Full wwPDB EM Validation Report ⓘ

Mar 22, 2025 – 07:28 am GMT

PDB ID	:	9F62
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 Full wwPDB EM Validation 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:

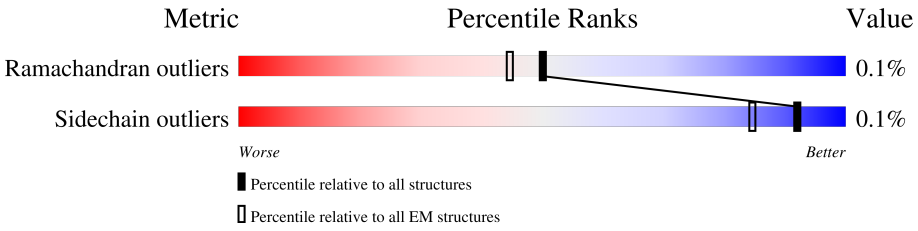
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	98%
1	1B	381	98%
1	6A	381	98%
1	6B	381	98%
2	1C	262	16% 79% 21%
2	1D	262	24% 79% 21%
2	6C	262	16% 79% 21%
2	6D	262	24% 79% 21%
3	1E	314	77% 23%

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Mol	Chain	Length	Quality of chain
3	1F	314	77% 23%
3	6E	314	77% 23%
3	6F	314	77% 23%
4	1G	60	98%
4	1H	60	98%
4	6G	60	98%
4	6H	60	98%
5	1I	69	99%
5	1J	69	12% 99%
5	6I	69	99%
5	6J	69	10% 99%
6	1K	73	96%
6	1L	73	96%
6	6K	73	96%
6	6L	73	96%
7	1M	495	94% 6%
7	1N	495	93% 6%
7	6M	495	94% 6%
7	6N	495	93% 6%
8	1O	59	81% 19%
8	1P	59	81% 19%
8	6O	59	81% 19%
8	6P	59	81% 19%
9	1Q	485	90% 9%
9	1S	485	90% 9%

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Mol	Chain	Length	Quality of chain
9	6Q	485	90% 9%
9	6S	485	90% 9%
10	1R	123	99%
10	1T	123	99%
10	6R	123	99%
10	6T	123	99%
11	2A	505	14% 100%
11	3A	505	100%
11	4A	505	35% 100%
11	7A	505	14% 100%
11	8A	505	100%
11	9A	505	34% 100%
12	2B	284	7% 50% 50%
12	3B	284	50% 50%
12	4B	284	23% 50% 50%
12	7B	284	7% 50% 50%
12	8B	284	50% 50%
12	9B	284	23% 50% 50%
13	2C	153	37% 100%
13	3C	153	19% 100%
13	4C	153	88% 100%
13	7C	153	37% 100%
13	8C	153	19% 100%
13	9C	153	89% 100%
14	2D	382	15% 70% 30%

