



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:50 PM JST

PDB ID : 8IB4 / pdb_00008ib4
EMDB ID : EMD-35331
Title : Respiratory complex CI:CIII2, type IA, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 4.30 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

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:

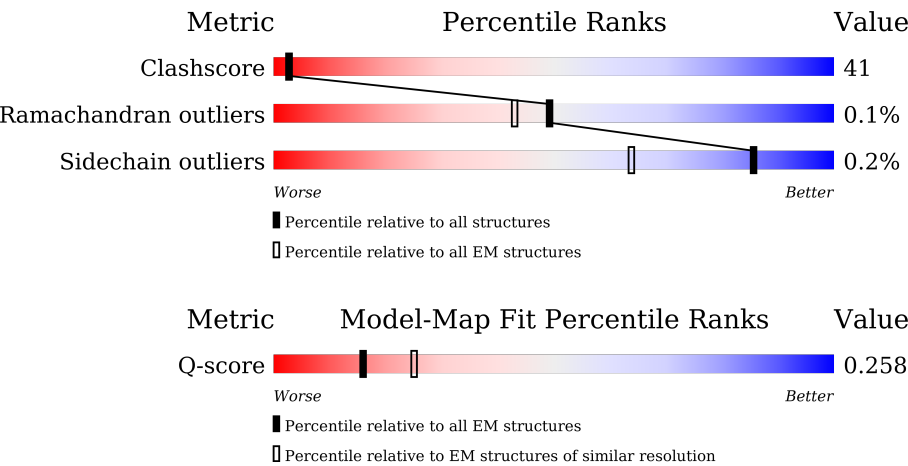
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 4.30 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	4585 (3.80 - 4.80)

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 ≥ 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	11% 17% 57% 7% 20%
2	B	224	6% 29% 34% 7% 30%
3	C	263	25% 36% 37% • 25%
4	D	463	13% 37% 50% 5% 8%

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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	
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	3PE	L	701	-	-	X	-
56	SF4	B	301	-	-	X	-
56	SF4	F	502	-	-	X	-
56	SF4	G	802	-	-	X	-
56	SF4	I	303	-	-	X	-
56	SF4	I	304	-	-	X	-
57	UQ1	B	302	-	-	X	-
59	FES	E	301	-	-	X	-
59	FES	G	803	-	-	X	-
62	CDL	a	101	-	-	X	-
70	HEC	AD	401	X	-	X	-
70	HEC	Ad	401	X	-	X	-

2 Entry composition

There are 71 unique types of molecules in this entry. The entry contains 97639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	424	Total	C	N	O	S	0	0
			3415	2182	587	622	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	314	Total	C	N	O	S	0	0
			2510	1687	380	421	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	174	Total	C	N	O	S	0	0
			1398	880	240	266	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	159	Total	C	N	O	S	0	0
			1205	814	171	205	15		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	458	Total	C	N	O	S	0	0
			3622	2402	566	615	39		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	340	Total	C	N	O	S	0	0
			2730	1765	479	479	7		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	84	Total	C	N	O	S	0	0
			678	438	100	135	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	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	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	119	Total	C	N	O	S	0	0
			988	646	170	164	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			863	546	158	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	55	Total	C	N	O	S	0	0
			475	310	84	79	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	136	Total	C	N	O	S	0	0
			1146	754	191	198	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	94	Total	C	N	O	S	0	0
			796	520	139	134	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	71	Total	C	N	O	S	0	0
			569	375	99	93	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	158	Total	C	N	O	S	0	0
			1328	858	221	238	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	127	Total	C	N	O		0	0
			1054	678	190	186			

- 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	120	Total	C	N	O	S	0	0
			1027	647	192	179	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1438	904	258	268	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	120	Total	C	N	O	S	0	0
			1004	645	178	177	4		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	14	Total	C	N	O	0	0
			115	75	17	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	400	Total	C	N	O	S	0	0
			3128	1952	557	603	16		

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
46	Ab	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	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
48	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	185	Total	C	N	O	S	0	0
			1427	902	250	268	7		
49	AI	51	Total	C	N	O		0	0
			345	221	64	60			
49	Ae	185	Total	C	N	O	S	0	0
			1432	905	250	270	7		

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

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

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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	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
51	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	65	Total	C	N	O	S	0	0
			535	327	99	104	5		
52	Ah	66	Total	C	N	O	S	0	0
			544	333	101	105	5		

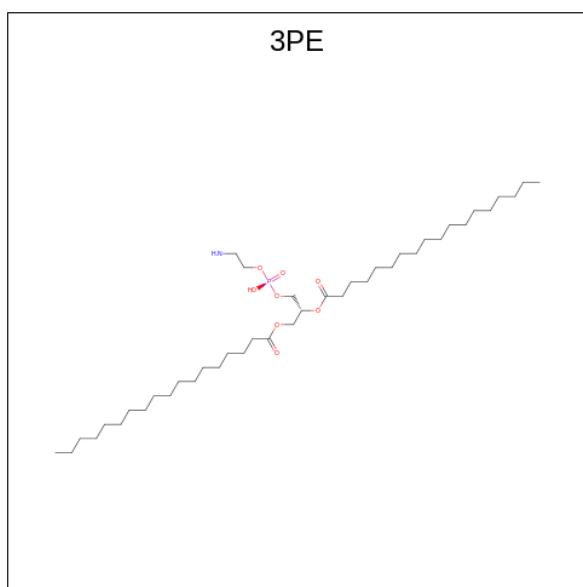
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
53	Aj	48	Total	C	N	O	0	0
			392	257	67	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	35	Total	C	N	O	S	0	0
			281	184	52	44	1		
54	Ak	44	Total	C	N	O	S	0	0
			357	236	63	57	1		

- Molecule 55 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



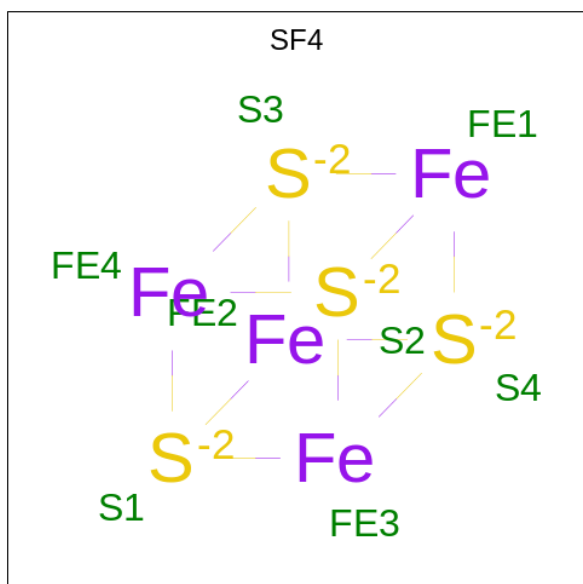
Mol	Chain	Residues	Atoms					AltConf
55	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
55	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
55	L	1	Total	C	N	O	P	0
			45	35	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
			51	41	1	8	1	
55	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
55	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
55	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
55	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
55	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	AF	1	Total	C	N	O	P	0
			42	32	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	
55	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
55	Ag	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



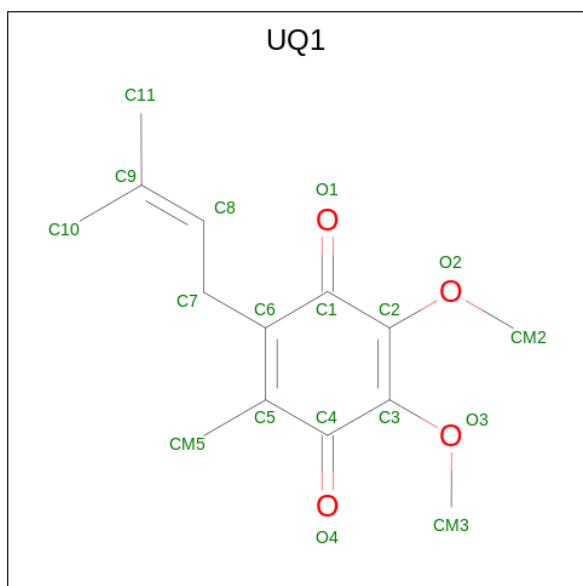
Mol	Chain	Residues	Atoms			AltConf
56	B	1	Total	Fe	S	0
			8	4	4	
56	F	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	G	1	Total	Fe	S	0
			8	4	4	
56	I	1	Total	Fe	S	0
			8	4	4	

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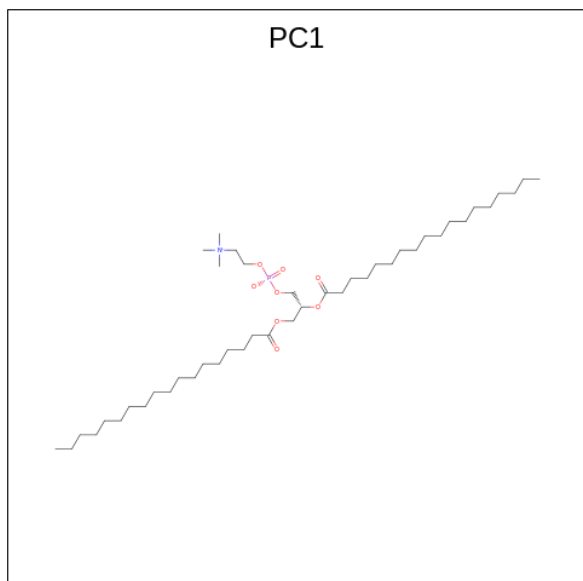
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
56	I	1	8	4	4	0

- Molecule 57 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



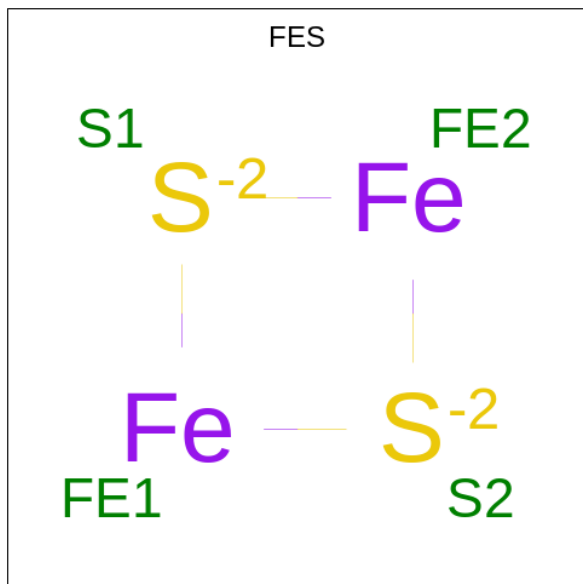
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
57	B	1	18	14	4	0

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



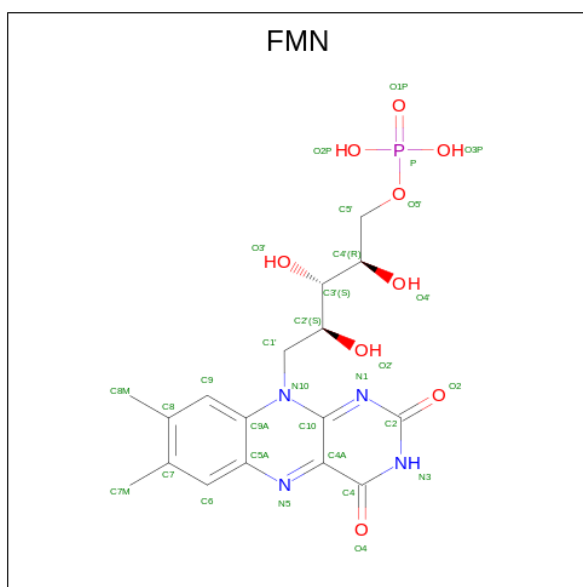
Mol	Chain	Residues	Atoms					AltConf
58	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	I	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	J	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



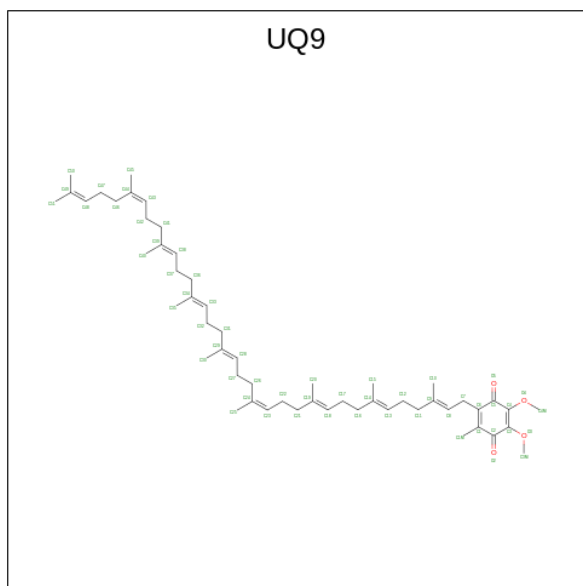
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



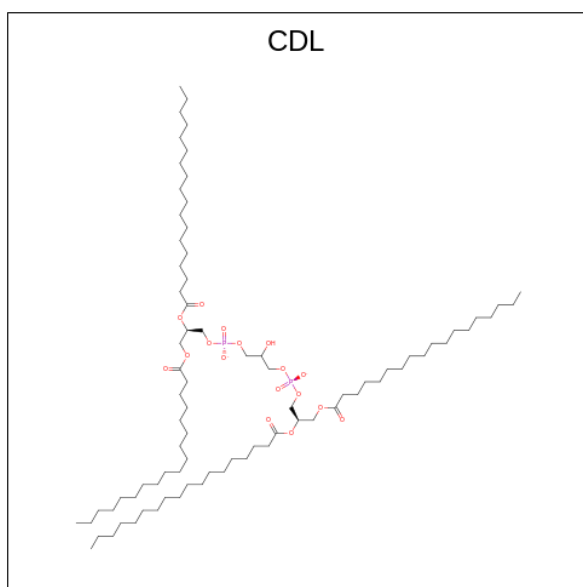
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



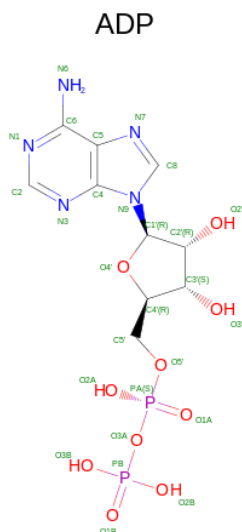
Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



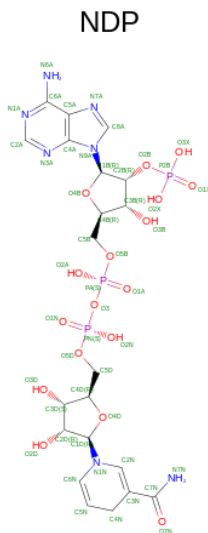
Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			77	58	17	2	
62	L	1	Total	C	O	P	0
			86	67	17	2	
62	X	1	Total	C	O	P	0
			67	48	17	2	
62	a	1	Total	C	O	P	0
			57	38	17	2	
62	h	1	Total	C	O	P	0
			70	51	17	2	
62	AC	1	Total	C	O	P	0
			56	37	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ac	1	Total	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: $C_{10}H_{15}N_5O_{10}P_2$).



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: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

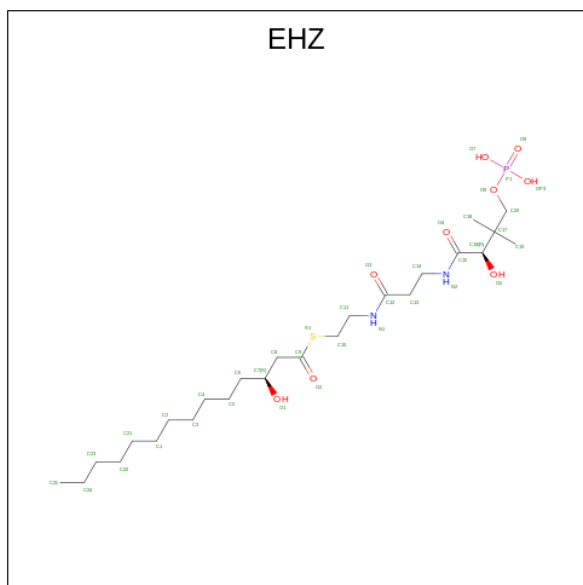


Mol	Chain	Residues	Atoms					AltConf
64	P	1	Total 48	C 21	N 7	O 17	P 3	0

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

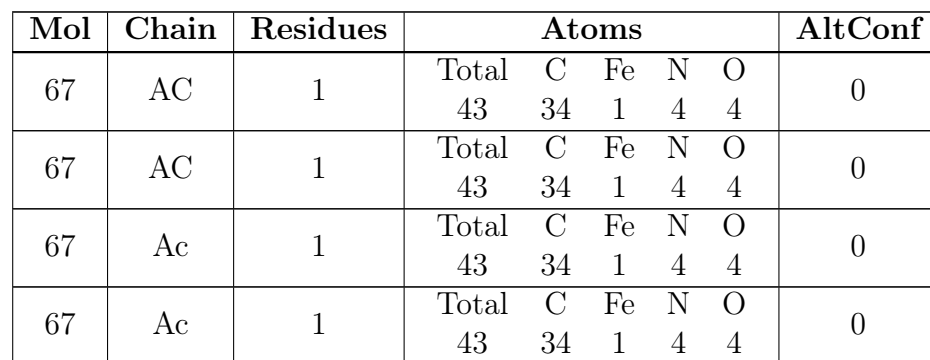
Mol	Chain	Residues	Atoms		AltConf
65	R	1	Total	Zn	0
			1	1	

- 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).



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

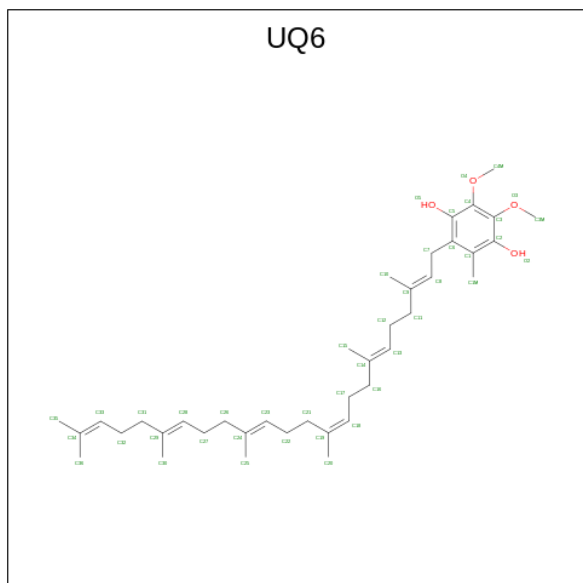
- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



- U10
-
- The chemical structure of U10 is a long-chain polyunsaturated fatty acid derivative. It consists of a long hydrocarbon chain with multiple double bonds and methyl branches, terminating in a substituted cyclohexene ring. The ring has two methoxy groups (OCH₃) and two hydroxyl groups (OH) attached to it.

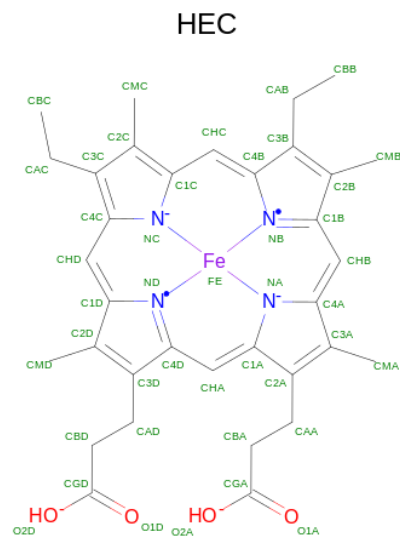
Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total	C	O	0
			23	19	4	
68	Ac	1	Total	C	O	0
			38	34	4	

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



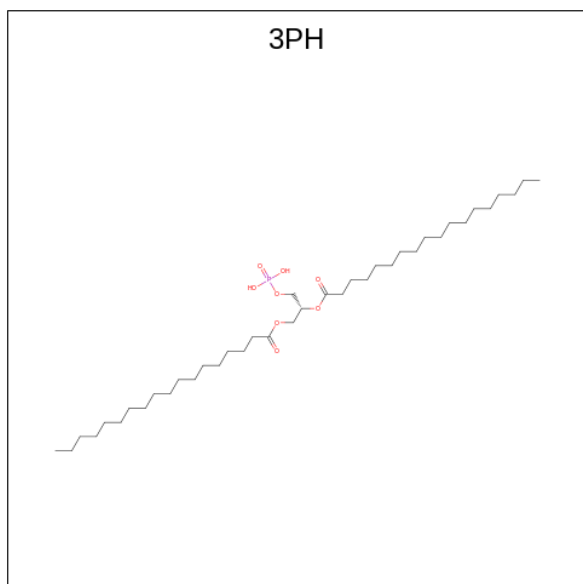
Mol	Chain	Residues	Atoms			AltConf
69	AC	1	Total	C	O	0
			28	24	4	
69	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 70 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 71 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).

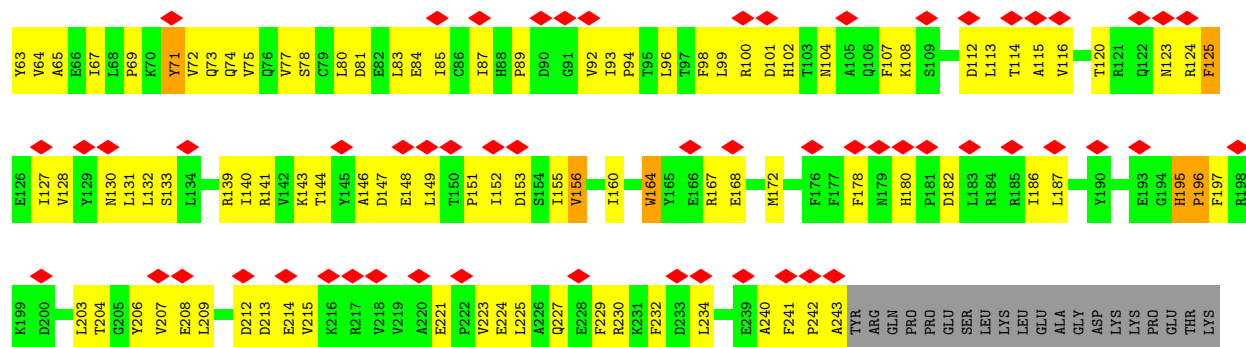


Mol	Chain	Residues	Atoms				AltConf
71	AD	1	Total	C	O	P	0
			36	27	8	1	

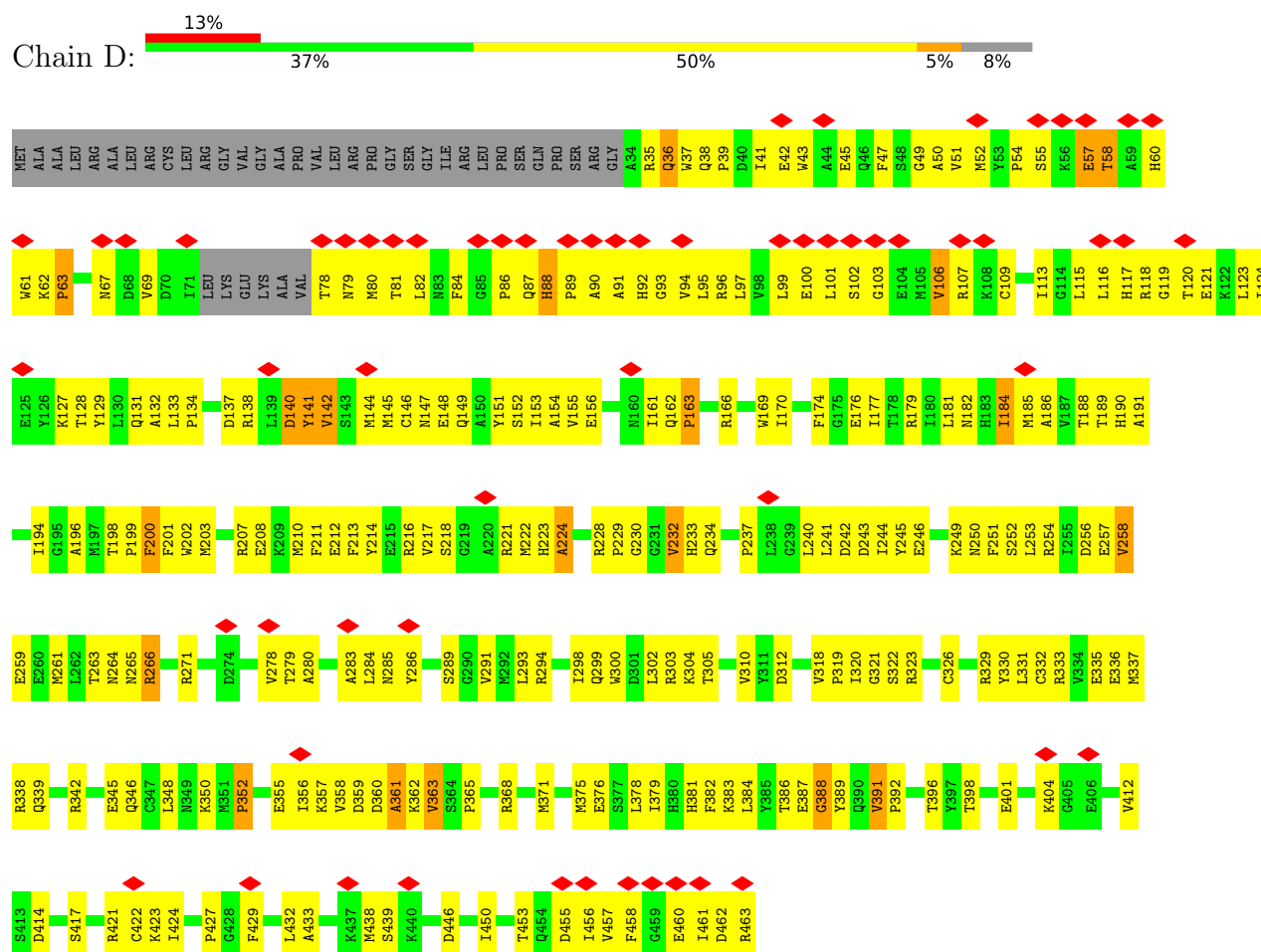
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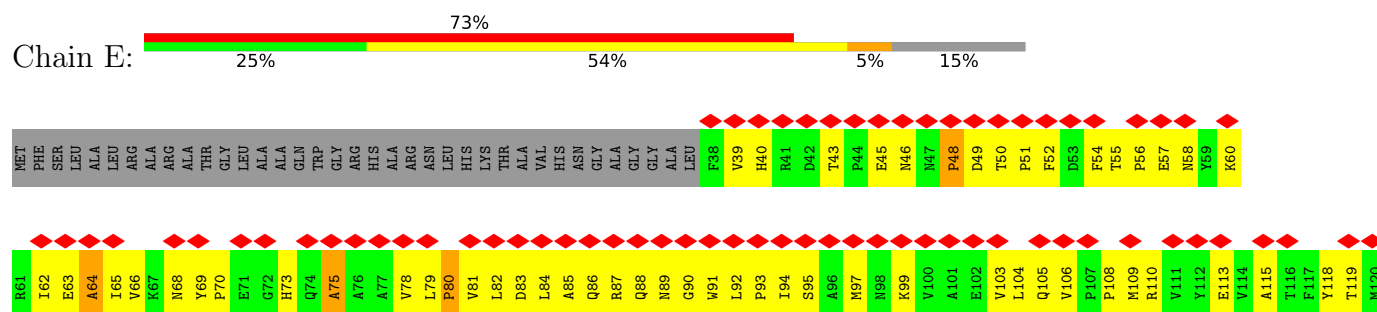
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
71	Ad	1	36	27	8	1	0



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



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

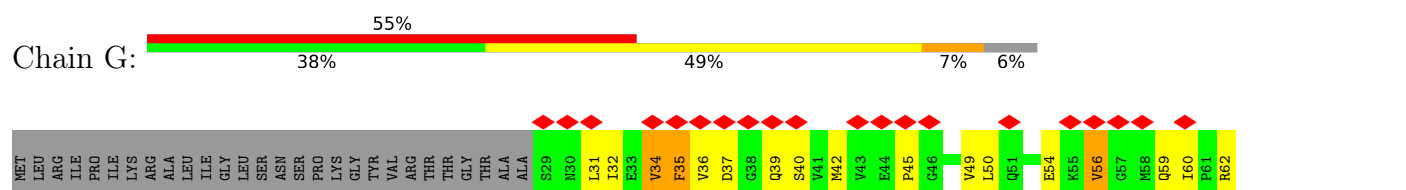


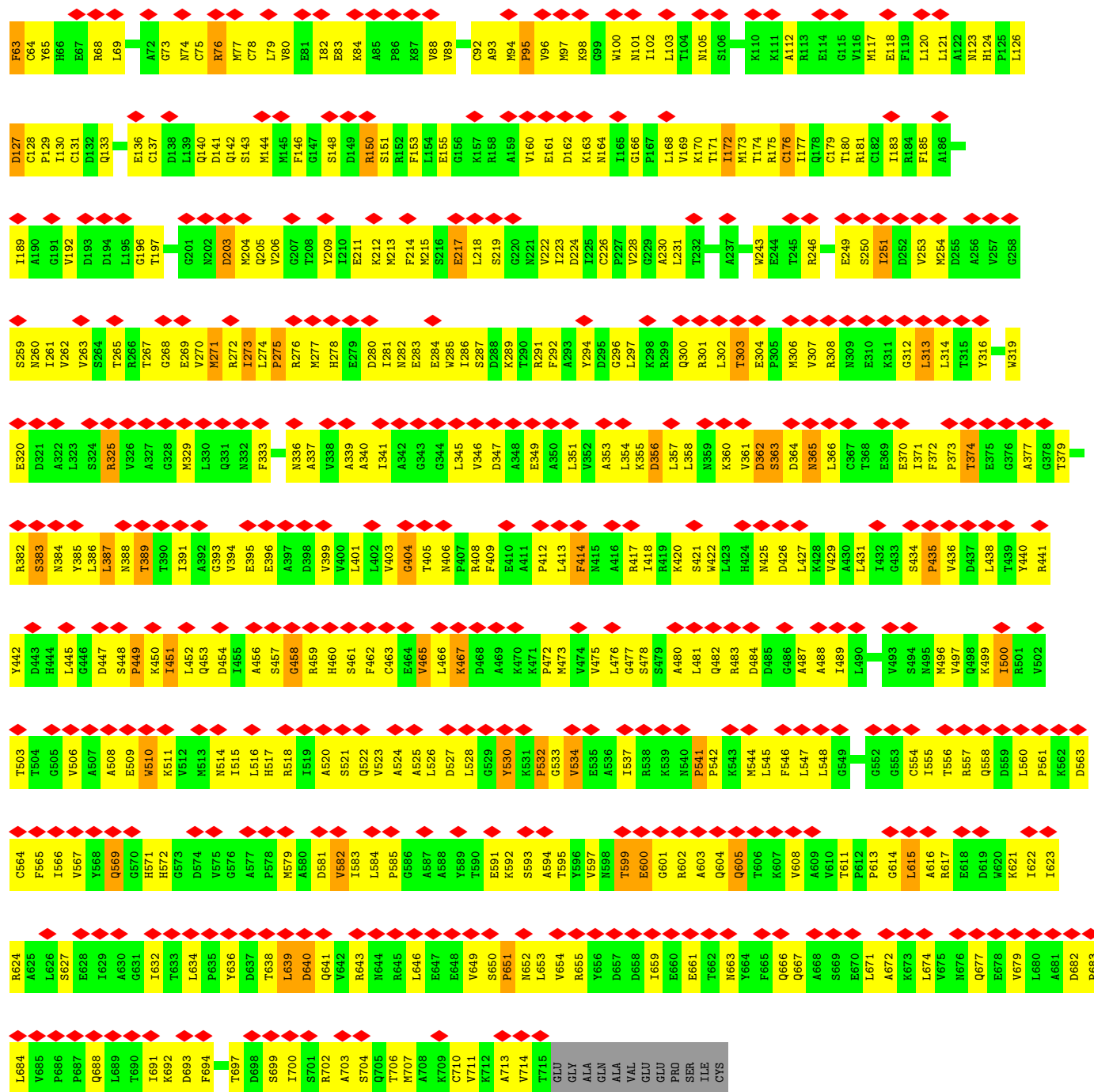


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

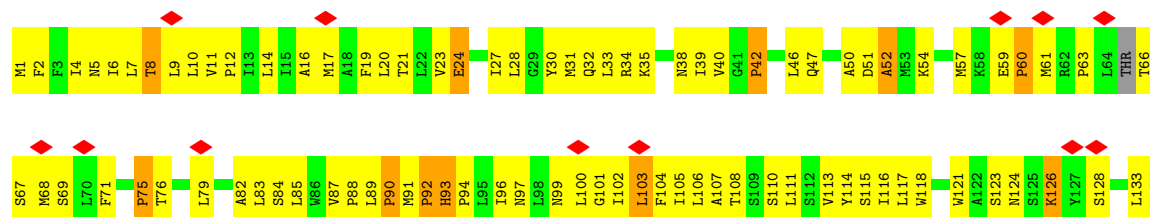


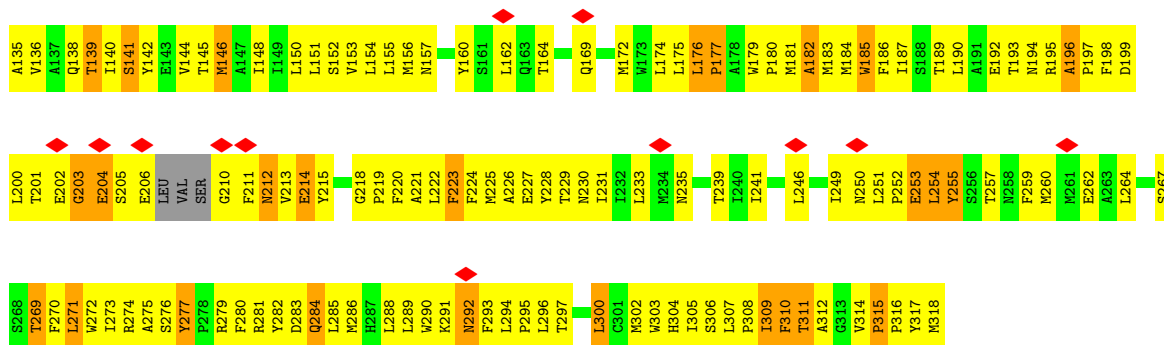
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



