



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 04:08 am BST

PDB ID : 9F62 / pdb_00009f62
EMDB ID : EMD-50210
Title : Subtomogram average of the Chlamydomonas reinhardtii mitochondrial respirasome I2 III4 IV6
Authors : Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on : 2024-04-30
Resolution : 5.44 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 : 1.8.4, 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

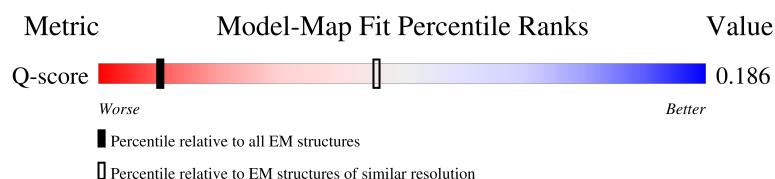
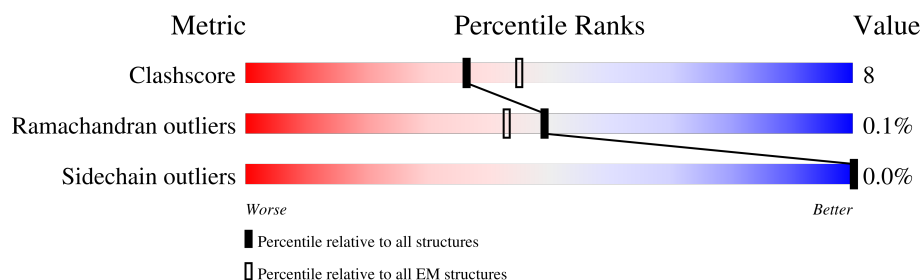
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.44 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	469 (4.94 - 5.94)

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	1A	381	
1	1B	381	
1	6A	381	
1	6B	381	

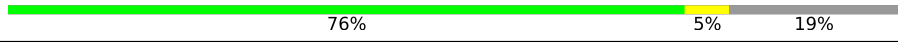
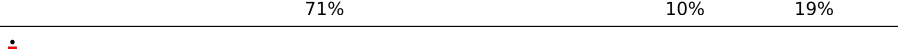
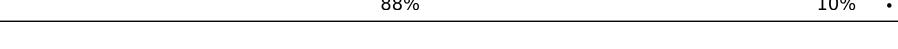
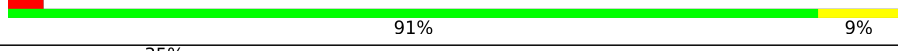
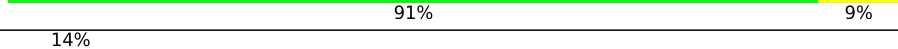
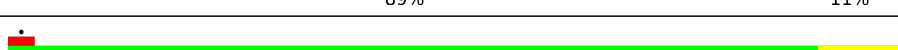
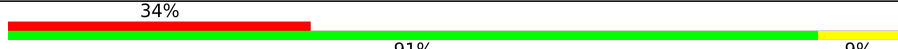
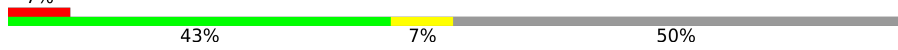
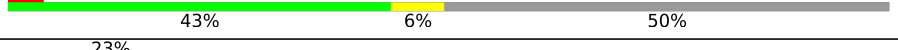
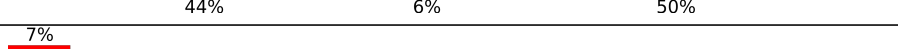
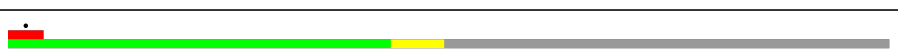
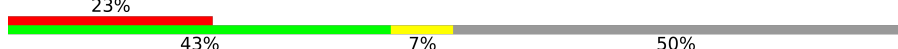
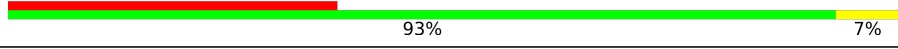
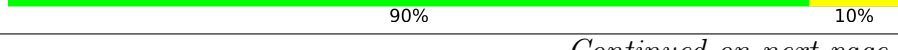
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Mol	Chain	Length	Quality of chain
2	1C	262	
2	1D	262	
2	6C	262	
2	6D	262	
3	1E	314	
3	1F	314	
3	6E	314	
3	6F	314	
4	1G	60	
4	1H	60	
4	6G	60	
4	6H	60	
5	1I	69	
5	1J	69	
5	6I	69	
5	6J	69	
6	1K	73	
6	1L	73	
6	6K	73	
6	6L	73	
7	1M	495	
7	1N	495	
7	6M	495	
7	6N	495	
8	1O	59	

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Mol	Chain	Length	Quality of chain
8	1P	59	
8	6O	59	
8	6P	59	
9	1Q	485	
9	1S	485	
9	6Q	485	
9	6S	485	
10	1R	123	
10	1T	123	
10	6R	123	
10	6T	123	
11	2A	505	
11	3A	505	
11	4A	505	
11	7A	505	
11	8A	505	
11	9A	505	
12	2B	284	
12	3B	284	
12	4B	284	
12	7B	284	
12	8B	284	
12	9B	284	
13	2C	153	
13	3C	153	

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Mol	Chain	Length	Quality of chain
13	4C	153	88% 90%10%
13	7C	153	37% 90%10%
13	8C	153	19% 90%10%
13	9C	153	89% 90%10%
14	2D	382	15% 64%6%30%
14	3D	382	8% 64%5%30%
14	4D	382	46% 64%6%30%
14	7D	382	15% 64%6%30%
14	8D	382	8% 64%5%30%
14	9D	382	47% 64%6%30%
15	2E	175	7% 49%..49%
15	3E	175	7% 49%.49%
15	4E	175	45% 49%.49%
15	7E	175	7% 49%..49%
15	8E	175	5% 49%.49%
15	9E	175	46% 48%.49%
16	2F	96	17% 81%8%10%
16	3F	96	18% 80%9%10%
16	4F	96	51% 83%6%10%
16	7F	96	18% 81%8%10%
16	8F	96	18% 80%9%10%
16	9F	96	50% 85%.10%
17	2G	125	27% 62%11%27%
17	3G	125	26% 65%8%27%
17	4G	125	58% 65%8%27%

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Mol	Chain	Length	Quality of chain
17	7G	125	
17	8G	125	
17	9G	125	
18	2H	148	
18	3H	148	
18	4H	148	
18	7H	148	
18	8H	148	
18	9H	148	
19	2I	101	
19	3I	101	
19	4I	101	
19	7I	101	
19	8I	101	
19	9I	101	
20	2J	105	
20	3J	105	
20	4J	105	
20	7J	105	
20	8J	105	
20	9J	105	
21	2K	58	
21	3K	58	
21	4K	58	
21	7K	58	

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Mol	Chain	Length	Quality of chain
21	8K	58	
21	9K	58	
22	2L	87	
22	3L	87	
22	4L	87	
22	7L	87	
22	8L	87	
22	9L	87	
23	5A	282	
23	A	282	
24	5B	484	
24	B	484	
25	5C	733	
25	C	733	
26	5D	282	
26	D	282	
27	5E	467	
27	E	467	
28	5F	164	
28	F	164	
29	5G	231	
29	G	231	
30	5H	118	
30	H	118	
31	5I	165	

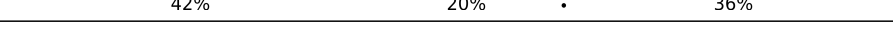
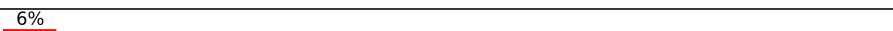
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Mol	Chain	Length	Quality of chain
31	I	165	
32	5J	128	
32	5r	128	
32	J	128	
32	r	128	
33	5K	138	
33	K	138	
34	5L	187	
34	L	187	
35	5M	154	
35	M	154	
36	5N	156	
36	N	156	
37	5O	101	
37	O	101	
38	5P	397	
38	P	397	
39	5Q	292	
39	Q	292	
40	5R	387	
40	R	387	
41	5S	279	
41	S	279	
42	5T	443	
42	T	443	

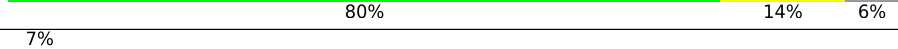
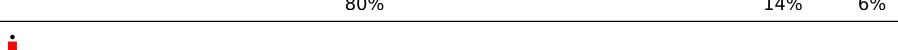
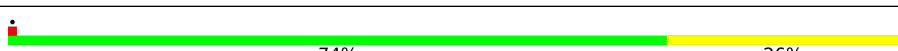
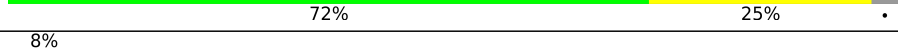
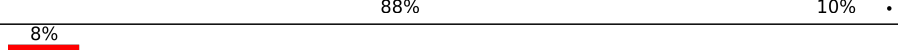
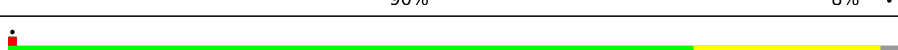
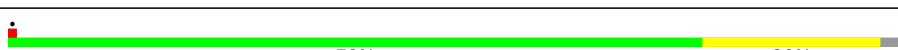
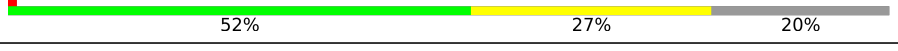
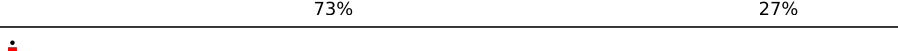
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Mol	Chain	Length	Quality of chain
43	5U	227	
43	U	227	
44	5V	546	
44	V	546	
45	5W	162	
45	W	162	
46	5X	149	
46	X	149	
47	5Y	64	
47	Y	64	
48	5Z	124	
48	Z	124	
49	5a	129	
49	a	129	
50	5b	172	
50	b	172	
51	5c	67	
51	c	67	
52	5d	86	
52	d	86	
53	5e	219	
53	e	219	
54	5f	65	
54	f	65	
55	5g	55	

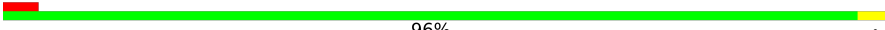
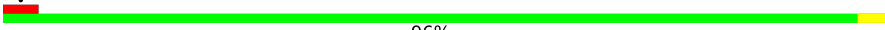
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Mol	Chain	Length	Quality of chain
55	g	55	
56	5h	142	
56	h	142	
57	5i	81	
57	i	81	
58	5j	86	
58	j	86	
59	5k	117	
59	k	117	
60	5l	121	
60	l	121	
61	5m	142	
61	m	142	
62	5n	106	
62	n	106	
63	5o	155	
63	o	155	
64	5p	130	
64	p	130	
65	5q	197	
65	q	197	
66	5s	312	
66	s	312	
67	5t	279	
67	t	279	

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Mol	Chain	Length	Quality of chain
68	5u	229	
68	u	229	
69	5v	45	
69	v	45	
70	5w	109	
70	w	109	
71	5x	157	
71	x	157	
72	5y	118	
72	y	118	

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
74	HEC	1E	401	X	-	-	-
74	HEC	1F	501	X	-	-	-
74	HEC	6E	401	X	-	-	-
74	HEC	6F	501	X	-	-	-
79	CUA	2C	301	-	-	X	-
79	CUA	3C	301	-	-	X	-
79	CUA	4C	301	-	-	X	-
79	CUA	7C	301	-	-	X	-
79	CUA	8C	301	-	-	X	-
79	CUA	9C	301	-	-	X	-
80	FES	5A	301	-	-	X	-
80	FES	A	301	-	-	X	-

2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 292492 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	1B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	6A	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		
1	6B	376	Total	C	N	O	S	0	0
			2958	1984	466	491	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	1D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	6C	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		
2	6D	207	Total	C	N	O	S	0	0
			1602	1017	279	299	7		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	1F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	6E	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		
3	6F	243	Total	C	N	O	S	0	0
			1898	1204	326	356	12		

- Molecule 4 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	1H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	6G	59	Total	C	N	O	S	0	0
			486	316	79	88	3		
4	6H	59	Total	C	N	O	S	0	0
			486	316	79	88	3		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	1J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	6I	68	Total	C	N	O	S	0	0
			550	347	92	105	6		
5	6J	68	Total	C	N	O	S	0	0
			550	347	92	105	6		

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	1L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	6K	70	Total	C	N	O	S	0	0
			594	386	104	103	1		
6	6L	70	Total	C	N	O	S	0	0
			594	386	104	103	1		

- Molecule 7 is a protein called MPP-Beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	1N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		
7	6M	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	6N	464	Total	C	N	O	S	0	0
			3646	2290	641	696	19		

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	1P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	6O	48	Total	C	N	O	S	0	0
			371	249	61	60	1		
8	6P	48	Total	C	N	O	S	0	0
			371	249	61	60	1		

- Molecule 9 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	1S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	6Q	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		
9	6S	441	Total	C	N	O	S	0	0
			3204	2018	562	619	5		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	1T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	6R	122	Total	C	N	O	S	0	0
			980	617	178	183	2		
10	6T	122	Total	C	N	O	S	0	0
			980	617	178	183	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	3A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	4A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	7A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	8A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		
11	9A	504	Total	C	N	O	S	0	0
			3888	2600	618	643	27		

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	3B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	4B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	7B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	8B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		
12	9B	141	Total	C	N	O	S	0	0
			1169	774	188	201	6		

- Molecule 13 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	3C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	4C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	7C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	8C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		
13	9C	153	Total	C	N	O	S	0	0
			1212	776	206	223	7		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	3D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	4D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	7D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	8D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		
14	9D	266	Total	C	N	O	S	0	0
			2079	1373	334	351	21		

- Molecule 15 is a protein called Cox5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	3E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	4E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	7E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	8E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		
15	9E	90	Total	C	N	O	S	0	0
			737	478	114	144	1		

- Molecule 16 is a protein called Cox5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	3F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	4F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	7F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		
16	8F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	9F	86	Total	C	N	O	S	0	0
			706	456	122	126	2		

- Molecule 17 is a protein called Cox6a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	3G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	4G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	7G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	8G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		
17	9G	91	Total	C	N	O	S	0	0
			733	484	120	124	5		

- Molecule 18 is a protein called Cox6b.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	3H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	4H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	7H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	8H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		
18	9H	114	Total	C	N	O	S	0	0
			954	606	159	185	4		

- Molecule 19 is a protein called Cox7c.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	2I	72	Total	C	N	O	0	0
			594	393	98	103		
19	3I	72	Total	C	N	O	0	0
			594	393	98	103		

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Mol	Chain	Residues	Atoms				AltConf	Trace
19	4I	72	Total	C	N	O	0	0
			594	393	98	103		
19	7I	72	Total	C	N	O	0	0
			594	393	98	103		
19	8I	72	Total	C	N	O	0	0
			594	393	98	103		
19	9I	72	Total	C	N	O	0	0
			594	393	98	103		

- Molecule 20 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	3J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	4J	101	Total	C	N	O	S	0	0
			790	506	140	141	3		
20	7J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	8J	104	Total	C	N	O	S	0	0
			816	522	144	147	3		
20	9J	101	Total	C	N	O	S	0	0
			790	506	140	141	3		

- Molecule 21 is a protein called Cox7a.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	2K	47	Total	C	N	O	0	0
			382	249	63	70		
21	3K	47	Total	C	N	O	0	0
			382	249	63	70		
21	4K	47	Total	C	N	O	0	0
			382	249	63	70		
21	7K	47	Total	C	N	O	0	0
			382	249	63	70		
21	8K	47	Total	C	N	O	0	0
			382	249	63	70		
21	9K	47	Total	C	N	O	0	0
			382	249	63	70		

- Molecule 22 is a protein called CoxIn.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2L	76	Total	C	N	O	S	0	0
			605	390	100	111	4		
22	3L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		
22	4L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		
22	7L	76	Total	C	N	O	S	0	0
			605	390	100	111	4		
22	8L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		
22	9L	78	Total	C	N	O	S	0	0
			627	405	104	114	4		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase 24 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		
23	A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		
24	B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase 78 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		
25	C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		
26	D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 49 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5E	386	Total	C	N	O	S	0	0
			3107	1986	540	558	23		
27	E	386	Total	C	N	O	S	0	0
			3107	1986	540	558	23		

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		
28	F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		

- Molecule 29 is a protein called NADH:ubiquinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		
29	G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		

- Molecule 30 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		
30	H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		

- Molecule 31 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
32	5r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		
32	J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
32	r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		
33	K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		
34	L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase 13 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		
35	M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		
36	N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		
37	O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		

- Molecule 38 is a protein called Putative NADH:ubiquinone oxidoreductase 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		
38	P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		
39	Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		
40	R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		
42	T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		

- Molecule 43 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		
43	U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		
44	V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		
45	W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		

- Molecule 46 is a protein called ASH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	5X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		
46	X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		

- Molecule 47 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		
47	Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		

- Molecule 48 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		
48	Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		

- Molecule 49 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		
49	a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		

- Molecule 50 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	5b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		
50	b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		

- Molecule 51 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	5c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		
51	c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		

- Molecule 52 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		
52	d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		

- Molecule 53 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		
53	e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		

- Molecule 54 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		
54	f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		

- Molecule 55 is a protein called Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		
55	g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		

- Molecule 56 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		
56	h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		

- Molecule 57 is a protein called NADH:ubiquinone oxidoreductase 15 kDa subunit-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		
57	i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	5j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		
58	j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	5k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		
59	k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		

- Molecule 60 is a protein called NADH:ubiquinone oxidoreductase 20,9 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	5l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		
60	l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	5m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		
61	m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		

- Molecule 62 is a protein called Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	5n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		
62	n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		

- Molecule 63 is a protein called Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		
63	o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		

- Molecule 64 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	5p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		
64	p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		

- Molecule 65 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	5q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		
65	q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		

- Molecule 66 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	5s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		
66	s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		

- Molecule 67 is a protein called CAG2 - CA-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	5t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		
67	t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		

- Molecule 68 is a protein called CAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	5u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		
68	u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		

- Molecule 69 is a protein called P10.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	5v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		
69	v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		

- Molecule 70 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	5w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		
70	w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		

- Molecule 71 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	5x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		
71	x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		

- Molecule 72 is a protein called NUOP7.

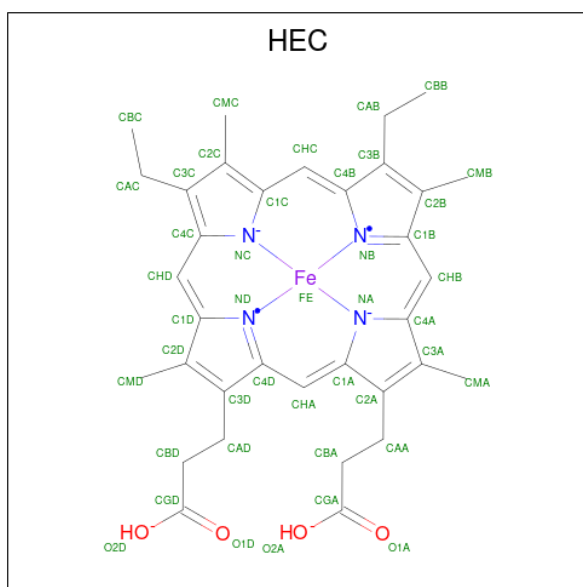
Mol	Chain	Residues	Atoms					AltConf	Trace
72	5y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
72	y	114	Total 932	C 615	N 154	O 161	S 2	0	0

- # HEM

- Molecule 74 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).

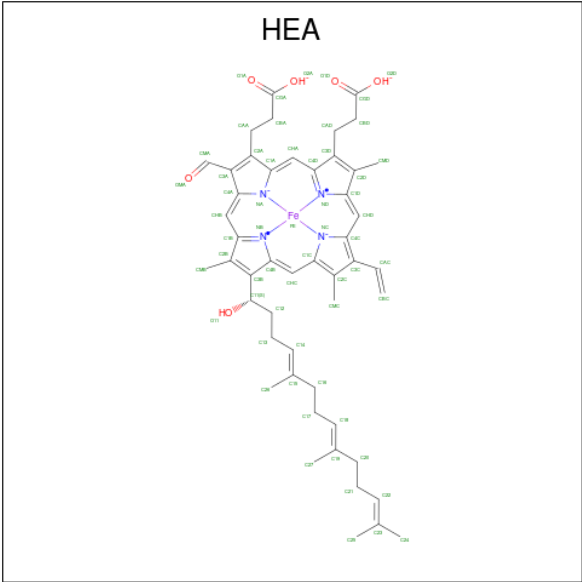


Mol	Chain	Residues	Atoms					AltConf
74	1E	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	1F	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	6E	1	Total 43	C 34	Fe 1	N 4	O 4	0
74	6F	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 75 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
75	1M	1	Total Zn 1 1	0
75	1N	1	Total Zn 1 1	0
75	5s	1	Total Zn 1 1	0
75	6M	1	Total Zn 1 1	0
75	6N	1	Total Zn 1 1	0
75	s	1	Total Zn 1 1	0

- Molecule 76 is HEME-A (CCD ID: HEA) (formula: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms					AltConf
76	2A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	2A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	3A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	3A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	7A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	7A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	9A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	9A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

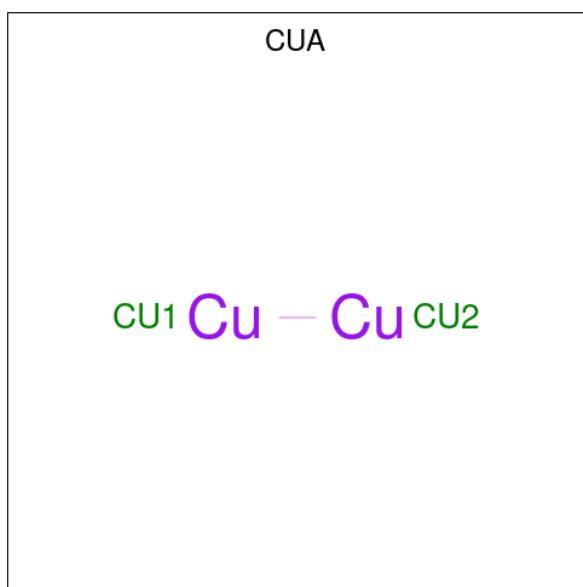
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
77	2A	1	Total 1	Cu 1	0
77	3A	1	Total 1	Cu 1	0
77	4A	1	Total 1	Cu 1	0
77	7A	1	Total 1	Cu 1	0
77	8A	1	Total 1	Cu 1	0
77	9A	1	Total 1	Cu 1	0

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

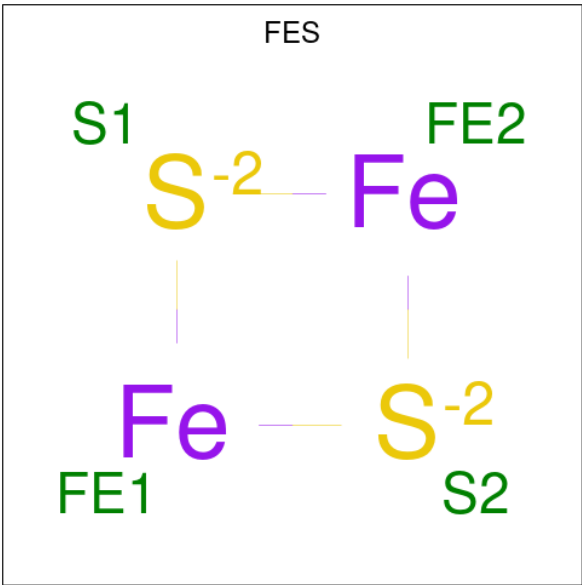
Mol	Chain	Residues	Atoms		AltConf
78	2A	1	Total 1	Mg 1	0
78	3A	1	Total 1	Mg 1	0
78	4A	1	Total 1	Mg 1	0
78	7A	1	Total 1	Mg 1	0
78	8A	1	Total 1	Mg 1	0
78	9A	1	Total 1	Mg 1	0

- Molecule 79 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



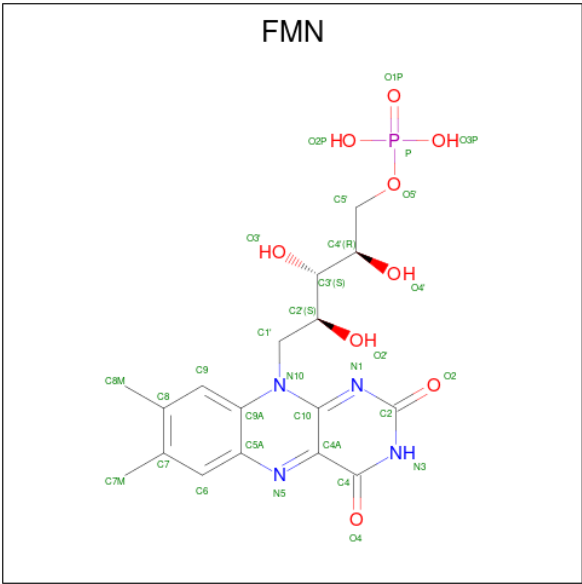
Mol	Chain	Residues	Atoms		AltConf
79	2C	1	Total 2	Cu 2	0
79	3C	1	Total 2	Cu 2	0
79	4C	1	Total 2	Cu 2	0
79	7C	1	Total 2	Cu 2	0
79	8C	1	Total 2	Cu 2	0
79	9C	1	Total 2	Cu 2	0

- Molecule 80 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



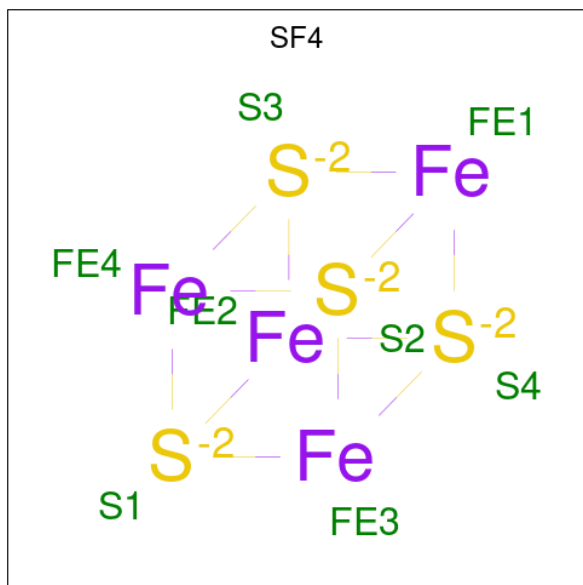
Mol	Chain	Residues	Atoms			AltConf
80	5A	1	Total	Fe	S	0
			4	2	2	
80	5C	1	Total	Fe	S	0
			4	2	2	
80	A	1	Total	Fe	S	0
			4	2	2	
80	C	1	Total	Fe	S	0
			4	2	2	

- Molecule 81 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					AltConf
81	5B	1	Total	C	N	O	P	0
			31	17	4	9	1	
81	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 82 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



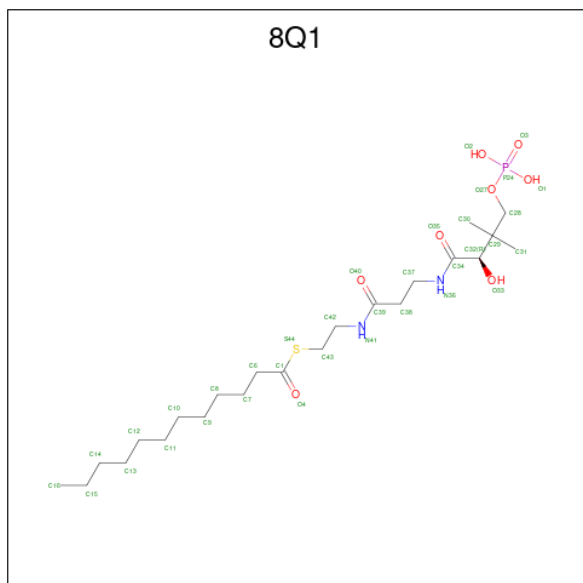
Mol	Chain	Residues	Atoms			AltConf
82	5B	1	Total	Fe	S	0
			8	4	4	
82	5C	1	Total	Fe	S	0
			8	4	4	
82	5C	1	Total	Fe	S	0
			8	4	4	
82	5F	1	Total	Fe	S	0
			8	4	4	
82	5G	1	Total	Fe	S	0
			8	4	4	
82	5G	1	Total	Fe	S	0
			8	4	4	
82	B	1	Total	Fe	S	0
			8	4	4	
82	C	1	Total	Fe	S	0
			8	4	4	
82	C	1	Total	Fe	S	0
			8	4	4	
82	F	1	Total	Fe	S	0
			8	4	4	

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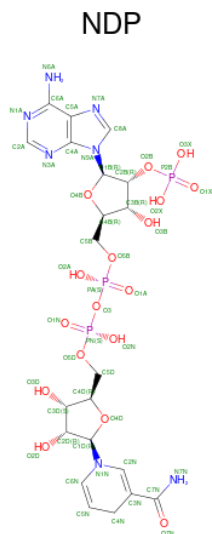
Mol	Chain	Residues	Atoms			AltConf
82	G	1	Total	Fe	S	0
			8	4	4	
82	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 83 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



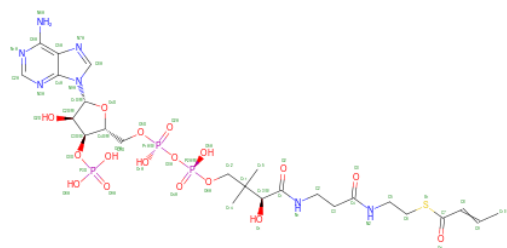
Mol	Chain	Residues	Atoms						AltConf
83	5J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
83	5k	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
83	J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
83	k	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 84 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
84	5P	1	Total 48	C 21	N 7	O 17	P 3	0
84	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 85 is CROTONYL COENZYME A (CCD ID: COO) (formula: $\text{C}_{25}\text{H}_{40}\text{N}_7\text{O}_{17}\text{P}_3\text{S}$).

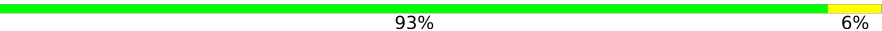


Mol	Chain	Residues	Atoms					AltConf	
85	5s	1	Total 53	C 25	N 7	O 17	P 3	S 1	0
85	s	1	Total 53	C 25	N 7	O 17	P 3	S 1	0

3 Residue-property plots [i](#)

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

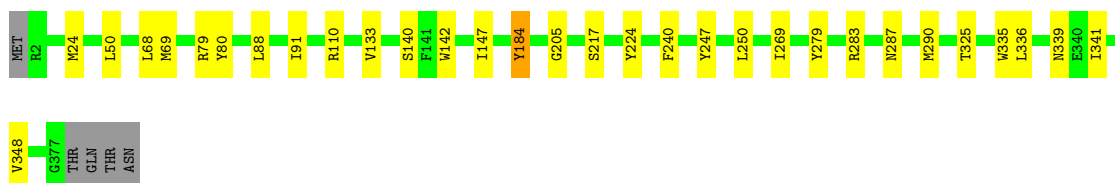
- Molecule 1: Cytochrome b

Chain 1A: 



- Molecule 1: Cytochrome b

Chain 1B: 



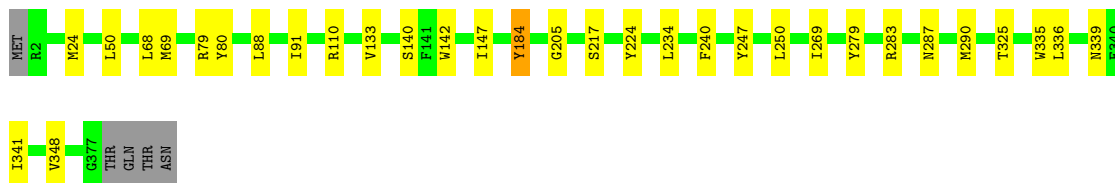
- Molecule 1: Cytochrome b

Chain 6A: 

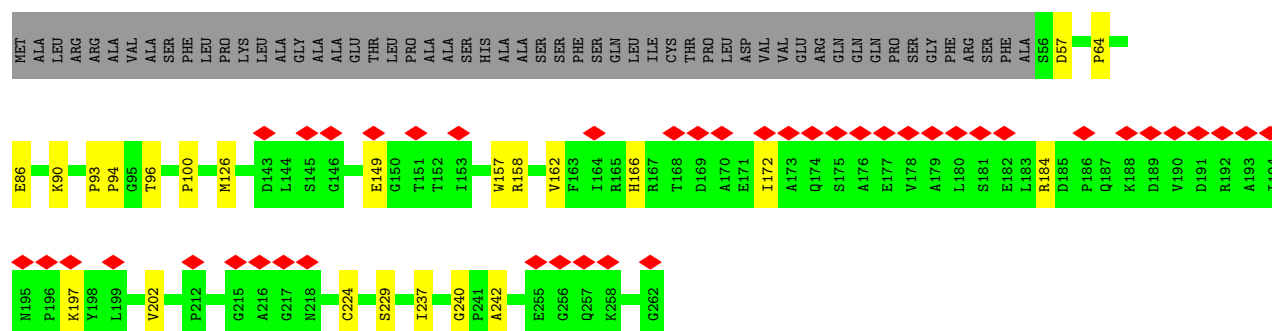


- Molecule 1: Cytochrome b

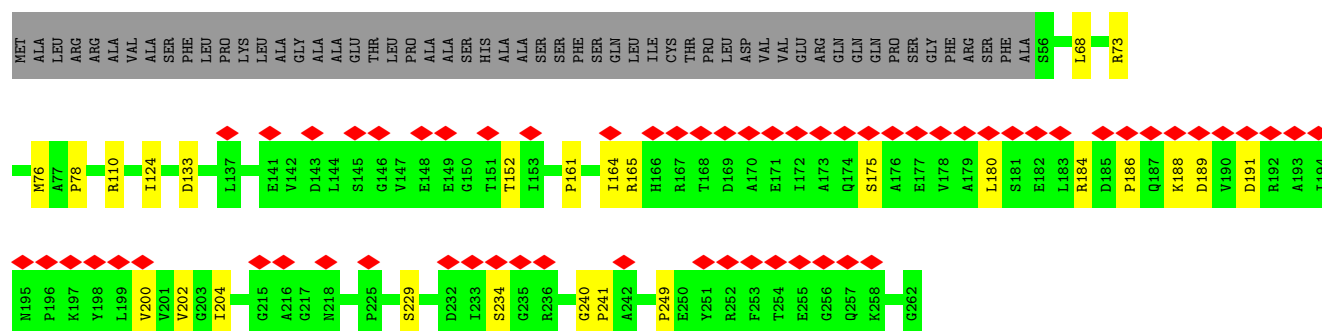
Chain 6B: 



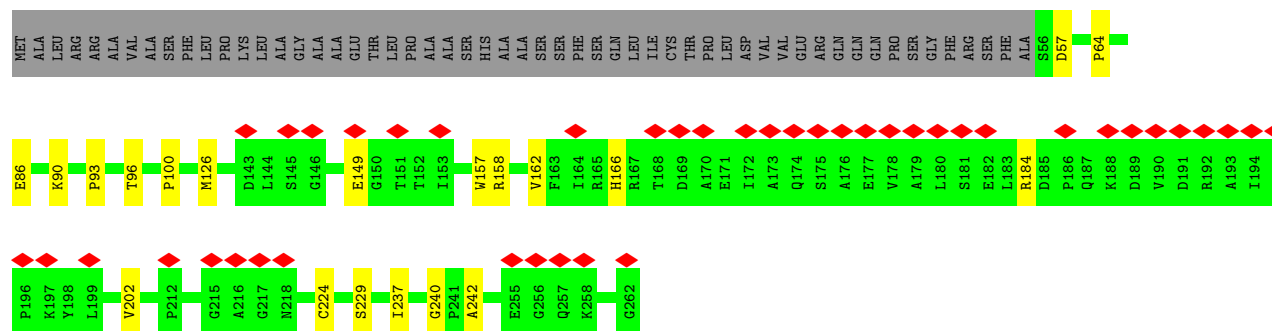
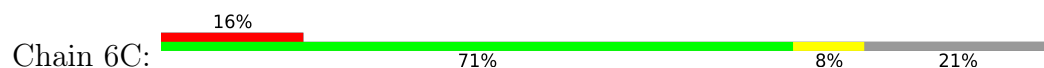
- Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



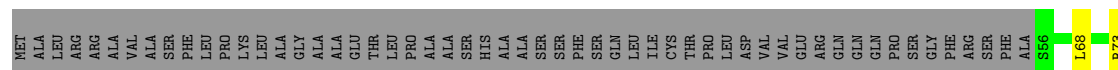
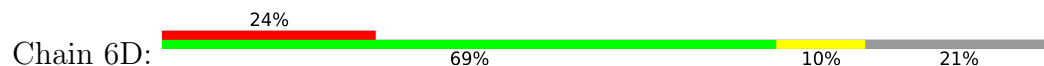
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

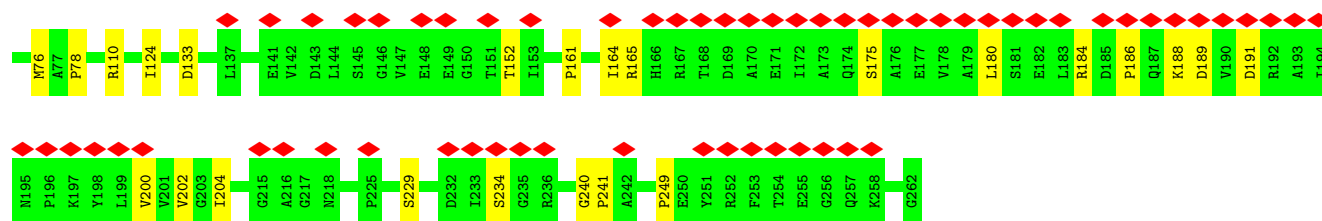


• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial



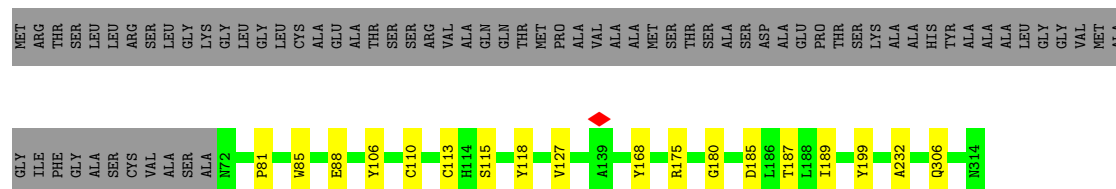
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial





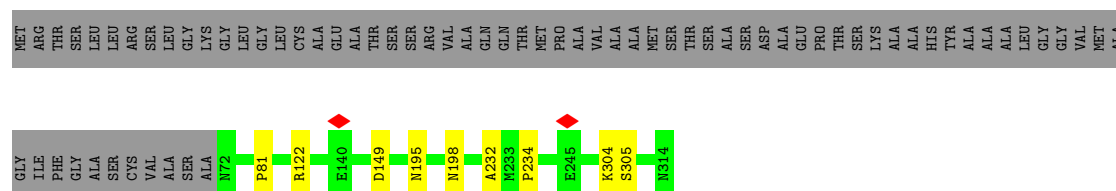
• Molecule 3: Cytochrome c1

Chain 1E: 72% 6% 23%



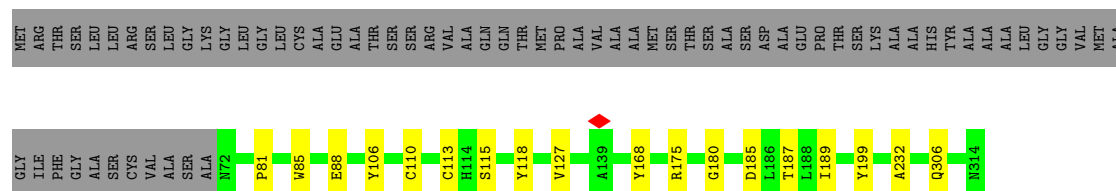
• Molecule 3: Cytochrome c1

Chain 1F: 75% 23%



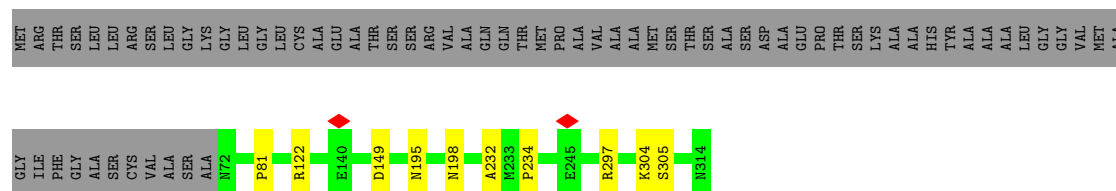
• Molecule 3: Cytochrome c1

Chain 6E: 72% 6% 23%



• Molecule 3: Cytochrome c1

Chain 6F: 74% 23%



• Molecule 4: Complex III subunit 9

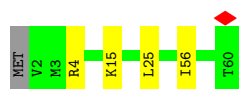
Chain 1G: 93% 5%



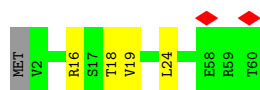
- Molecule 4: Complex III subunit 9



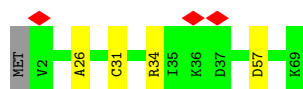
- Molecule 4: Complex III subunit 9



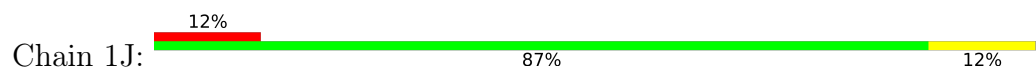
- Molecule 4: Complex III subunit 9



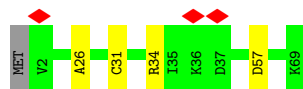
- Molecule 5: Cytochrome b-c1 complex subunit 6



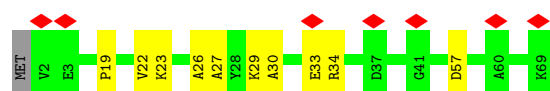
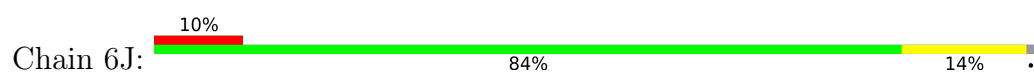
- Molecule 5: Cytochrome b-c1 complex subunit 6



- Molecule 5: Cytochrome b-c1 complex subunit 6



- Molecule 5: Cytochrome b-c1 complex subunit 6



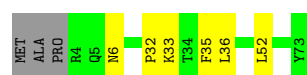
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



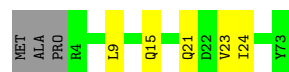
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



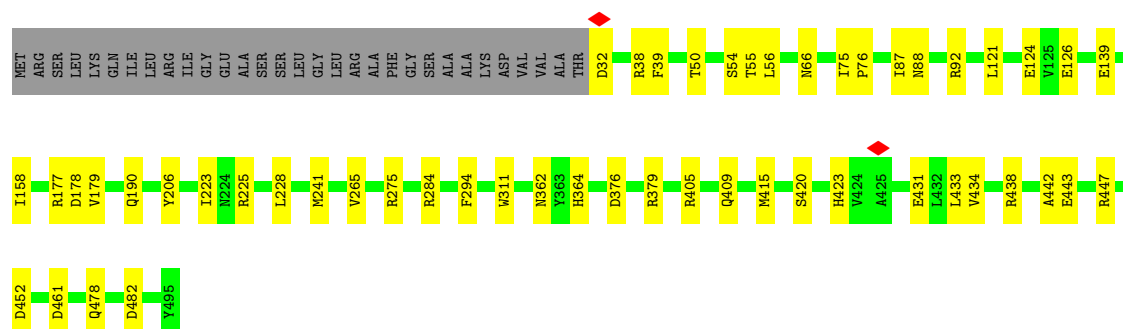
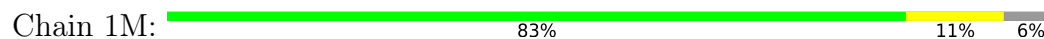
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



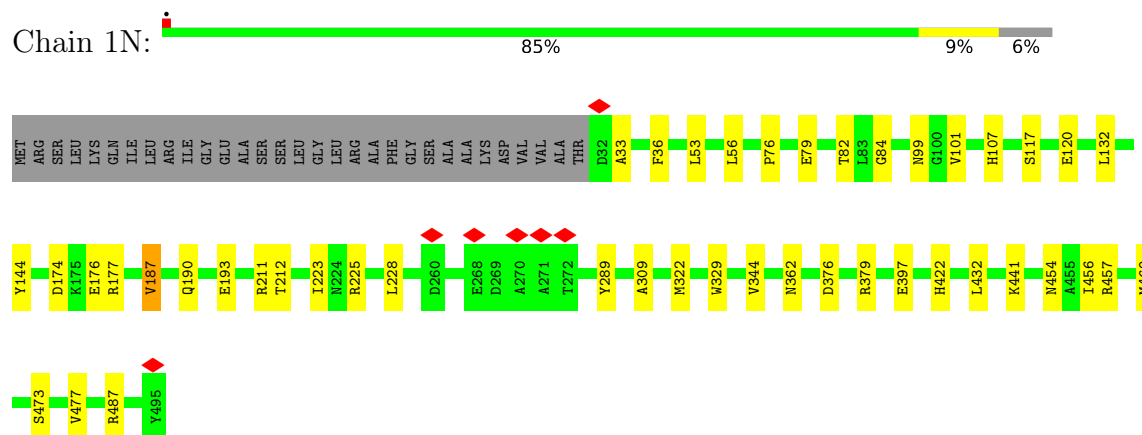
- Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8



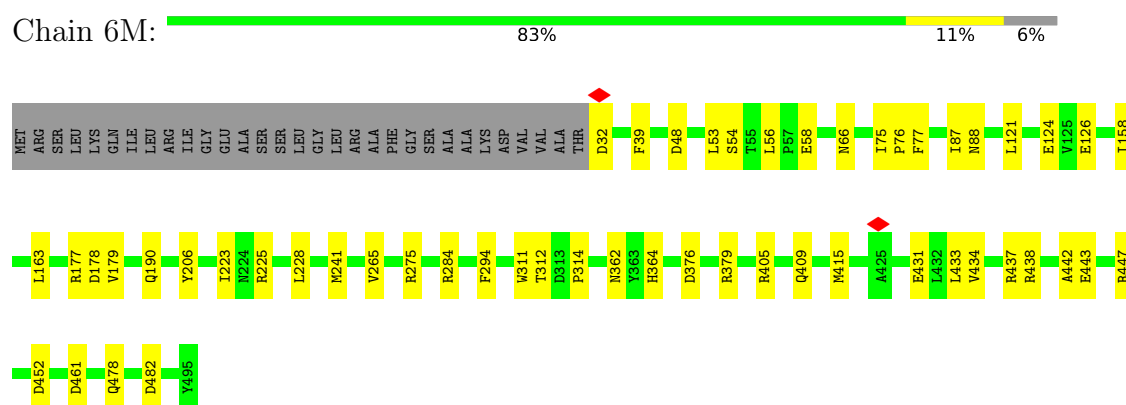
- Molecule 7: MPP-Beta



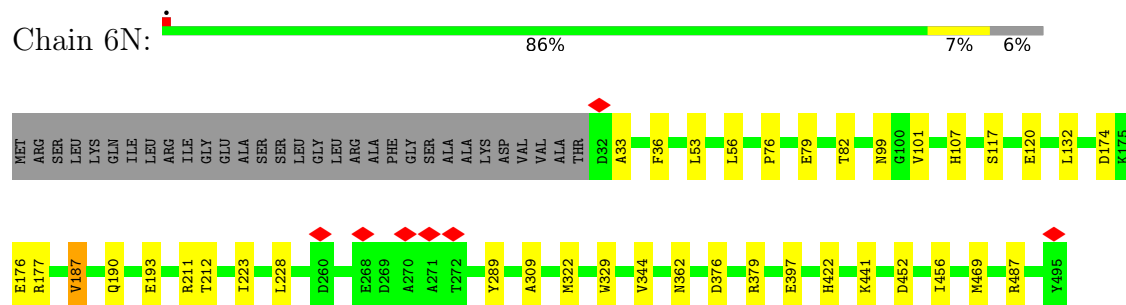
- Molecule 7: MPP-Beta



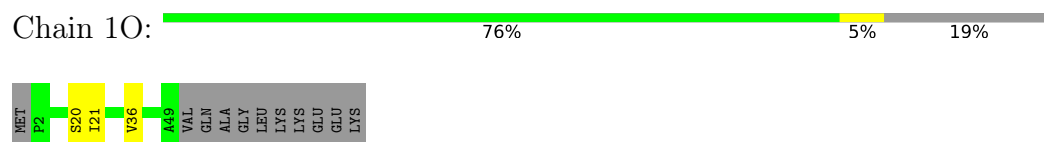
- Molecule 7: MPP-Beta



- Molecule 7: MPP-Beta

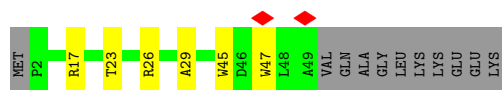


- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

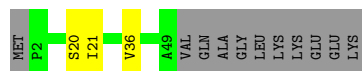
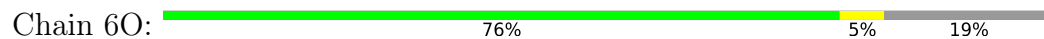


- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

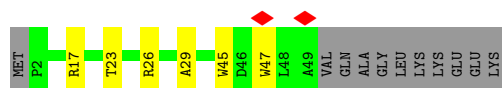




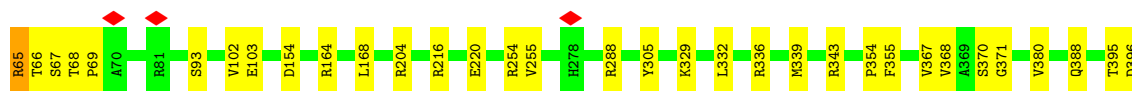
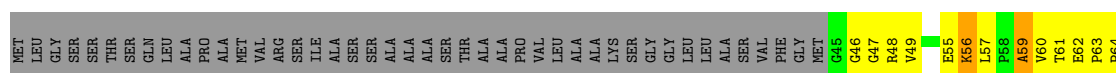
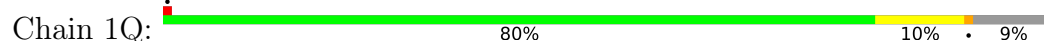
- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



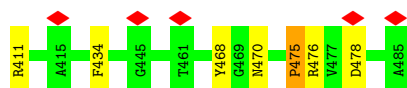
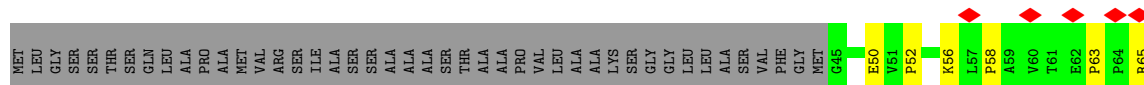
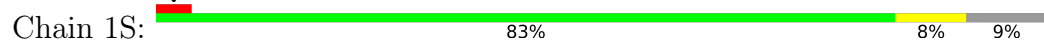
- Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10



- Molecule 9: Alpha-MPP

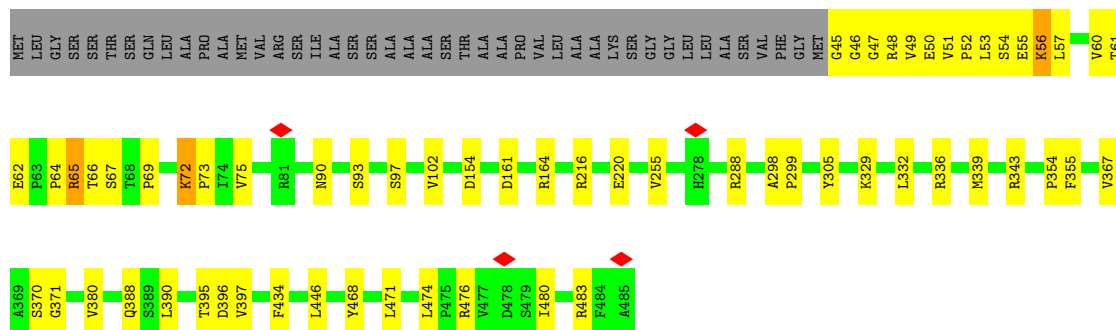


- Molecule 9: Alpha-MPP



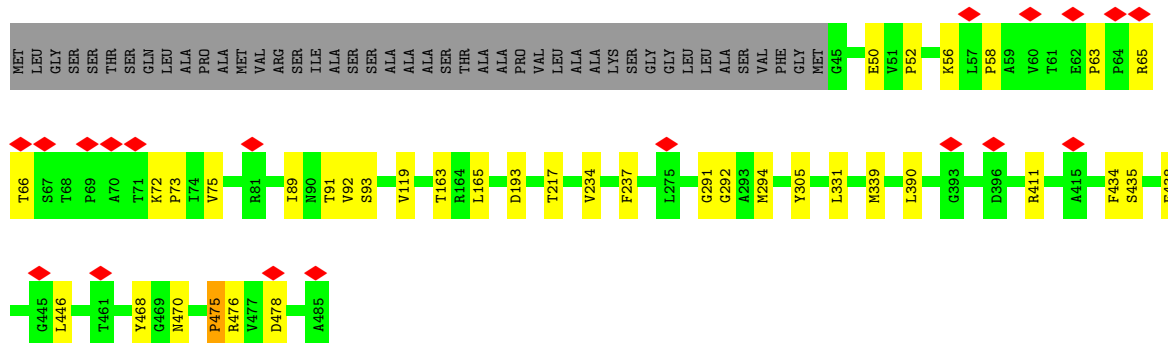
- Molecule 9: Alpha-MPP

Chain 6Q:  78% 12% 9%



• Molecule 9: Alpha-MPP

Chain 6S:  83% 8% 9%



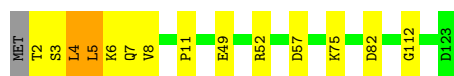
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1R:  86% 11% ..



• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1T:  88% 10% ..



• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 6R:  86% 11% ..



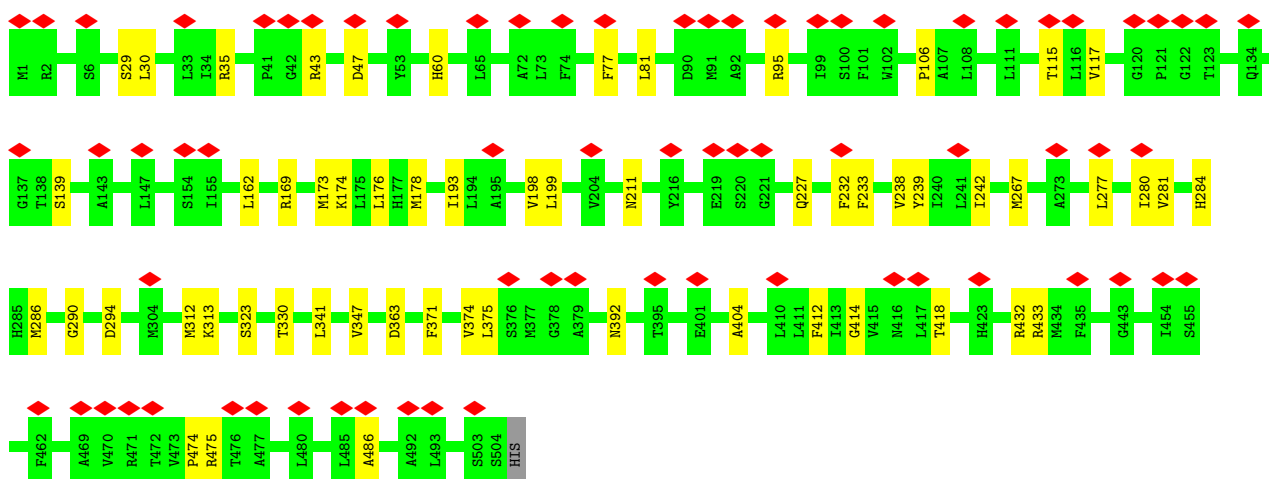
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 6T:  88% 10% ..



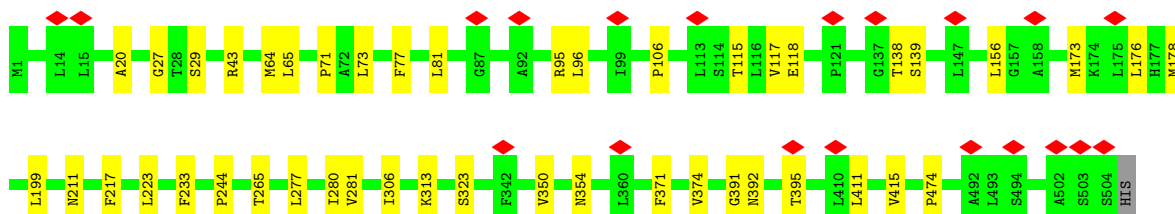
• Molecule 11: Cytochrome c oxidase subunit 1

Chain 2A:  14% 89% 11%



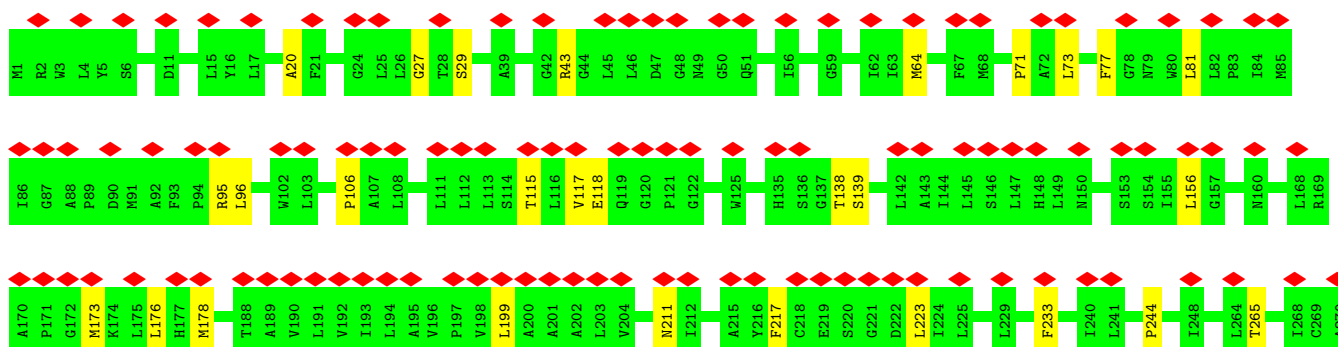
• Molecule 11: Cytochrome c oxidase subunit 1

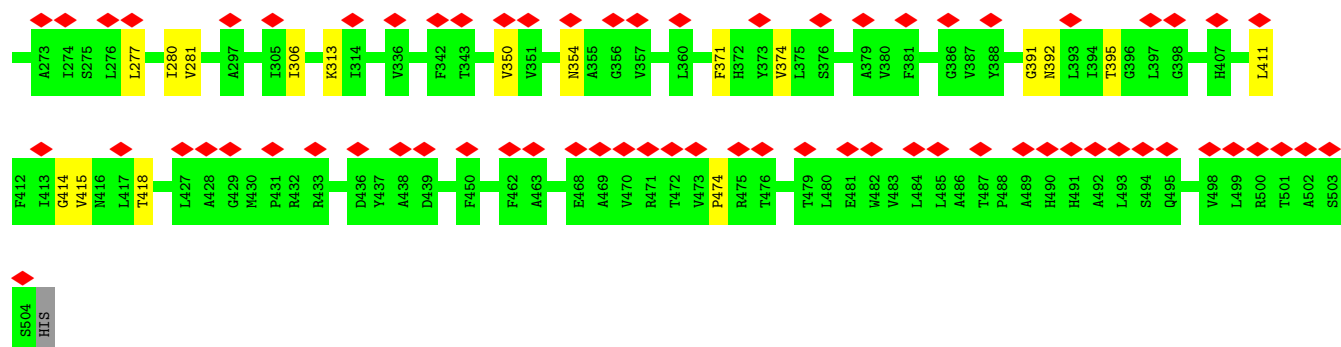
Chain 3A:  91% 9%



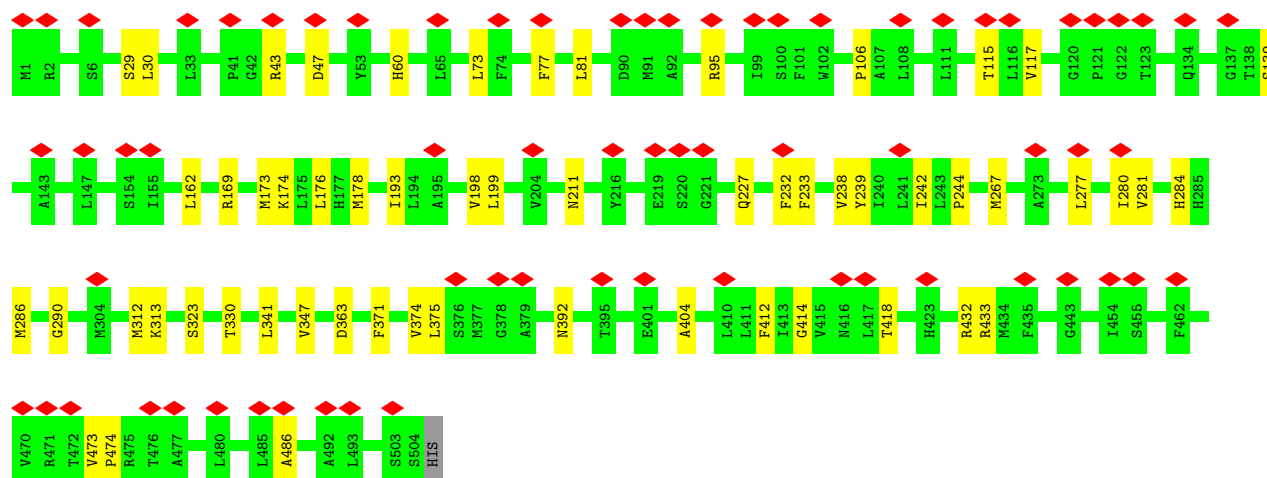
• Molecule 11: Cytochrome c oxidase subunit 1

Chain 4A:  35% 91% 9%

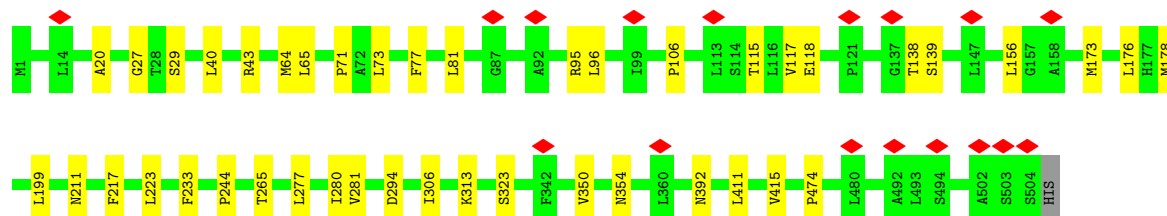




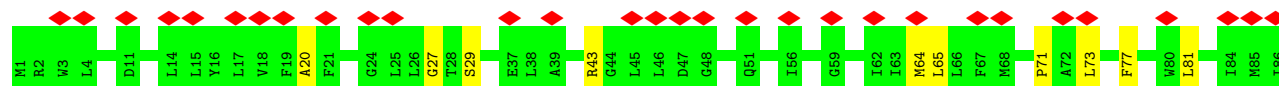
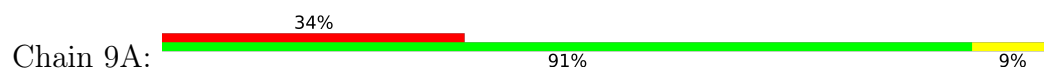
• Molecule 11: Cytochrome c oxidase subunit 1

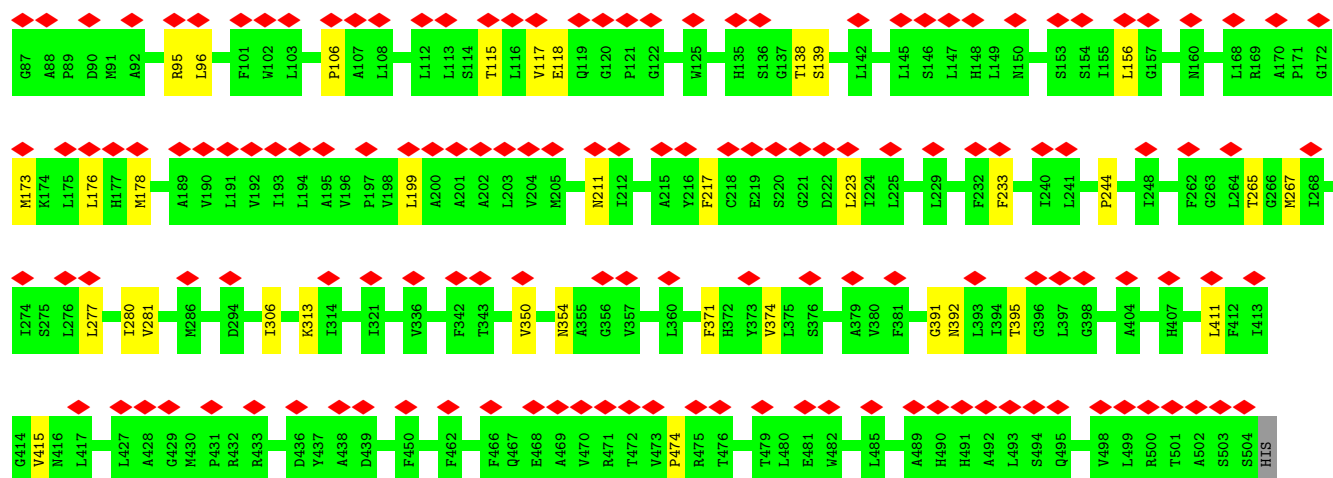


• Molecule 11: Cytochrome c oxidase subunit 1

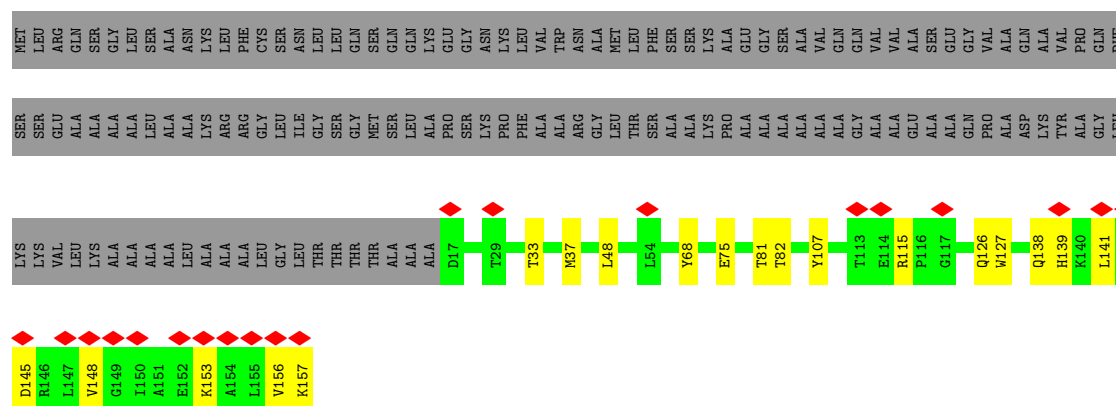
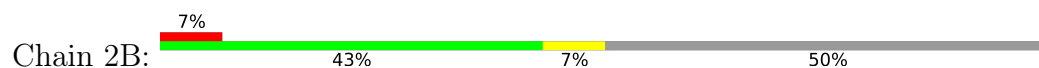


• Molecule 11: Cytochrome c oxidase subunit 1





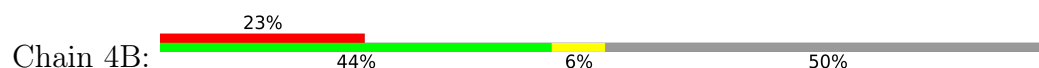
• Molecule 12: Cytochrome c oxidase polypeptide II



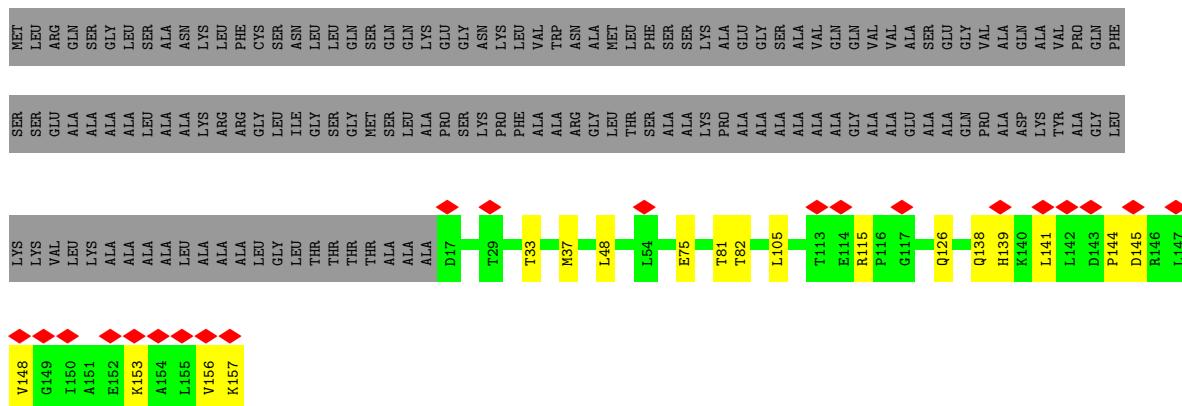
• Molecule 12: Cytochrome c oxidase polypeptide II



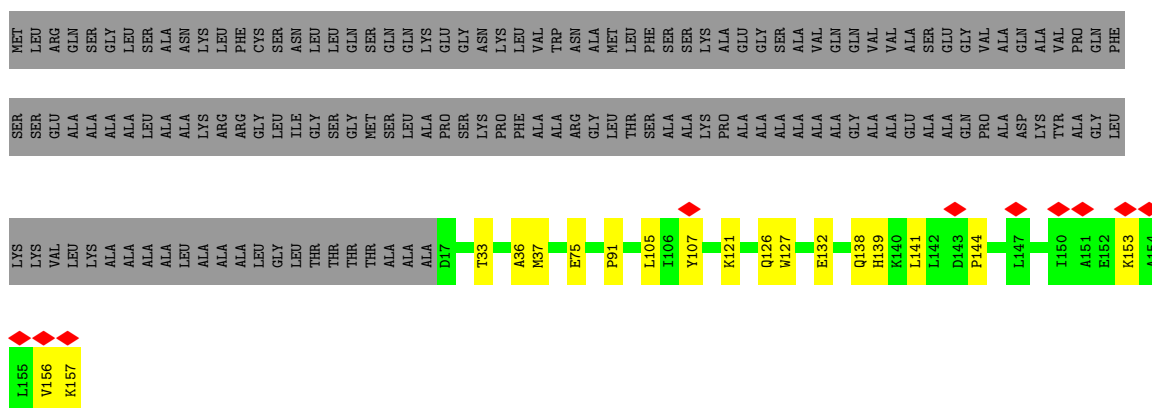
• Molecule 12: Cytochrome c oxidase polypeptide II



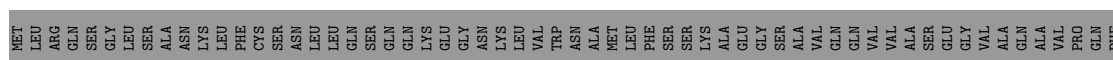
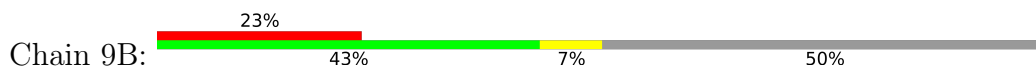
- Molecule 12: Cytochrome c oxidase polypeptide II

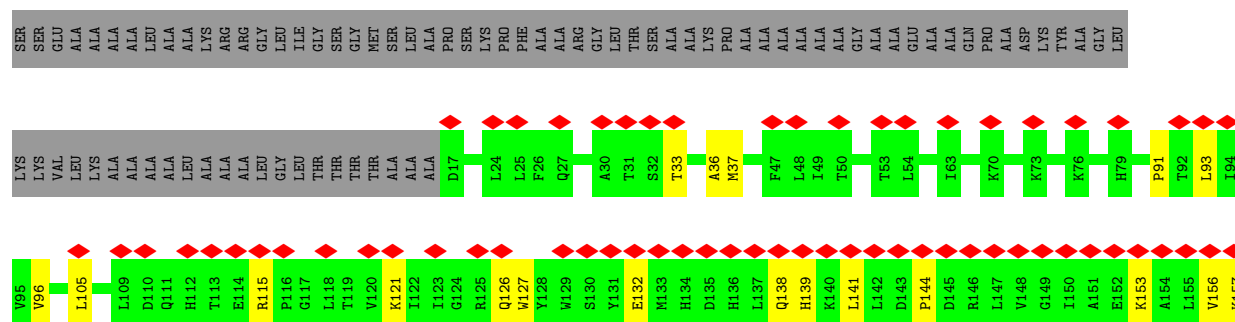


- Molecule 12: Cytochrome c oxidase polypeptide II

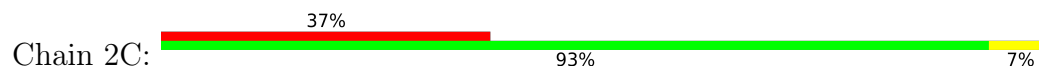


- Molecule 12: Cytochrome c oxidase polypeptide II

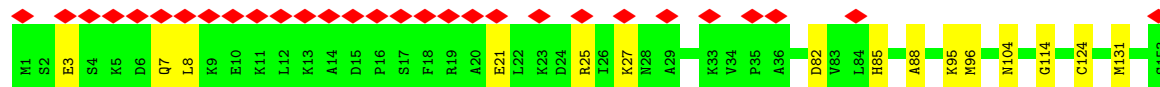




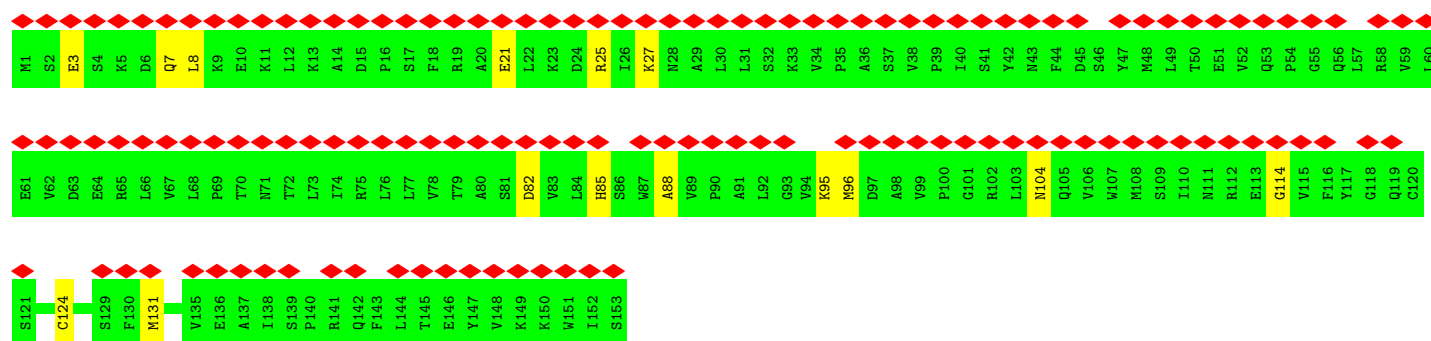
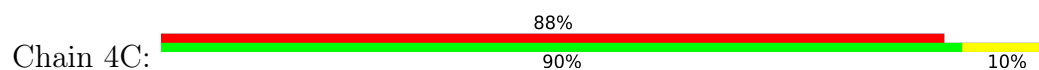
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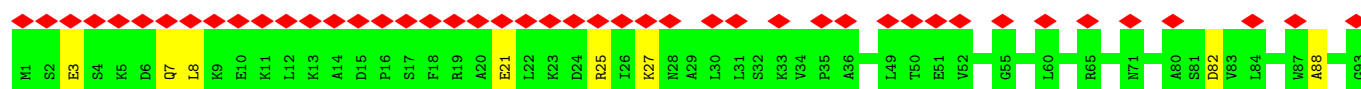
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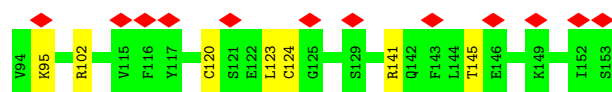


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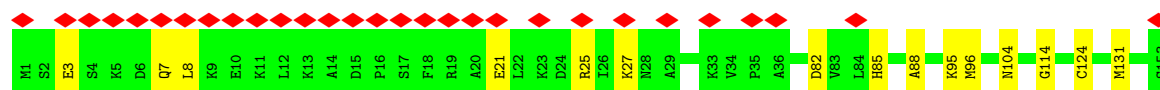


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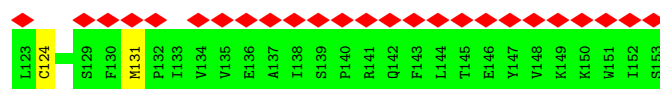
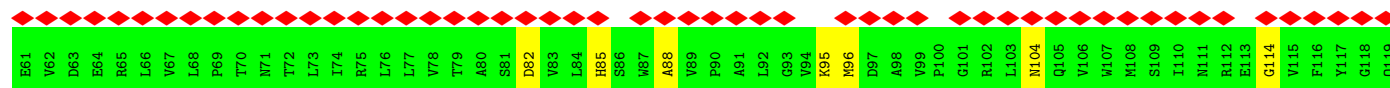
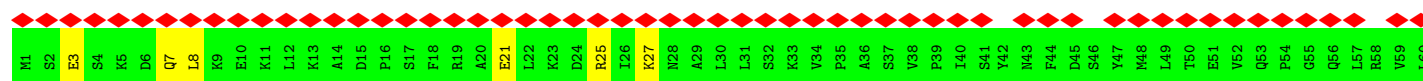
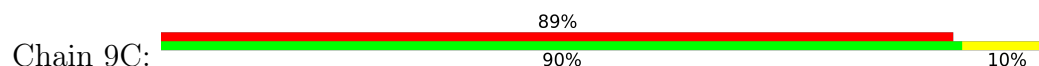




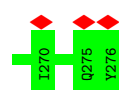
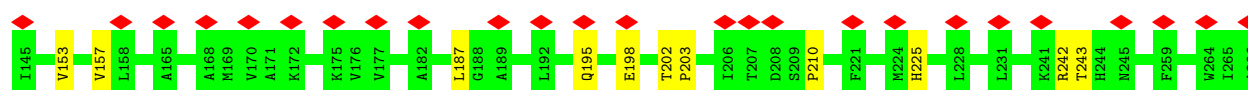
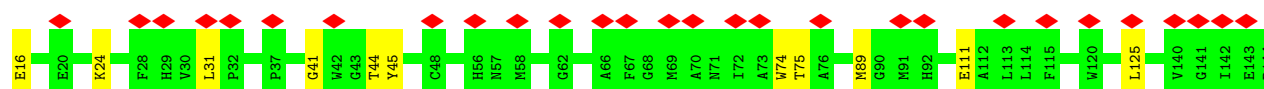
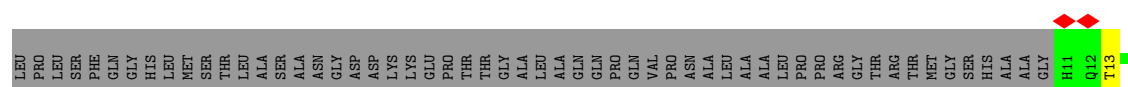
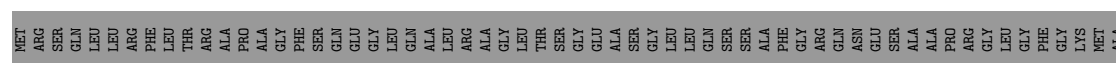
- Molecule 13: cytochrome-c oxidase



- Molecule 13: cytochrome-c oxidase

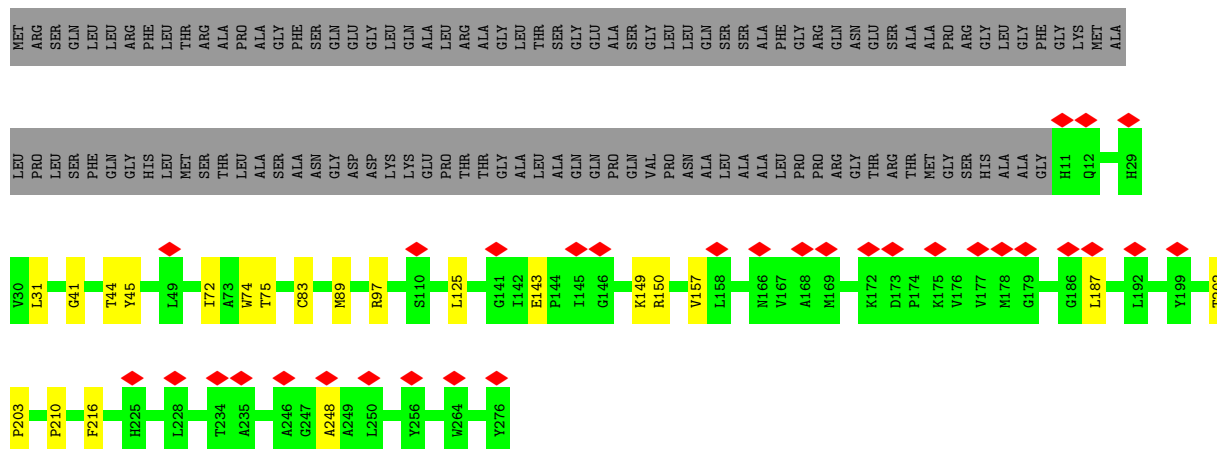


- Molecule 14: Cytochrome c oxidase subunit 3

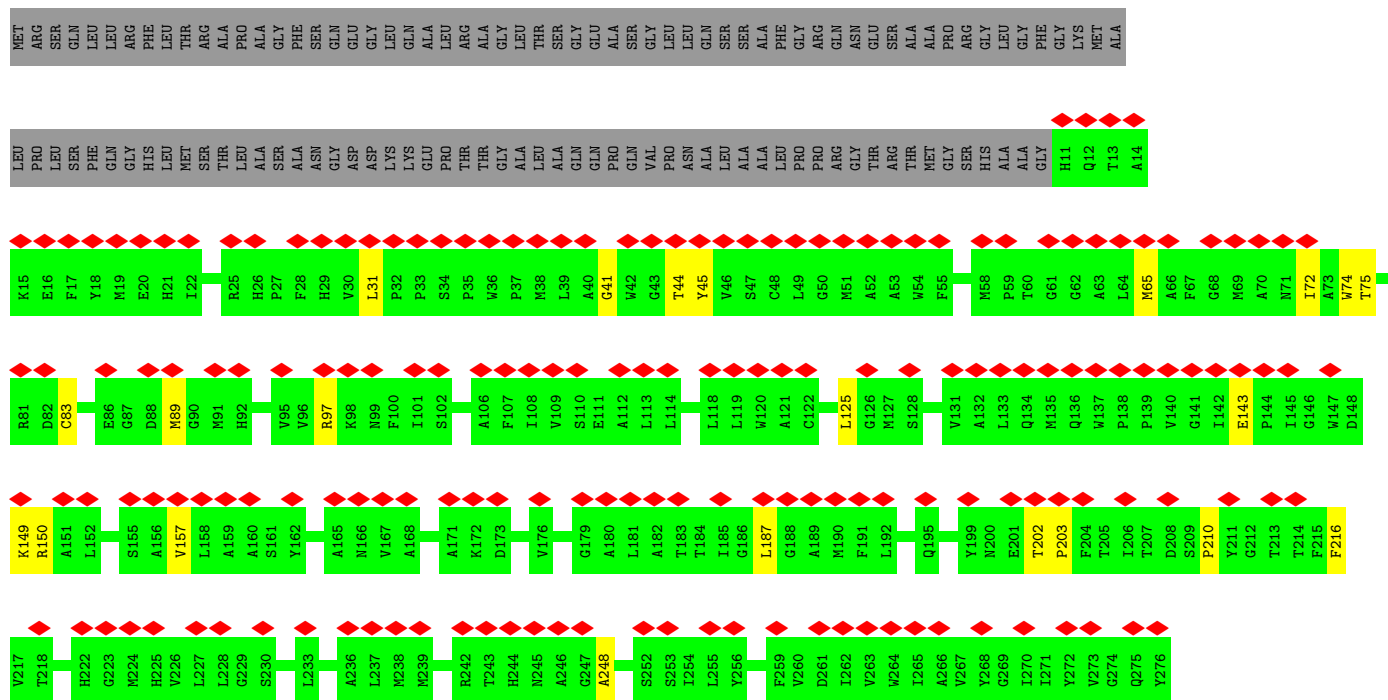


- Molecule 14: Cytochrome c oxidase subunit 3

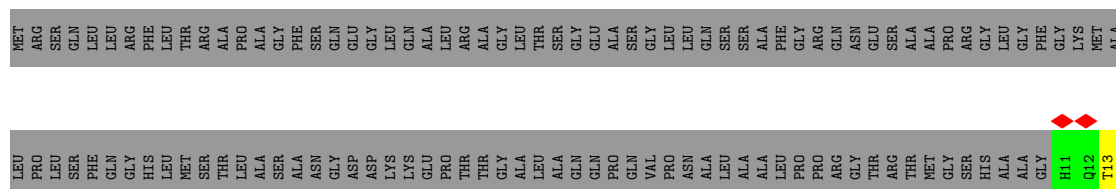


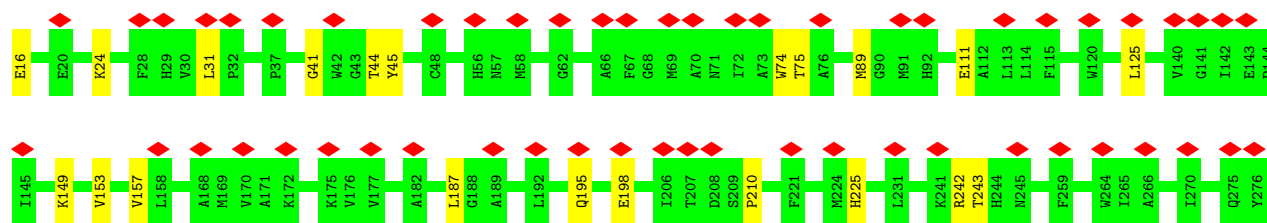


• Molecule 14: Cytochrome c oxidase subunit 3

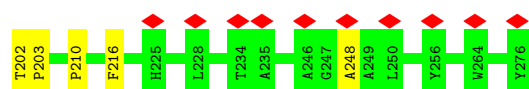
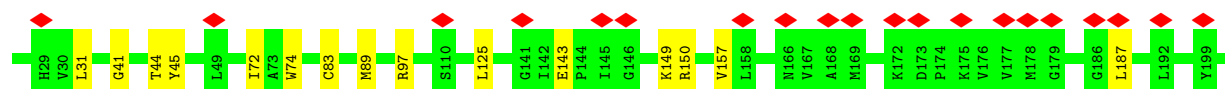
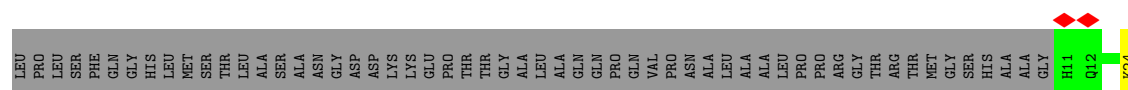
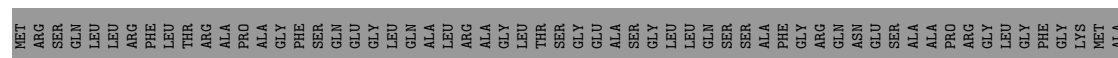


• Molecule 14: Cytochrome c oxidase subunit 3

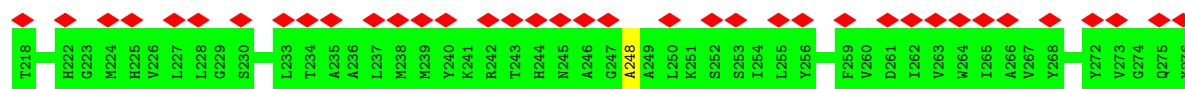
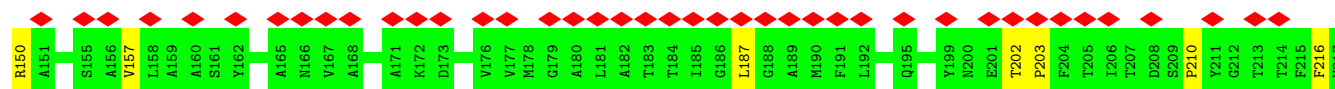
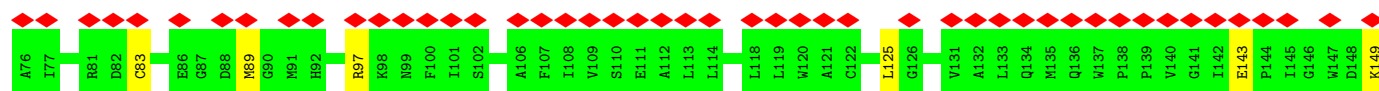
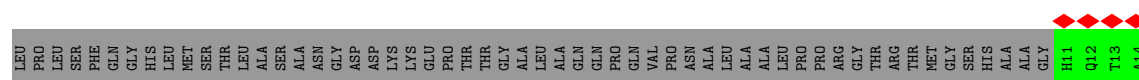




• Molecule 14: Cytochrome c oxidase subunit 3



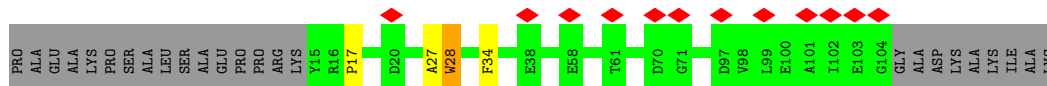
• Molecule 14: Cytochrome c oxidase subunit 3



• Molecule 15: Cox5b



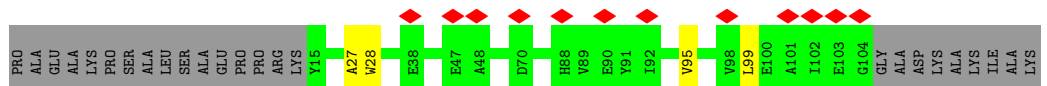
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• Molecule 15: Cox5b



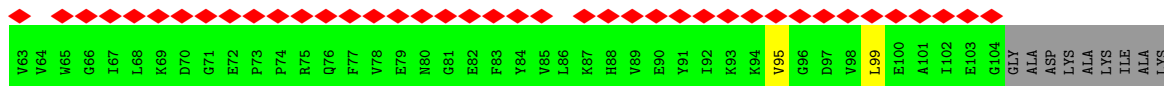
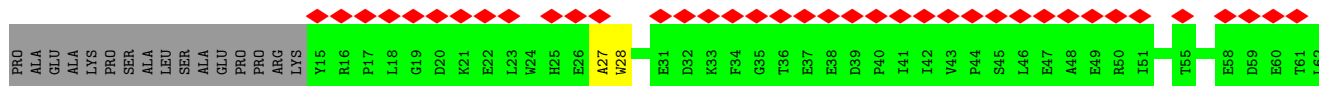
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• Molecule 15: Cox5b



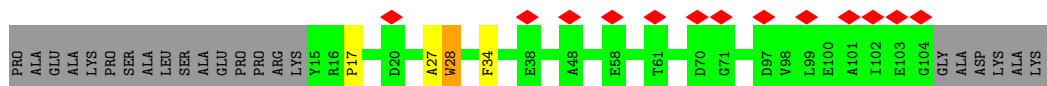
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• Molecule 15: Cox5b



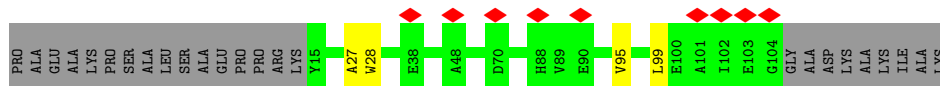
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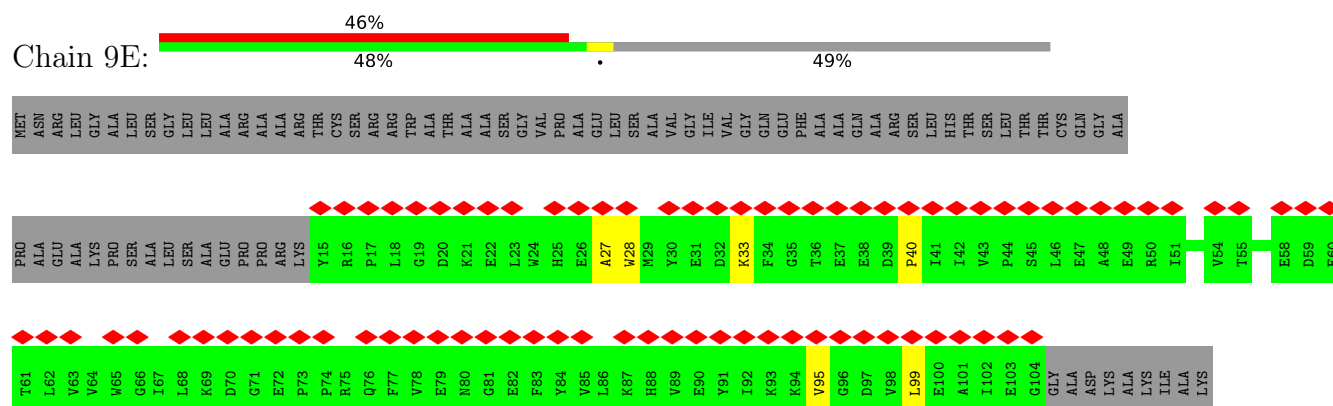
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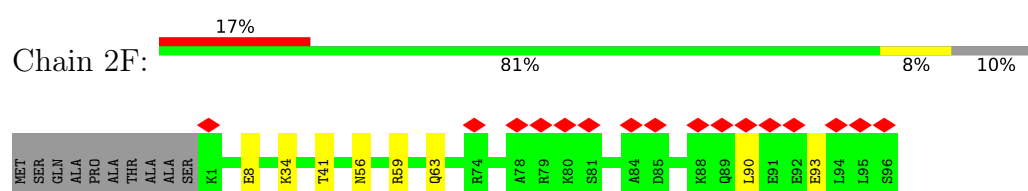
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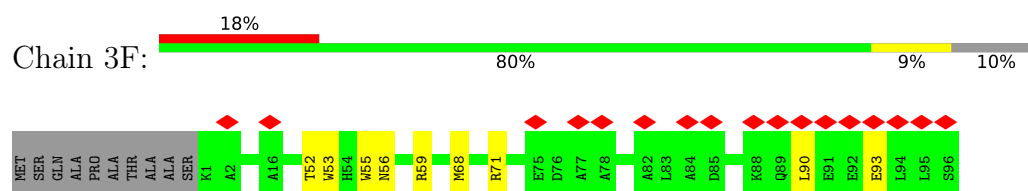
- Molecule 15: Cox5b



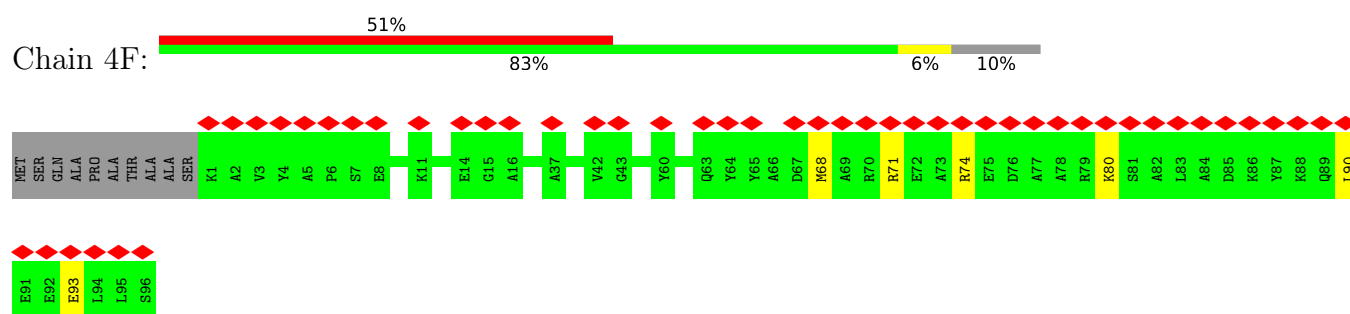
- Molecule 16: Cox5c



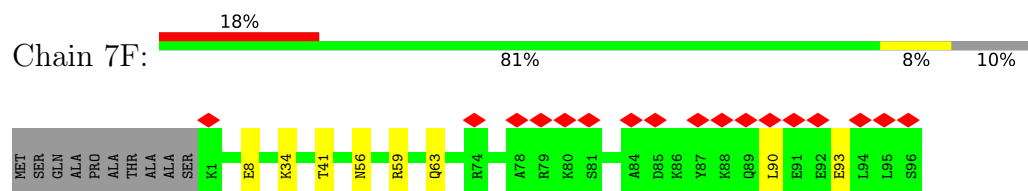
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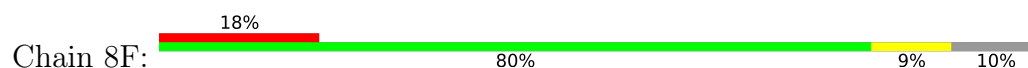
- Molecule 16: Cox5c



- Molecule 16: Cox5c

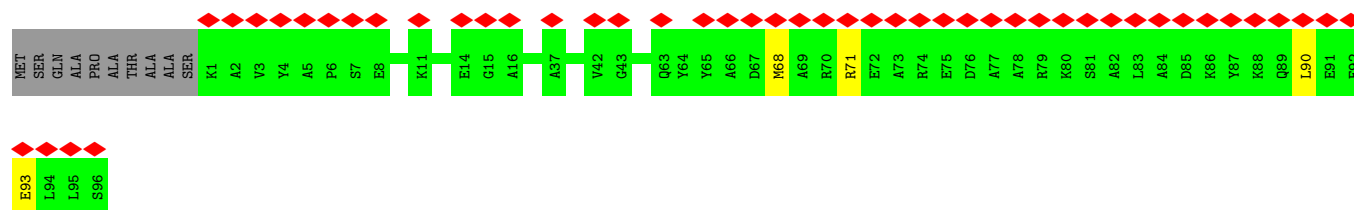
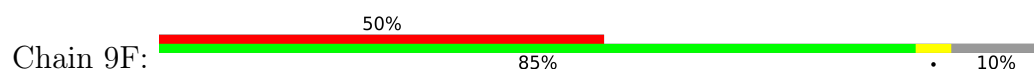


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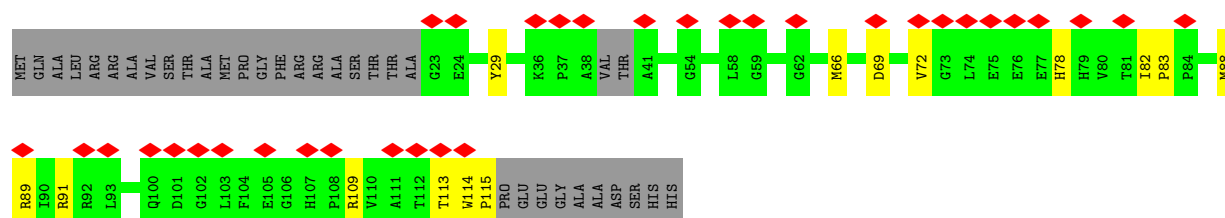




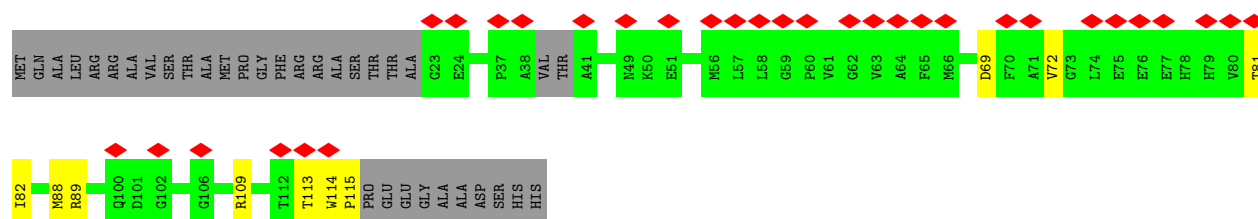
- Molecule 16: Cox5c



- Molecule 17: Cox6a



- Molecule 17: Cox6a

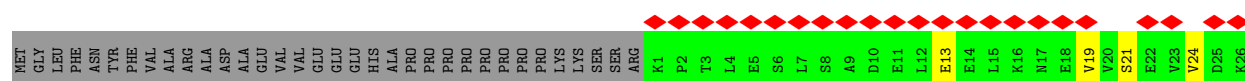


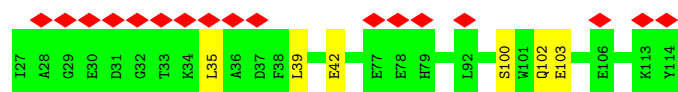
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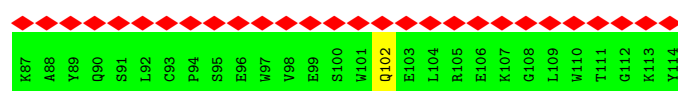
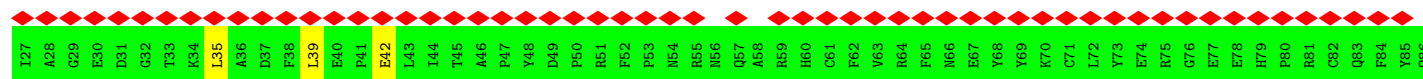
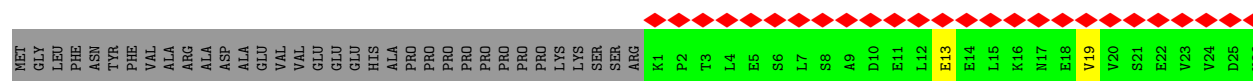
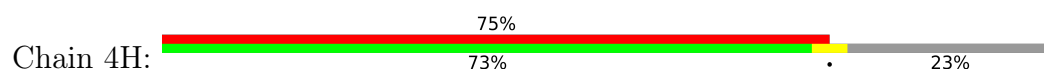
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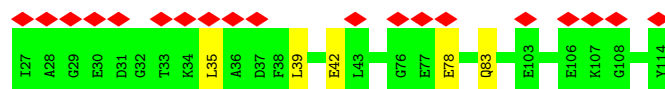
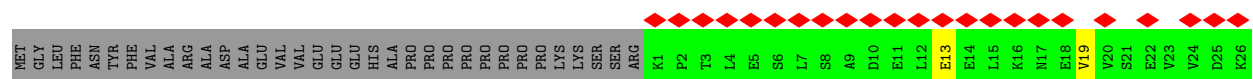
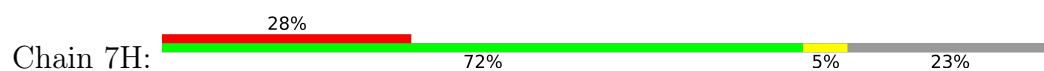




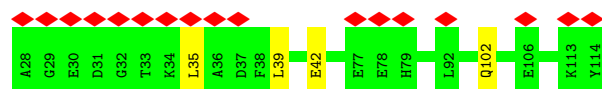
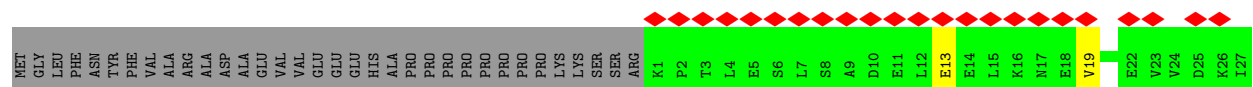
• Molecule 18: Cox6b



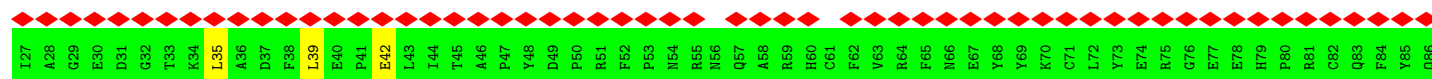
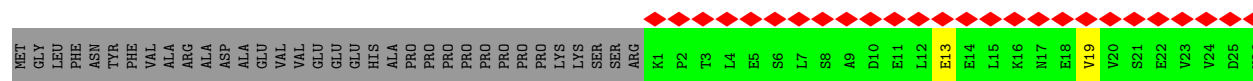
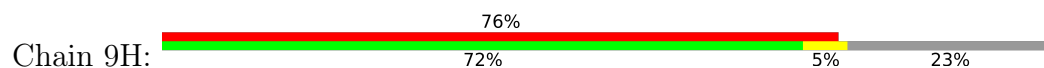
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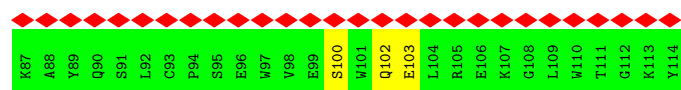


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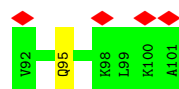
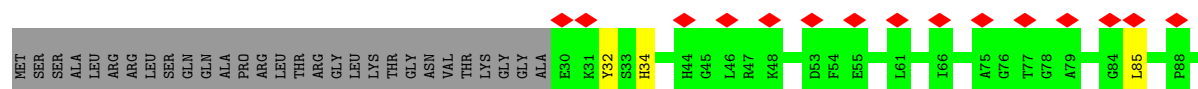


• Molecule 18: Cox6b

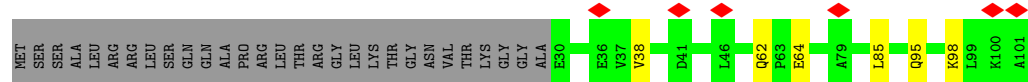




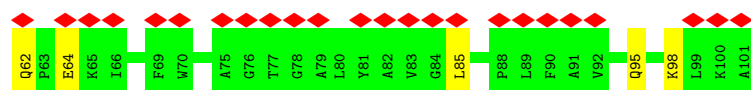
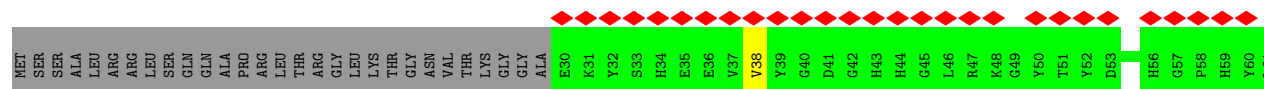
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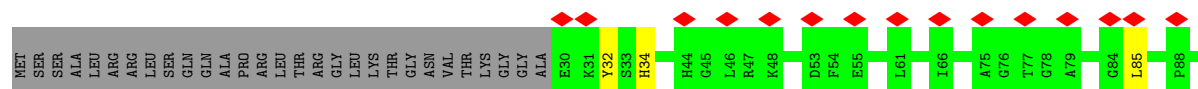
• Molecule 19: Cox7c