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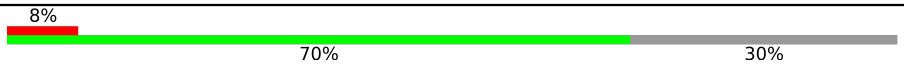
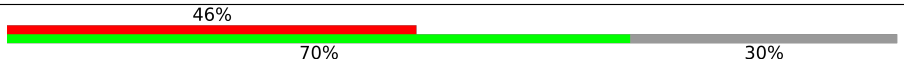
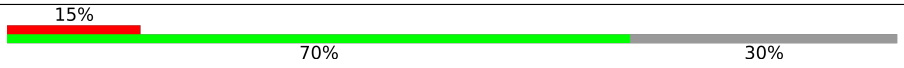
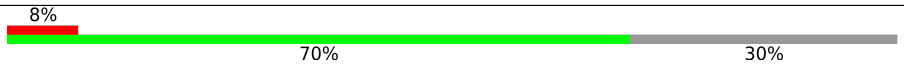
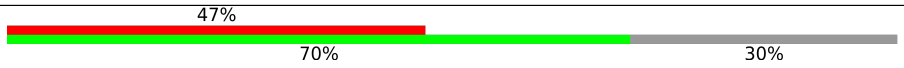
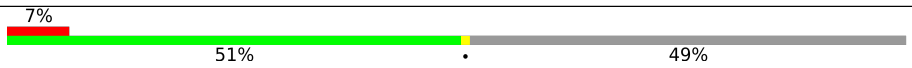
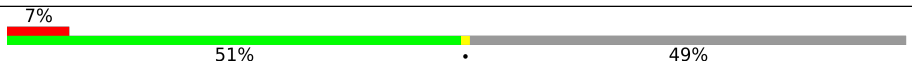
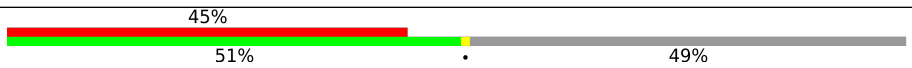
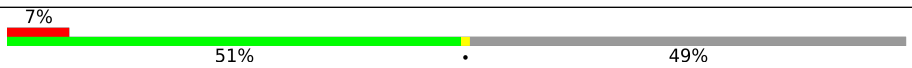
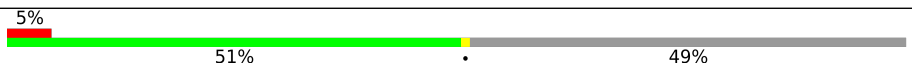
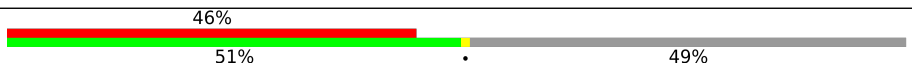
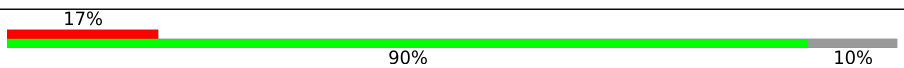
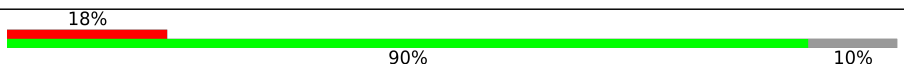
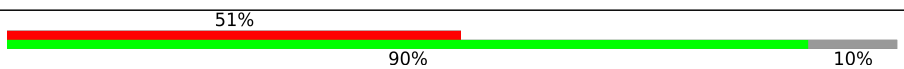
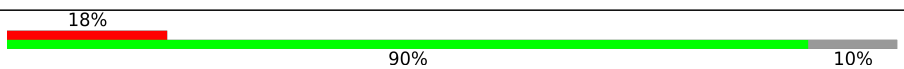
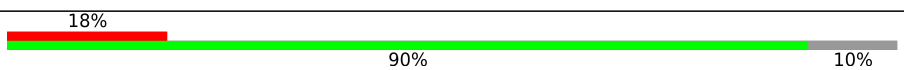
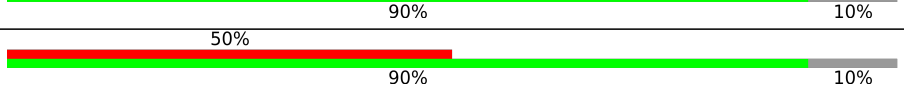
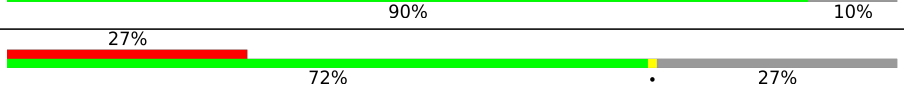
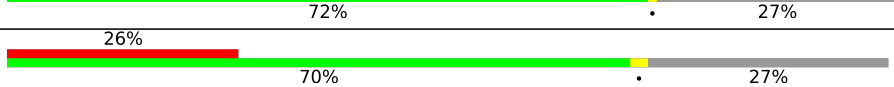
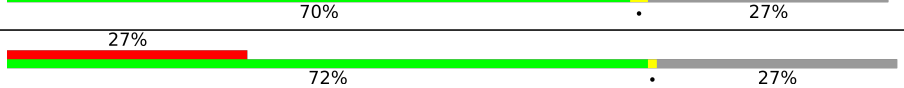
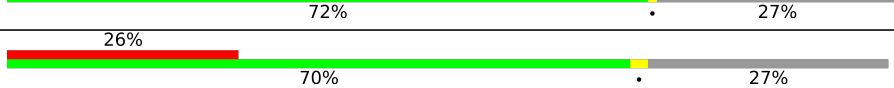
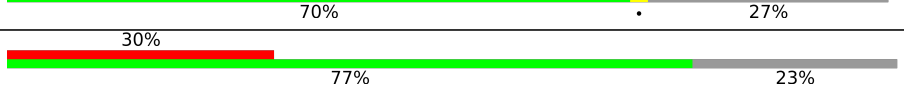
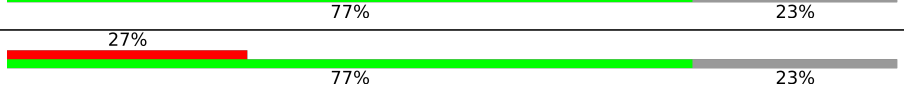
Mol	Chain	Length	Quality of chain
14	3D	382	
14	4D	382	
14	7D	382	
14	8D	382	
14	9D	382	
15	2E	175	
15	3E	175	
15	4E	175	
15	7E	175	
15	8E	175	
15	9E	175	
16	2F	96	
16	3F	96	
16	4F	96	
16	7F	96	
16	8F	96	
16	9F	96	
17	2G	125	
17	3G	125	
17	4G	125	
17	7G	125	
17	8G	125	
17	9G	125	
18	2H	148	
18	3H	148	