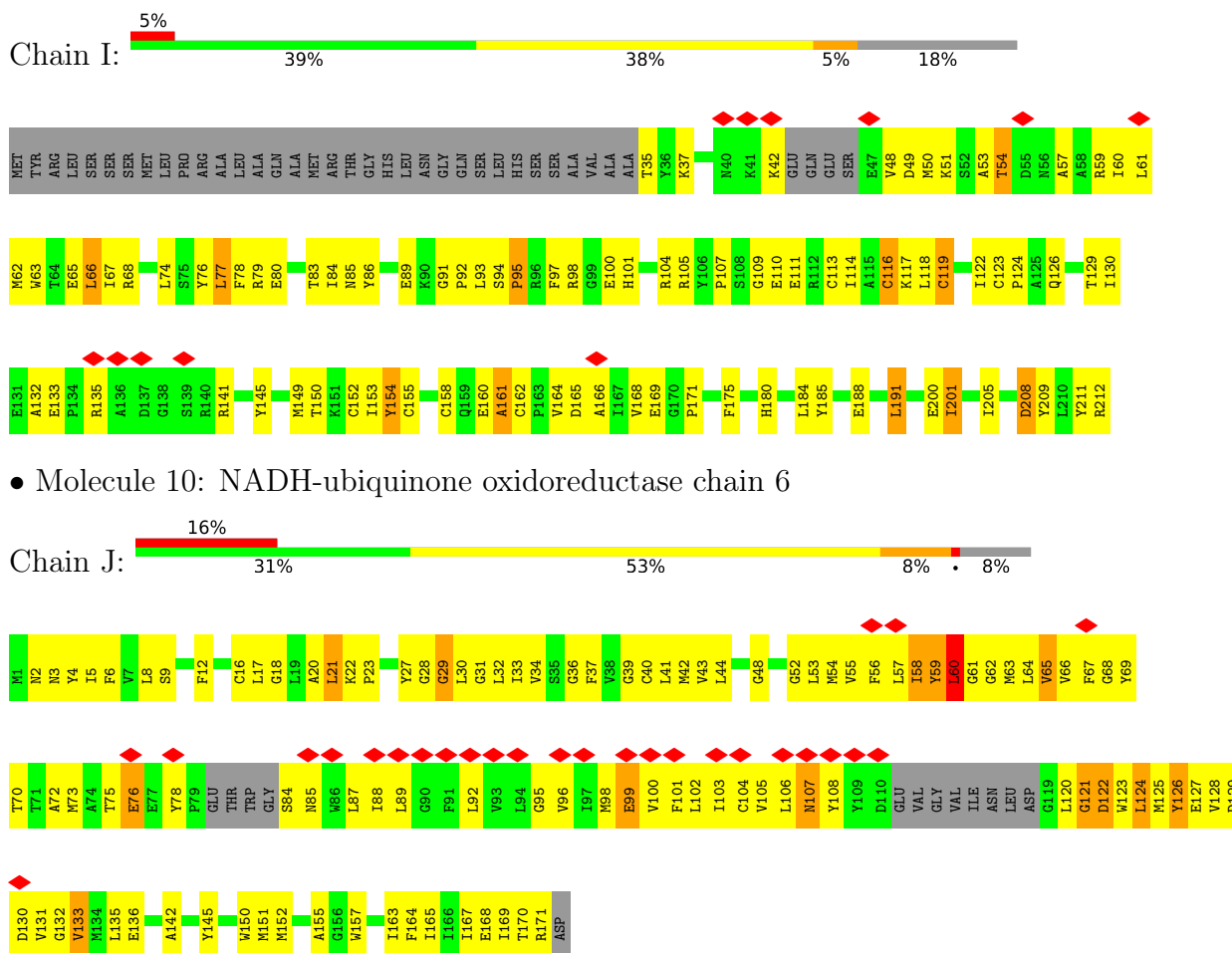


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

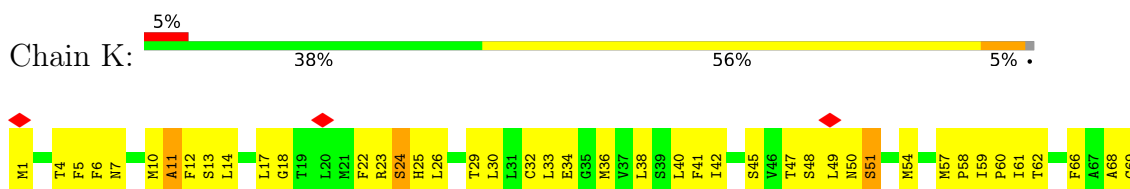


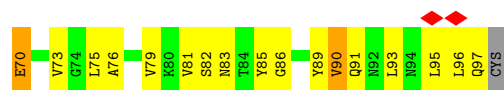


- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



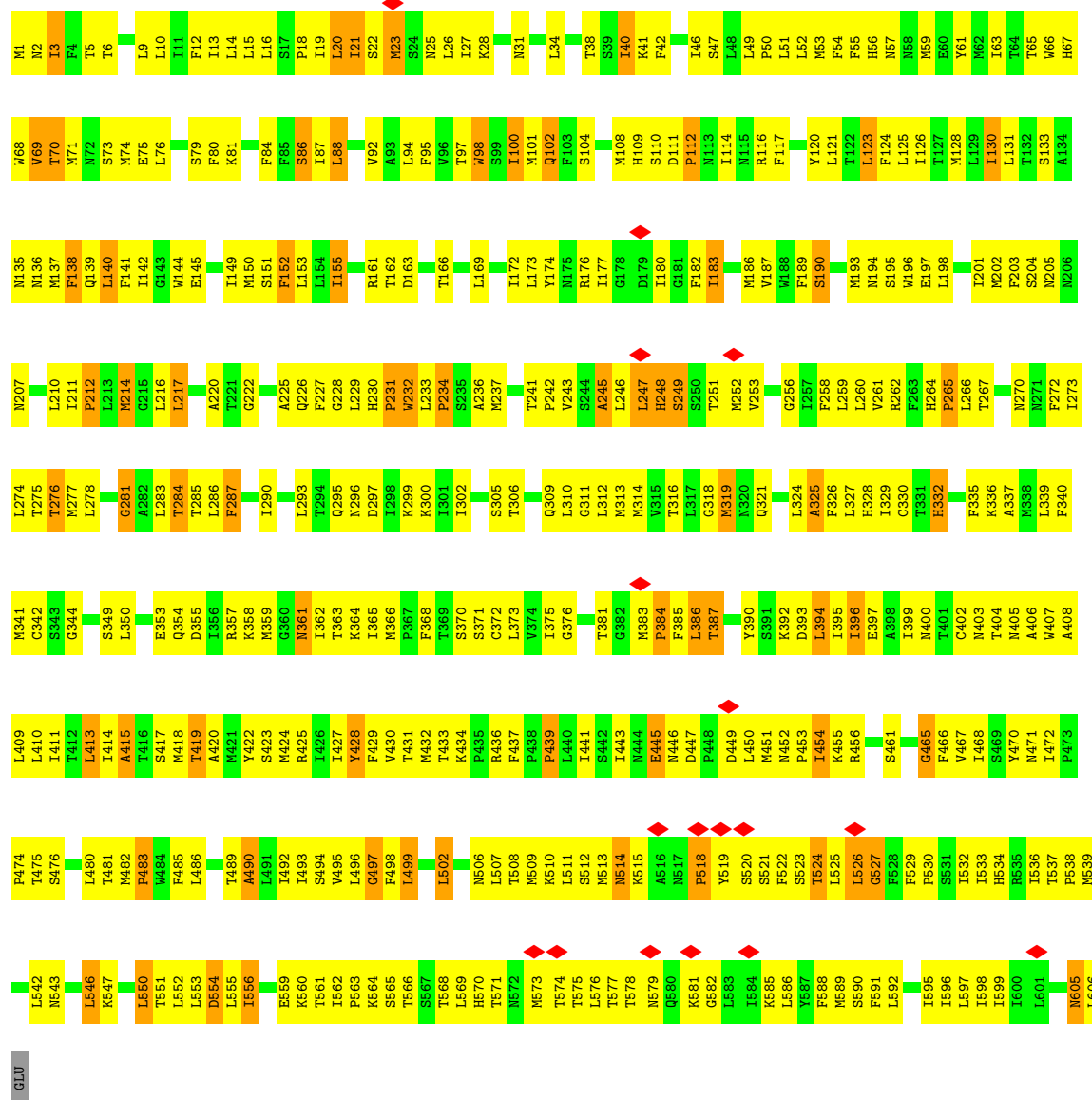
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L





• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 33% 56% 11%

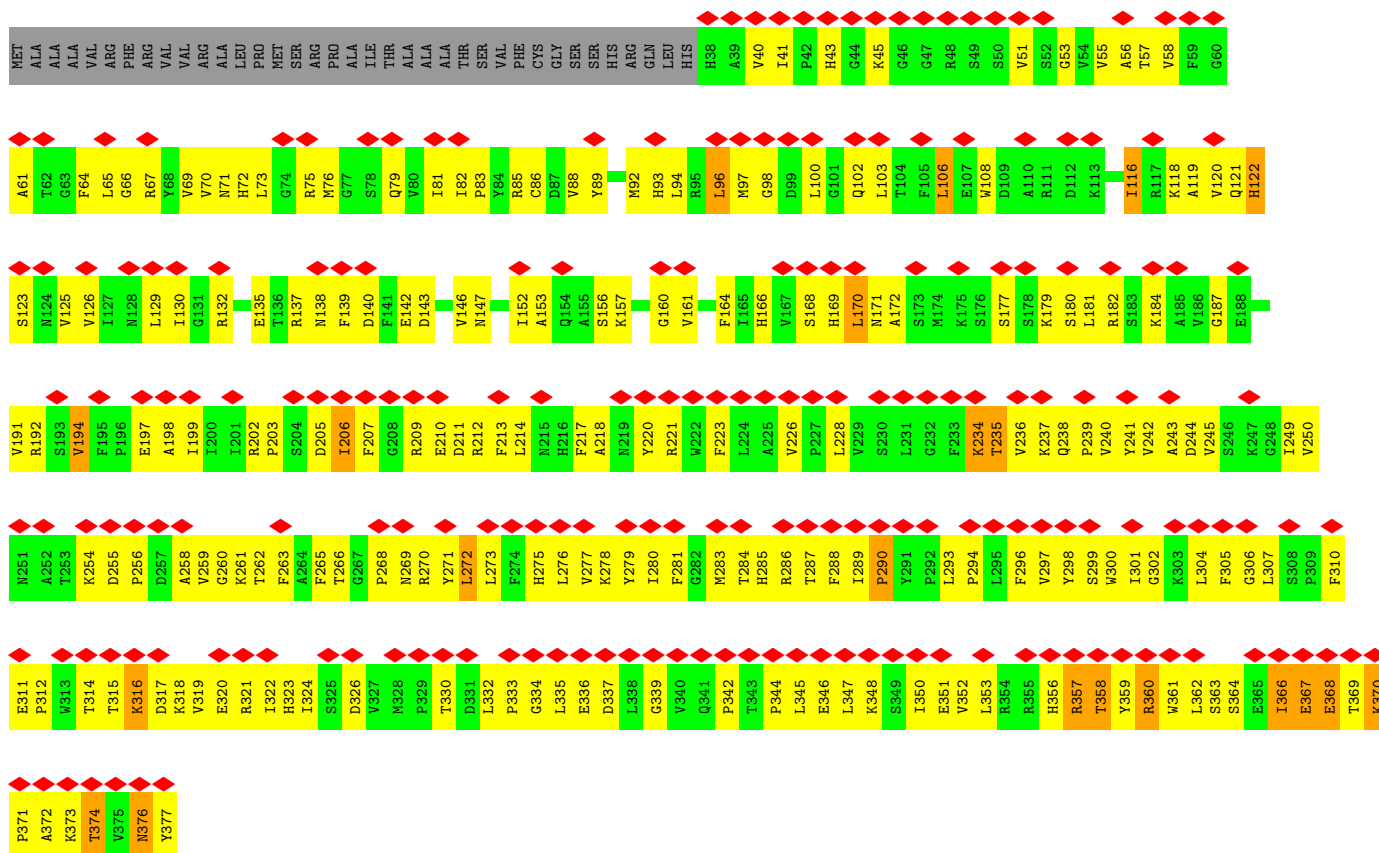


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

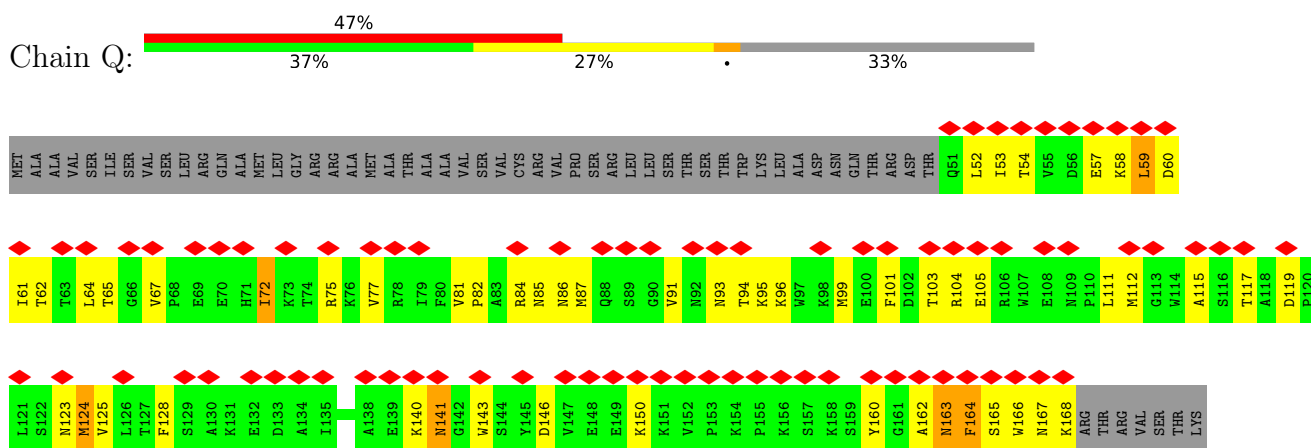
Chain M: 28% 60% 12%



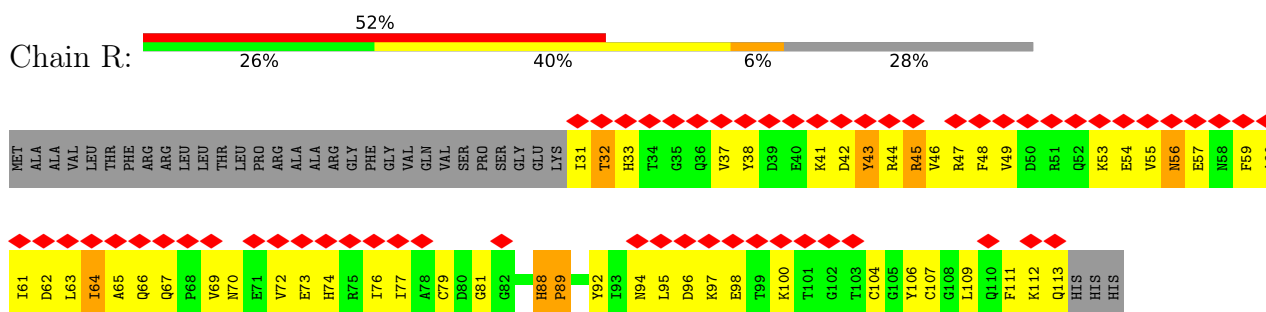




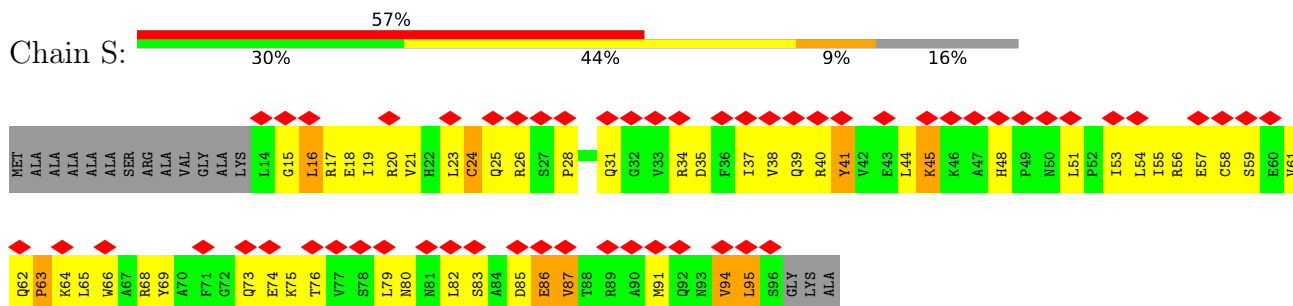
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



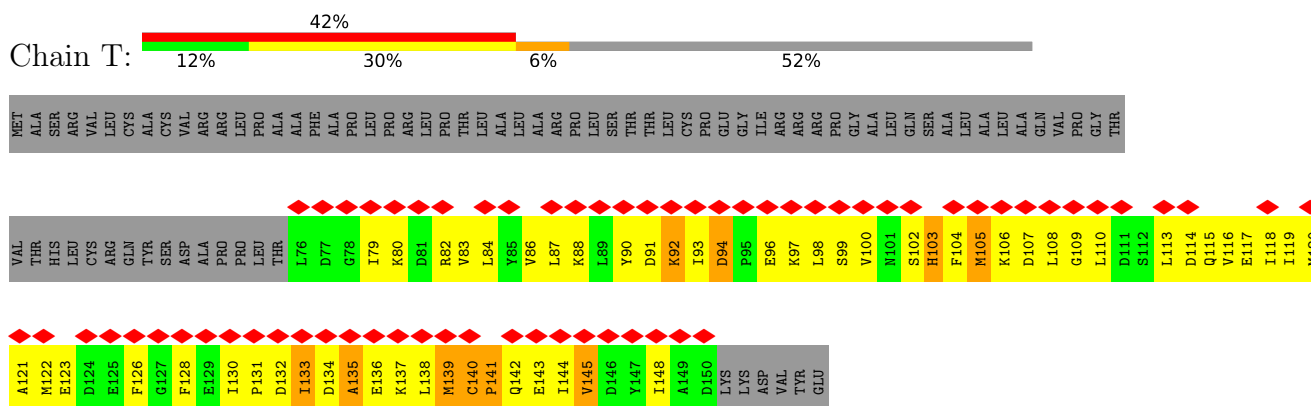
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



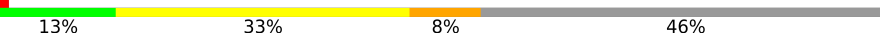
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

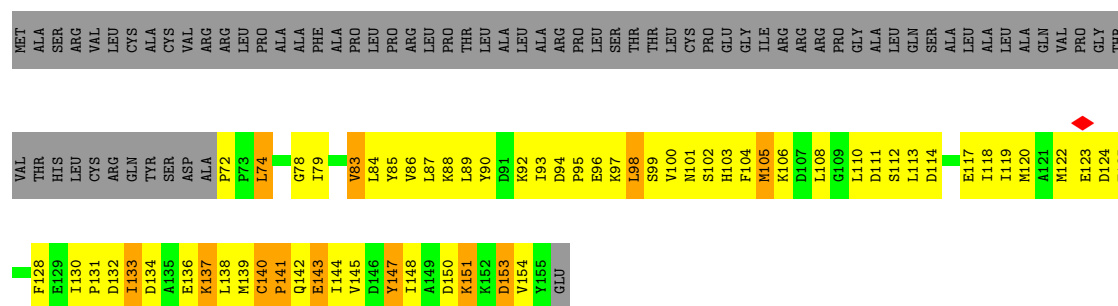


- Molecule 20: Acyl carrier protein, mitochondrial



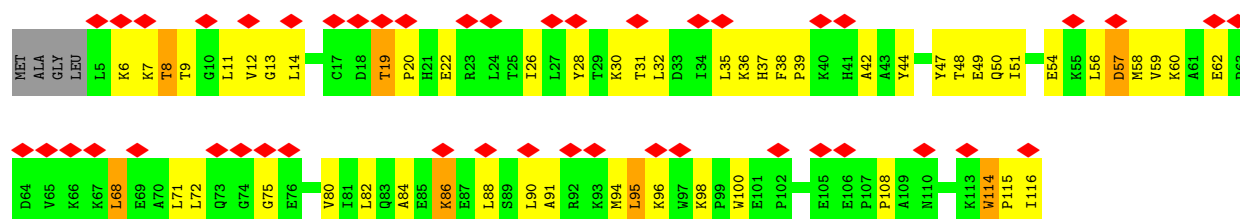
- Molecule 20: Acyl carrier protein, mitochondrial

Chain U: 



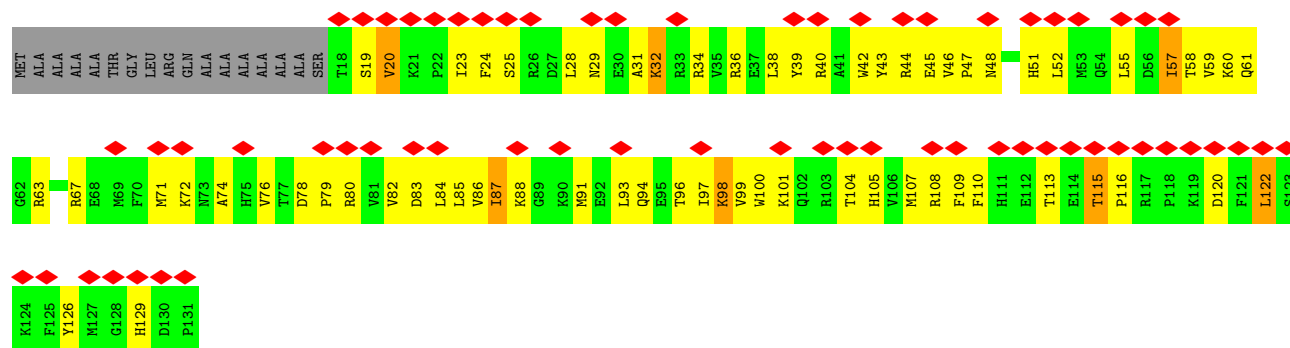
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V: 



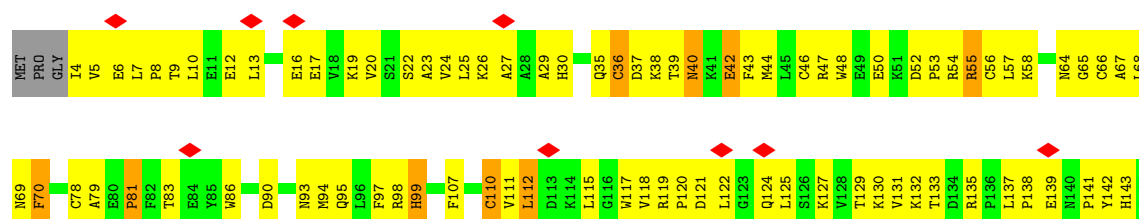
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

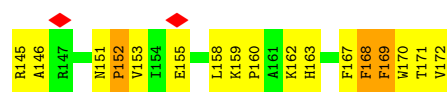
Chain W: 



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

Chain X: 

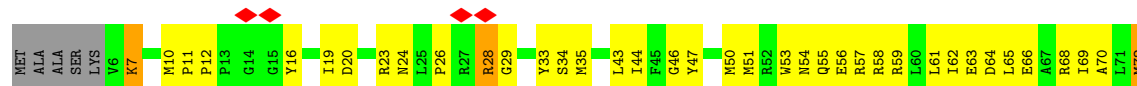




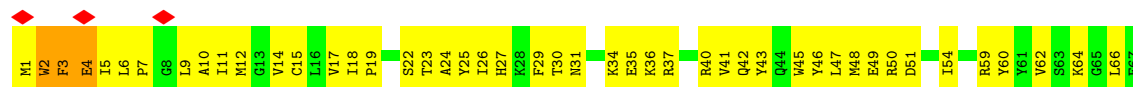
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



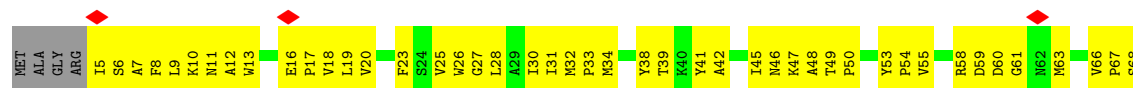
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



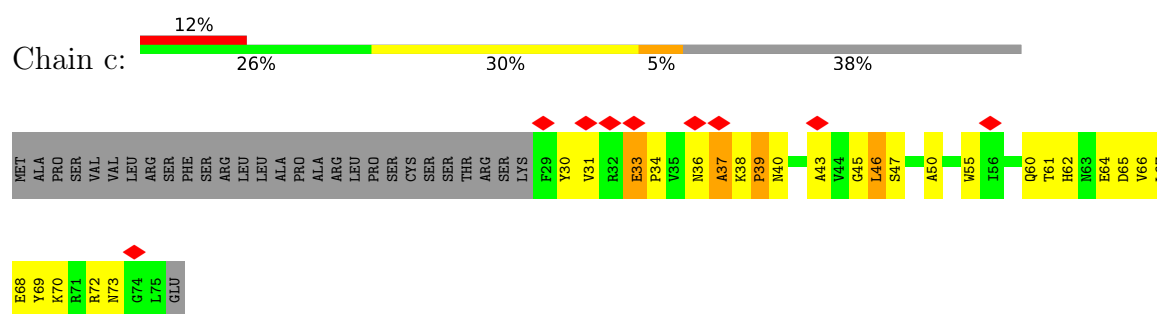
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



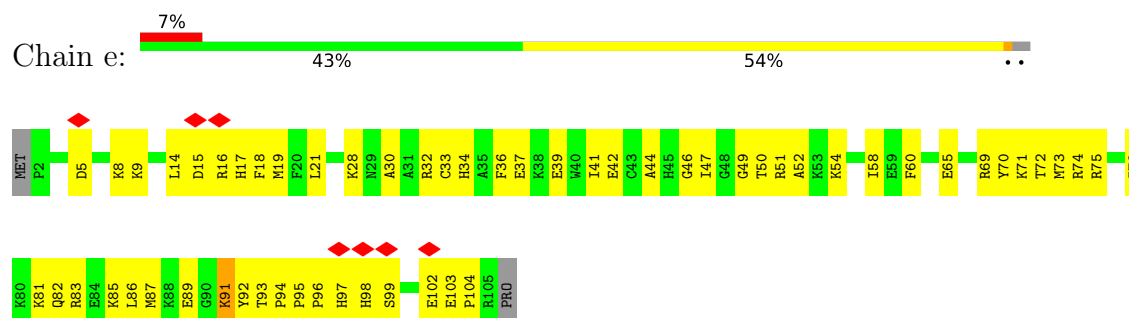
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



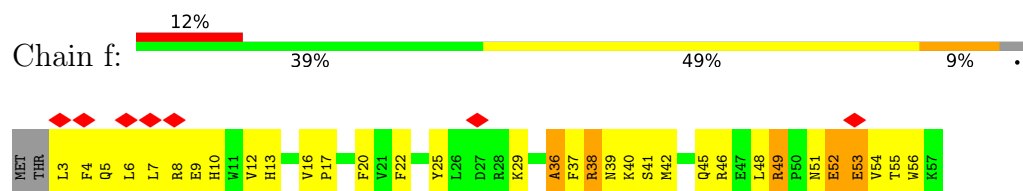
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



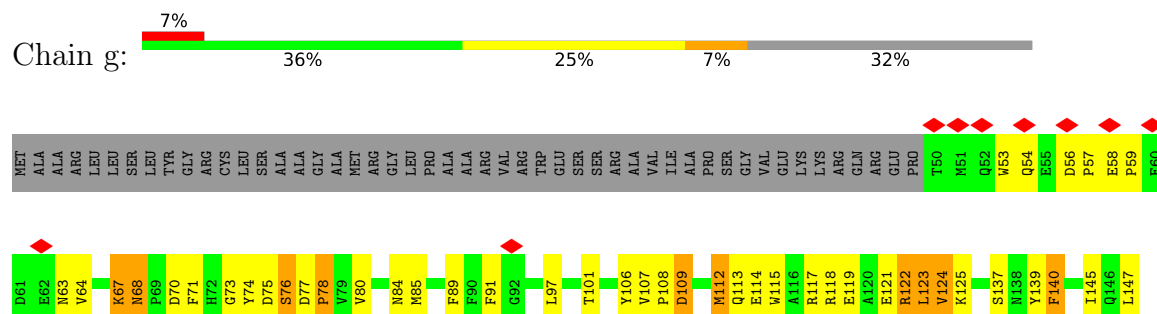
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



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

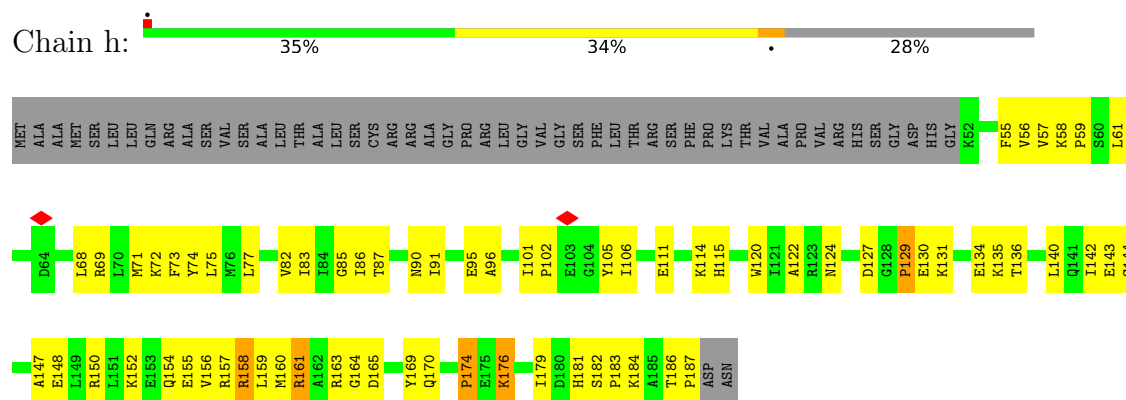


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

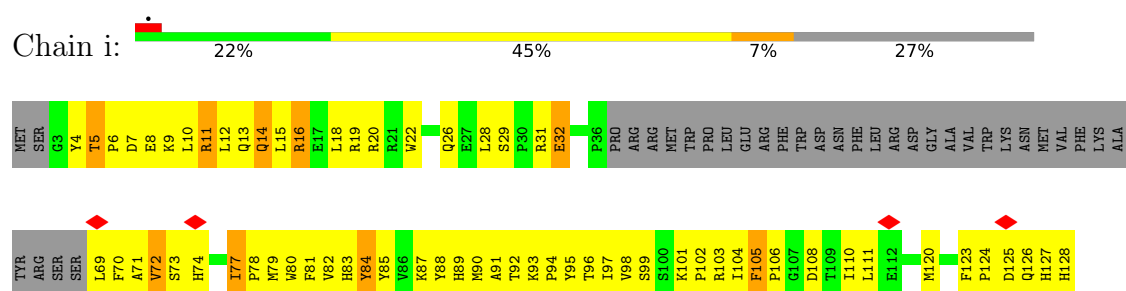




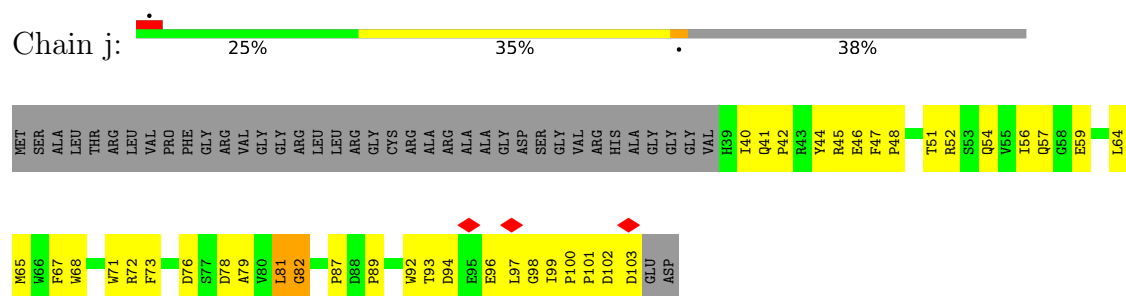
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



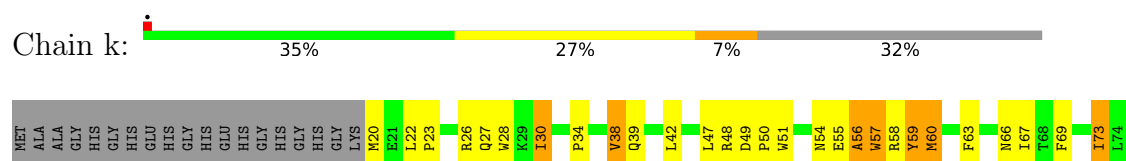
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



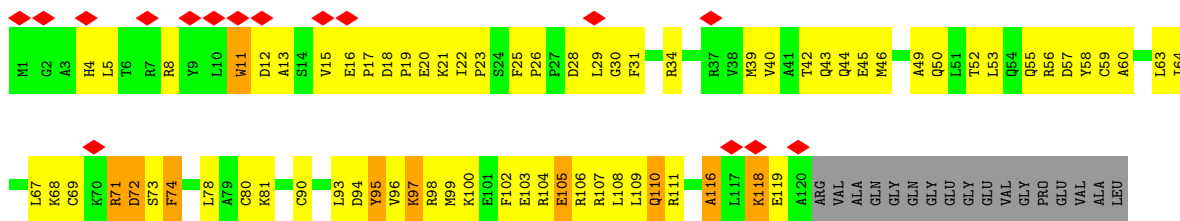
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



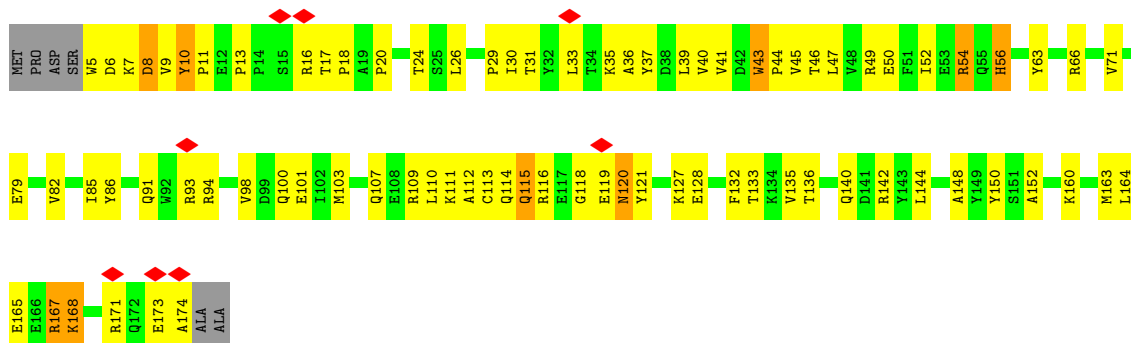
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



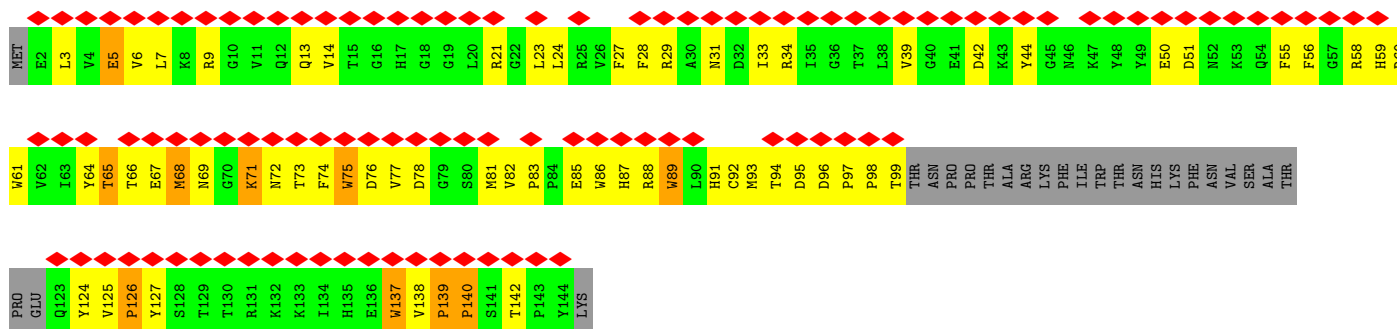
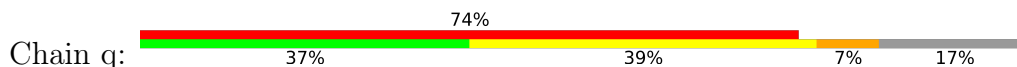




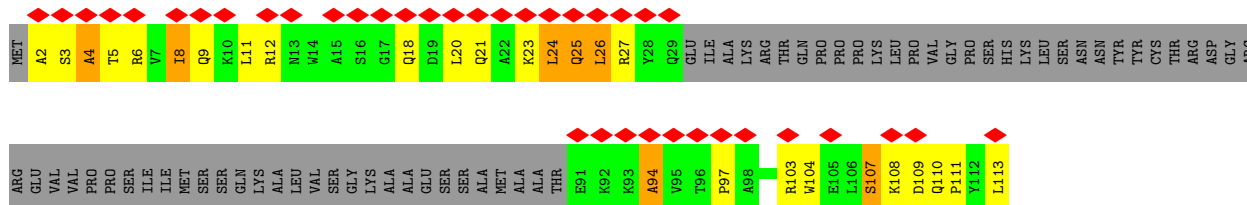
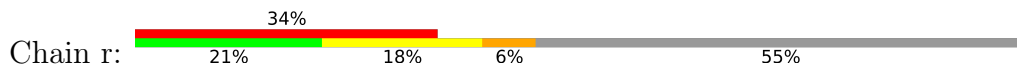
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



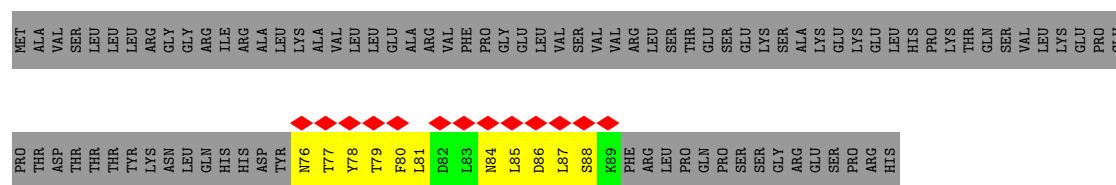
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



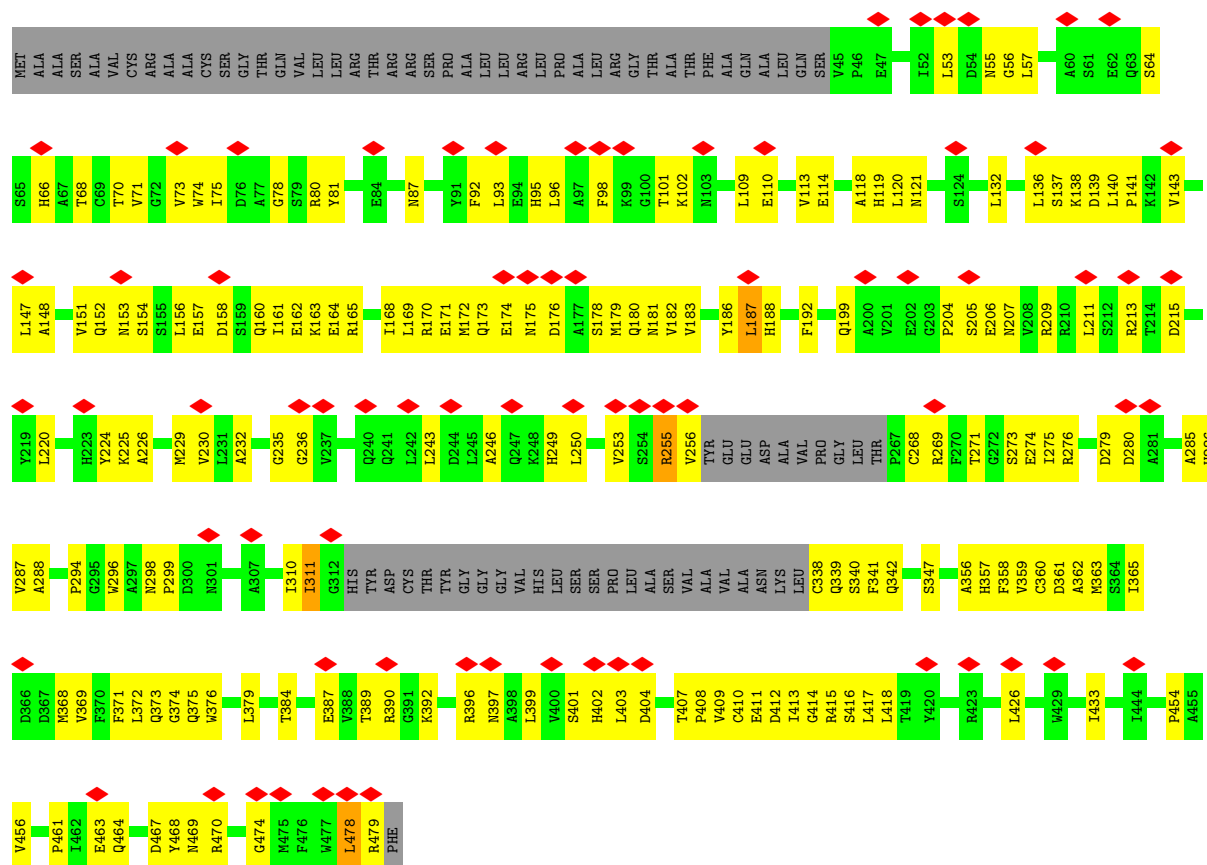
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



