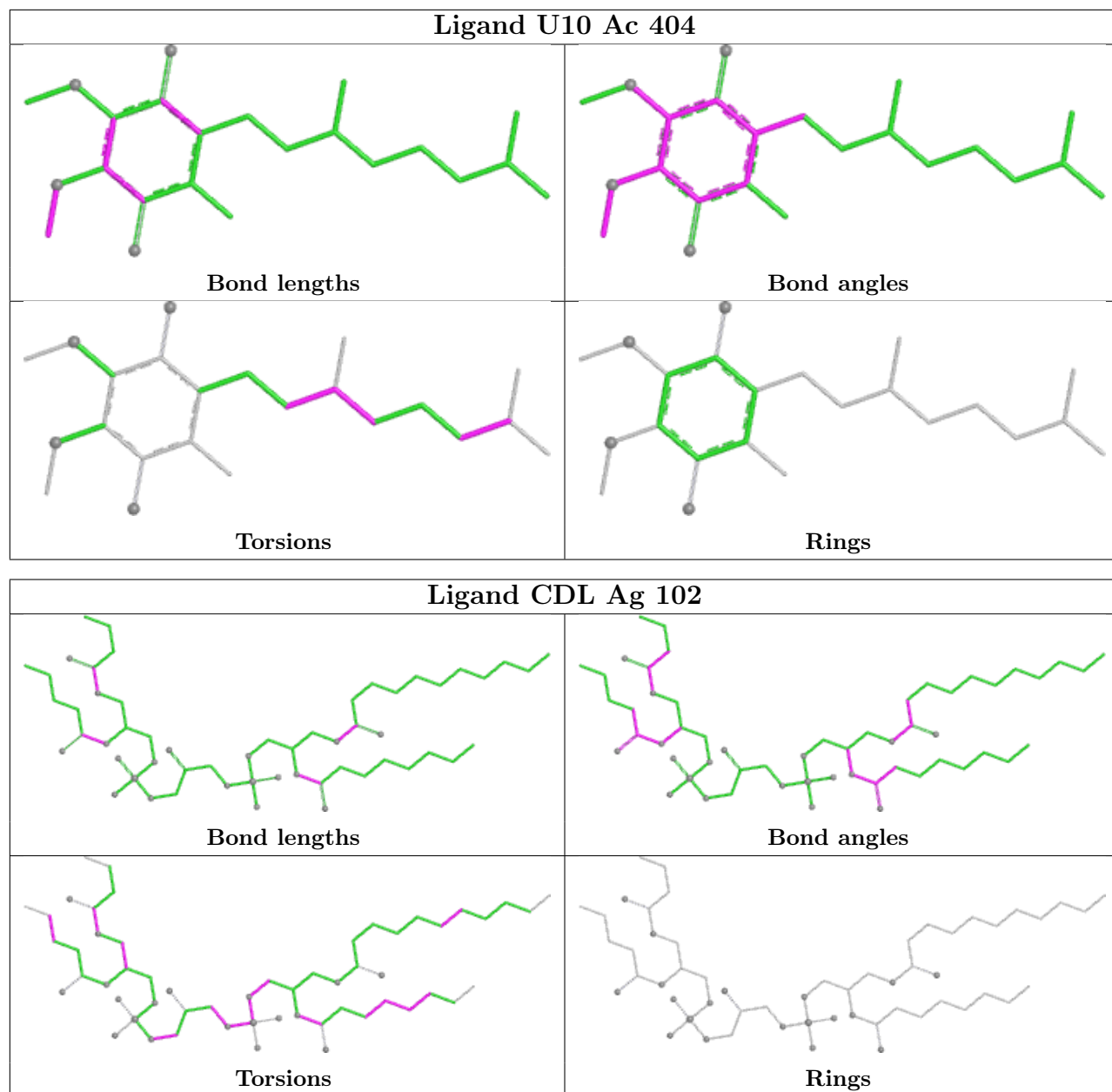
Ligand SF4 I 303



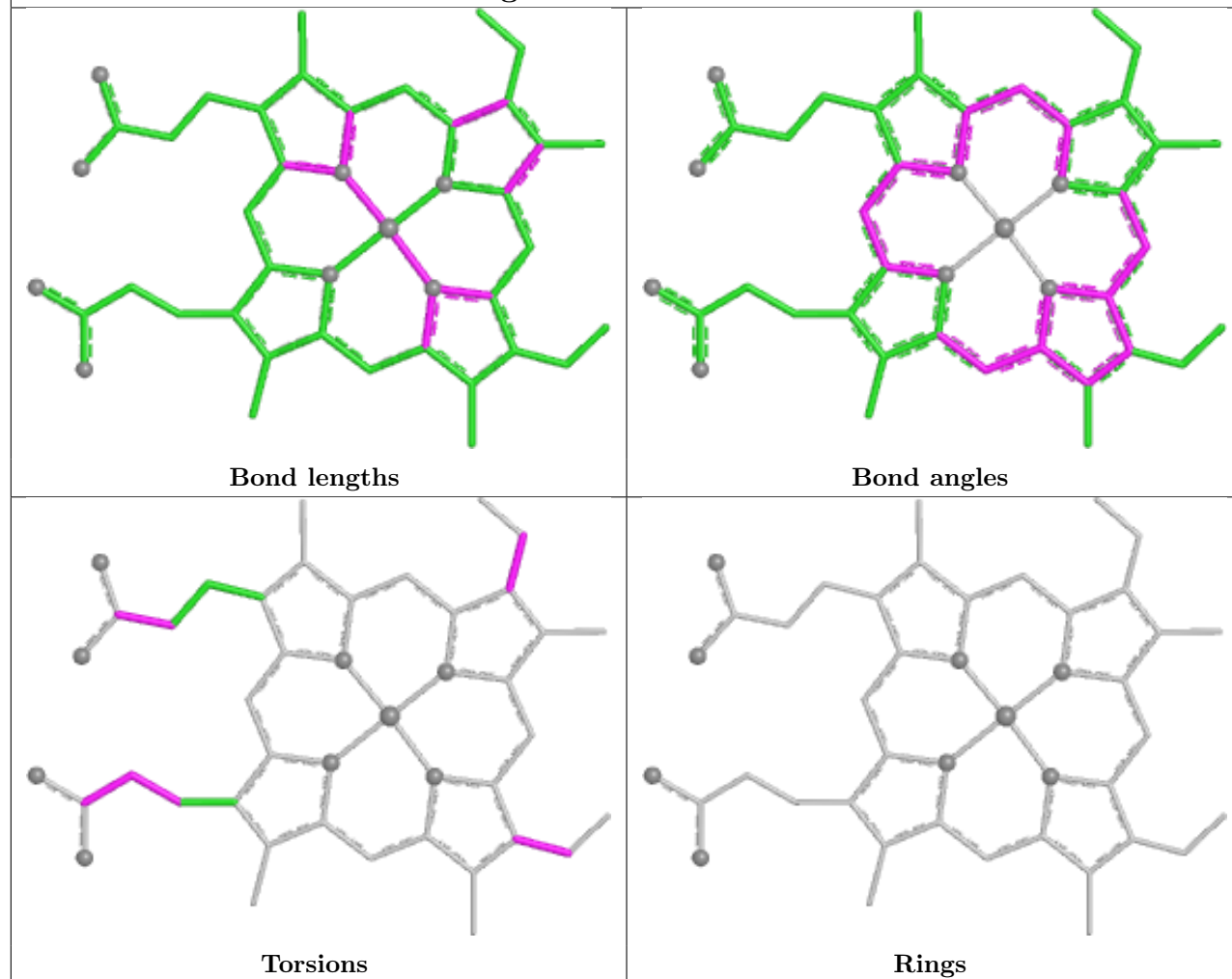
Ligand SF4 B 301



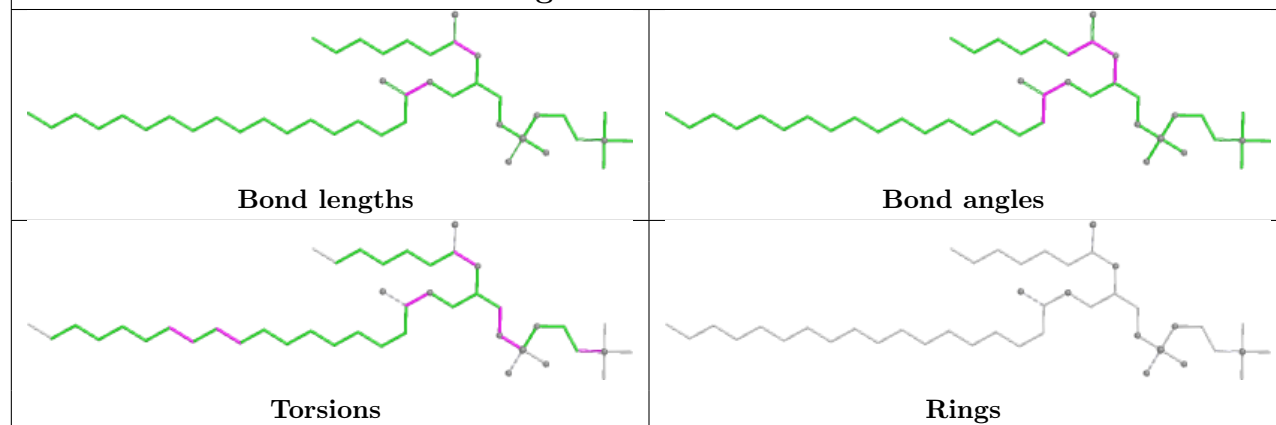