• Molecule 19: Cox7c

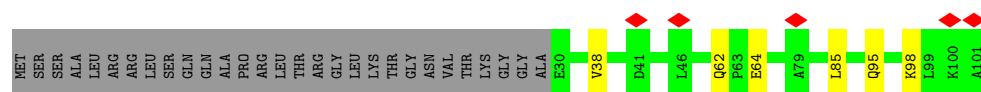


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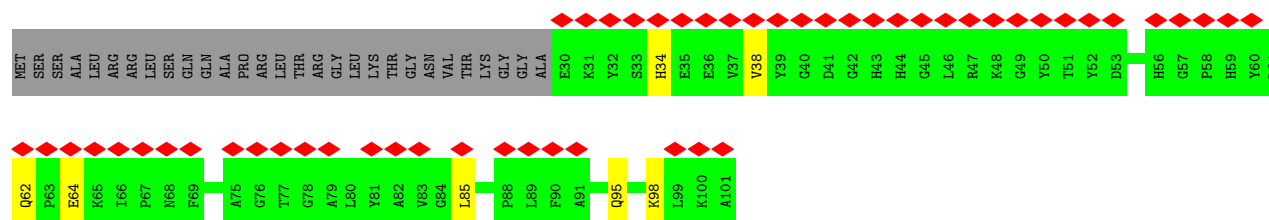


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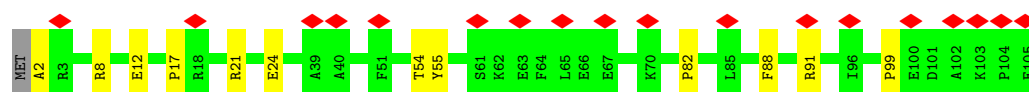




- Molecule 19: Cox7c



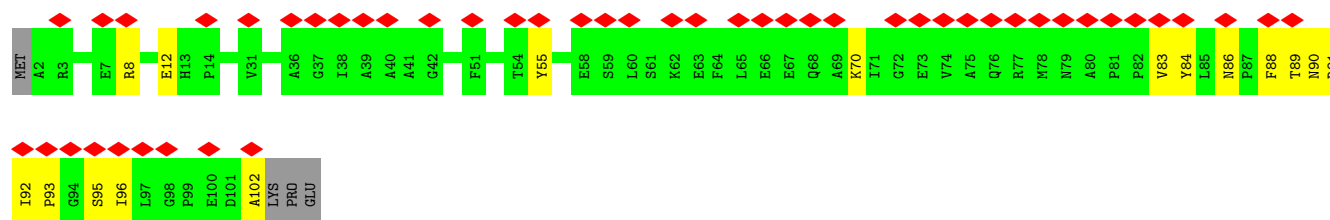
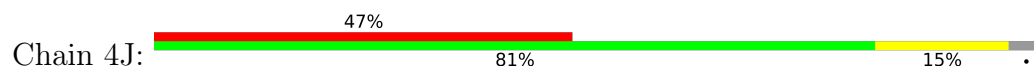
- Molecule 20: Cytochrome c oxidase subunit



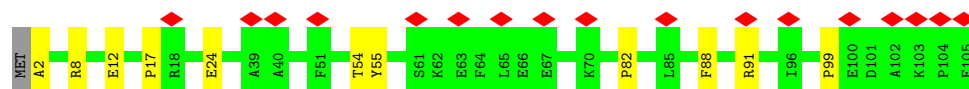
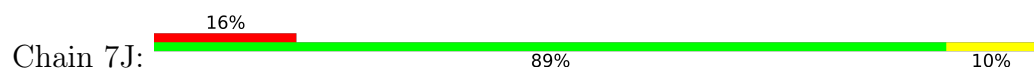
- Molecule 20: Cytochrome c oxidase subunit



- Molecule 20: Cytochrome c oxidase subunit



- Molecule 20: Cytochrome c oxidase subunit



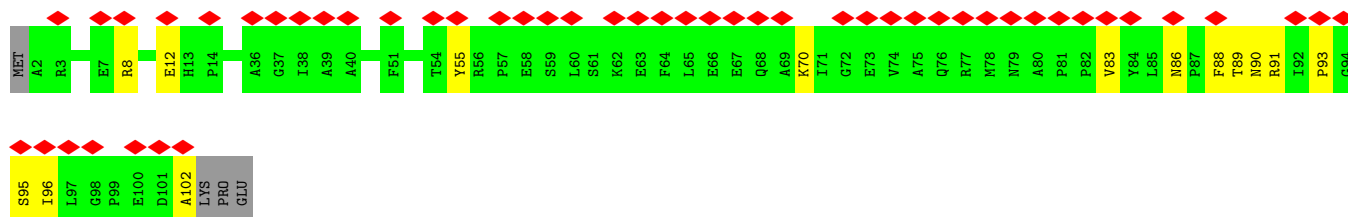
- Molecule 20: Cytochrome c oxidase subunit

Chain 8J:  91% 8%



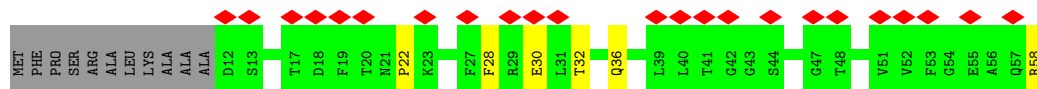
- Molecule 20: Cytochrome c oxidase subunit

Chain 9J:  48% 83% 13%



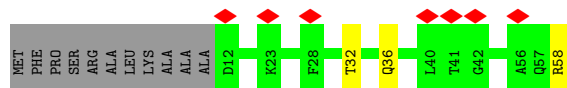
- Molecule 21: Cox7a

Chain 2K:  40% 71% 10% 19%



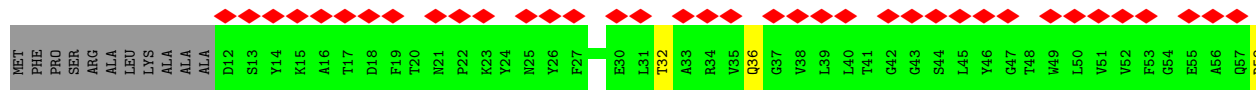
- Molecule 21: Cox7a

Chain 3K:  12% 76% 5% 19%



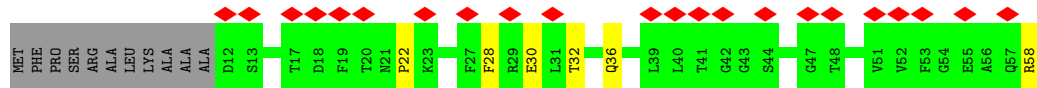
- Molecule 21: Cox7a

Chain 4K:  64% 76% 5% 19%



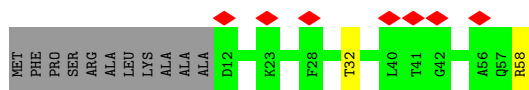
- Molecule 21: Cox7a

Chain 7K:  38% 71% 10% 19%

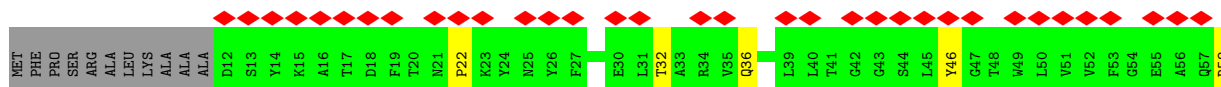


- Molecule 21: Cox7a

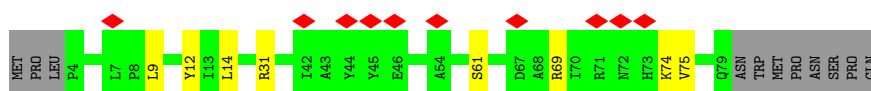
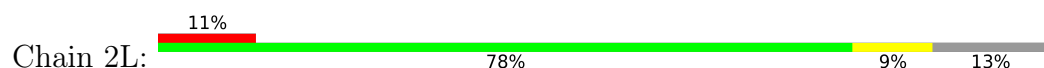
Chain 8K:  12% 78% 19%



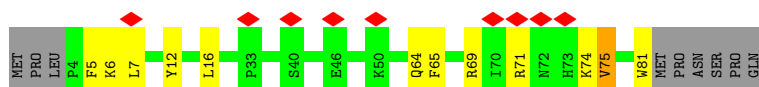
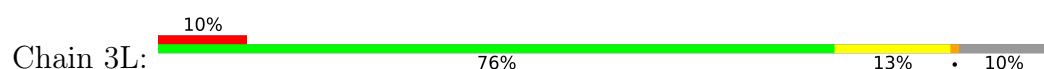
• Molecule 21: Cox7a



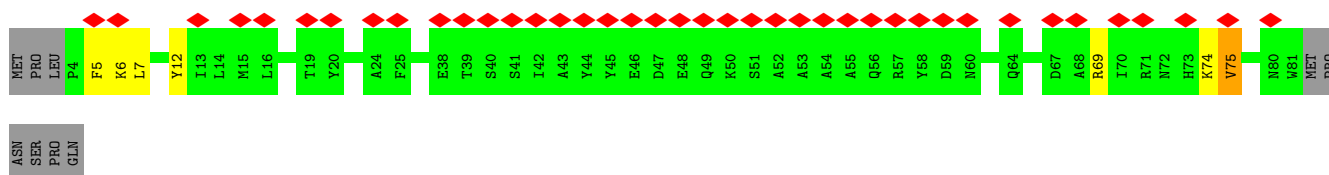
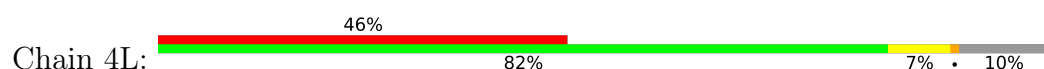
• Molecule 22: CoxIn



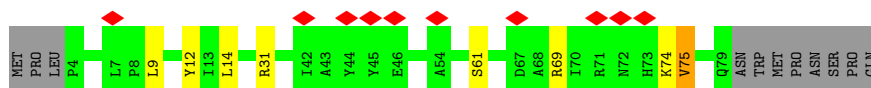
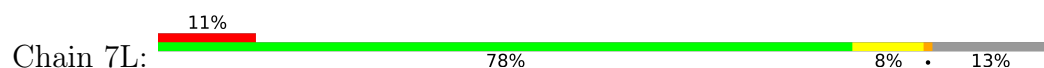
• Molecule 22: CoxIn



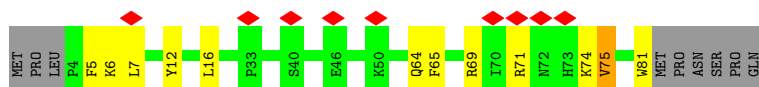
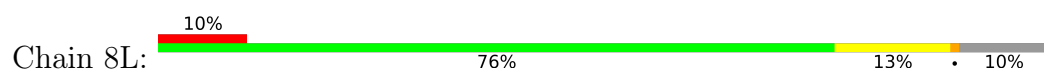
• Molecule 22: CoxIn



• Molecule 22: CoxIn

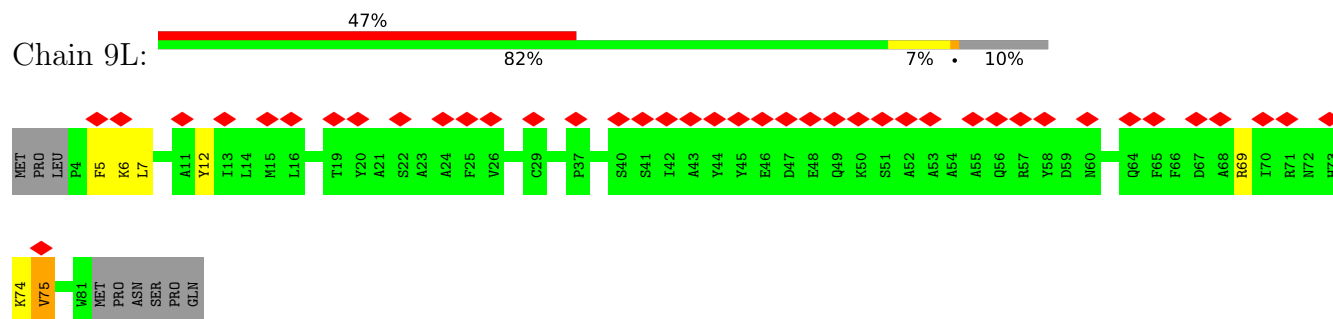


• Molecule 22: CoxIn



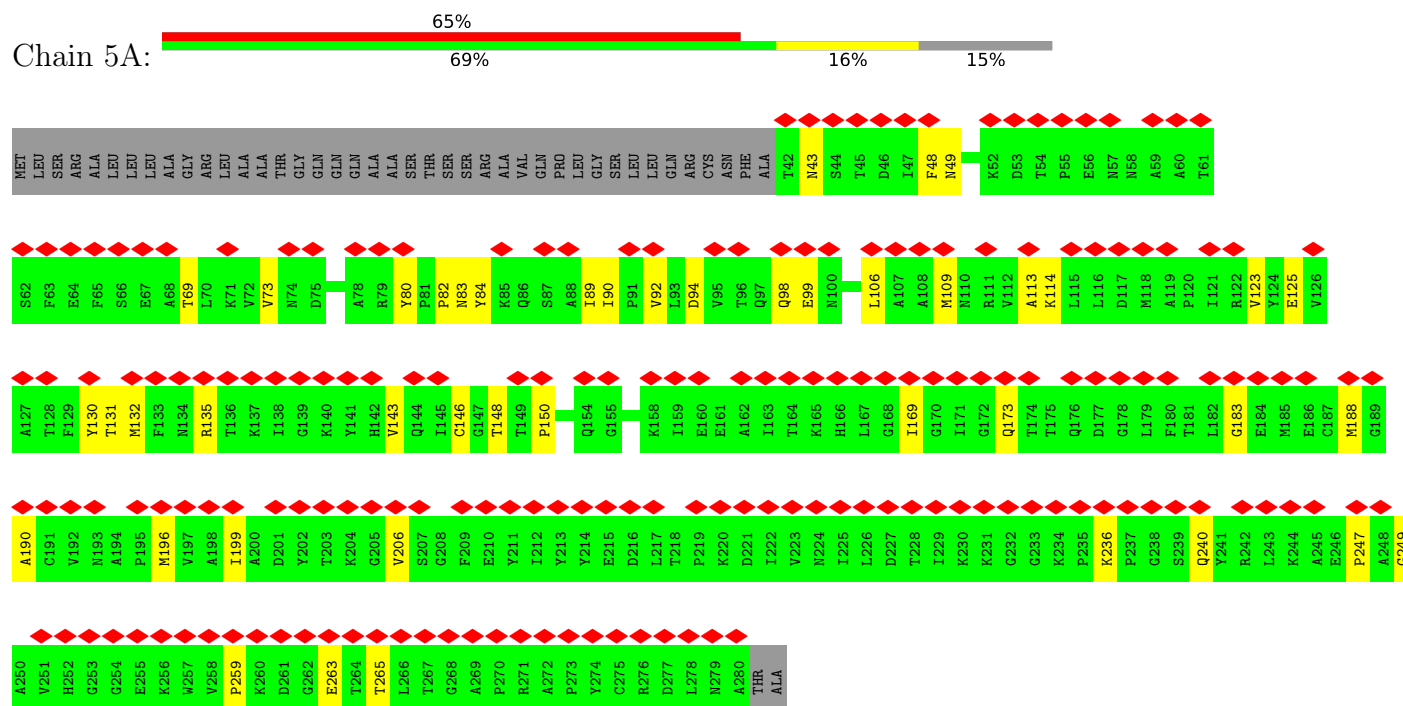
- Molecule 22: CoxIn

Chain 9L:



- Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

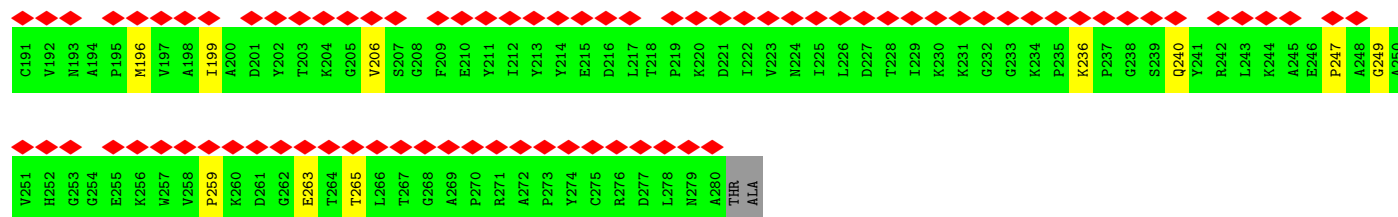
Chain 5A:



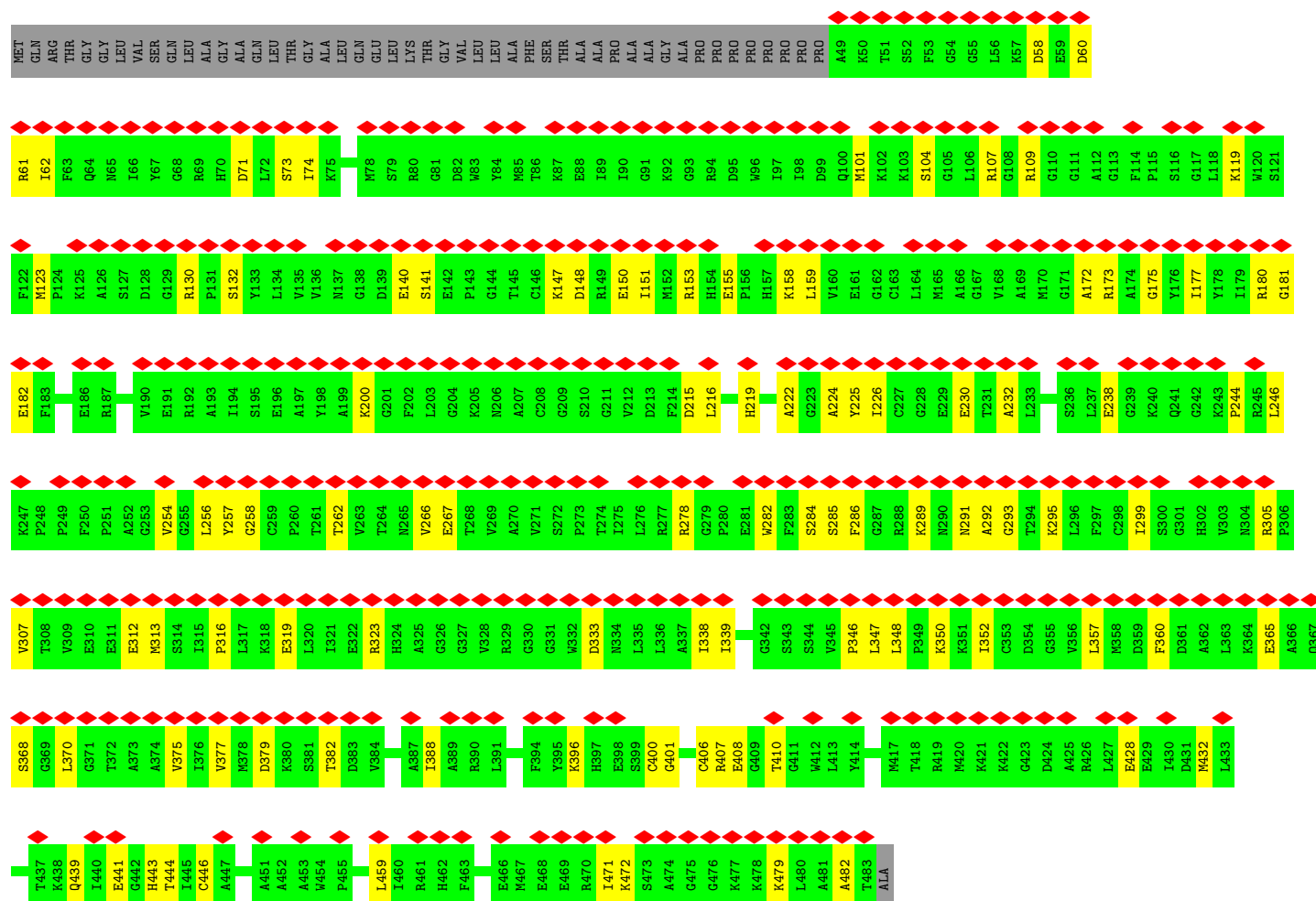
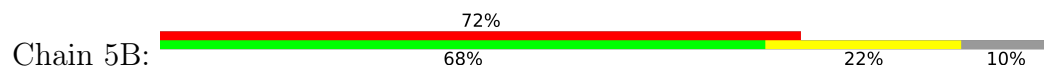
- Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

Chain A:

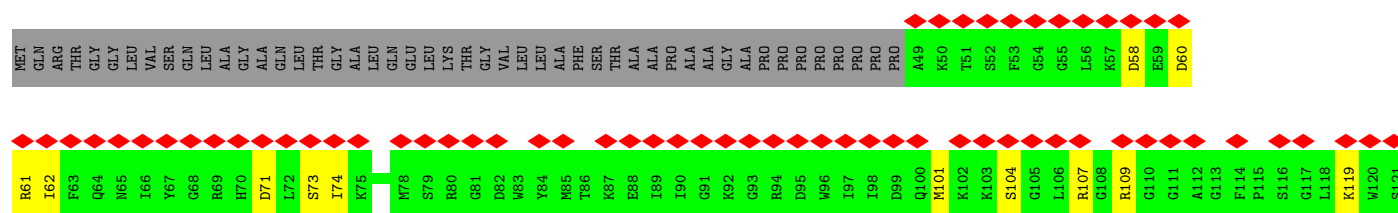


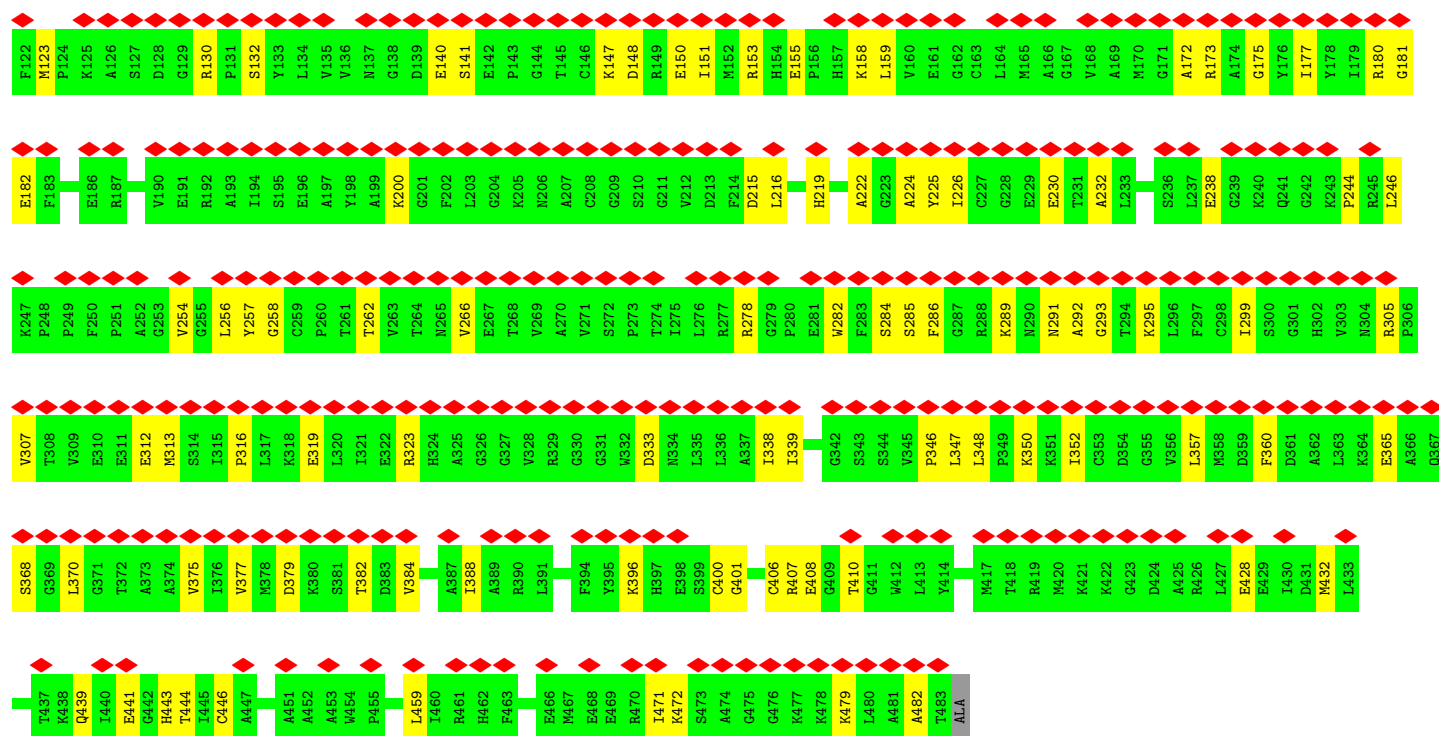


• Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

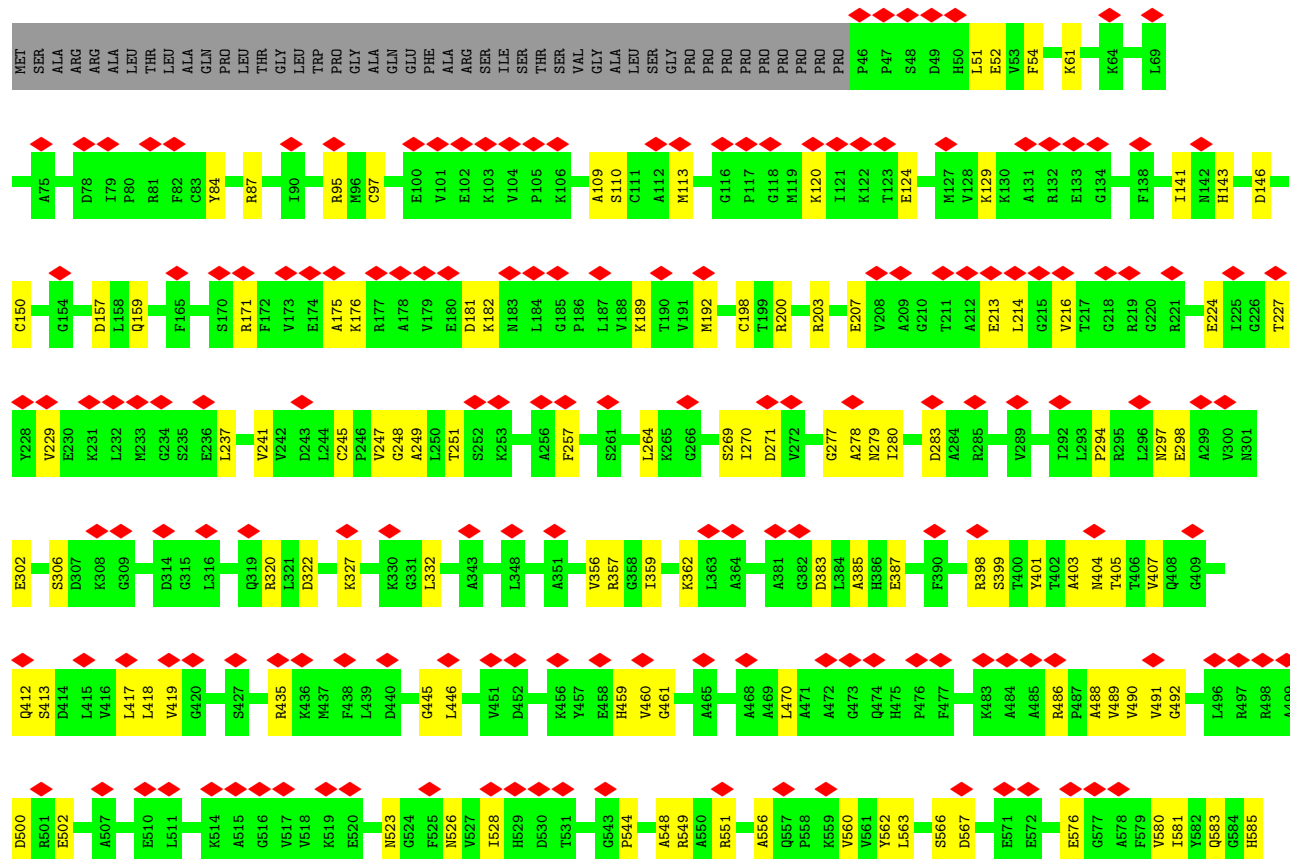
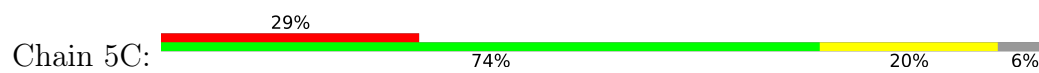


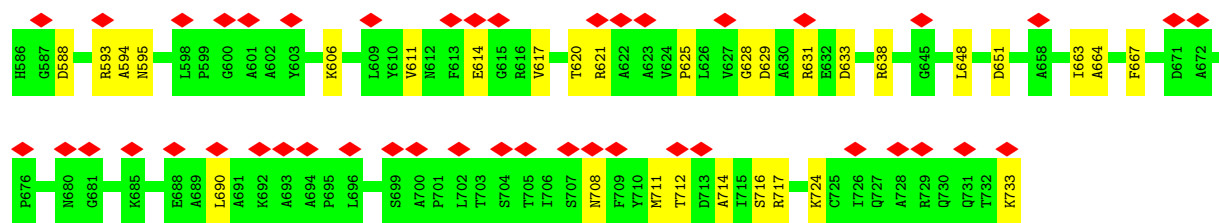
• Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



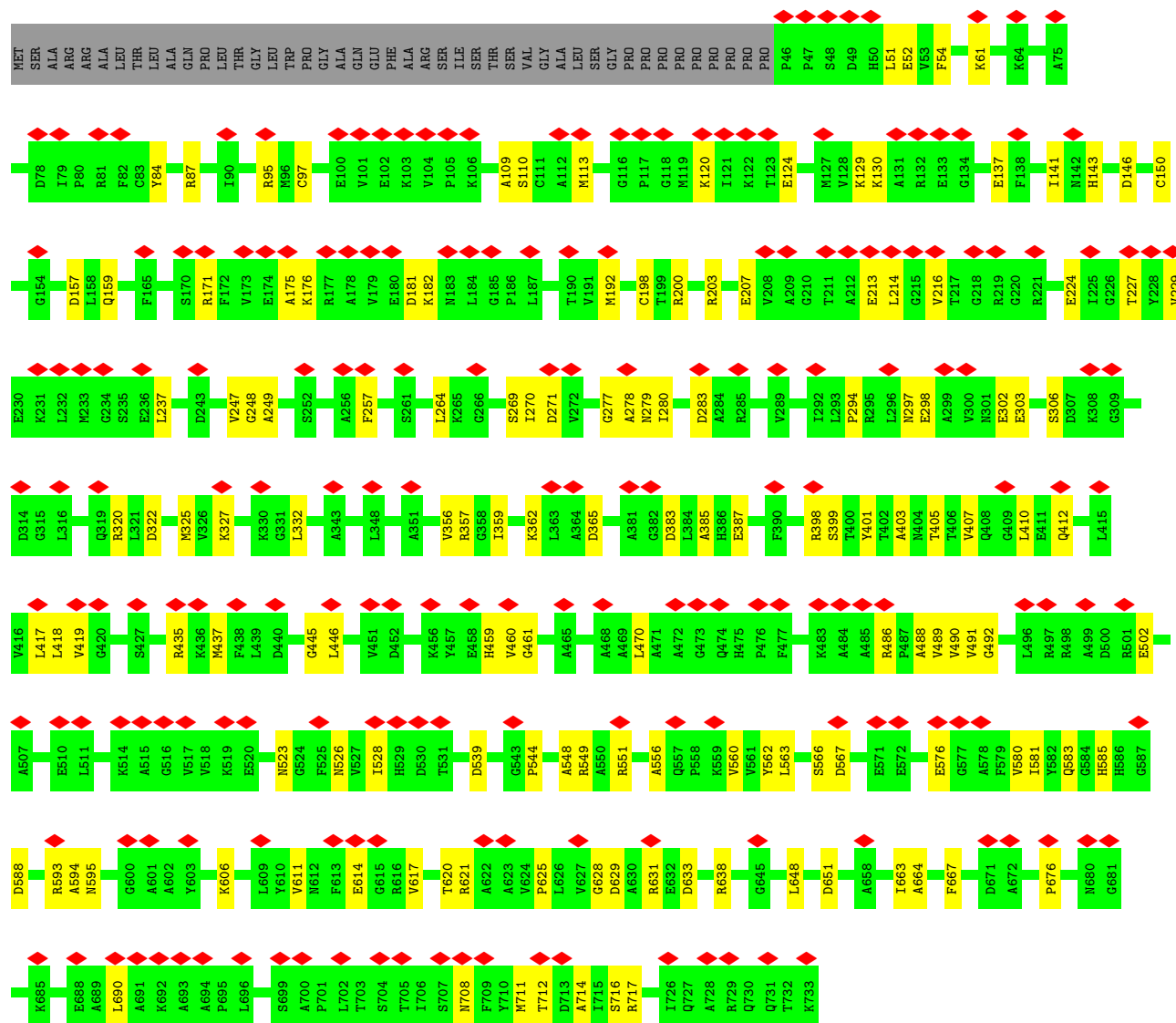
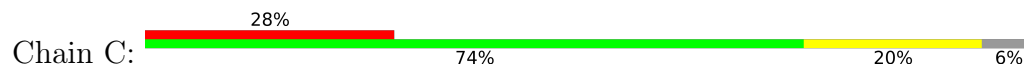


• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

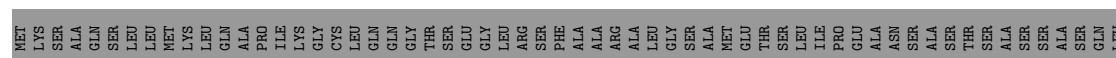


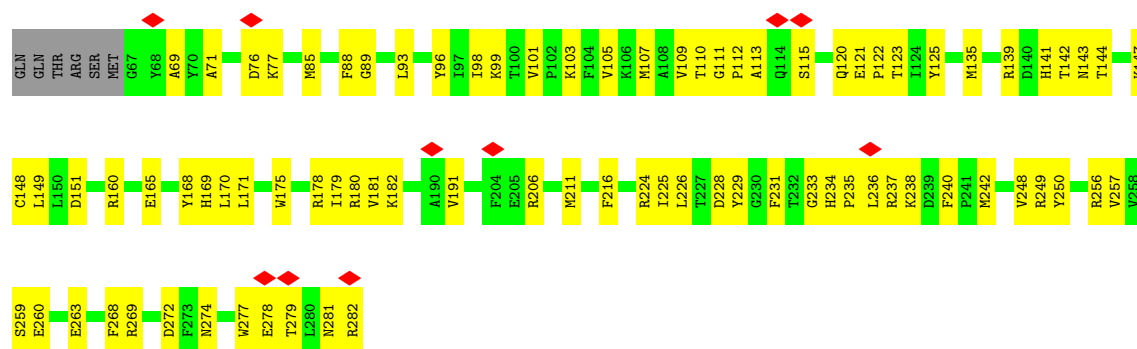


• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

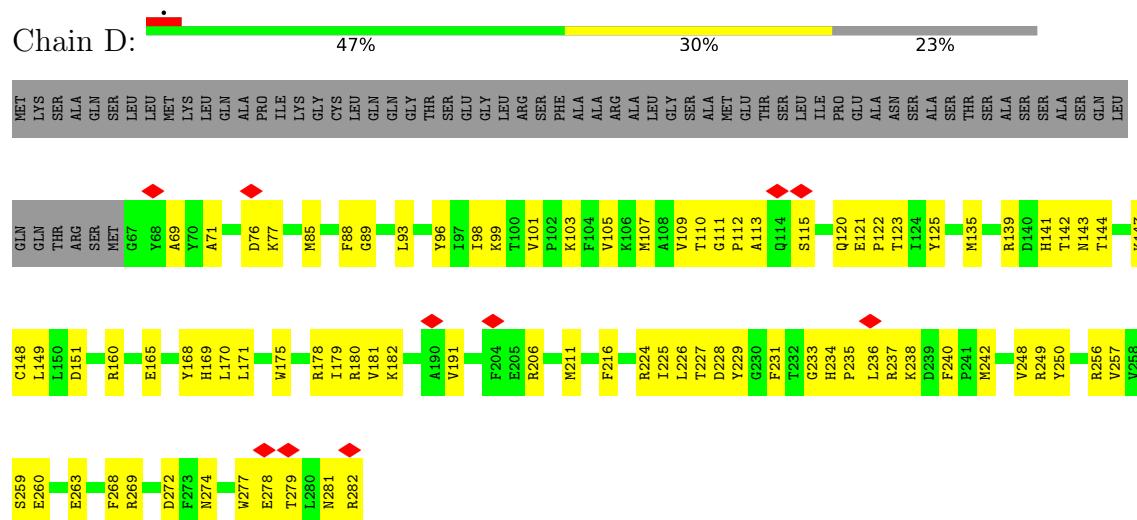


• Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

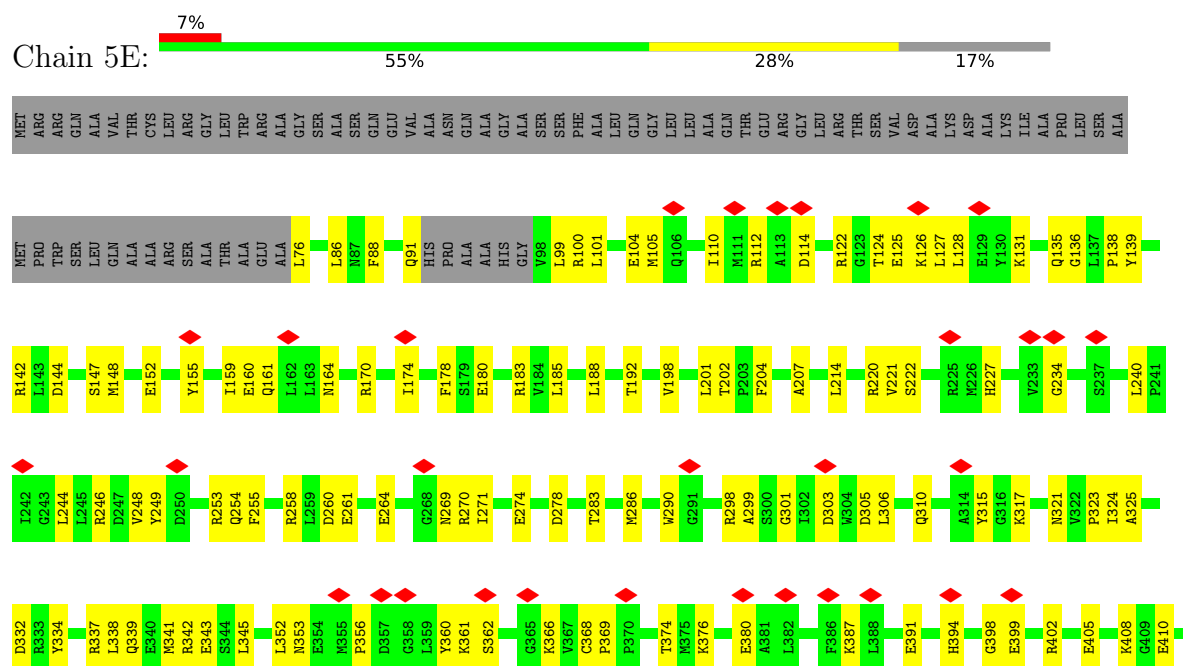


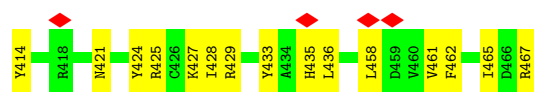


- Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

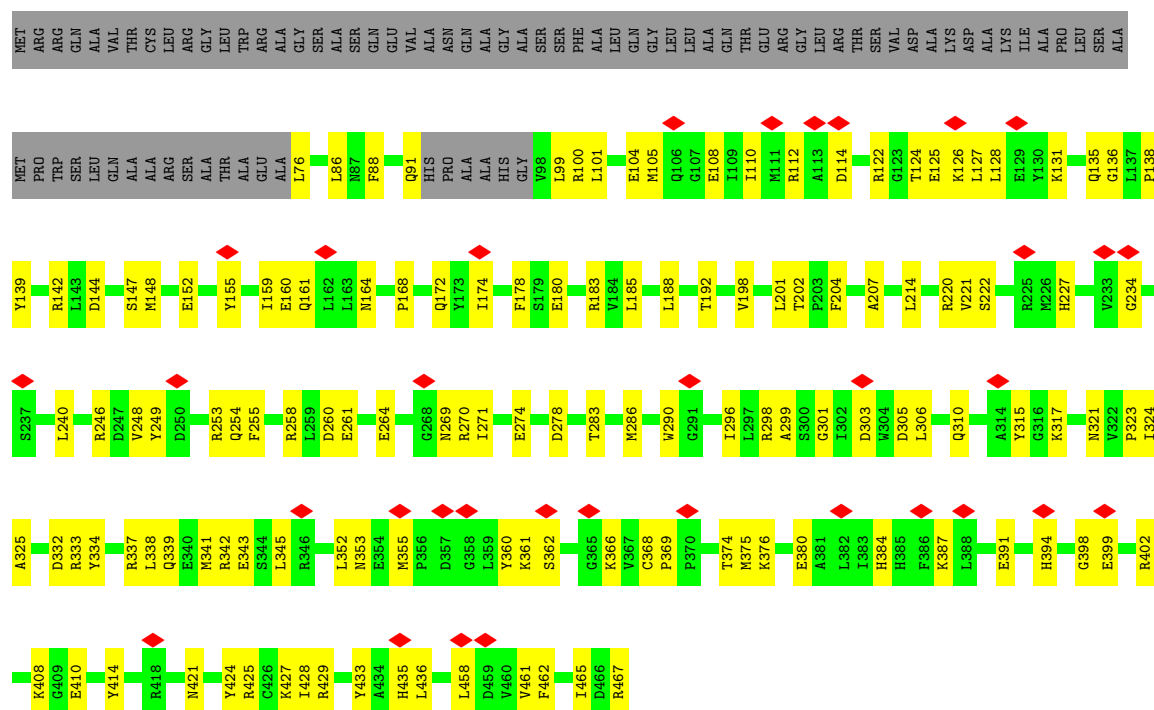


- Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit

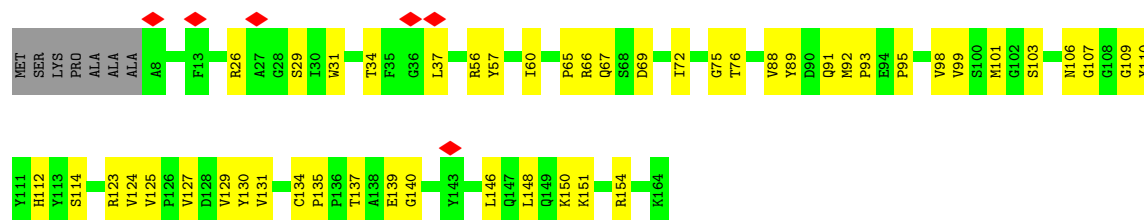




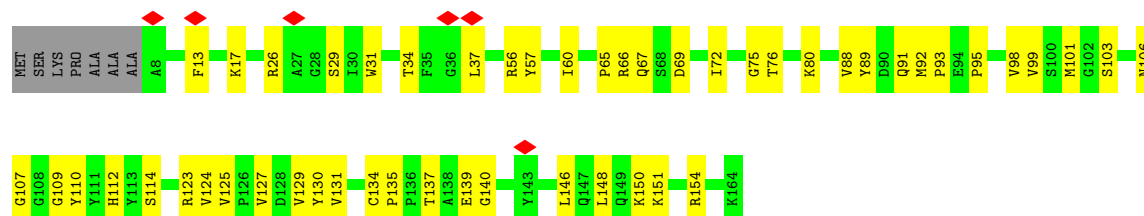
- Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit



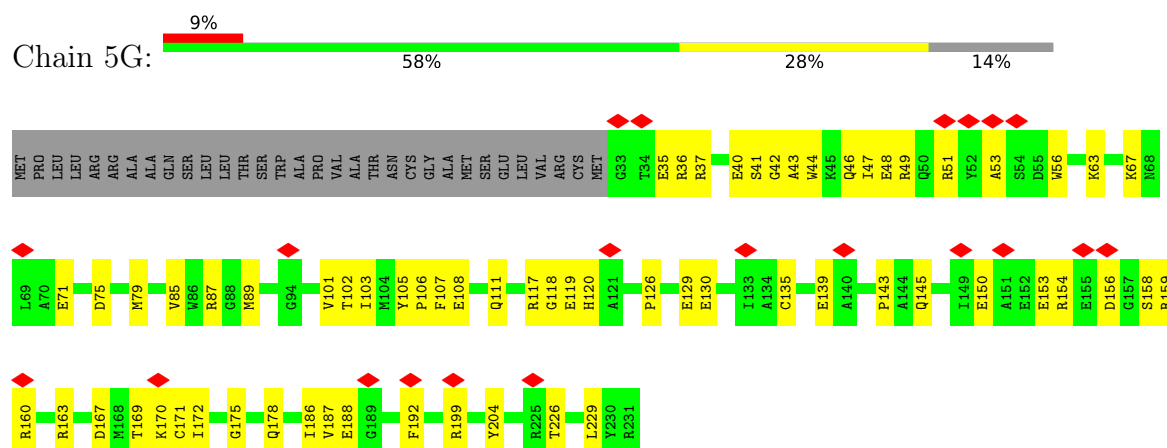
- Molecule 28: NADH:ubiquinone oxidoreductase subunit 10



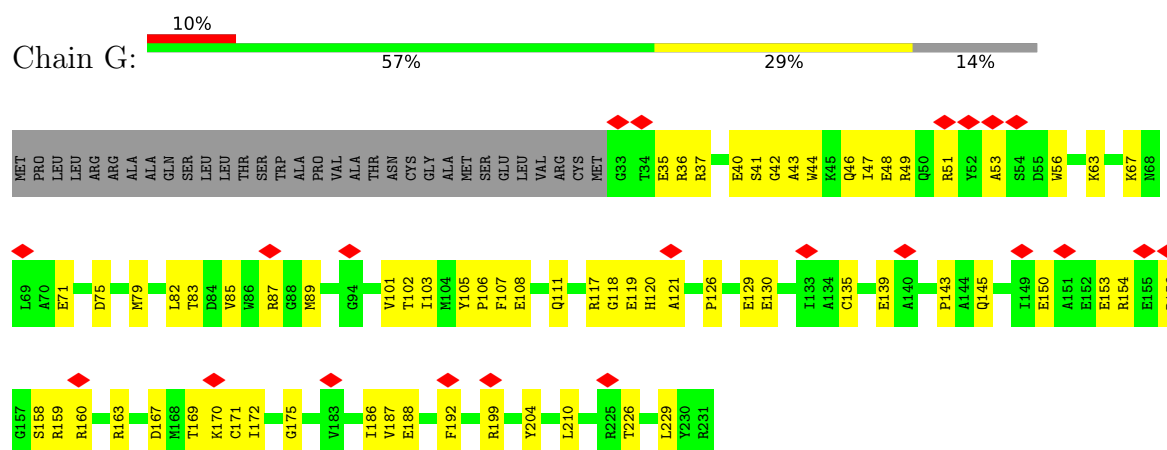
- Molecule 28: NADH:ubiquinone oxidoreductase subunit 10



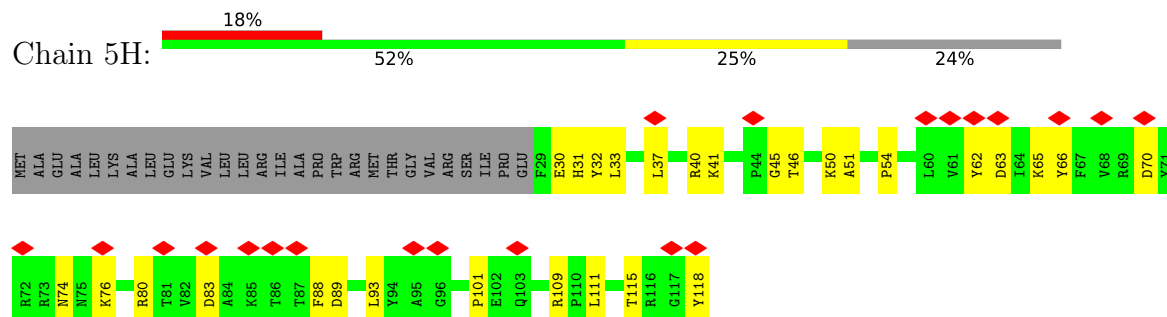
- Molecule 29: NADH:ubiquinone oxidoreductase subunit 8



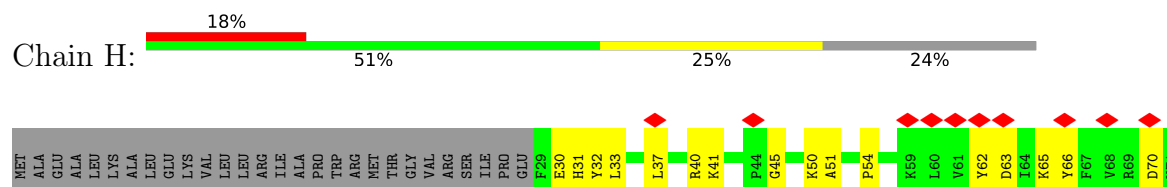
- Molecule 29: NADH:ubiquinone oxidoreductase subunit 8

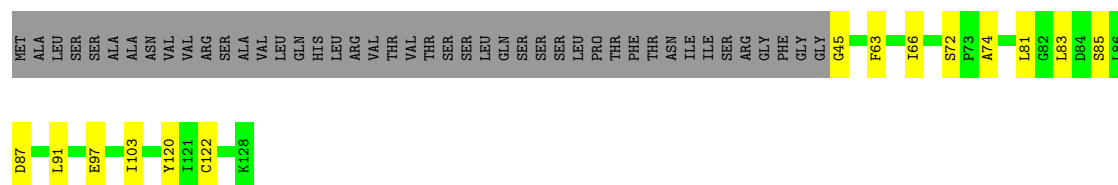


- Molecule 30: B14.5a

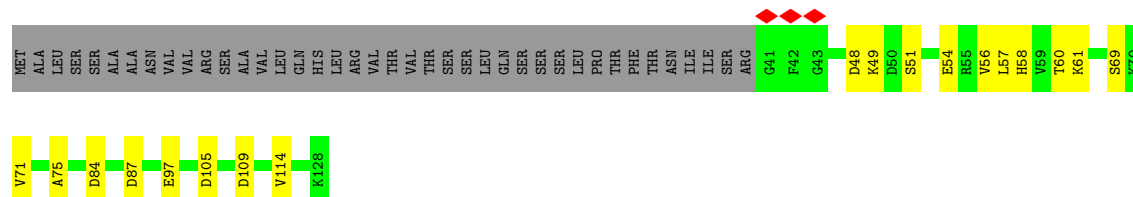


- Molecule 30: B14.5a

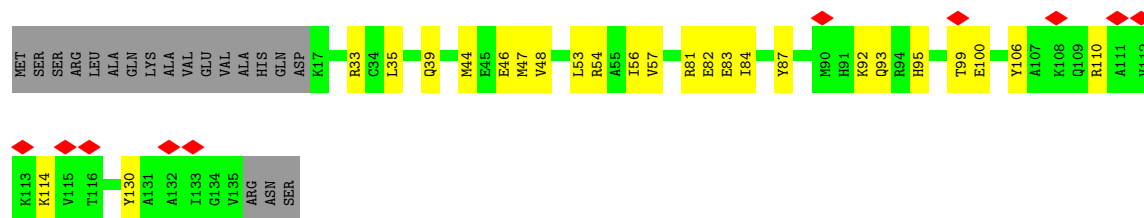




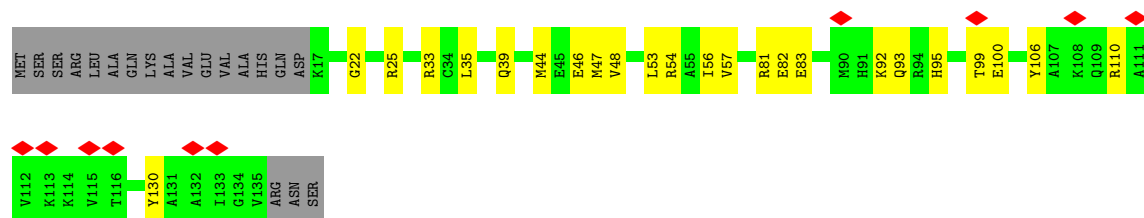
- Molecule 32: Acyl carrier protein



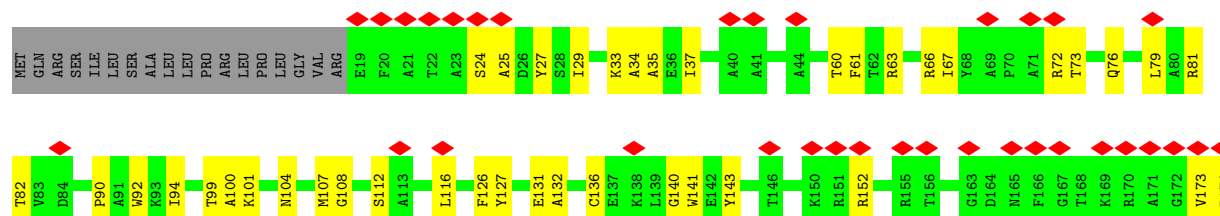
- Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