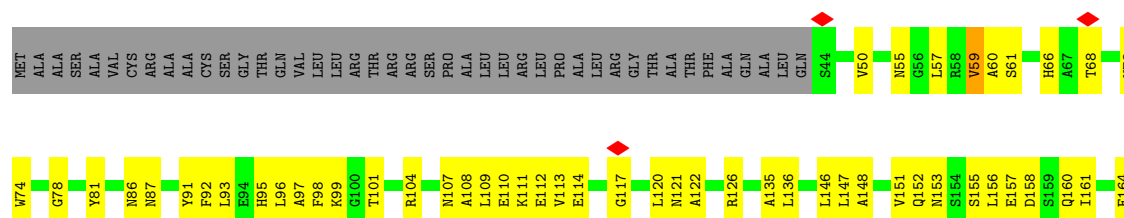
- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

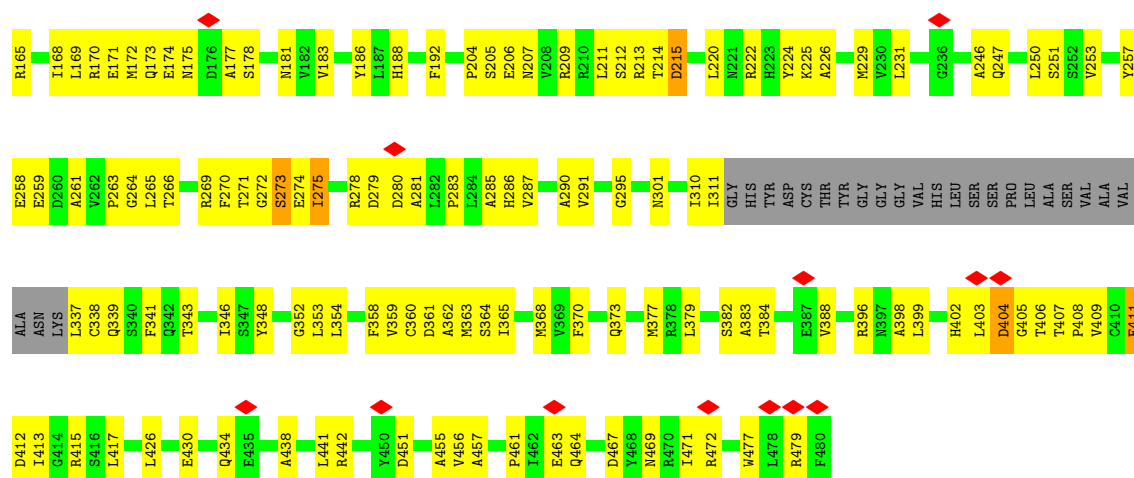


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

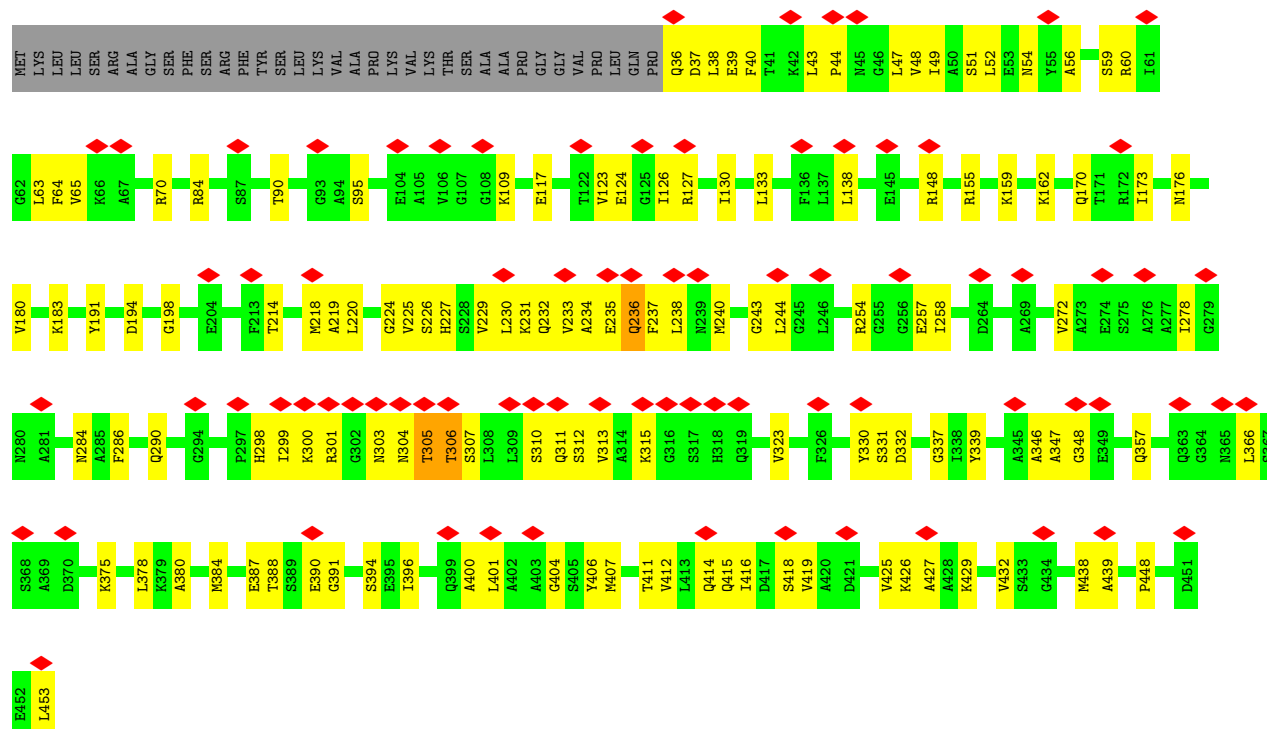


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

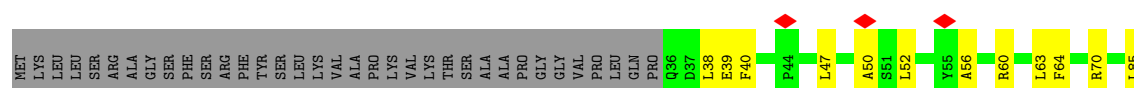


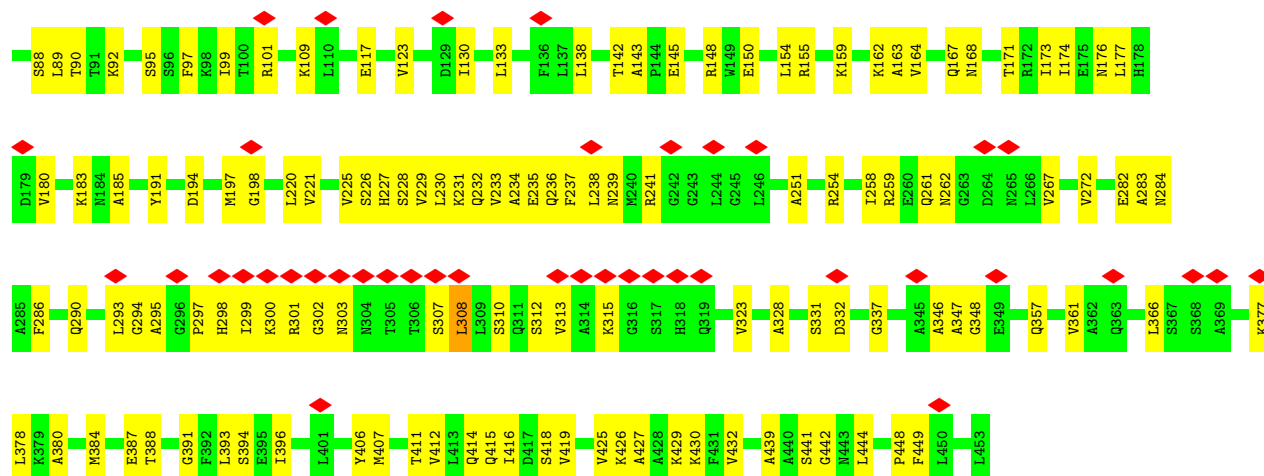


- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial



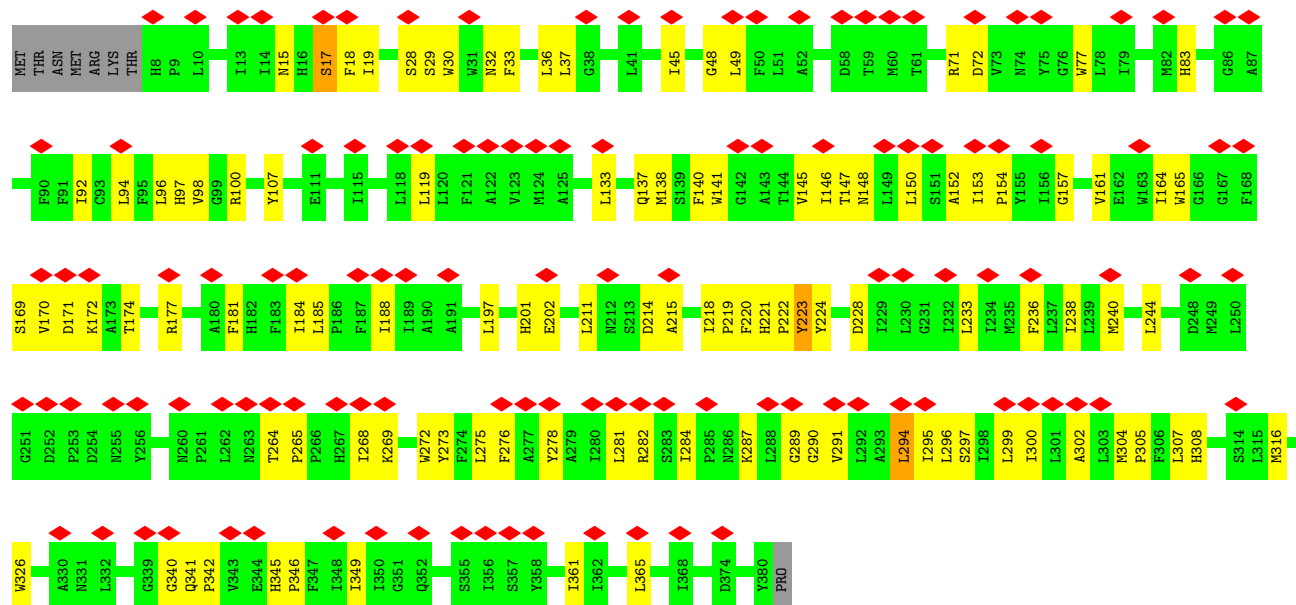
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial





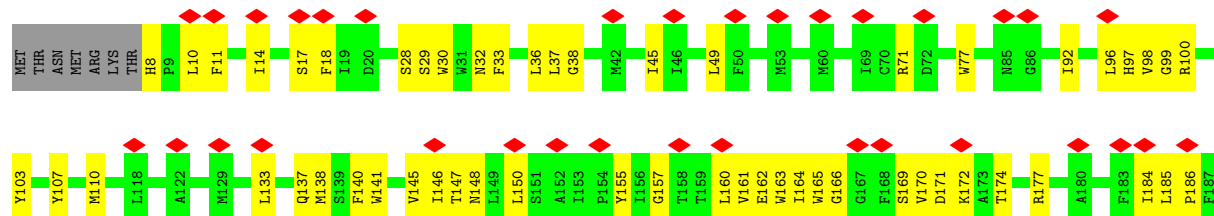
• Molecule 47: Cytochrome b

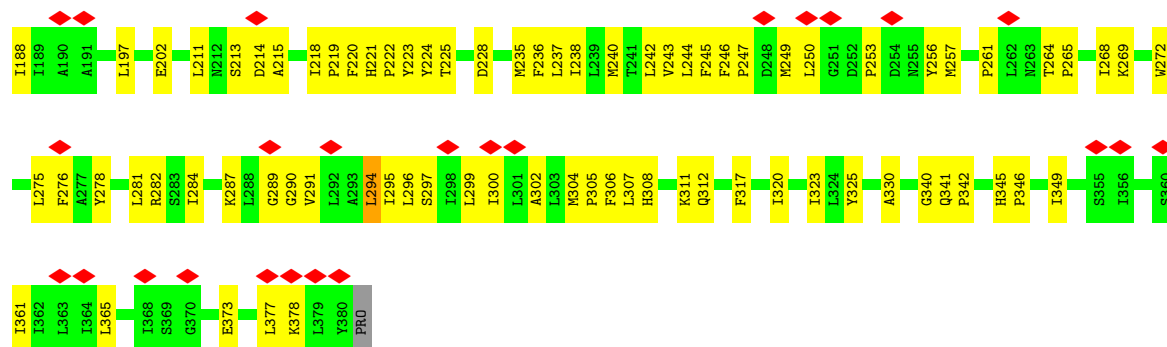
Chain AC: 32% 69% 28% ..



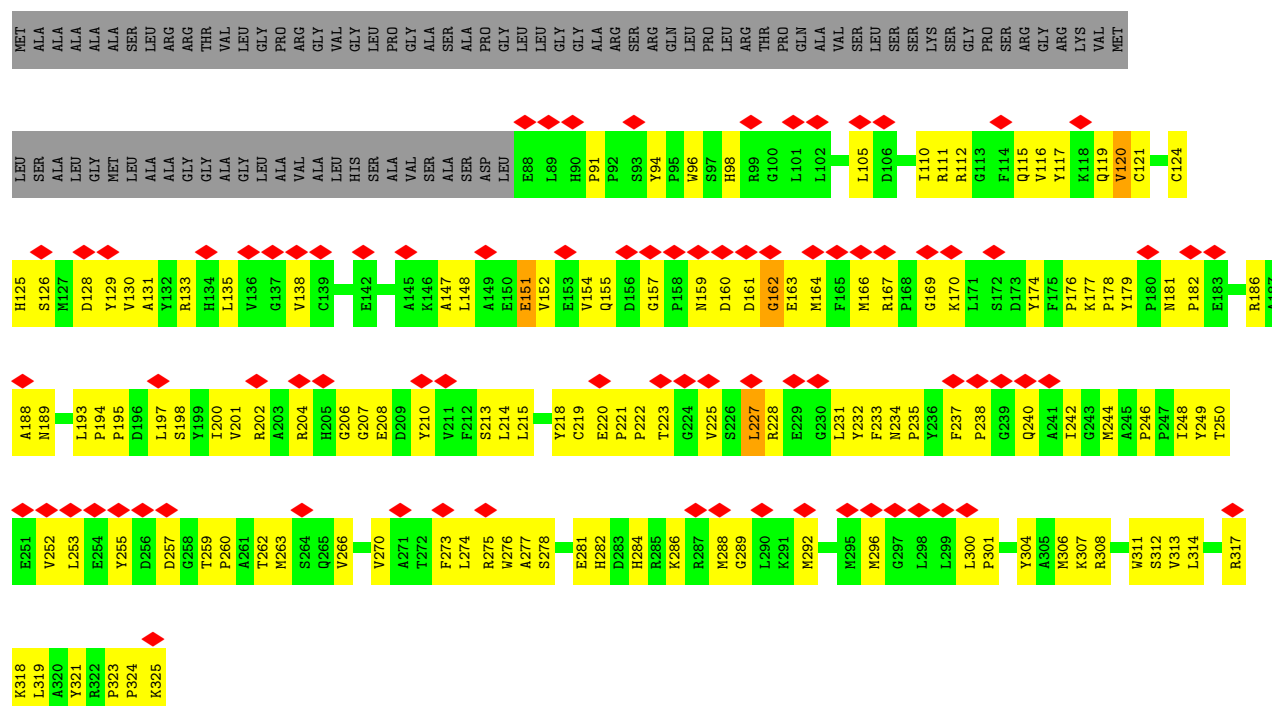
• Molecule 47: Cytochrome b

Chain AC: 15% 63% 35% .

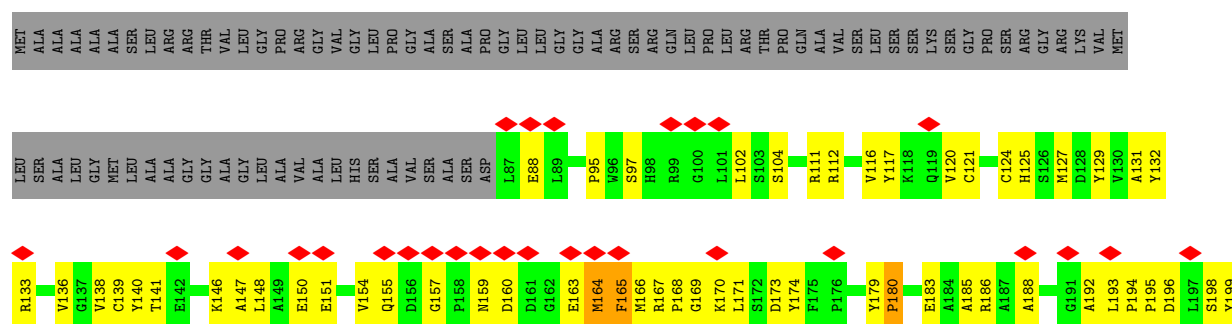


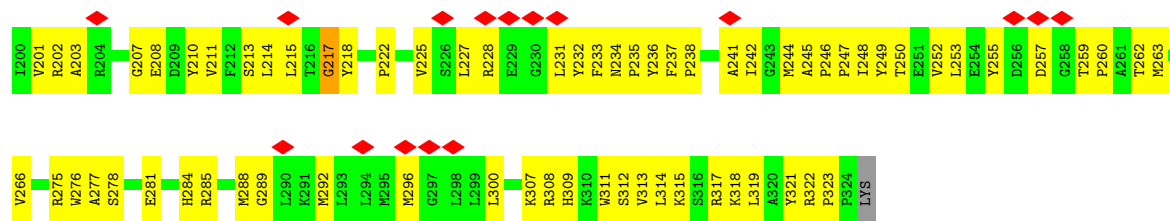


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

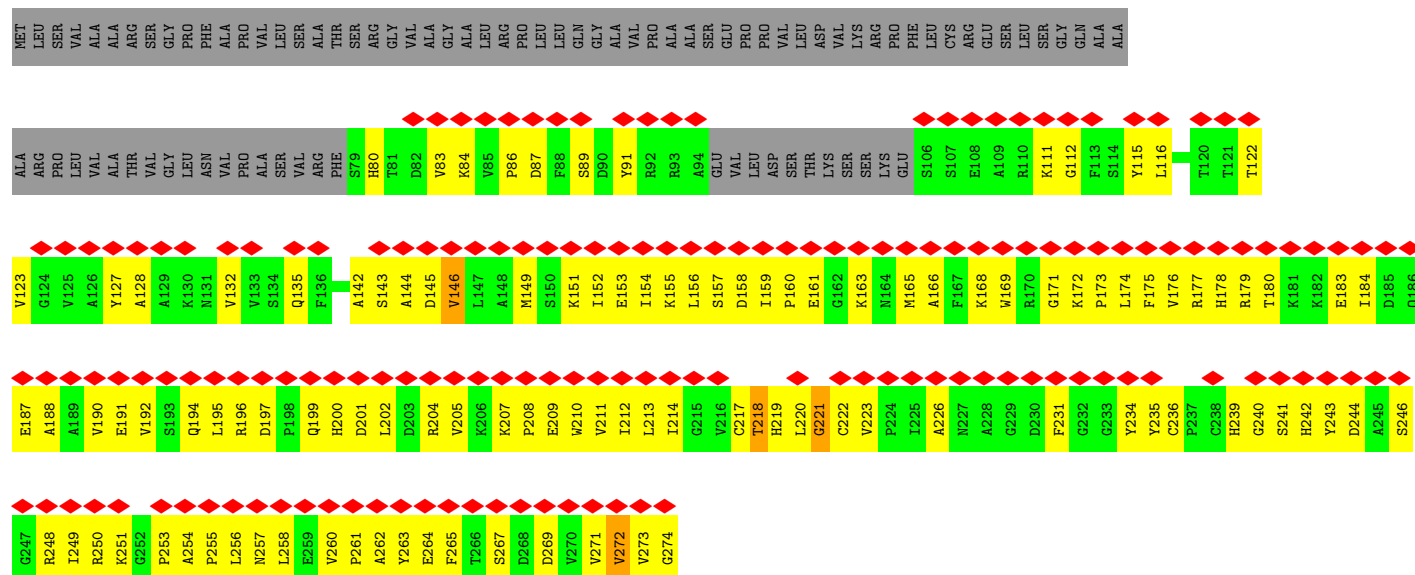


- Molecule 48: Cytochrome c1, heme protein, mitochondrial

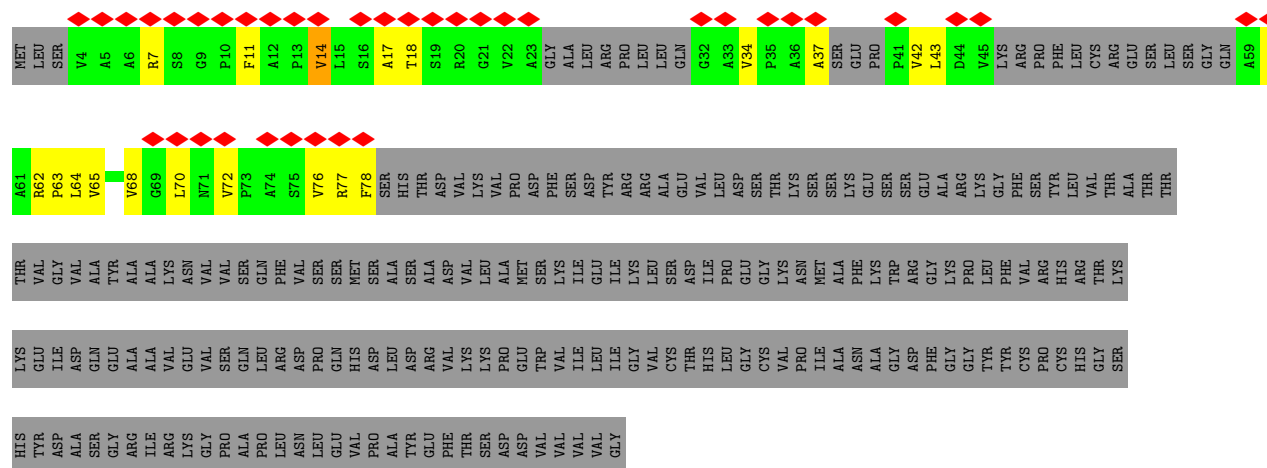




• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

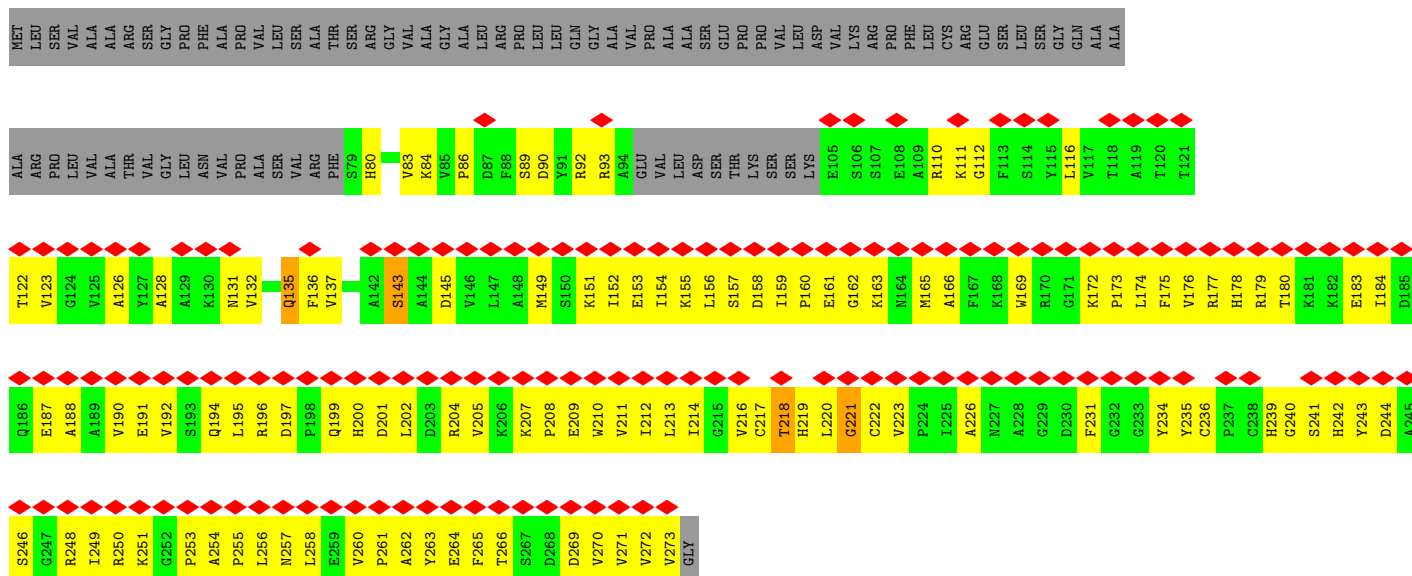


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

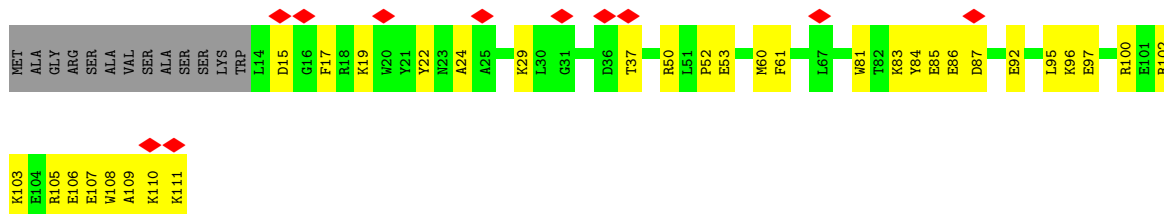


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

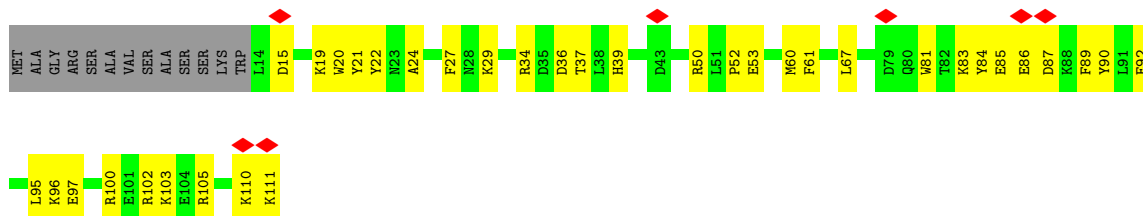




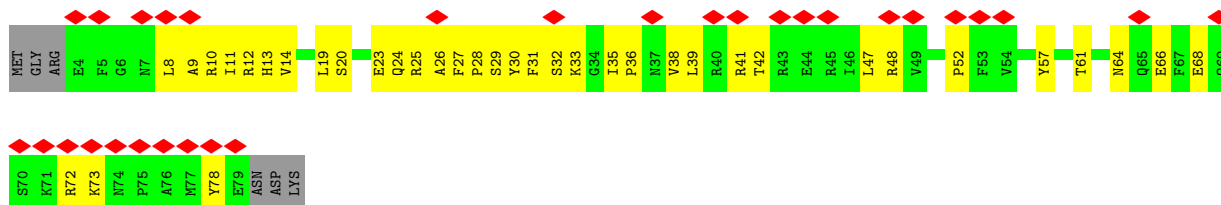
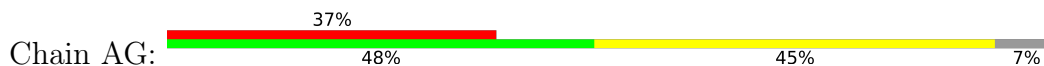
- Molecule 50: Cytochrome b-c1 complex subunit 7



- Molecule 50: Cytochrome b-c1 complex subunit 7

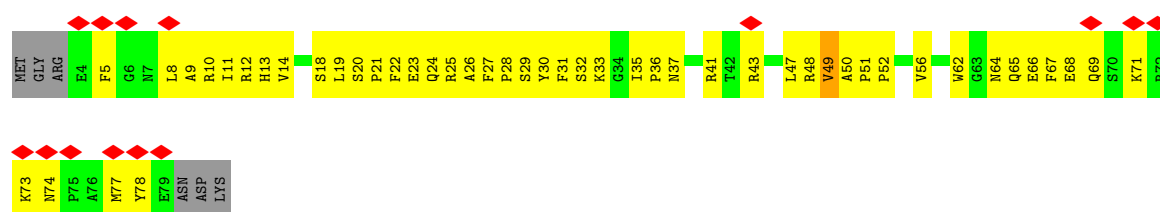


- Molecule 51: Cytochrome b-c1 complex subunit 8

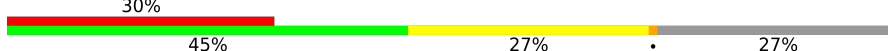


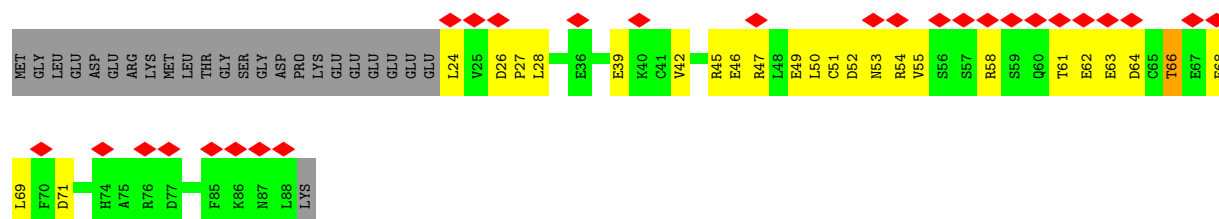
- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain Ag: 

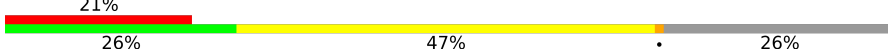


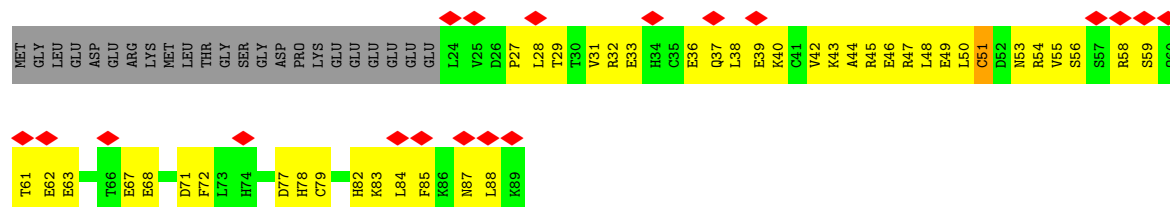
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH: 

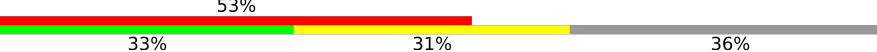


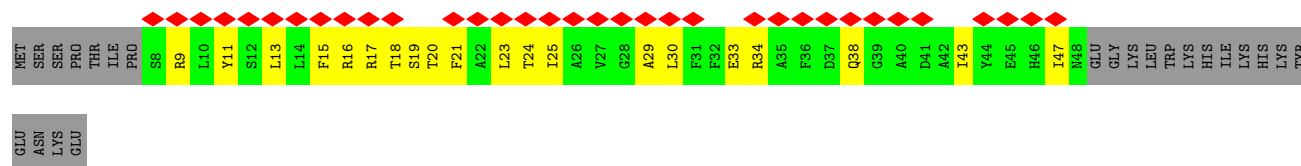
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah: 

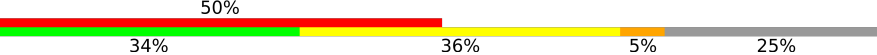


- Molecule 53: Cytochrome b-c1 complex subunit 9

Chain AJ: 



- Molecule 53: Cytochrome b-c1 complex subunit 9

Chain Aj: 



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49613	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	0.080	Depositor
Minimum map value	-0.033	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: SF4, CDL, NDP, PC1, U10, HEC, UQ6, ZN, EHZ, 3PH, FMN, 3PE, ADP, FES, UQ1, UQ9, HEM

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	0.83	0/774	1.33	11/1056 (1.0%)
2	B	0.97	1/1289 (0.1%)	1.45	18/1744 (1.0%)
3	C	0.87	1/1687 (0.1%)	1.31	14/2297 (0.6%)
4	D	0.96	9/3504 (0.3%)	1.38	34/4747 (0.7%)
5	E	0.86	3/1675 (0.2%)	1.35	24/2282 (1.1%)
6	F	0.96	6/3363 (0.2%)	1.54	64/4543 (1.4%)
7	G	0.92	10/5374 (0.2%)	1.60	109/7281 (1.5%)
8	H	0.98	5/2585 (0.2%)	1.52	59/3529 (1.7%)
9	I	0.93	1/1427 (0.1%)	1.54	18/1927 (0.9%)
10	J	0.78	0/1233	1.35	16/1672 (1.0%)
11	K	0.90	0/740	1.54	13/1005 (1.3%)
12	L	0.99	8/4921 (0.2%)	1.59	114/6696 (1.7%)
13	M	1.01	7/3709 (0.2%)	1.56	85/5052 (1.7%)
14	N	1.01	4/2756 (0.1%)	1.56	62/3751 (1.7%)
15	O	1.02	9/2666 (0.3%)	1.44	43/3615 (1.2%)
16	P	0.88	4/2804 (0.1%)	1.35	43/3802 (1.1%)
17	Q	0.87	1/980 (0.1%)	1.29	12/1324 (0.9%)
18	R	0.87	1/671 (0.1%)	1.22	10/903 (1.1%)
19	S	1.09	3/678 (0.4%)	1.74	20/915 (2.2%)
20	T	1.03	1/613 (0.2%)	1.56	13/826 (1.6%)
20	U	0.96	1/690 (0.1%)	1.49	22/931 (2.4%)
21	V	0.86	0/937	1.47	14/1270 (1.1%)
22	W	0.80	0/993	1.32	15/1335 (1.1%)
23	X	0.87	2/1422 (0.1%)	1.42	26/1921 (1.4%)
24	Y	0.88	0/1054	0.97	2/1429 (0.1%)
25	Z	0.76	0/1183	1.10	7/1597 (0.4%)
26	a	0.83	0/561	1.47	7/755 (0.9%)
27	b	0.70	0/651	0.91	1/895 (0.1%)
28	c	0.92	1/400 (0.2%)	1.48	13/544 (2.4%)
29	d	1.02	2/1020 (0.2%)	1.15	11/1377 (0.8%)
30	e	0.63	0/885	0.91	1/1178 (0.1%)
31	f	0.92	1/488 (0.2%)	1.30	10/657 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.88	3/886 (0.3%)	1.35	20/1207 (1.7%)
33	h	0.76	1/1181 (0.1%)	1.27	8/1599 (0.5%)
34	i	0.79	0/823	1.31	13/1119 (1.2%)
35	j	0.82	0/588	1.32	8/805 (1.0%)
36	k	0.86	0/587	1.40	11/794 (1.4%)
37	l	0.97	3/1384 (0.2%)	1.24	11/1889 (0.6%)
38	m	0.79	1/1083 (0.1%)	1.17	14/1468 (1.0%)
39	n	0.89	1/1596 (0.1%)	1.27	17/2162 (0.8%)
40	o	0.83	0/1052	1.29	14/1411 (1.0%)
41	p	0.64	1/1471 (0.1%)	1.03	15/1988 (0.8%)
42	q	1.07	2/1037 (0.2%)	1.52	17/1408 (1.2%)
43	r	1.04	2/426 (0.5%)	1.57	11/573 (1.9%)
44	s	0.98	0/116	1.78	3/157 (1.9%)
45	AA	0.58	1/3187 (0.0%)	0.82	5/4320 (0.1%)
45	Aa	0.60	2/3288 (0.1%)	0.84	10/4462 (0.2%)
46	AB	0.44	1/3187 (0.0%)	0.67	5/4308 (0.1%)
46	Ab	0.45	0/3187	0.66	2/4308 (0.0%)
47	AC	0.43	1/3089 (0.0%)	0.69	3/4221 (0.1%)
47	Ac	0.45	0/3089	0.73	4/4221 (0.1%)
48	AD	0.53	0/1955	0.83	4/2655 (0.2%)
48	Ad	0.58	2/1954 (0.1%)	0.81	3/2655 (0.1%)
49	AE	0.66	0/1459	1.05	4/1976 (0.2%)
49	AI	0.75	0/349	1.15	2/476 (0.4%)
49	Ae	0.67	1/1464 (0.1%)	1.04	3/1983 (0.2%)
50	AF	0.38	0/884	0.52	0/1184
50	Af	0.38	0/884	0.53	0/1184
51	AG	0.50	0/662	0.87	1/895 (0.1%)
51	Ag	0.65	0/662	1.00	2/895 (0.2%)
52	AH	0.38	0/542	0.80	2/728 (0.3%)
52	Ah	0.71	0/551	0.99	3/739 (0.4%)
53	AJ	0.53	0/339	0.71	0/457
53	Aj	0.65	0/402	1.01	3/541 (0.6%)
54	AK	0.48	0/291	0.83	1/399 (0.3%)
54	Ak	0.68	1/371 (0.3%)	0.92	1/511 (0.2%)
All	All	0.81	104/97759 (0.1%)	1.25	1131/132554 (0.9%)

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	247	PRO	N-CD	16.66	1.71	1.47
18	R	89	PRO	N-CD	-15.05	1.26	1.47
29	d	115	PRO	N-CD	-13.98	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	265	PRO	N-CD	13.84	1.67	1.47
14	N	255	PRO	N-CD	-13.54	1.28	1.47

The worst 5 of 1131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.24	132.39	110.65
4	D	142	VAL	N-CA-C	-19.04	92.53	110.42
7	G	174	THR	N-CA-C	-16.81	89.08	114.64
6	F	125	CYS	N-CA-C	-15.64	93.46	113.17
6	F	332	CYS	N-CA-C	15.63	130.09	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	814	187	0
2	B	1258	0	1270	160	0
3	C	1641	0	1596	134	0
4	D	3415	0	3353	341	0
5	E	1635	0	1626	185	0
6	F	3288	0	3243	357	0
7	G	5287	0	5323	551	0
8	H	2510	0	2593	430	0
9	I	1398	0	1359	151	0
10	J	1205	0	1229	260	0
11	K	729	0	764	112	0
12	L	4798	0	4986	623	0
13	M	3622	0	3845	543	0
14	N	2694	0	2896	399	0
15	O	2599	0	2552	266	0
16	P	2730	0	2747	233	0
17	Q	957	0	949	74	0
18	R	660	0	639	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	667	0	685	72	0
20	T	604	0	596	92	0
20	U	678	0	677	90	0
21	V	915	0	954	82	0
22	W	970	0	991	78	0
23	X	1385	0	1366	111	0
24	Y	1030	0	1015	82	0
25	Z	1152	0	1148	145	0
26	a	548	0	562	83	0
27	b	628	0	628	93	0
28	c	389	0	385	27	0
29	d	988	0	989	90	0
30	e	863	0	850	105	0
31	f	475	0	472	42	0
32	g	858	0	787	70	0
33	h	1146	0	1153	124	0
34	i	796	0	797	122	0
35	j	563	0	510	67	0
36	k	569	0	568	53	0
37	l	1328	0	1218	89	0
38	m	1054	0	1064	97	0
39	n	1541	0	1470	139	0
40	o	1027	0	1018	101	0
41	p	1438	0	1404	124	0
42	q	1004	0	962	83	0
43	r	418	0	434	44	0
44	s	115	0	113	14	0
45	AA	3128	0	3052	191	0
45	Aa	3225	0	3141	196	0
46	AB	3137	0	3143	138	0
46	Ab	3137	0	3143	154	0
47	AC	2988	0	3045	145	0
47	Ac	2988	0	3045	162	0
48	AD	1896	0	1846	155	0
48	Ad	1895	0	1844	175	0
49	AE	1427	0	1409	180	0
49	AI	345	0	364	44	0
49	Ae	1432	0	1412	239	0
50	AF	864	0	854	31	0
50	Af	864	0	854	34	0
51	AG	643	0	643	57	0
51	Ag	643	0	643	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AH	535	0	518	27	0
52	Ah	544	0	529	39	0
53	AJ	332	0	324	29	0
53	Aj	392	0	388	43	0
54	AK	281	0	277	19	0
54	Ak	357	0	347	38	0
55	A	46	0	69	12	0
55	AC	35	0	44	12	0
55	AF	42	0	61	7	0
55	Ac	58	0	64	6	0
55	Ag	39	0	52	9	0
55	I	51	0	82	14	0
55	J	46	0	66	5	0
55	L	225	0	332	54	0
55	M	153	0	246	26	0
55	N	37	0	48	14	0
55	O	31	0	36	5	0
55	Y	40	0	54	20	0
55	b	46	0	69	16	0
56	B	8	0	0	6	0
56	F	8	0	0	10	0
56	G	16	0	0	5	0
56	I	16	0	0	16	0
57	B	18	0	18	13	0
58	B	35	0	44	7	0
58	I	47	0	71	9	0
58	J	42	0	58	8	0
59	E	4	0	0	5	0
59	G	4	0	0	4	0
60	F	31	0	19	1	0
61	H	35	0	43	4	0
62	AC	56	0	56	4	0
62	Aa	46	0	36	8	0
62	Ac	42	0	28	3	0
62	Ag	56	0	56	9	0
62	L	163	0	217	38	0
62	X	67	0	81	9	0
62	a	57	0	58	22	0
62	h	70	0	87	15	0
63	O	27	0	12	6	0
64	P	48	0	26	7	0
65	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	W	32	0	0	7	0
66	n	32	0	0	0	0
67	AC	86	0	60	7	0
67	Ac	86	0	60	9	0
68	AC	23	0	23	4	0
68	Ac	38	0	47	5	0
69	AC	28	0	31	14	0
69	Ac	28	0	31	12	0
70	AD	43	0	32	24	0
70	Ad	43	0	32	25	0
71	AD	36	0	45	13	0
71	Ad	36	0	45	19	0
All	All	97639	0	97960	7968	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 41.