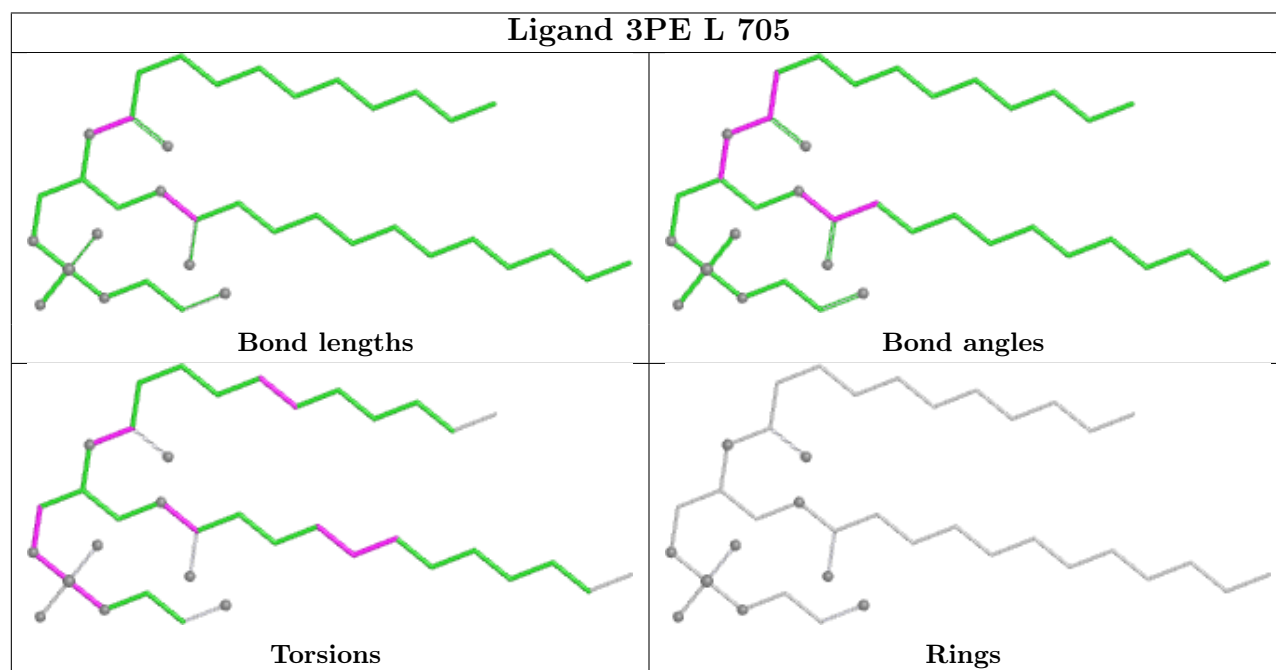
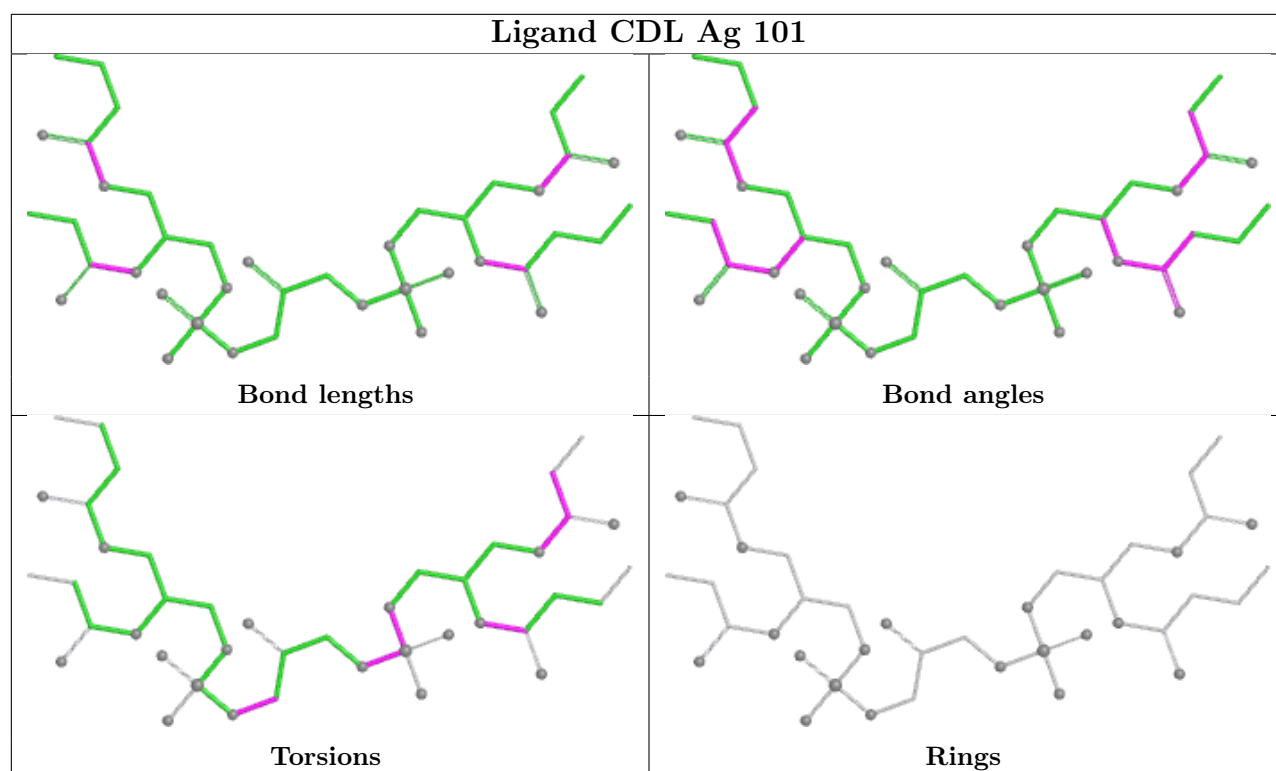


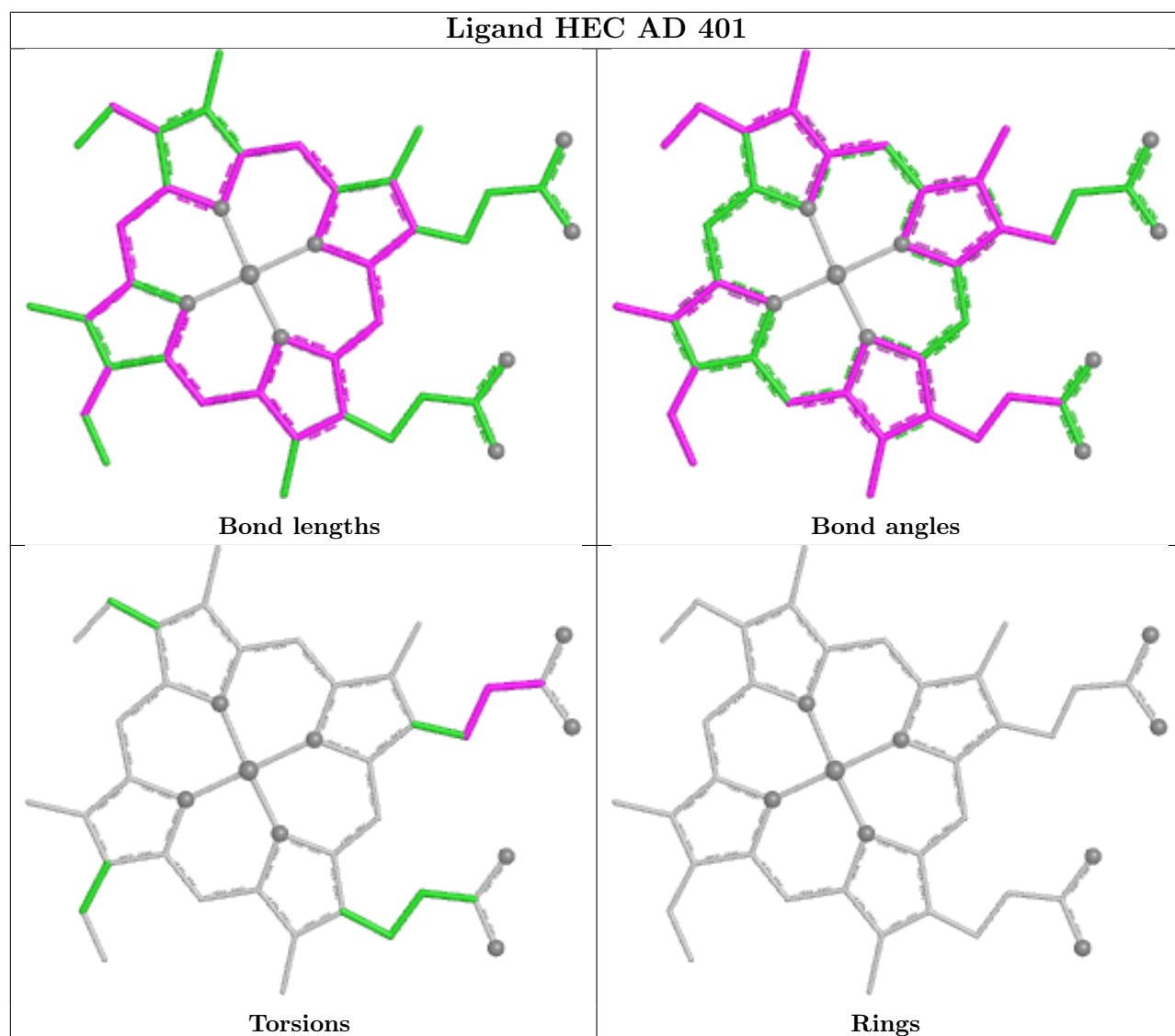
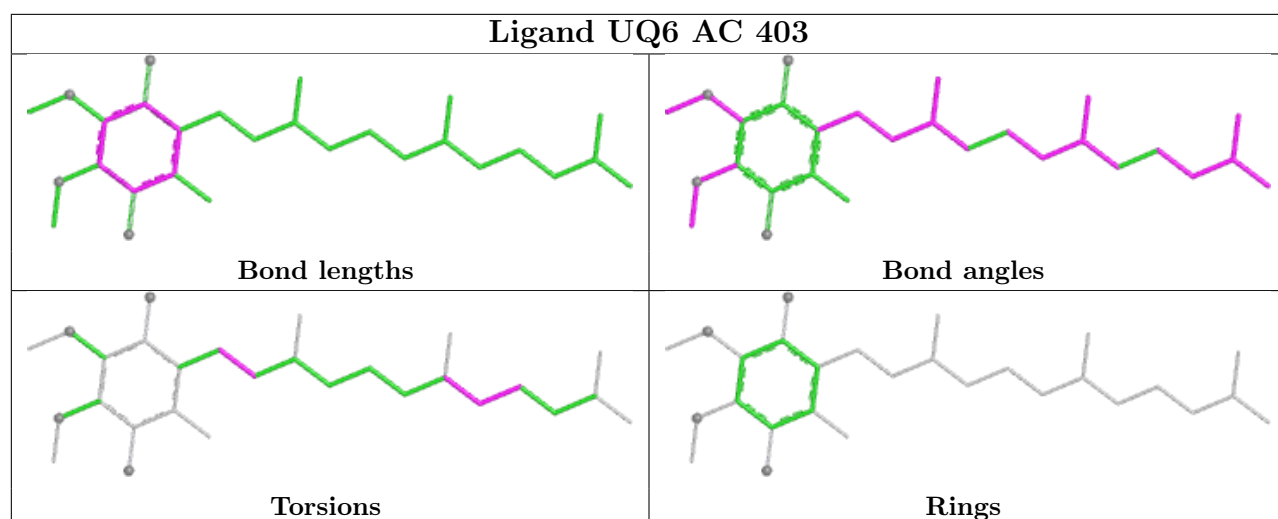
Ligand HEM Ac 401