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Mol	Chain	Length	Quality of chain
18	4H	148	75% 77% 23%
18	7H	148	28% 77% 23%
18	8H	148	27% 77% 23%
18	9H	148	76% 77% 23%
19	2I	101	19% 71% 29%
19	3I	101	6% 71% 29%
19	4I	101	51% 71% 29%
19	7I	101	19% 71% 29%
19	8I	101	5% 71% 29%
19	9I	101	52% 71% 29%
20	2J	105	17% 99%
20	3J	105	99%
20	4J	105	47% 96%
20	7J	105	16% 99%
20	8J	105	99%
20	9J	105	48% 96%
21	2K	58	40% 81% 19%
21	3K	58	12% 81% 19%
21	4K	58	64% 81% 19%
21	7K	58	38% 81% 19%
21	8K	58	12% 81% 19%
21	9K	58	59% 81% 19%
22	2L	87	11% 87% 13%
22	3L	87	10% 90% 10%
22	4L	87	46% 90% 10%

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Mol	Chain	Length	Quality of chain
22	7L	87	11% 87% 13%
22	8L	87	10% 90% 10%
22	9L	87	47% 90% 10%
23	5A	282	65% 85% 15%
23	A	282	65% 85% 15%
24	5B	484	72% 90% 10%
24	B	484	72% 90% 10%
25	5C	733	29% 94% 6%
25	C	733	28% 94% 6%
26	5D	282	77% 23%
26	D	282	77% 23%
27	5E	467	7% 83% 17%
27	E	467	7% 83% 17%
28	5F	164	96%
28	F	164	96%
29	5G	231	9% 86% 14%
29	G	231	10% 86% 14%
30	5H	118	18% 76% 24%
30	H	118	18% 76% 24%
31	5I	165	8% 82% 18%
31	I	165	8% 82% 18%
32	5J	128	66% 34%
32	5r	128	69% 31%
32	J	128	66% 34%
32	r	128	69% 31%