The worst 5 of 7968 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)
15:O:247:PRO:CD	15:O:247:PRO:N	1.71	1.39
48:Ad:170:LYS:CD	49:Ae:151:LYS:HD2	1.57	1.33
12:L:302:ILE:HG22	12:L:340:PHE:CZ	1.64	1.31
11:K:66:PHE:HZ	14:N:35:PHE:CZ	1.49	1.29
12:L:358:LYS:HG3	39:n:80:TYR:CZ	1.66	1.29

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	21	58
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100	100
4	D	420/463 (91%)	391 (93%)	29 (7%)	0	100	100
5	E	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
6	F	424/464 (91%)	408 (96%)	16 (4%)	0	100	100
7	G	685/727 (94%)	629 (92%)	56 (8%)	0	100	100
8	H	308/318 (97%)	288 (94%)	19 (6%)	1 (0%)	36	71
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	J	153/172 (89%)	144 (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%)	30 (5%)	1 (0%)	43	77
13	M	456/459 (99%)	438 (96%)	18 (4%)	0	100	100
14	N	342/345 (99%)	330 (96%)	11 (3%)	1 (0%)	36	71
15	O	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
16	P	338/377 (90%)	317 (94%)	21 (6%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	77 (95%)	4 (5%)	0	100	100
19	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	82/156 (53%)	76 (93%)	6 (7%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
23	X	167/172 (97%)	155 (93%)	12 (7%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
25	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
26	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
27	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
30	e	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
31	f	53/57 (93%)	50 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
33	h	134/189 (71%)	127 (95%)	7 (5%)	0	100	100
34	i	90/128 (70%)	76 (84%)	13 (14%)	1 (1%)	11	45
35	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
36	k	69/104 (66%)	67 (97%)	2 (3%)	0	100	100
37	l	156/186 (84%)	143 (92%)	13 (8%)	0	100	100
38	m	125/129 (97%)	117 (94%)	8 (6%)	0	100	100
39	n	176/179 (98%)	162 (92%)	13 (7%)	1 (1%)	21	58
40	o	118/137 (86%)	109 (92%)	9 (8%)	0	100	100
41	p	168/176 (96%)	153 (91%)	15 (9%)	0	100	100
42	q	116/145 (80%)	115 (99%)	1 (1%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
44	s	12/104 (12%)	12 (100%)	0	0	100	100
45	AA	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
45	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
46	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
46	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
47	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
47	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100
49	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100
49	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100
49	Ae	181/274 (66%)	166 (92%)	15 (8%)	0	100	100
50	AF	96/111 (86%)	96 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	74/82 (90%)	74 (100%)	0	0	100	100
51	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
52	AH	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
52	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
54	AK	33/56 (59%)	33 (100%)	0	0	100	100
54	AK	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	11769/14118 (83%)	11186 (95%)	577 (5%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
14	N	109	ALA
34	i	124	PRO
2	B	195	PRO
39	n	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	77
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	366/395 (93%)	365 (100%)	1 (0%)	86	84
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	81
6	F	341/370 (92%)	341 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	276/280 (99%)	276 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	J	127/138 (92%)	125 (98%)	2 (2%)	55	69
11	K	87/88 (99%)	87 (100%)	0	100	100
12	L	549/550 (100%)	547 (100%)	2 (0%)	84	82
13	M	414/415 (100%)	413 (100%)	1 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	307/308 (100%)	306 (100%)	1 (0%)	86	84
15	O	283/309 (92%)	283 (100%)	0	100	100
16	P	297/325 (91%)	296 (100%)	1 (0%)	86	84
17	Q	105/153 (69%)	104 (99%)	1 (1%)	68	76
18	R	70/96 (73%)	69 (99%)	1 (1%)	59	71
19	S	74/80 (92%)	73 (99%)	1 (1%)	59	71
20	T	69/135 (51%)	68 (99%)	1 (1%)	59	71
20	U	78/135 (58%)	78 (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	77
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	106/107 (99%)	106 (100%)	0	100	100
30	e	91/94 (97%)	90 (99%)	1 (1%)	65	74
31	f	51/53 (96%)	51 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	121/162 (75%)	121 (100%)	0	100	100
34	i	89/120 (74%)	88 (99%)	1 (1%)	65	74
35	j	61/87 (70%)	61 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	142/161 (88%)	142 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	163/164 (99%)	163 (100%)	0	100	100
40	o	110/121 (91%)	110 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	108/131 (82%)	108 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	s	14/95 (15%)	14 (100%)	0	100	100
45	AA	338/398 (85%)	337 (100%)	1 (0%)	86	84
45	Aa	349/398 (88%)	349 (100%)	0	100	100
46	AB	328/356 (92%)	328 (100%)	0	100	100
46	Ab	328/356 (92%)	328 (100%)	0	100	100
47	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
47	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	203/260 (78%)	203 (100%)	0	100	100
49	AE	155/224 (69%)	154 (99%)	1 (1%)	78	80
49	AI	34/224 (15%)	33 (97%)	1 (3%)	37	58
49	Ae	156/224 (70%)	155 (99%)	1 (1%)	78	80
50	AF	90/99 (91%)	90 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	69/74 (93%)	69 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	62/83 (75%)	62 (100%)	0	100	100
52	Ah	63/83 (76%)	63 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	39/55 (71%)	39 (100%)	0	100	100
54	AK	26/46 (56%)	26 (100%)	0	100	100
54	Ak	34/46 (74%)	34 (100%)	0	100	100
All	All	10334/12037 (86%)	10310 (100%)	24 (0%)	85	85

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	103	HIS
34	i	72	VAL
30	e	91	LYS
45	AA	478	LEU
12	L	3	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 250 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	43	HIS
45	Aa	173	GLN
29	d	59	HIS
45	Aa	103	ASN
47	Ac	260	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 60 ligands modelled in this entry, 1 is monoatomic - leaving 59 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	$\# Z > 2$
66	EHZ	n	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.85	11 (29%)
55	3PE	M	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.11	3 (5%)
55	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
56	SF4	G	802	7	0,12,12	-	-	-	-	-
71	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)
55	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
59	FES	G	803	7	0,4,4	-	-	-	-	-
62	CDL	X	201	-	66,66,99	1.09	4 (6%)	72,78,111	1.26	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	SF4	I	303	9	0,12,12	-	-	-		
55	3PE	L	703	-	50,50,50	0.90	2 (4%)	53,55,55	1.12	3 (5%)
58	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)
68	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
69	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
71	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
55	3PE	L	707	-	44,44,50	0.96	2 (4%)	47,49,55	1.08	3 (6%)
55	3PE	M	502	-	50,50,50	0.89	2 (4%)	53,55,55	1.15	4 (7%)
62	CDL	h	201	-	69,69,99	1.08	4 (5%)	75,81,111	1.21	6 (8%)
55	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
62	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)
64	NDP	P	401	-	49,52,52	1.21	5 (10%)	66,80,80	1.68	11 (16%)
55	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
62	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
56	SF4	I	304	9	0,12,12	-	-	-		
56	SF4	G	801	7	0,12,12	-	-	-		
69	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
55	3PE	M	501	-	50,50,50	0.91	2 (4%)	53,55,55	1.11	4 (7%)
56	SF4	B	301	2	0,12,12	-	-	-		
66	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
70	HEC	AD	401	48	50,50,50	2.80	26 (52%)	68,82,82	2.48	30 (44%)
63	ADP	O	402	-	27,29,29	1.37	4 (14%)	42,45,45	1.98	11 (26%)
55	3PE	A	401	-	45,45,50	0.94	2 (4%)	48,50,55	1.01	2 (4%)
55	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0
55	3PE	O	401	-	30,30,50	1.16	2 (6%)	33,35,55	1.27	3 (9%)
55	3PE	L	701	-	41,41,50	0.99	2 (4%)	44,46,55	1.03	2 (4%)
55	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
61	UQ9	H	400	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
67	HEM	AC	402	47	50,50,50	1.69	11 (22%)	66,82,82	2.17	23 (34%)
67	HEM	Ac	402	47	50,50,50	1.63	9 (18%)	66,82,82	1.98	16 (24%)
56	SF4	F	502	6	0,12,12	-	-	-		
55	3PE	L	702	-	39,39,50	1.03	2 (5%)	42,44,55	1.10	4 (9%)
62	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
55	3PE	J	202	-	45,45,50	0.96	2 (4%)	48,50,55	1.06	3 (6%)
55	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
58	PC1	J	201	-	41,41,53	1.07	2 (4%)	47,49,61	1.08	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	FES	E	301	5	0,4,4	-	-	-		
60	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)
62	CDL	a	101	-	56,56,99	1.20	4 (7%)	62,68,111	1.28	6 (9%)
62	CDL	L	706	-	85,85,99	0.99	4 (4%)	91,97,111	1.13	5 (5%)
67	HEM	AC	401	47	50,50,50	1.58	8 (16%)	66,82,82	1.76	14 (21%)
67	HEM	Ac	403	47	50,50,50	1.65	10 (20%)	66,82,82	1.70	13 (19%)
58	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	3 (7%)
62	CDL	L	705	-	76,76,99	1.02	4 (5%)	82,88,111	1.17	5 (6%)
62	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
55	3PE	L	704	-	46,46,50	0.95	2 (4%)	49,51,55	1.08	3 (6%)
70	HEC	Ad	401	48	50,50,50	2.80	25 (50%)	68,82,82	2.44	26 (38%)
68	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
55	3PE	Y	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.14	3 (7%)
57	UQ1	B	302	-	18,18,18	1.07	2 (11%)	22,25,25	0.70	0
55	3PE	N	401	-	36,36,50	1.06	2 (5%)	39,41,55	1.18	4 (10%)

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
66	EHZ	n	201	-	-	21/39/39/45	-
55	3PE	M	503	-	-	17/54/54/54	-
55	3PE	Ag	102	-	-	5/42/42/54	-
56	SF4	G	802	7	-	-	0/6/5/5
71	3PH	AD	402	-	-	8/37/37/49	-
55	3PE	AC	403	-	-	12/38/38/54	-
59	FES	G	803	7	-	-	0/1/1/1
62	CDL	X	201	-	-	27/77/77/110	-
56	SF4	I	303	9	-	-	0/6/5/5
55	3PE	L	703	-	-	13/54/54/54	-
58	PC1	I	302	-	-	13/50/50/57	-
68	U10	AC	404	-	-	0/15/39/87	0/1/1/1
69	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
71	3PH	Ad	402	-	-	8/37/37/49	-
55	3PE	L	707	-	-	13/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	3PE	M	502	-	-	14/54/54/54	-
62	CDL	h	201	-	-	23/80/80/110	-
55	3PE	I	301	-	-	17/54/54/54	-
62	CDL	Ag	101	-	-	12/66/66/110	-
64	NDP	P	401	-	-	6/34/77/77	0/5/5/5
55	3PE	AF	201	-	-	9/45/45/54	-
62	CDL	Aa	501	-	-	16/56/56/110	-
56	SF4	I	304	9	-	-	0/6/5/5
56	SF4	G	801	7	-	-	0/6/5/5
69	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1
55	3PE	M	501	-	-	15/54/54/54	-
66	EHZ	W	201	-	-	22/39/39/45	-
70	HEC	AD	401	48	1/1/3/7	7/14/54/54	-
56	SF4	B	301	2	-	-	0/6/5/5
63	ADP	O	402	-	-	5/16/32/32	0/3/3/3
55	3PE	A	401	-	-	14/49/49/54	-
55	3PE	O	401	-	-	10/34/34/54	-
55	3PE	Ac	401	-	-	10/26/26/54	-
55	3PE	L	701	-	-	13/45/45/54	-
55	3PE	b	201	-	-	8/49/49/54	-
61	UQ9	H	400	-	-	13/30/54/81	0/1/1/1
67	HEM	AC	402	47	-	6/14/54/54	-
67	HEM	Ac	402	47	-	5/14/54/54	-
56	SF4	F	502	6	-	-	0/6/5/5
55	3PE	L	702	-	-	8/43/43/54	-
62	CDL	Ac	407	-	-	11/52/52/110	-
55	3PE	J	202	-	-	12/49/49/54	-
55	3PE	Ac	404	-	-	8/38/38/54	-
58	PC1	J	201	-	-	14/45/45/57	-
60	FMN	F	501	-	-	4/18/18/18	0/3/3/3
62	CDL	a	101	-	-	14/67/67/110	-
59	FES	E	301	5	-	-	0/1/1/1
62	CDL	L	706	-	-	27/96/96/110	-
67	HEM	AC	401	47	-	8/14/54/54	-
67	HEM	Ac	403	47	-	10/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PC1	B	303	-	-	11/38/38/57	-
62	CDL	L	705	-	-	24/87/87/110	-
62	CDL	AC	406	-	-	18/66/66/110	-
55	3PE	L	704	-	-	13/50/50/54	-
70	HEC	Ad	401	48	1/1/3/7	7/14/54/54	-
68	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
55	3PE	Y	201	-	-	5/43/43/54	-
57	UQ1	B	302	-	-	3/9/33/33	0/1/1/1
55	3PE	N	401	-	-	8/40/40/54	-

The worst 5 of 217 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	404	U10	C6-C1	7.59	1.49	1.35
68	Ac	405	U10	C6-C1	7.42	1.48	1.35
69	AC	405	UQ6	C2-C3	5.95	1.49	1.39
69	Ac	406	UQ6	C2-C3	5.90	1.49	1.39
69	Ac	406	UQ6	C5-C4	5.87	1.48	1.39

The worst 5 of 333 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
63	O	402	ADP	C5-C4-N3	-6.41	118.39	126.75
66	W	201	EHZ	C8-C9-S1	6.32	121.44	113.63
66	n	201	EHZ	C8-C9-S1	6.30	121.43	113.63
67	AC	402	HEM	CHC-C4B-NB	6.28	131.24	124.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
70	AD	401	HEC	NA
70	Ad	401	HEC	NA

5 of 586 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	401	3PE	C12-C11-O13-P
55	A	401	3PE	O32-C31-O31-C3
55	A	401	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
55	I	301	3PE	C11-O13-P-O12
55	L	701	3PE	C1-O11-P-O12

There are no ring outliers.

57 monomers are involved in 537 short contacts:

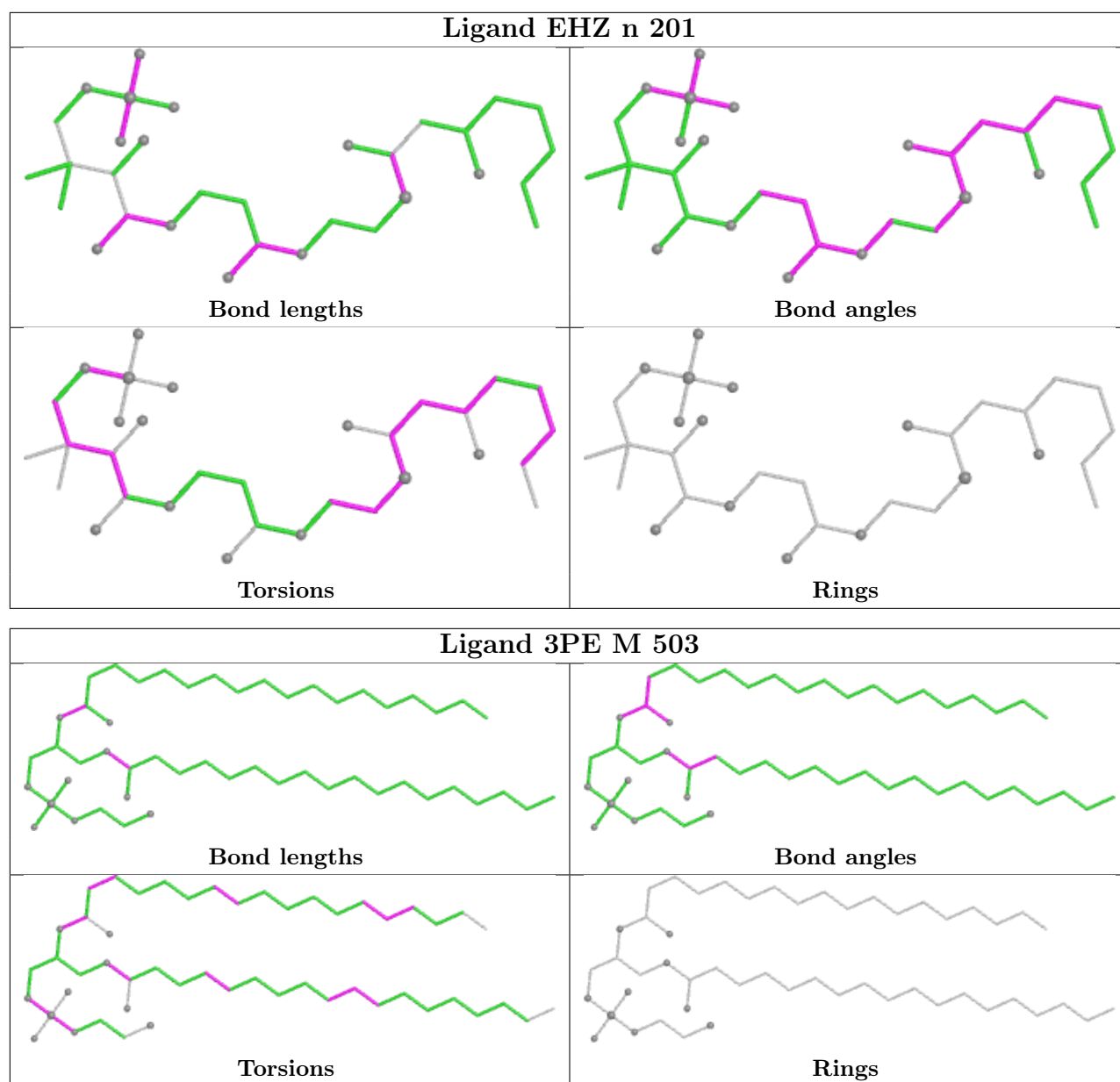
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	M	503	3PE	6	0
55	Ag	102	3PE	9	0
56	G	802	SF4	5	0
71	AD	402	3PH	13	0
55	AC	403	3PE	12	0
59	G	803	FES	4	0
62	X	201	CDL	9	0
56	I	303	SF4	11	0
55	L	703	3PE	10	0
58	I	302	PC1	9	0
68	AC	404	U10	4	0
69	AC	405	UQ6	14	0
71	Ad	402	3PH	19	0
55	L	707	3PE	10	0
55	M	502	3PE	14	0
62	h	201	CDL	15	0
55	I	301	3PE	14	0
62	Ag	101	CDL	9	0
64	P	401	NDP	7	0
55	AF	201	3PE	7	0
62	Aa	501	CDL	8	0
56	I	304	SF4	5	0
69	Ac	406	UQ6	12	0
55	M	501	3PE	6	0
56	B	301	SF4	6	0
66	W	201	EHZ	7	0
70	AD	401	HEC	24	0
63	O	402	ADP	6	0
55	A	401	3PE	12	0
55	Ac	401	3PE	3	0
55	O	401	3PE	5	0
55	L	701	3PE	23	0
55	b	201	3PE	16	0
61	H	400	UQ9	4	0
67	AC	402	HEM	4	0

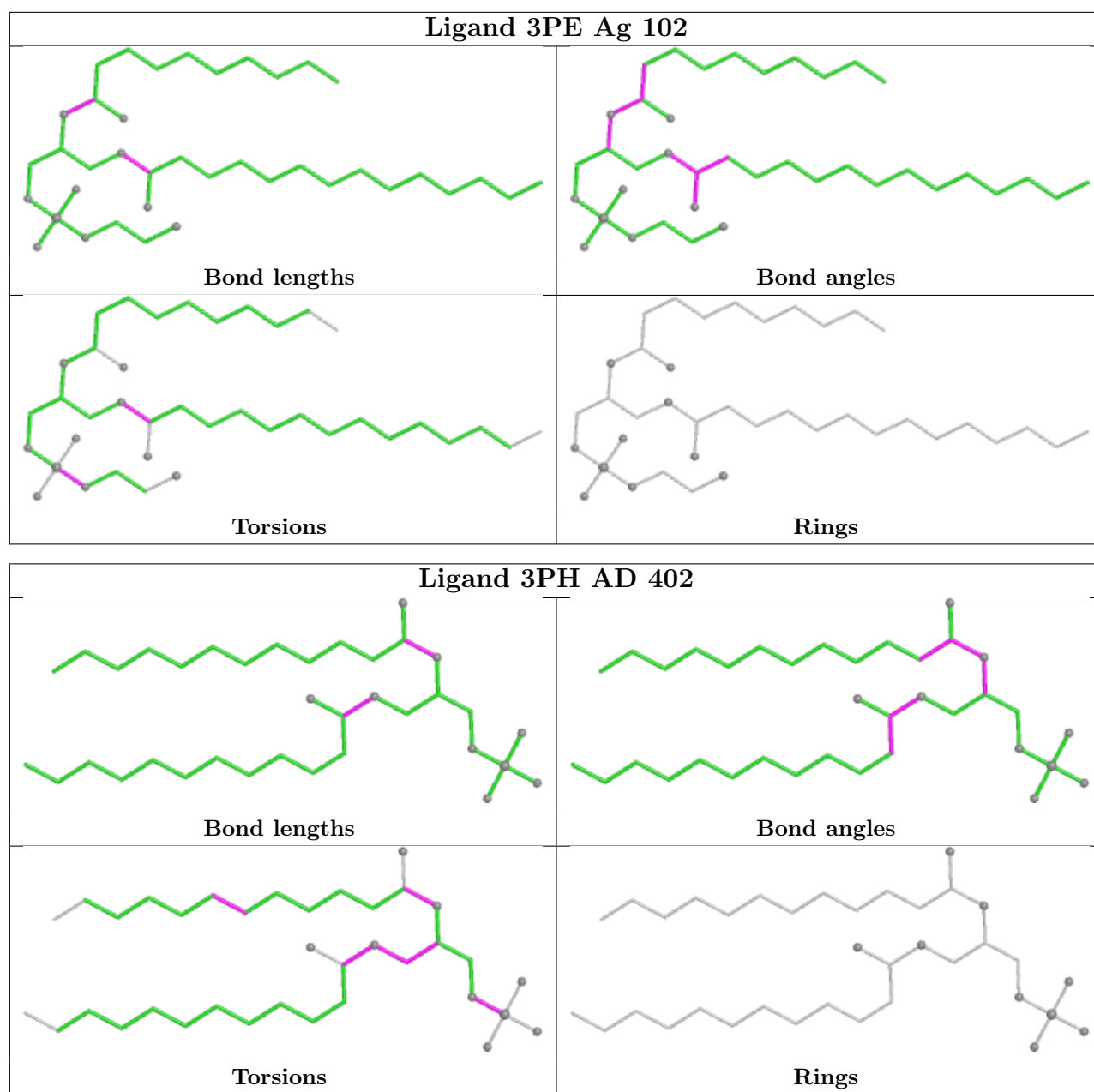
Continued on next page...

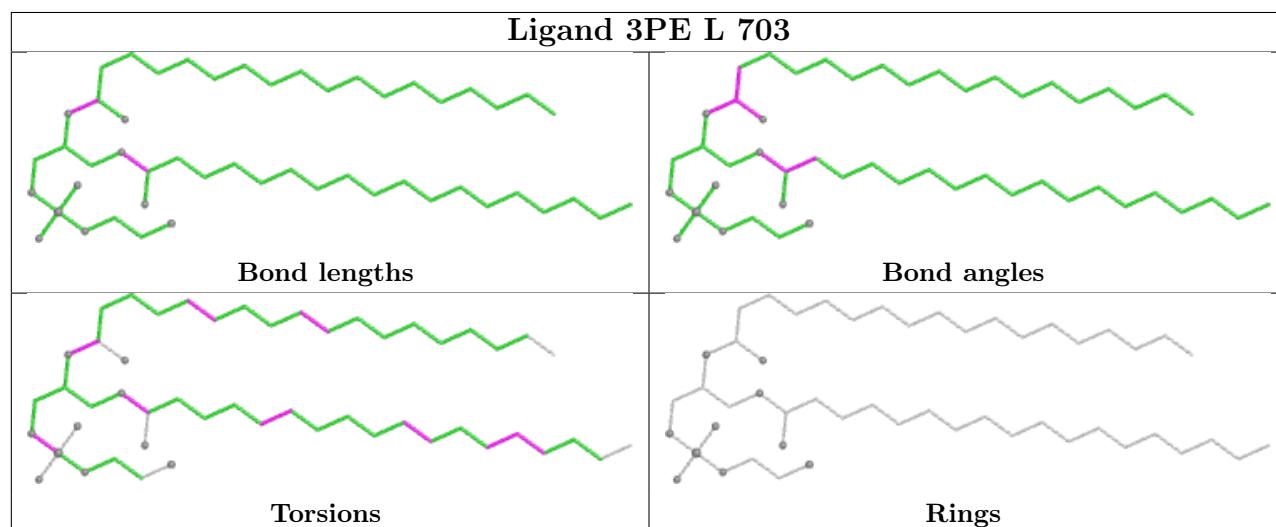
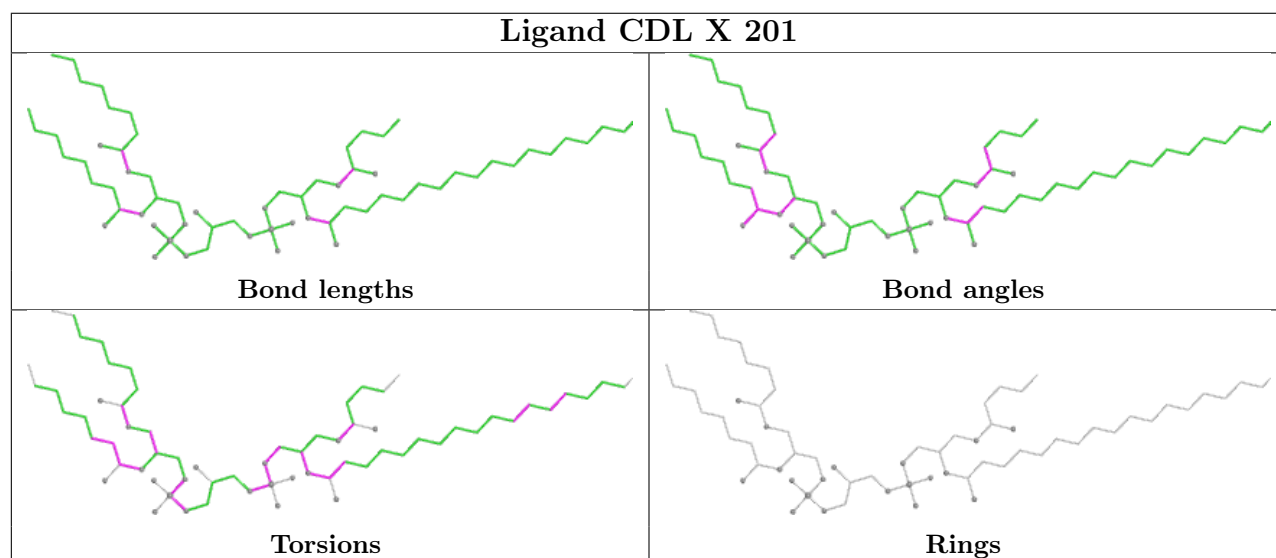
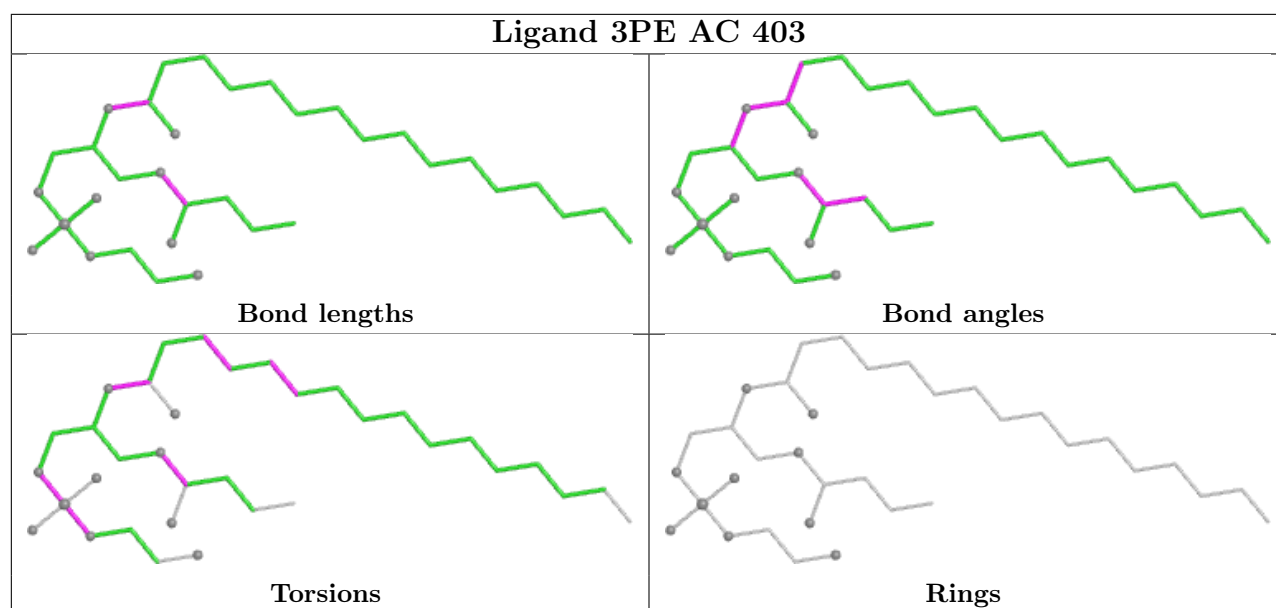
Continued from previous page...