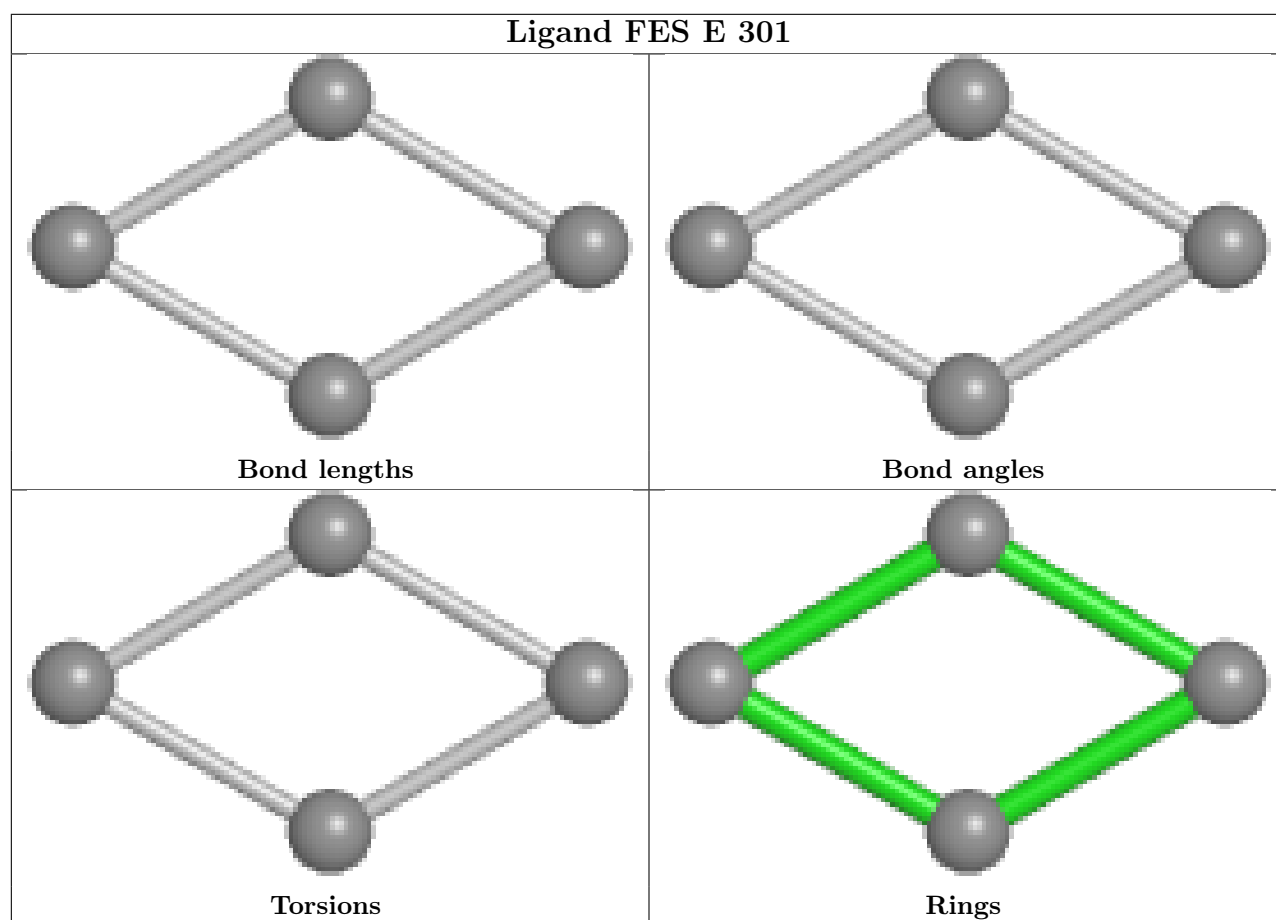
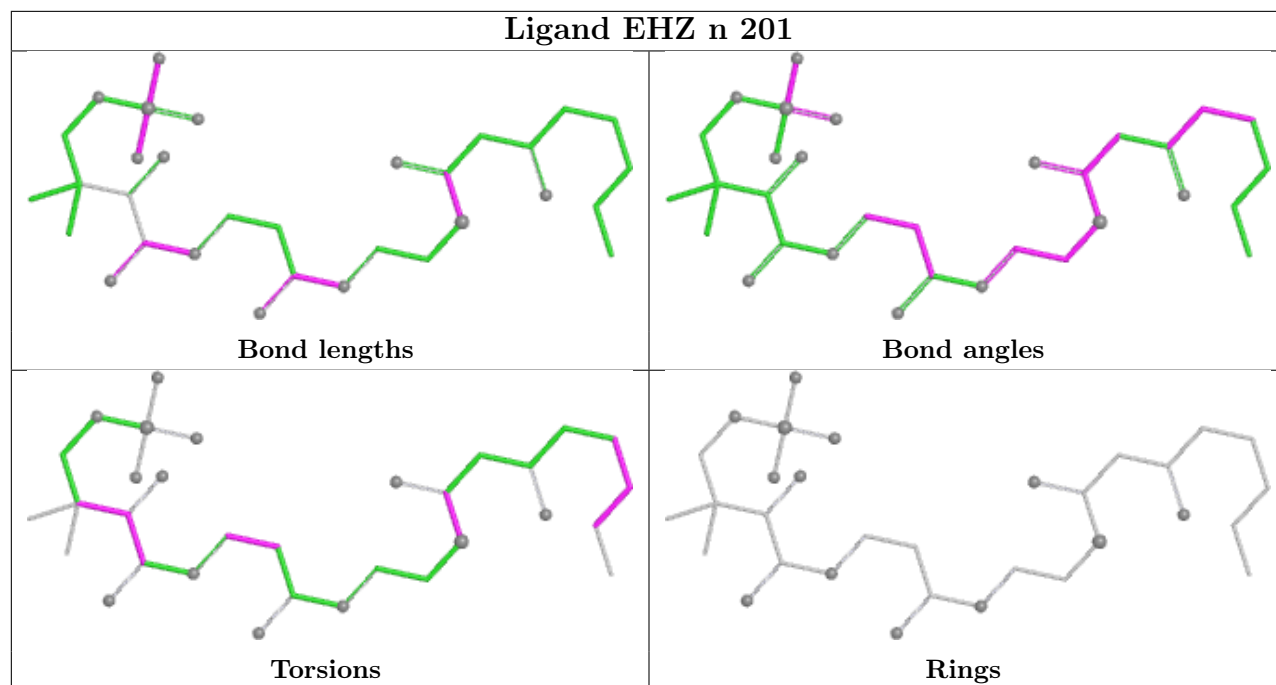


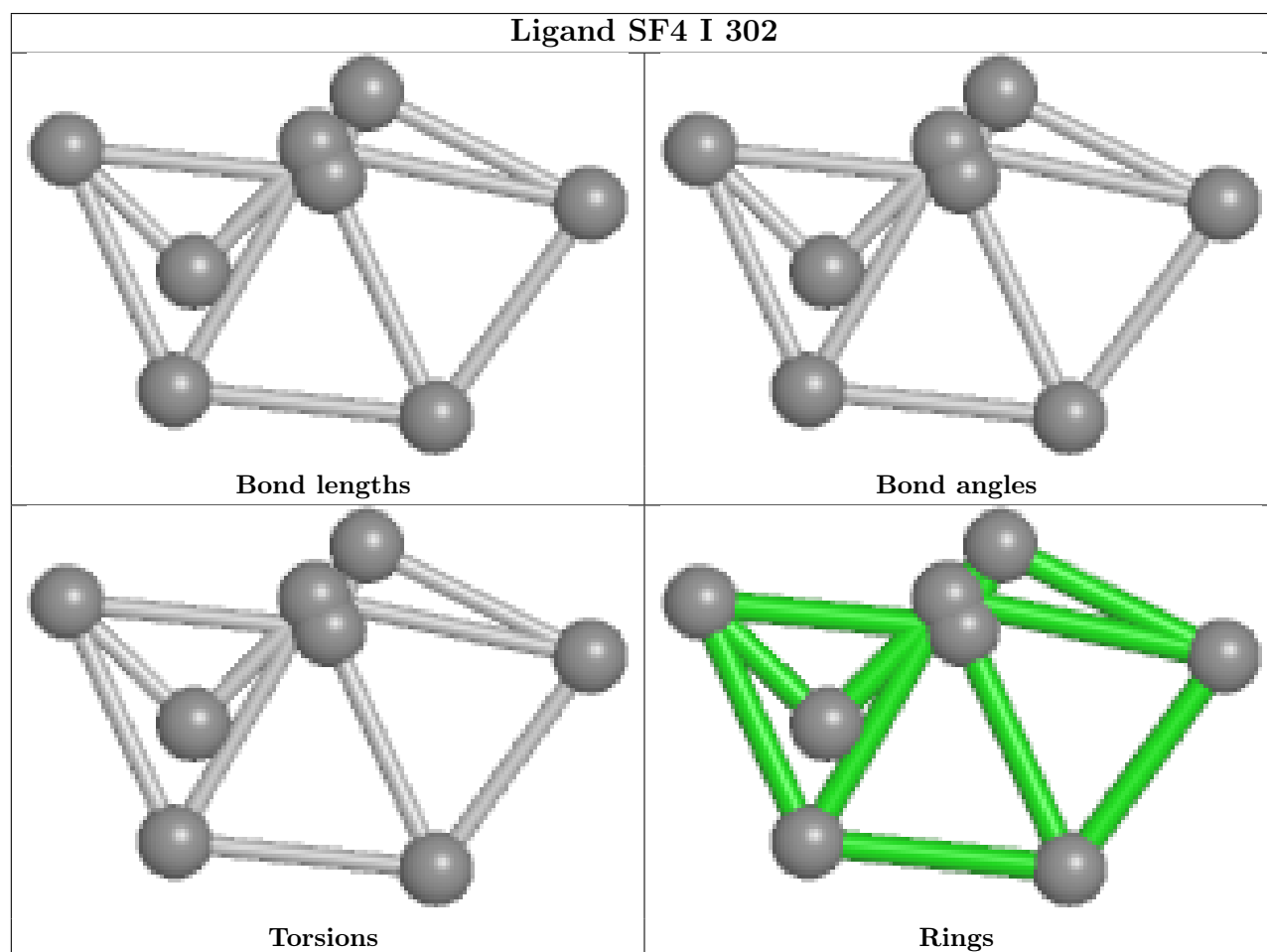
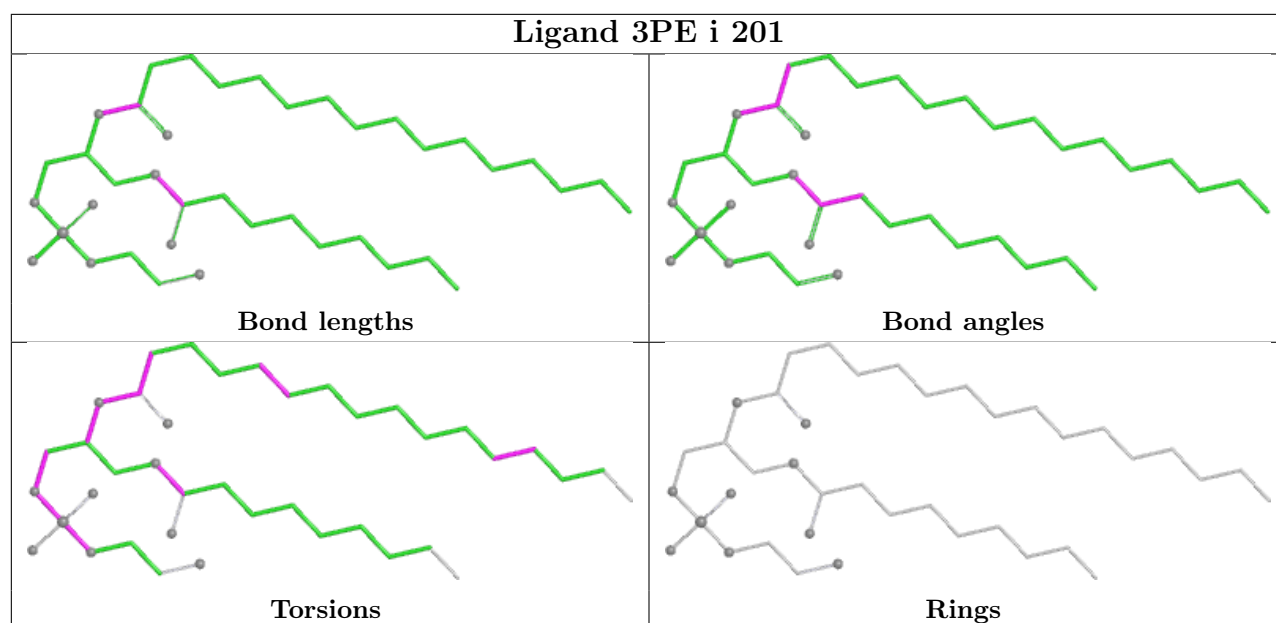
Ligand PC1 B 304