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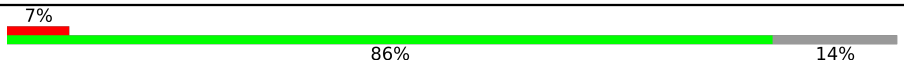
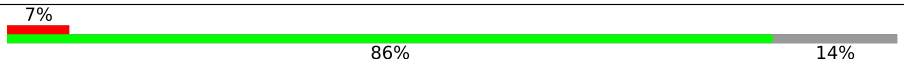
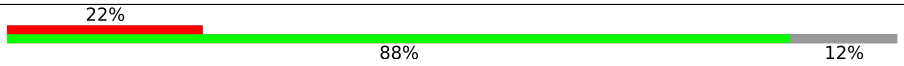
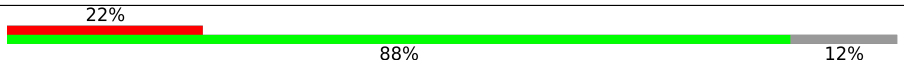
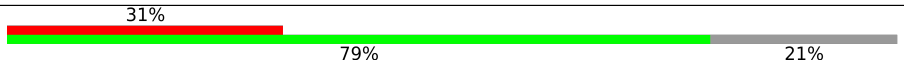
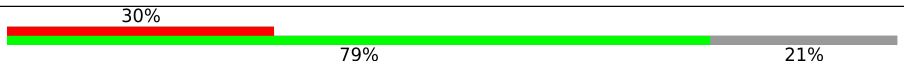
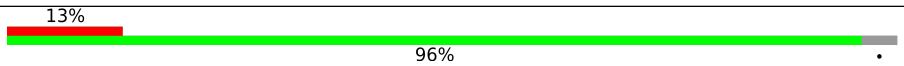
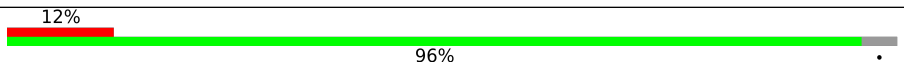
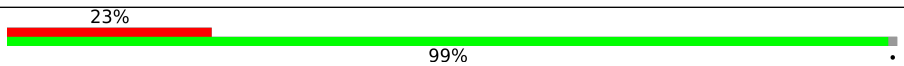
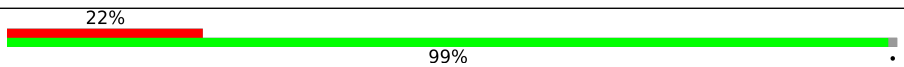
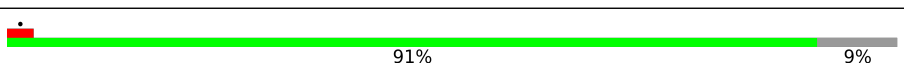
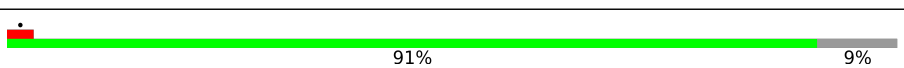
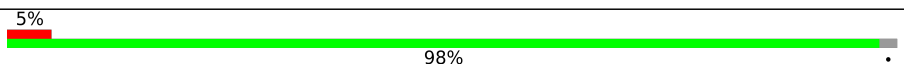
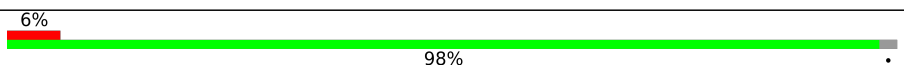
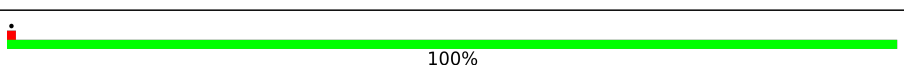