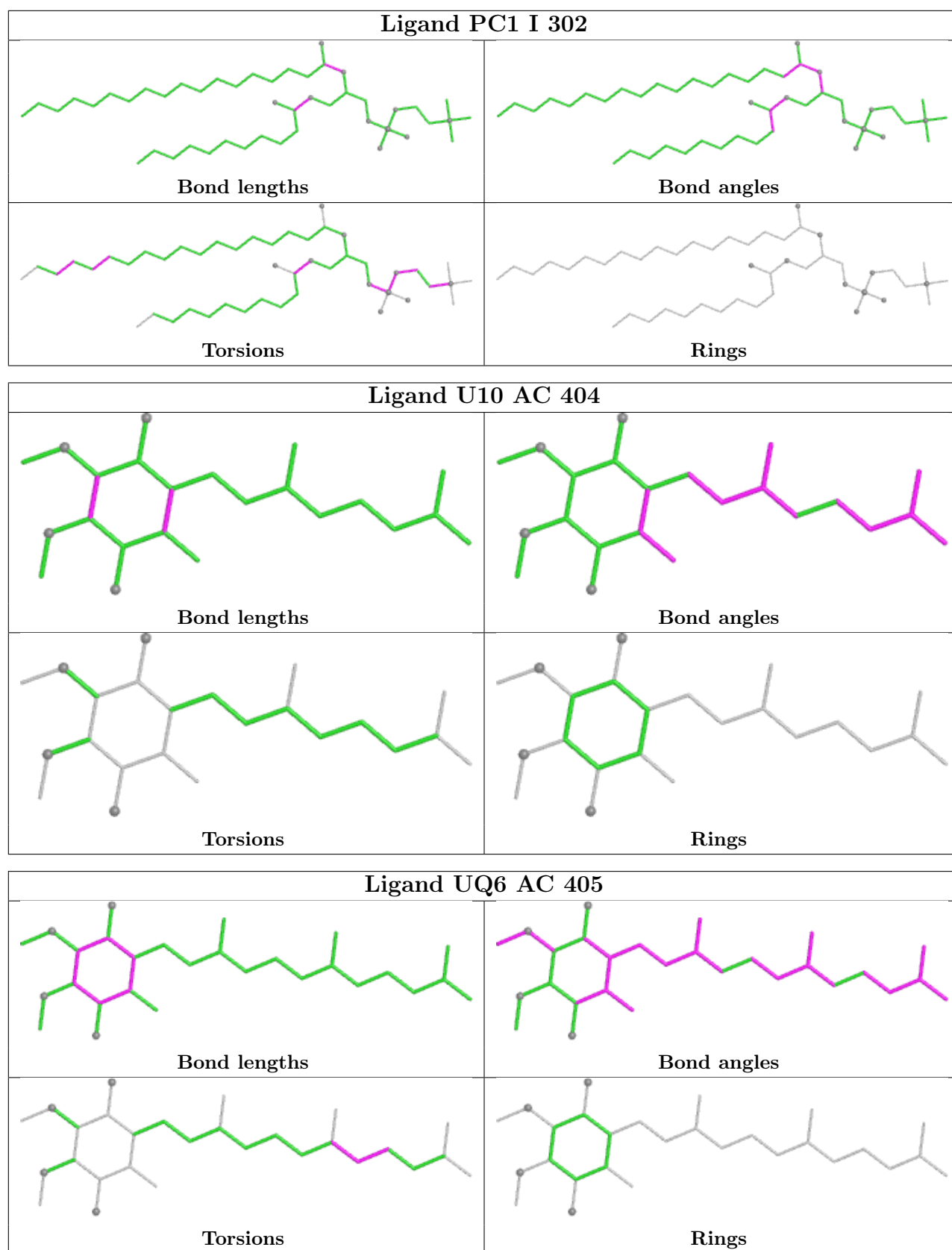
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Ac	402	HEM	3	0
56	F	502	SF4	10	0
55	L	702	3PE	6	0
62	Ac	407	CDL	3	0
55	J	202	3PE	5	0
55	Ac	404	3PE	3	0
58	J	201	PC1	8	0
59	E	301	FES	5	0
60	F	501	FMN	1	0
62	a	101	CDL	22	0
62	L	706	CDL	19	0
67	AC	401	HEM	3	0
67	Ac	403	HEM	6	0
58	B	303	PC1	7	0
62	L	705	CDL	19	0
62	AC	406	CDL	4	0
55	L	704	3PE	8	0
70	Ad	401	HEC	25	0
68	Ac	405	U10	5	0
55	Y	201	3PE	20	0
57	B	302	UQ1	13	0
55	N	401	3PE	14	0

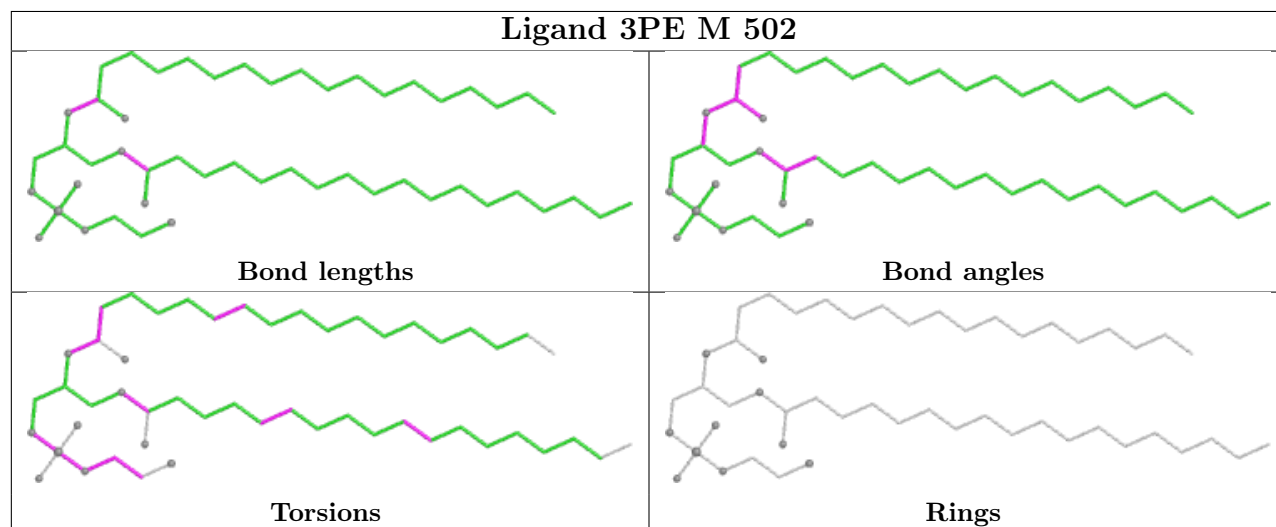
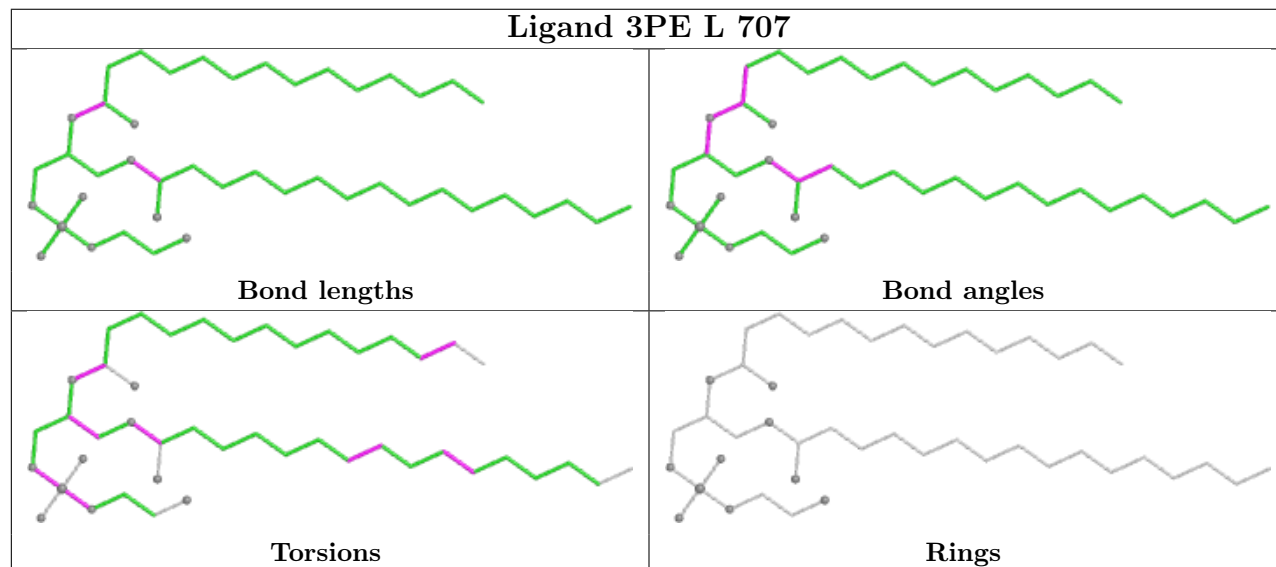
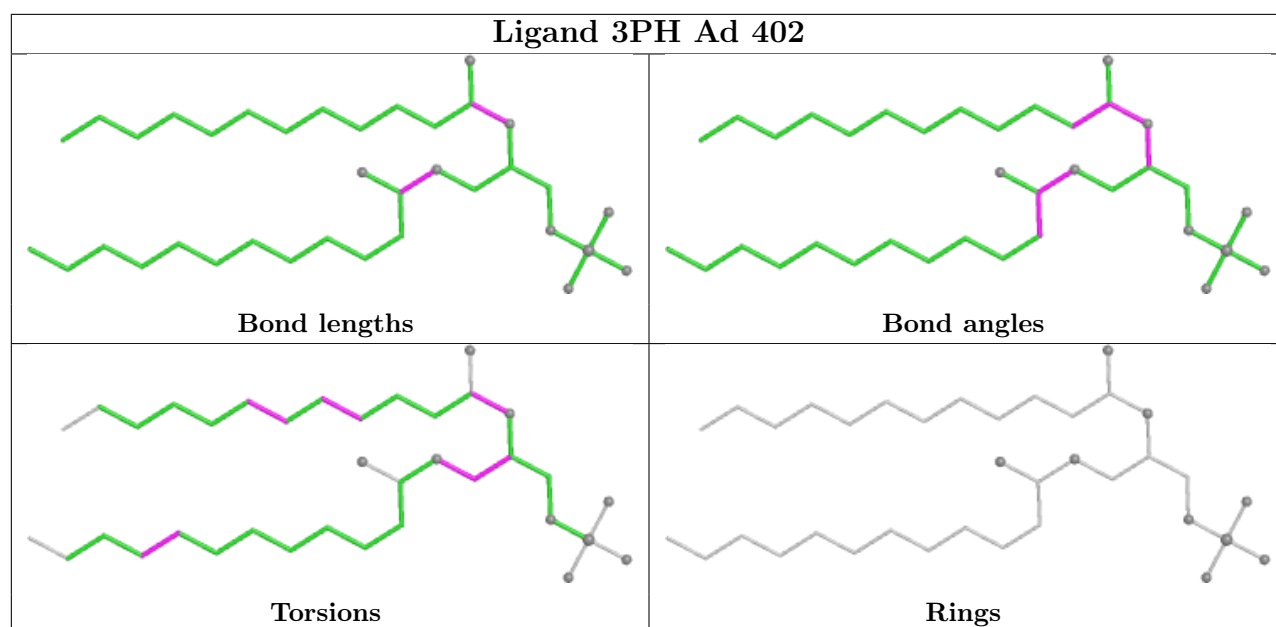
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

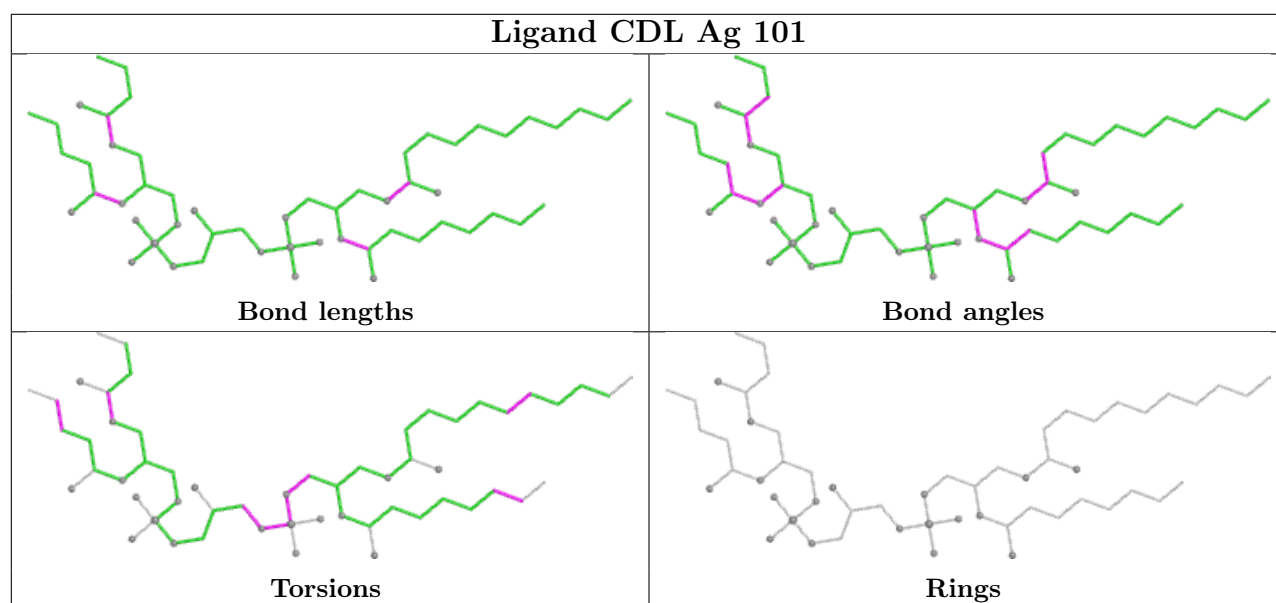
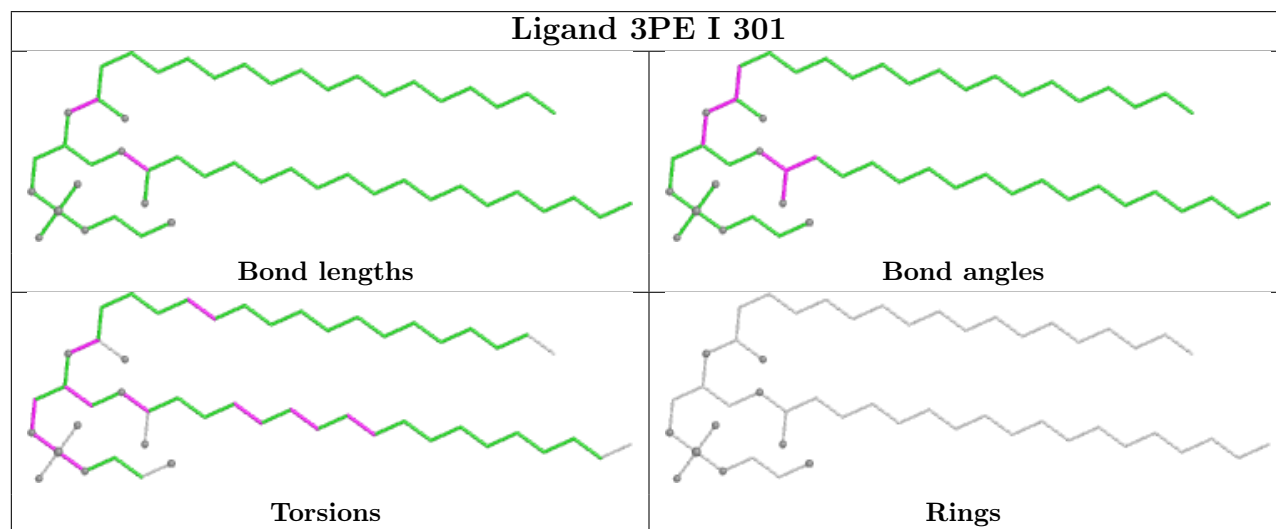
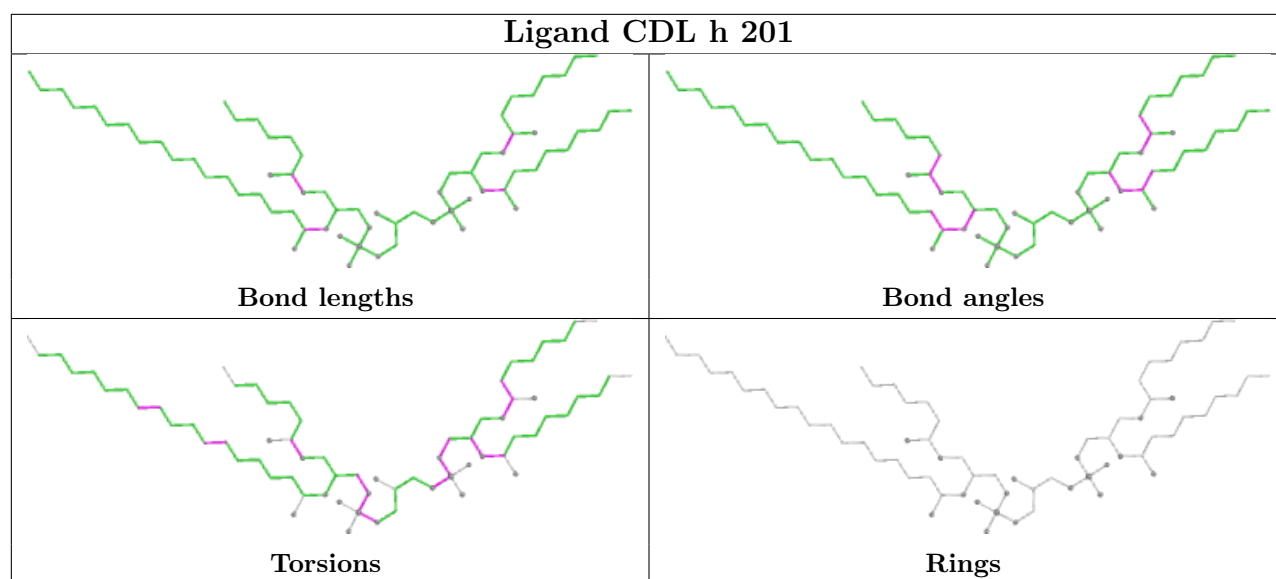


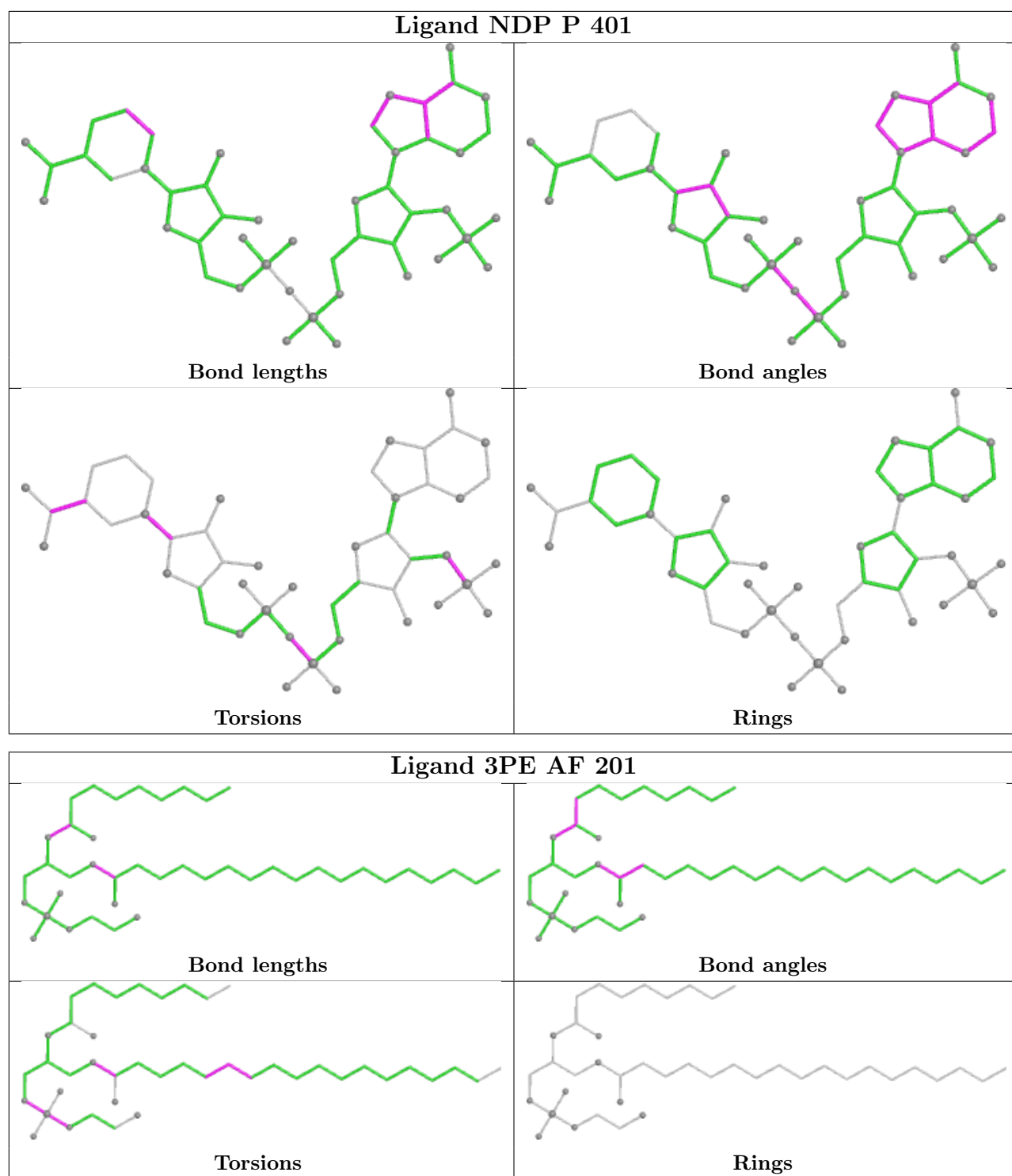


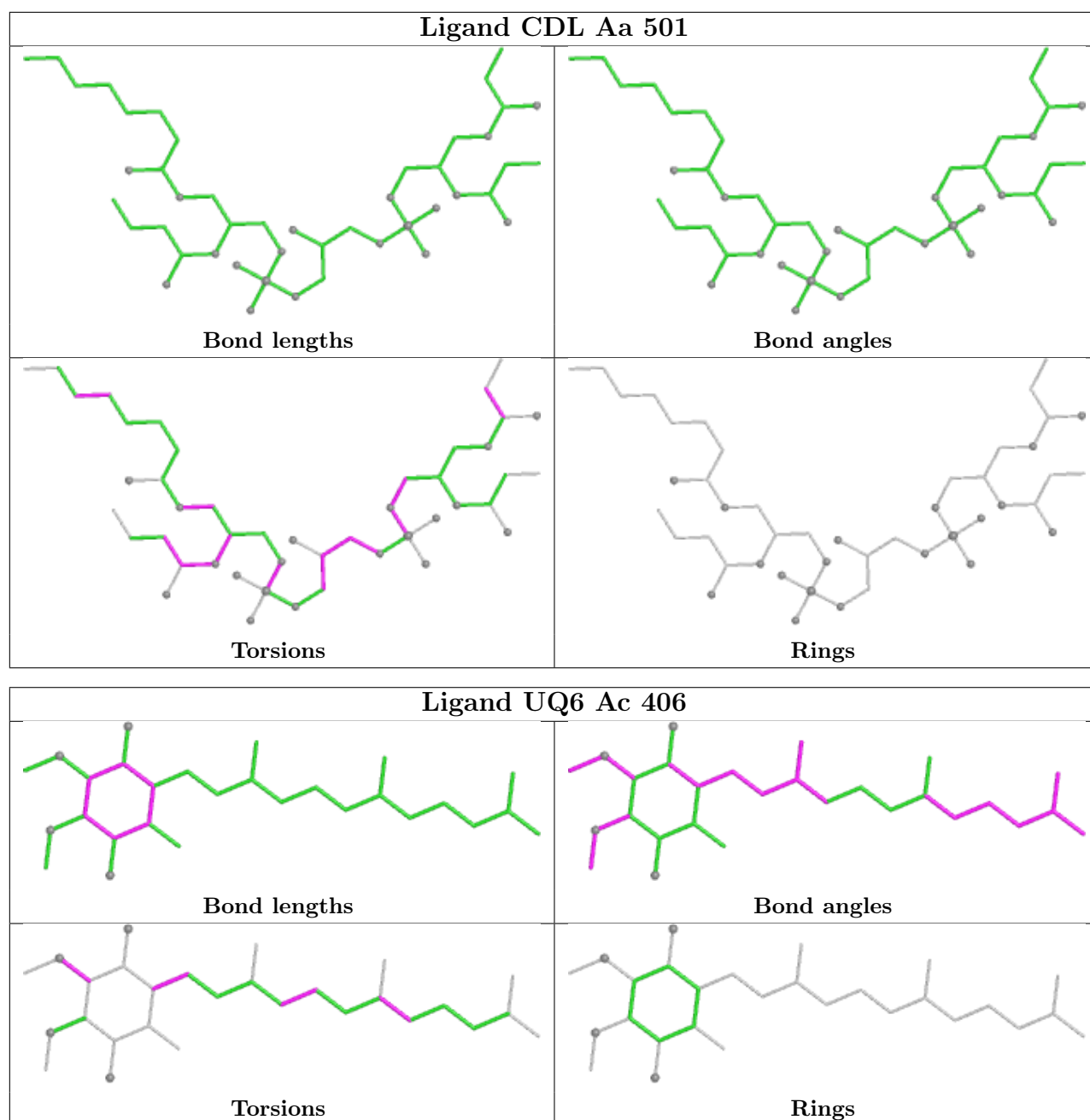


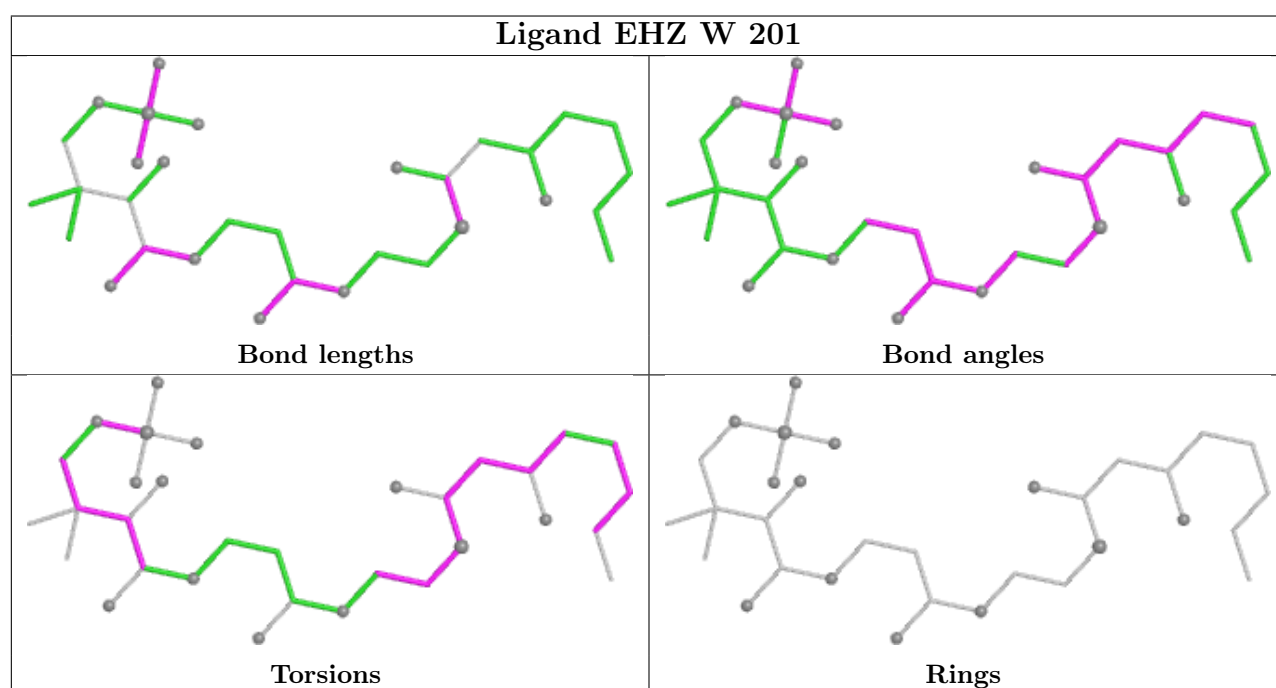
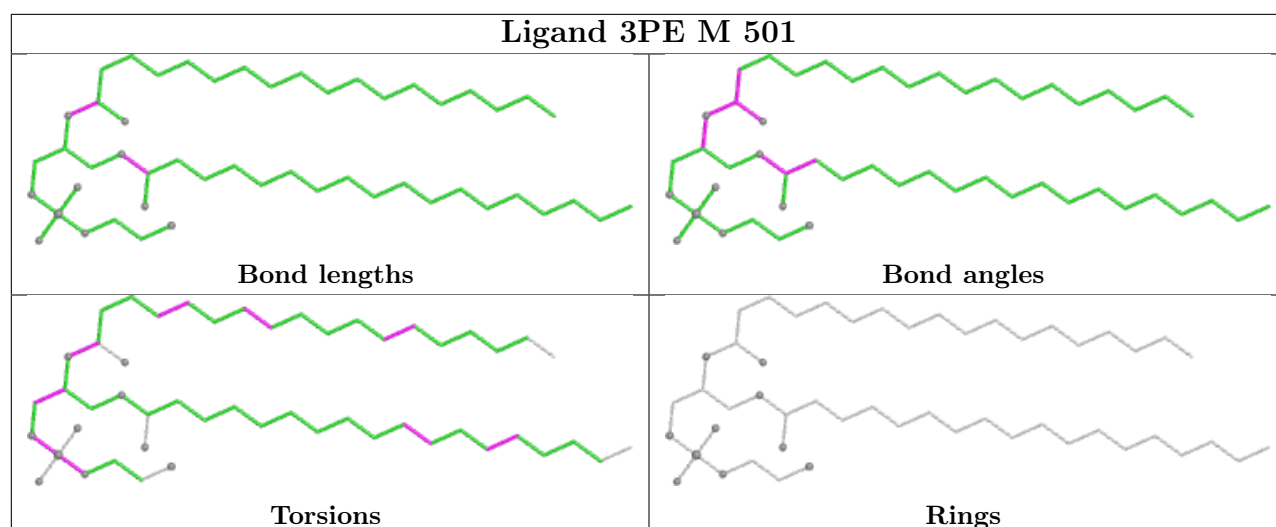




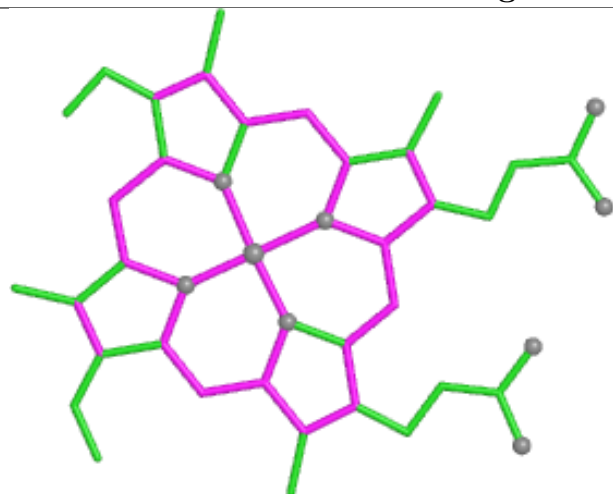




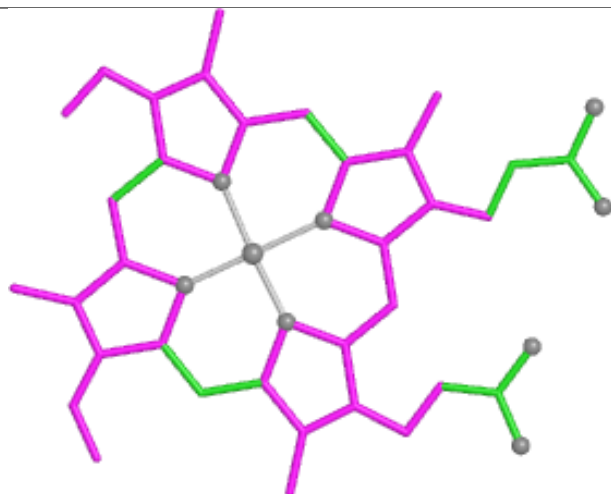




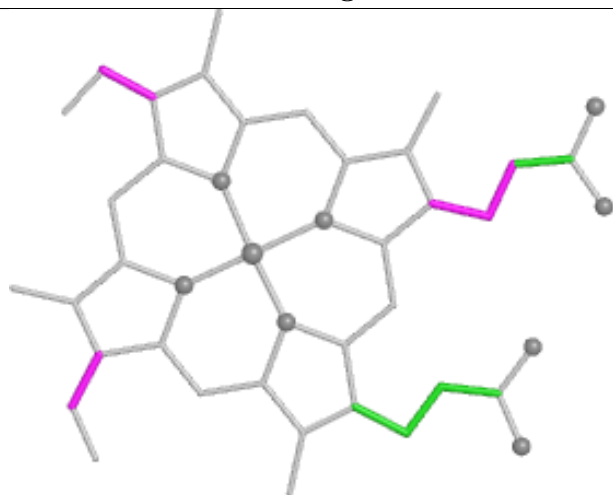
Ligand HEC AD 401



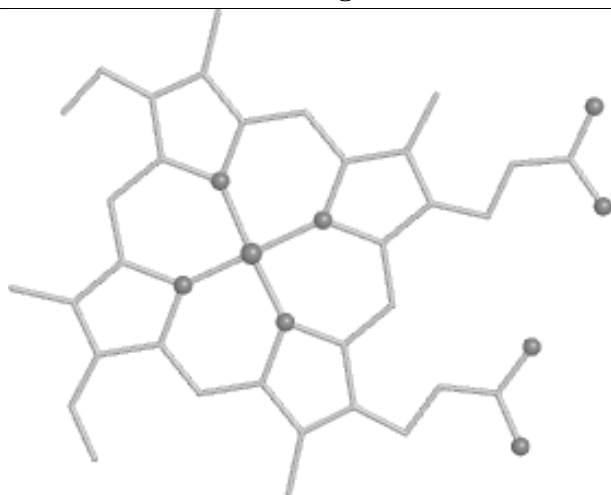
Bond lengths



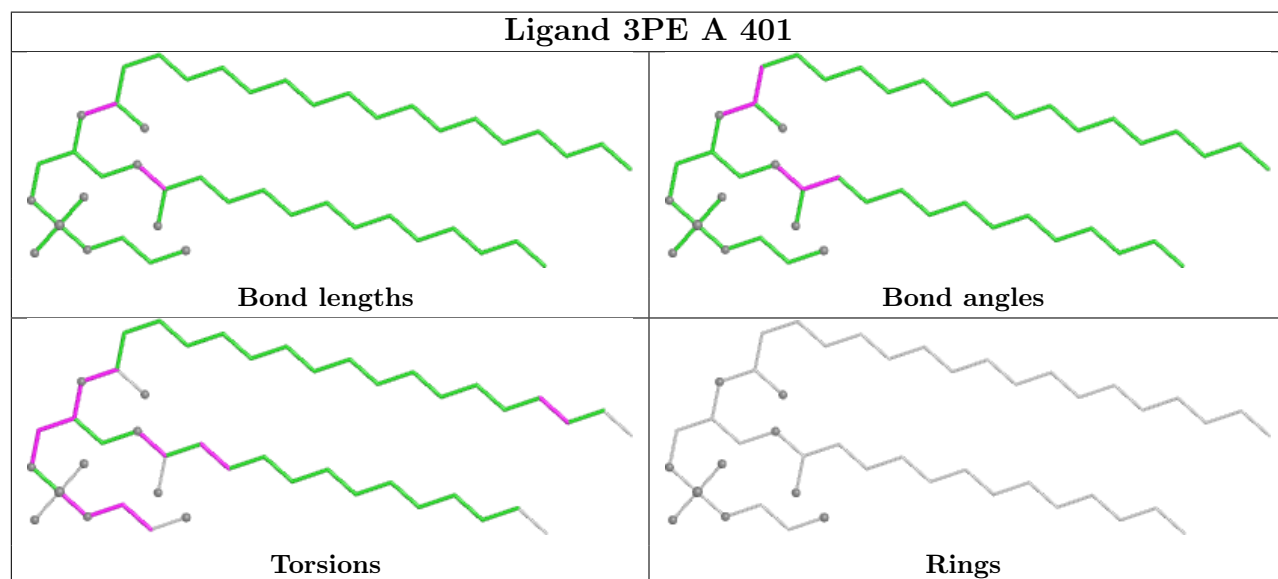
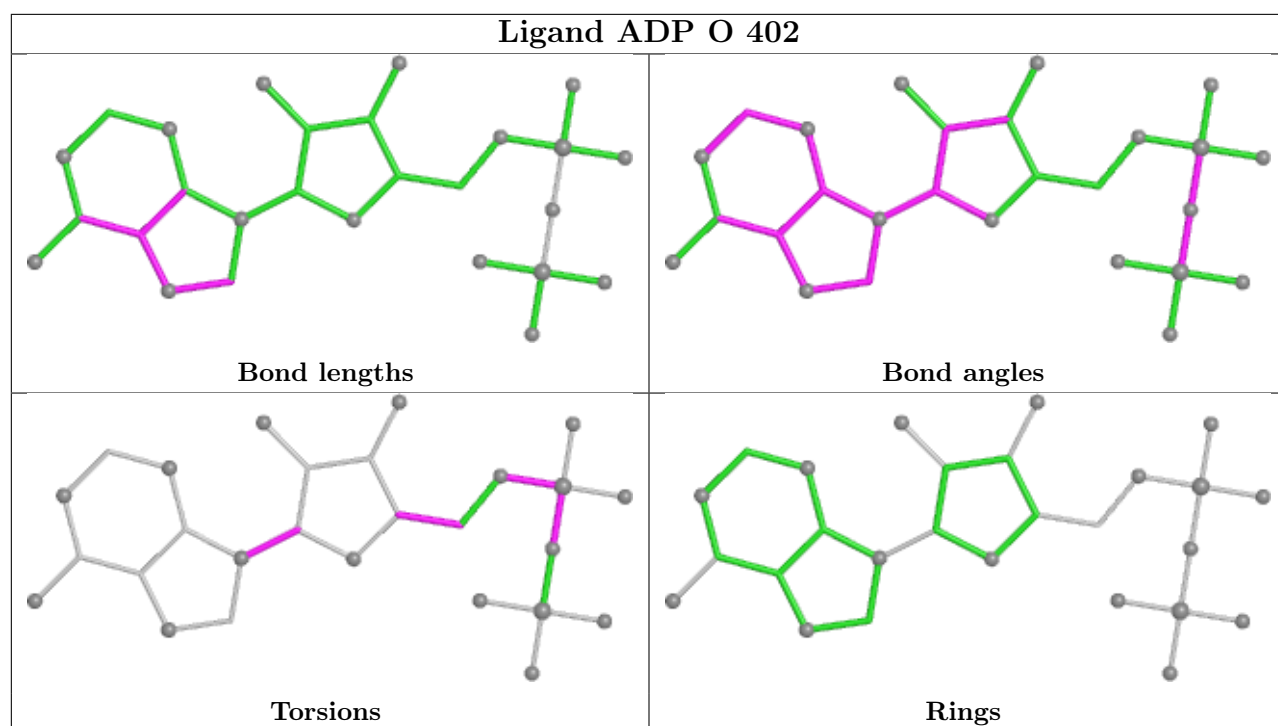
Bond angles