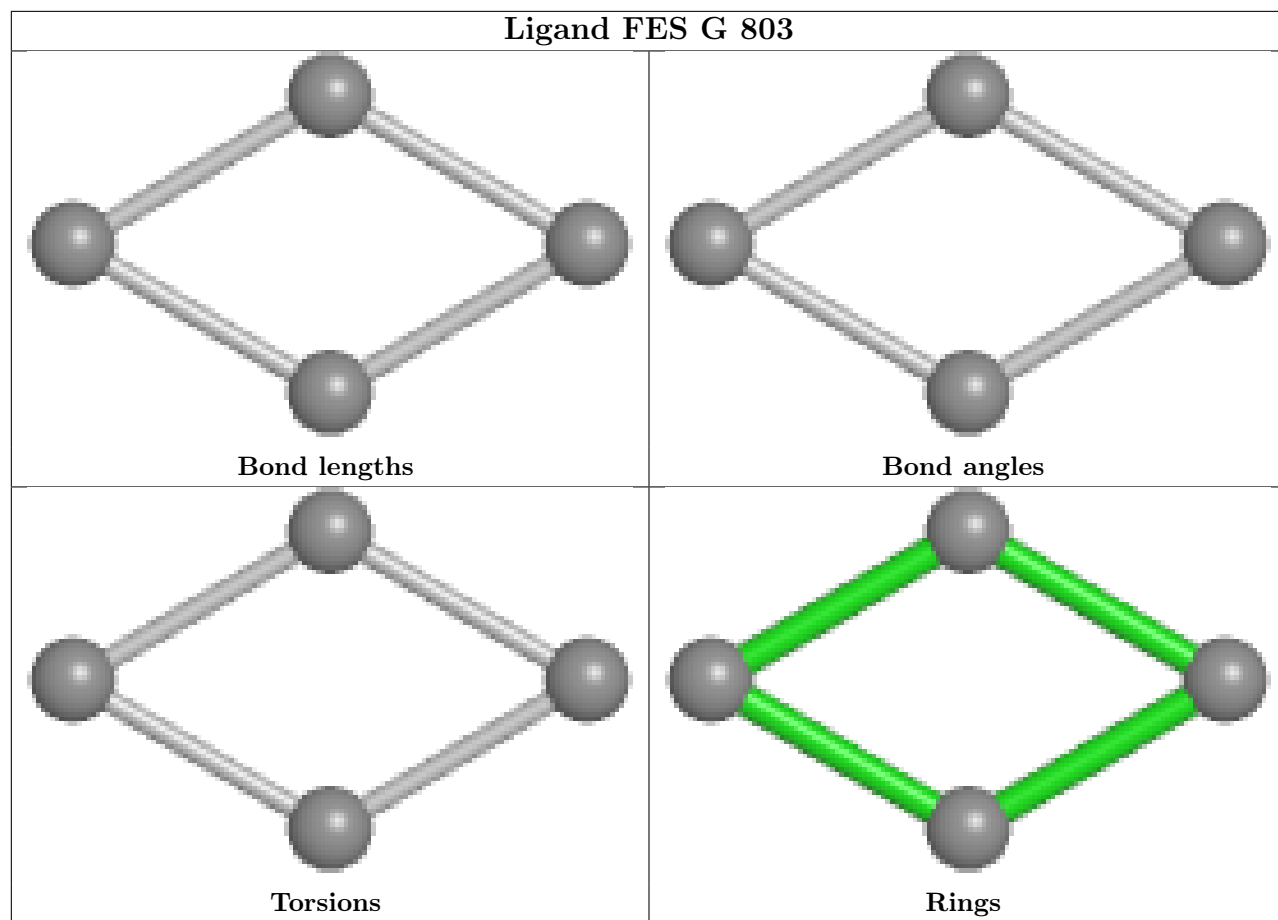




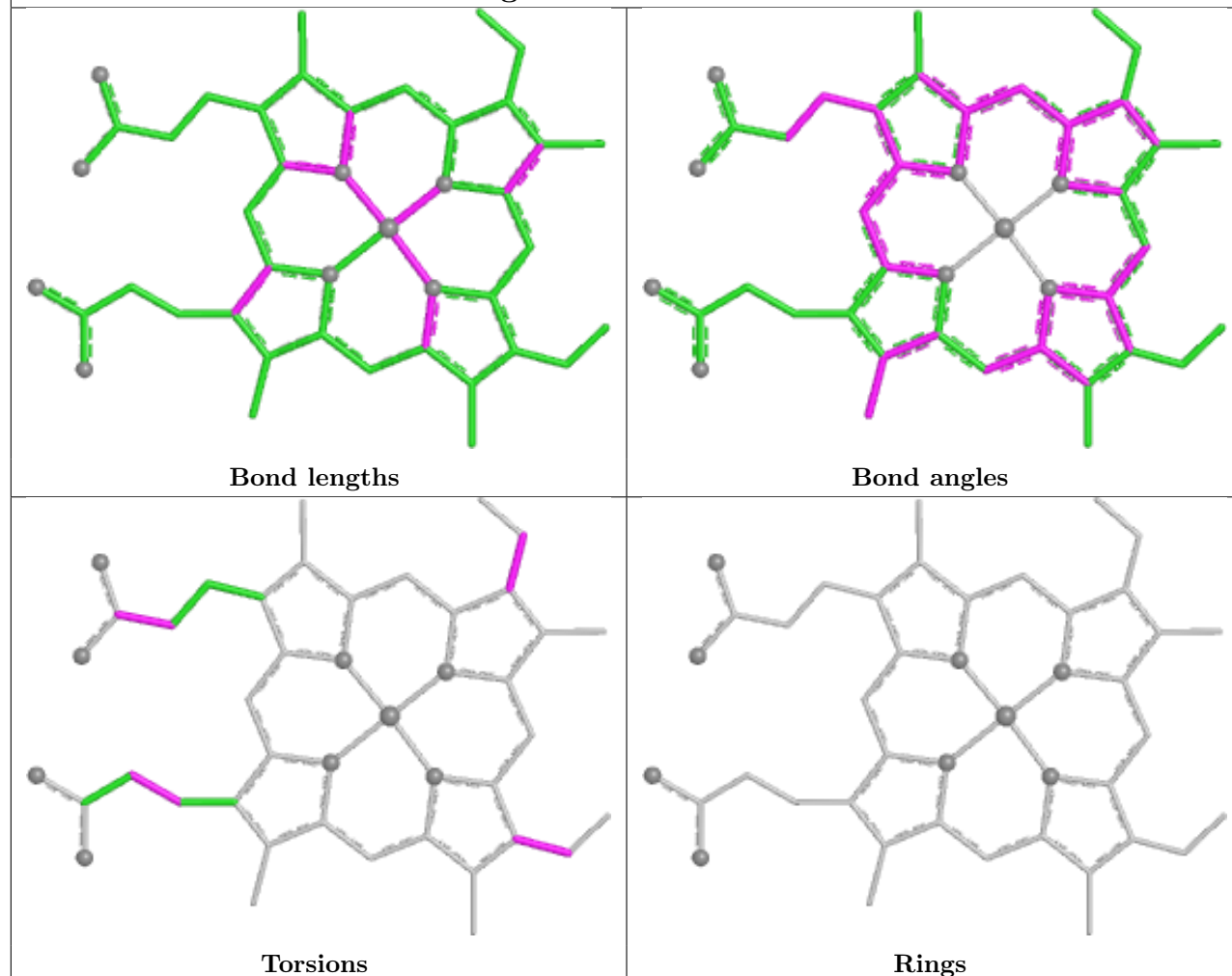




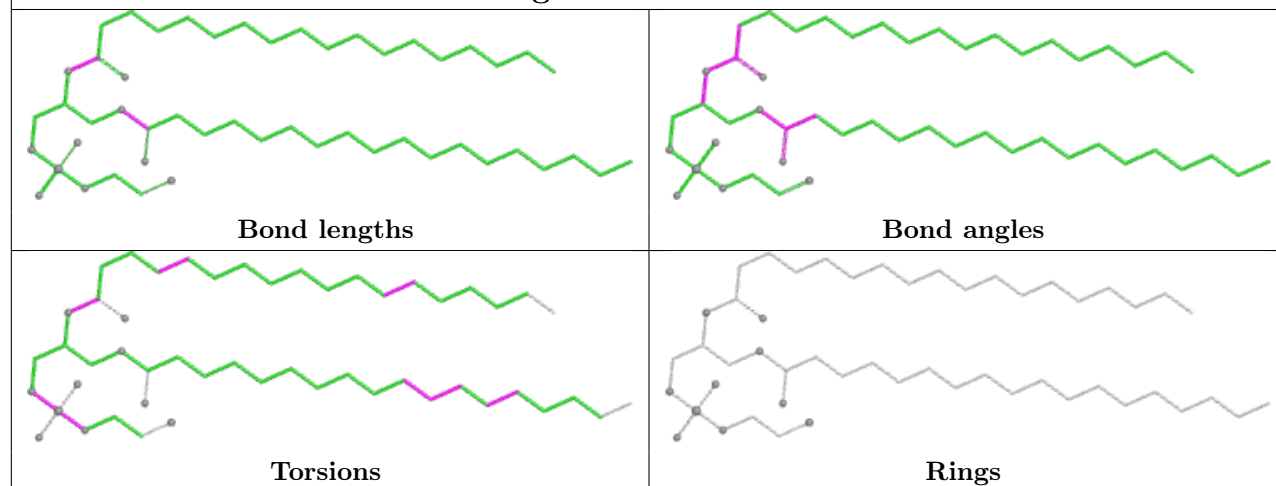


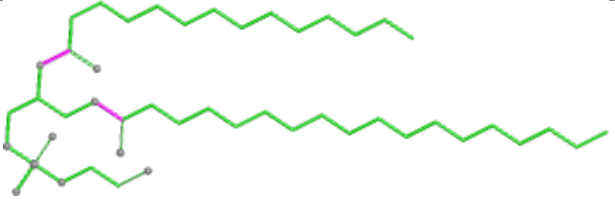
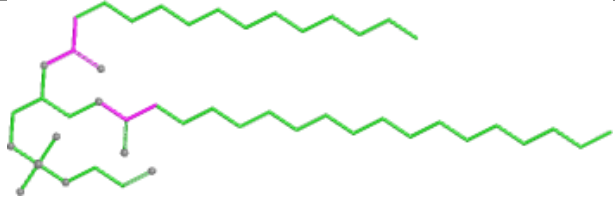
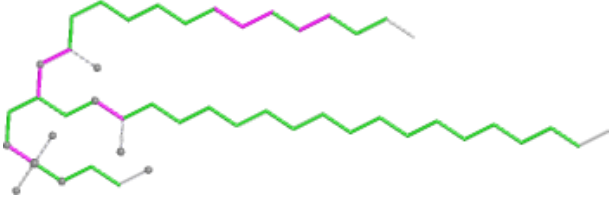
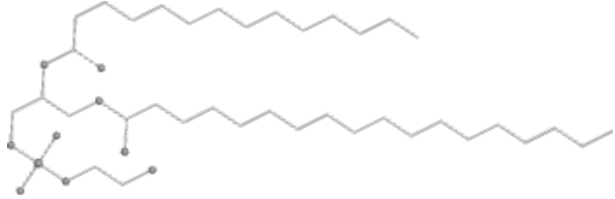
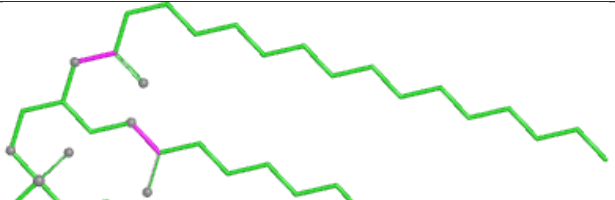
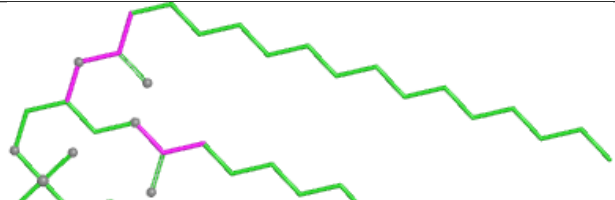
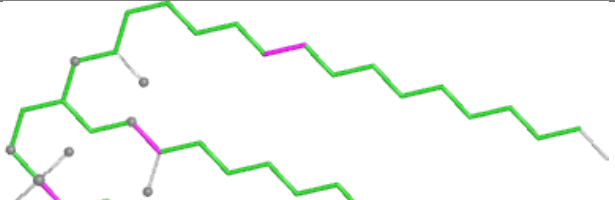
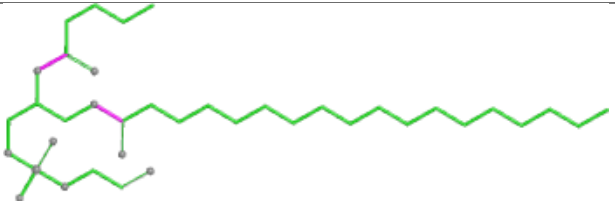
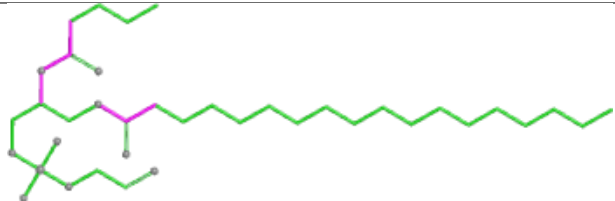
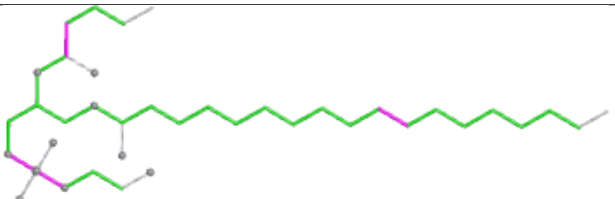
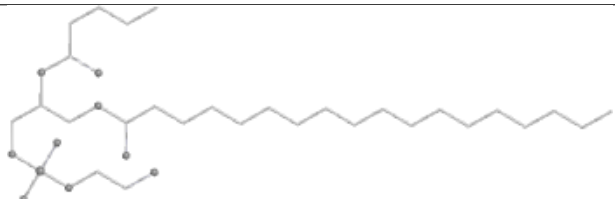