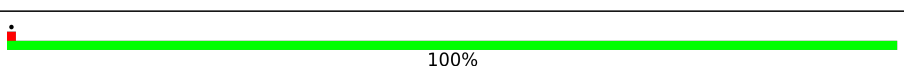
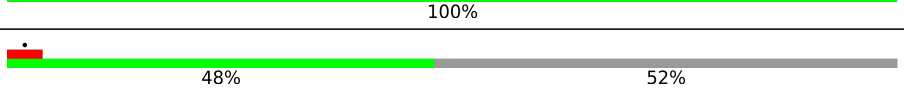
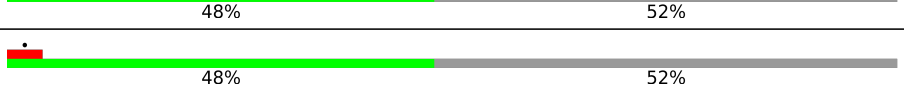
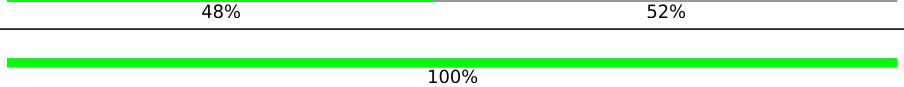
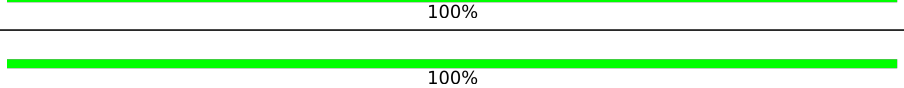
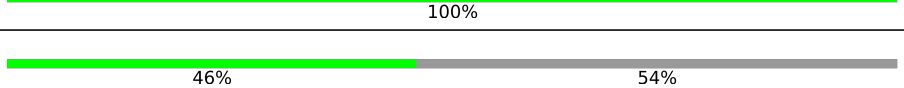
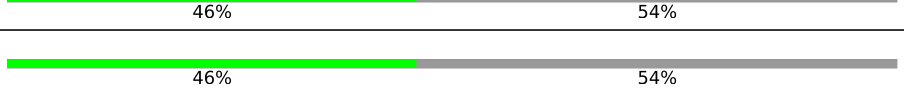
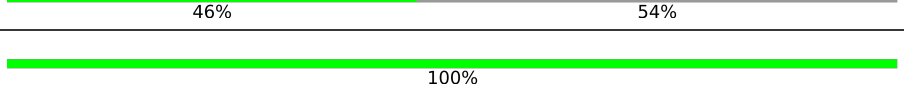
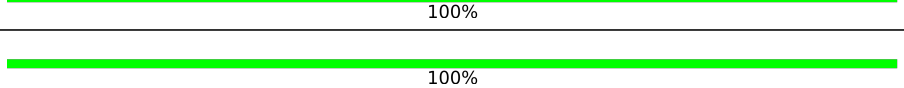
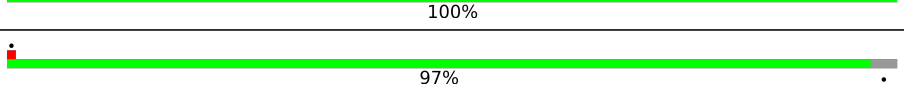
Mol	Chain	Length	Quality of chain
33	5K	138	
33	K	138	
34	5L	187	
34	L	187	
35	5M	154	
35	M	154	
36	5N	156	
36	N	156	
37	5O	101	
37	O	101	
38	5P	397	
38	P	397	
39	5Q	292	
39	Q	292	
40	5R	387	
40	R	387	
41	5S	279	
41	S	279	
42	5T	443	
42	T	443	
43	5U	227	
43	U	227	
44	5V	546	
44	V	546	
45	5W	162	