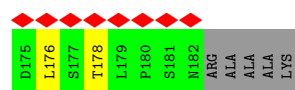


- Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

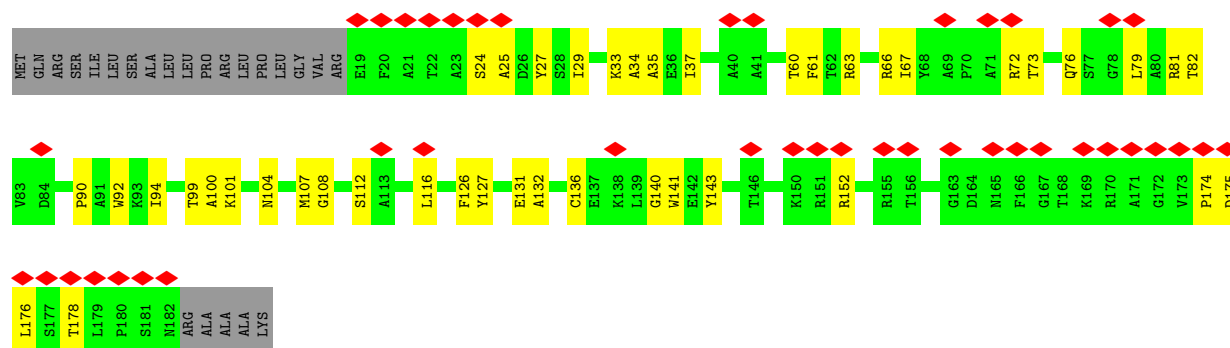


- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

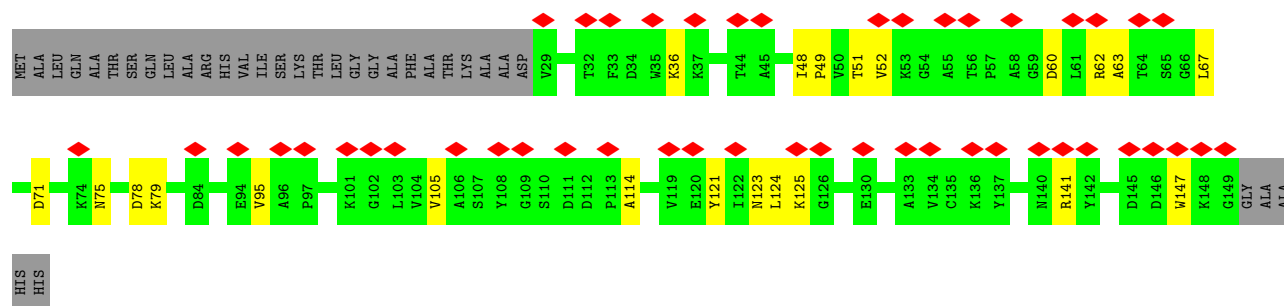




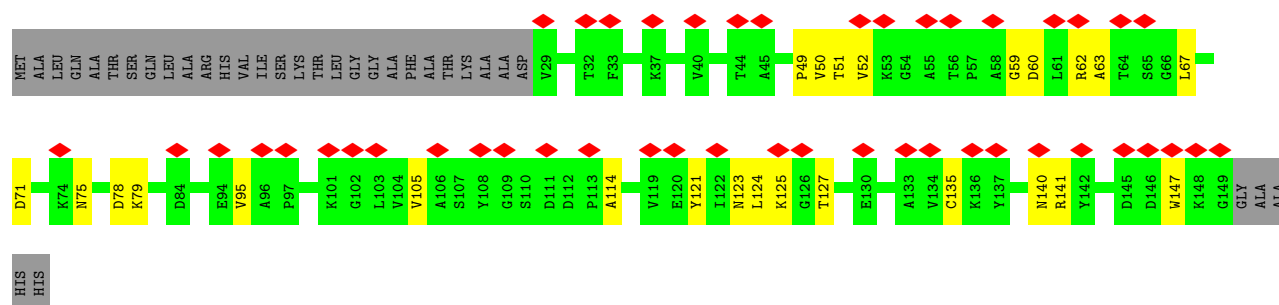
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



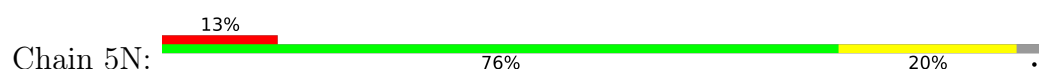
- Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit

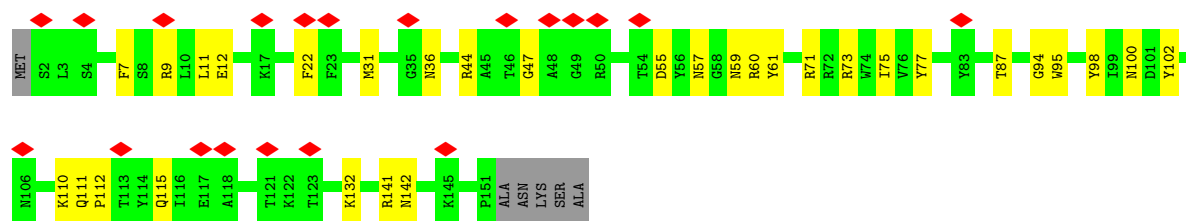


- Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit

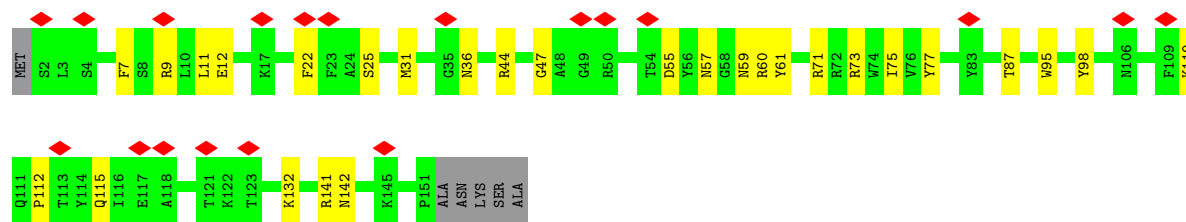
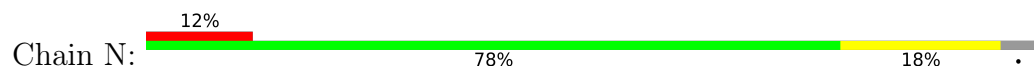


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

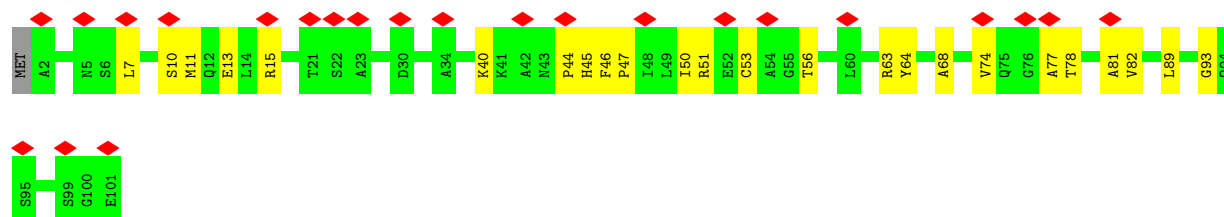
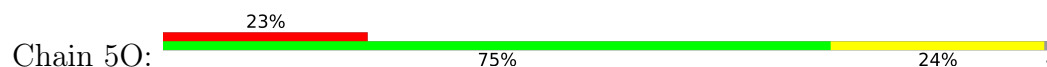




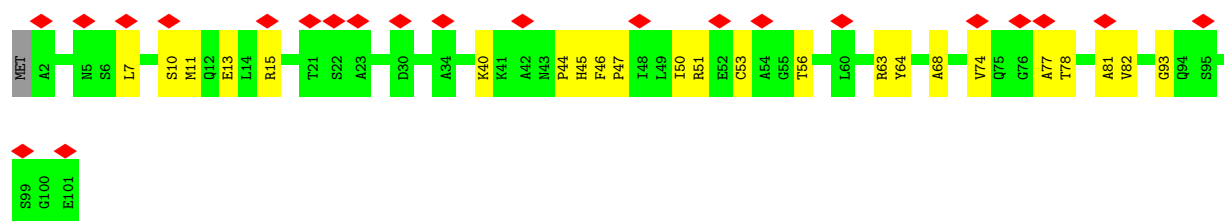
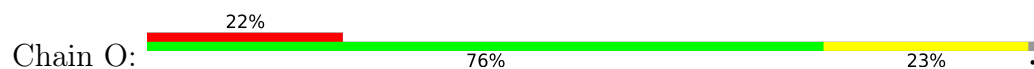
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



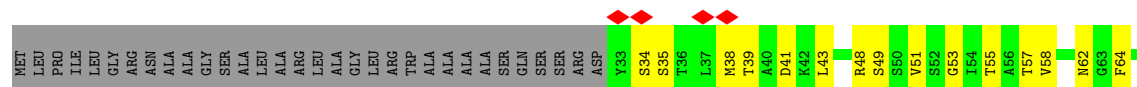
- Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit

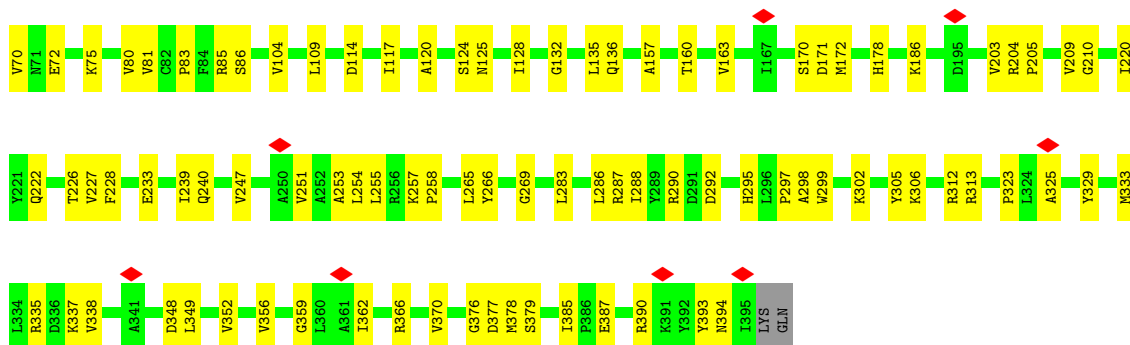


- Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit



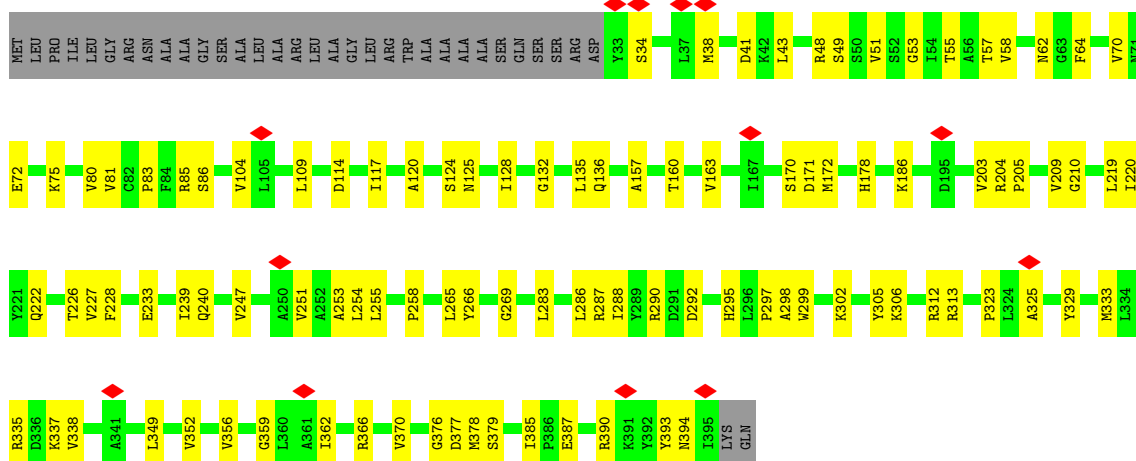
- Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit





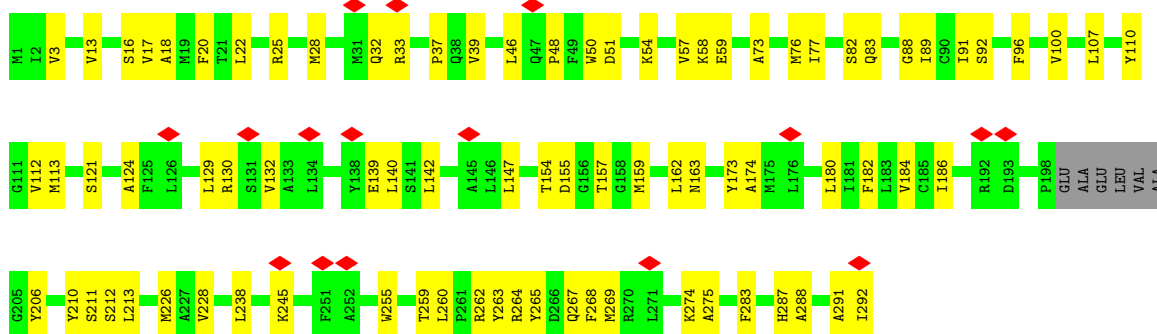
- Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

Chain P: 66% 25% 9%



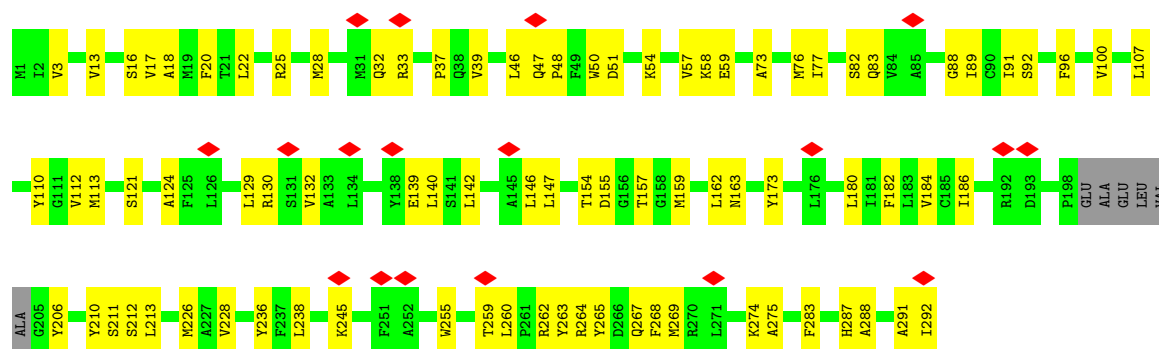
- Molecule 39: NADH-ubiquinone oxidoreductase chain 1

Chain 5Q: 5% 70% 28%



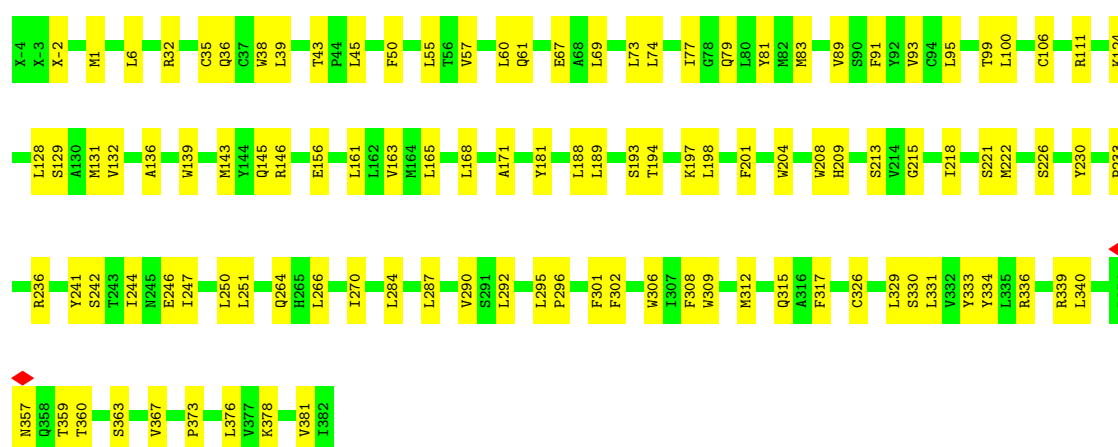
- Molecule 39: NADH-ubiquinone oxidoreductase chain 1

Chain Q: 6% 69% 29%



• Molecule 40: NADH-ubiquinone oxidoreductase chain 2

Chain 5R: 72% 28%



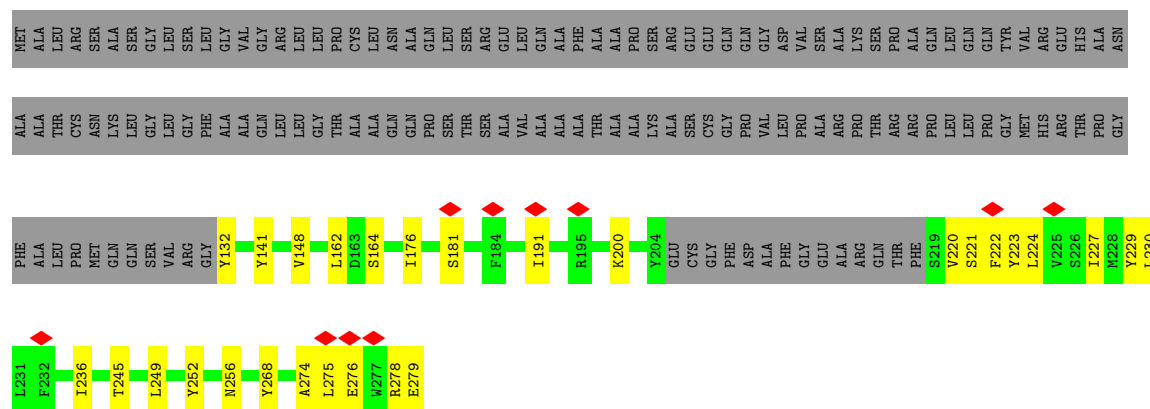
• Molecule 40: NADH-ubiquinone oxidoreductase chain 2

Chain R: 70% 30%

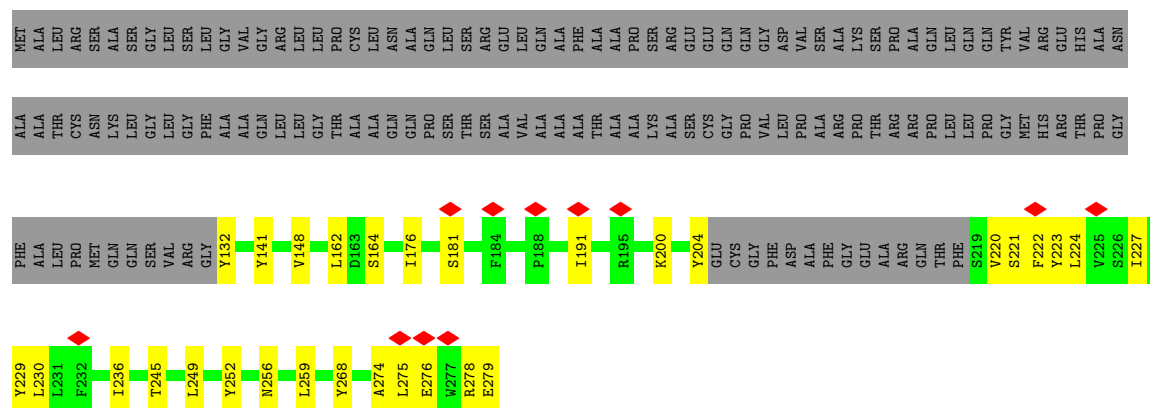
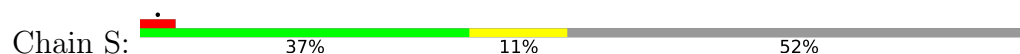


• Molecule 41: NADH-ubiquinone oxidoreductase chain 3

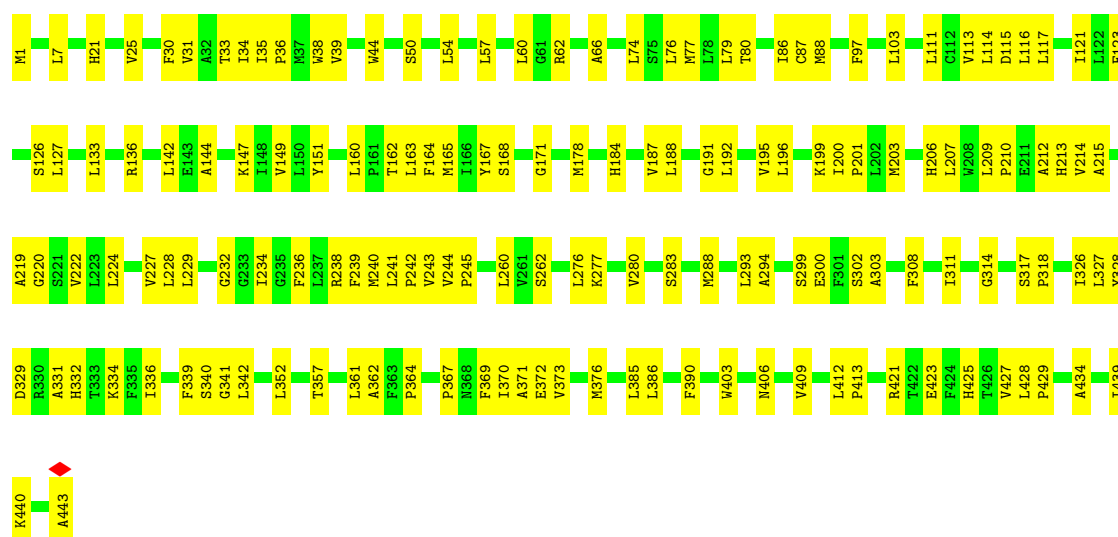
Chain 5S: 38% 10% 52%



• Molecule 41: NADH-ubiquinone oxidoreductase chain 3



• Molecule 42: NADH-ubiquinone oxidoreductase chain 4



• Molecule 42: NADH-ubiquinone oxidoreductase chain 4

- Molecule 43: NADH dehydrogenase subunit 4L

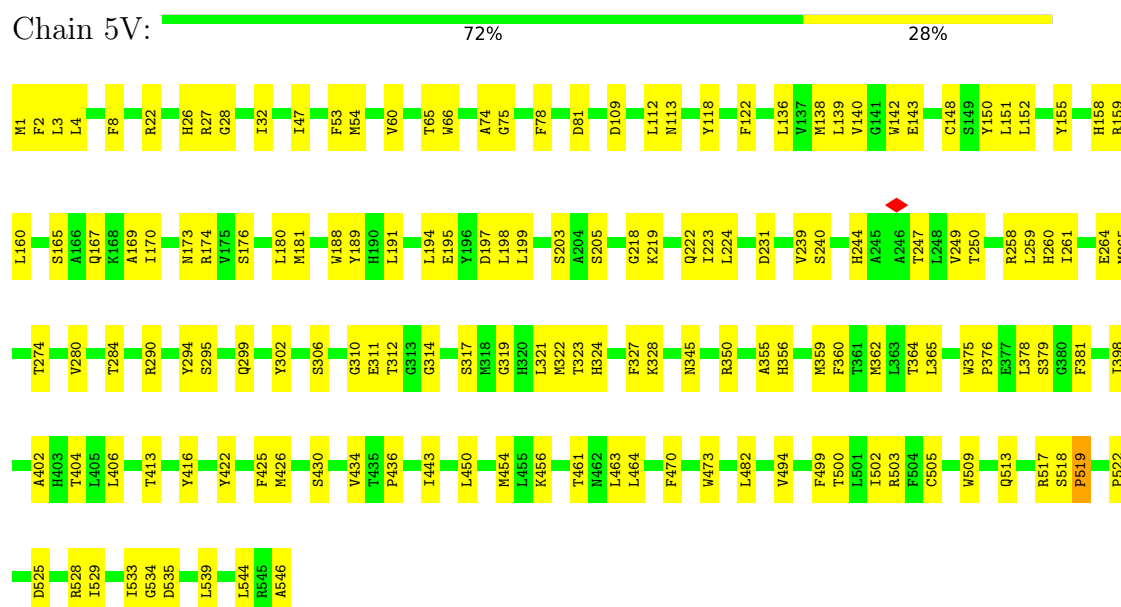
[illegible]

- Molecule 43: NADH dehydrogenase subunit 4L

L226	K227	ARG	Y123	Y136	M141	F142	W143	I146	V150	R154	N155	L156	I157	I158	A163	E164	M167	L168	A169	M172	A178	N182	D183	I184	T185	G186	A187	I191	T192	A198	C199	E200	T201	A202	I203	G204	L205	F212	S216	D219	V220	E221	A222	W226																	
PHE	ALA	ASN	ILE	VAL	ASN	ARG	PRO	MET	ARG	VAL	PRO	LEU	ALA	THR	THR	GLY	PHE	ALA	ALA	PHE	SER	PRO	LEU	MET	GLN	THR	ALA	PRO	VAL	ALA	ASN	GLY	LEU	GLN	GLY	ALA	GLN	LYS	GLN	GLN	GLY	SER	GLN	PRO	ALA	SER	SER	ALA	LEU	VAL	ALA										
MET	SER	ARG	THR	GLN	LEU	LEU	ARG	LEU	PRO	GLY	VAL	PRO	PRO	THR	ALA	ALA	GLY	PHE	ALA	ALA	SER	SER	GLN	SER	CYS	THR	ALA	VAL	PRO	ALA	ASN	GLY	LEU	GLN	GLN	GLY	CYS	PHE	PHE	SER	SER	HIS	GLU	GLU	GLU	GLN	GLN	LYS	GLN	GLN	SER	SER	GLN	PRO	ALA	SER	SER	ALA	LEU	VAL	GLN

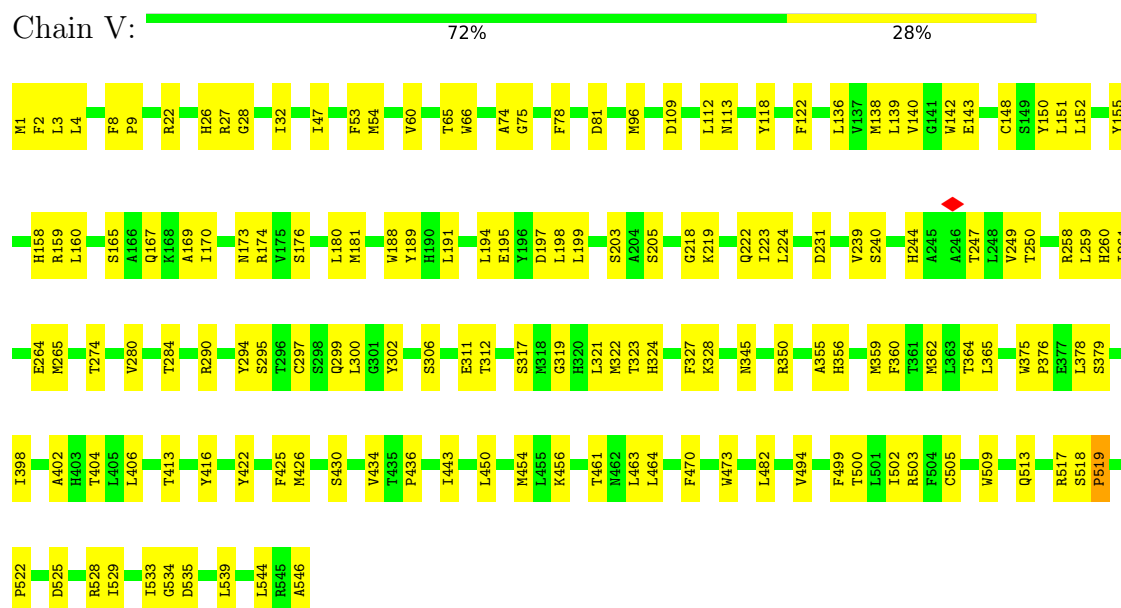
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain 5V:



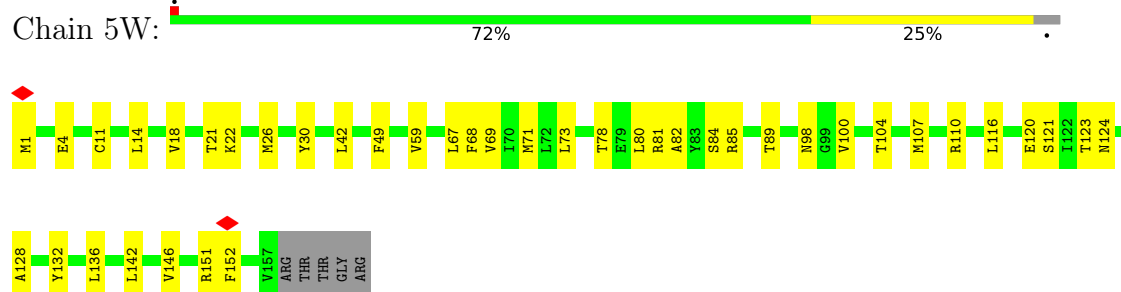
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain V:



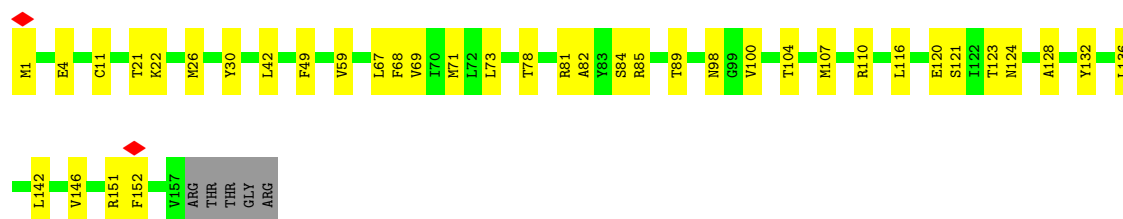
- Molecule 45: NADH-ubiquinone oxidoreductase chain 6

Chain 5W:



- Molecule 45: NADH-ubiquinone oxidoreductase chain 6

Chain W:  73% 23%



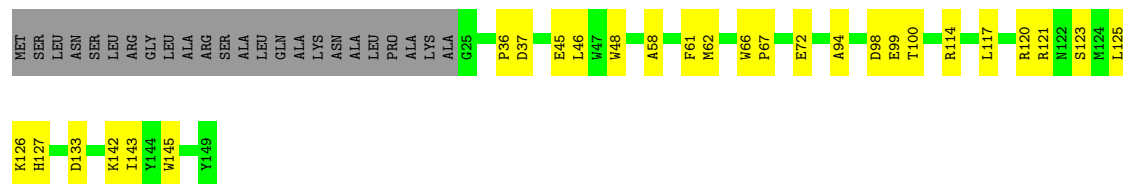
- Molecule 46: ASHI

Chain 5X:  64% 19% 16%



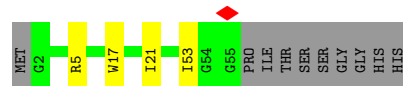
- Molecule 46: ASHI

Chain X:  66% 18% 16%



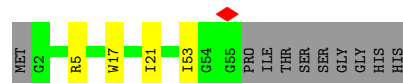
- Molecule 47: P9

Chain 5Y:  78% 6% 16%



- Molecule 47: P9

Chain Y:  78% 6% 16%

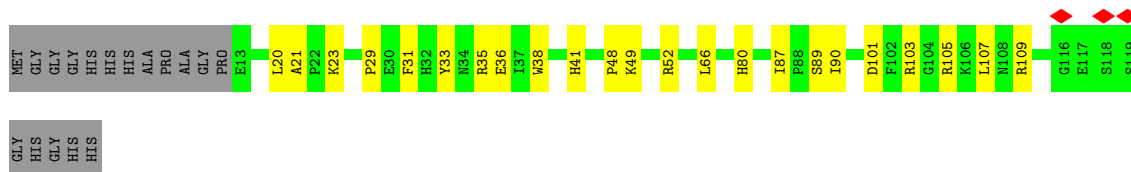


- Molecule 48: KFYI

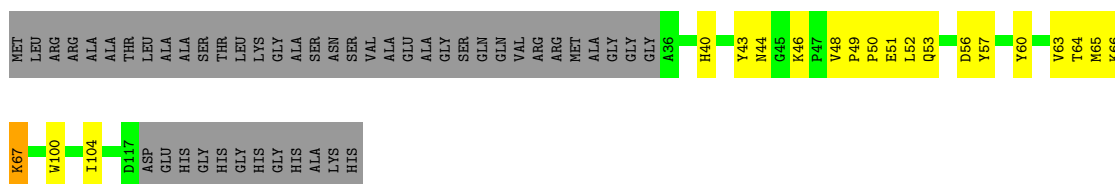
Chain 5Z:  71% 15% 14%



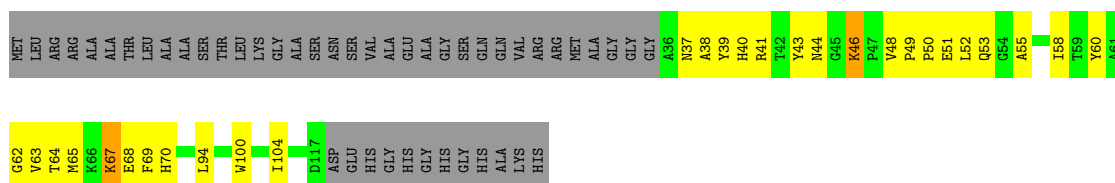
• Molecule 48: KFYI



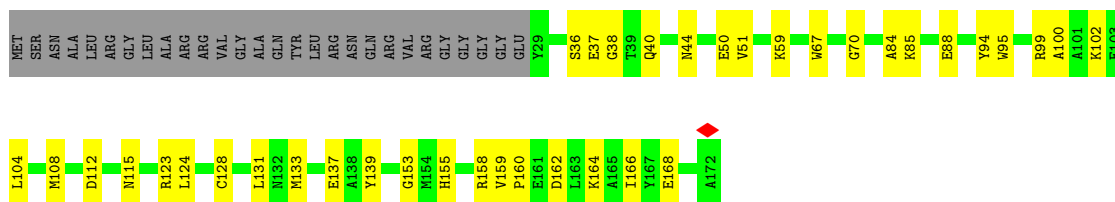
• Molecule 49: AGGG



• Molecule 49: AGGG



• Molecule 50: ESSS

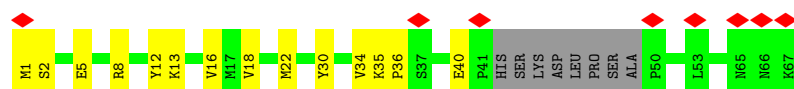


• Molecule 50: ESSS

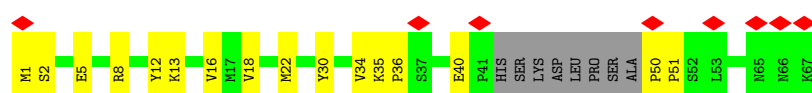




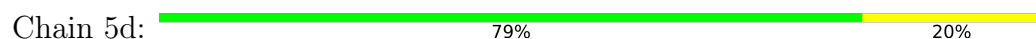
- Molecule 51: B9



- Molecule 51: B9



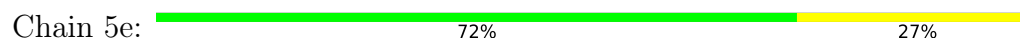
- Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit



- Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit

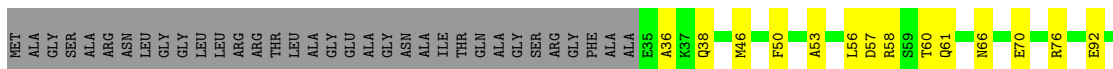


- Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit



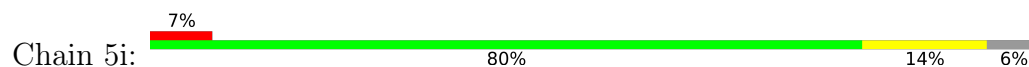
- Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit



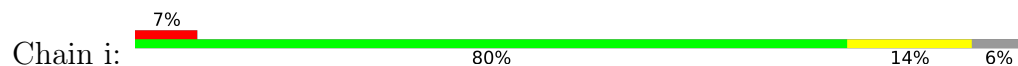




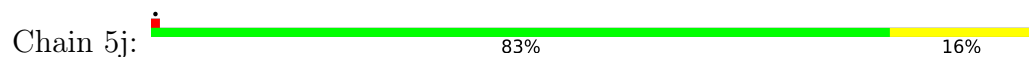
- Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like



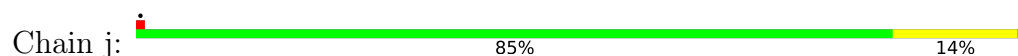
- Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like



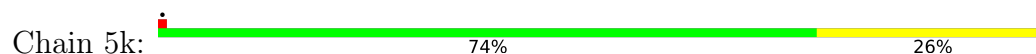
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



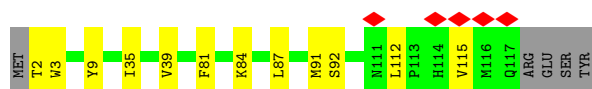
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





- Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

Chain 5l: 86% 10%



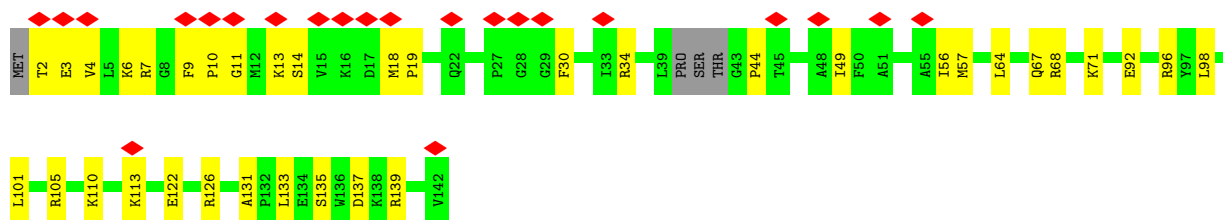
- Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

Chain l: 85% 11%



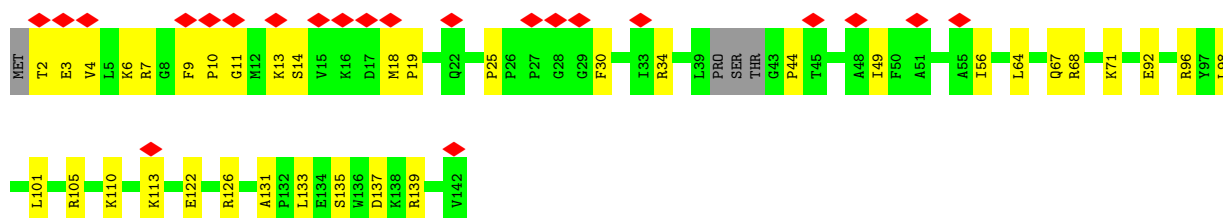
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain 5m: 15% 72% 25%



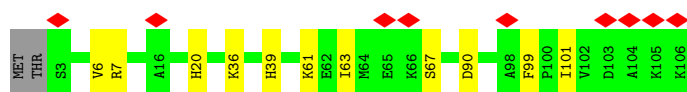
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain m: 15% 72% 25%

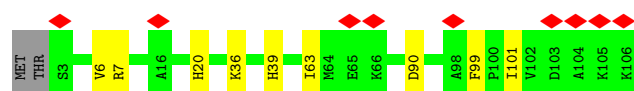
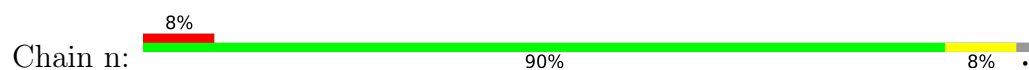


- Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

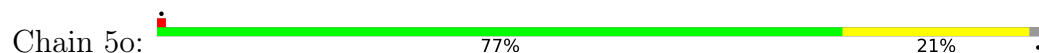
Chain 5n: 8% 88% 10%



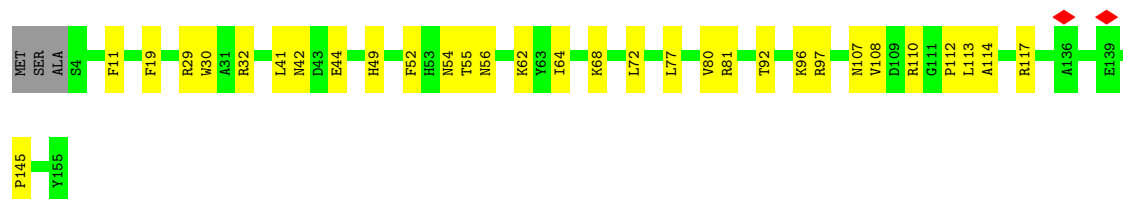
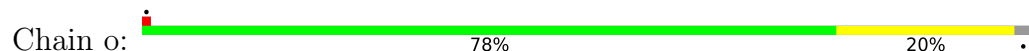
- Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit



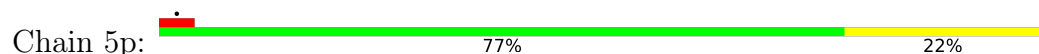
- Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit



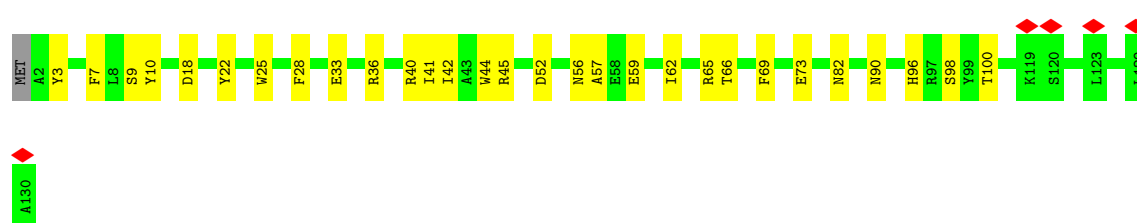
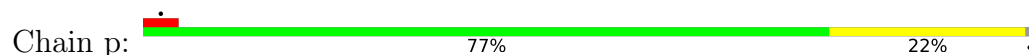
- Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit



- Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

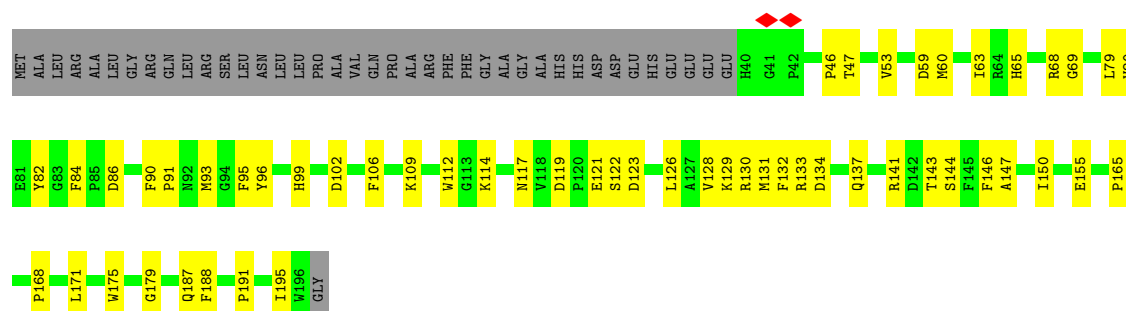


- Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

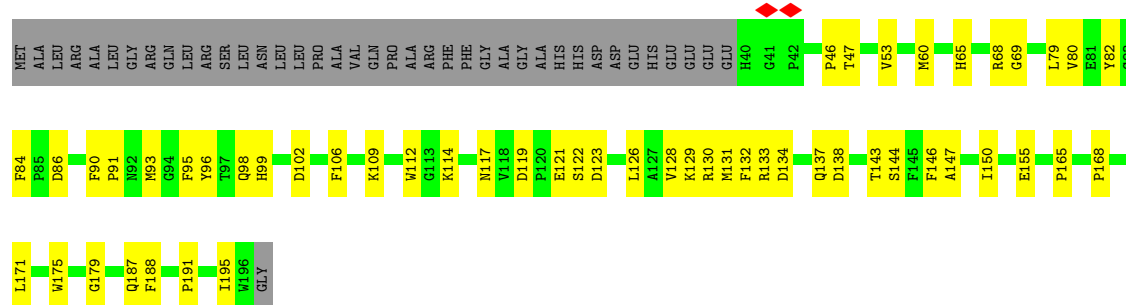


- Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

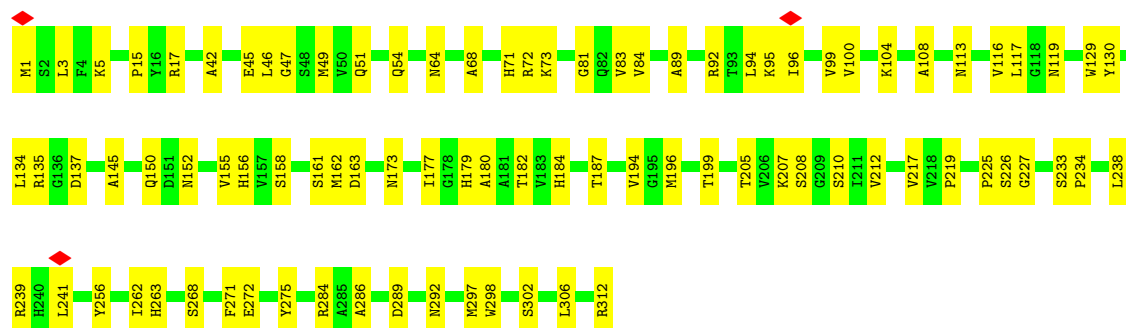




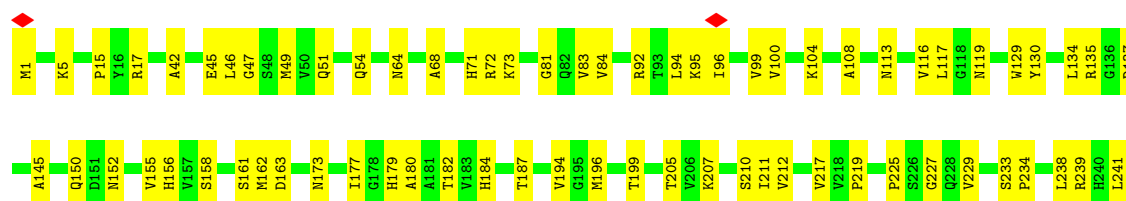
- Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

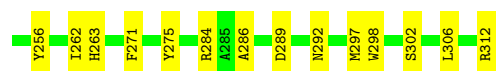


- Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

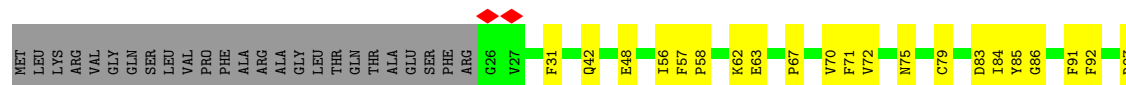


- Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

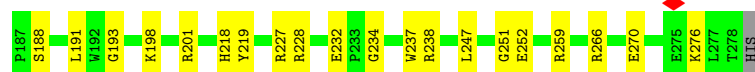




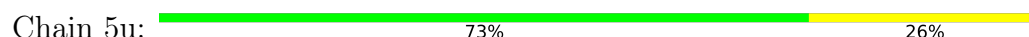
• Molecule 67: CAG2 - CA-like



• Molecule 67: CAG2 - CA-like



• Molecule 68: CAG1

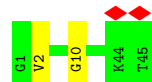


• Molecule 68: CAG1

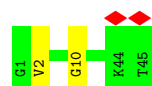




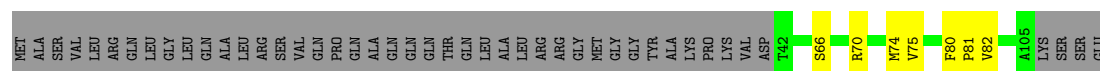
- Molecule 69: P10



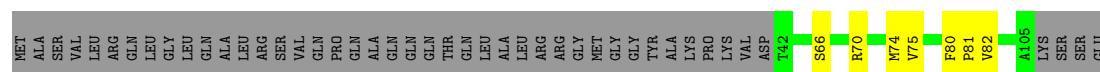
- Molecule 69: P10



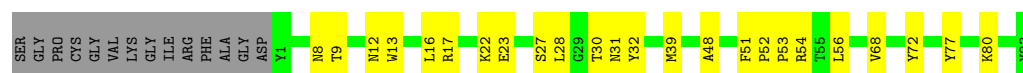
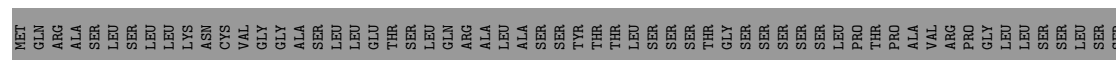
- Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit



- Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit



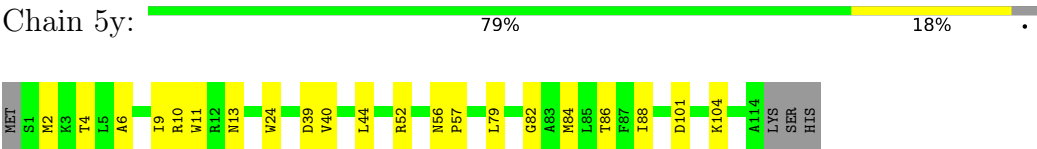
- Molecule 71: NUOP8



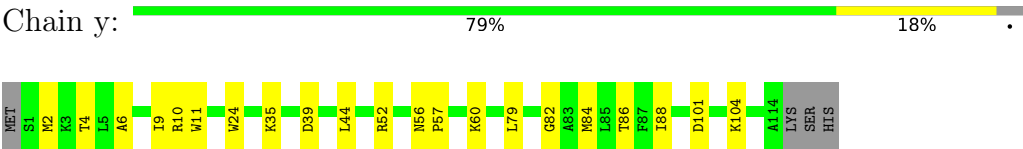
- Molecule 71: NUOP8



● Molecule 72: NUOP7



● Molecule 72: NUOP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	14488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	143.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	64000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.803	Depositor
Minimum map value	-0.297	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	550.08, 550.08, 550.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.9100001, 1.9100001, 1.9100001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, HEA, COO, NDP, CUA, SF4, HEC, MG, CU, ZN, 8Q1, HEM, FES

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	1A	0.25	0/3060	0.48	1/4187 (0.0%)
1	1B	0.26	0/3060	0.48	1/4187 (0.0%)
1	6A	0.26	0/3060	0.48	1/4187 (0.0%)
1	6B	0.26	0/3060	0.48	1/4187 (0.0%)
2	1C	0.18	0/1643	0.36	0/2233
2	1D	0.17	0/1643	0.34	0/2233
2	6C	0.19	0/1643	0.36	0/2233
2	6D	0.18	0/1643	0.33	0/2233
3	1E	0.24	0/1953	0.43	1/2654 (0.0%)
3	1F	0.22	0/1953	0.38	0/2654
3	6E	0.24	0/1953	0.43	1/2654 (0.0%)
3	6F	0.22	0/1953	0.38	0/2654
4	1G	0.23	0/496	0.41	0/667
4	1H	0.22	0/496	0.39	0/667
4	6G	0.24	0/496	0.41	0/667
4	6H	0.22	0/496	0.39	0/667
5	1I	0.23	0/567	0.45	0/766
5	1J	0.21	0/567	0.39	0/766
5	6I	0.23	0/567	0.45	0/766
5	6J	0.21	0/567	0.39	0/766
6	1K	0.26	0/609	0.44	0/817
6	1L	0.22	0/609	0.42	0/817
6	6K	0.26	0/609	0.44	0/817
6	6L	0.22	0/609	0.42	0/817
7	1M	0.23	0/3723	0.42	0/5046
7	1N	0.22	0/3723	0.38	0/5046
7	6M	0.23	0/3723	0.42	0/5046
7	6N	0.22	0/3723	0.39	0/5046
8	1O	0.20	0/385	0.44	0/531
8	1P	0.21	0/385	0.52	0/531
8	6O	0.20	0/385	0.43	0/531
8	6P	0.21	0/385	0.51	0/531

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	1Q	0.30	0/3258	0.51	1/4439 (0.0%)
9	1S	0.21	0/3258	0.43	1/4439 (0.0%)
9	6Q	0.29	0/3258	0.49	0/4439
9	6S	0.21	0/3258	0.43	1/4439 (0.0%)
10	1R	0.28	0/996	0.59	3/1349 (0.2%)
10	1T	0.28	0/996	0.50	2/1349 (0.1%)
10	6R	0.28	0/996	0.59	3/1349 (0.2%)
10	6T	0.28	0/996	0.50	2/1349 (0.1%)
11	2A	0.26	0/4011	0.51	3/5484 (0.1%)
11	3A	0.27	0/4011	0.54	1/5484 (0.0%)
11	4A	0.27	0/4011	0.54	1/5484 (0.0%)
11	7A	0.26	0/4011	0.51	3/5484 (0.1%)
11	8A	0.27	0/4011	0.54	1/5484 (0.0%)
11	9A	0.28	0/4011	0.54	1/5484 (0.0%)
12	2B	0.24	0/1204	0.45	0/1641
12	3B	0.24	0/1204	0.46	0/1641
12	4B	0.24	0/1204	0.46	0/1641
12	7B	0.24	0/1204	0.45	0/1641
12	8B	0.24	0/1204	0.46	0/1641
12	9B	0.24	0/1204	0.46	0/1641
13	2C	0.21	0/1237	0.41	0/1676
13	3C	0.25	0/1237	0.46	0/1676
13	4C	0.25	0/1237	0.46	0/1676
13	7C	0.21	0/1237	0.41	0/1676
13	8C	0.24	0/1237	0.46	0/1676
13	9C	0.25	0/1237	0.46	0/1676
14	2D	0.24	0/2152	0.47	0/2937
14	3D	0.24	0/2152	0.49	0/2937
14	4D	0.24	0/2152	0.49	0/2937
14	7D	0.24	0/2152	0.47	0/2937
14	8D	0.24	0/2152	0.49	0/2937
14	9D	0.25	0/2152	0.49	0/2937
15	2E	0.24	0/757	0.62	3/1029 (0.3%)
15	3E	0.24	0/757	0.61	2/1029 (0.2%)
15	4E	0.25	0/757	0.61	2/1029 (0.2%)
15	7E	0.24	0/757	0.62	3/1029 (0.3%)
15	8E	0.25	0/757	0.61	2/1029 (0.2%)
15	9E	0.25	0/757	0.61	2/1029 (0.2%)
16	2F	0.19	0/726	0.35	0/974
16	3F	0.19	0/726	0.38	0/974
16	4F	0.19	0/726	0.38	0/974
16	7F	0.19	0/726	0.35	0/974
16	8F	0.19	0/726	0.38	0/974