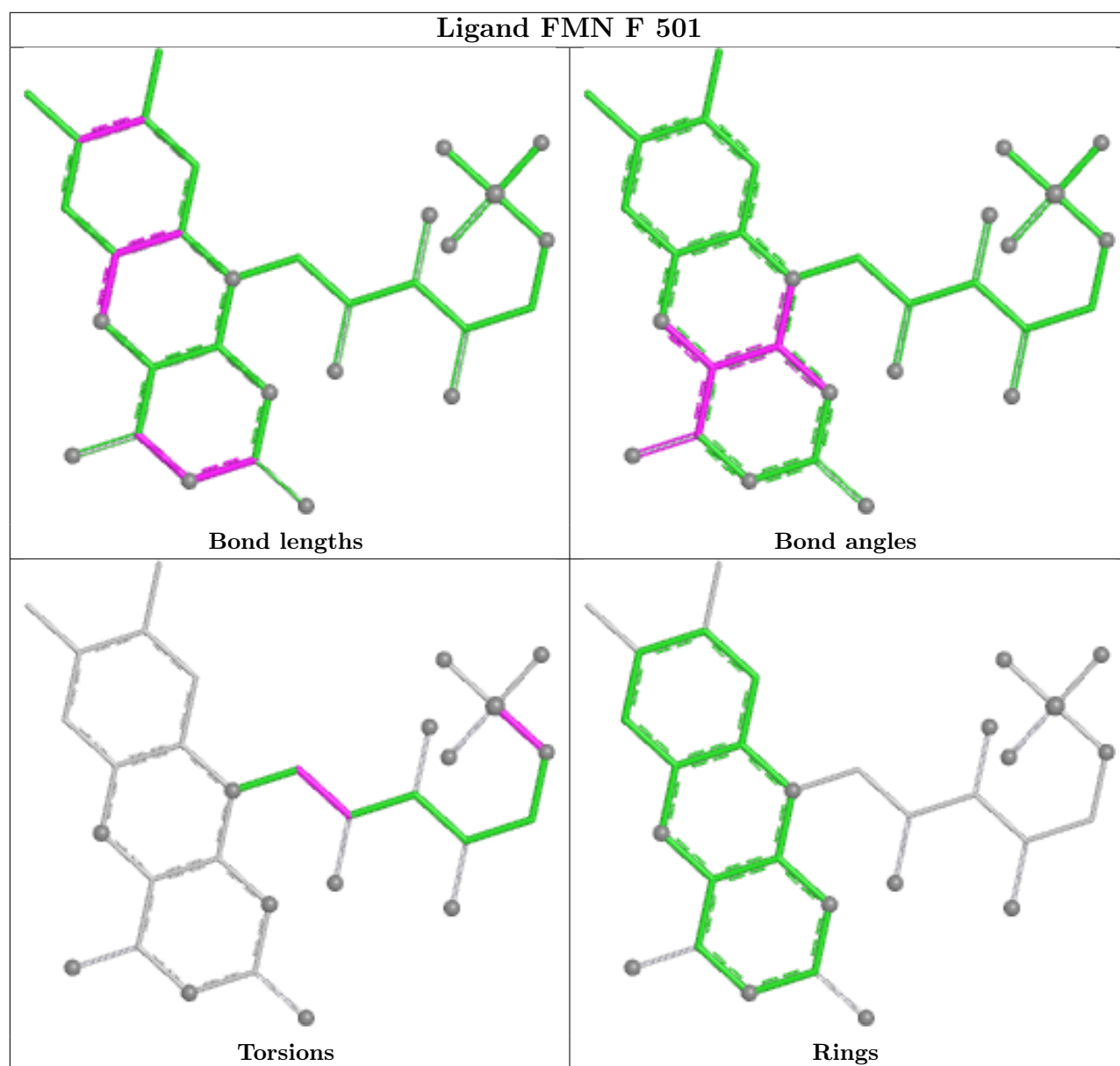
Ligand HEM Ac 402



Ligand 3PE M 502



Ligand 3PE m 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 3PE L 703	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 3PE Ag 103	
 Bond lengths	 Bond angles
 Torsions	 Rings



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.

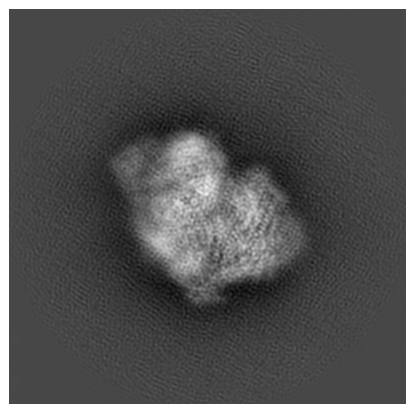
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35340. These allow visual inspection of the internal detail of the map and identification of artifacts.

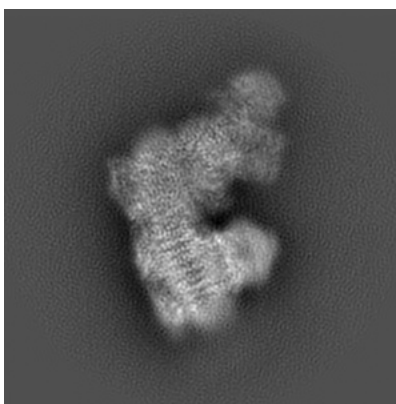
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

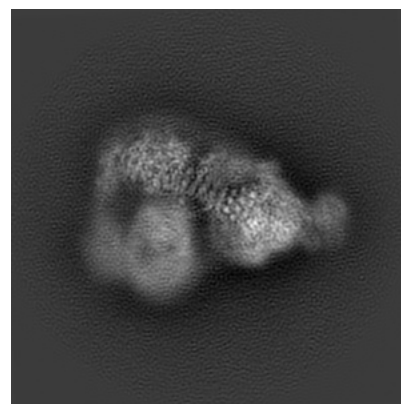
6.1.1 Primary map



X

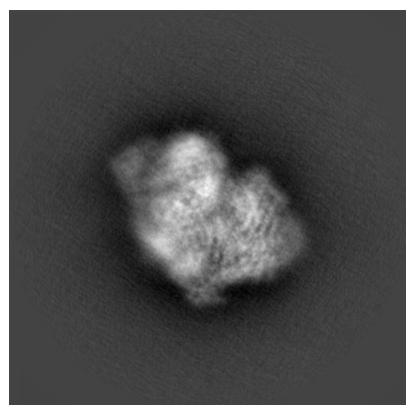


Y

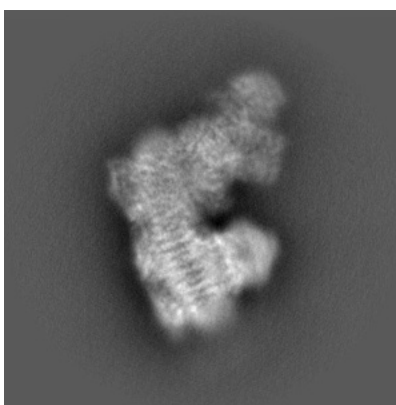


Z

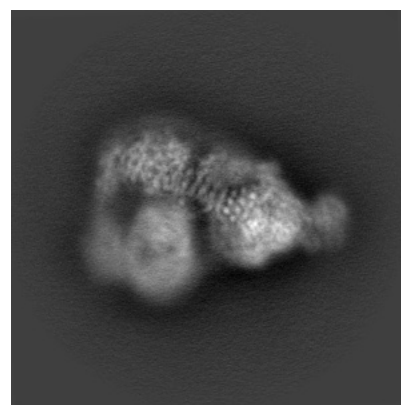
6.1.2 Raw map



X



Y

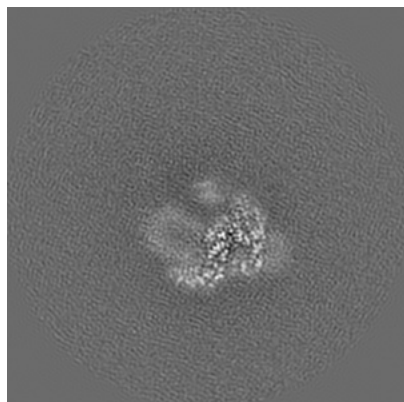


Z

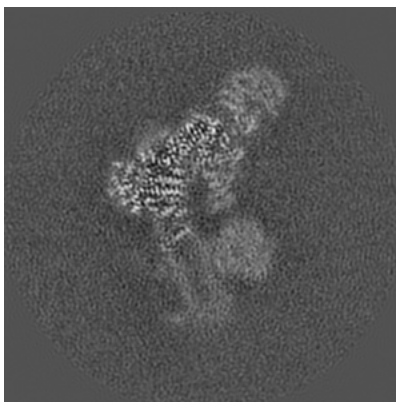
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

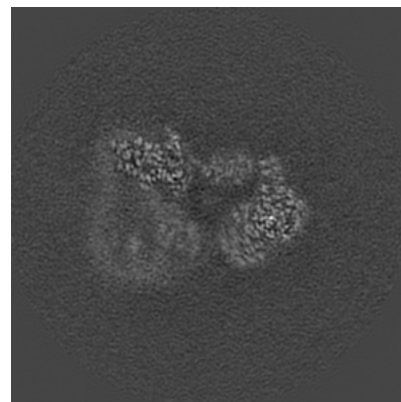
6.2.1 Primary map



X Index: 192

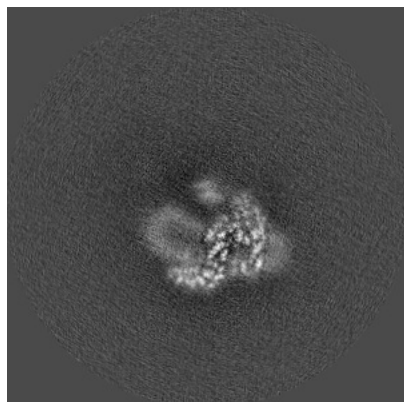


Y Index: 192

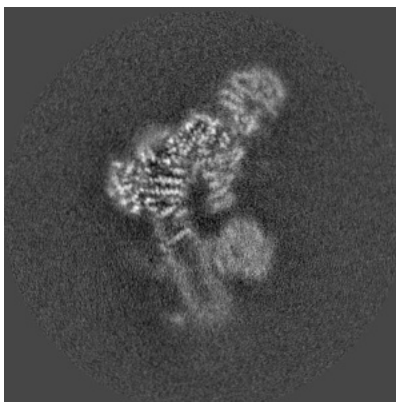


Z Index: 192

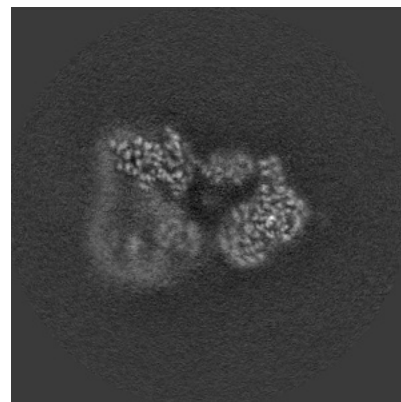
6.2.2 Raw map



X Index: 192



Y Index: 192

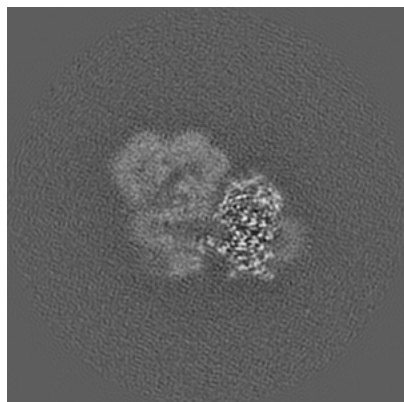


Z Index: 192

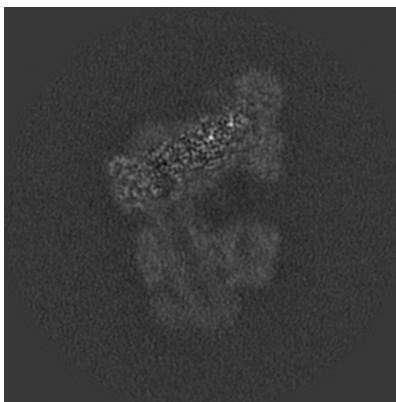
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