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Mol	Chain	Length	Quality of chain
45	W	162	97%
46	5X	149	84% 16%
46	X	149	84% 16%
47	5Y	64	84% 16%
47	Y	64	84% 16%
48	5Z	124	86% 14%
48	Z	124	86% 14%
49	5a	129	63% 36%
49	a	129	62% 36%
50	5b	172	84% 16%
50	b	172	84% 16%
51	5c	67	12% 88% 12%
51	c	67	12% 88% 12%
52	5d	86	99%
52	d	86	99%
53	5e	219	99%
53	e	219	99%
54	5f	65	6% 98%
54	f	65	8% 98%
55	5g	55	91% 9%
55	g	55	91% 9%
56	5h	142	76% 24%
56	h	142	76% 24%
57	5i	81	7% 94% 6%
57	i	81	7% 94% 6%

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Mol	Chain	Length	Quality of chain
58	5j	86	99%
58	j	86	99%
59	5k	117	100%
59	k	117	100%
60	5l	121	95%
60	l	121	95%
61	5m	142	15% 97%
61	m	142	15% 97%
62	5n	106	8% 98%
62	n	106	8% 98%
63	5o	155	98%
63	o	155	98%
64	5p	130	99%
64	p	130	99%
65	5q	197	80% 20%
65	q	197	80% 20%
66	5s	312	100%
66	s	312	100%
67	5t	279	91% 9%
67	t	279	91% 9%
68	5u	229	99%
68	u	229	99%
69	5v	45	100%
69	v	45	100%
70	5w	109	59% 41%

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Mol	Chain	Length	Quality of chain
70	w	109	59% 41%
71	5x	157	53% 47%
71	x	157	53% 47%
72	5y	118	97% .
72	y	118	97% .

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 ASHI.

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 subunit.

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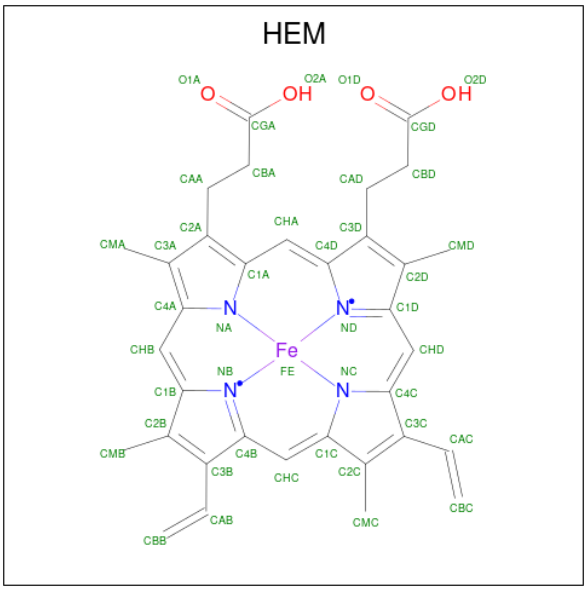
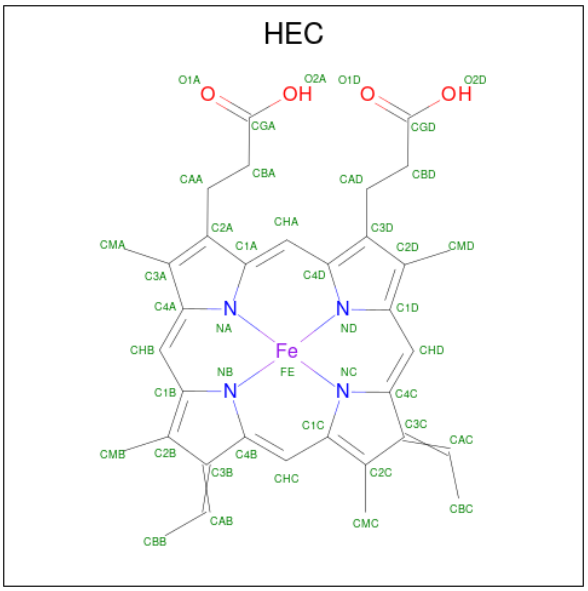
Mol	Chain	Residues	Atoms					AltConf	Trace
72	y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

- Molecule 73 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
73	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	1A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	1B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
73	6B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 74 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