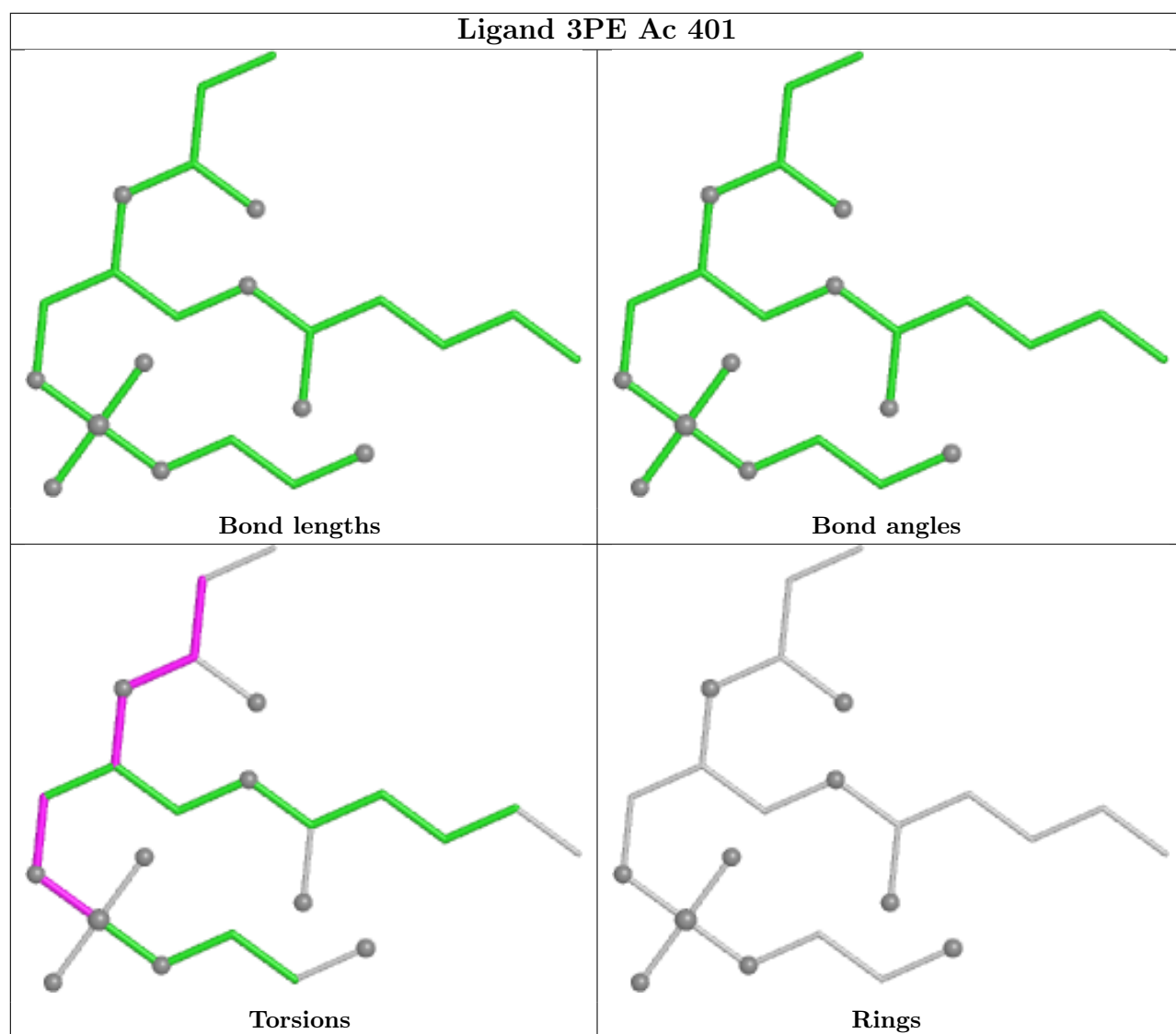


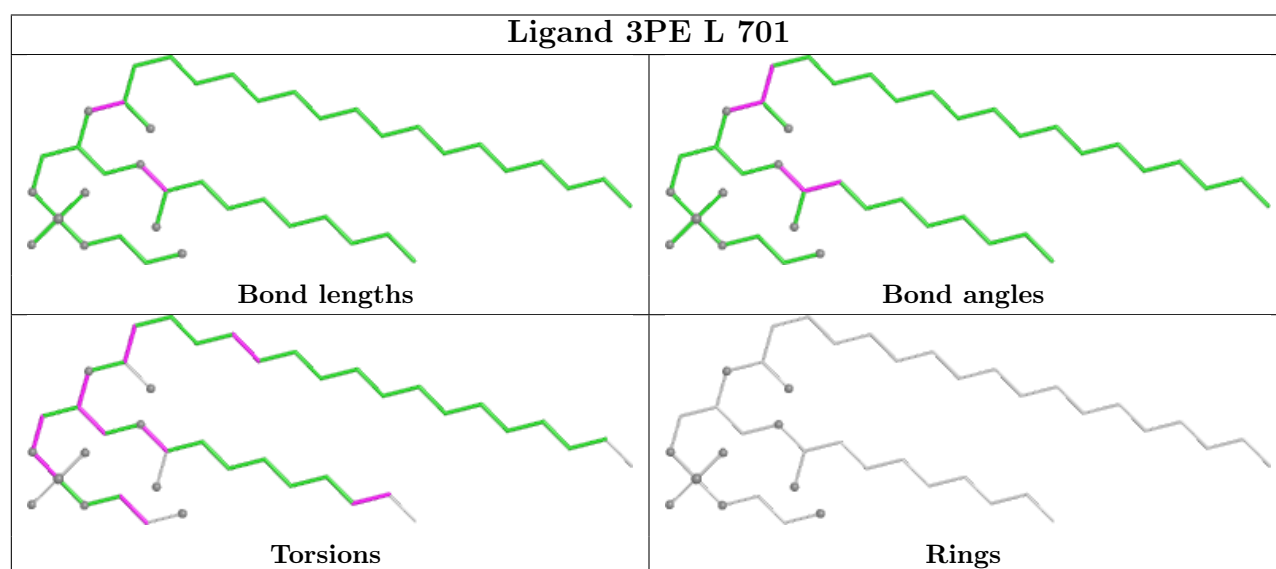
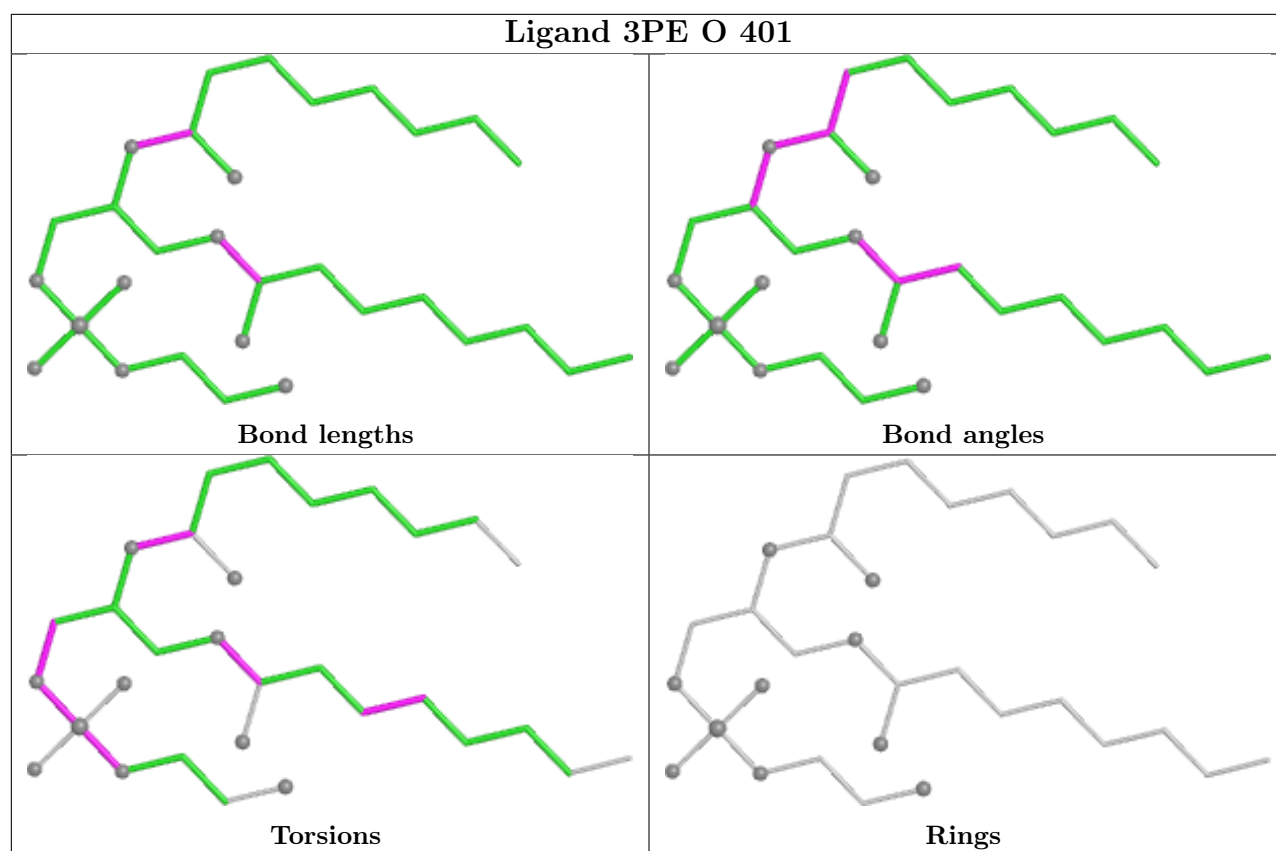
Torsions

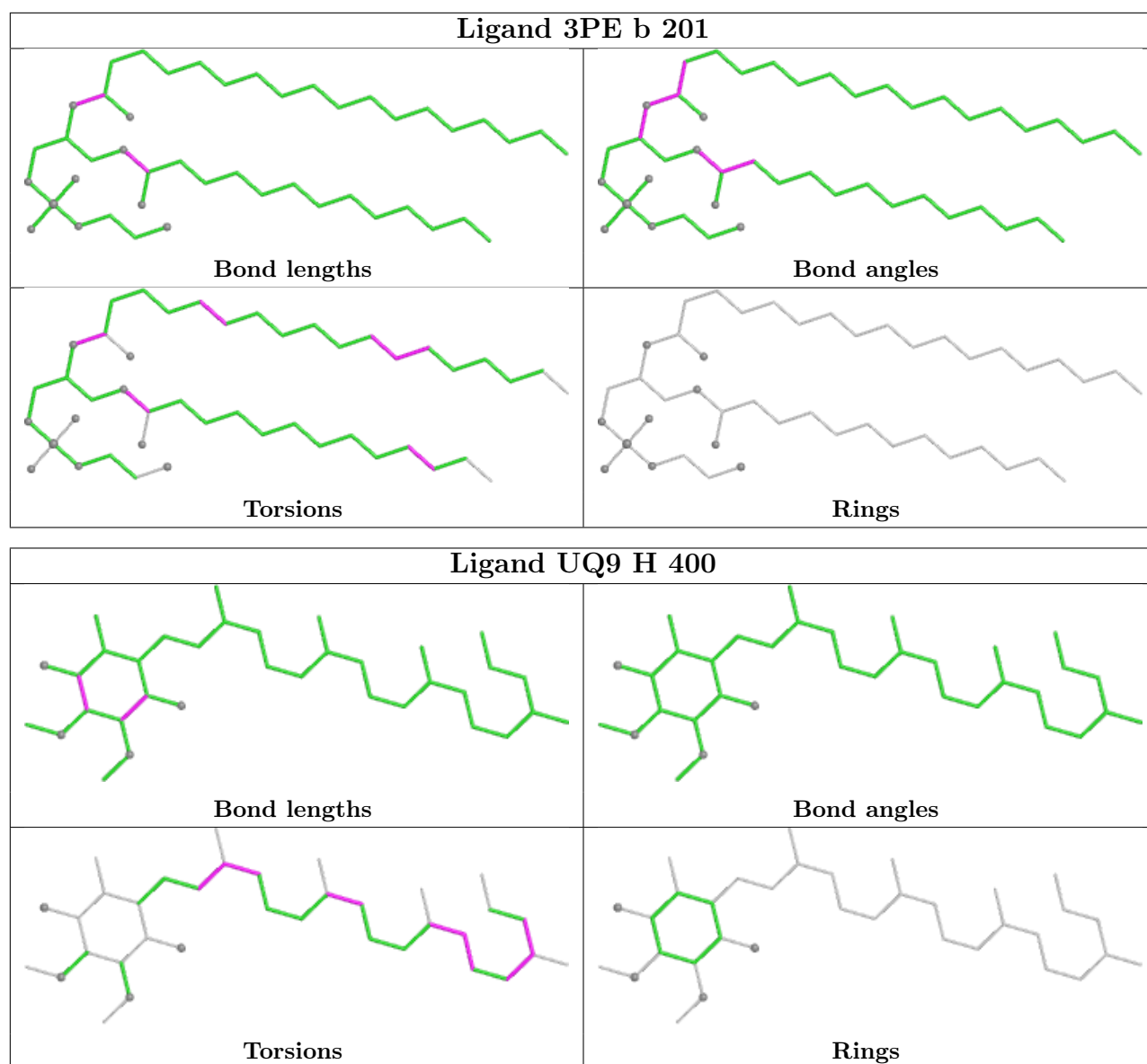


Rings

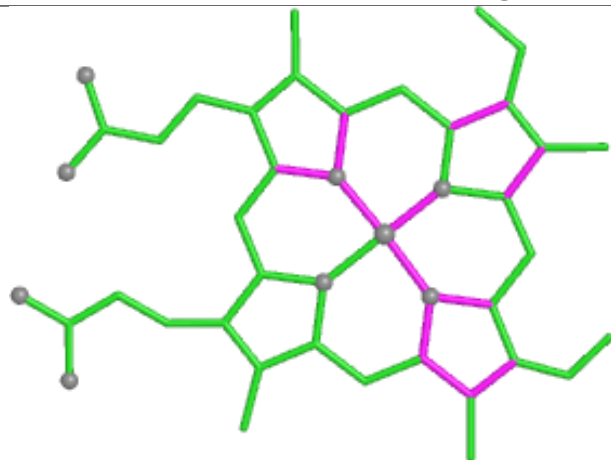




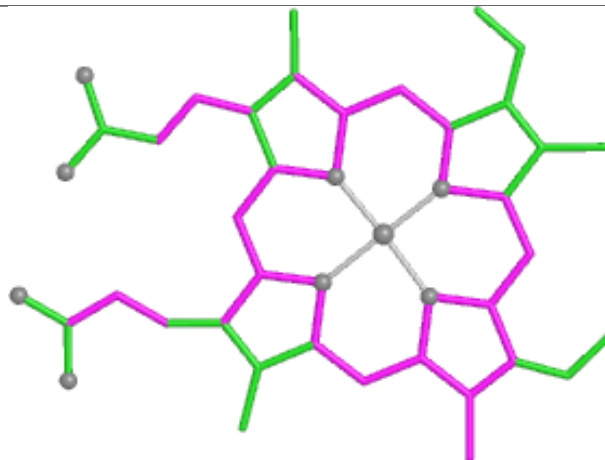




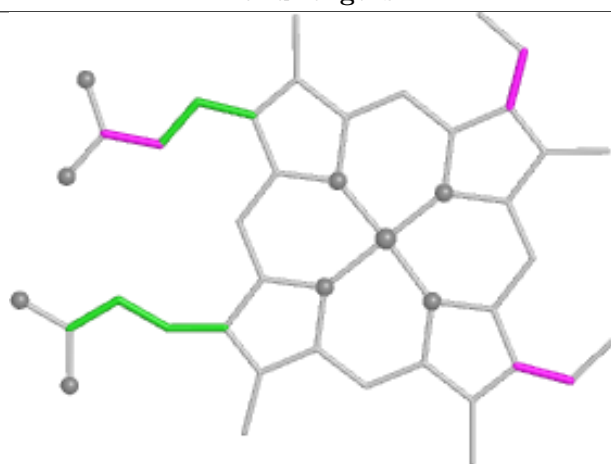
Ligand HEM AC 402



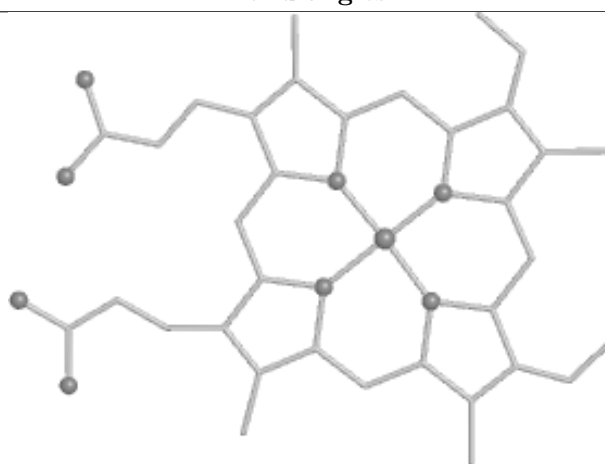
Bond lengths



Bond angles

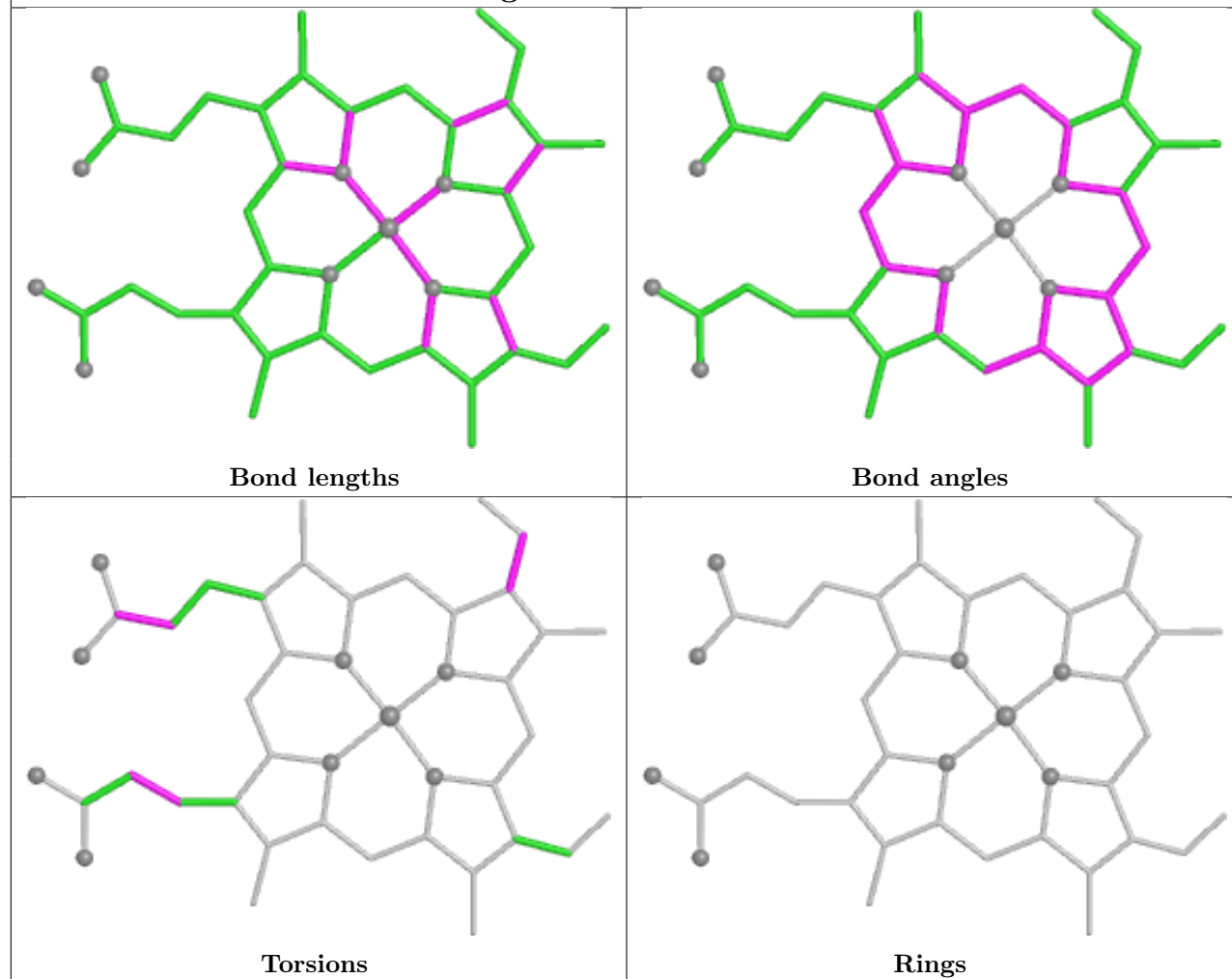


Torsions

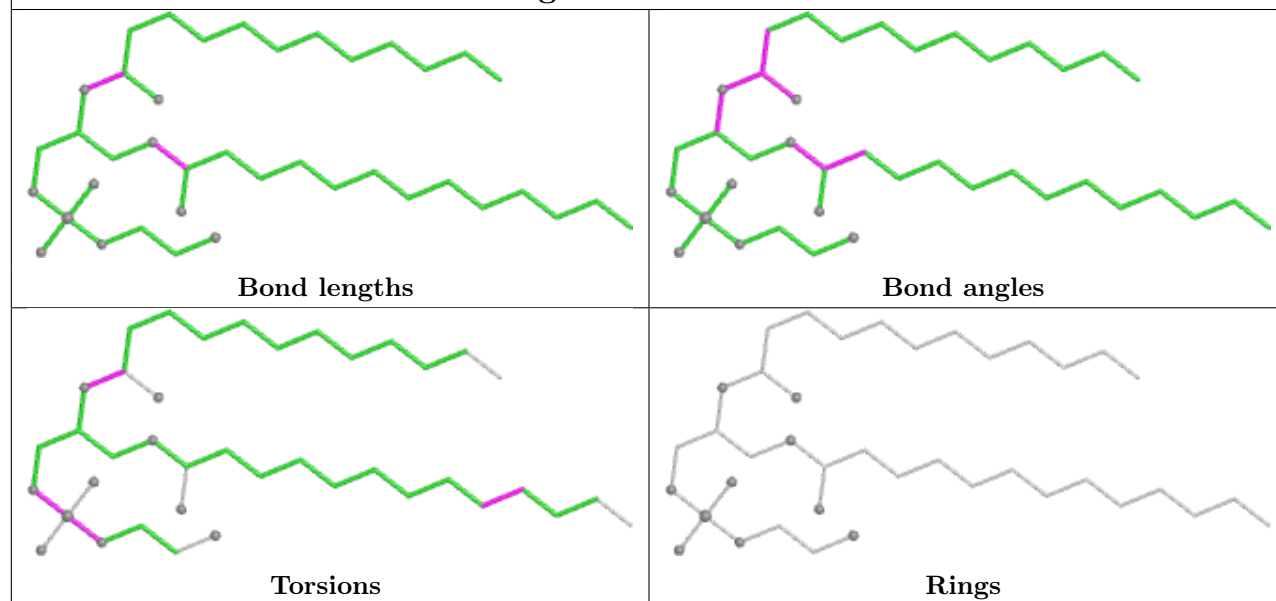


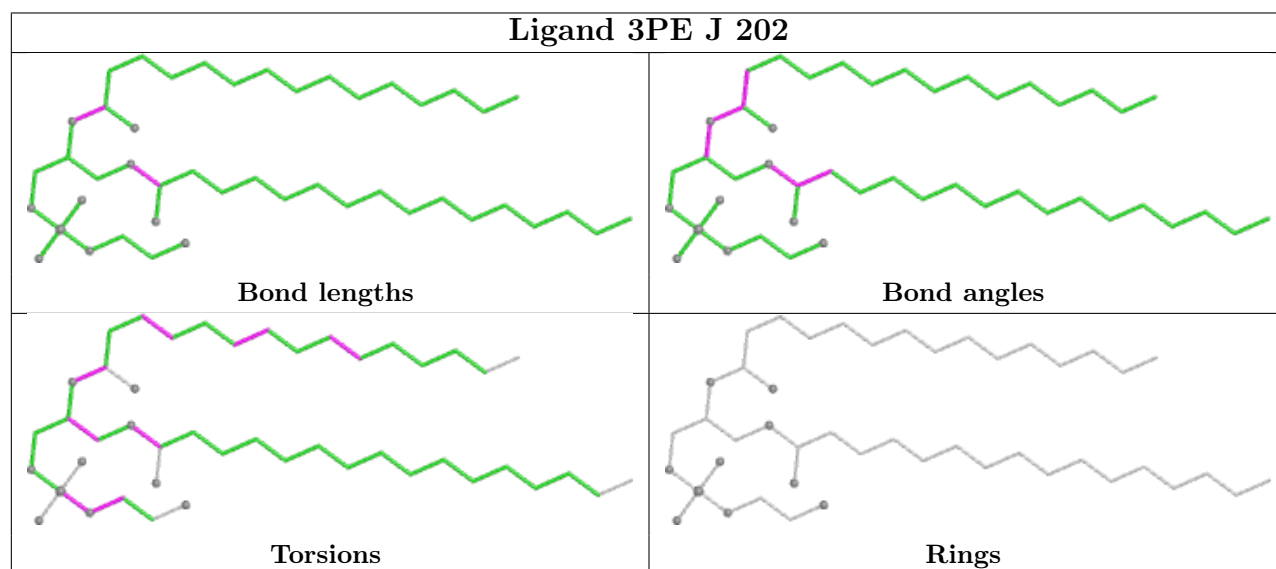
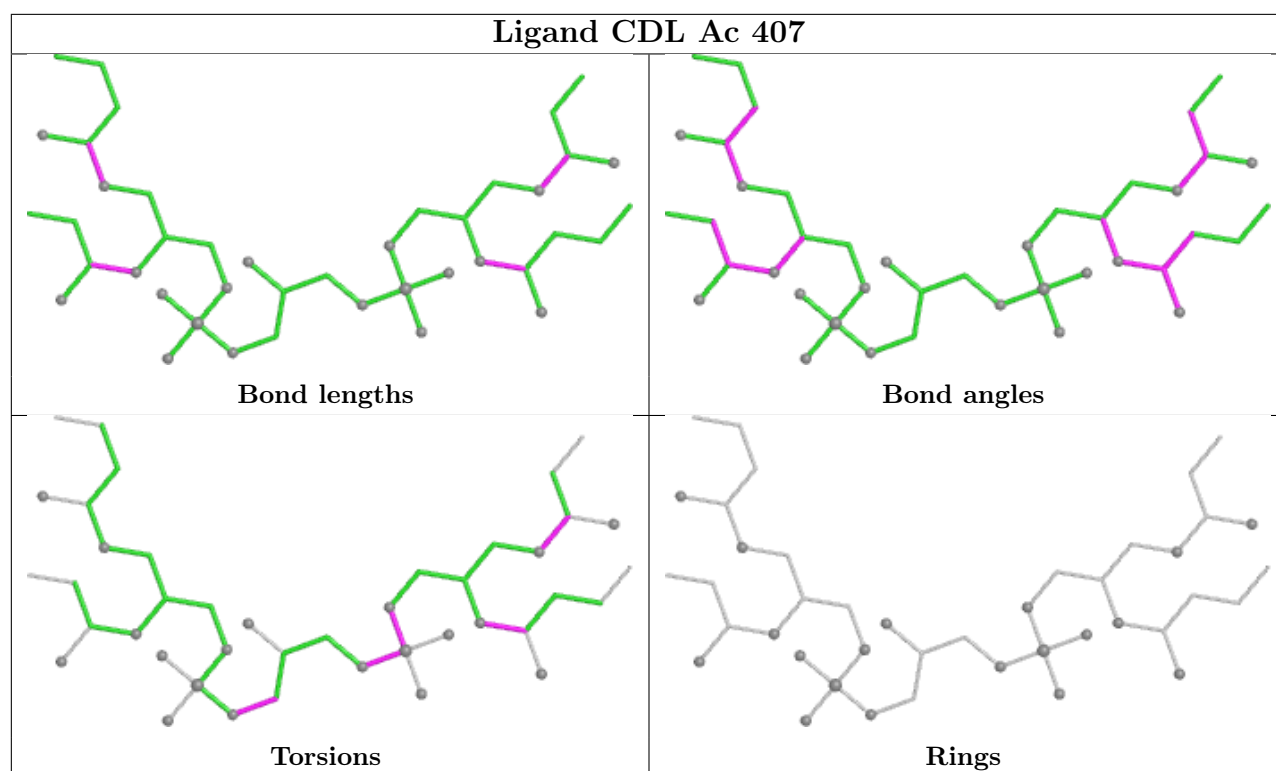
Rings

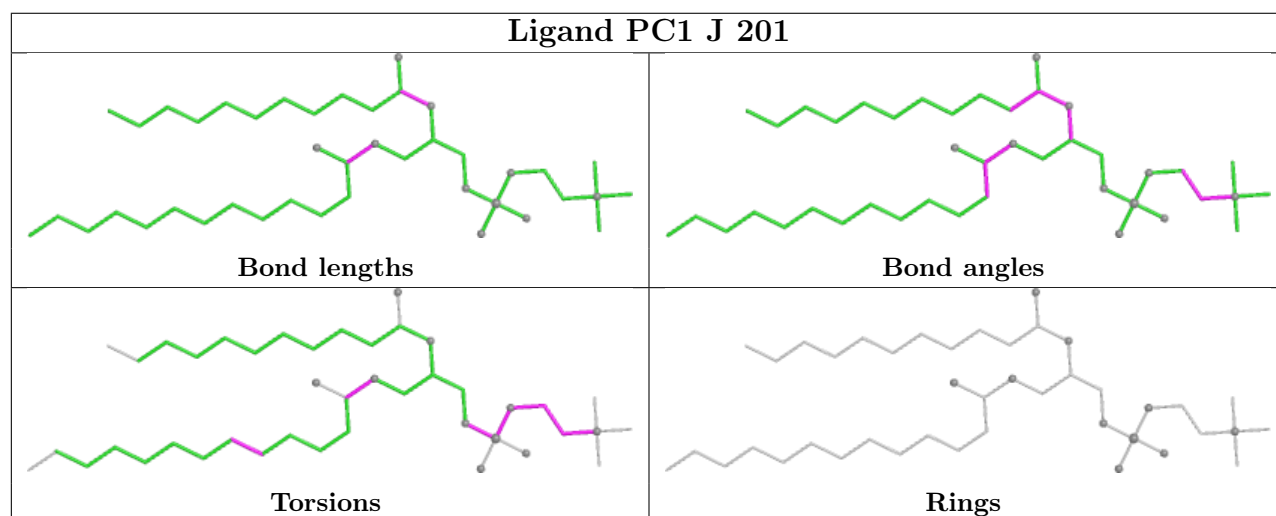
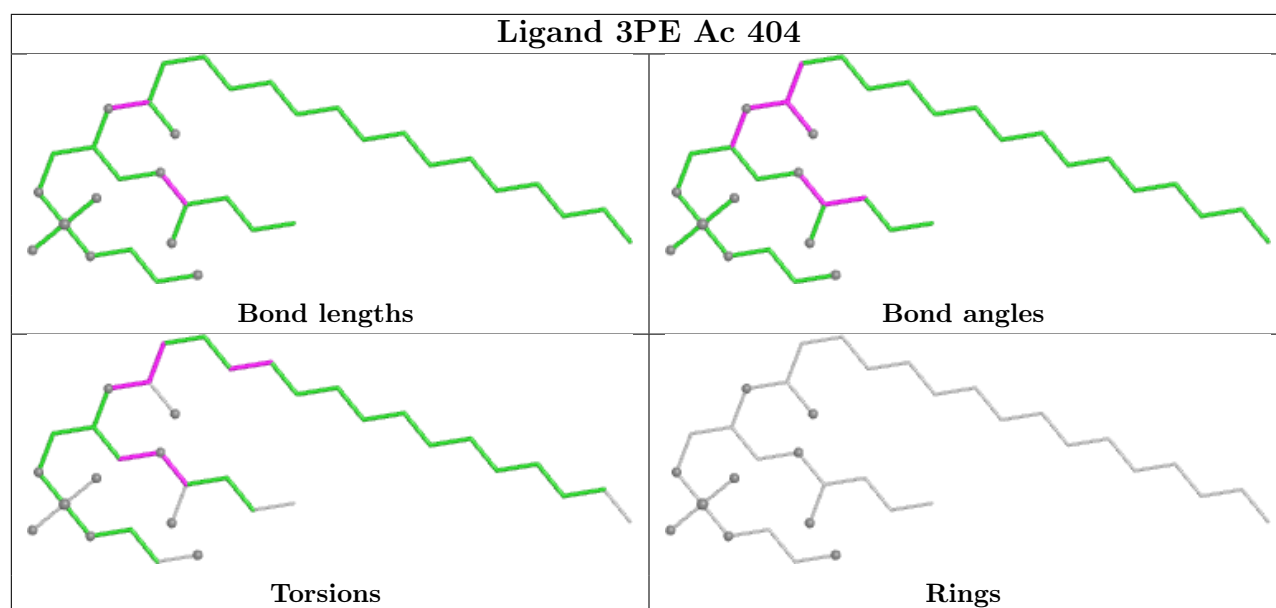
Ligand HEM Ac 402