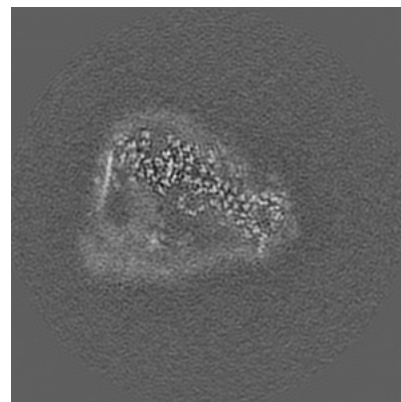
6.3.1 Primary map



X Index: 157

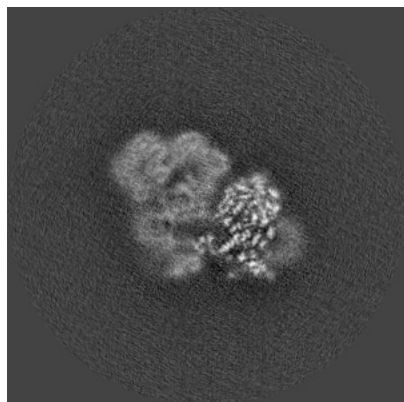


Y Index: 176

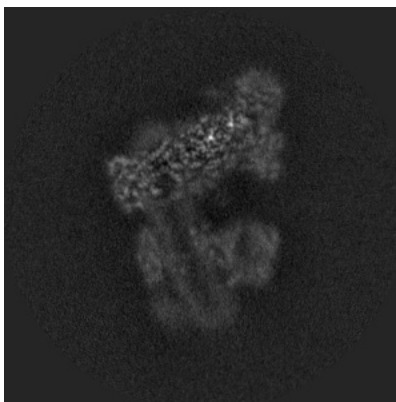


Z Index: 167

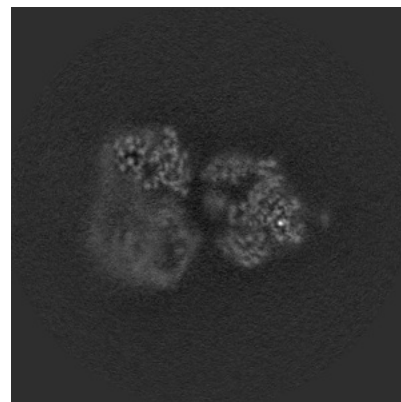
6.3.2 Raw map



X Index: 159



Y Index: 176

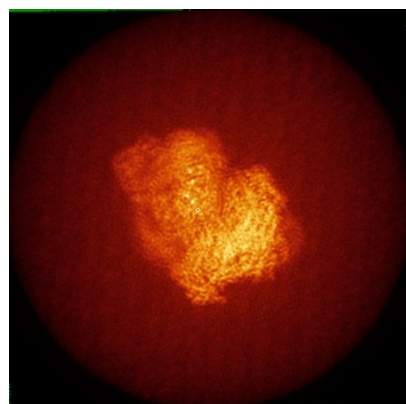


Z Index: 198

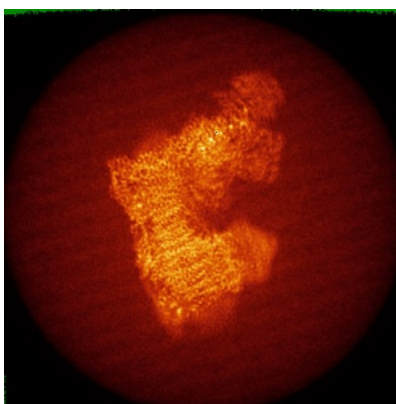
The images above show the largest variance slices of the map in three orthogonal directions.

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

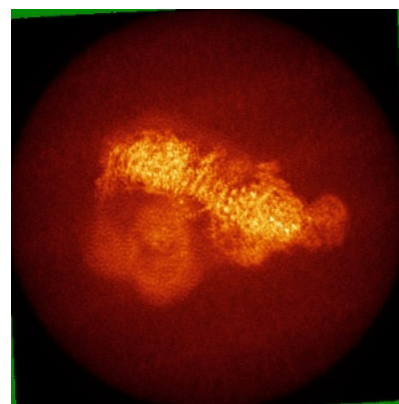
6.4.1 Primary map



X

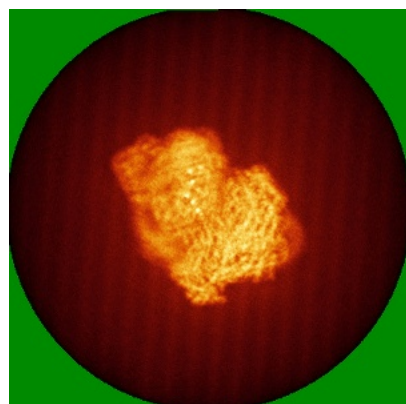


Y

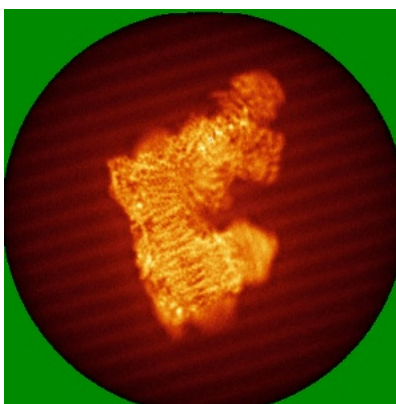


Z

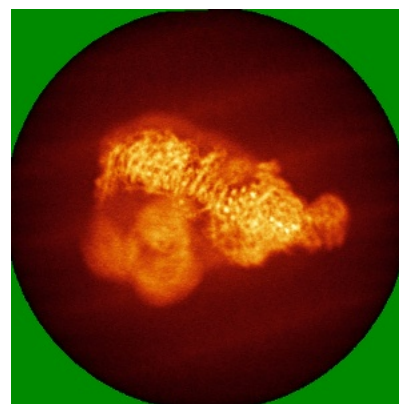
6.4.2 Raw map



X



Y

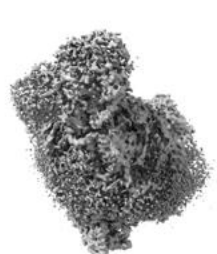


Z

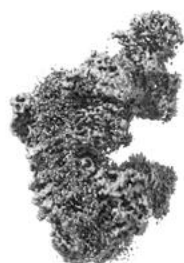
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



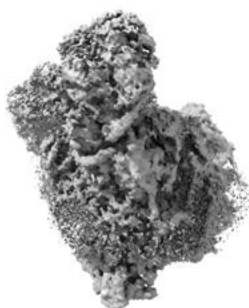
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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



X



Y



Z

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.

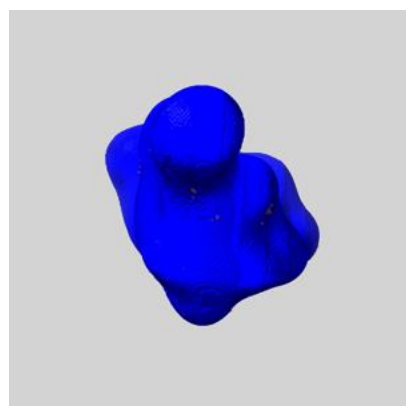
6.6 Mask visualisation [i](#)

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

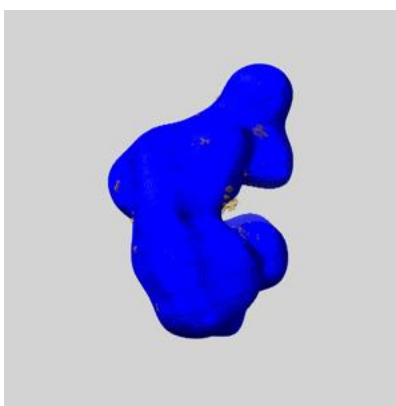
A mask typically either:

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

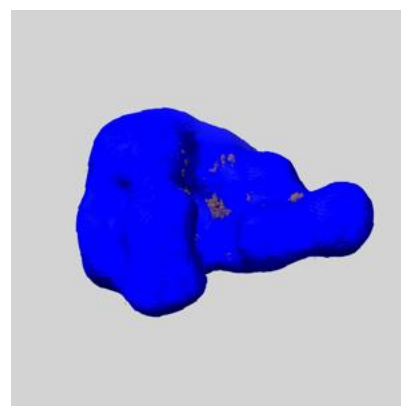
6.6.1 emd_35340_msk_1.map [i](#)