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	9F	0.19	0/726	0.38	0/974
17	2G	0.27	0/762	0.57	0/1038
17	3G	0.27	0/762	0.52	0/1038
17	4G	0.27	0/762	0.52	0/1038
17	7G	0.27	0/762	0.57	0/1038
17	8G	0.27	0/762	0.52	0/1038
17	9G	0.27	0/762	0.52	0/1038
18	2H	0.20	0/980	0.42	0/1325
18	3H	0.23	0/980	0.52	1/1325 (0.1%)
18	4H	0.23	0/980	0.52	1/1325 (0.1%)
18	7H	0.20	0/980	0.42	0/1325
18	8H	0.23	0/980	0.52	1/1325 (0.1%)
18	9H	0.23	0/980	0.52	1/1325 (0.1%)
19	2I	0.24	0/619	0.46	0/839
19	3I	0.21	0/619	0.45	0/839
19	4I	0.22	0/619	0.45	0/839
19	7I	0.24	0/619	0.47	0/839
19	8I	0.21	0/619	0.45	0/839
19	9I	0.22	0/619	0.45	0/839
20	2J	0.21	0/839	0.39	0/1143
20	3J	0.23	0/839	0.43	0/1143
20	4J	0.23	0/812	0.42	0/1108
20	7J	0.22	0/839	0.39	0/1143
20	8J	0.23	0/839	0.43	0/1143
20	9J	0.23	0/812	0.42	0/1108
21	2K	0.20	0/392	0.39	0/531
21	3K	0.24	0/392	0.40	0/531
21	4K	0.24	0/392	0.41	0/531
21	7K	0.20	0/392	0.39	0/531
21	8K	0.24	0/392	0.40	0/531
21	9K	0.24	0/392	0.41	0/531
22	2L	0.25	0/621	0.58	1/841 (0.1%)
22	3L	0.27	0/645	0.57	1/875 (0.1%)
22	4L	0.28	0/645	0.57	1/875 (0.1%)
22	7L	0.26	0/621	0.58	1/841 (0.1%)
22	8L	0.27	0/645	0.57	1/875 (0.1%)
22	9L	0.27	0/645	0.57	1/875 (0.1%)
23	5A	0.11	0/1878	0.28	0/2549
23	A	0.11	0/1878	0.29	0/2549
24	5B	0.11	0/3400	0.26	0/4573
24	B	0.10	0/3400	0.27	0/4573
25	5C	0.11	0/5272	0.27	0/7143
25	C	0.11	0/5272	0.27	0/7143

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	5D	0.11	0/1843	0.31	0/2506
26	D	0.11	0/1843	0.31	0/2506
27	5E	0.12	0/3181	0.29	0/4303
27	E	0.11	0/3181	0.29	0/4303
28	5F	0.12	0/1258	0.31	0/1706
28	F	0.11	0/1258	0.31	0/1706
29	5G	0.12	0/1648	0.31	0/2222
29	G	0.11	0/1648	0.31	0/2222
30	5H	0.10	0/773	0.31	0/1046
30	H	0.10	0/773	0.31	0/1046
31	5I	0.10	0/1061	0.27	0/1441
31	I	0.10	0/1061	0.27	0/1441
32	5J	0.12	0/649	0.31	0/875
32	5r	0.11	0/673	0.27	0/906
32	J	0.12	0/649	0.31	0/875
32	r	0.10	0/673	0.27	0/906
33	5K	0.11	0/1007	0.30	0/1348
33	K	0.11	0/1007	0.30	0/1348
34	5L	0.11	0/1306	0.30	0/1769
34	L	0.10	0/1306	0.30	0/1769
35	5M	0.11	0/936	0.27	0/1276
35	M	0.10	0/936	0.27	0/1276
36	5N	0.10	0/1277	0.26	0/1735
36	N	0.10	0/1277	0.26	0/1735
37	5O	0.11	0/772	0.31	0/1037
37	O	0.11	0/772	0.31	0/1037
38	5P	0.12	0/2879	0.31	0/3905
38	P	0.12	0/2879	0.31	0/3905
39	5Q	0.15	0/2234	0.36	0/3034
39	Q	0.15	0/2234	0.36	0/3034
40	5R	0.14	0/3075	0.36	0/4191
40	R	0.14	0/3075	0.36	0/4191
41	5S	0.14	0/1106	0.32	0/1512
41	S	0.14	0/1106	0.32	0/1512
42	5T	0.13	0/3533	0.31	0/4825
42	T	0.13	0/3533	0.31	0/4825
43	5U	0.13	0/819	0.31	0/1112
43	U	0.13	0/819	0.30	0/1112
44	5V	0.13	0/4258	0.31	0/5792
44	V	0.12	0/4258	0.31	0/5792
45	5W	0.13	0/1239	0.36	0/1686
45	W	0.13	0/1239	0.36	0/1686
46	5X	0.12	0/1081	0.33	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
46	X	0.11	0/1081	0.33	0/1479
47	5Y	0.12	0/411	0.30	0/557
47	Y	0.11	0/411	0.31	0/557
48	5Z	0.11	0/894	0.28	0/1218
48	Z	0.11	0/894	0.28	0/1218
49	5a	0.41	0/698	0.57	0/949
49	a	0.44	0/698	0.59	0/949
50	5b	0.12	0/1201	0.30	0/1623
50	b	0.11	0/1201	0.31	0/1623
51	5c	0.12	0/463	0.29	0/623
51	c	0.11	0/463	0.29	0/623
52	5d	0.18	0/721	0.33	0/968
52	d	0.18	0/721	0.33	0/968
53	5e	0.13	0/1688	0.30	0/2301
53	e	0.13	0/1688	0.30	0/2301
54	5f	0.11	0/547	0.23	0/740
54	f	0.10	0/547	0.23	0/740
55	5g	0.27	0/433	0.54	0/587
55	g	0.11	0/433	0.32	0/587
56	5h	0.12	0/948	0.30	0/1285
56	h	0.11	0/948	0.30	0/1285
57	5i	0.10	0/644	0.25	0/860
57	i	0.10	0/644	0.25	0/860
58	5j	0.09	0/732	0.26	0/983
58	j	0.09	0/732	0.26	0/983
59	5k	0.12	0/1011	0.27	0/1361
59	k	0.11	0/1011	0.27	0/1361
60	5l	0.12	0/936	0.29	0/1278
60	l	0.11	0/936	0.29	0/1278
61	5m	0.11	0/1155	0.26	0/1558
61	m	0.11	0/1155	0.26	0/1558
62	5n	0.11	0/886	0.24	0/1188
62	n	0.10	0/886	0.24	0/1188
63	5o	0.12	0/1265	0.33	0/1705
63	o	0.12	0/1265	0.33	0/1705
64	5p	0.12	0/1095	0.29	0/1480
64	p	0.12	0/1095	0.29	0/1480
65	5q	0.12	0/1308	0.30	0/1779
65	q	0.12	0/1308	0.30	0/1779
66	5s	0.12	0/2353	0.30	0/3202
66	s	0.12	0/2353	0.30	0/3202
67	5t	0.11	0/2043	0.28	0/2778
67	t	0.11	0/2043	0.28	0/2778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
68	5u	0.13	0/1730	0.31	0/2341
68	u	0.13	0/1730	0.31	0/2341
69	5v	0.11	0/369	0.26	0/498
69	v	0.11	0/369	0.26	0/498
70	5w	0.12	0/521	0.30	0/702
70	w	0.12	0/521	0.30	0/702
71	5x	0.12	0/727	0.28	0/994
71	x	0.12	0/727	0.28	0/994
72	5y	0.15	0/963	0.30	0/1313
72	y	0.14	0/963	0.30	0/1313
All	All	0.20	0/298402	0.40	53/405254 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1A	0	1
1	1B	0	1
1	6A	0	1
1	6B	0	1
17	3G	0	1
17	4G	0	1
17	8G	0	1
17	9G	0	1
53	5e	0	1
53	e	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1R	10	LEU	CA-C-N	-10.11	107.20	119.84
10	1R	10	LEU	C-N-CA	-10.11	107.20	119.84
10	6R	10	LEU	CA-C-N	-10.07	107.25	119.84
10	6R	10	LEU	C-N-CA	-10.07	107.25	119.84
9	1Q	59	ALA	N-CA-C	-9.56	95.01	109.83

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1A	184	TYR	Sidechain
1	1B	184	TYR	Sidechain
17	3G	114	TRP	Peptide
17	4G	114	TRP	Peptide
53	5e	147	MET	Peptide

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	1A	2958	0	2955	13	0
1	1B	2958	0	2955	18	0
1	6A	2958	0	2955	15	0
1	6B	2958	0	2955	19	0
2	1C	1602	0	1577	14	0
2	1D	1602	0	1577	16	0
2	6C	1602	0	1577	12	0
2	6D	1602	0	1577	16	0
3	1E	1898	0	1800	11	0
3	1F	1898	0	1800	8	0
3	6E	1898	0	1800	11	0
3	6F	1898	0	1800	9	0
4	1G	486	0	490	3	0
4	1H	486	0	490	3	0
4	6G	486	0	490	4	0
4	6H	486	0	490	3	0
5	1I	550	0	501	6	0
5	1J	550	0	501	20	0
5	6I	550	0	501	6	0
5	6J	550	0	501	58	0
6	1K	594	0	590	8	0
6	1L	594	0	590	4	0
6	6K	594	0	590	8	0
6	6L	594	0	590	5	0
7	1M	3646	0	3555	52	0
7	1N	3646	0	3555	29	0
7	6M	3646	0	3555	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	6N	3646	0	3555	25	0
8	1O	371	0	372	2	0
8	1P	371	0	372	5	0
8	6O	371	0	372	2	0
8	6P	371	0	372	5	0
9	1Q	3204	0	3271	95	0
9	1S	3204	0	3271	26	0
9	6Q	3204	0	3271	130	0
9	6S	3204	0	3271	24	0
10	1R	980	0	1005	17	0
10	1T	980	0	1005	26	0
10	6R	980	0	1005	18	0
10	6T	980	0	1005	26	0
11	2A	3888	0	3936	38	0
11	3A	3888	0	3936	36	0
11	4A	3888	0	3936	35	0
11	7A	3888	0	3936	37	0
11	8A	3888	0	3936	36	0
11	9A	3888	0	3936	36	0
12	2B	1169	0	1191	25	0
12	3B	1169	0	1191	14	0
12	4B	1169	0	1191	13	0
12	7B	1169	0	1191	23	0
12	8B	1169	0	1191	15	0
12	9B	1169	0	1191	15	0
13	2C	1212	0	1243	12	0
13	3C	1212	0	1243	12	0
13	4C	1212	0	1243	12	0
13	7C	1212	0	1243	14	0
13	8C	1212	0	1243	12	0
13	9C	1212	0	1243	12	0
14	2D	2079	0	2039	15	0
14	3D	2079	0	2039	14	0
14	4D	2079	0	2039	15	0
14	7D	2079	0	2039	15	0
14	8D	2079	0	2039	14	0
14	9D	2079	0	2039	16	0
15	2E	737	0	706	21	0
15	3E	737	0	706	1	0
15	4E	737	0	706	1	0
15	7E	737	0	706	21	0
15	8E	737	0	706	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	9E	737	0	706	2	0
16	2F	706	0	683	26	0
16	3F	706	0	685	37	0
16	4F	706	0	685	5	0
16	7F	706	0	683	27	0
16	8F	706	0	685	37	0
16	9F	706	0	685	2	0
17	2G	733	0	708	11	0
17	3G	733	0	708	5	0
17	4G	733	0	708	5	0
17	7G	733	0	708	10	0
17	8G	733	0	708	8	0
17	9G	733	0	708	6	0
18	2H	954	0	900	7	0
18	3H	954	0	900	7	0
18	4H	954	0	900	5	0
18	7H	954	0	900	6	0
18	8H	954	0	900	6	0
18	9H	954	0	900	7	0
19	2I	594	0	553	4	0
19	3I	594	0	553	5	0
19	4I	594	0	553	5	0
19	7I	594	0	553	4	0
19	8I	594	0	553	5	0
19	9I	594	0	553	6	0
20	2J	816	0	807	10	0
20	3J	816	0	807	6	0
20	4J	790	0	781	60	0
20	7J	816	0	807	8	0
20	8J	816	0	807	6	0
20	9J	790	0	781	25	0
21	2K	382	0	367	6	0
21	3K	382	0	367	3	0
21	4K	382	0	367	3	0
21	7K	382	0	367	6	0
21	8K	382	0	367	3	0
21	9K	382	0	367	5	0
22	2L	605	0	588	12	0
22	3L	627	0	604	48	0
22	4L	627	0	604	14	0
22	7L	605	0	588	13	0
22	8L	627	0	604	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	9L	627	0	604	14	0
23	5A	1839	0	1827	36	0
23	A	1839	0	1827	33	0
24	5B	3331	0	3328	76	0
24	B	3331	0	3328	75	0
25	5C	5175	0	5182	97	0
25	C	5175	0	5182	98	0
26	5D	1790	0	1740	72	0
26	D	1790	0	1740	75	0
27	5E	3107	0	3083	112	0
27	E	3107	0	3083	114	0
28	5F	1225	0	1224	38	0
28	F	1225	0	1224	41	0
29	5G	1615	0	1551	67	0
29	G	1615	0	1551	69	0
30	5H	750	0	751	26	0
30	H	750	0	751	26	0
31	5I	1044	0	1046	23	0
31	I	1044	0	1046	23	0
32	5J	640	0	629	11	0
32	5r	663	0	647	32	0
32	J	640	0	629	10	0
32	r	663	0	647	29	0
33	5K	986	0	1017	23	0
33	K	986	0	1017	24	0
34	5L	1275	0	1243	36	0
34	L	1275	0	1243	38	0
35	5M	913	0	909	15	0
35	M	913	0	909	16	0
36	5N	1235	0	1161	22	0
36	N	1235	0	1161	20	0
37	5O	761	0	759	18	0
37	O	761	0	759	17	0
38	5P	2823	0	2854	71	0
38	P	2823	0	2854	70	0
39	5Q	2179	0	2241	74	0
39	Q	2179	0	2241	75	0
40	5R	3014	0	3082	89	0
40	R	3014	0	3082	94	0
41	5S	1071	0	1035	34	0
41	S	1071	0	1035	37	0
42	5T	3434	0	3590	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	T	3434	0	3590	109	0
43	5U	805	0	812	30	0
43	U	805	0	812	29	0
44	5V	4152	0	4212	107	0
44	V	4152	0	4212	110	0
45	5W	1210	0	1275	48	0
45	W	1210	0	1275	46	0
46	5X	1037	0	981	27	0
46	X	1037	0	981	25	0
47	5Y	405	0	404	7	0
47	Y	405	0	404	7	0
48	5Z	861	0	826	14	0
48	Z	861	0	826	17	0
49	5a	674	0	620	28	0
49	a	674	0	620	45	0
50	5b	1169	0	1144	32	0
50	b	1169	0	1144	30	0
51	5c	453	0	475	10	0
51	c	453	0	475	11	0
52	5d	699	0	670	16	0
52	d	699	0	670	17	0
53	5e	1639	0	1618	61	0
53	e	1639	0	1618	63	0
54	5f	532	0	524	12	0
54	f	532	0	524	11	0
55	5g	416	0	402	53	0
55	g	416	0	400	65	0
56	5h	915	0	866	20	0
56	h	915	0	866	19	0
57	5i	633	0	612	8	0
57	i	633	0	612	9	0
58	5j	712	0	684	11	0
58	j	712	0	684	9	0
59	5k	984	0	980	30	0
59	k	984	0	980	26	0
60	5l	904	0	875	7	0
60	l	904	0	875	8	0
61	5m	1126	0	1148	30	0
61	m	1126	0	1148	30	0
62	5n	864	0	839	10	0
62	n	864	0	839	8	0
63	5o	1240	0	1222	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	o	1240	0	1222	29	0
64	5p	1069	0	1014	63	0
64	p	1069	0	1014	64	0
65	5q	1268	0	1209	42	0
65	q	1268	0	1209	42	0
66	5s	2302	0	2299	105	0
66	s	2302	0	2299	101	0
67	5t	1997	0	1985	60	0
67	t	1997	0	1985	57	0
68	5u	1698	0	1686	46	0
68	u	1698	0	1686	44	0
69	5v	361	0	359	2	0
69	v	361	0	359	2	0
70	5w	508	0	494	7	0
70	w	508	0	494	7	0
71	5x	699	0	662	29	0
71	x	699	0	662	31	0
72	5y	932	0	950	19	0
72	y	932	0	950	21	0
73	1A	86	0	60	0	0
73	1B	86	0	60	2	0
73	6A	86	0	60	1	0
73	6B	86	0	60	2	0
74	1E	43	0	32	3	0
74	1F	43	0	32	2	0
74	6E	43	0	32	3	0
74	6F	43	0	32	2	0
75	1M	1	0	0	0	0
75	1N	1	0	0	0	0
75	5s	1	0	0	0	0
75	6M	1	0	0	0	0
75	6N	1	0	0	0	0
75	s	1	0	0	0	0
76	2A	120	0	108	2	0
76	3A	120	0	108	3	0
76	4A	120	0	108	3	0
76	7A	120	0	108	2	0
76	8A	120	0	108	3	0
76	9A	120	0	108	3	0
77	2A	1	0	0	0	0
77	3A	1	0	0	0	0
77	4A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
77	7A	1	0	0	0	0
77	8A	1	0	0	0	0
77	9A	1	0	0	0	0
78	2A	1	0	0	0	0
78	3A	1	0	0	0	0
78	4A	1	0	0	0	0
78	7A	1	0	0	0	0
78	8A	1	0	0	0	0
78	9A	1	0	0	0	0
79	2C	2	0	0	3	0
79	3C	2	0	0	2	0
79	4C	2	0	0	2	0
79	7C	2	0	0	3	0
79	8C	2	0	0	2	0
79	9C	2	0	0	2	0
80	5A	4	0	0	2	0
80	5C	4	0	0	1	0
80	A	4	0	0	2	0
80	C	4	0	0	1	0
81	5B	31	0	19	2	0
81	B	31	0	19	2	0
82	5B	8	0	0	0	0
82	5C	16	0	0	1	0
82	5F	8	0	0	1	0
82	5G	16	0	0	1	0
82	B	8	0	0	0	0
82	C	16	0	0	1	0
82	F	8	0	0	1	0
82	G	16	0	0	1	0
83	5J	35	0	0	1	0
83	5k	35	0	0	0	0
83	J	35	0	0	1	0
83	k	35	0	0	0	0
84	5P	48	0	26	4	0
84	P	48	0	26	4	0
85	5s	53	0	37	8	0
85	s	53	0	37	9	0
All	All	292492	0	289480	4480	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 4480 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)
66:5s:92:ARG:CD	15:7E:34:PHE:CD2	1.77	1.68
64:5p:10:TYR:CD2	16:8F:59:ARG:HD3	1.24	1.65
16:3F:59:ARG:HD3	64:p:10:TYR:CD2	1.24	1.65
9:6Q:60:VAL:CG2	55:g:11:ARG:HG2	1.22	1.62
11:8A:265:THR:HG21	22:8L:5:PHE:CE2	1.39	1.58

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	1A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	1B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
1	6A	374/381 (98%)	363 (97%)	11 (3%)	0	100	100
1	6B	374/381 (98%)	366 (98%)	8 (2%)	0	100	100
2	1C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	1D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
2	6C	205/262 (78%)	194 (95%)	11 (5%)	0	100	100
2	6D	205/262 (78%)	201 (98%)	4 (2%)	0	100	100
3	1E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	1F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
3	6E	241/314 (77%)	236 (98%)	5 (2%)	0	100	100
3	6F	241/314 (77%)	235 (98%)	6 (2%)	0	100	100
4	1G	57/60 (95%)	57 (100%)	0	0	100	100
4	1H	57/60 (95%)	57 (100%)	0	0	100	100
4	6G	57/60 (95%)	57 (100%)	0	0	100	100
4	6H	57/60 (95%)	57 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1I	66/69 (96%)	66 (100%)	0	0	100	100
5	1J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
5	6I	66/69 (96%)	66 (100%)	0	0	100	100
5	6J	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	1K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	1L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
6	6K	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
6	6L	68/73 (93%)	65 (96%)	3 (4%)	0	100	100
7	1M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	1N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	77
7	6M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	6N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	43	77
8	1O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	1P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
8	6O	46/59 (78%)	43 (94%)	3 (6%)	0	100	100
8	6P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
9	1Q	439/485 (90%)	419 (95%)	19 (4%)	1 (0%)	43	77
9	1S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	24	63
9	6Q	439/485 (90%)	416 (95%)	22 (5%)	1 (0%)	43	77
9	6S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	24	63
10	1R	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
10	1T	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
10	6R	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
10	6T	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
11	2A	502/505 (99%)	487 (97%)	15 (3%)	0	100	100
11	3A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
11	4A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
11	7A	502/505 (99%)	488 (97%)	14 (3%)	0	100	100
11	8A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
11	9A	502/505 (99%)	490 (98%)	12 (2%)	0	100	100
12	2B	139/284 (49%)	136 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	3B	139/284 (49%)	134 (96%)	5 (4%)	0	100	100
12	4B	139/284 (49%)	134 (96%)	5 (4%)	0	100	100
12	7B	139/284 (49%)	136 (98%)	3 (2%)	0	100	100
12	8B	139/284 (49%)	134 (96%)	5 (4%)	0	100	100
12	9B	139/284 (49%)	135 (97%)	4 (3%)	0	100	100
13	2C	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
13	3C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
13	4C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
13	7C	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
13	8C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
13	9C	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
14	2D	264/382 (69%)	255 (97%)	9 (3%)	0	100	100
14	3D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
14	4D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
14	7D	264/382 (69%)	255 (97%)	9 (3%)	0	100	100
14	8D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
14	9D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
15	2E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	3E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	4E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	7E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	8E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
15	9E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	11	45
16	2F	84/96 (88%)	81 (96%)	3 (4%)	0	100	100
16	3F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
16	4F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
16	7F	84/96 (88%)	81 (96%)	3 (4%)	0	100	100
16	8F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
16	9F	84/96 (88%)	80 (95%)	4 (5%)	0	100	100
17	2G	87/125 (70%)	78 (90%)	9 (10%)	0	100	100
17	3G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	4G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
17	7G	87/125 (70%)	78 (90%)	9 (10%)	0	100	100
17	8G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
17	9G	87/125 (70%)	80 (92%)	7 (8%)	0	100	100
18	2H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	3H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	4H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	7H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	8H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
18	9H	112/148 (76%)	108 (96%)	4 (4%)	0	100	100
19	2I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	3I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	4I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	7I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	8I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
19	9I	70/101 (69%)	67 (96%)	3 (4%)	0	100	100
20	2J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	3J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	4J	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
20	7J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	8J	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
20	9J	99/105 (94%)	98 (99%)	1 (1%)	0	100	100
21	2K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	3K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	4K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	7K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	8K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
21	9K	45/58 (78%)	44 (98%)	1 (2%)	0	100	100
22	2L	74/87 (85%)	70 (95%)	4 (5%)	0	100	100
22	3L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
22	4L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	7L	74/87 (85%)	70 (95%)	4 (5%)	0	100	100
22	8L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
22	9L	76/87 (87%)	72 (95%)	4 (5%)	0	100	100
23	5A	237/282 (84%)	232 (98%)	5 (2%)	0	100	100
23	A	237/282 (84%)	232 (98%)	5 (2%)	0	100	100
24	5B	433/484 (90%)	425 (98%)	8 (2%)	0	100	100
24	B	433/484 (90%)	425 (98%)	8 (2%)	0	100	100
25	5C	686/733 (94%)	668 (97%)	18 (3%)	0	100	100
25	C	686/733 (94%)	668 (97%)	18 (3%)	0	100	100
26	5D	214/282 (76%)	204 (95%)	10 (5%)	0	100	100
26	D	214/282 (76%)	205 (96%)	9 (4%)	0	100	100
27	5E	382/467 (82%)	367 (96%)	15 (4%)	0	100	100
27	E	382/467 (82%)	367 (96%)	15 (4%)	0	100	100
28	5F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
28	F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
29	5G	197/231 (85%)	190 (96%)	7 (4%)	0	100	100
29	G	197/231 (85%)	190 (96%)	7 (4%)	0	100	100
30	5H	88/118 (75%)	83 (94%)	5 (6%)	0	100	100
30	H	88/118 (75%)	83 (94%)	5 (6%)	0	100	100
31	5I	133/165 (81%)	131 (98%)	2 (2%)	0	100	100
31	I	133/165 (81%)	131 (98%)	2 (2%)	0	100	100
32	5J	82/128 (64%)	79 (96%)	3 (4%)	0	100	100
32	5r	86/128 (67%)	81 (94%)	5 (6%)	0	100	100
32	J	82/128 (64%)	80 (98%)	2 (2%)	0	100	100
32	r	86/128 (67%)	81 (94%)	5 (6%)	0	100	100
33	5K	117/138 (85%)	114 (97%)	3 (3%)	0	100	100
33	K	117/138 (85%)	114 (97%)	3 (3%)	0	100	100
34	5L	162/187 (87%)	157 (97%)	5 (3%)	0	100	100
34	L	162/187 (87%)	157 (97%)	5 (3%)	0	100	100
35	5M	119/154 (77%)	114 (96%)	5 (4%)	0	100	100
35	M	119/154 (77%)	114 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	5N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
36	N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
37	5O	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	O	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	5P	361/397 (91%)	351 (97%)	9 (2%)	1 (0%)	36	71
38	P	361/397 (91%)	351 (97%)	9 (2%)	1 (0%)	36	71
39	5Q	282/292 (97%)	272 (96%)	10 (4%)	0	100	100
39	Q	282/292 (97%)	272 (96%)	10 (4%)	0	100	100
40	5R	381/387 (98%)	365 (96%)	16 (4%)	0	100	100
40	R	381/387 (98%)	366 (96%)	15 (4%)	0	100	100
41	5S	130/279 (47%)	129 (99%)	1 (1%)	0	100	100
41	S	130/279 (47%)	129 (99%)	1 (1%)	0	100	100
42	5T	441/443 (100%)	428 (97%)	13 (3%)	0	100	100
42	T	441/443 (100%)	428 (97%)	13 (3%)	0	100	100
43	5U	103/227 (45%)	101 (98%)	2 (2%)	0	100	100
43	U	103/227 (45%)	101 (98%)	2 (2%)	0	100	100
44	5V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	43	77
44	V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	43	77
45	5W	155/162 (96%)	148 (96%)	7 (4%)	0	100	100
45	W	155/162 (96%)	149 (96%)	6 (4%)	0	100	100
46	5X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
46	X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
47	5Y	52/64 (81%)	52 (100%)	0	0	100	100
47	Y	52/64 (81%)	52 (100%)	0	0	100	100
48	5Z	105/124 (85%)	103 (98%)	2 (2%)	0	100	100
48	Z	105/124 (85%)	103 (98%)	2 (2%)	0	100	100
49	5a	80/129 (62%)	79 (99%)	0	1 (1%)	9	40
49	a	80/129 (62%)	78 (98%)	1 (1%)	1 (1%)	9	40
50	5b	142/172 (83%)	140 (99%)	2 (1%)	0	100	100
50	b	142/172 (83%)	141 (99%)	1 (1%)	0	100	100
51	5c	55/67 (82%)	51 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	c	55/67 (82%)	51 (93%)	4 (7%)	0	100	100
52	5d	83/86 (96%)	83 (100%)	0	0	100	100
52	d	83/86 (96%)	83 (100%)	0	0	100	100
53	5e	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
53	e	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
54	5f	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	f	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
55	5g	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
55	g	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
56	5h	106/142 (75%)	98 (92%)	8 (8%)	0	100	100
56	h	106/142 (75%)	98 (92%)	8 (8%)	0	100	100
57	5i	74/81 (91%)	74 (100%)	0	0	100	100
57	i	74/81 (91%)	74 (100%)	0	0	100	100
58	5j	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
58	j	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
59	5k	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
59	k	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
60	5l	114/121 (94%)	113 (99%)	1 (1%)	0	100	100
60	l	114/121 (94%)	113 (99%)	1 (1%)	0	100	100
61	5m	134/142 (94%)	132 (98%)	2 (2%)	0	100	100
61	m	134/142 (94%)	132 (98%)	2 (2%)	0	100	100
62	5n	102/106 (96%)	102 (100%)	0	0	100	100
62	n	102/106 (96%)	102 (100%)	0	0	100	100
63	5o	150/155 (97%)	144 (96%)	6 (4%)	0	100	100
63	o	150/155 (97%)	144 (96%)	6 (4%)	0	100	100
64	5p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
64	p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
65	5q	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
65	q	155/197 (79%)	150 (97%)	5 (3%)	0	100	100
66	5s	310/312 (99%)	299 (96%)	11 (4%)	0	100	100
66	s	310/312 (99%)	299 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	5t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
67	t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
68	5u	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
68	u	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
69	5v	43/45 (96%)	43 (100%)	0	0	100	100
69	v	43/45 (96%)	43 (100%)	0	0	100	100
70	5w	62/109 (57%)	62 (100%)	0	0	100	100
70	w	62/109 (57%)	62 (100%)	0	0	100	100
71	5x	81/157 (52%)	81 (100%)	0	0	100	100
71	x	81/157 (52%)	81 (100%)	0	0	100	100
72	5y	112/118 (95%)	112 (100%)	0	0	100	100
72	y	112/118 (95%)	112 (100%)	0	0	100	100
All	All	36512/43212 (84%)	35417 (97%)	1075 (3%)	20 (0%)	49	82

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	1Q	396	ASP
15	2E	28	TRP
15	3E	28	TRP
15	4E	28	TRP
9	6Q	396	ASP

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	1A	312/317 (98%)	312 (100%)	0	100	100
1	1B	312/317 (98%)	312 (100%)	0	100	100
1	6A	312/317 (98%)	312 (100%)	0	100	100
1	6B	312/317 (98%)	312 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1C	171/213 (80%)	171 (100%)	0	100	100
2	1D	171/213 (80%)	171 (100%)	0	100	100
2	6C	171/213 (80%)	171 (100%)	0	100	100
2	6D	171/213 (80%)	171 (100%)	0	100	100
3	1E	191/238 (80%)	191 (100%)	0	100	100
3	1F	191/238 (80%)	191 (100%)	0	100	100
3	6E	191/238 (80%)	191 (100%)	0	100	100
3	6F	191/238 (80%)	191 (100%)	0	100	100
4	1G	52/53 (98%)	52 (100%)	0	100	100
4	1H	52/53 (98%)	52 (100%)	0	100	100
4	6G	52/53 (98%)	52 (100%)	0	100	100
4	6H	52/53 (98%)	52 (100%)	0	100	100
5	1I	58/59 (98%)	58 (100%)	0	100	100
5	1J	58/59 (98%)	58 (100%)	0	100	100
5	6I	58/59 (98%)	58 (100%)	0	100	100
5	6J	58/59 (98%)	58 (100%)	0	100	100
6	1K	62/64 (97%)	62 (100%)	0	100	100
6	1L	62/64 (97%)	62 (100%)	0	100	100
6	6K	62/64 (97%)	62 (100%)	0	100	100
6	6L	62/64 (97%)	62 (100%)	0	100	100
7	1M	390/413 (94%)	390 (100%)	0	100	100
7	1N	390/413 (94%)	390 (100%)	0	100	100
7	6M	390/413 (94%)	390 (100%)	0	100	100
7	6N	390/413 (94%)	390 (100%)	0	100	100
8	1O	38/47 (81%)	38 (100%)	0	100	100
8	1P	38/47 (81%)	38 (100%)	0	100	100
8	6O	38/47 (81%)	38 (100%)	0	100	100
8	6P	38/47 (81%)	38 (100%)	0	100	100
9	1Q	333/362 (92%)	331 (99%)	2 (1%)	78	81
9	1S	333/362 (92%)	333 (100%)	0	100	100
9	6Q	333/362 (92%)	330 (99%)	3 (1%)	70	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	6S	333/362 (92%)	333 (100%)	0	100	100
10	1R	106/107 (99%)	106 (100%)	0	100	100
10	1T	106/107 (99%)	106 (100%)	0	100	100
10	6R	106/107 (99%)	106 (100%)	0	100	100
10	6T	106/107 (99%)	106 (100%)	0	100	100
11	2A	408/409 (100%)	408 (100%)	0	100	100
11	3A	408/409 (100%)	408 (100%)	0	100	100
11	4A	408/409 (100%)	408 (100%)	0	100	100
11	7A	408/409 (100%)	408 (100%)	0	100	100
11	8A	408/409 (100%)	408 (100%)	0	100	100
11	9A	408/409 (100%)	408 (100%)	0	100	100
12	2B	132/224 (59%)	132 (100%)	0	100	100
12	3B	132/224 (59%)	132 (100%)	0	100	100
12	4B	132/224 (59%)	132 (100%)	0	100	100
12	7B	132/224 (59%)	132 (100%)	0	100	100
12	8B	132/224 (59%)	132 (100%)	0	100	100
12	9B	132/224 (59%)	132 (100%)	0	100	100
13	2C	137/137 (100%)	137 (100%)	0	100	100
13	3C	137/137 (100%)	137 (100%)	0	100	100
13	4C	137/137 (100%)	137 (100%)	0	100	100
13	7C	137/137 (100%)	137 (100%)	0	100	100
13	8C	137/137 (100%)	137 (100%)	0	100	100
13	9C	137/137 (100%)	137 (100%)	0	100	100
14	2D	211/294 (72%)	211 (100%)	0	100	100
14	3D	211/294 (72%)	211 (100%)	0	100	100
14	4D	211/294 (72%)	211 (100%)	0	100	100
14	7D	211/294 (72%)	211 (100%)	0	100	100
14	8D	211/294 (72%)	211 (100%)	0	100	100
14	9D	211/294 (72%)	211 (100%)	0	100	100
15	2E	79/137 (58%)	79 (100%)	0	100	100
15	3E	79/137 (58%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	4E	79/137 (58%)	79 (100%)	0	100	100
15	7E	79/137 (58%)	79 (100%)	0	100	100
15	8E	79/137 (58%)	79 (100%)	0	100	100
15	9E	79/137 (58%)	79 (100%)	0	100	100
16	2F	66/72 (92%)	66 (100%)	0	100	100
16	3F	66/72 (92%)	66 (100%)	0	100	100
16	4F	66/72 (92%)	66 (100%)	0	100	100
16	7F	66/72 (92%)	66 (100%)	0	100	100
16	8F	66/72 (92%)	66 (100%)	0	100	100
16	9F	66/72 (92%)	66 (100%)	0	100	100
17	2G	75/100 (75%)	75 (100%)	0	100	100
17	3G	75/100 (75%)	75 (100%)	0	100	100
17	4G	75/100 (75%)	75 (100%)	0	100	100
17	7G	75/100 (75%)	75 (100%)	0	100	100
17	8G	75/100 (75%)	75 (100%)	0	100	100
17	9G	75/100 (75%)	75 (100%)	0	100	100
18	2H	103/132 (78%)	103 (100%)	0	100	100
18	3H	103/132 (78%)	103 (100%)	0	100	100
18	4H	103/132 (78%)	103 (100%)	0	100	100
18	7H	103/132 (78%)	103 (100%)	0	100	100
18	8H	103/132 (78%)	103 (100%)	0	100	100
18	9H	103/132 (78%)	103 (100%)	0	100	100
19	2I	58/80 (72%)	58 (100%)	0	100	100
19	3I	58/80 (72%)	58 (100%)	0	100	100
19	4I	58/80 (72%)	58 (100%)	0	100	100
19	7I	58/80 (72%)	58 (100%)	0	100	100
19	8I	58/80 (72%)	58 (100%)	0	100	100
19	9I	58/80 (72%)	58 (100%)	0	100	100
20	2J	83/84 (99%)	83 (100%)	0	100	100
20	3J	83/84 (99%)	83 (100%)	0	100	100
20	4J	80/84 (95%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	7J	83/84 (99%)	83 (100%)	0	100	100
20	8J	83/84 (99%)	83 (100%)	0	100	100
20	9J	80/84 (95%)	80 (100%)	0	100	100
21	2K	39/46 (85%)	39 (100%)	0	100	100
21	3K	39/46 (85%)	39 (100%)	0	100	100
21	4K	39/46 (85%)	39 (100%)	0	100	100
21	7K	39/46 (85%)	39 (100%)	0	100	100
21	8K	39/46 (85%)	39 (100%)	0	100	100
21	9K	39/46 (85%)	39 (100%)	0	100	100
22	2L	63/74 (85%)	63 (100%)	0	100	100
22	3L	65/74 (88%)	65 (100%)	0	100	100
22	4L	65/74 (88%)	65 (100%)	0	100	100
22	7L	63/74 (85%)	63 (100%)	0	100	100
22	8L	65/74 (88%)	65 (100%)	0	100	100
22	9L	65/74 (88%)	65 (100%)	0	100	100
23	5A	197/228 (86%)	197 (100%)	0	100	100
23	A	197/228 (86%)	197 (100%)	0	100	100
24	5B	344/377 (91%)	344 (100%)	0	100	100
24	B	344/377 (91%)	344 (100%)	0	100	100
25	5C	537/572 (94%)	537 (100%)	0	100	100
25	C	537/572 (94%)	537 (100%)	0	100	100
26	5D	196/248 (79%)	196 (100%)	0	100	100
26	D	196/248 (79%)	196 (100%)	0	100	100
27	5E	332/388 (86%)	332 (100%)	0	100	100
27	E	332/388 (86%)	332 (100%)	0	100	100
28	5F	129/133 (97%)	129 (100%)	0	100	100
28	F	129/133 (97%)	129 (100%)	0	100	100
29	5G	172/198 (87%)	172 (100%)	0	100	100
29	G	172/198 (87%)	172 (100%)	0	100	100
30	5H	82/105 (78%)	82 (100%)	0	100	100
30	H	82/105 (78%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	5I	111/134 (83%)	111 (100%)	0	100	100
31	I	111/134 (83%)	111 (100%)	0	100	100
32	5J	71/108 (66%)	71 (100%)	0	100	100
32	5r	72/108 (67%)	72 (100%)	0	100	100
32	J	71/108 (66%)	71 (100%)	0	100	100
32	r	72/108 (67%)	72 (100%)	0	100	100
33	5K	106/122 (87%)	106 (100%)	0	100	100
33	K	106/122 (87%)	106 (100%)	0	100	100
34	5L	130/148 (88%)	130 (100%)	0	100	100
34	L	130/148 (88%)	130 (100%)	0	100	100
35	5M	100/121 (83%)	100 (100%)	0	100	100
35	M	100/121 (83%)	100 (100%)	0	100	100
36	5N	128/132 (97%)	128 (100%)	0	100	100
36	N	128/132 (97%)	128 (100%)	0	100	100
37	5O	80/81 (99%)	80 (100%)	0	100	100
37	O	80/81 (99%)	80 (100%)	0	100	100
38	5P	305/327 (93%)	305 (100%)	0	100	100
38	P	305/327 (93%)	305 (100%)	0	100	100
39	5Q	230/234 (98%)	230 (100%)	0	100	100
39	Q	230/234 (98%)	230 (100%)	0	100	100
40	5R	321/321 (100%)	321 (100%)	0	100	100
40	R	321/321 (100%)	321 (100%)	0	100	100
41	5S	111/217 (51%)	111 (100%)	0	100	100
41	S	111/217 (51%)	111 (100%)	0	100	100
42	5T	374/374 (100%)	374 (100%)	0	100	100
42	T	374/374 (100%)	374 (100%)	0	100	100
43	5U	84/180 (47%)	84 (100%)	0	100	100
43	U	84/180 (47%)	84 (100%)	0	100	100
44	5V	439/439 (100%)	439 (100%)	0	100	100
44	V	439/439 (100%)	439 (100%)	0	100	100
45	5W	131/135 (97%)	131 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	W	131/135 (97%)	131 (100%)	0	100	100
46	5X	105/122 (86%)	105 (100%)	0	100	100
46	X	105/122 (86%)	105 (100%)	0	100	100
47	5Y	38/46 (83%)	38 (100%)	0	100	100
47	Y	38/46 (83%)	38 (100%)	0	100	100
48	5Z	93/102 (91%)	93 (100%)	0	100	100
48	Z	93/102 (91%)	93 (100%)	0	100	100
49	5a	68/98 (69%)	67 (98%)	1 (2%)	57	70
49	a	68/98 (69%)	66 (97%)	2 (3%)	37	57
50	5b	119/138 (86%)	119 (100%)	0	100	100
50	b	119/138 (86%)	119 (100%)	0	100	100
51	5c	49/56 (88%)	49 (100%)	0	100	100
51	c	49/56 (88%)	49 (100%)	0	100	100
52	5d	63/64 (98%)	63 (100%)	0	100	100
52	d	63/64 (98%)	63 (100%)	0	100	100
53	5e	163/164 (99%)	163 (100%)	0	100	100
53	e	163/164 (99%)	163 (100%)	0	100	100
54	5f	52/53 (98%)	52 (100%)	0	100	100
54	f	52/53 (98%)	52 (100%)	0	100	100
55	5g	40/45 (89%)	40 (100%)	0	100	100
55	g	40/45 (89%)	40 (100%)	0	100	100
56	5h	91/110 (83%)	91 (100%)	0	100	100
56	h	91/110 (83%)	91 (100%)	0	100	100
57	5i	65/67 (97%)	65 (100%)	0	100	100
57	i	65/67 (97%)	65 (100%)	0	100	100
58	5j	72/73 (99%)	72 (100%)	0	100	100
58	j	72/73 (99%)	72 (100%)	0	100	100
59	5k	102/102 (100%)	102 (100%)	0	100	100
59	k	102/102 (100%)	102 (100%)	0	100	100
60	5l	94/99 (95%)	94 (100%)	0	100	100
60	l	94/99 (95%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	5m	118/122 (97%)	118 (100%)	0	100	100
61	m	118/122 (97%)	118 (100%)	0	100	100
62	5n	92/94 (98%)	92 (100%)	0	100	100
62	n	92/94 (98%)	92 (100%)	0	100	100
63	5o	130/132 (98%)	130 (100%)	0	100	100
63	o	130/132 (98%)	130 (100%)	0	100	100
64	5p	109/110 (99%)	109 (100%)	0	100	100
64	p	109/110 (99%)	109 (100%)	0	100	100
65	5q	135/165 (82%)	135 (100%)	0	100	100
65	q	135/165 (82%)	135 (100%)	0	100	100
66	5s	243/243 (100%)	243 (100%)	0	100	100
66	s	243/243 (100%)	243 (100%)	0	100	100
67	5t	212/233 (91%)	212 (100%)	0	100	100
67	t	212/233 (91%)	212 (100%)	0	100	100
68	5u	180/181 (99%)	179 (99%)	1 (1%)	78	81
68	u	180/181 (99%)	179 (99%)	1 (1%)	78	81
69	5v	38/38 (100%)	38 (100%)	0	100	100
69	v	38/38 (100%)	38 (100%)	0	100	100
70	5w	55/91 (60%)	55 (100%)	0	100	100
70	w	55/91 (60%)	55 (100%)	0	100	100
71	5x	70/130 (54%)	70 (100%)	0	100	100
71	x	70/130 (54%)	70 (100%)	0	100	100
72	5y	102/106 (96%)	102 (100%)	0	100	100
72	y	102/106 (96%)	102 (100%)	0	100	100
All	All	30538/35054 (87%)	30528 (100%)	10 (0%)	100	100

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	a	46	LYS
49	a	67	LYS
68	u	43	ASN
68	5u	43	ASN
9	6Q	56	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 249 such sidechains are listed below:

Mol	Chain	Res	Type
64	5p	90	ASN
45	W	54	ASN
5	6J	20	HIS
44	V	113	ASN
63	o	54	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 74 ligands modelled in this entry, 18 are monoatomic - leaving 56 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	$\# Z > 2$
79	CUA	2C	301	-	0,1,1	-	-	-		
82	SF4	C	802	25	0,12,12	-	-	-		
82	SF4	5G	301	29	0,12,12	-	-	-		
73	HEM	1B	402	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	9 (13%)
73	HEM	6B	402	1	50,50,50	1.37	7 (14%)	66,82,82	1.24	9 (13%)
76	HEA	9A	603	11	66,67,67	2.40	23 (34%)	78,103,103	2.60	31 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	8Q1	k	200	-	31,34,34	1.74	5 (16%)	40,43,43	1.68	7 (17%)
76	HEA	4A	602	11	66,67,67	2.39	23 (34%)	78,103,103	2.58	30 (38%)
76	HEA	4A	604	11	66,67,67	2.39	26 (39%)	78,103,103	2.55	33 (42%)
82	SF4	5B	502	24	0,12,12	-	-	-	-	-
74	HEC	6F	501	3	50,50,50	1.76	4 (8%)	68,82,82	1.53	12 (17%)
73	HEM	1A	401	1	50,50,50	1.49	7 (14%)	66,82,82	1.38	7 (10%)
74	HEC	6E	401	3	50,50,50	1.84	5 (10%)	68,82,82	1.45	7 (10%)
79	CUA	3C	301	13	0,1,1	-	-	-	-	-
81	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.17	7 (14%)
82	SF4	5G	302	29	0,12,12	-	-	-	-	-
76	HEA	2A	601	11	66,67,67	2.46	23 (34%)	78,103,103	2.58	32 (41%)
85	COO	s	401	-	48,55,55	1.10	4 (8%)	68,81,81	4.02	17 (25%)
76	HEA	7A	602	11	66,67,67	2.46	24 (36%)	78,103,103	2.59	32 (41%)
80	FES	5C	801	25	0,4,4	-	-	-	-	-
82	SF4	B	501	24	0,12,12	-	-	-	-	-
80	FES	C	803	25	0,4,4	-	-	-	-	-
74	HEC	1F	501	3	50,50,50	1.77	4 (8%)	68,82,82	1.53	12 (17%)
76	HEA	2A	602	11	66,67,67	2.44	26 (39%)	78,103,103	2.54	32 (41%)
84	NDP	P	401	-	49,52,52	2.22	5 (10%)	66,80,80	1.65	13 (19%)
82	SF4	G	301	29	0,12,12	-	-	-	-	-
73	HEM	6B	401	1	50,50,50	1.43	8 (16%)	66,82,82	1.37	10 (15%)
74	HEC	1E	401	3	50,50,50	1.84	5 (10%)	68,82,82	1.44	8 (11%)
76	HEA	7A	601	11	66,67,67	2.44	26 (39%)	78,103,103	2.54	30 (38%)
80	FES	A	301	23	0,4,4	-	-	-	-	-
76	HEA	9A	602	11	66,67,67	2.39	24 (36%)	78,103,103	2.55	33 (42%)
82	SF4	5C	803	25	0,12,12	-	-	-	-	-
73	HEM	1B	401	1	50,50,50	1.43	8 (16%)	66,82,82	1.36	10 (15%)
76	HEA	8A	604	11	66,67,67	2.39	24 (36%)	78,103,103	2.54	33 (42%)
79	CUA	8C	301	13	0,1,1	-	-	-	-	-
76	HEA	3A	604	11	66,67,67	2.40	23 (34%)	78,103,103	2.60	30 (38%)
83	8Q1	5J	200	-	31,34,34	1.72	5 (16%)	40,43,43	1.54	5 (12%)
76	HEA	8A	601	11	66,67,67	2.40	23 (34%)	78,103,103	2.59	30 (38%)
83	8Q1	5k	200	-	31,34,34	1.75	6 (19%)	40,43,43	1.68	7 (17%)
76	HEA	3A	601	11	66,67,67	2.39	25 (37%)	78,103,103	2.54	33 (42%)
82	SF4	F	201	28	0,12,12	-	-	-	-	-
73	HEM	6A	402	1	50,50,50	1.49	7 (14%)	66,82,82	1.39	8 (12%)
82	SF4	C	801	25	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	COO	5s	401	-	48,55,55	1.10	4 (8%)	68,81,81	4.01	17 (25%)
82	SF4	5F	201	28	0,12,12	-	-	-	-	-
84	NDP	5P	401	-	49,52,52	2.22	6 (12%)	66,80,80	1.65	13 (19%)
81	FMN	5B	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.16	7 (14%)
82	SF4	G	302	29	0,12,12	-	-	-	-	-
73	HEM	1A	402	1	50,50,50	1.31	7 (14%)	66,82,82	1.30	8 (12%)
80	FES	5A	301	23	0,4,4	-	-	-	-	-
82	SF4	5C	802	25	0,12,12	-	-	-	-	-
83	8Q1	J	200	-	31,34,34	1.72	6 (19%)	40,43,43	1.55	5 (12%)
79	CUA	4C	301	13	0,1,1	-	-	-	-	-
79	CUA	7C	301	-	0,1,1	-	-	-	-	-
79	CUA	9C	301	13	0,1,1	-	-	-	-	-
73	HEM	6A	401	1	50,50,50	1.31	7 (14%)	66,82,82	1.29	7 (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
82	SF4	C	802	25	-	-	0/6/5/5
82	SF4	5G	301	29	-	-	0/6/5/5
73	HEM	1B	402	1	-	4/14/54/54	-
73	HEM	6B	402	1	-	4/14/54/54	-
76	HEA	9A	603	11	-	4/36/76/76	-
83	8Q1	k	200	-	-	21/41/41/41	-
76	HEA	4A	602	11	-	4/36/76/76	-
76	HEA	4A	604	11	-	9/36/76/76	-
82	SF4	5B	502	24	-	-	0/6/5/5
74	HEC	6E	401	3	1/1/3/7	2/14/54/54	-
73	HEM	1A	401	1	-	3/14/54/54	-
74	HEC	6F	501	3	1/1/3/7	2/14/54/54	-
81	FMN	B	502	-	-	5/18/18/18	0/3/3/3
85	COO	s	401	-	-	22/54/70/70	0/3/3/3
82	SF4	5G	302	29	-	-	0/6/5/5
76	HEA	2A	601	11	-	7/36/76/76	-
76	HEA	7A	602	11	-	7/36/76/76	-
80	FES	5C	801	25	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SF4	B	501	24	-	-	0/6/5/5
80	FES	C	803	25	-	-	0/1/1/1
74	HEC	1F	501	3	1/1/3/7	2/14/54/54	-
76	HEA	2A	602	11	-	10/36/76/76	-
84	NDP	P	401	-	-	8/34/77/77	0/5/5/5
82	SF4	G	301	29	-	-	0/6/5/5
73	HEM	6B	401	1	-	4/14/54/54	-
74	HEC	1E	401	3	1/1/3/7	2/14/54/54	-
76	HEA	7A	601	11	-	10/36/76/76	-
80	FES	A	301	23	-	-	0/1/1/1
76	HEA	9A	602	11	-	9/36/76/76	-
82	SF4	5C	803	25	-	-	0/6/5/5
73	HEM	1B	401	1	-	4/14/54/54	-
76	HEA	8A	604	11	-	9/36/76/76	-
76	HEA	3A	604	11	-	4/36/76/76	-
83	8Q1	5J	200	-	-	7/41/41/41	-
76	HEA	8A	601	11	-	4/36/76/76	-
83	8Q1	5k	200	-	-	21/41/41/41	-
76	HEA	3A	601	11	-	9/36/76/76	-
82	SF4	F	201	28	-	-	0/6/5/5
73	HEM	6A	402	1	-	3/14/54/54	-
82	SF4	C	801	25	-	-	0/6/5/5
82	SF4	5F	201	28	-	-	0/6/5/5
84	NDP	5P	401	-	-	8/34/77/77	0/5/5/5
81	FMN	5B	501	-	-	5/18/18/18	0/3/3/3
82	SF4	G	302	29	-	-	0/6/5/5
73	HEM	1A	402	1	-	4/14/54/54	-
80	FES	5A	301	23	-	-	0/1/1/1
82	SF4	5C	802	25	-	-	0/6/5/5
83	8Q1	J	200	-	-	7/41/41/41	-
85	COO	5s	401	-	-	22/54/70/70	0/3/3/3
73	HEM	6A	401	1	-	4/14/54/54	-

The worst 5 of 411 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	P	401	NDP	P2B-O2B	12.50	1.82	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	5P	401	NDP	P2B-O2B	12.47	1.82	1.59
74	1E	401	HEC	C3D-C2D	7.84	1.53	1.36
74	6E	401	HEC	C3D-C2D	7.83	1.53	1.36
74	1F	501	HEC	C3D-C2D	7.75	1.53	1.36

The worst 5 of 584 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	s	401	COO	C15-C11-C12	-19.15	77.00	108.23
85	5s	401	COO	C15-C11-C12	-19.15	77.00	108.23
85	s	401	COO	C15-C11-C13	-16.74	79.80	108.82
85	5s	401	COO	C15-C11-C13	-16.71	79.86	108.82
85	s	401	COO	C15-C11-C14	-15.20	78.19	109.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
74	1E	401	HEC	NA
74	1F	501	HEC	NA
74	6E	401	HEC	NA
74	6F	501	HEC	NA

5 of 250 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
76	2A	601	HEA	C3B-C11-C12-C13
76	2A	601	HEA	O11-C11-C12-C13
76	2A	601	HEA	C15-C16-C17-C18
76	2A	602	HEA	C2A-C3A-CMA-OMA
76	3A	604	HEA	C3B-C11-C12-C13

There are no ring outliers.