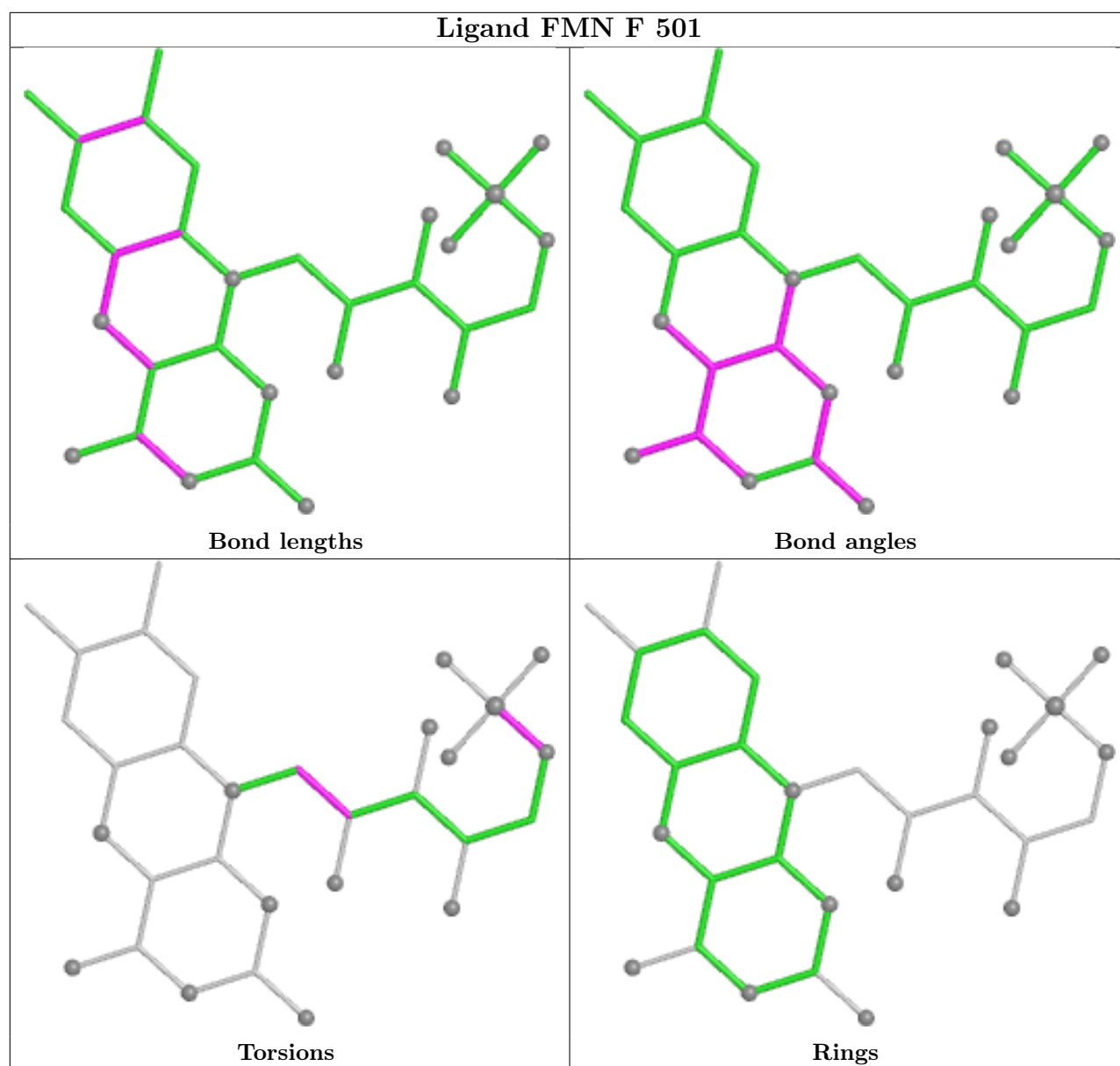


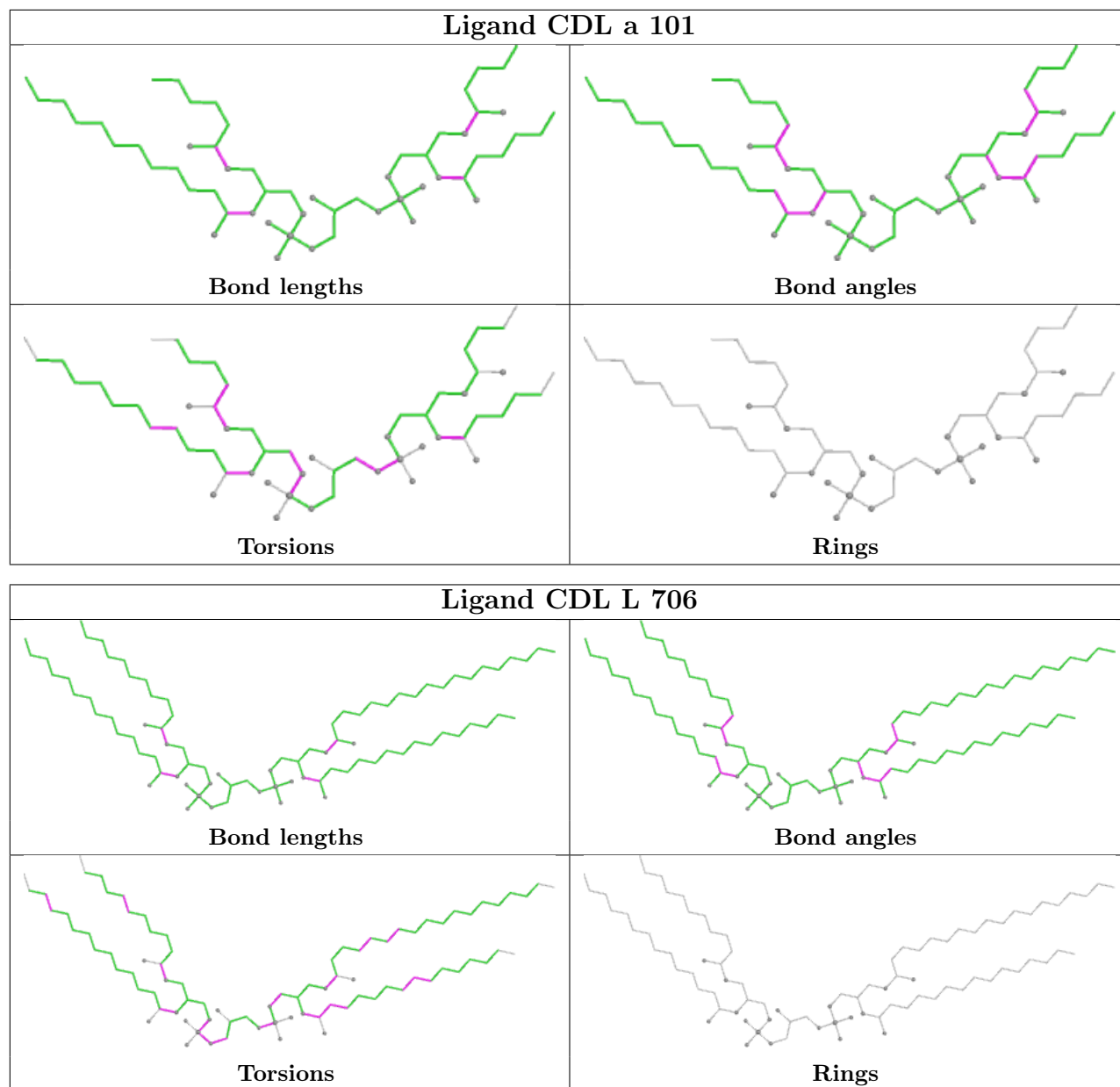
Ligand 3PE L 702



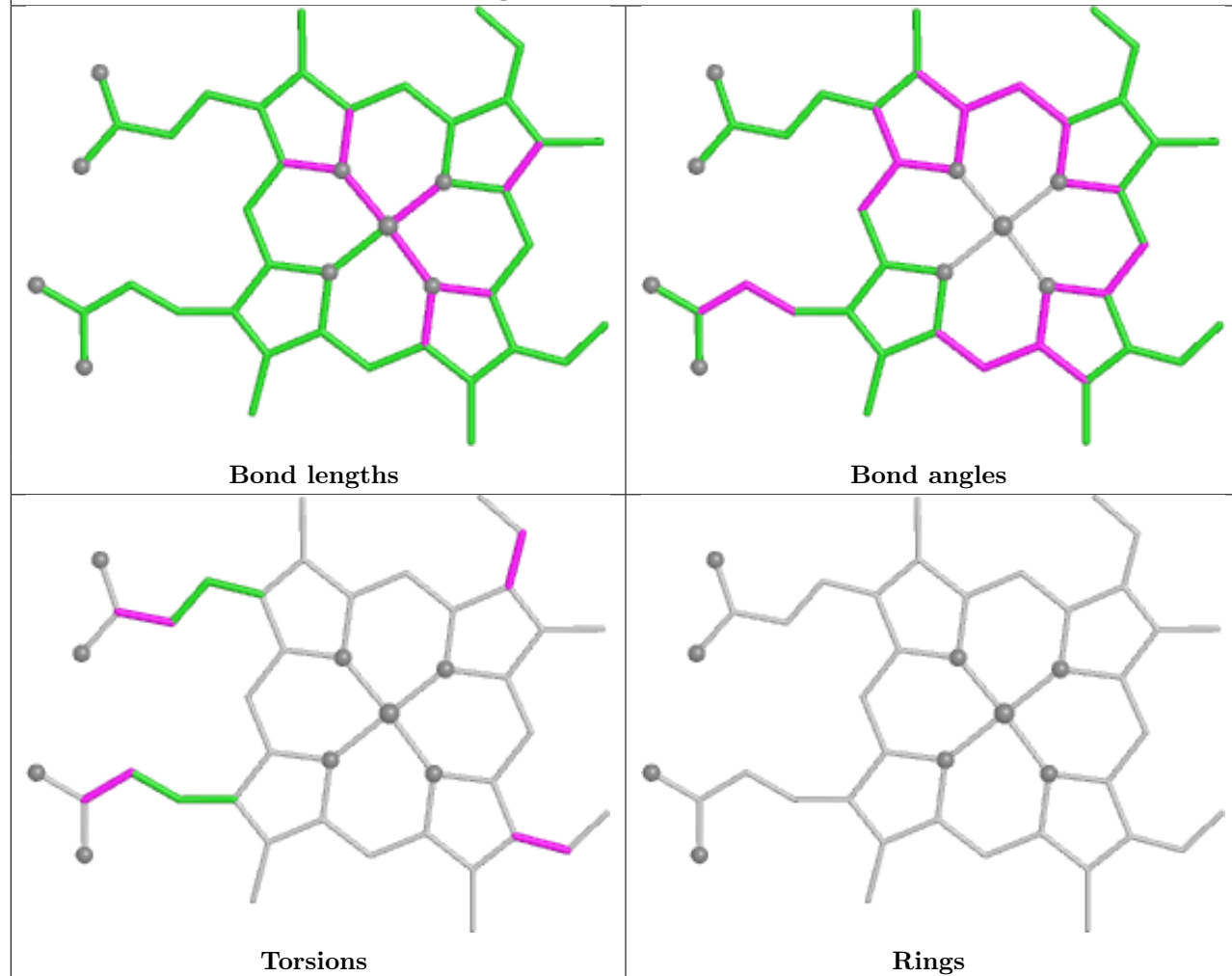




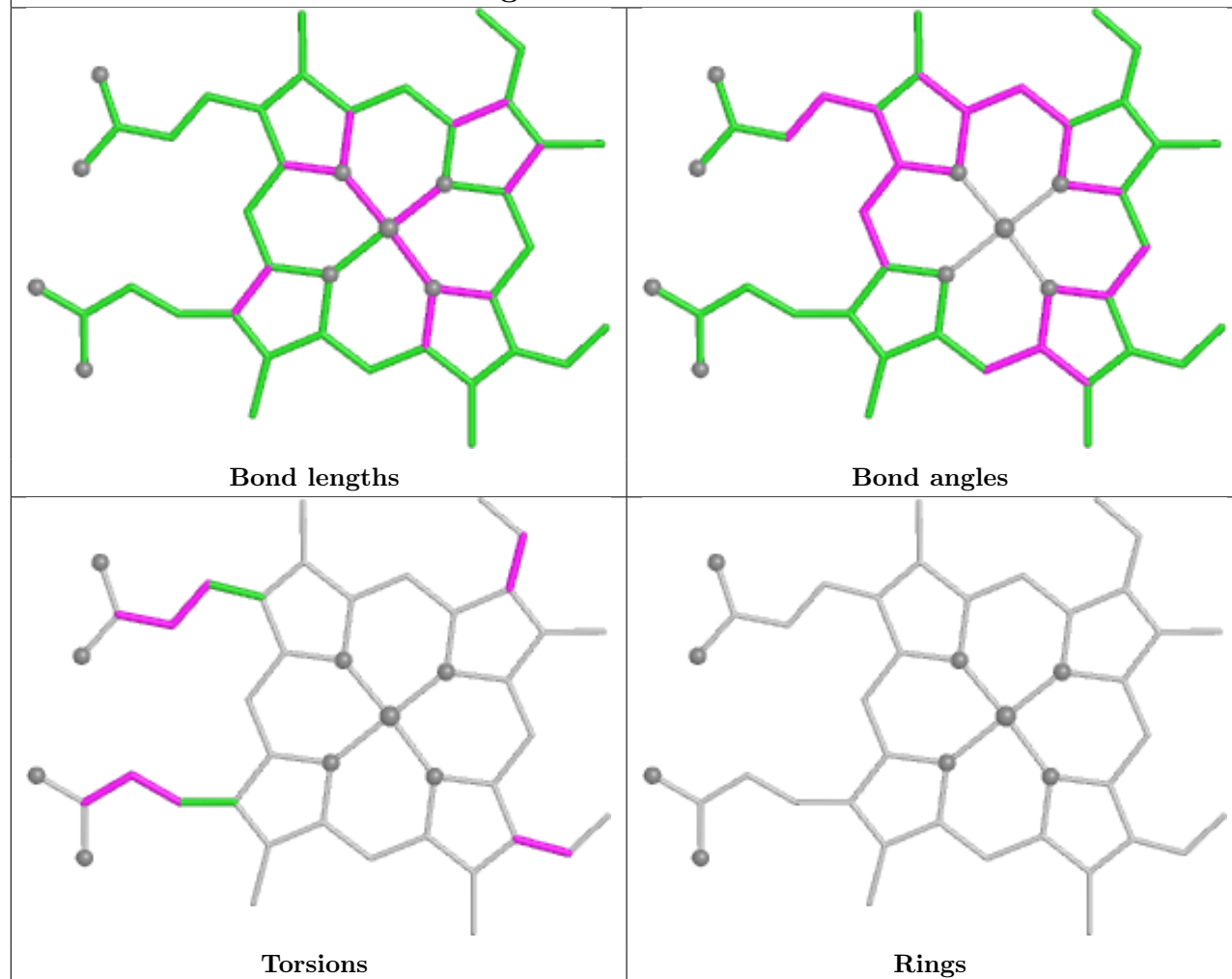




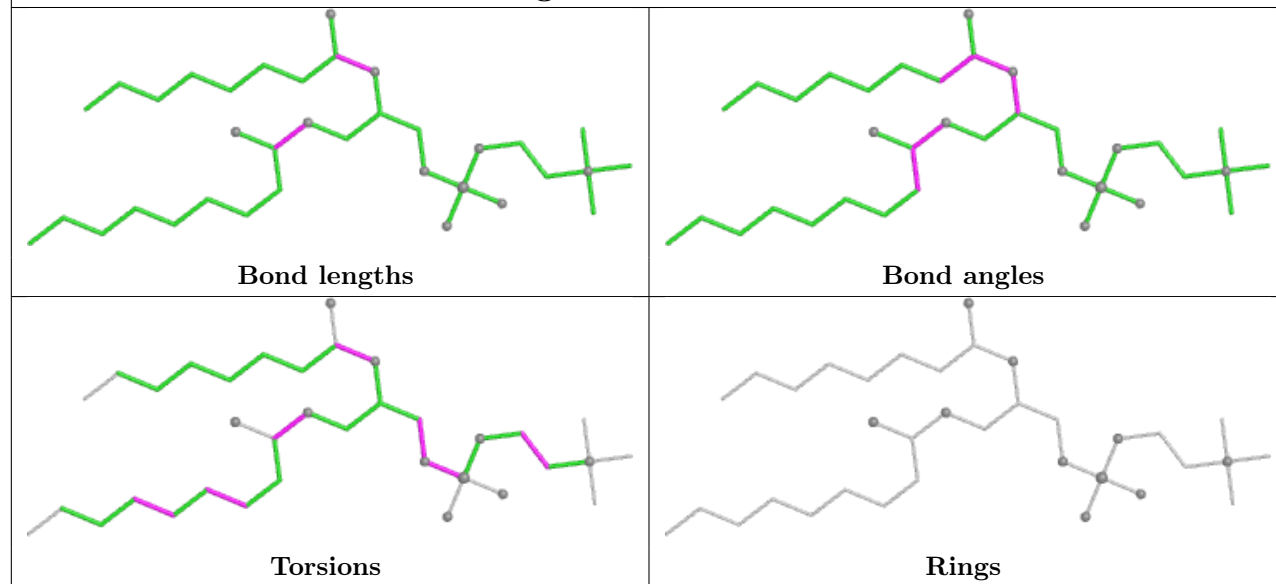
Ligand HEM AC 401

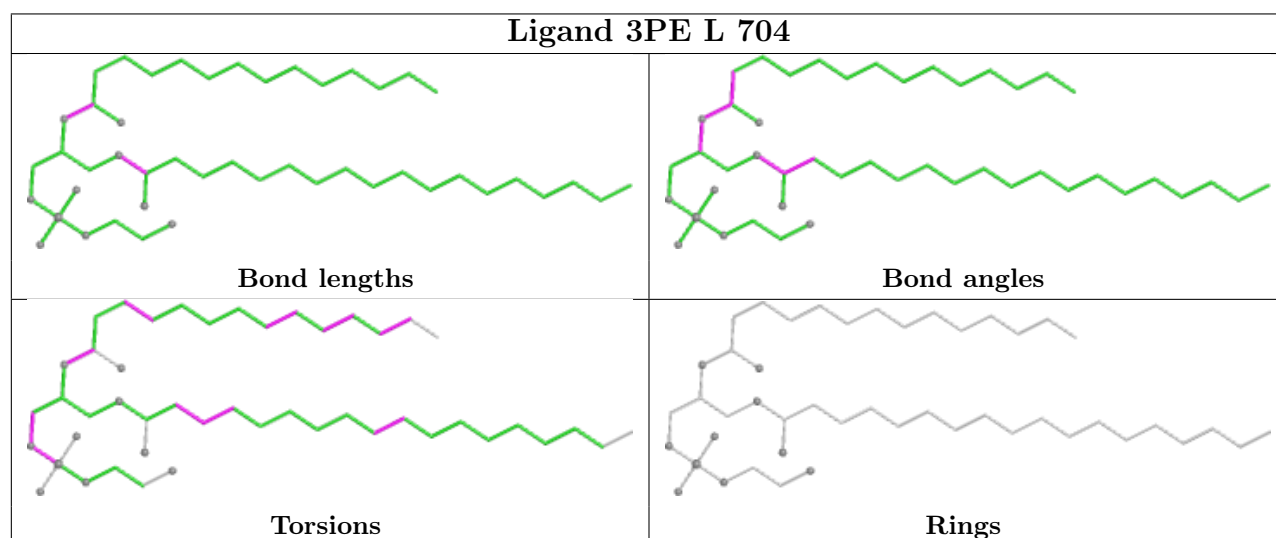
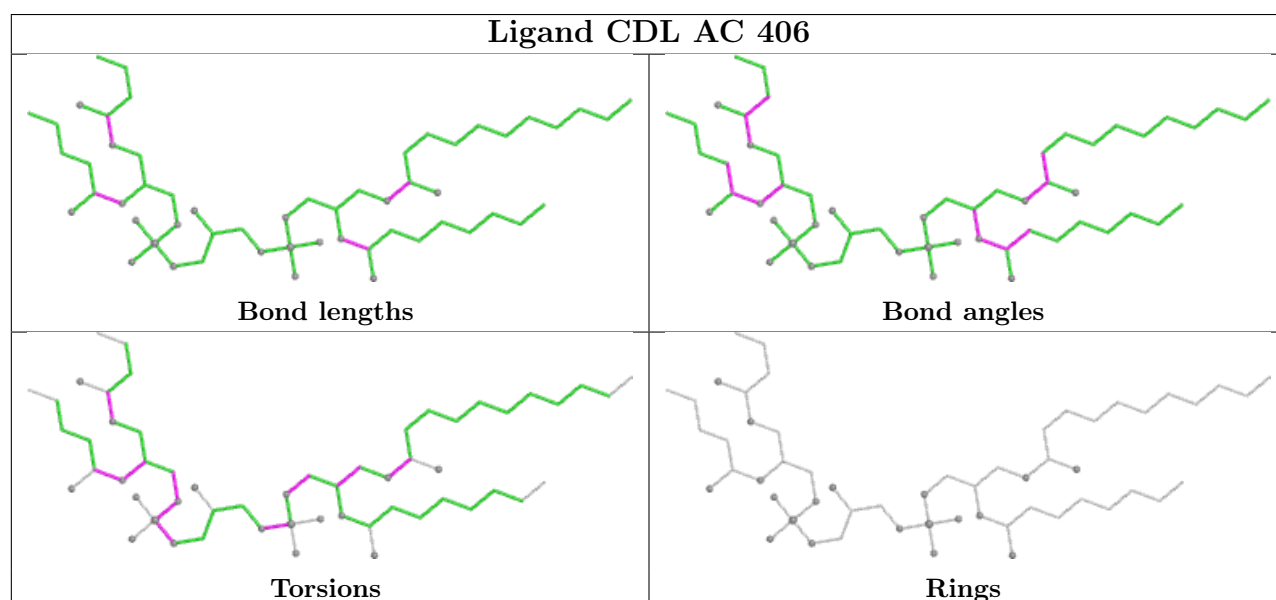
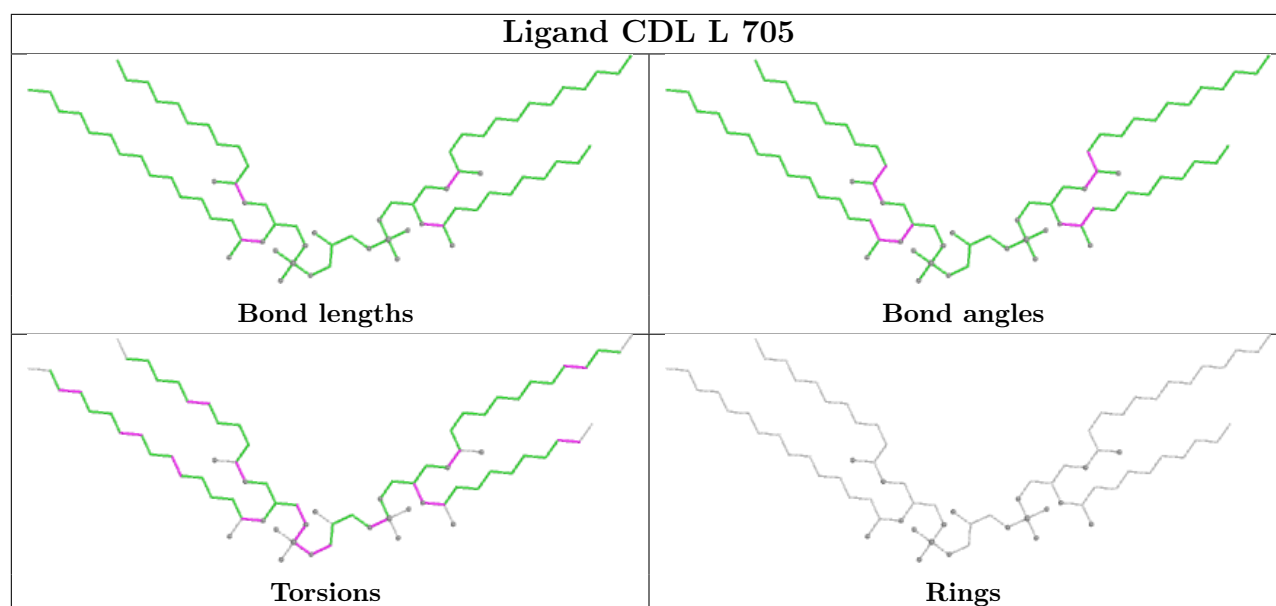


Ligand HEM Ac 403

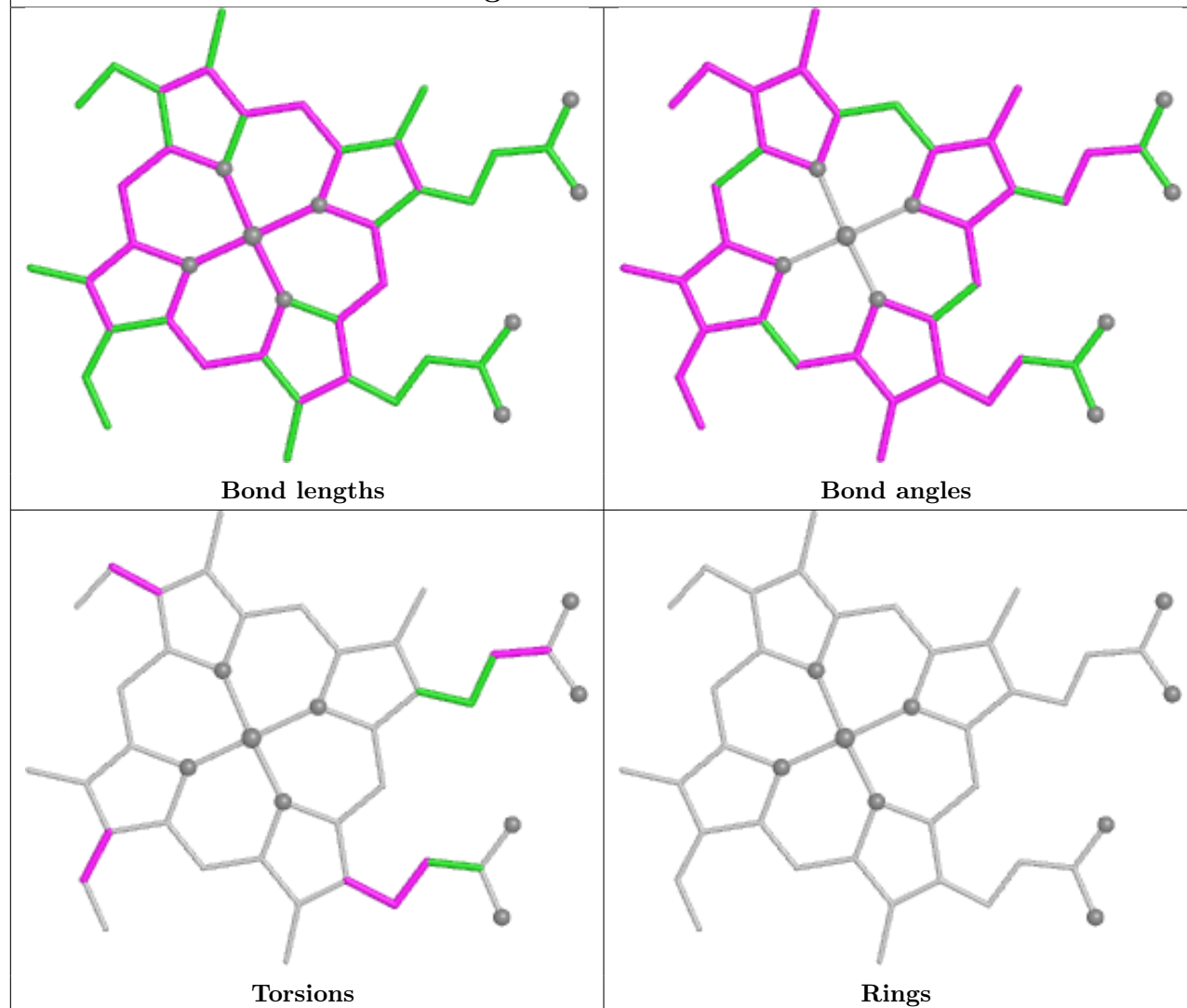


Ligand PC1 B 303

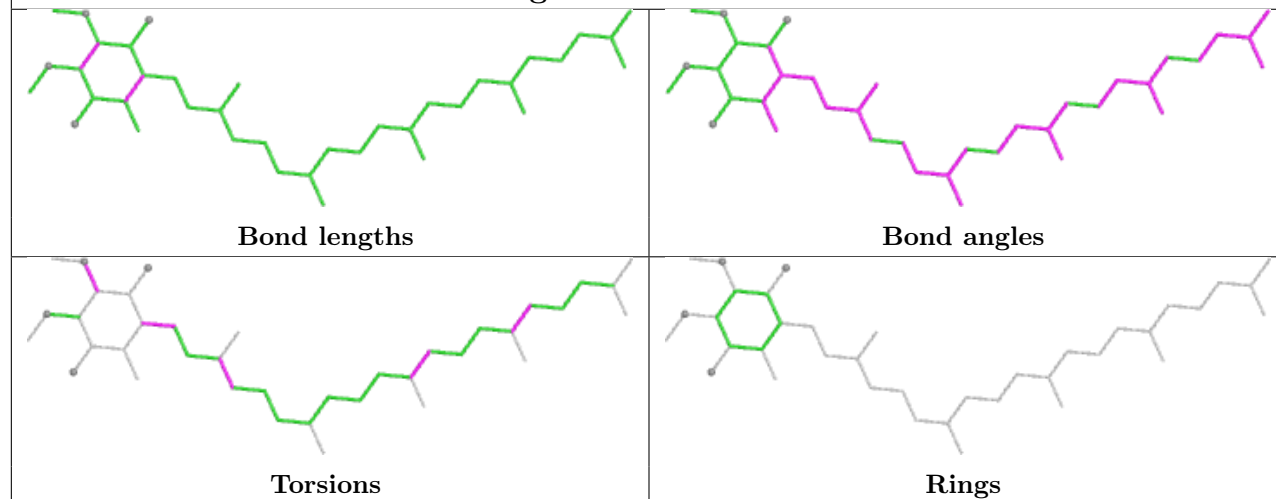




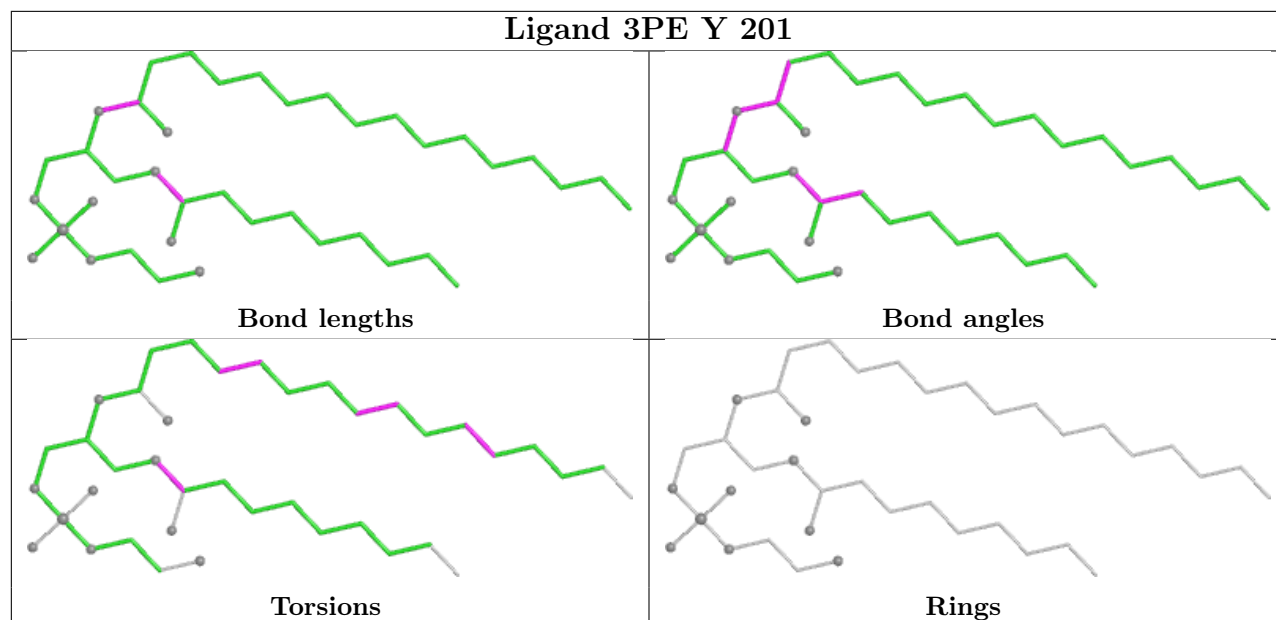
Ligand HEC Ad 401



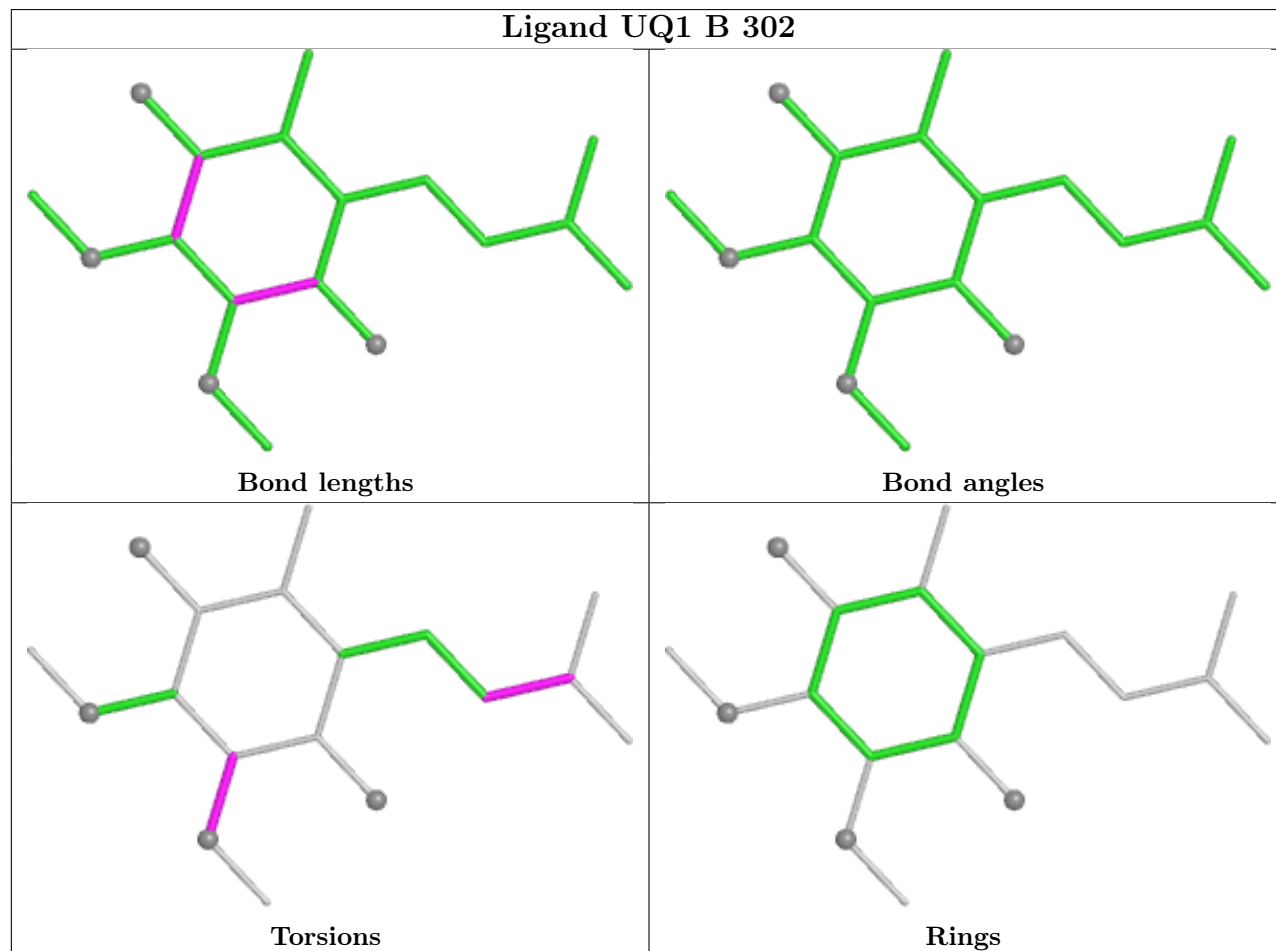
Ligand U10 Ac 405

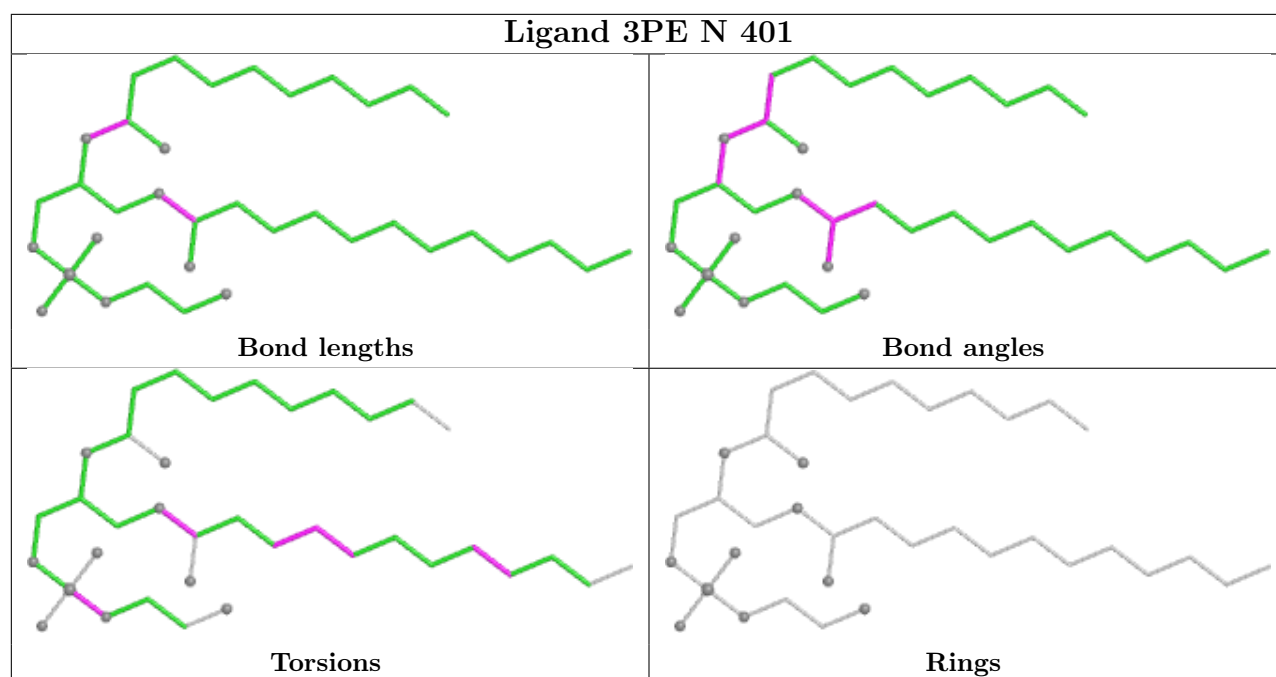


Ligand 3PE Y 201



Ligand UQ1 B 302





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.

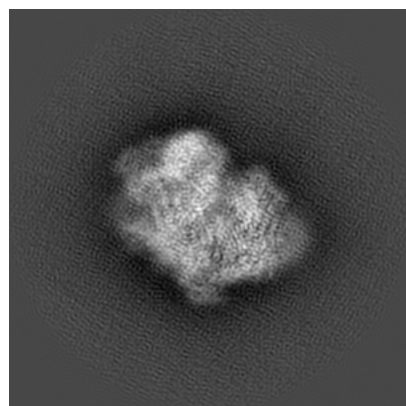
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35331. These allow visual inspection of the internal detail of the map and identification of artifacts.

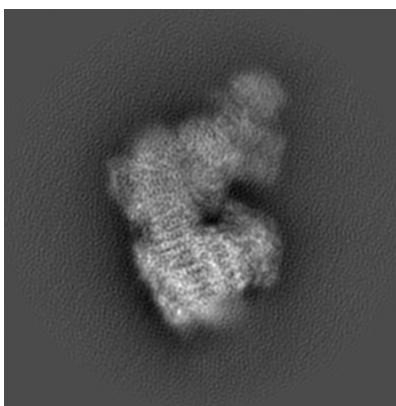
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

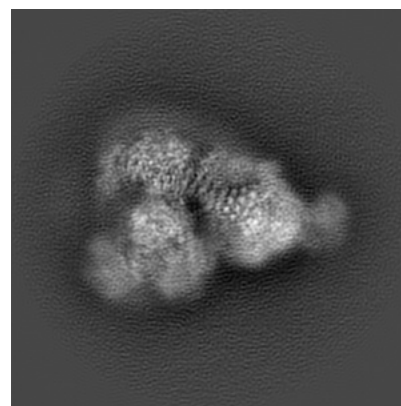
6.1.1 Primary map



X

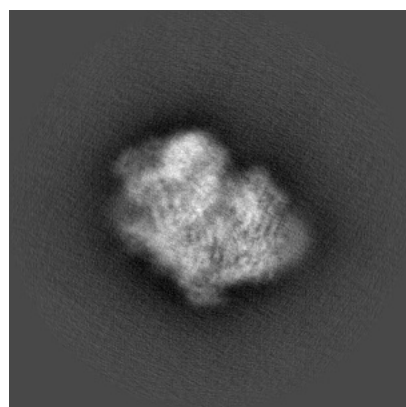


Y

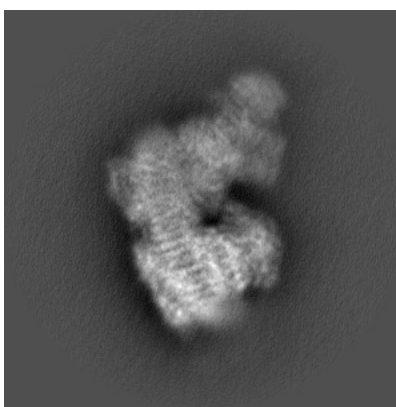


Z

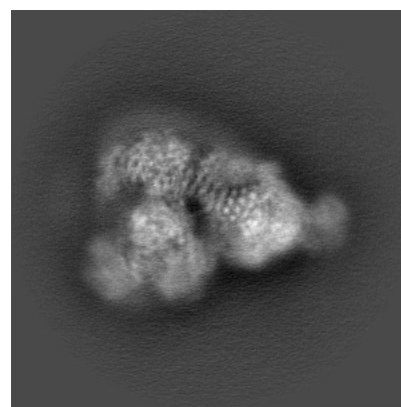
6.1.2 Raw map



X



Y

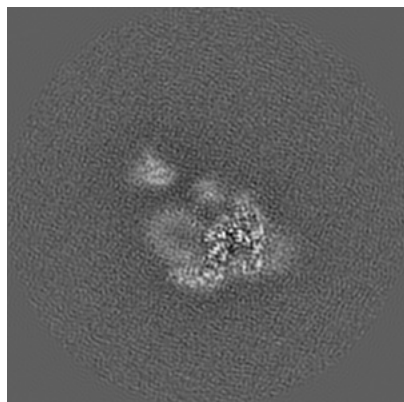


Z

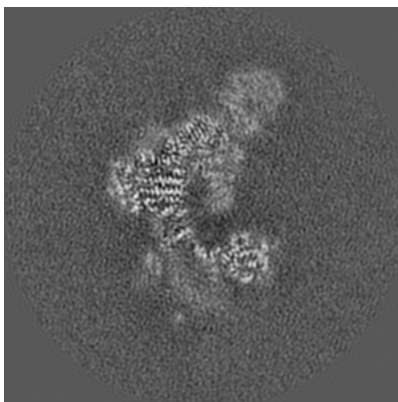
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

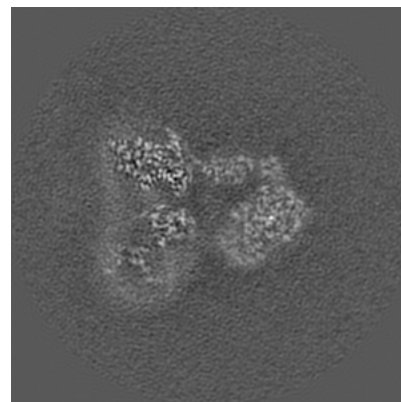
6.2.1 Primary map



X Index: 192

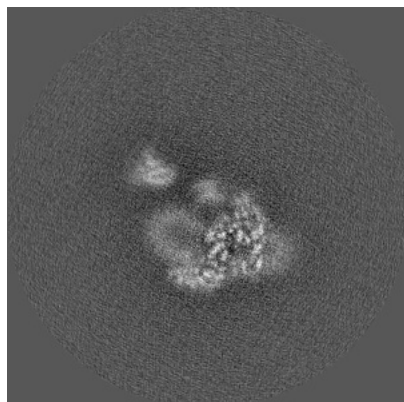


Y Index: 192

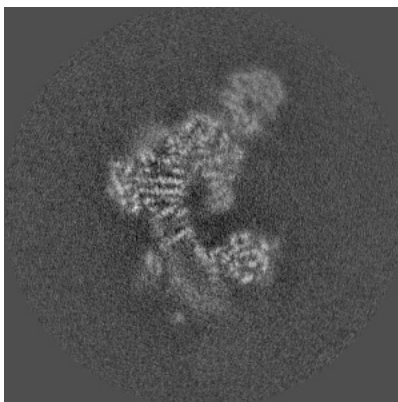


Z Index: 192

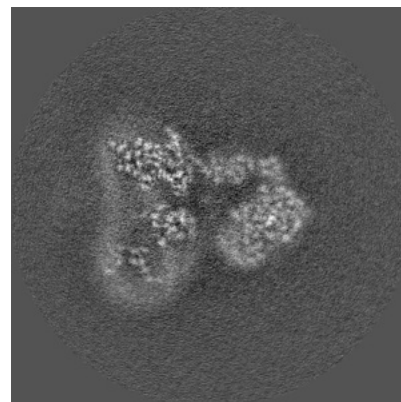
6.2.2 Raw map



X Index: 192



Y Index: 192

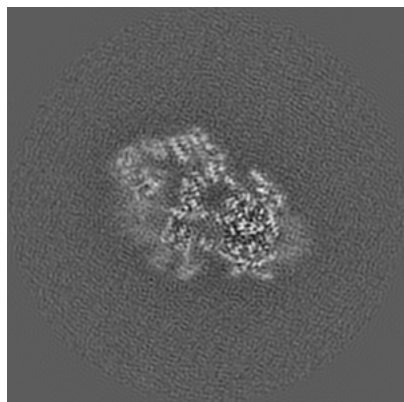


Z Index: 192

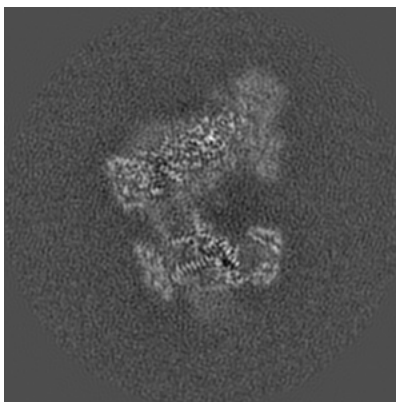
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

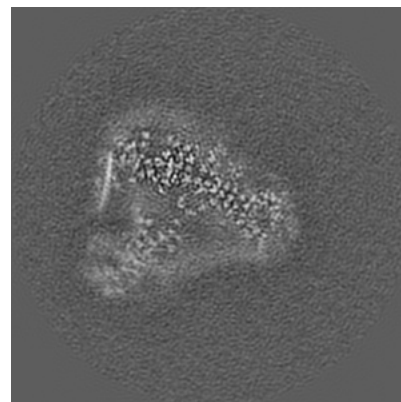
6.3.1 Primary map



X Index: 154

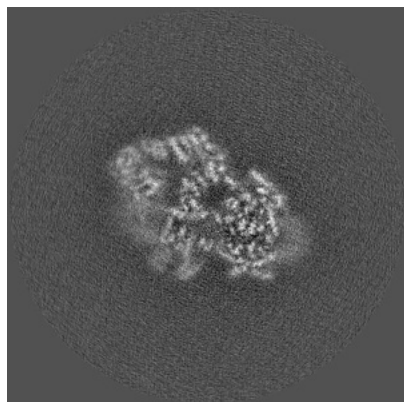


Y Index: 177

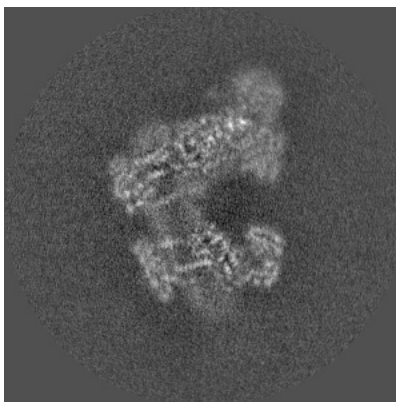


Z Index: 167

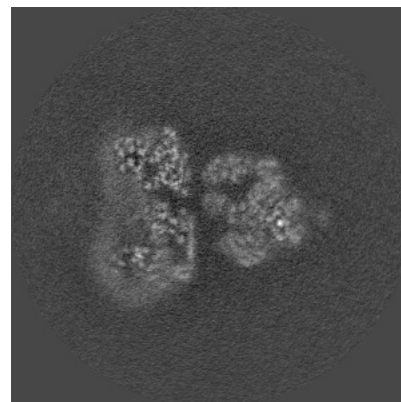
6.3.2 Raw map



X Index: 154



Y Index: 174

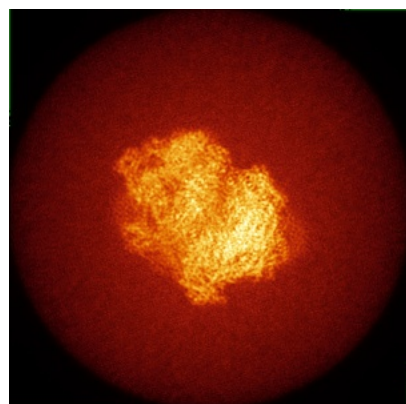


Z Index: 198

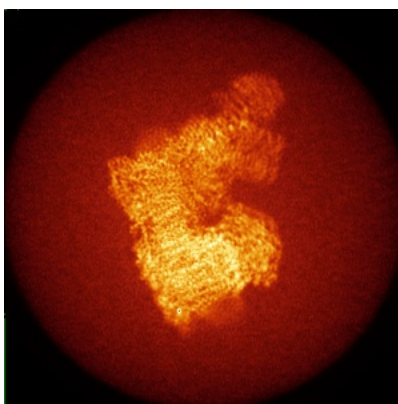
The images above show the largest variance slices of the map in three orthogonal directions.