X



Y

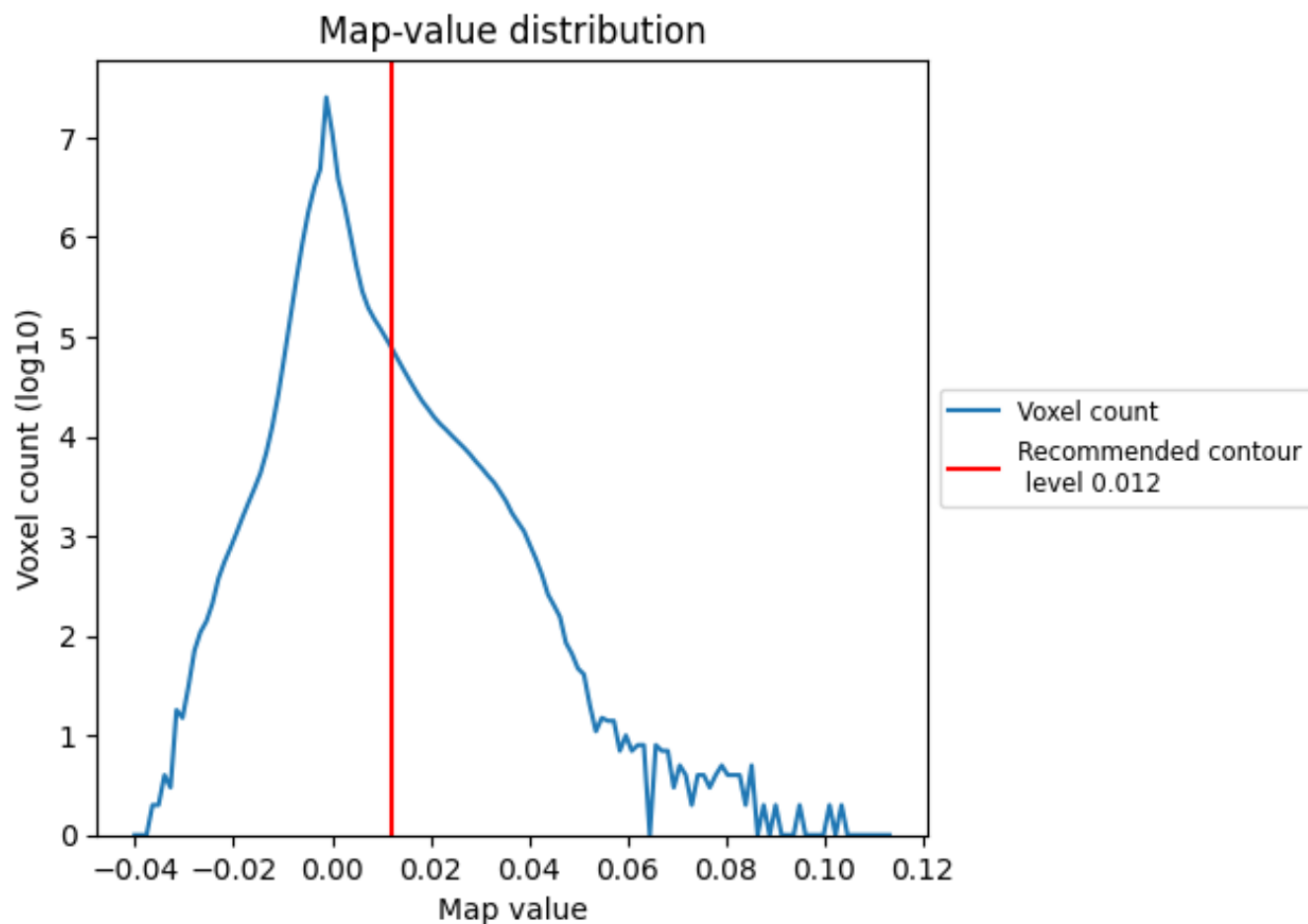


Z

7 Map analysis [i](#)

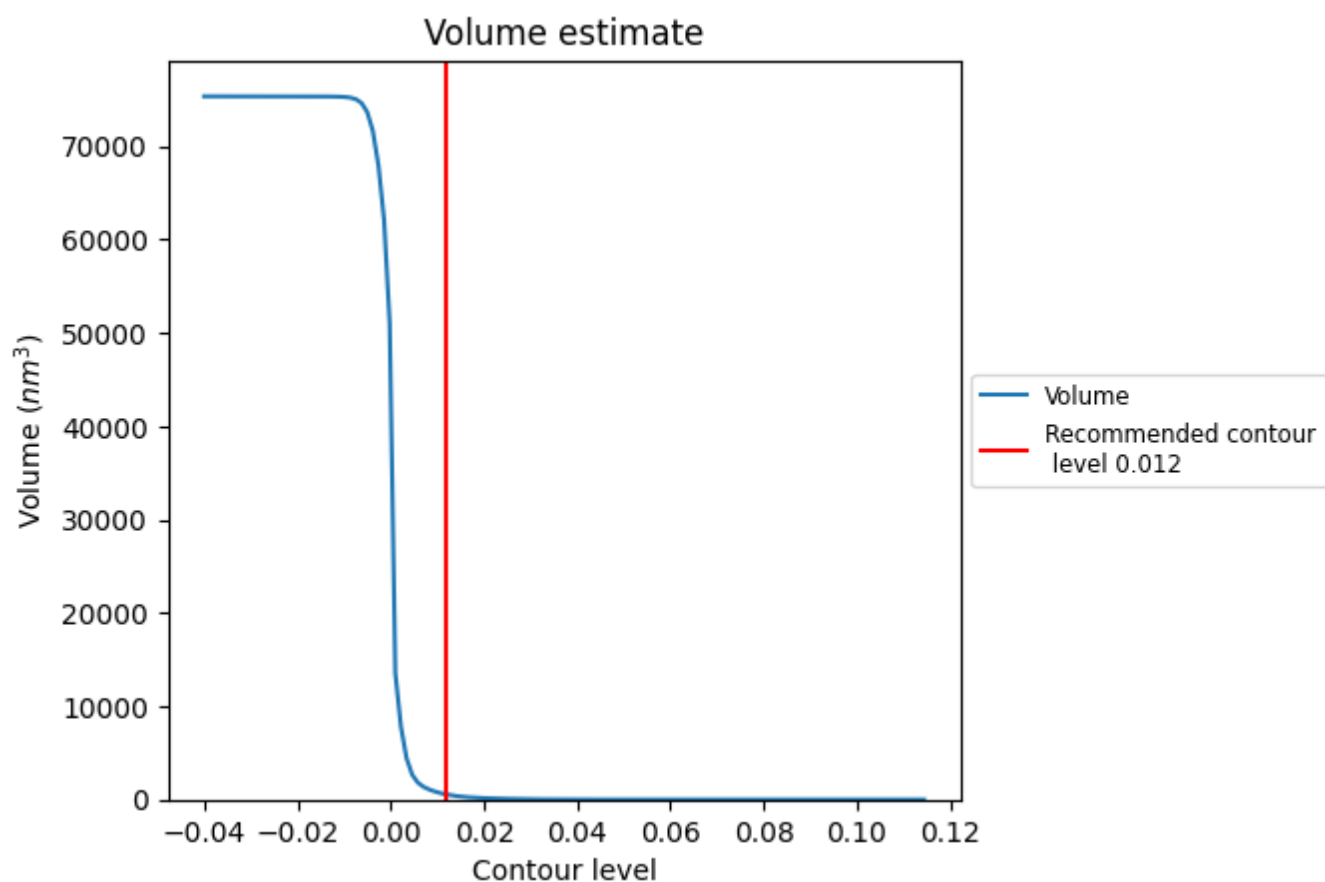
This section contains the results of statistical analysis of the map.

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.

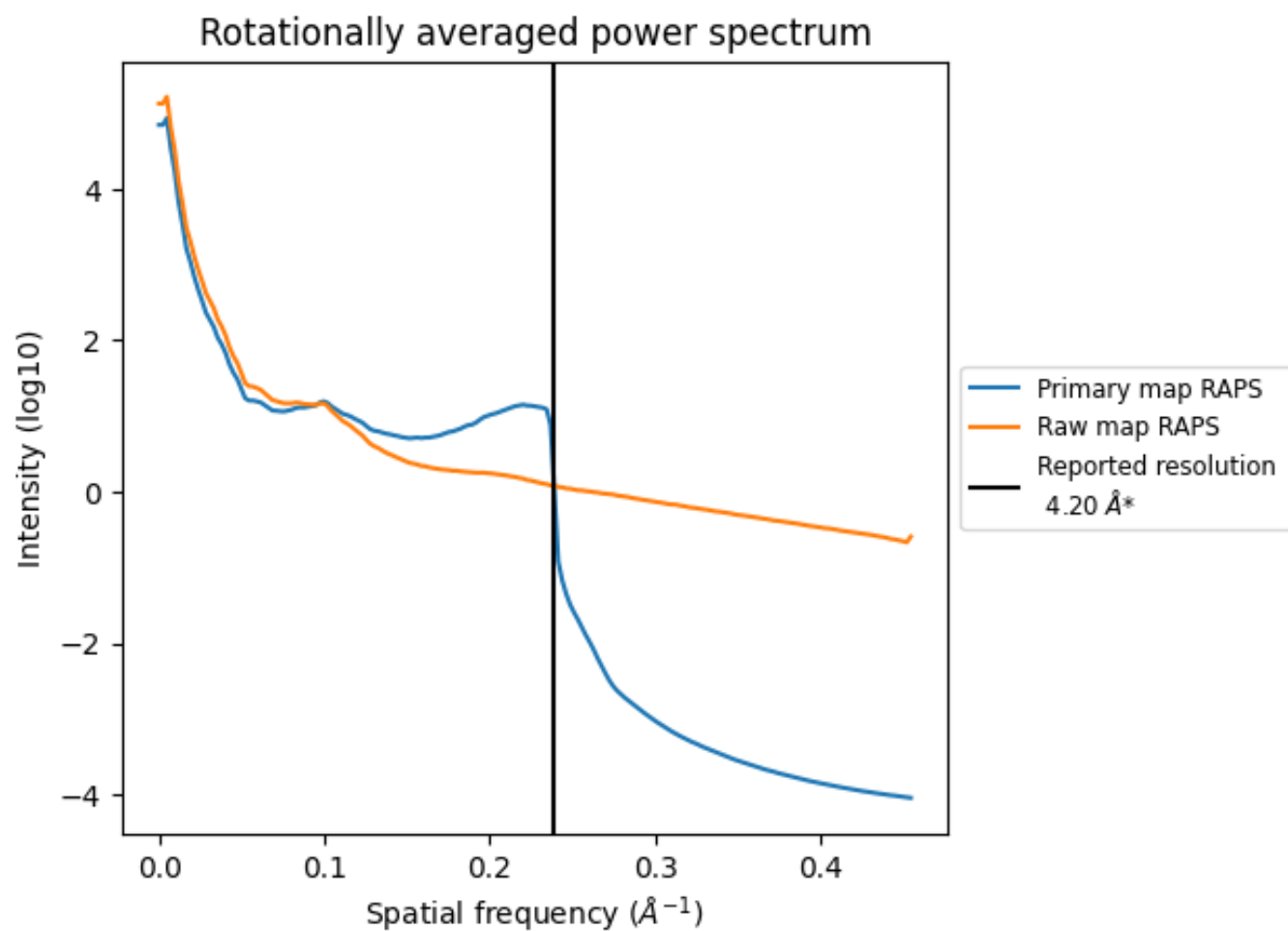
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 542 nm³; this corresponds to an approximate mass of 490 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