43 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
79	2C	301	CUA	3	0
76	9A	603	HEA	2	0
76	4A	602	HEA	2	0
76	4A	604	HEA	1	0
74	6F	501	HEC	2	0
74	6E	401	HEC	3	0

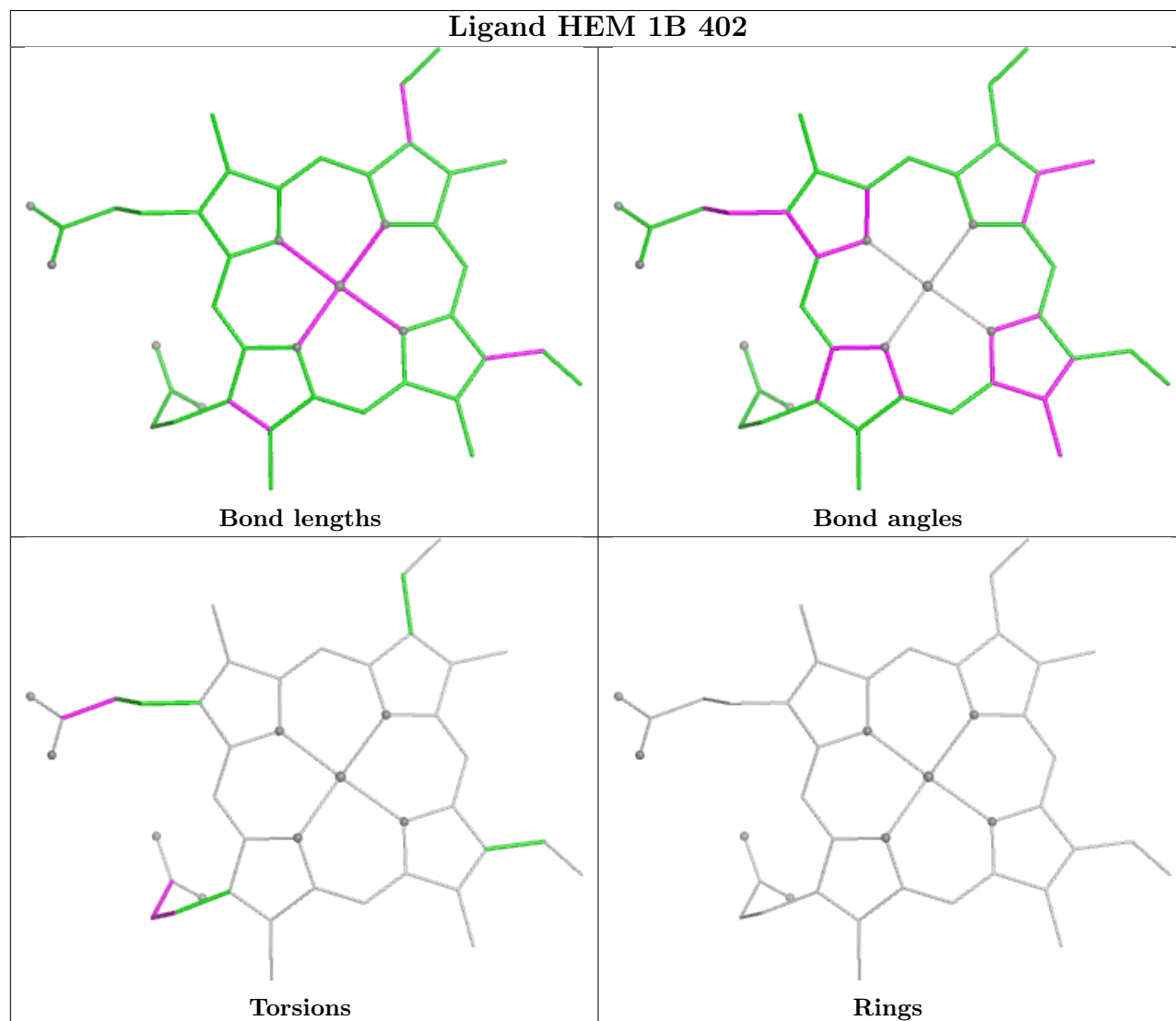
Continued on next page...

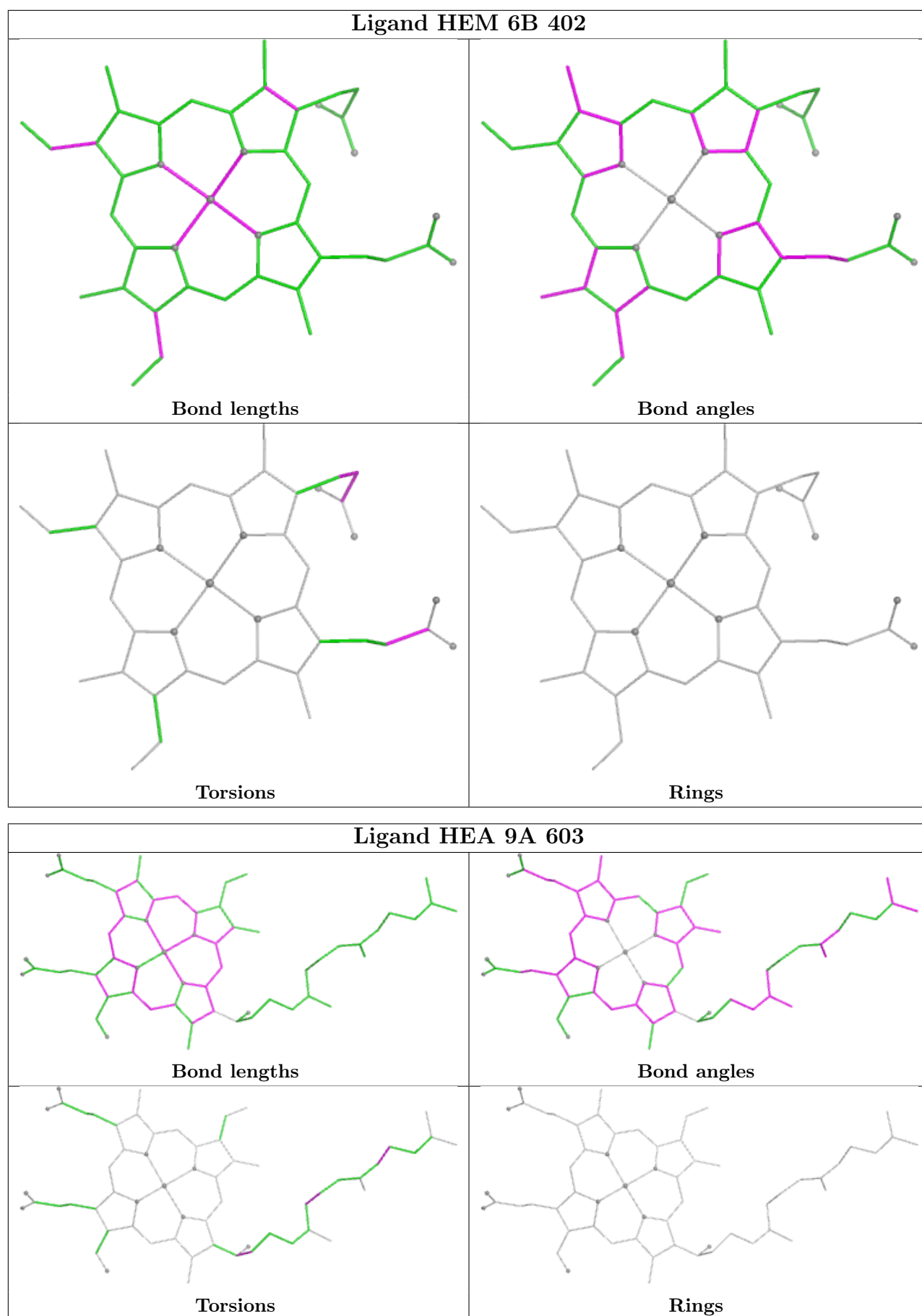
Continued from previous page...

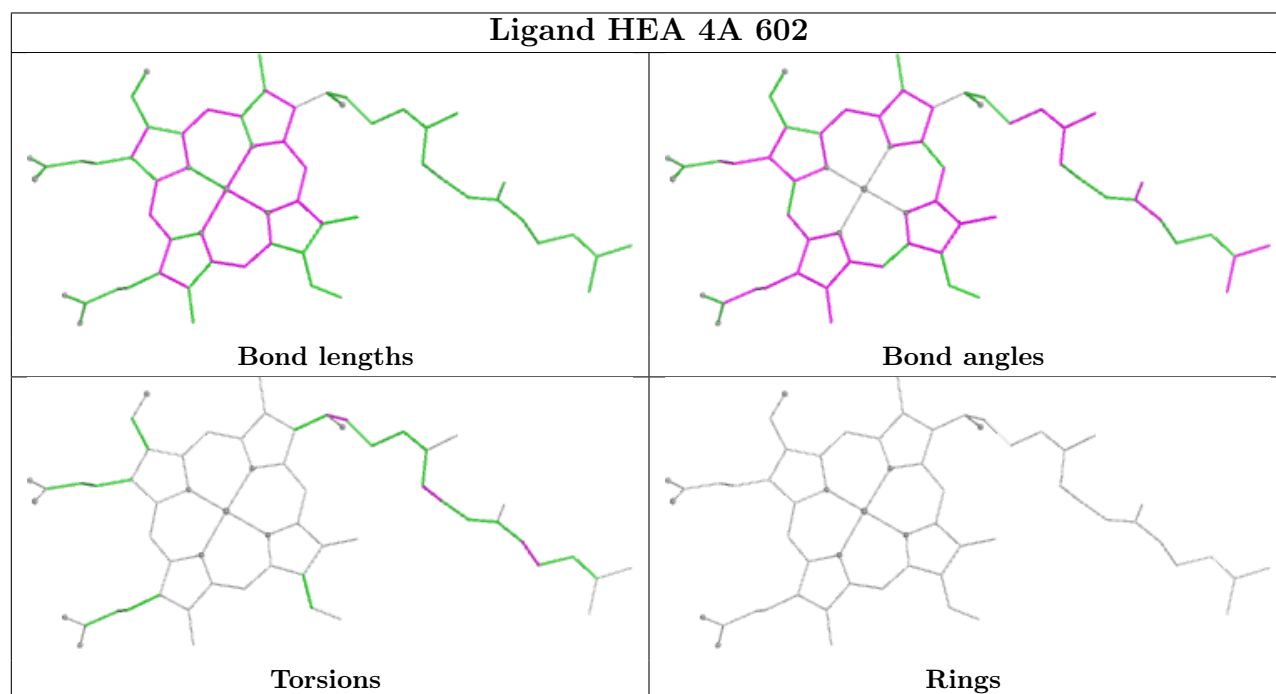
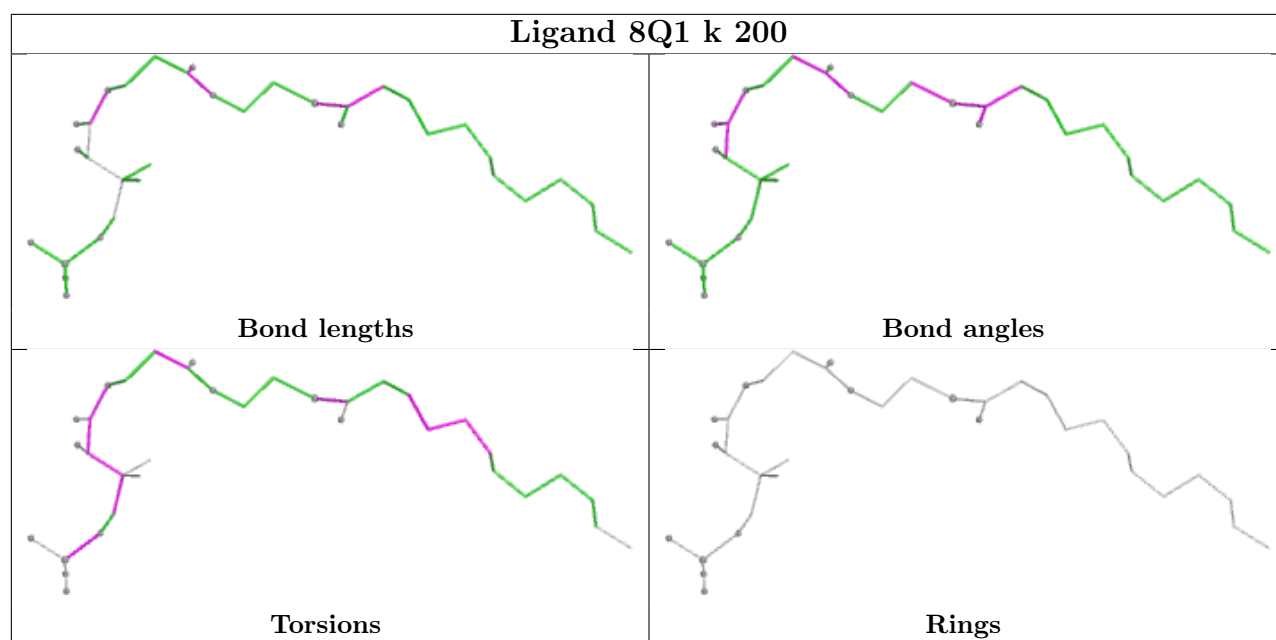
Mol	Chain	Res	Type	Clashes	Symm-Clashes
79	3C	301	CUA	2	0
81	B	502	FMN	2	0
82	5G	302	SF4	1	0
76	2A	601	HEA	1	0
85	s	401	COO	9	0
76	7A	602	HEA	1	0
80	5C	801	FES	1	0
80	C	803	FES	1	0
74	1F	501	HEC	2	0
76	2A	602	HEA	1	0
84	P	401	NDP	4	0
73	6B	401	HEM	2	0
74	1E	401	HEC	3	0
76	7A	601	HEA	1	0
80	A	301	FES	2	0
76	9A	602	HEA	1	0
82	5C	803	SF4	1	0
73	1B	401	HEM	2	0
76	8A	604	HEA	1	0
79	8C	301	CUA	2	0
76	3A	604	HEA	2	0
83	5J	200	8Q1	1	0
76	8A	601	HEA	2	0
76	3A	601	HEA	1	0
82	F	201	SF4	1	0
82	C	801	SF4	1	0
85	5s	401	COO	8	0
82	5F	201	SF4	1	0
84	5P	401	NDP	4	0
81	5B	501	FMN	2	0
82	G	302	SF4	1	0
80	5A	301	FES	2	0
83	J	200	8Q1	1	0
79	4C	301	CUA	2	0
79	7C	301	CUA	3	0
79	9C	301	CUA	2	0
73	6A	401	HEM	1	0

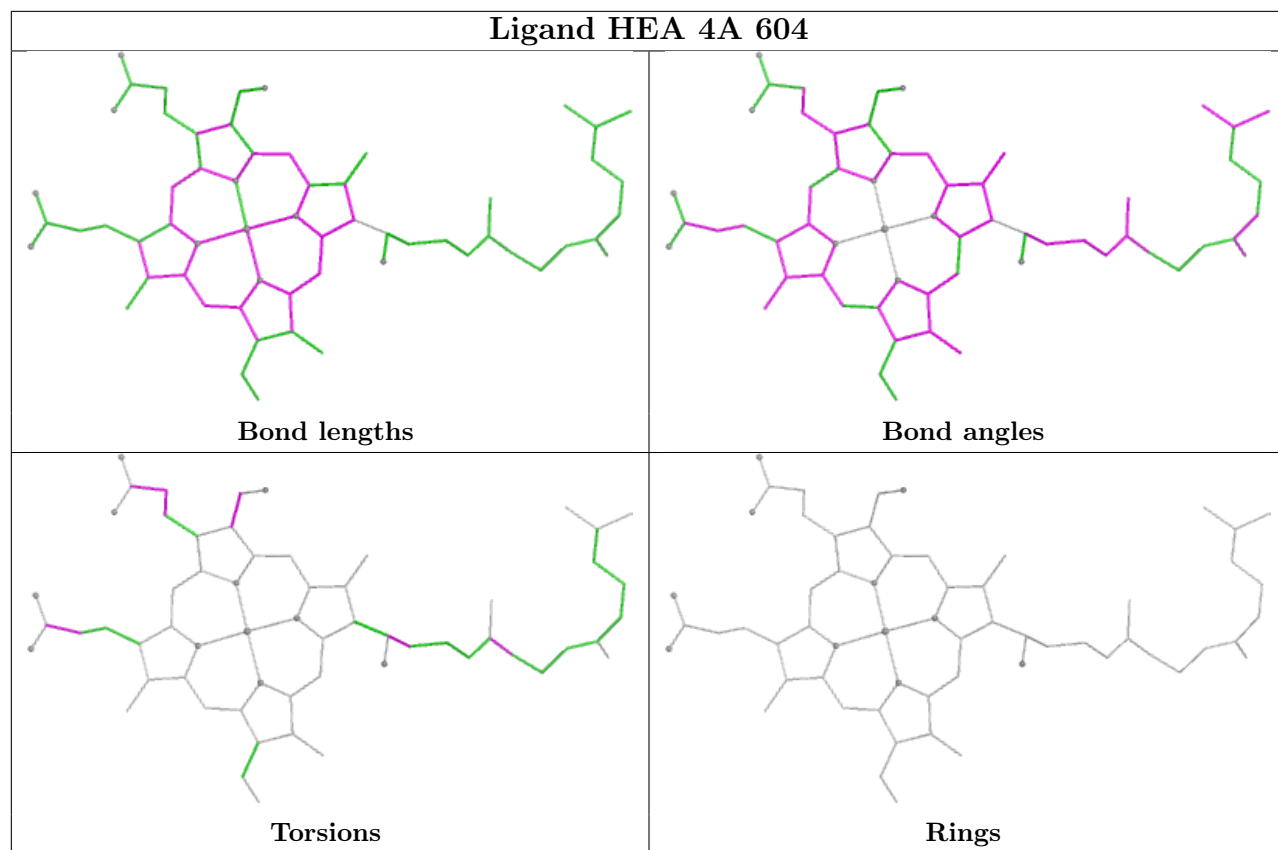
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

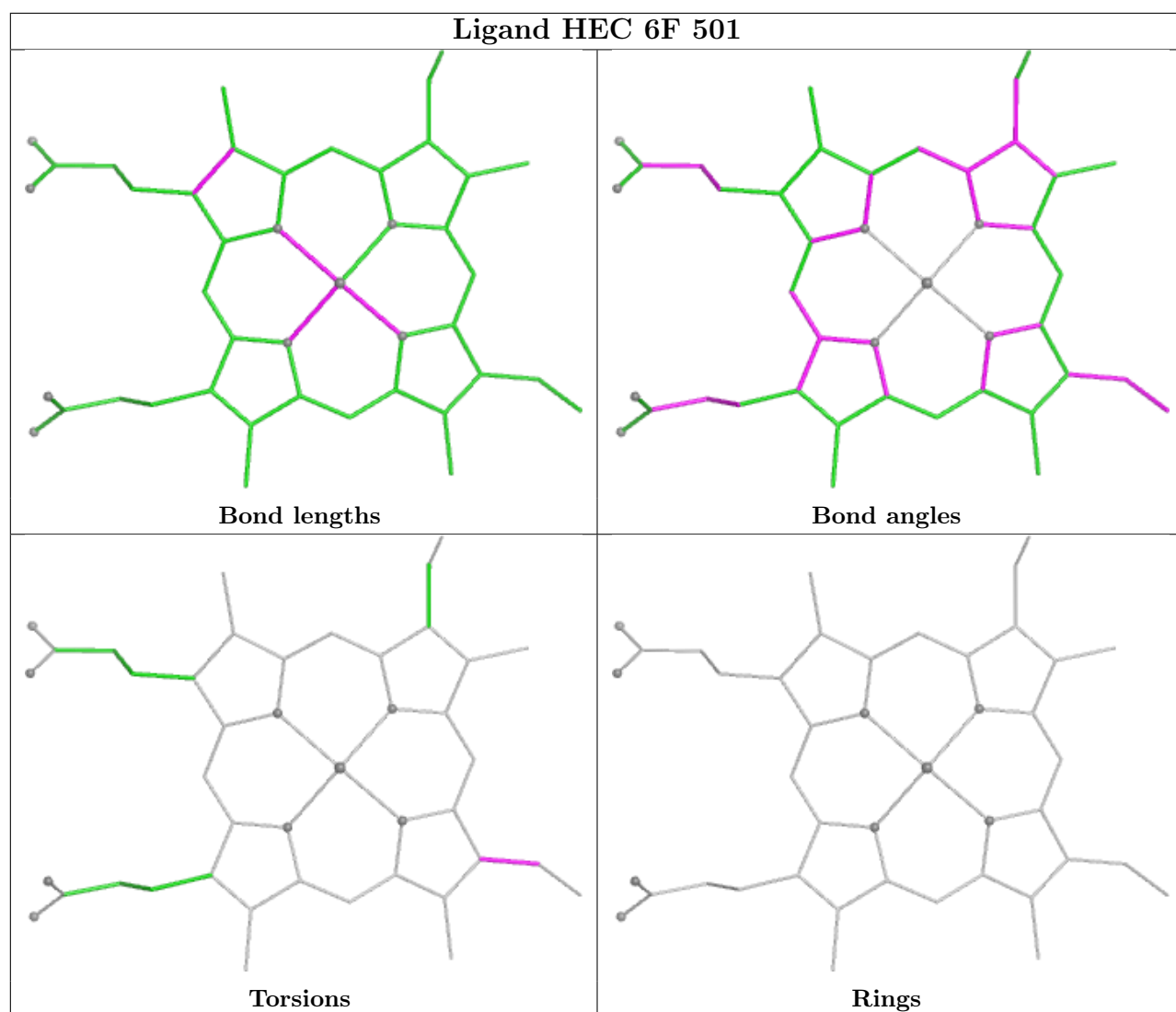
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



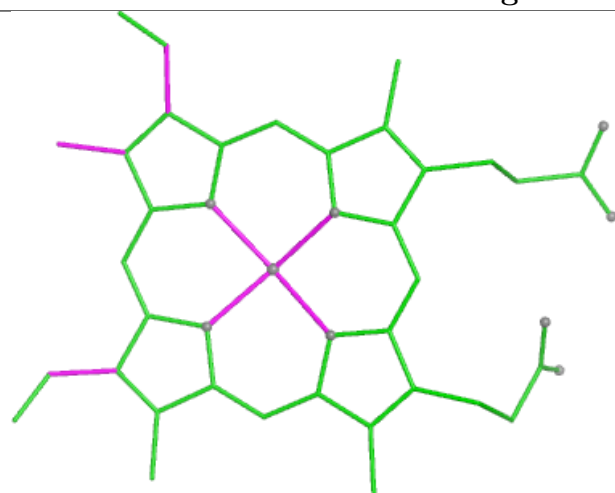




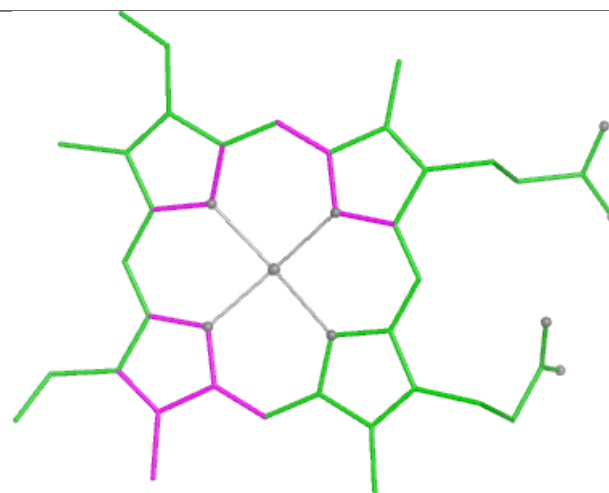




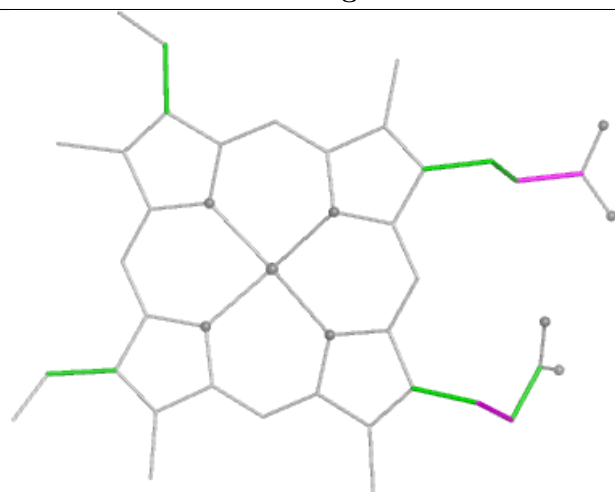
Ligand HEM 1A 401



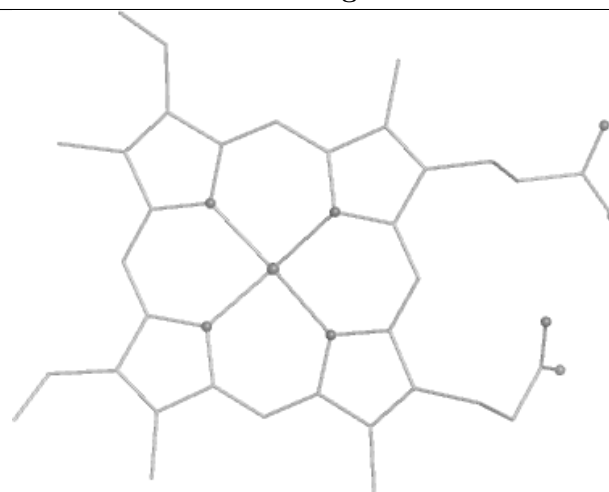
Bond lengths



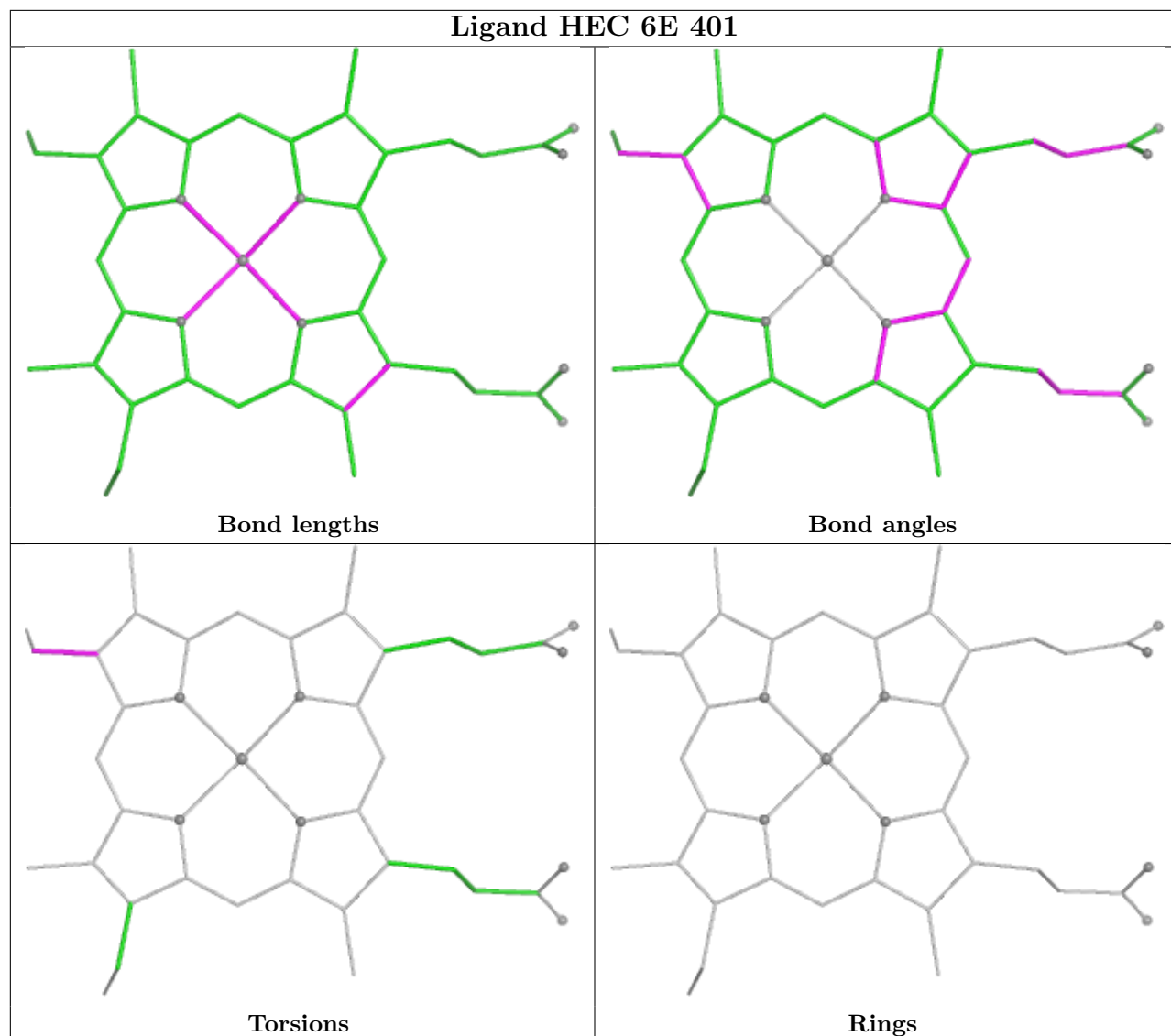
Bond angles

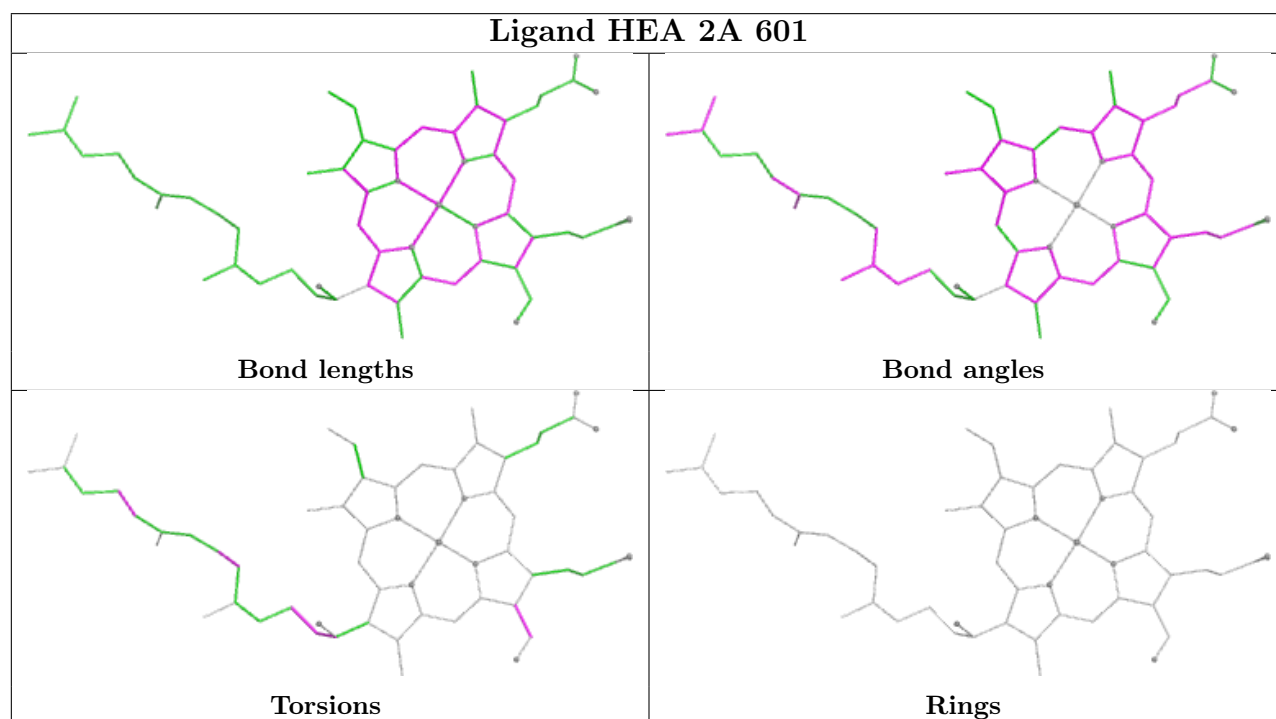
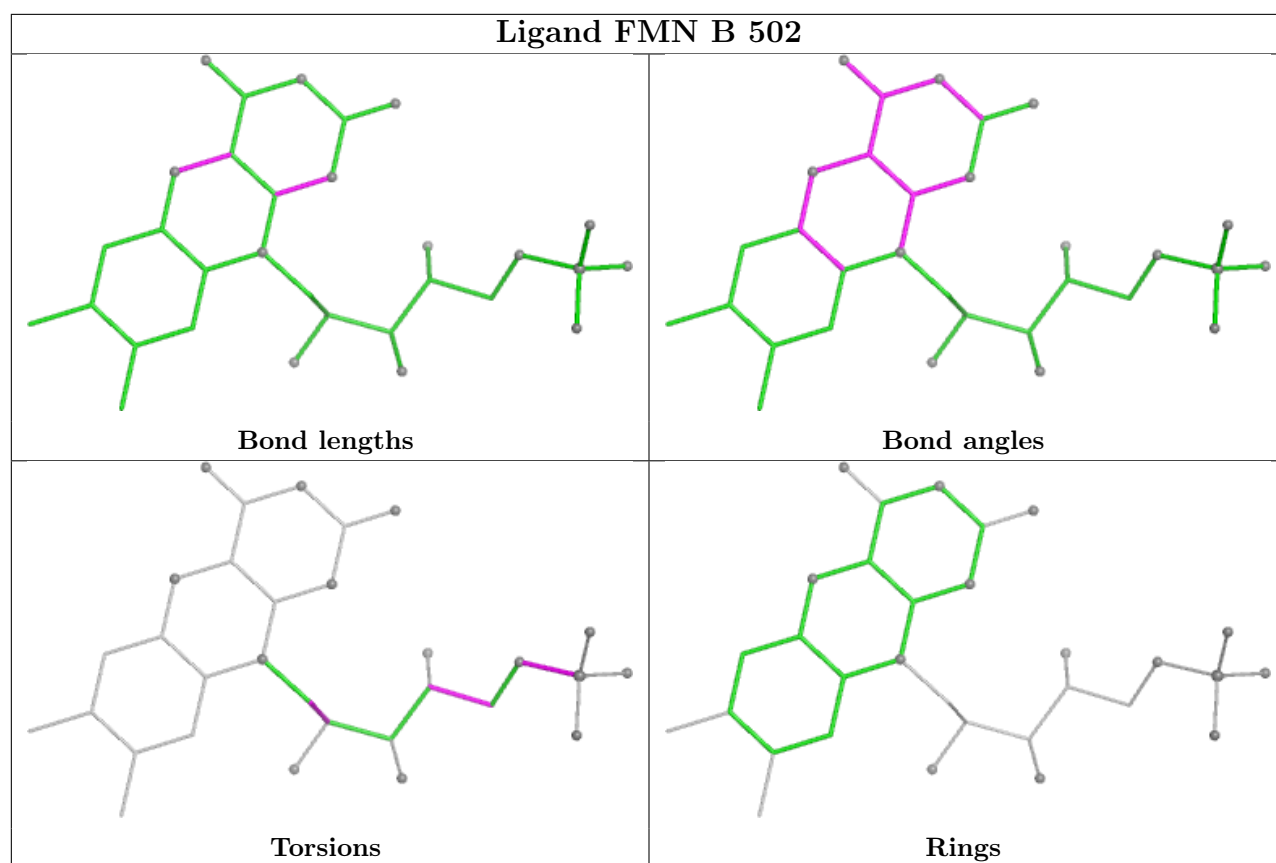


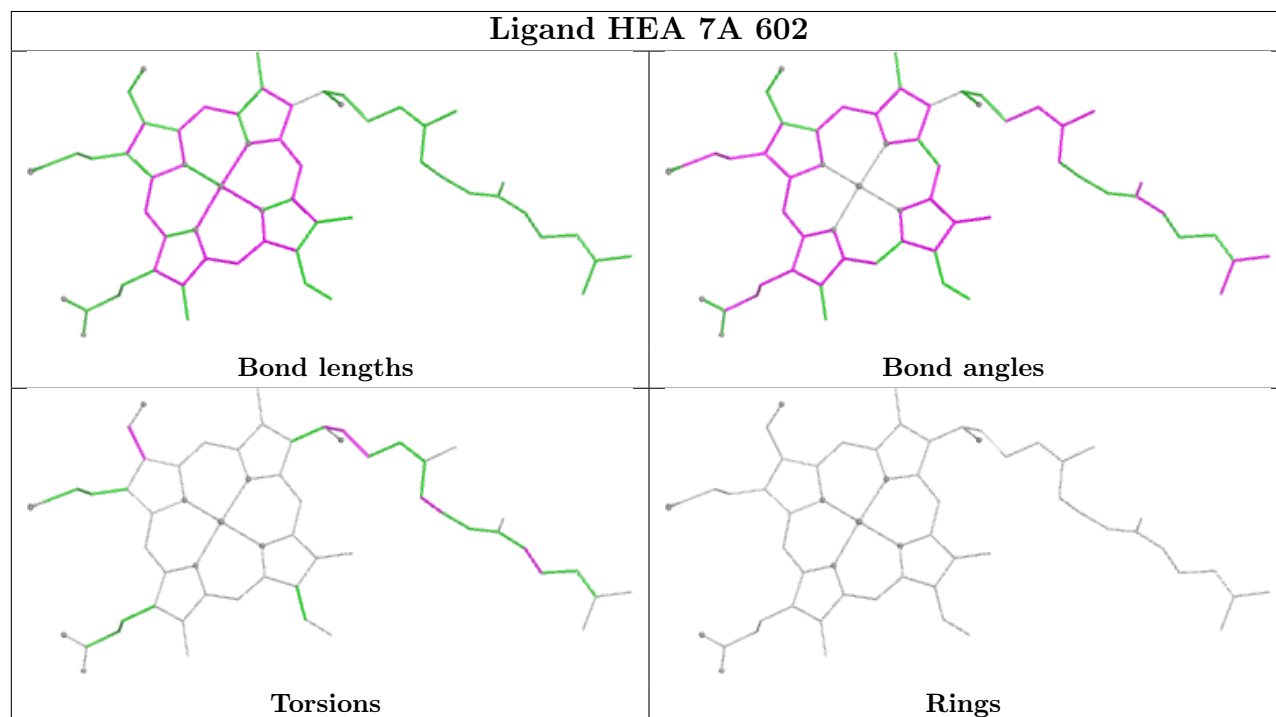
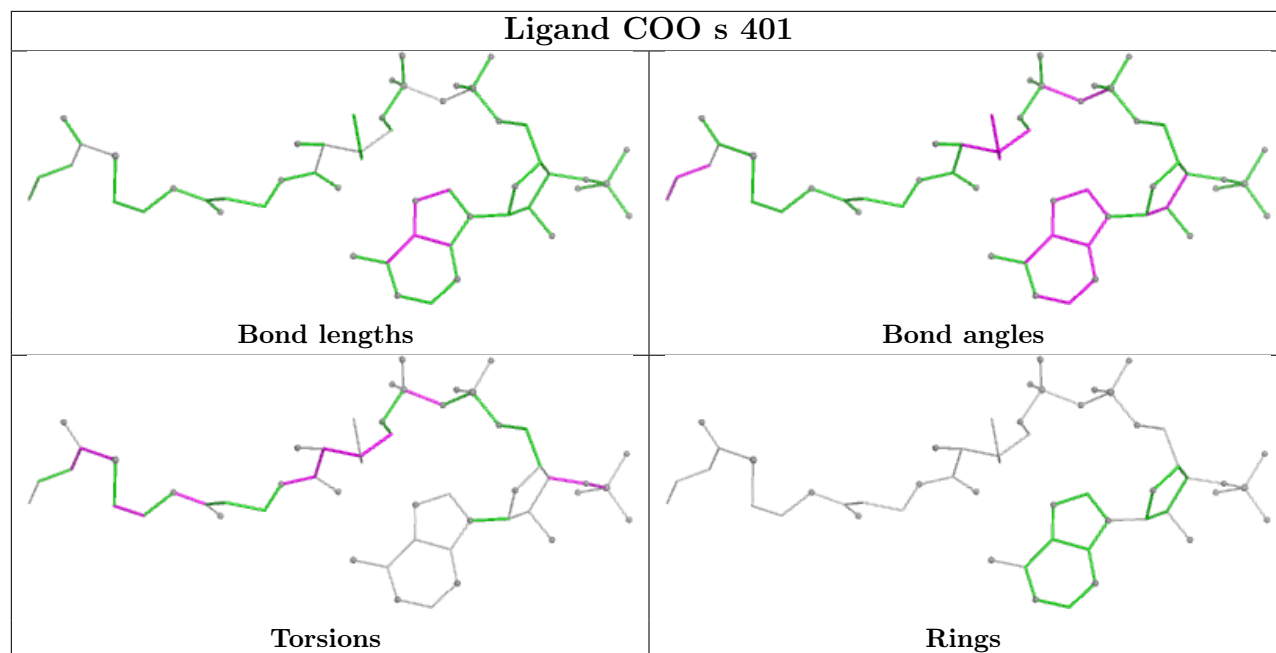
Torsions

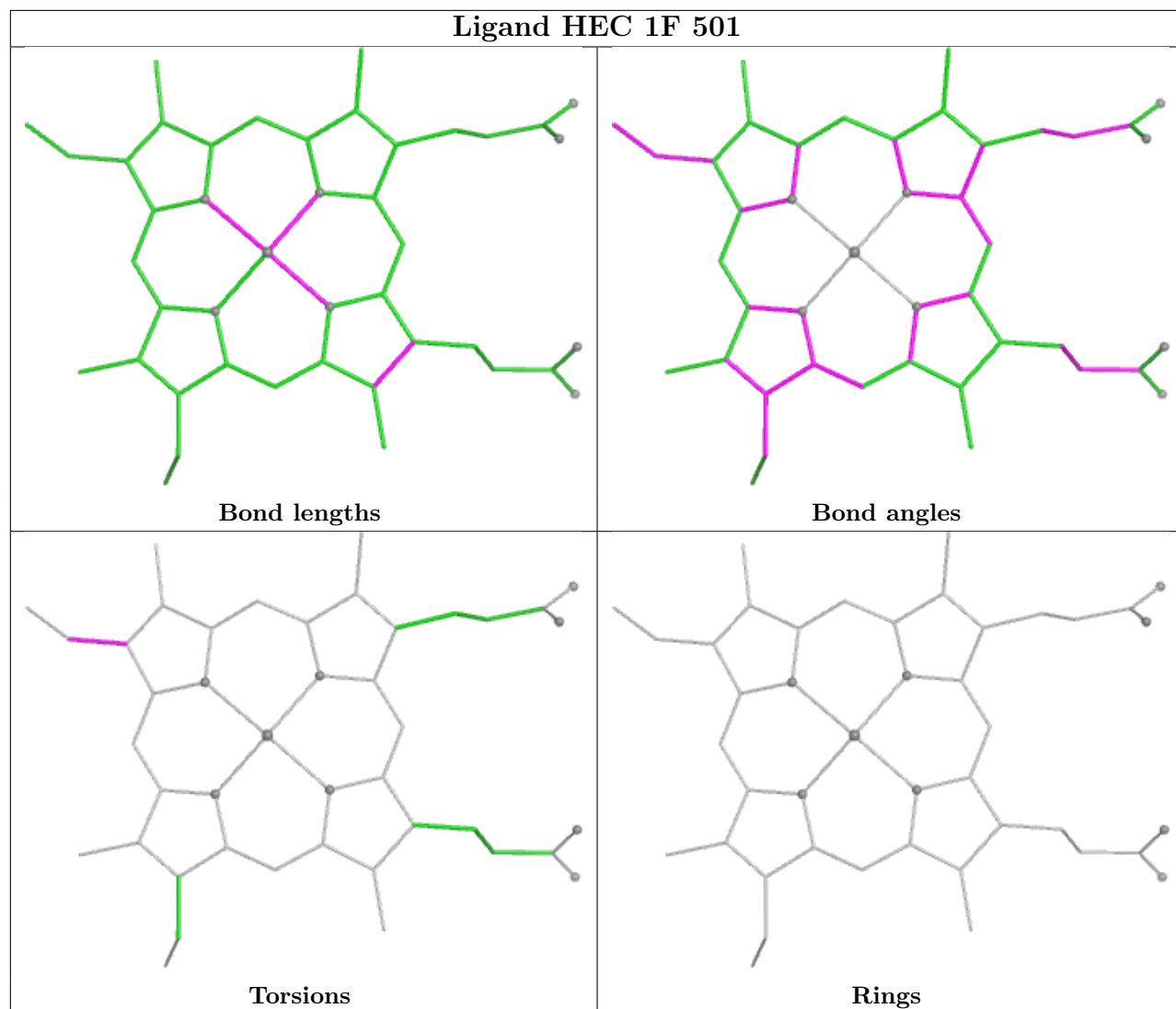


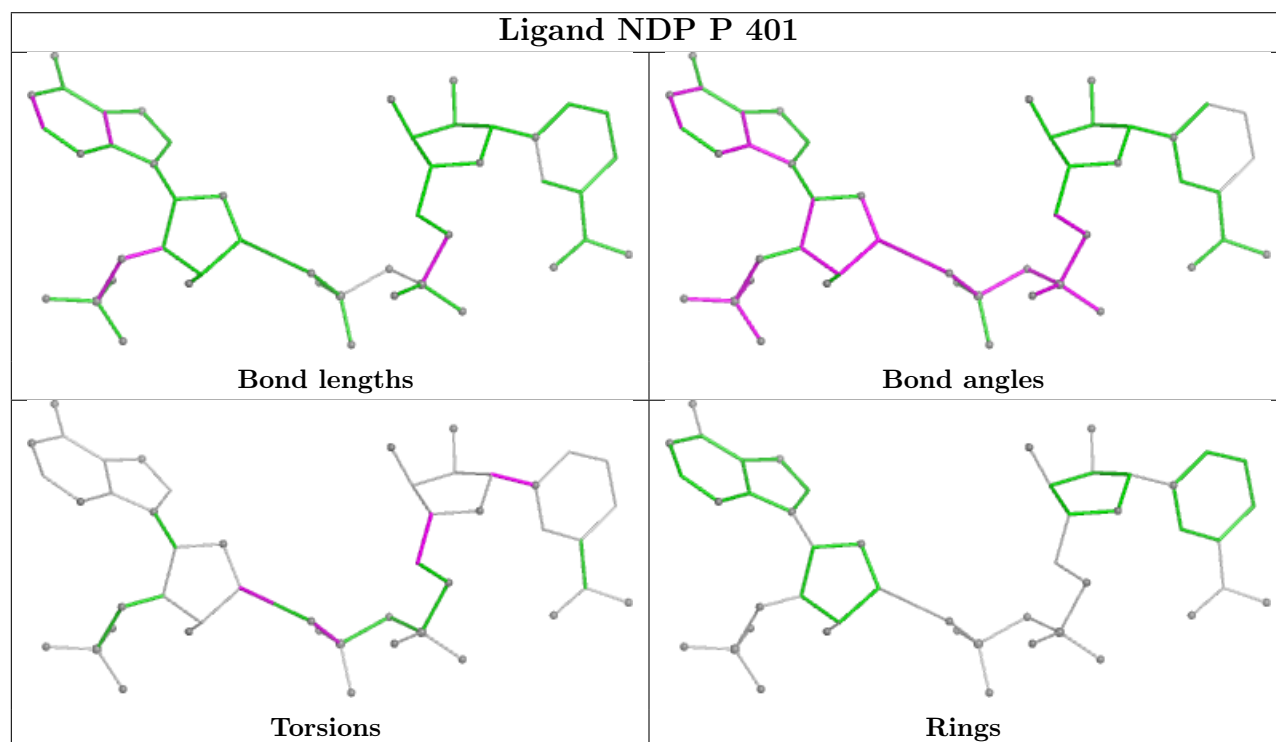
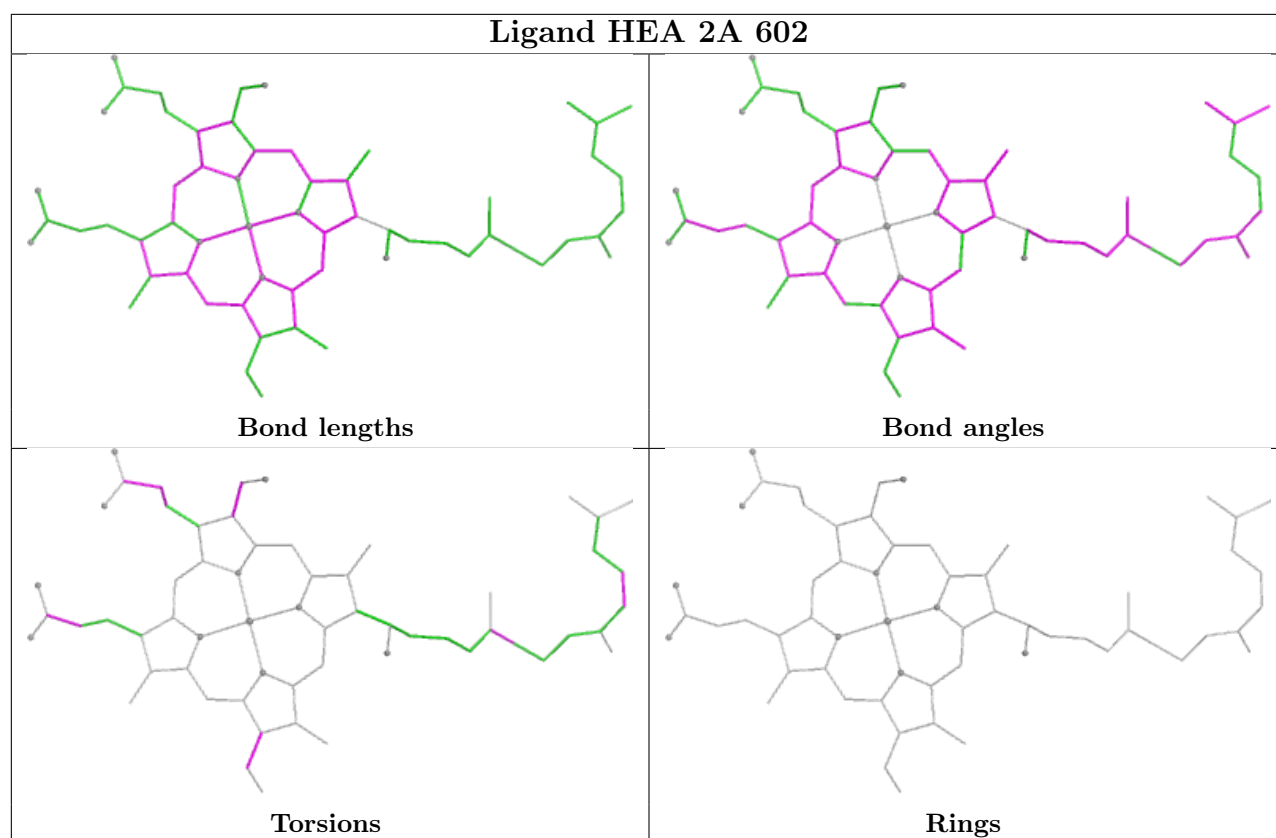
Rings