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

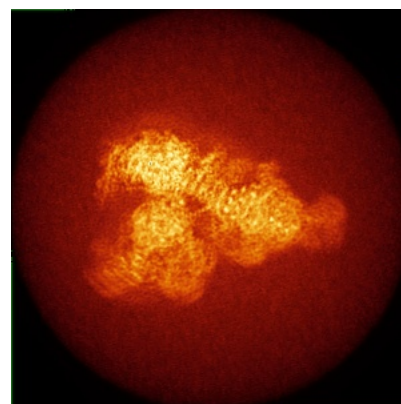
6.4.1 Primary map



X

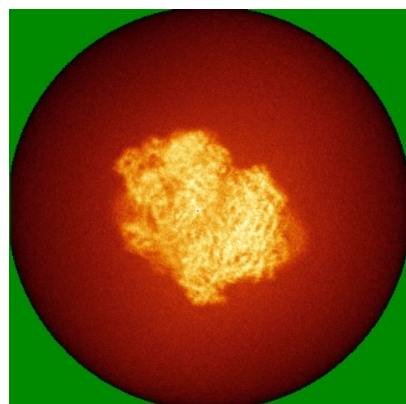


Y

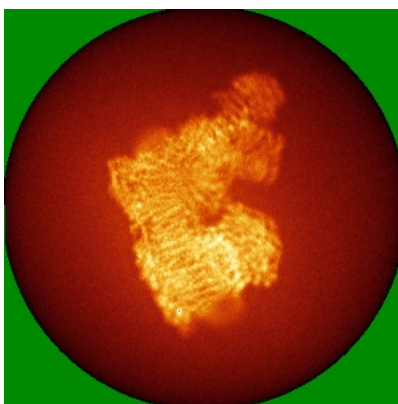


Z

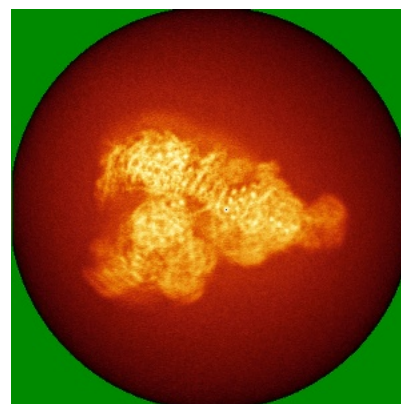
6.4.2 Raw map



X



Y

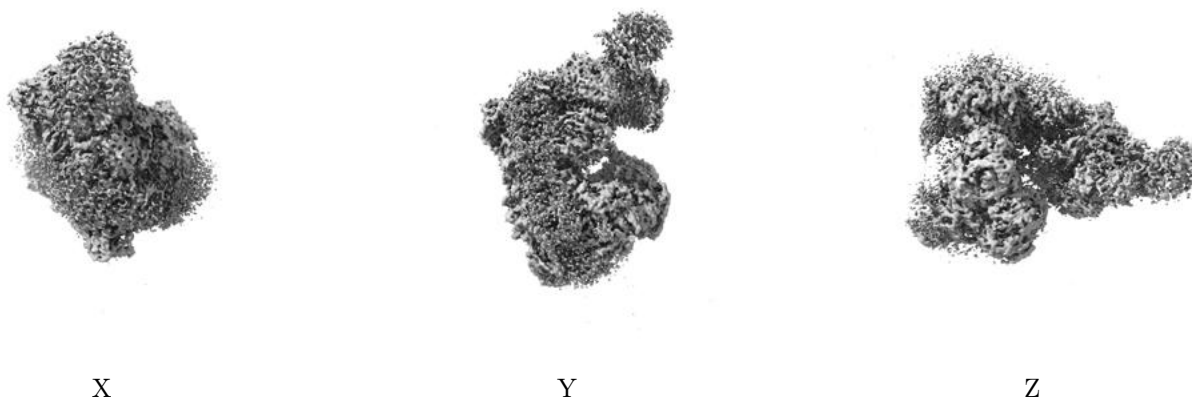


Z

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

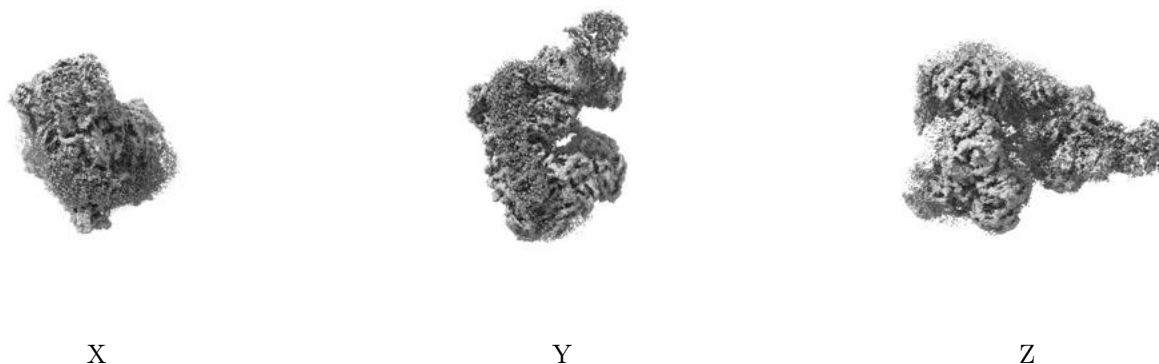
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

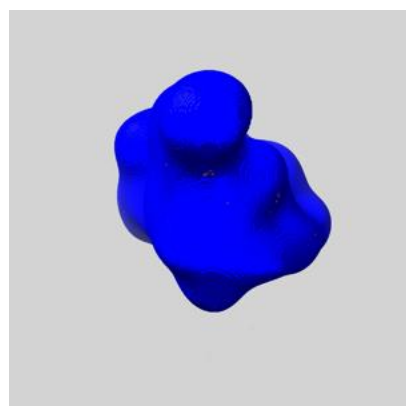
6.6 Mask visualisation [i](#)

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

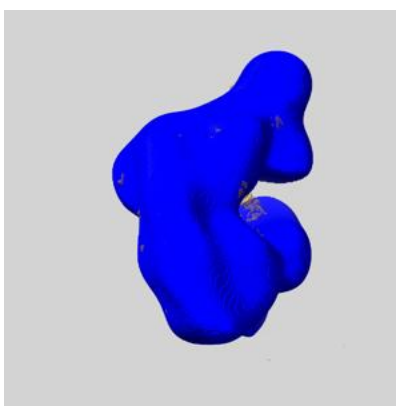
A mask typically either:

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

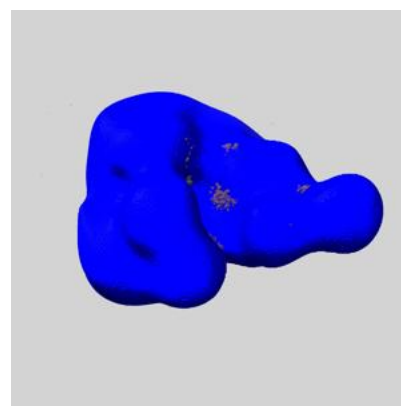
6.6.1 emd_35331_msk_1.map [i](#)



X



Y

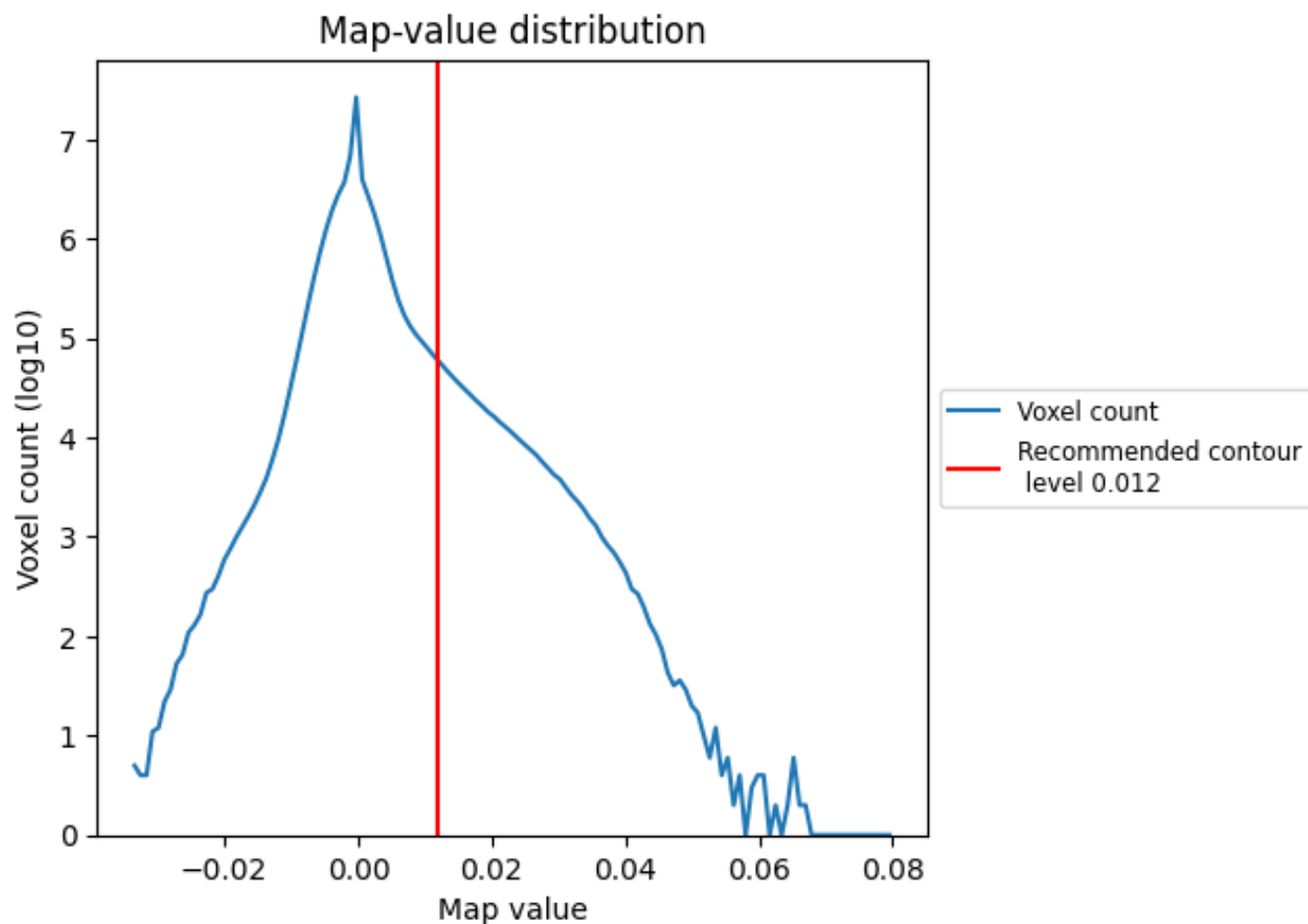


Z

7 Map analysis [i](#)

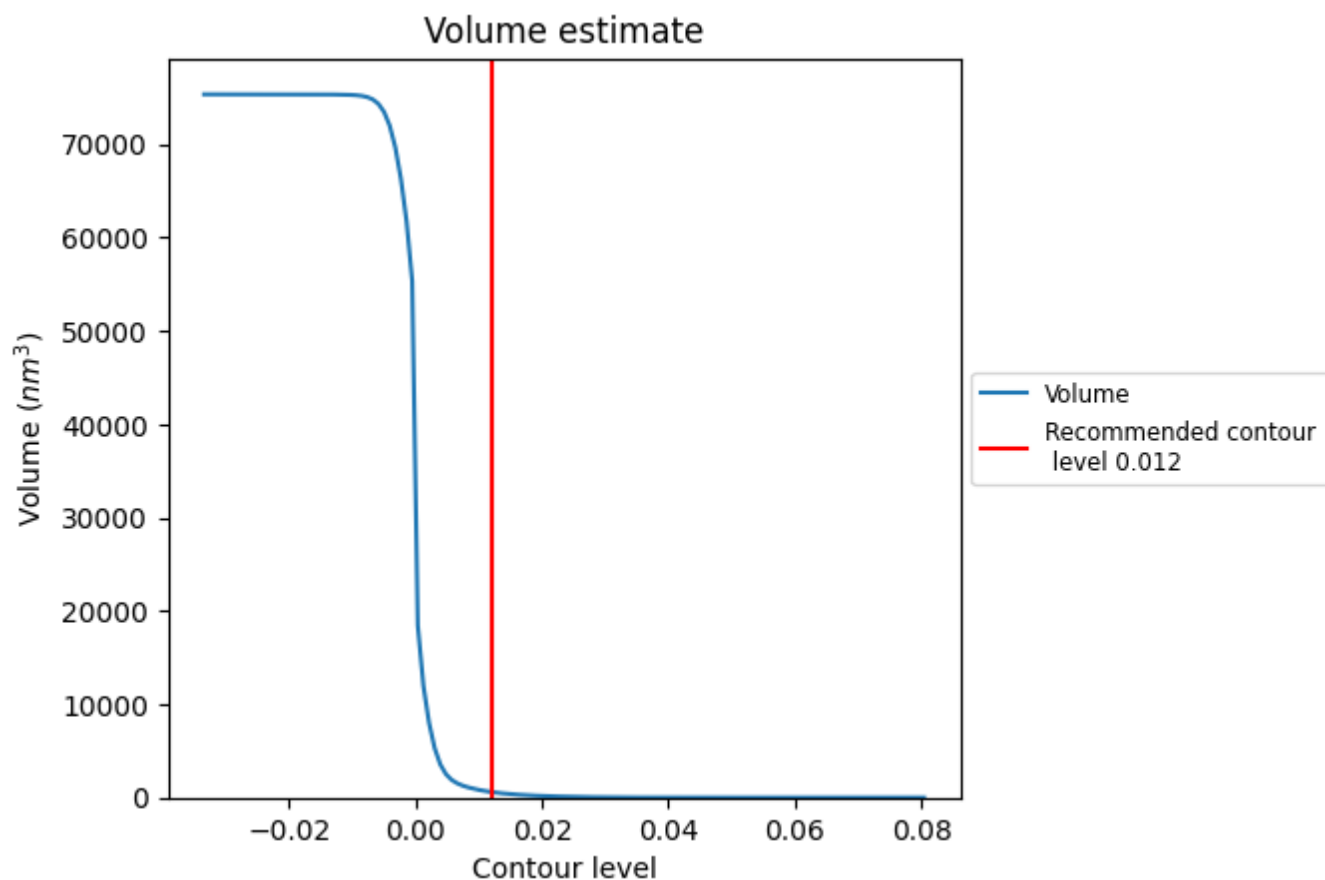
This section contains the results of statistical analysis of the map.

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.

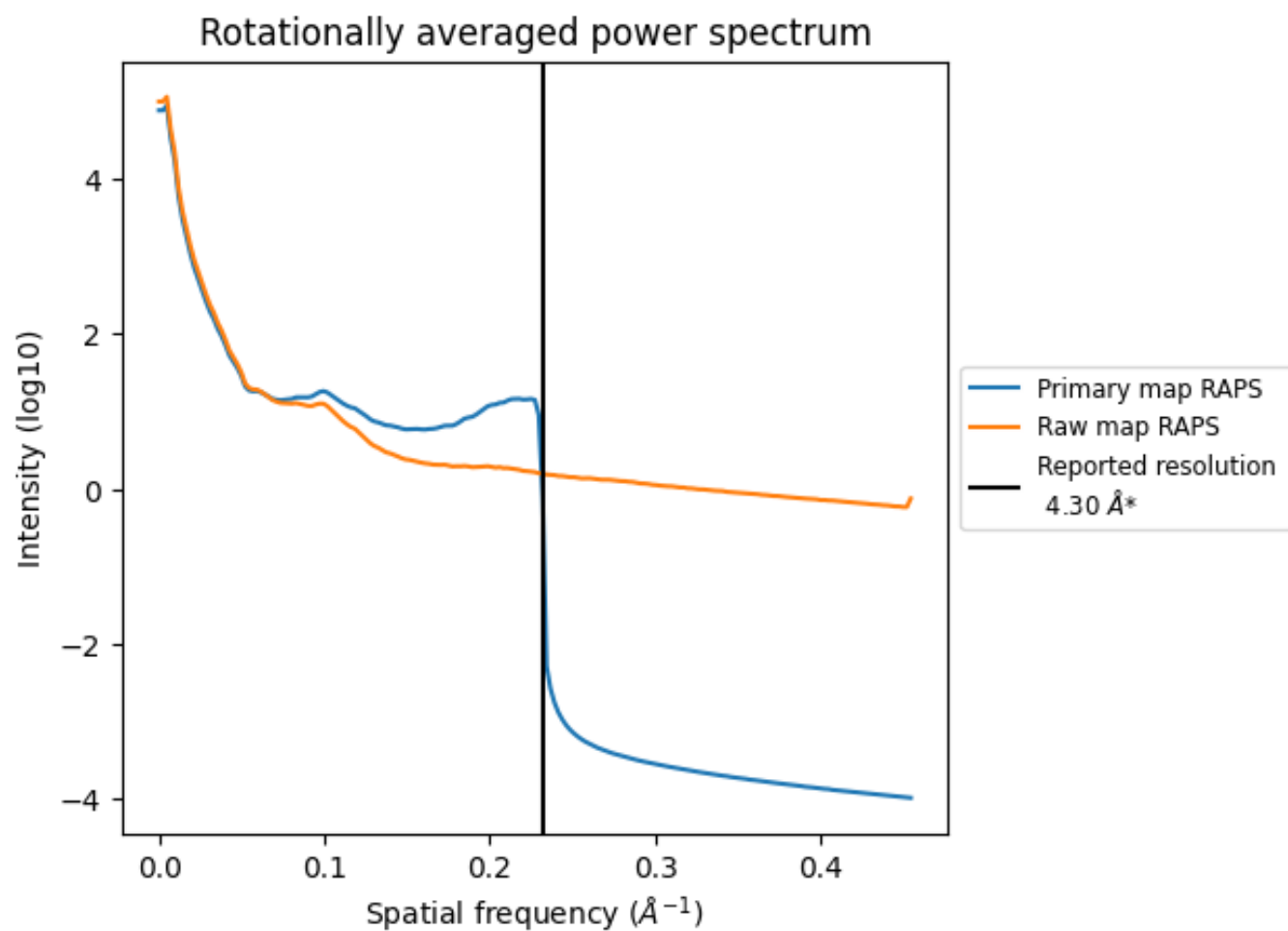
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 593 nm³; this corresponds to an approximate mass of 536 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 ⓘ

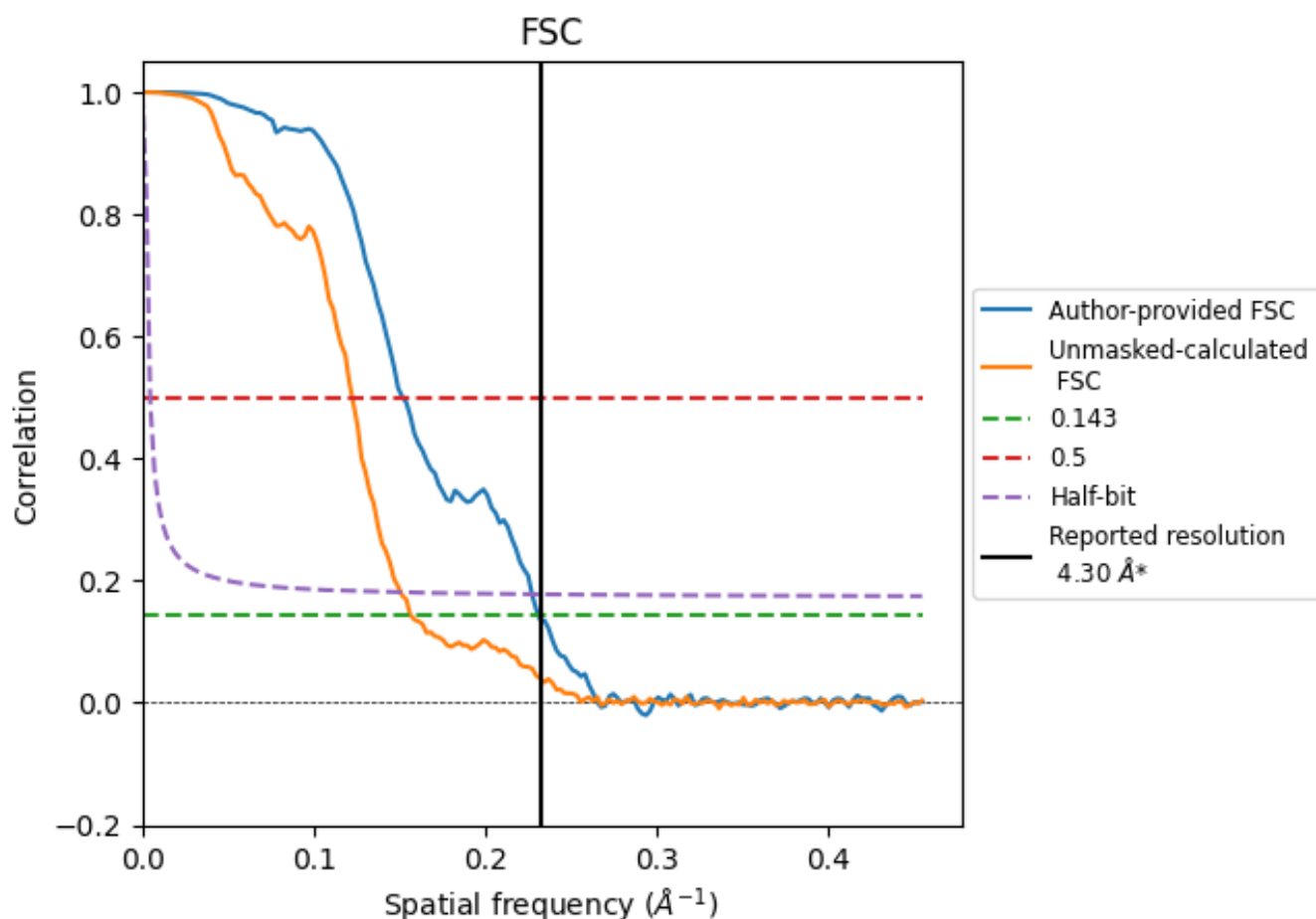


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 $0.233 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

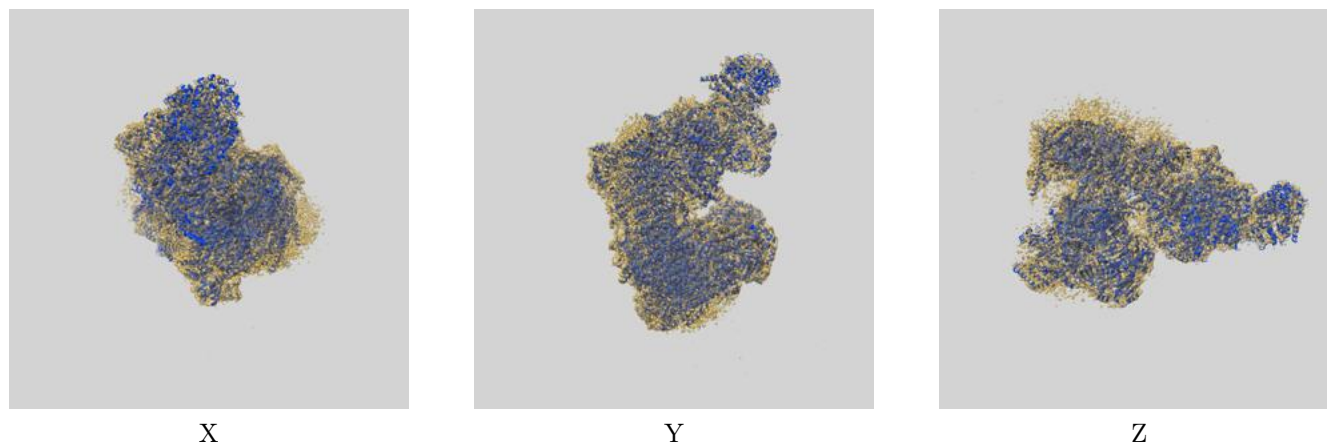
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	6.59	4.40
Unmasked-calculated*	6.39	8.17	6.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

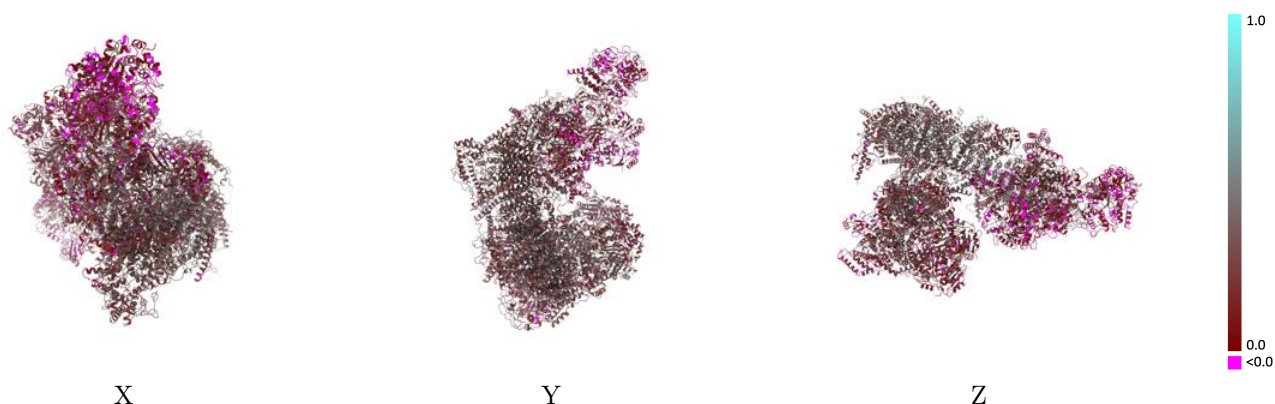
This section contains information regarding the fit between EMDB map EMD-35331 and PDB model 8IB4. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



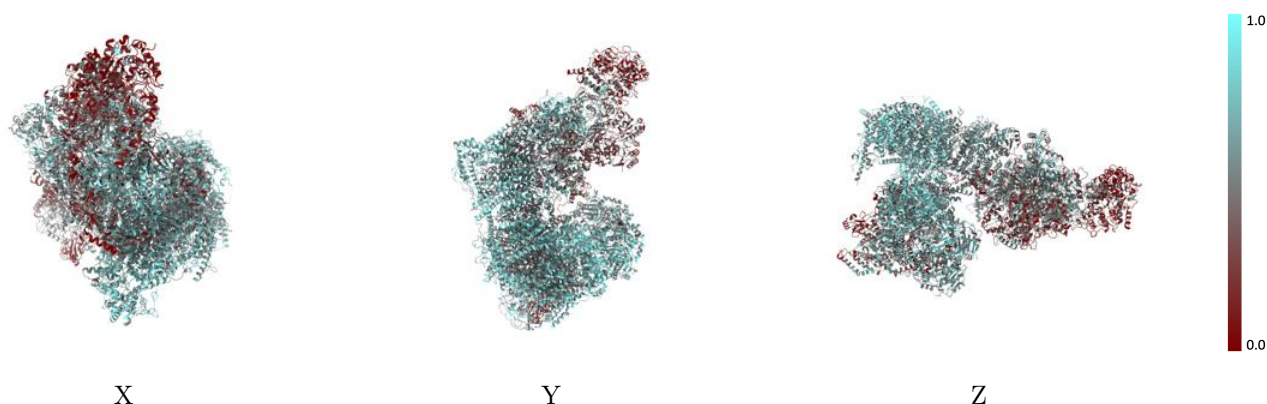
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



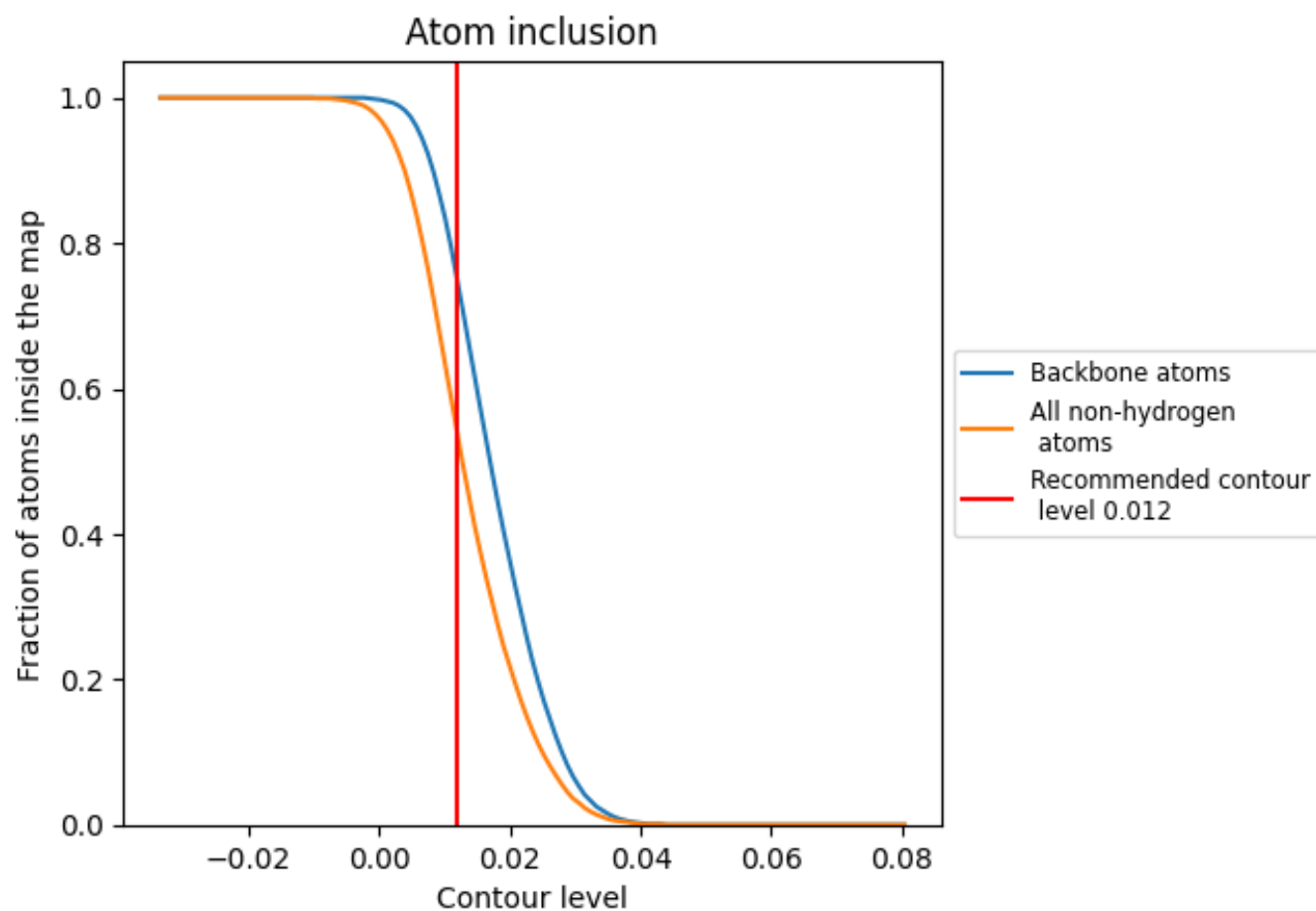
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 54% 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	 0.5370	 0.2580
A	 0.5630	 0.3210
AA	 0.5930	 0.2210
AB	 0.5900	 0.2290
AC	 0.4970	 0.2570
AD	 0.5020	 0.1900
AE	 0.1630	 0.1300
AF	 0.6180	 0.2580
AG	 0.4350	 0.1990
AH	 0.4400	 0.1220
AI	 0.2820	 0.2100
AJ	 0.1830	 0.1680
AK	 0.1720	 0.1620
Aa	 0.6900	 0.3210
Ab	 0.6560	 0.2690
Ac	 0.5620	 0.2860
Ad	 0.5900	 0.2170
Ae	 0.1790	 0.1480
Af	 0.6290	 0.2990
Ag	 0.5350	 0.2910
Ah	 0.5510	 0.1690
Aj	 0.3540	 0.2340
Ak	 0.1580	 0.1740
B	 0.6170	 0.3110
C	 0.5140	 0.2050
D	 0.6100	 0.3010
E	 0.1830	 0.0850
F	 0.2410	 0.1140
G	 0.3630	 0.1480
H	 0.6240	 0.3380
I	 0.6400	 0.2880
J	 0.5270	 0.2930
K	 0.6230	 0.3560
L	 0.6340	 0.3490
M	 0.6740	 0.3770



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Chain	Atom inclusion	Q-score
N	 0.6600	 0.3700
O	 0.5300	 0.2840
P	 0.3430	 0.1390
Q	 0.3060	 0.1770
R	 0.2130	 0.1200
S	 0.2980	 0.1030
T	 0.2020	 0.0800
U	 0.7410	 0.3560
V	 0.4580	 0.1640
W	 0.3570	 0.1420
X	 0.6760	 0.2990
Y	 0.6030	 0.3310
Z	 0.6950	 0.3090
a	 0.6500	 0.3120
b	 0.6520	 0.2950
c	 0.5930	 0.2730
d	 0.7040	 0.3470
e	 0.6680	 0.3140
f	 0.6080	 0.2920
g	 0.6530	 0.3140
h	 0.6790	 0.3300
i	 0.7090	 0.3220
j	 0.6840	 0.3020
k	 0.7380	 0.3450
l	 0.7390	 0.3840
m	 0.7130	 0.3500
n	 0.7500	 0.3470
o	 0.6400	 0.2640
p	 0.7140	 0.3320
q	 0.1600	 0.1780
r	 0.2320	 0.1530
s	 0.1050	 0.0160