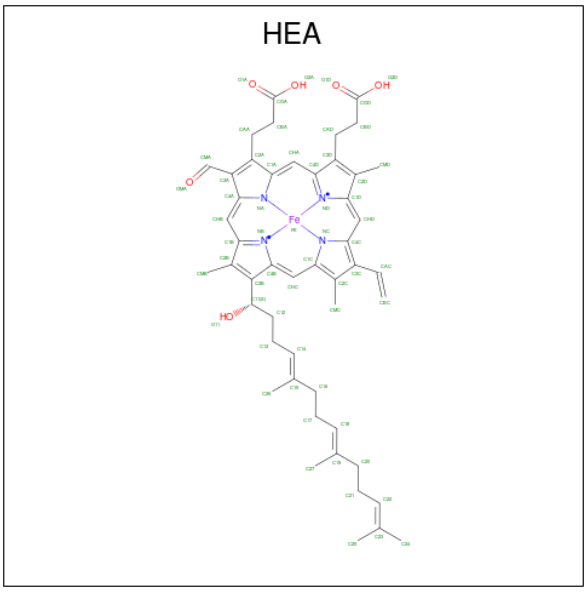


Mol	Chain	Residues	Atoms					AltConf
74	1E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	1F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	6E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	6F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 75 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 76 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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	

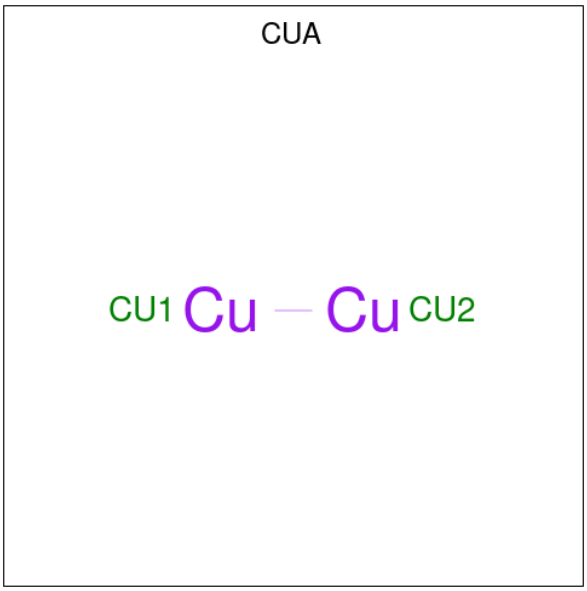
- Molecule 77 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

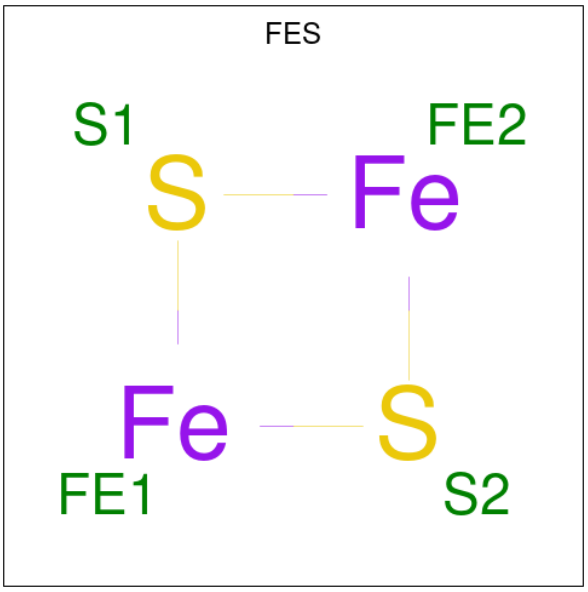
Mol	Chain	Residues	Atoms	AltConf
78	2A	1	Total Mg 1 1	0
78	3A	1	Total Mg 1 1	0
78	4A	1	Total Mg 1 1	0
78	7A	1	Total Mg 1 1	0
78	8A	1	Total Mg 1 1	0
78	9A	1	Total Mg 1 1	0