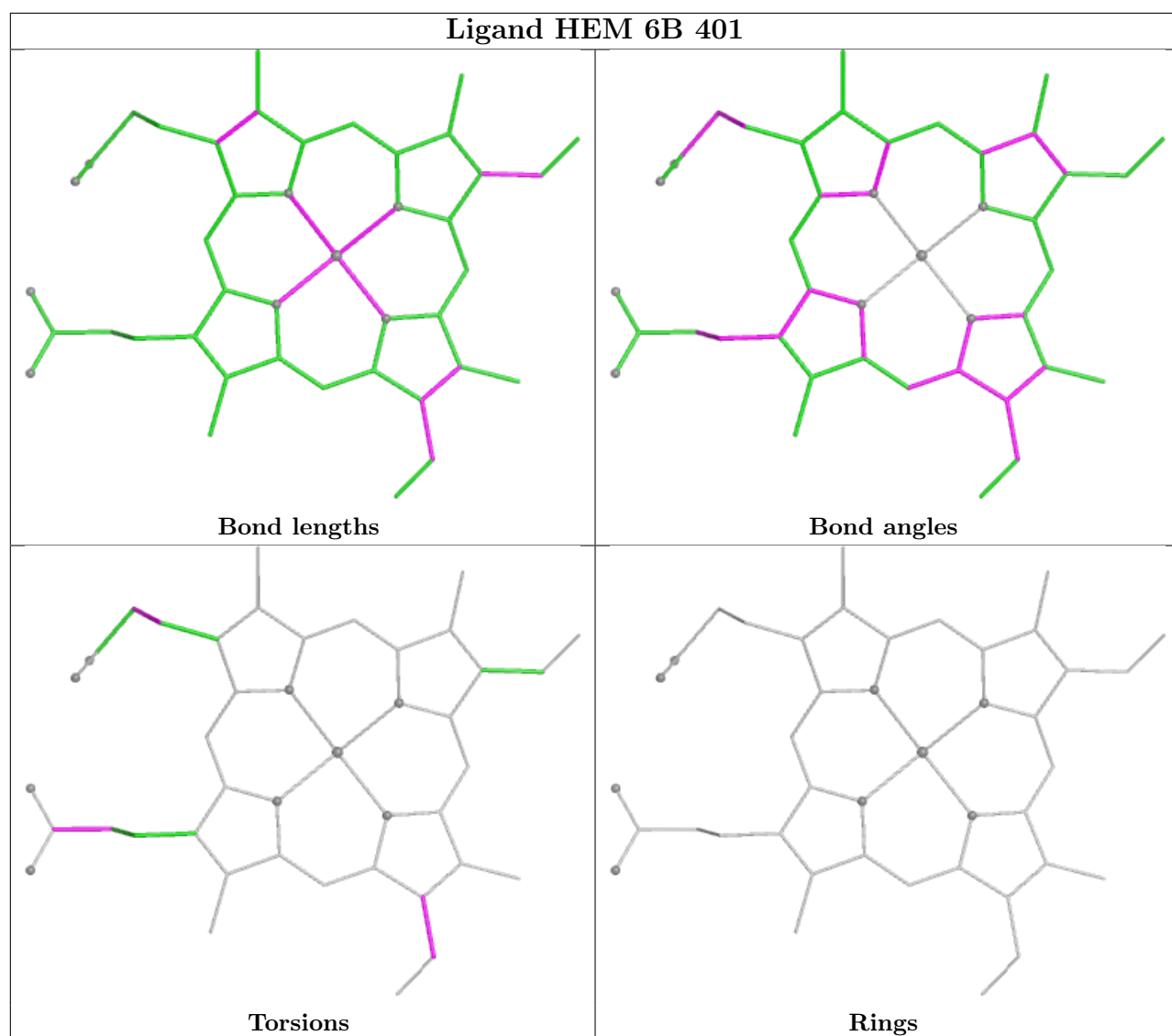


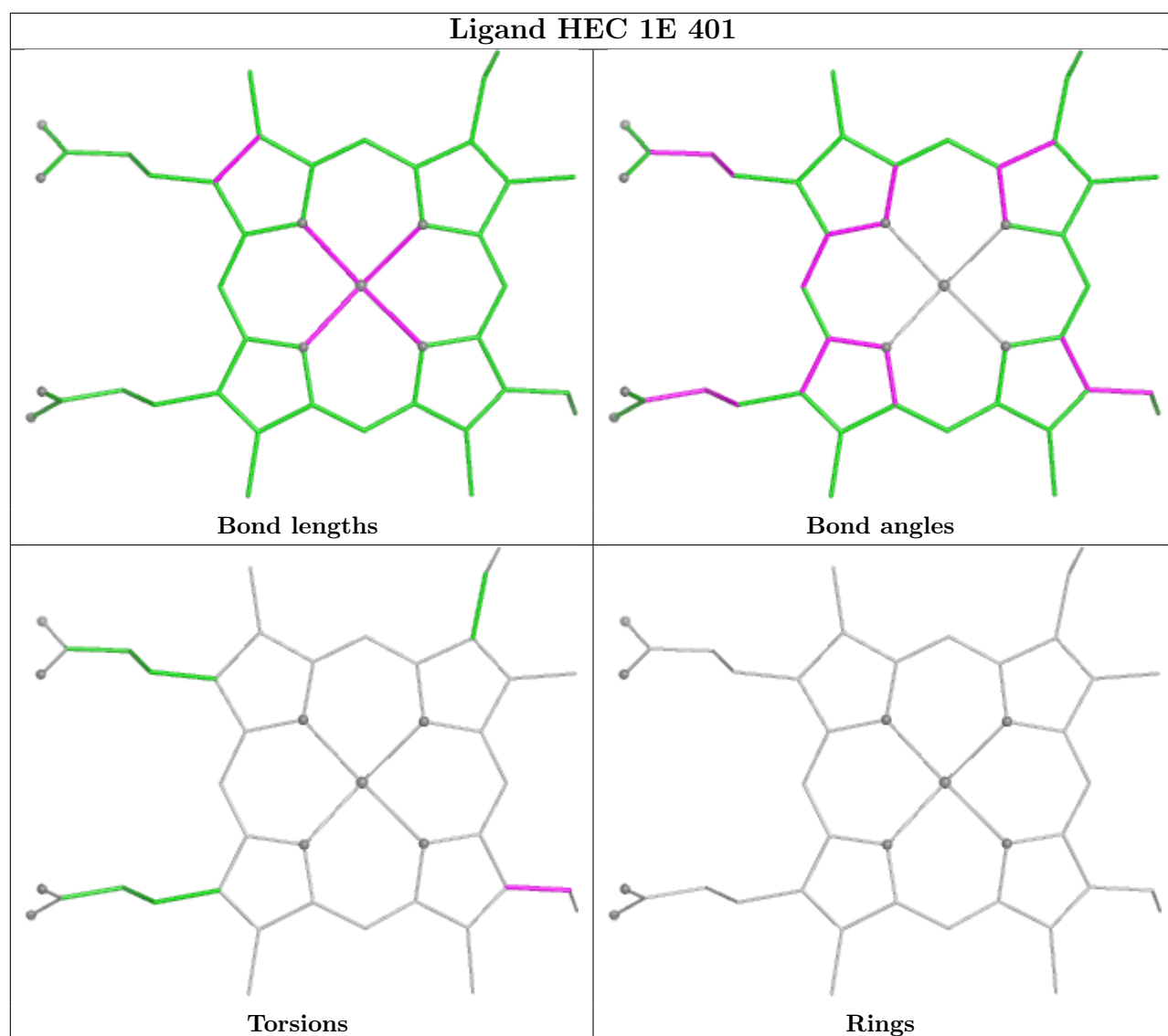


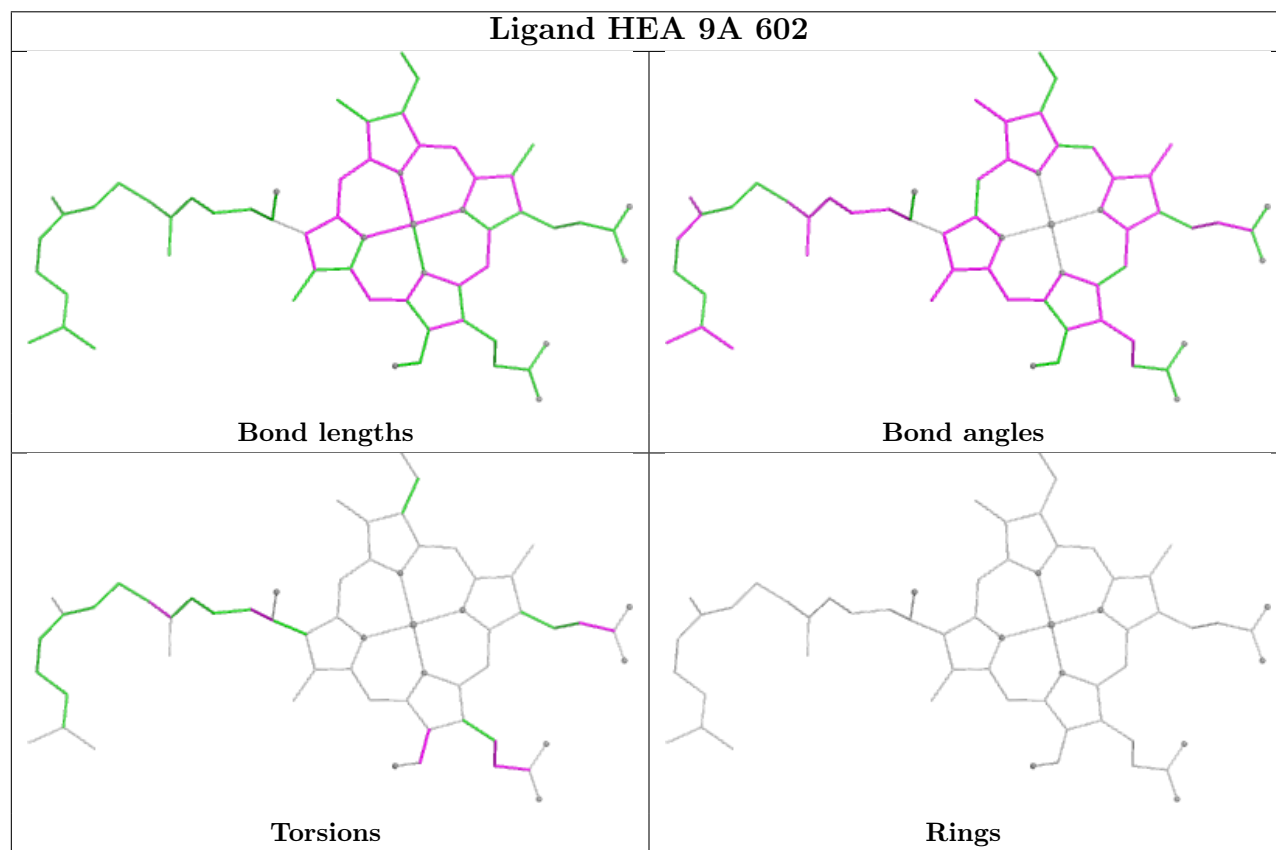
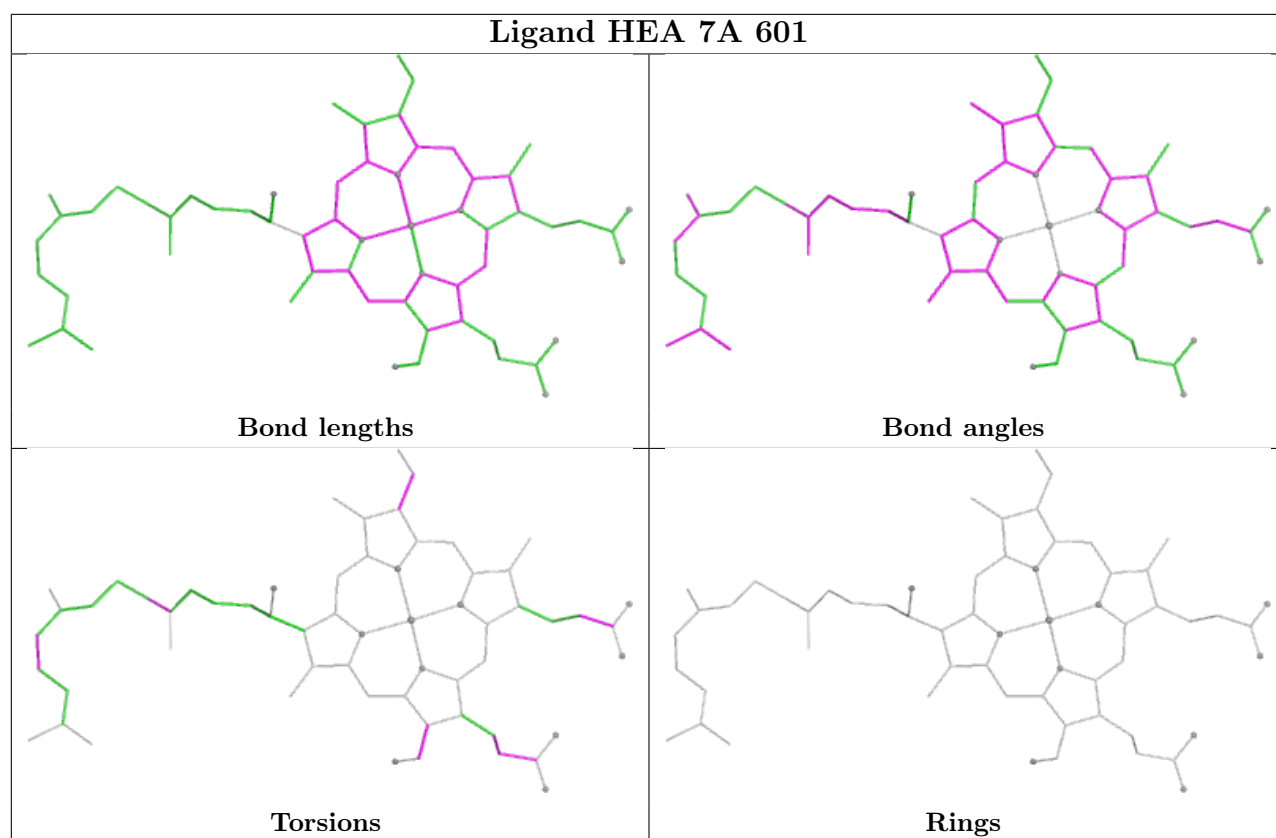




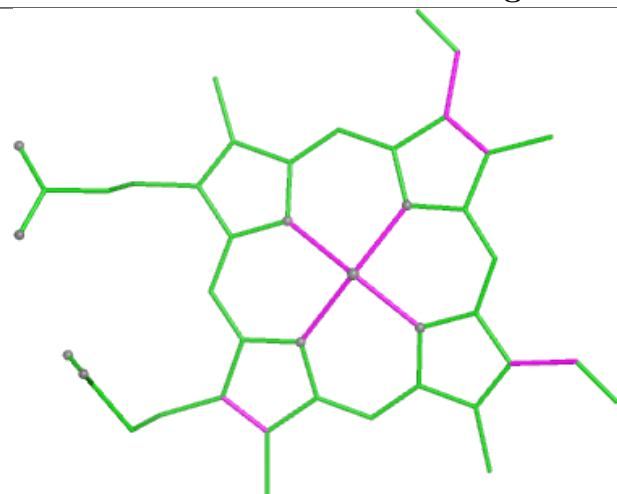




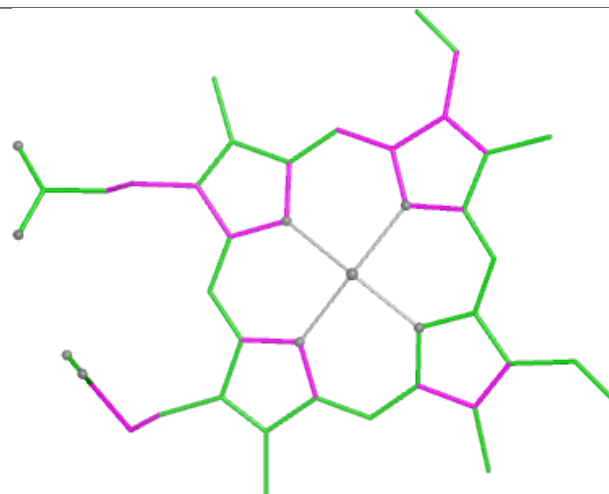




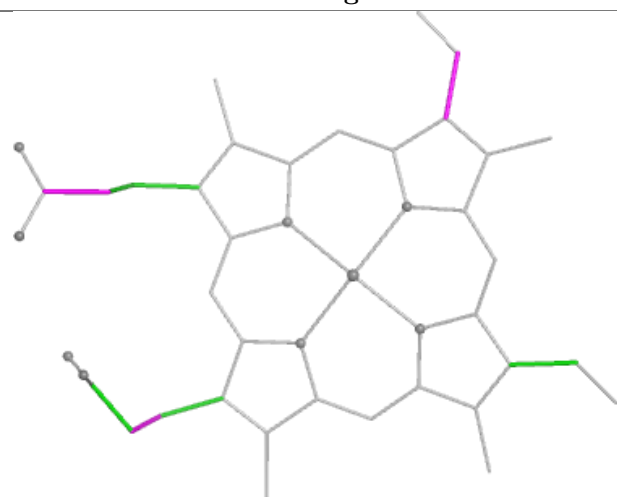
Ligand HEM 1B 401



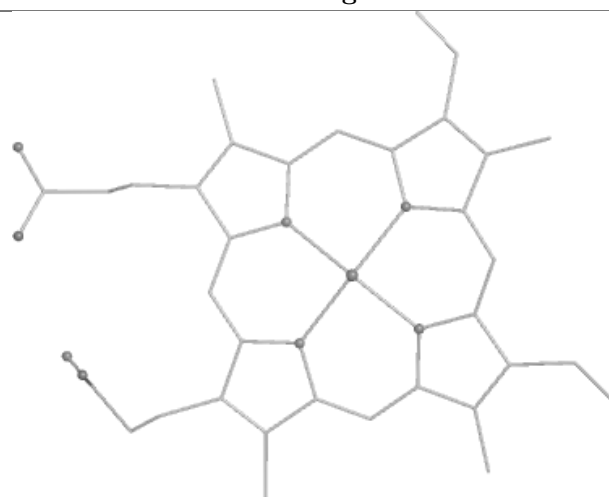
Bond lengths



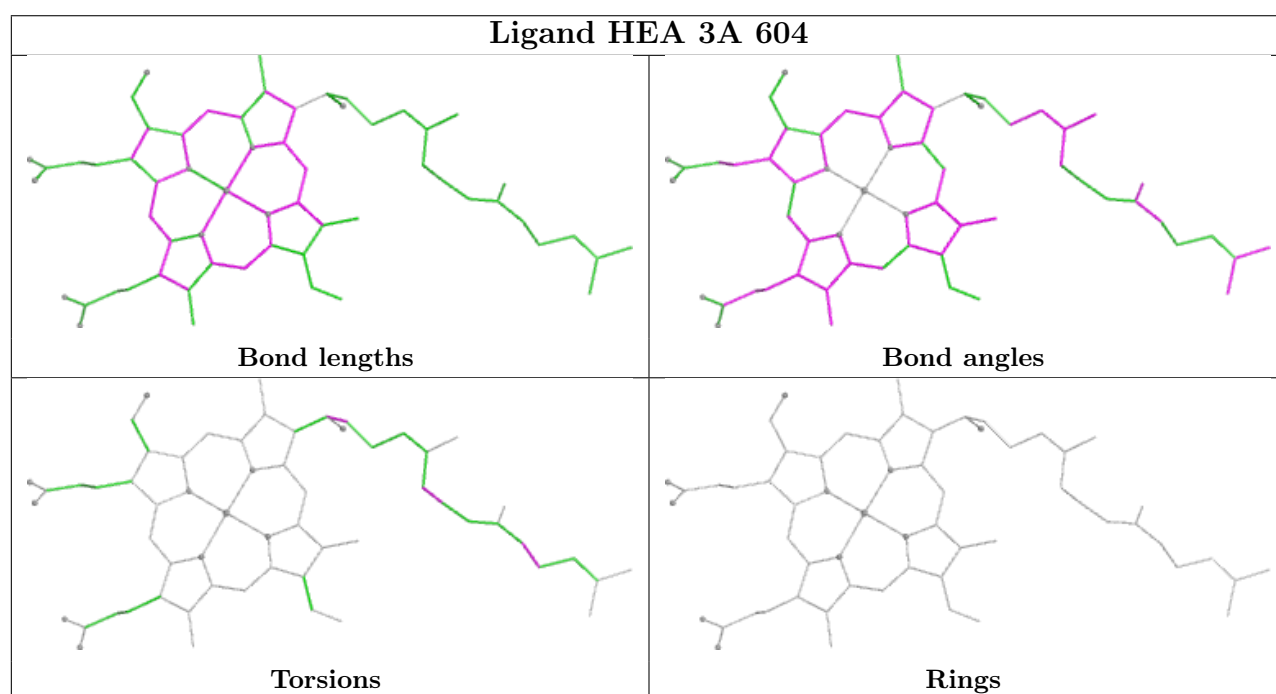
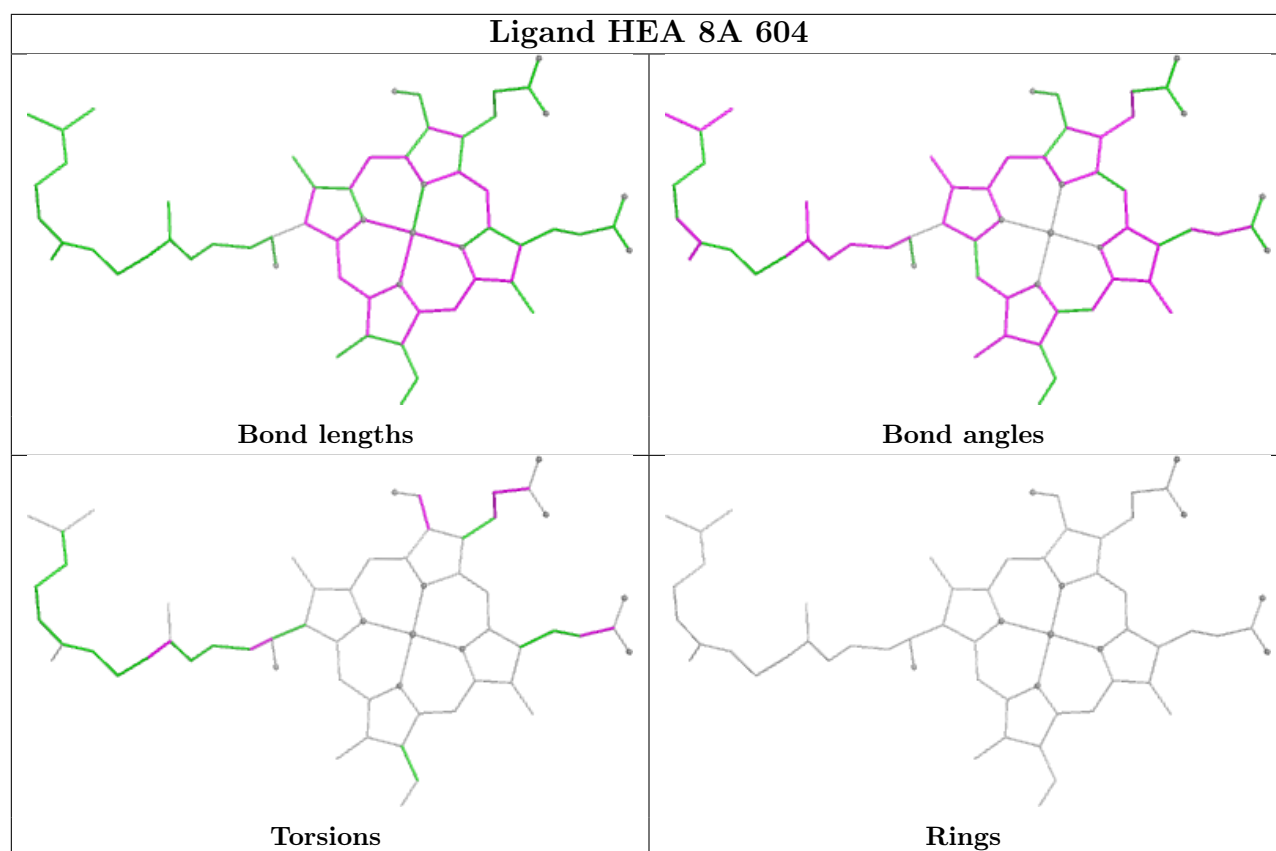
Bond angles

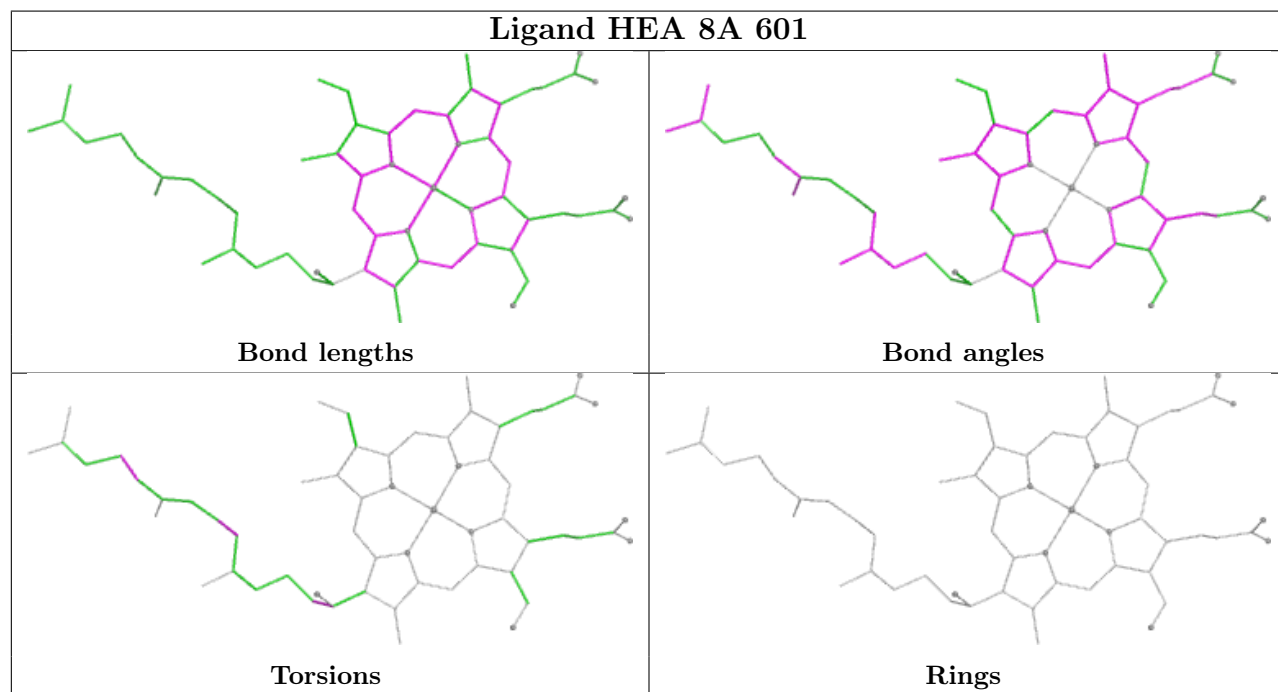
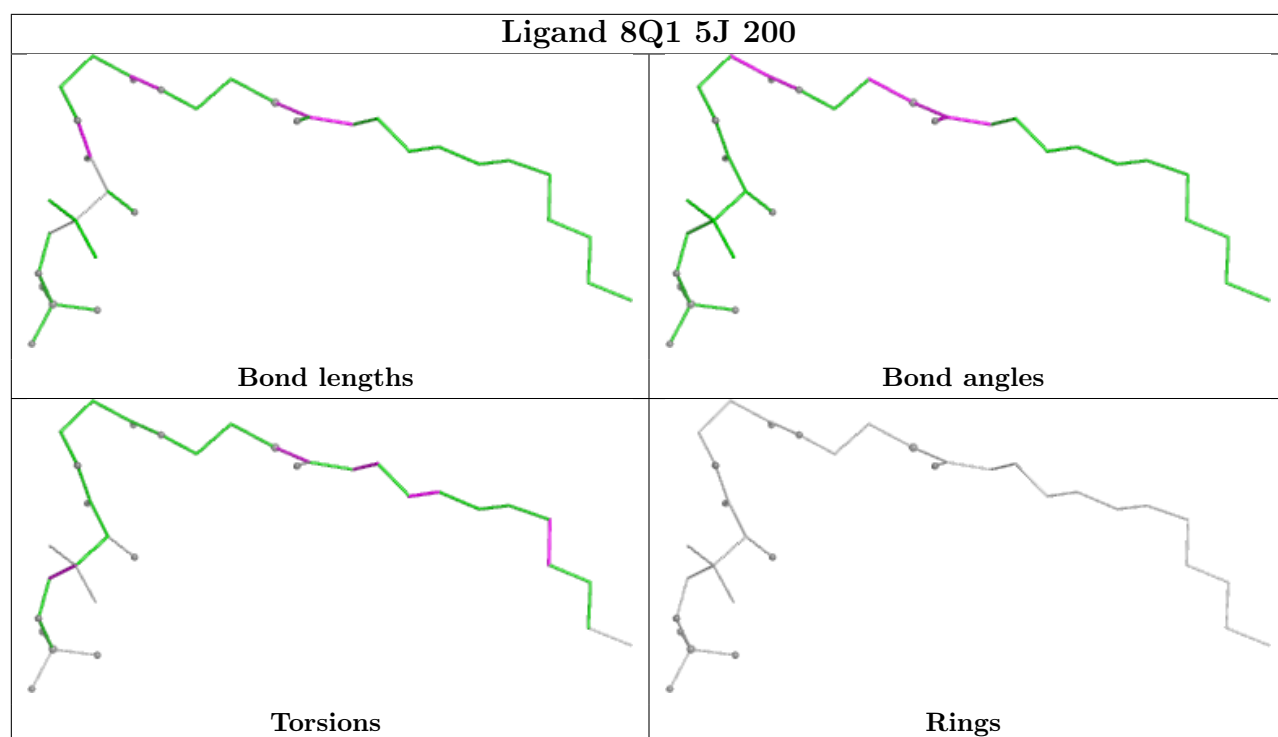


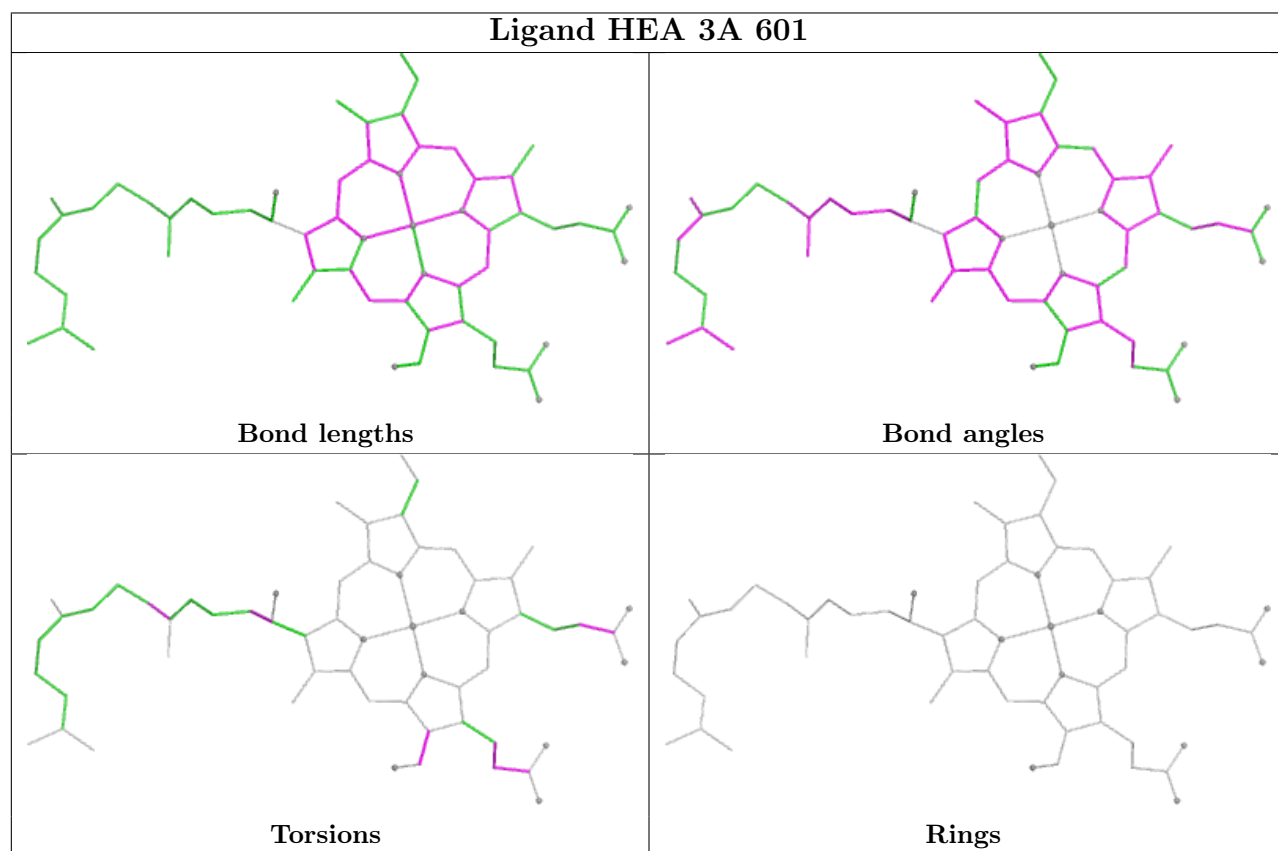
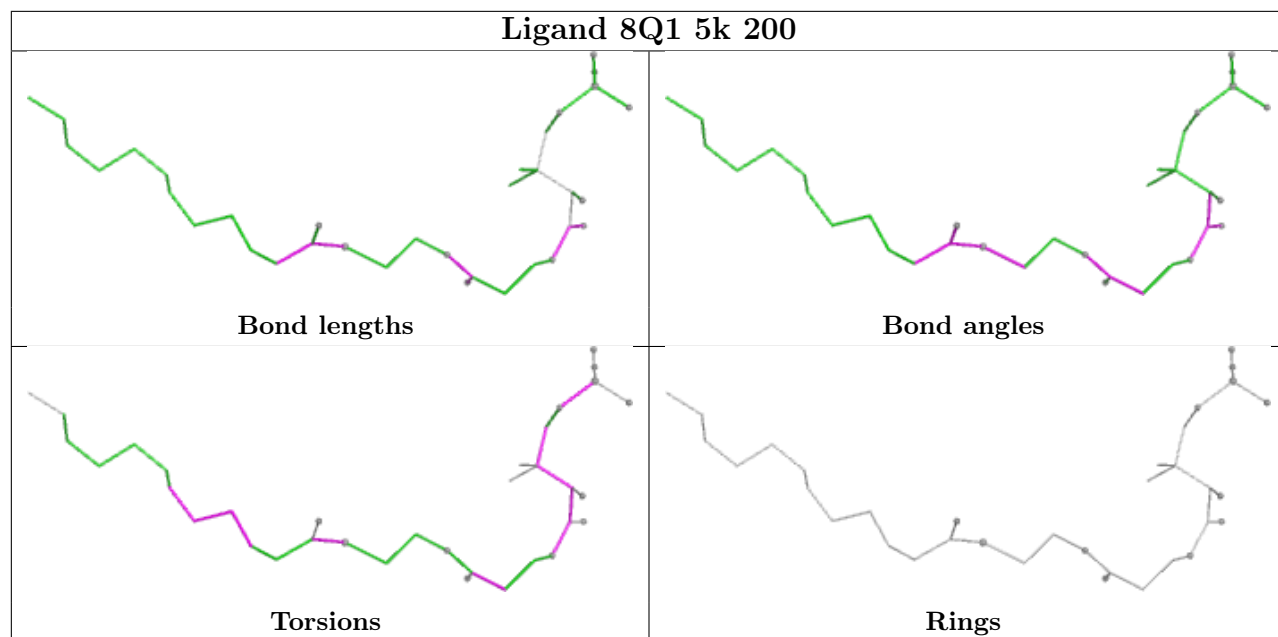
Torsions



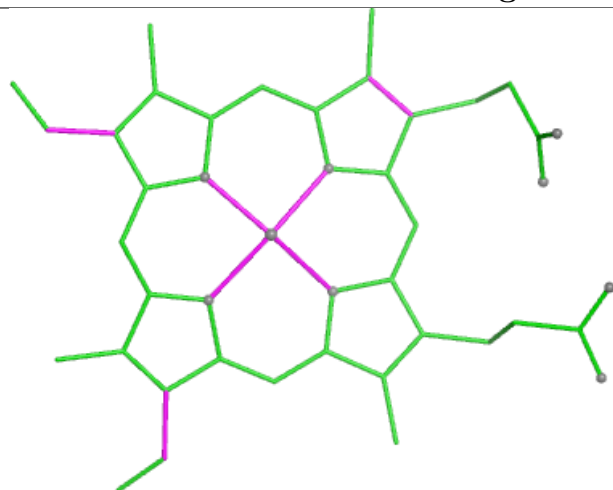
Rings



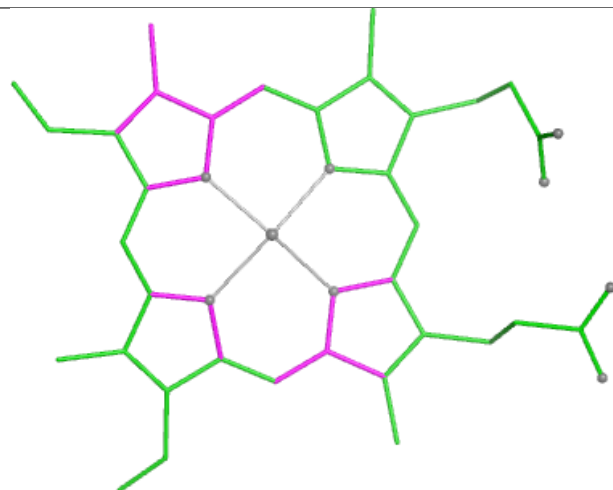




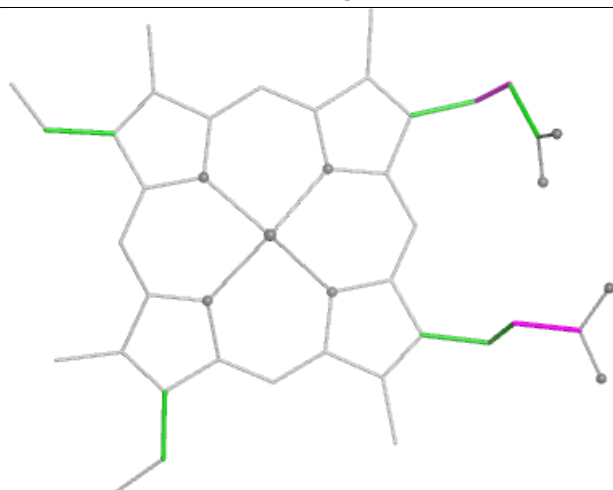
Ligand HEM 6A 402



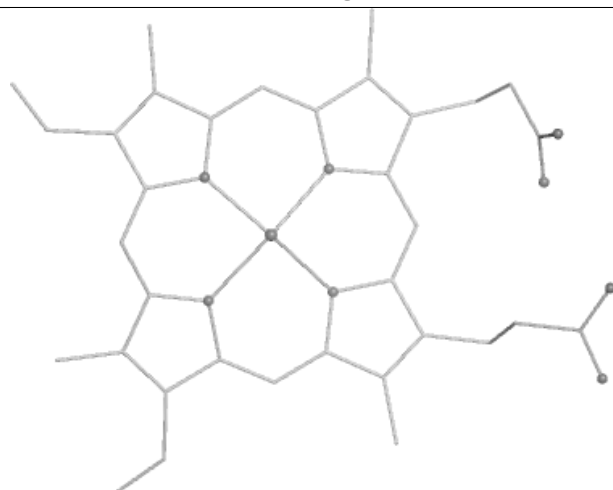
Bond lengths



Bond angles

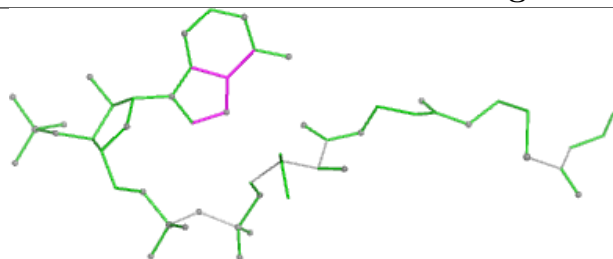


Torsions

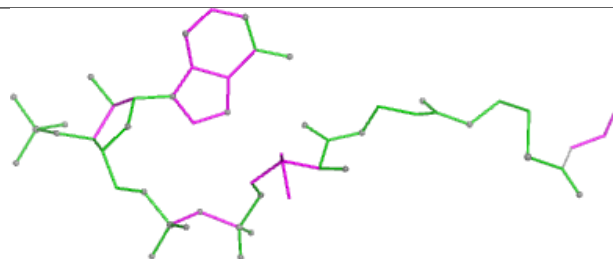


Rings

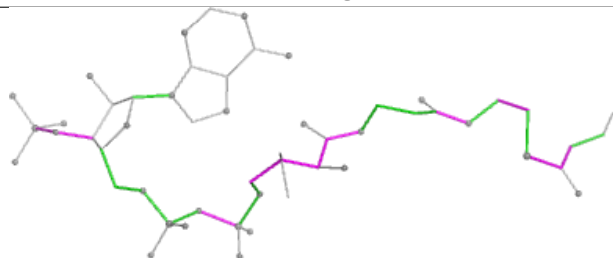
Ligand COO 5s 401



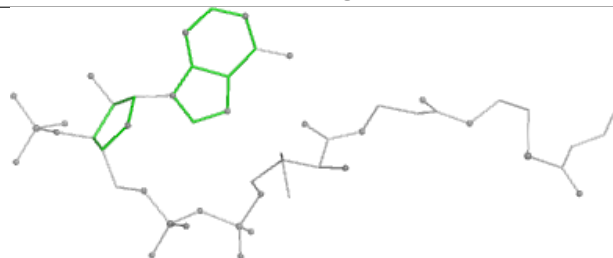
Bond lengths



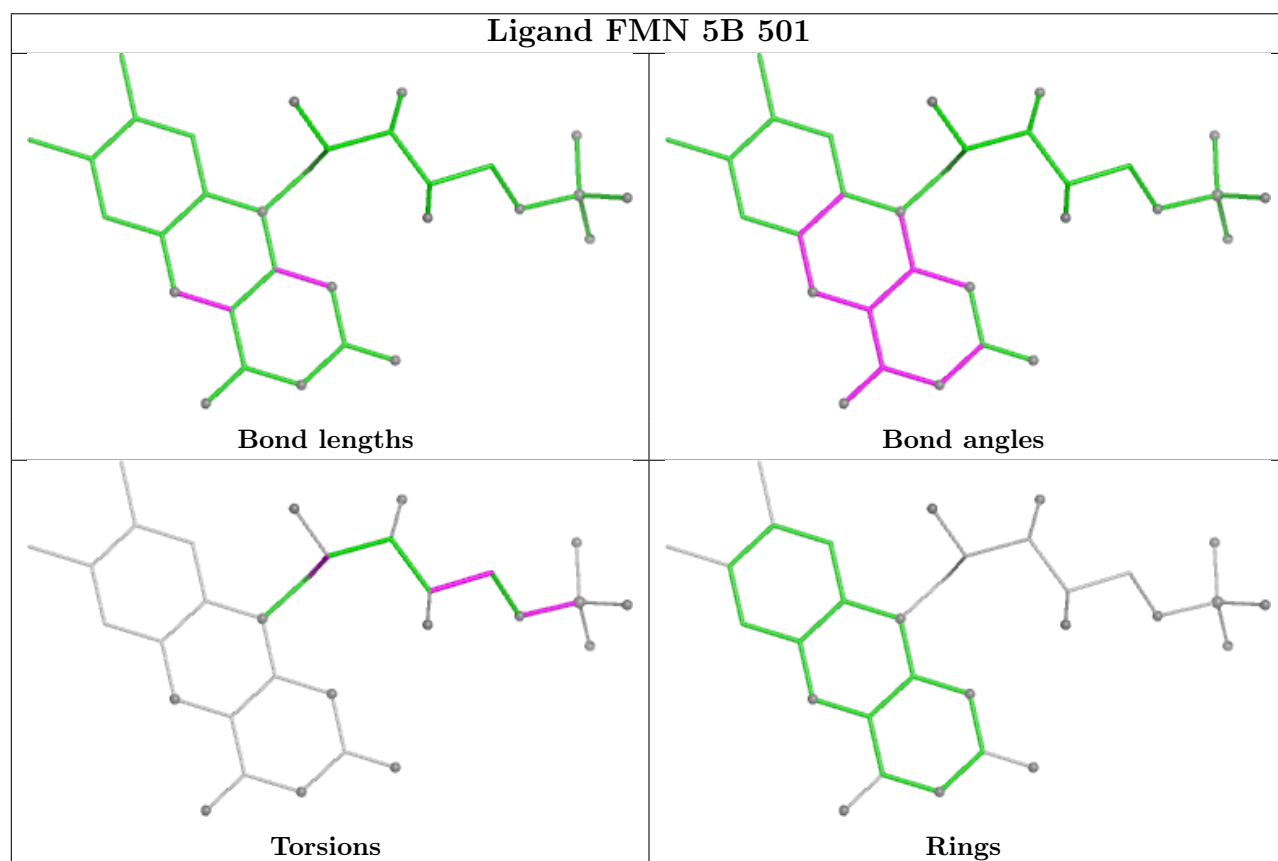
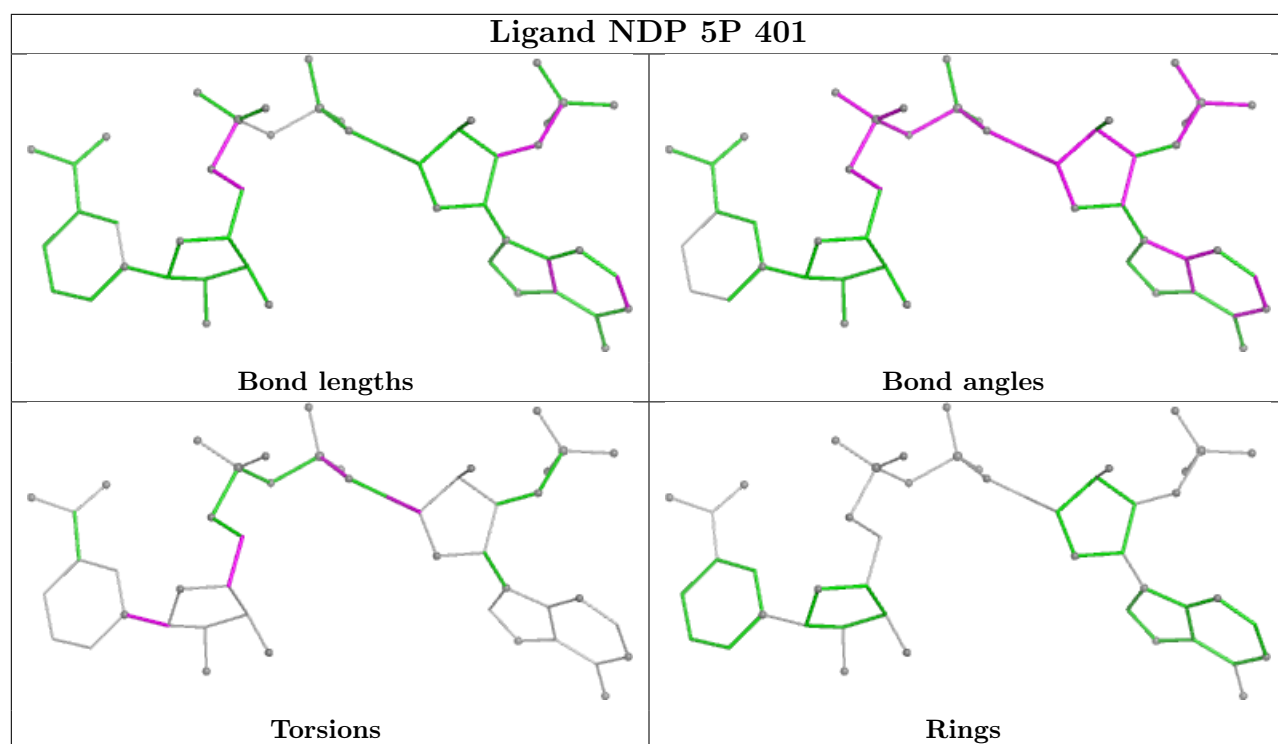
Bond angles



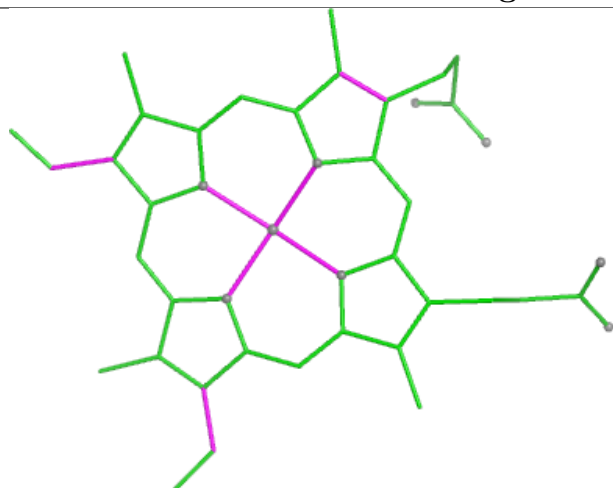
Torsions



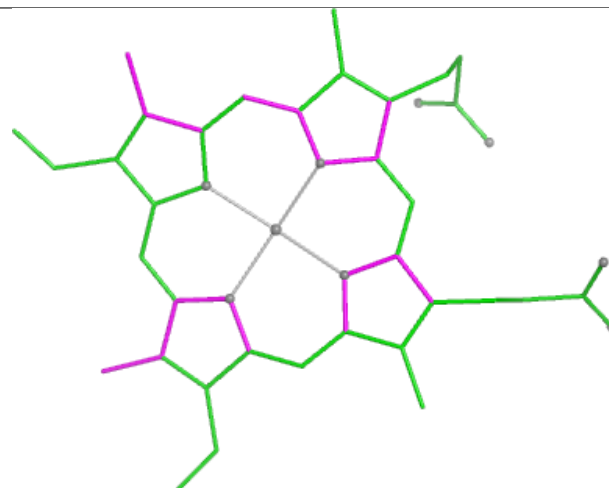
Rings



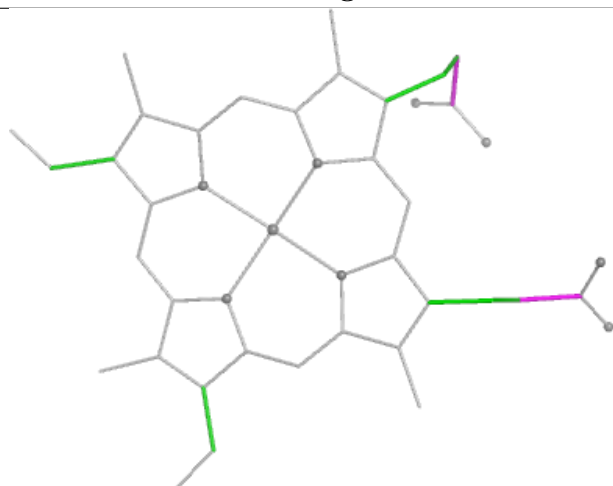
Ligand HEM 1A 402



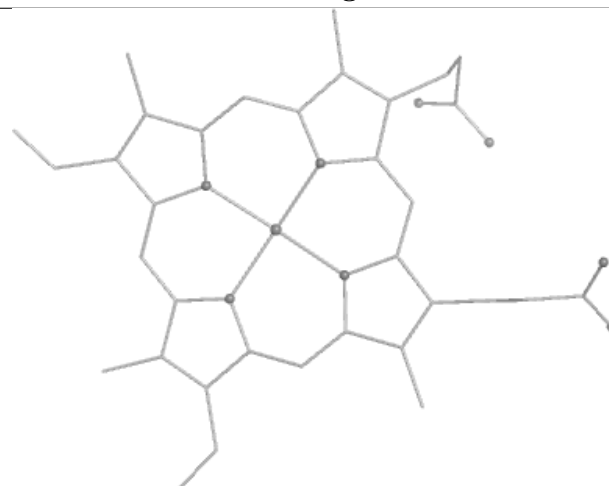
Bond lengths



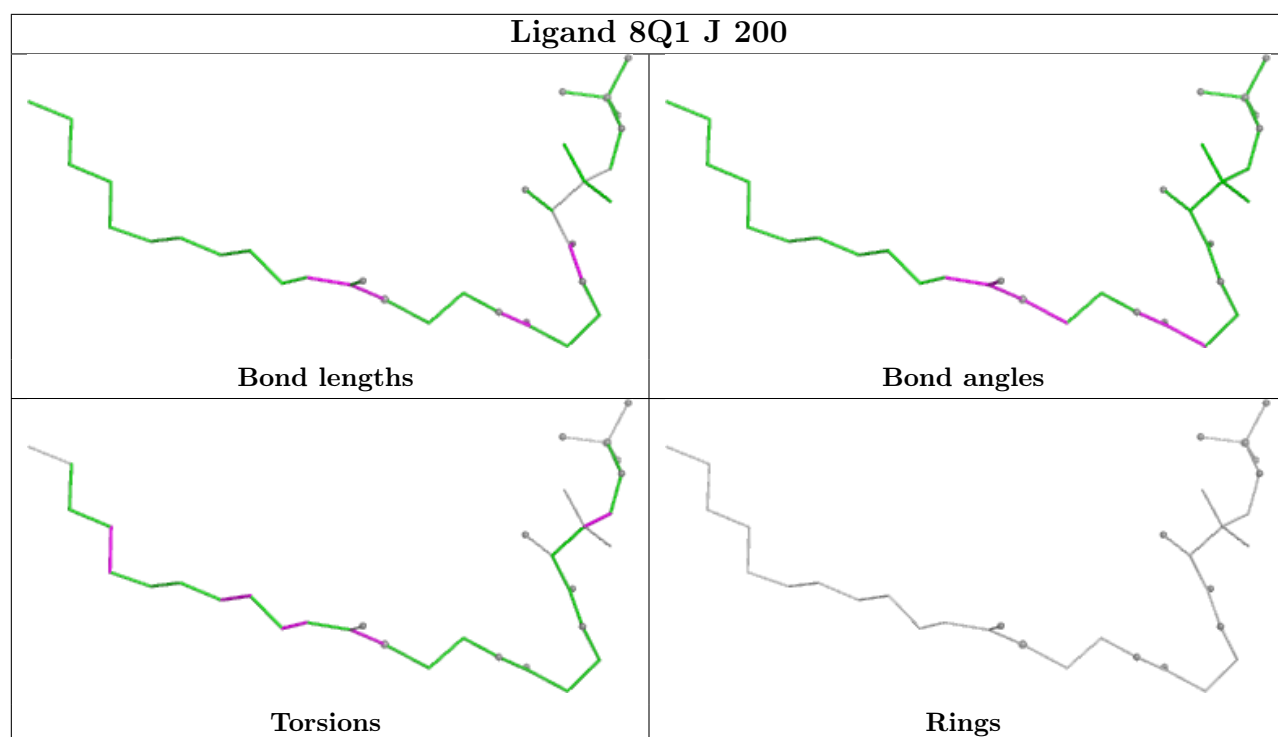
Bond angles

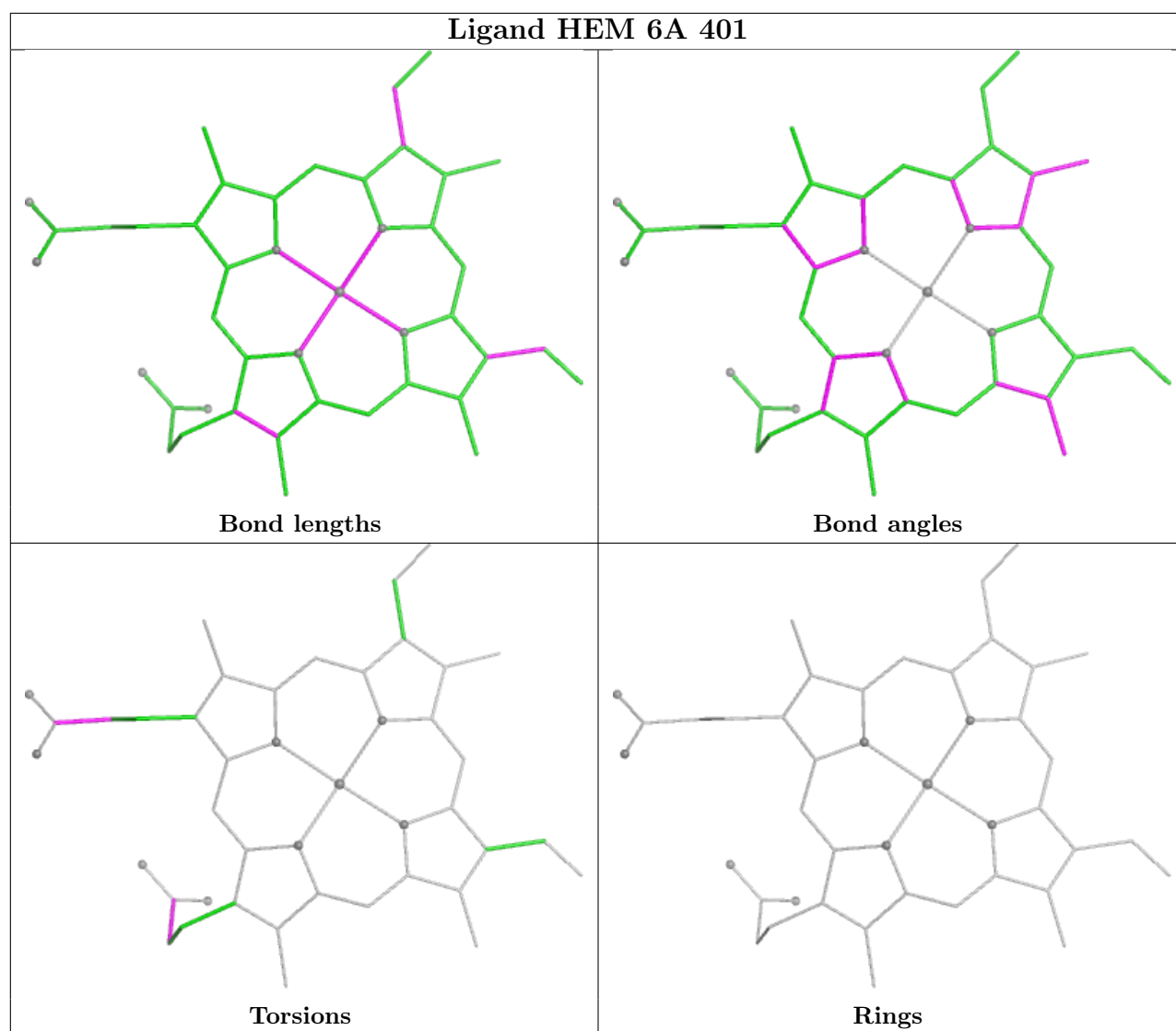


Torsions



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.