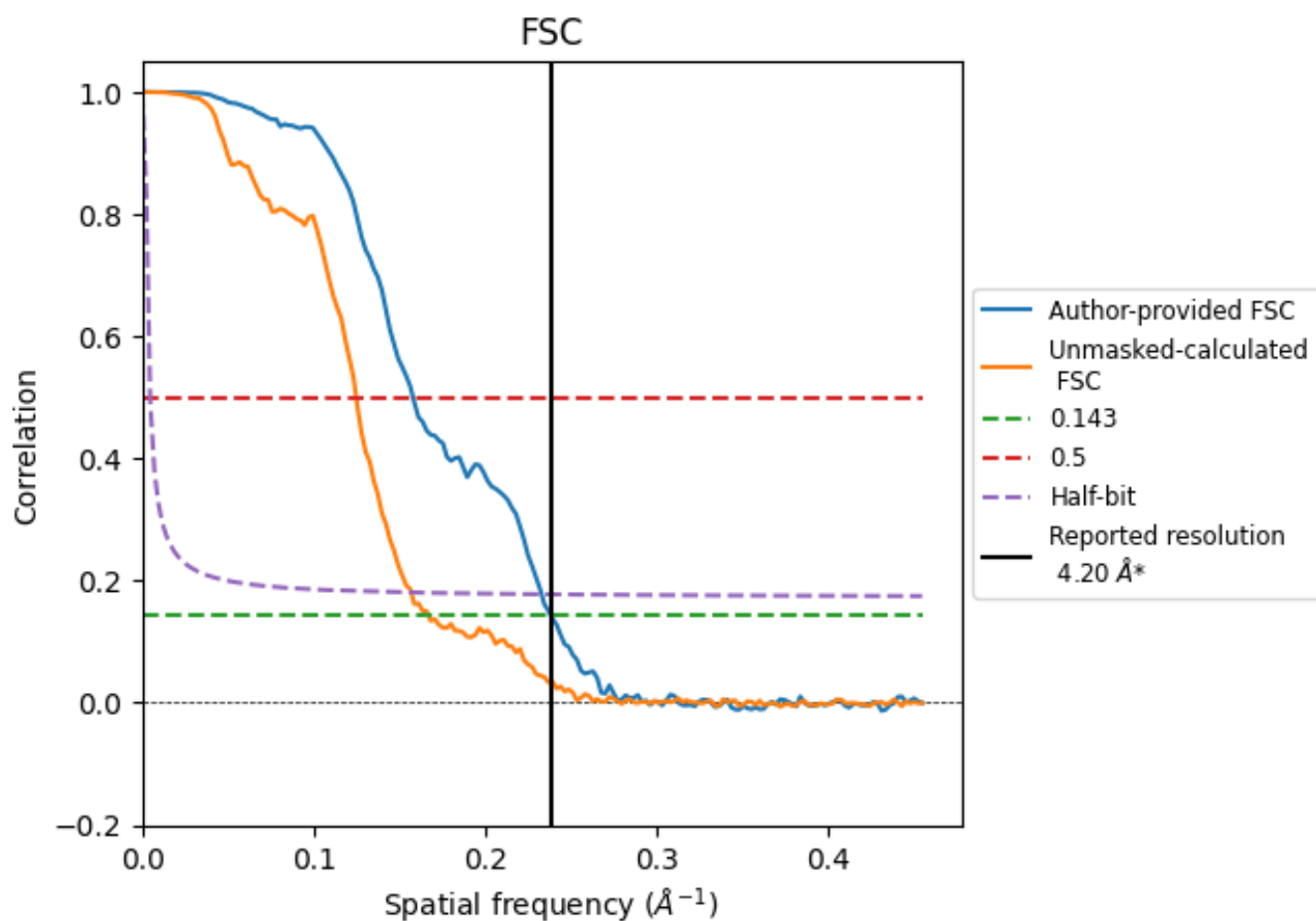


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

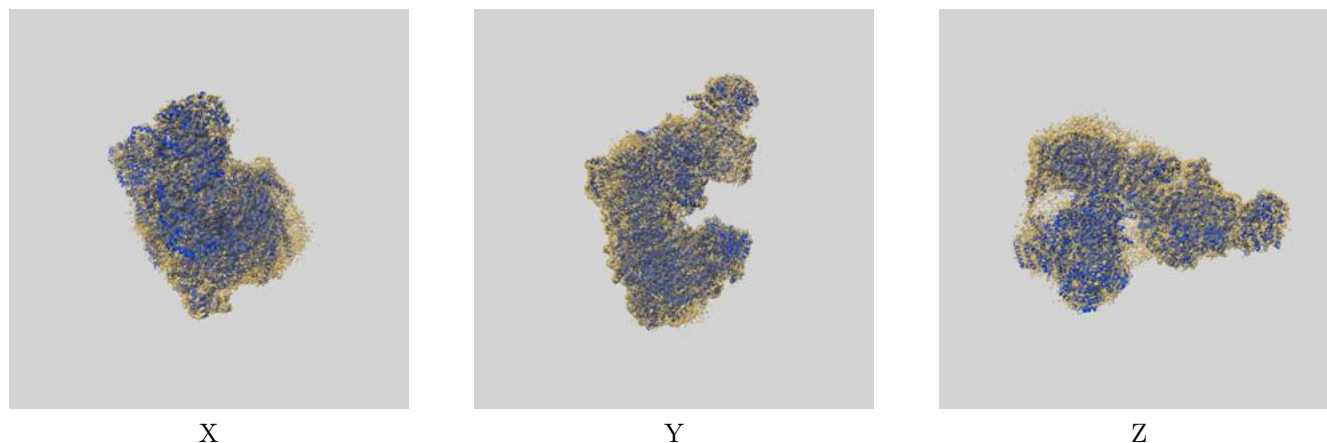
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.34	4.30
Unmasked-calculated*	6.00	8.02	6.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.00 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

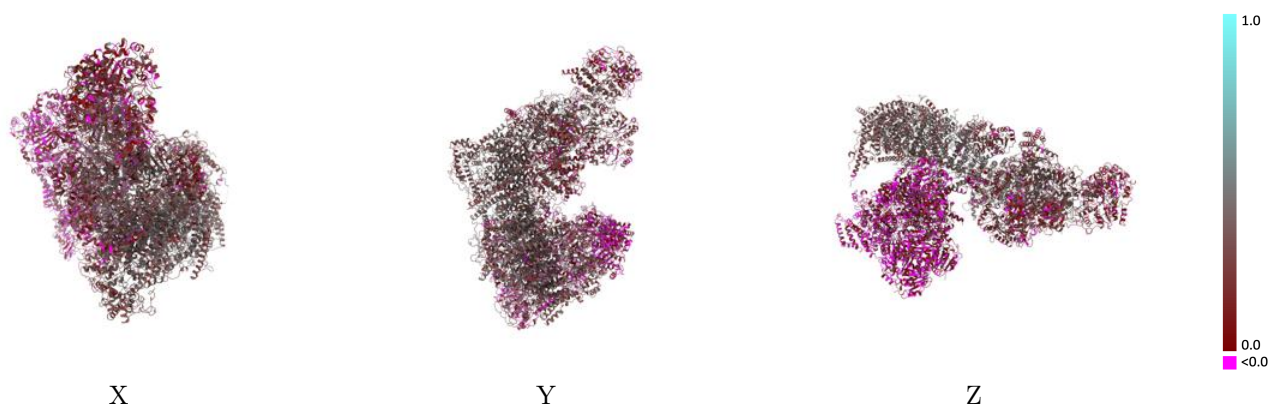
This section contains information regarding the fit between EMDB map EMD-35340 and PDB model 8IBD. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



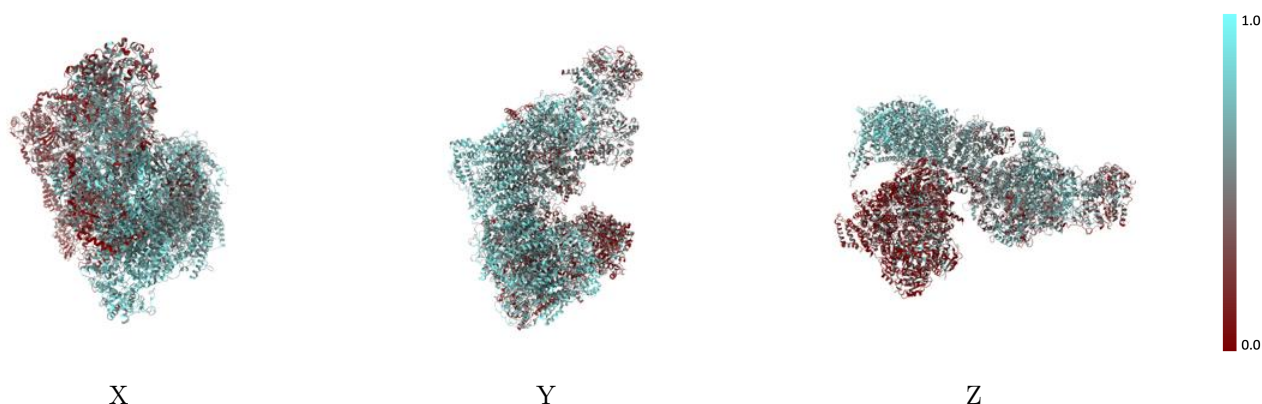
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



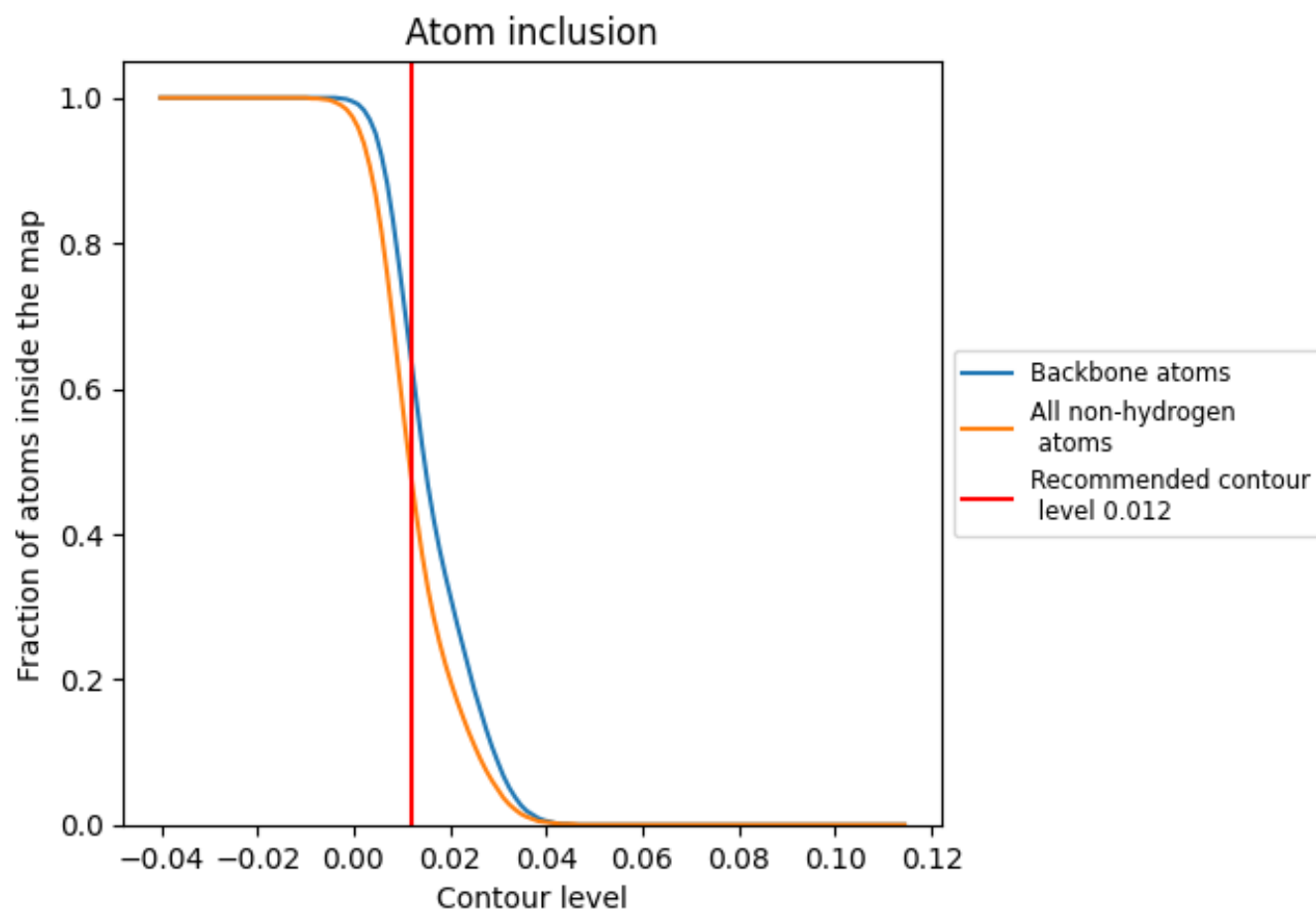
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 48% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4760	 0.2320
A	 0.5720	 0.3400
AA	 0.2260	 0.0500
AB	 0.2790	 0.0900
AC	 0.1360	 0.0600
AD	 0.1840	 0.0400
AE	 0.0400	 0.0110
AF	 0.2120	 0.0620
AG	 0.1030	 0.0200
AH	 0.1380	 0.0390
AI	 0.0610	 0.0570
AJ	 0.0870	 -0.0090
AK	 0.0170	 -0.0420
Aa	 0.2460	 0.0880
Ab	 0.2610	 0.0640
Ac	 0.2520	 0.1320
Ad	 0.3300	 0.1260
Ae	 0.0650	 0.0450
Af	 0.2580	 0.1320
Ag	 0.1940	 0.1060
Ah	 0.2590	 0.0910
Ai	 0.0400	 0.0720
Aj	 0.1070	 0.1090
Ak	 0.0240	 0.0290
B	 0.6760	 0.3570
C	 0.6330	 0.2840
D	 0.6690	 0.3480
E	 0.3820	 0.1930
F	 0.4370	 0.1890
G	 0.5440	 0.2330
H	 0.6730	 0.3720
I	 0.7440	 0.3600
J	 0.5640	 0.3220
K	 0.6160	 0.3800
L	 0.6650	 0.3660



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Chain	Atom inclusion	Q-score
M	 0.7000	 0.3940
N	 0.6830	 0.3940
O	 0.4740	 0.2590
P	 0.4870	 0.2060
Q	 0.4780	 0.2770
R	 0.2910	 0.1840
S	 0.4200	 0.1130
T	 0.2970	 0.1400
U	 0.7030	 0.3250
V	 0.5450	 0.2120
W	 0.4600	 0.1940
X	 0.7290	 0.3370
Y	 0.5570	 0.3280
Z	 0.7300	 0.3220
a	 0.6740	 0.3380
b	 0.7270	 0.3520
c	 0.6160	 0.2950
d	 0.6980	 0.3570
e	 0.7060	 0.3520
f	 0.6930	 0.3500
g	 0.6790	 0.3590
h	 0.7020	 0.3620
i	 0.6860	 0.3330
j	 0.7040	 0.3200
k	 0.7240	 0.3210
l	 0.7000	 0.3590
m	 0.6240	 0.3380
n	 0.7220	 0.3400
o	 0.6530	 0.2710
p	 0.7140	 0.3460
q	 0.1400	 0.1820
r	 0.1940	 0.1580
s	 0.1220	 0.1140