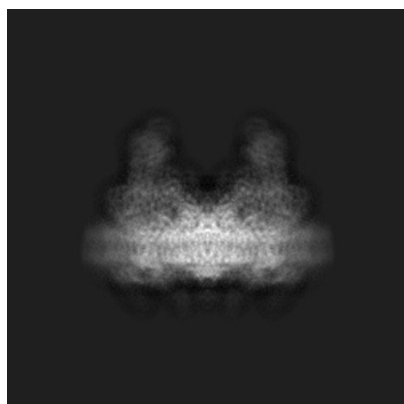
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50210. These allow visual inspection of the internal detail of the map and identification of artifacts.

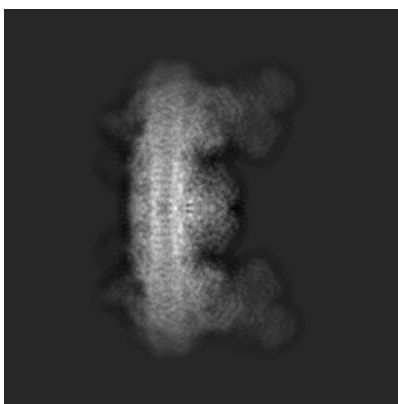
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

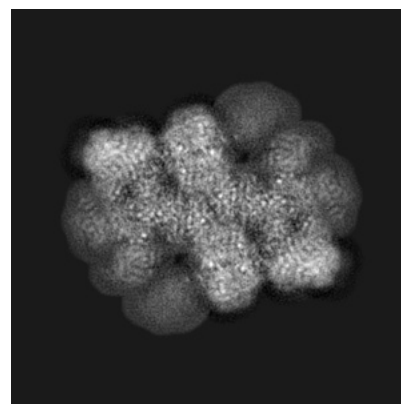
6.1.1 Primary map



X

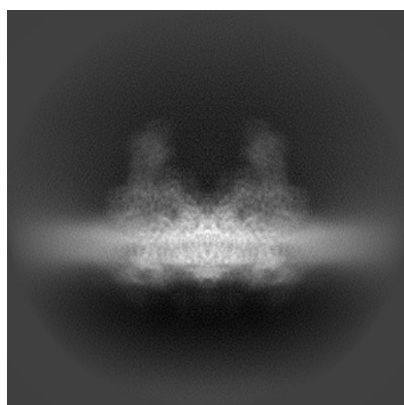


Y

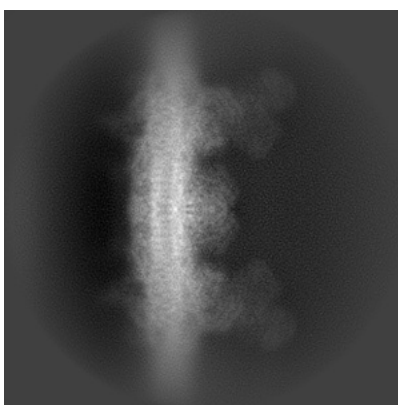


Z

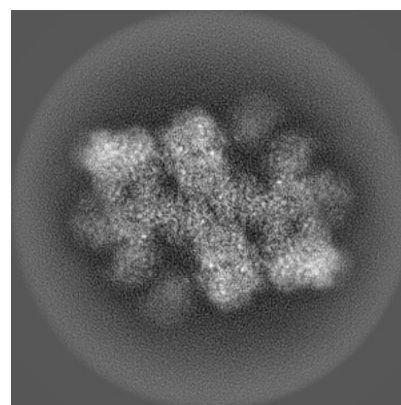
6.1.2 Raw map



X



Y

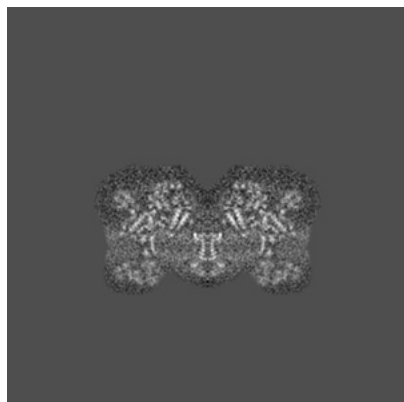


Z

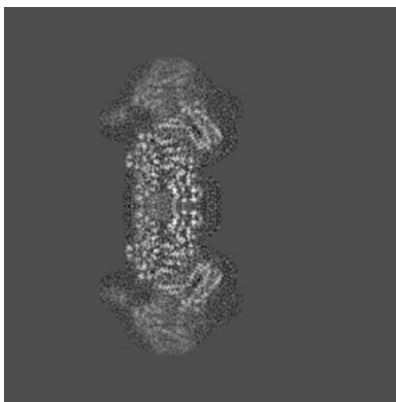
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

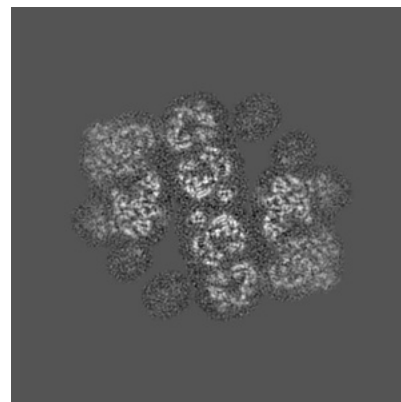
6.2.1 Primary map



X Index: 144

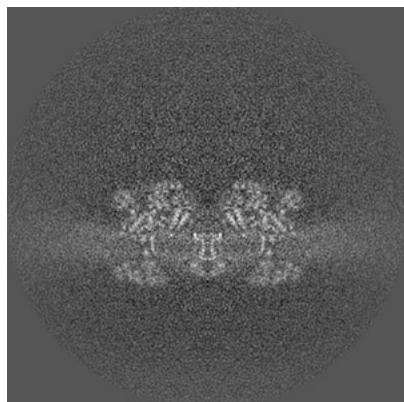


Y Index: 144

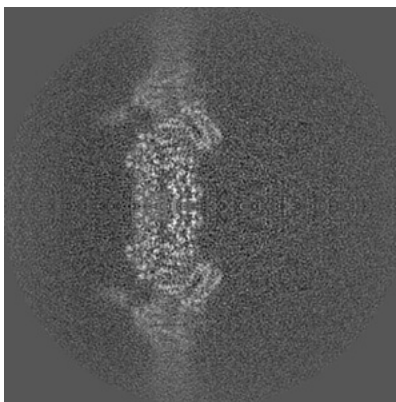


Z Index: 144

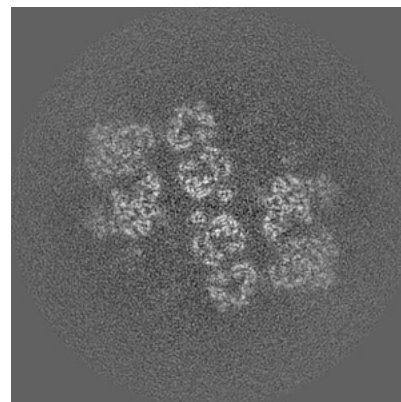
6.2.2 Raw map



X Index: 144



Y Index: 144

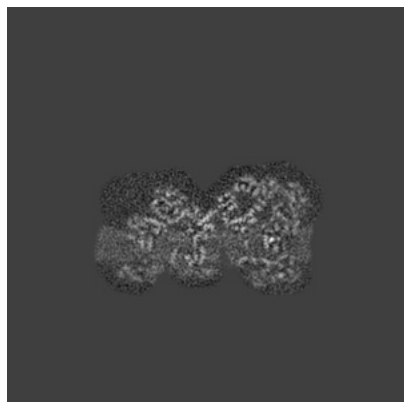


Z Index: 144

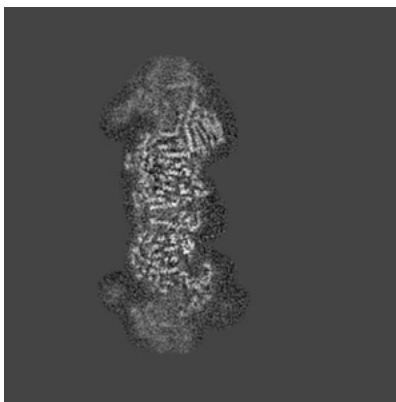
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

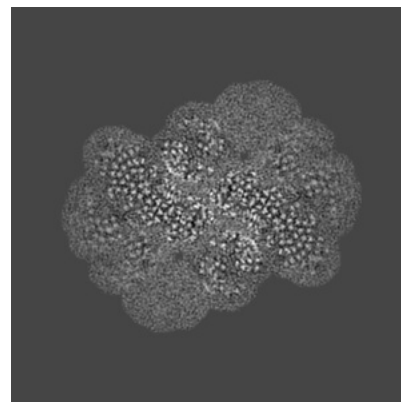
6.3.1 Primary map



X Index: 139

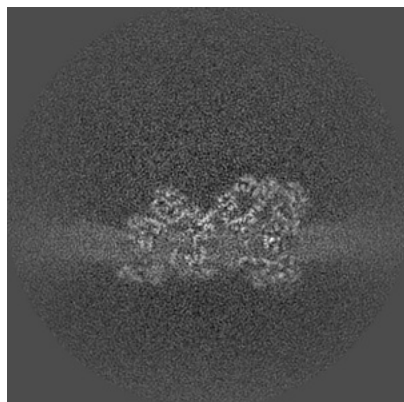


Y Index: 148

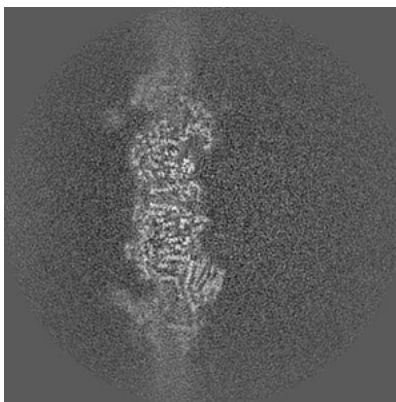


Z Index: 123

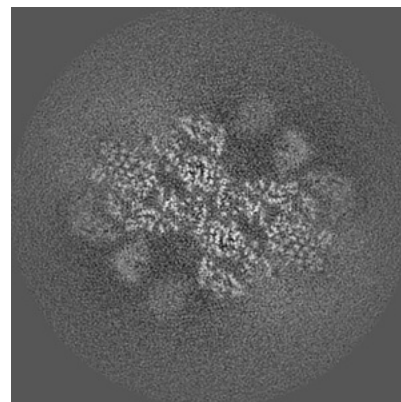
6.3.2 Raw map



X Index: 139



Y Index: 140

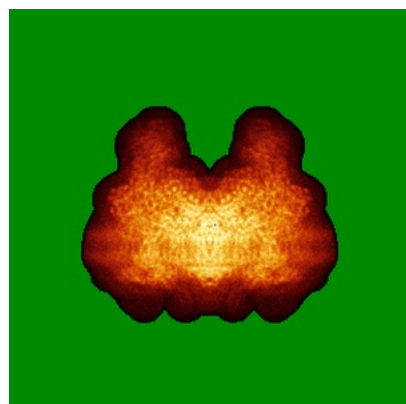


Z Index: 134

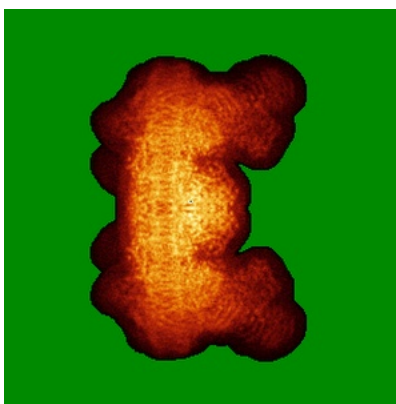
The images above show the largest variance slices of the map in three orthogonal directions.

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

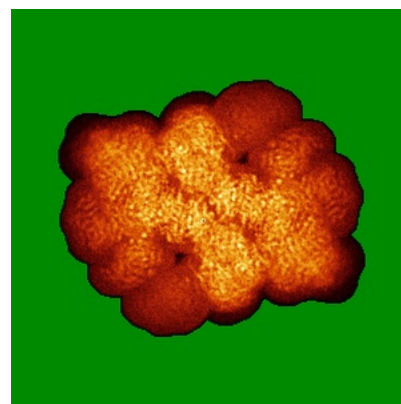
6.4.1 Primary map



X

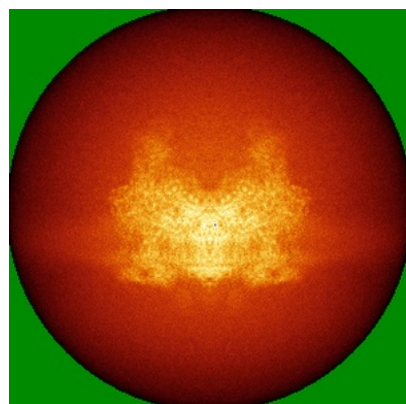


Y

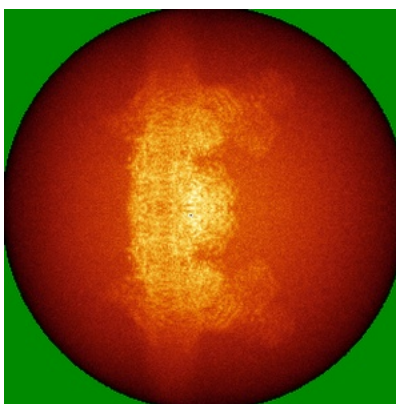


Z

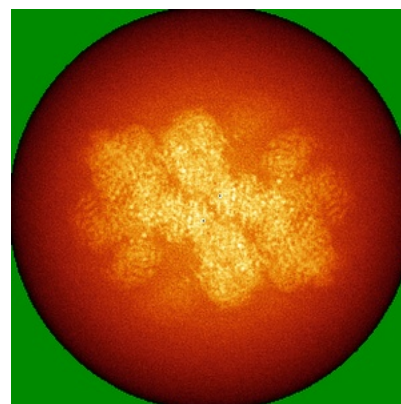
6.4.2 Raw map



X



Y

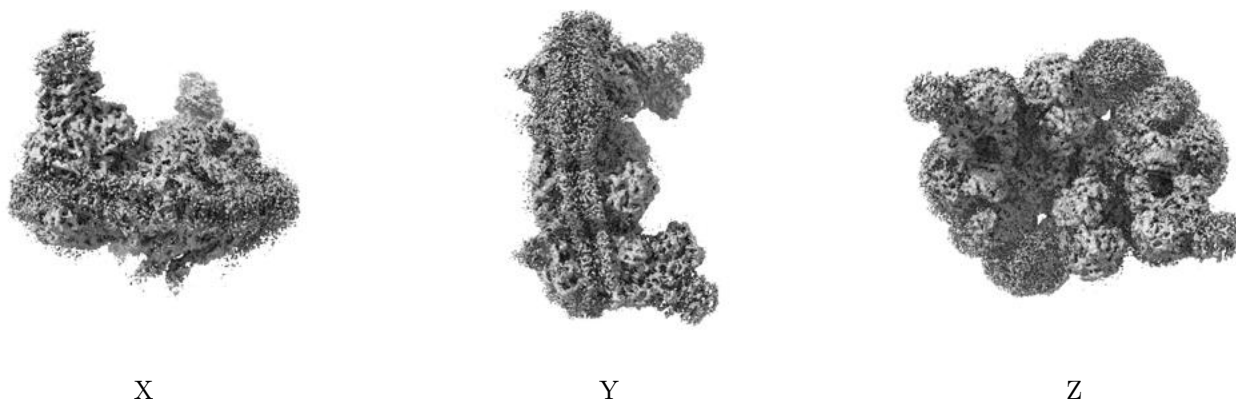


Z

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.

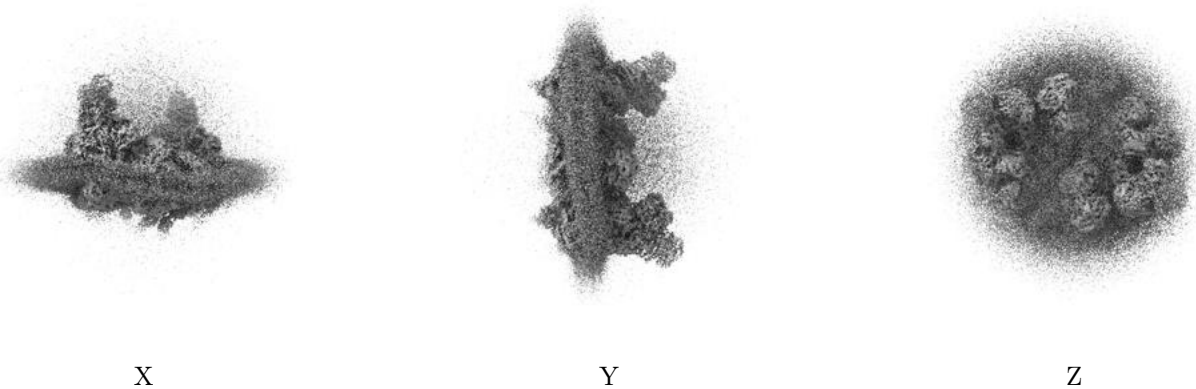
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

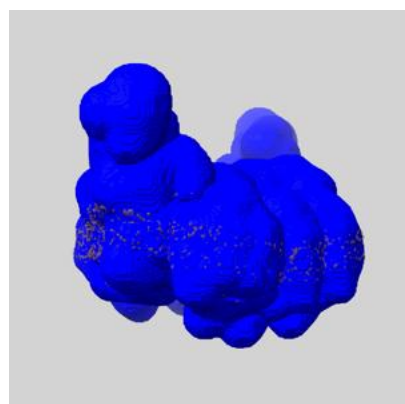
6.6 Mask visualisation [i](#)

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

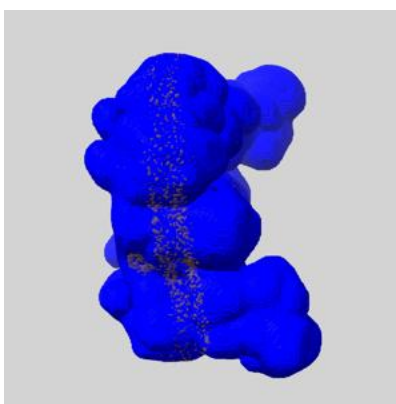
A mask typically either:

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

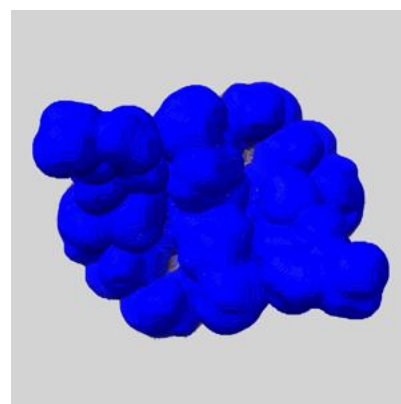
6.6.1 emd_50210_msk_1.map [i](#)



X



Y

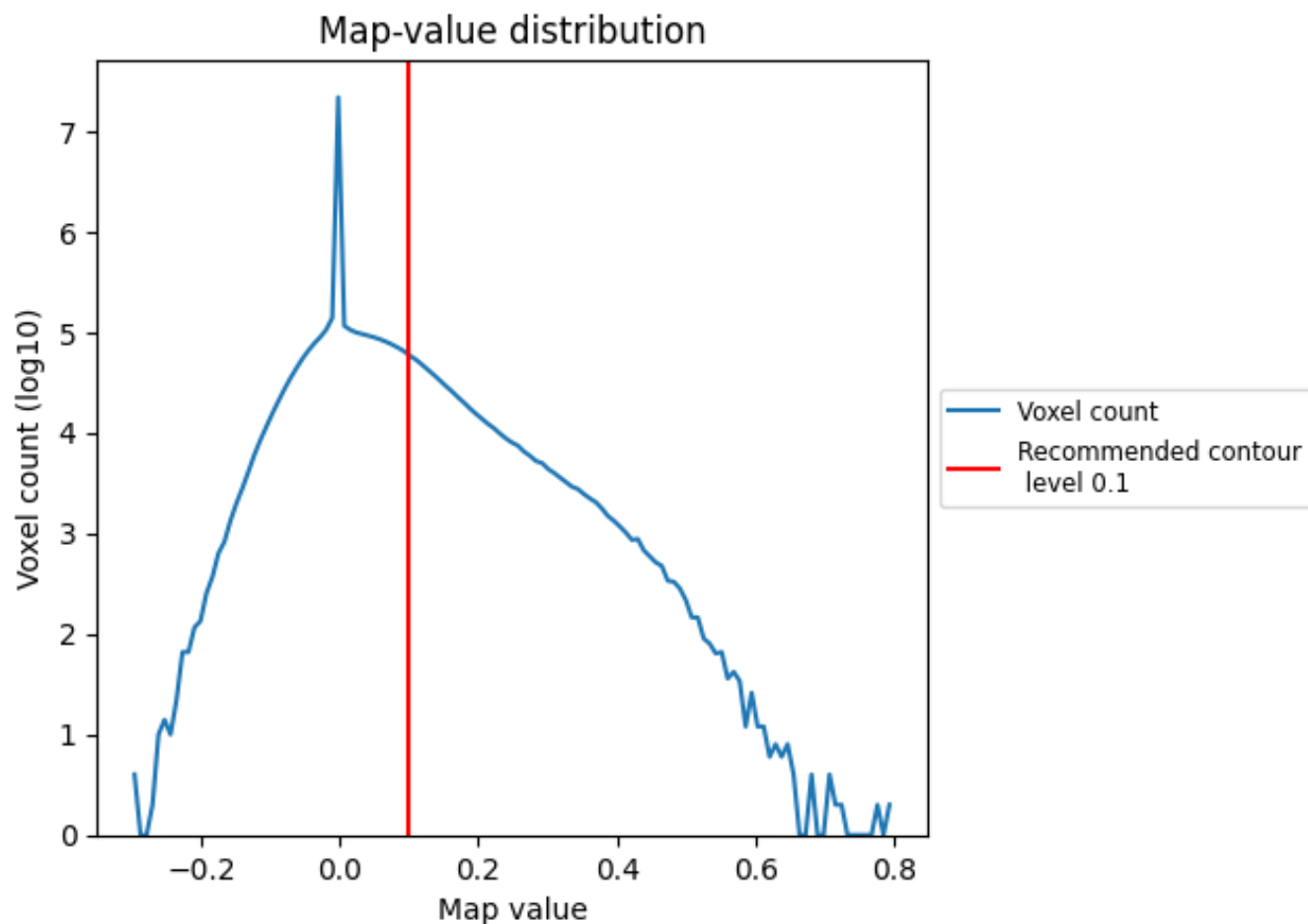


Z

7 Map analysis [i](#)

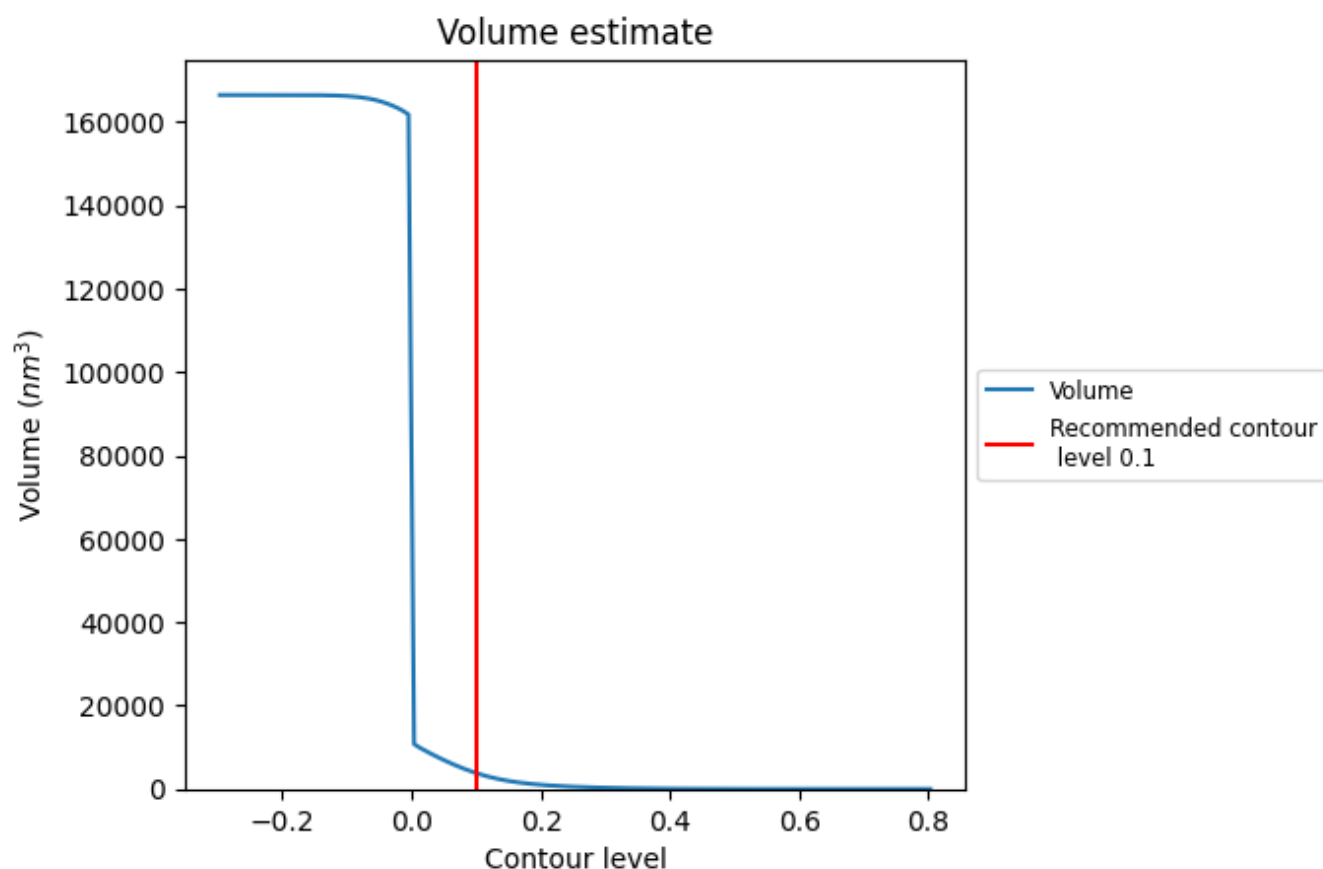
This section contains the results of statistical analysis of the map.

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.

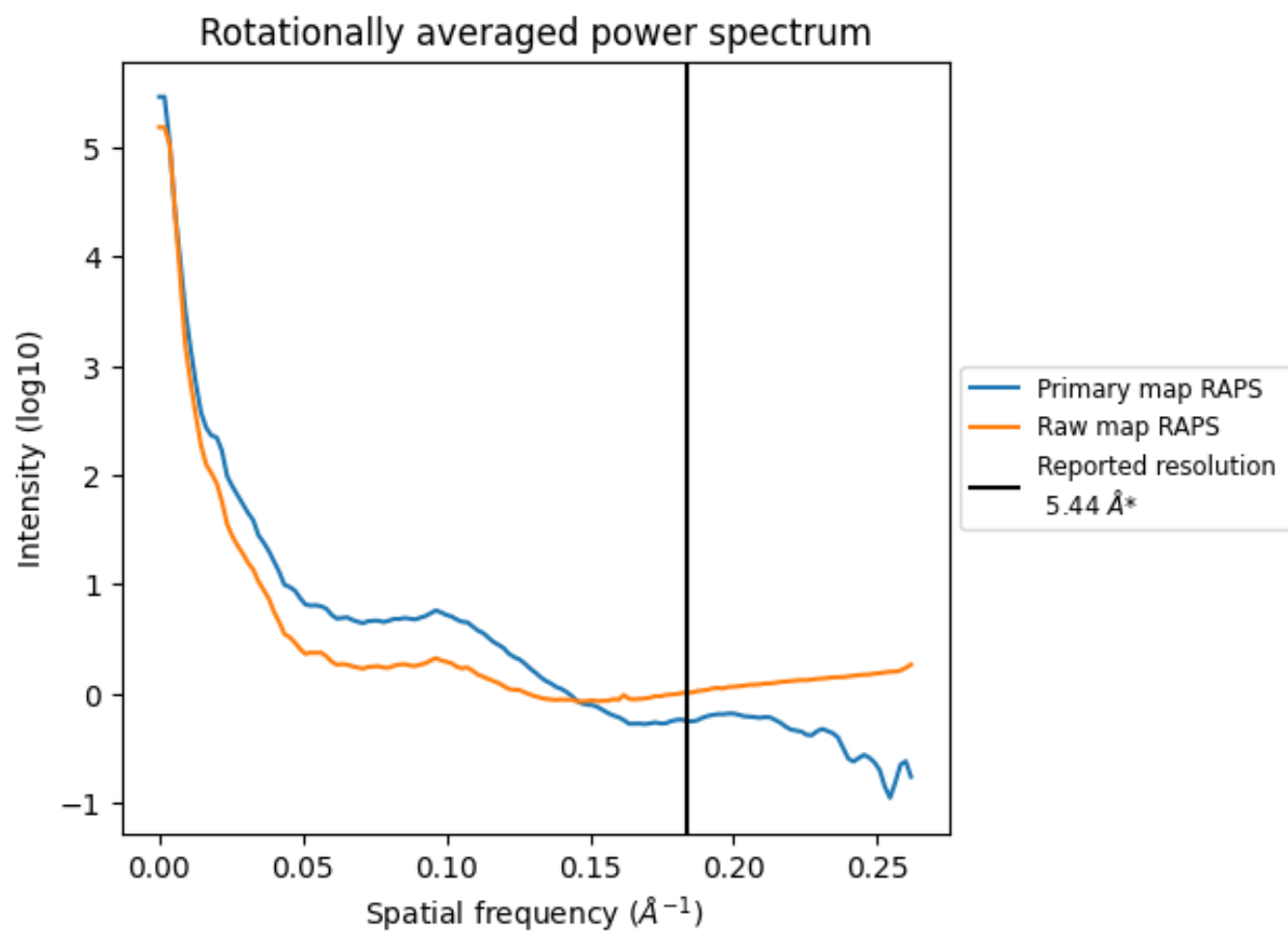
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3804 nm³; this corresponds to an approximate mass of 3437 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 ⓘ

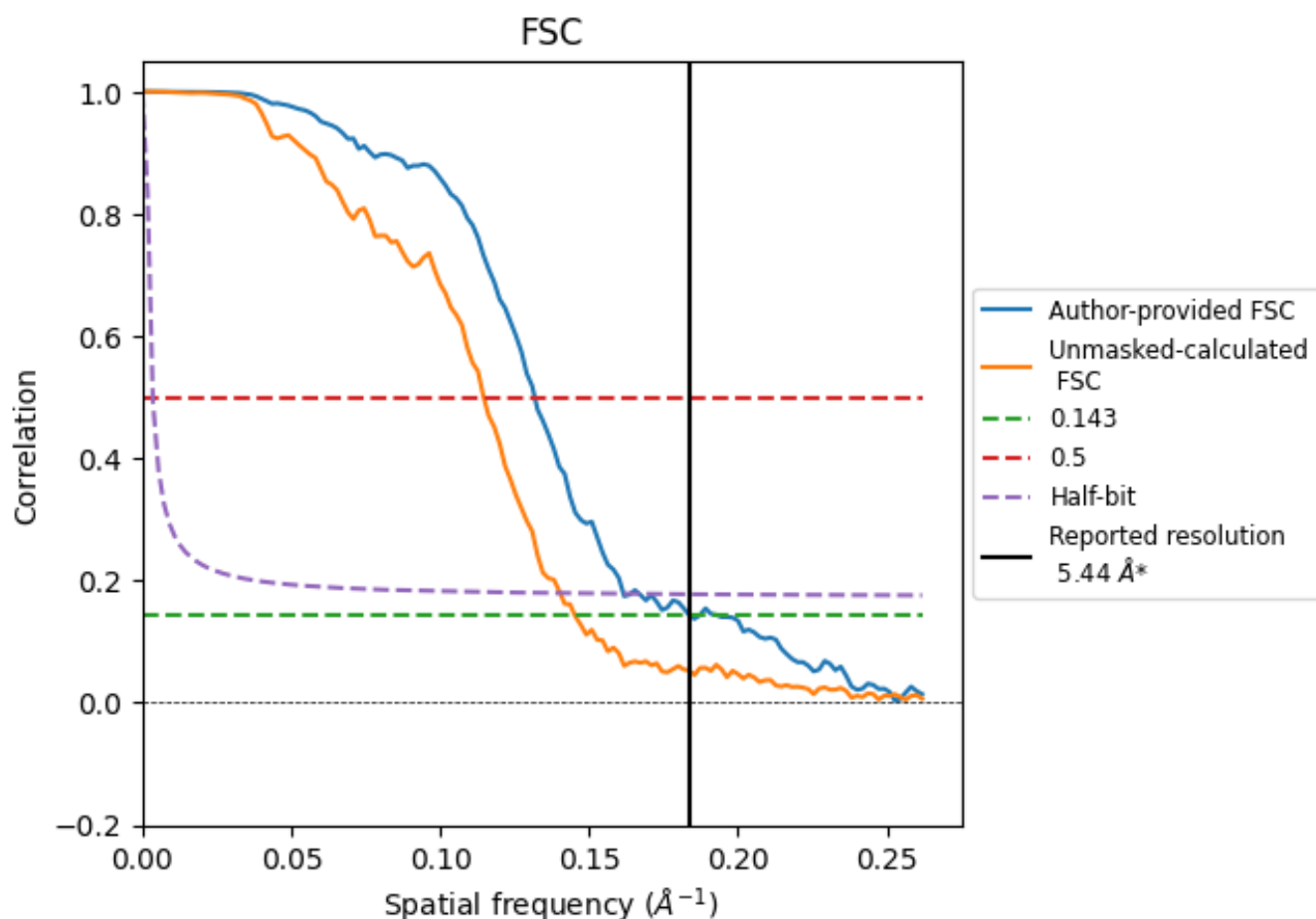


*Reported resolution corresponds to spatial frequency of 0.184 Å⁻¹

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 0.184 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

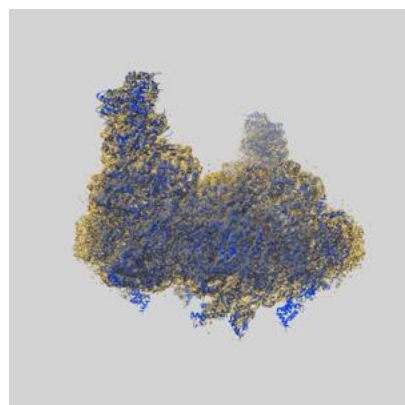
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.44	-	-
Author-provided FSC curve	5.45	7.59	6.19
Unmasked-calculated*	6.88	8.73	7.13

*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 6.88 differs from the reported value 5.44 by more than 10 %

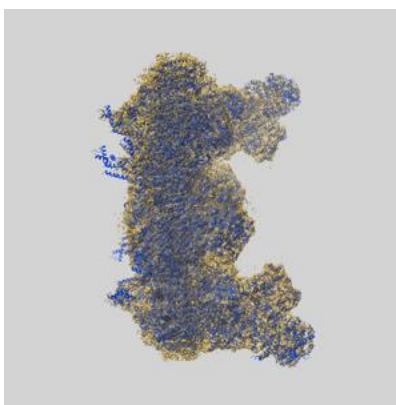
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50210 and PDB model 9F62. Per-residue inclusion information can be found in section 3 on page 38.

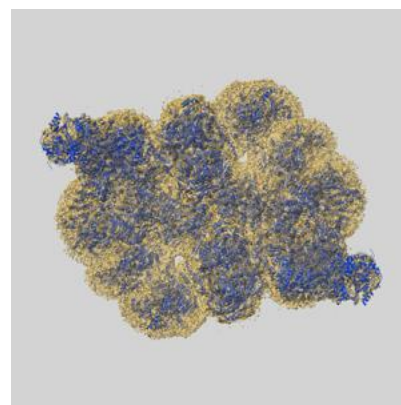
9.1 Map-model overlay [i](#)



X



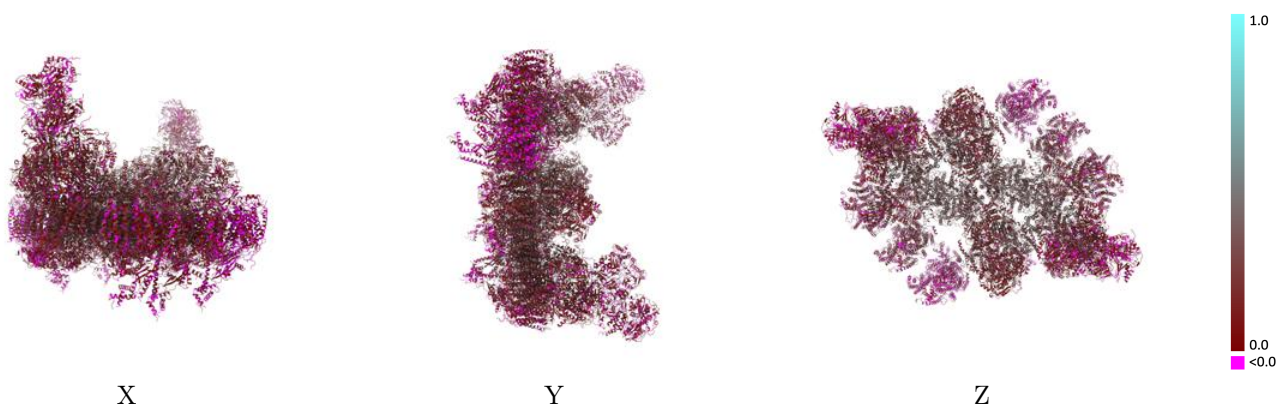
Y



Z

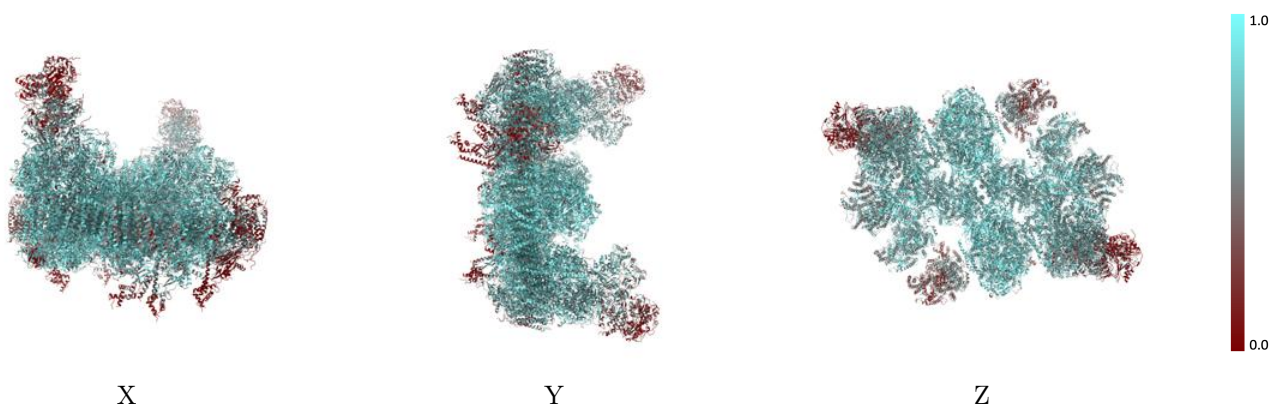
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



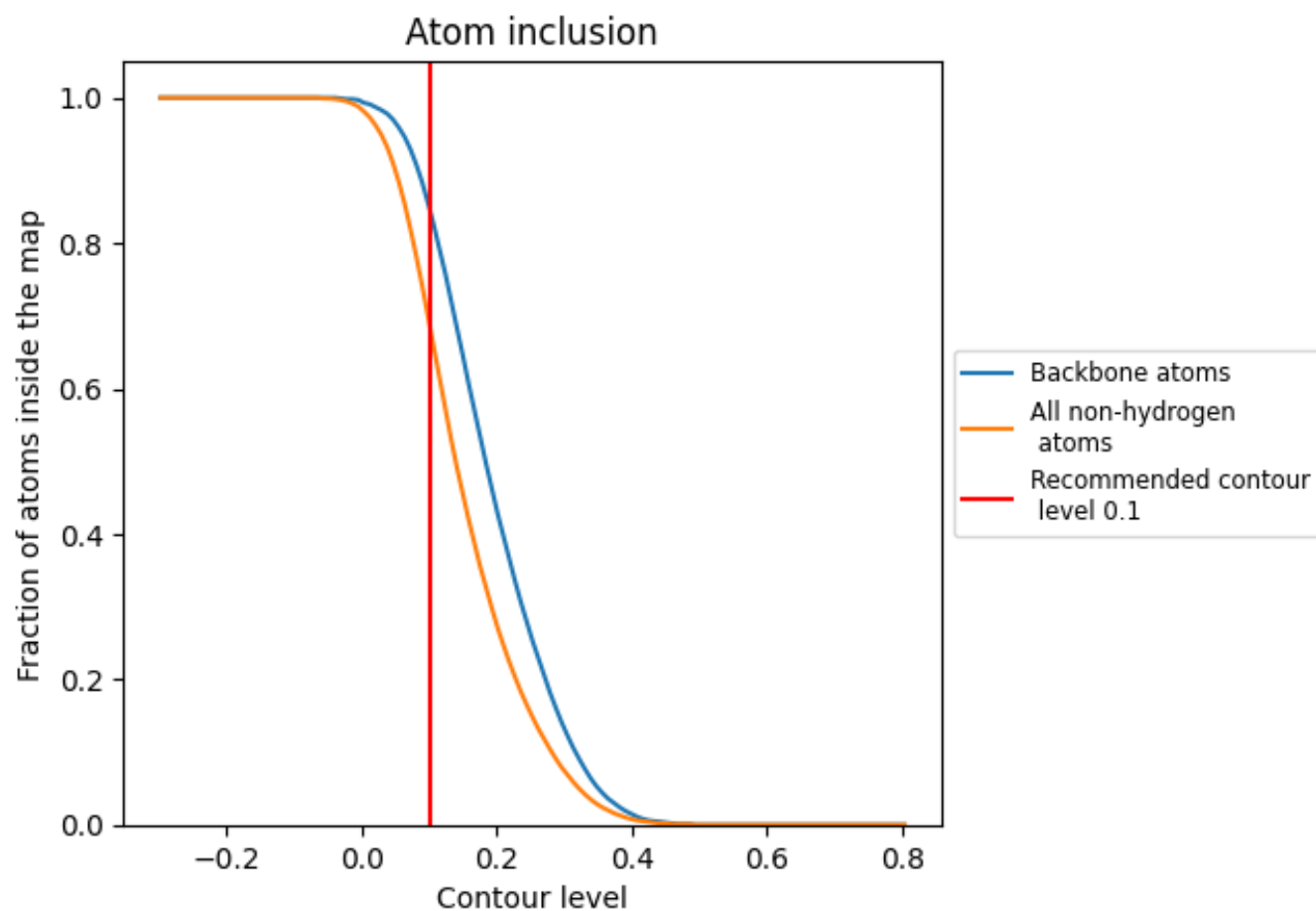
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 69% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.1860
1A	 0.8300	 0.2440
1B	 0.8460	 0.2770
1C	 0.6800	 0.1370
1D	 0.5770	 0.0990
1E	 0.8530	 0.2330
1F	 0.8120	 0.1950
1G	 0.8560	 0.2470
1H	 0.8220	 0.2080
1I	 0.8030	 0.1970
1J	 0.6890	 0.1300
1K	 0.8600	 0.2700
1L	 0.8030	 0.2010
1M	 0.8730	 0.2800
1N	 0.7910	 0.2110
1O	 0.8970	 0.2540
1P	 0.8370	 0.2270
1Q	 0.8430	 0.2440
1R	 0.8460	 0.2440
1S	 0.7830	 0.2070
1T	 0.8510	 0.2610
2A	 0.6240	 0.1410
2B	 0.6420	 0.1470
2C	 0.4820	 0.0880
2D	 0.5830	 0.1110
2E	 0.6350	 0.1480
2F	 0.6460	 0.1490
2G	 0.4980	 0.0960
2H	 0.4590	 0.0850
2I	 0.5360	 0.1070
2J	 0.6200	 0.1390
2K	 0.4070	 0.0790
2L	 0.6350	 0.1370
3A	 0.7430	 0.1530
3B	 0.7470	 0.1620



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Chain	Atom inclusion	Q-score
3C	 0.6530	 0.1570
3D	 0.6860	 0.1270
3E	 0.6960	 0.1110
3F	 0.6850	 0.1660
3G	 0.5420	 0.0910
3H	 0.4920	 0.0710
3I	 0.7410	 0.1140
3J	 0.8140	 0.1650
3K	 0.6580	 0.0910
3L	 0.6510	 0.1210
4A	 0.5160	 0.0480
4B	 0.4480	 0.0510
4C	 0.1580	 0.0530
4D	 0.3330	 0.0310
4E	 0.1600	 0.0580
4F	 0.3750	 0.1140
4G	 0.1930	 0.0230
4H	 0.0700	 0.0190
4I	 0.2660	 0.0090
4J	 0.4530	 0.0970
4K	 0.2340	 -0.0030
4L	 0.3770	 0.0120
5A	 0.2210	 0.1040
5B	 0.2100	 0.0750
5C	 0.5440	 0.1320
5D	 0.7210	 0.2010
5E	 0.6690	 0.1800
5F	 0.7330	 0.2060
5G	 0.6710	 0.1570
5H	 0.5780	 0.1630
5I	 0.6690	 0.1690
5J	 0.7740	 0.2420
5K	 0.7000	 0.1730
5L	 0.5610	 0.1690
5M	 0.4520	 0.1210
5N	 0.6910	 0.1840
5O	 0.6280	 0.1230
5P	 0.7620	 0.2020
5Q	 0.7000	 0.1810
5R	 0.8110	 0.2780
5S	 0.7140	 0.1920
5T	 0.8470	 0.3010

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Chain	Atom inclusion	Q-score
5U	 0.7940	 0.2470
5V	 0.8670	 0.2840
5W	 0.7650	 0.2310
5X	 0.9150	 0.3130
5Y	 0.8200	 0.2410
5Z	 0.8940	 0.2740
5a	 0.8880	 0.2630
5b	 0.8560	 0.2740
5c	 0.6960	 0.1900
5d	 0.8570	 0.2770
5e	 0.8920	 0.2900
5f	 0.7080	 0.1910
5g	 0.8570	 0.2170
5h	 0.9190	 0.3150
5i	 0.7980	 0.1940
5j	 0.8750	 0.2410
5k	 0.8810	 0.2970
5l	 0.8000	 0.2340
5m	 0.6540	 0.1690
5n	 0.6620	 0.1590
5o	 0.8560	 0.2530
5p	 0.8300	 0.2420
5q	 0.8920	 0.3070
5r	 0.8550	 0.2790
5s	 0.8380	 0.2330
5t	 0.8450	 0.2780
5u	 0.8500	 0.2590
5v	 0.8420	 0.2510
5w	 0.8890	 0.2930
5x	 0.8670	 0.2910
5y	 0.8940	 0.3060
6A	 0.8300	 0.2460
6B	 0.8460	 0.2780
6C	 0.6800	 0.1380
6D	 0.5780	 0.1010
6E	 0.8530	 0.2320
6F	 0.8160	 0.1990
6G	 0.8580	 0.2420
6H	 0.8250	 0.2090
6I	 0.7970	 0.1980
6J	 0.6960	 0.1340
6K	 0.8600	 0.2700

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Chain	Atom inclusion	Q-score
6L	 0.8040	 0.2080
6M	 0.8730	 0.2760
6N	 0.7920	 0.2110
6O	 0.8950	 0.2560
6P	 0.8390	 0.2230
6Q	 0.8430	 0.2420
6R	 0.8480	 0.2460
6S	 0.7840	 0.2060
6T	 0.8510	 0.2590
7A	 0.6240	 0.1410
7B	 0.6410	 0.1440
7C	 0.4840	 0.0880
7D	 0.5860	 0.1120
7E	 0.6330	 0.1540
7F	 0.6470	 0.1490
7G	 0.4960	 0.0920
7H	 0.4580	 0.0820
7I	 0.5450	 0.1100
7J	 0.6210	 0.1370
7K	 0.4070	 0.0860
7L	 0.6380	 0.1370
8A	 0.7430	 0.1550
8B	 0.7450	 0.1630
8C	 0.6500	 0.1610
8D	 0.6870	 0.1310
8E	 0.7040	 0.1150
8F	 0.6840	 0.1660
8G	 0.5370	 0.0930
8H	 0.4930	 0.0710
8I	 0.7440	 0.1130
8J	 0.8150	 0.1690
8K	 0.6580	 0.0900
8L	 0.6520	 0.1220
9A	 0.5170	 0.0460
9B	 0.4390	 0.0480
9C	 0.1540	 0.0600
9D	 0.3310	 0.0250
9E	 0.1620	 0.0610
9F	 0.3860	 0.1180
9G	 0.1990	 0.0270
9H	 0.0760	 0.0280
9I	 0.2770	 0.0130

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Chain	Atom inclusion	Q-score
9J	 0.4660	 0.1080
9K	 0.2670	 0.0010
9L	 0.3690	 0.0120
A	 0.2220	 0.1040
B	 0.2100	 0.0750
C	 0.5440	 0.1300
D	 0.7220	 0.2000
E	 0.6700	 0.1780
F	 0.7330	 0.2070
G	 0.6700	 0.1570
H	 0.5770	 0.1660
I	 0.6730	 0.1710
J	 0.7740	 0.2400
K	 0.7000	 0.1740
L	 0.5610	 0.1690
M	 0.4600	 0.1220
N	 0.6900	 0.1820
O	 0.6260	 0.1240
P	 0.7620	 0.2030
Q	 0.6980	 0.1810
R	 0.8110	 0.2780
S	 0.7130	 0.1940
T	 0.8480	 0.3000
U	 0.7930	 0.2490
V	 0.8670	 0.2800
W	 0.7630	 0.2330
X	 0.9160	 0.3100
Y	 0.8120	 0.2390
Z	 0.8950	 0.2740
a	 0.8960	 0.2610
b	 0.8590	 0.2740
c	 0.6980	 0.1940
d	 0.8540	 0.2740
e	 0.8920	 0.2910
f	 0.7000	 0.1870
g	 0.8690	 0.2330
h	 0.9190	 0.3140
i	 0.7880	 0.1910
j	 0.8700	 0.2390
k	 0.8810	 0.2960
l	 0.7990	 0.2350
m	 0.6570	 0.1750

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Chain	Atom inclusion	Q-score
n	 0.6620	 0.1630
o	 0.8540	 0.2530
p	 0.8280	 0.2440
q	 0.8930	 0.3050
r	 0.8560	 0.2790
s	 0.8390	 0.2360
t	 0.8470	 0.2810
u	 0.8510	 0.2620
v	 0.8480	 0.2420
w	 0.8970	 0.2890
x	 0.8670	 0.2900
y	 0.8940	 0.3020