- Molecule 79 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



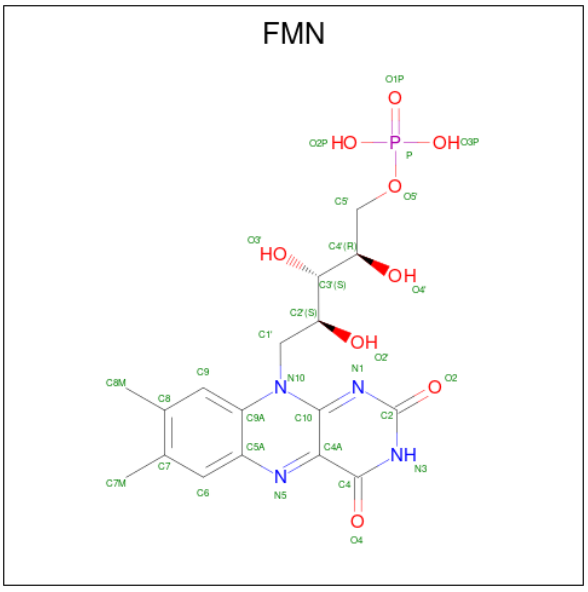
Mol	Chain	Residues	Atoms	AltConf
79	2C	1	Total Cu 2 2	0
79	3C	1	Total Cu 2 2	0
79	4C	1	Total Cu 2 2	0
79	7C	1	Total Cu 2 2	0
79	8C	1	Total Cu 2 2	0
79	9C	1	Total Cu 2 2	0

- Molecule 80 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



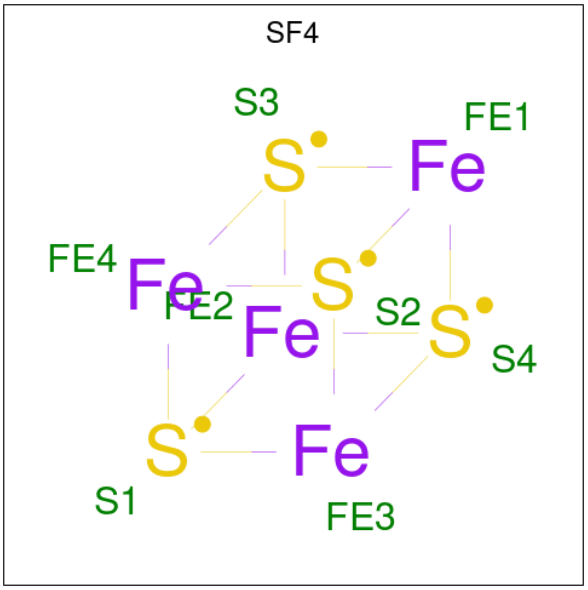
Mol	Chain	Residues	Atoms	AltConf
80	5A	1	Total Fe S 4 2 2	0
80	5C	1	Total Fe S 4 2 2	0
80	A	1	Total Fe S 4 2 2	0
80	C	1	Total Fe S 4 2 2	0

- Molecule 81 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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 (three-letter code: 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	

Continued on next page...

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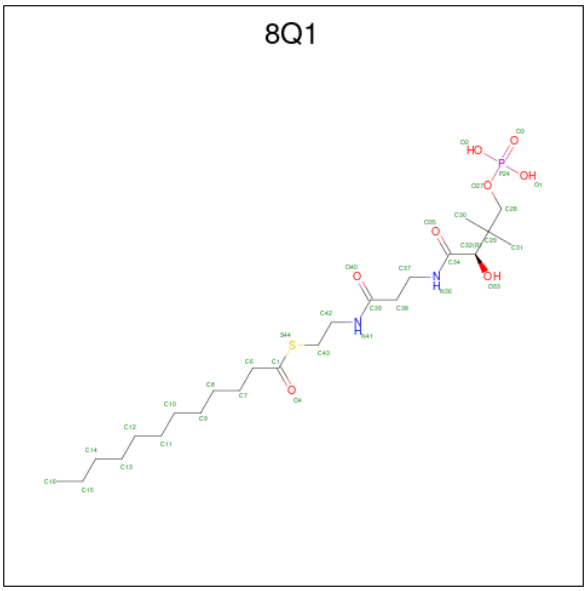
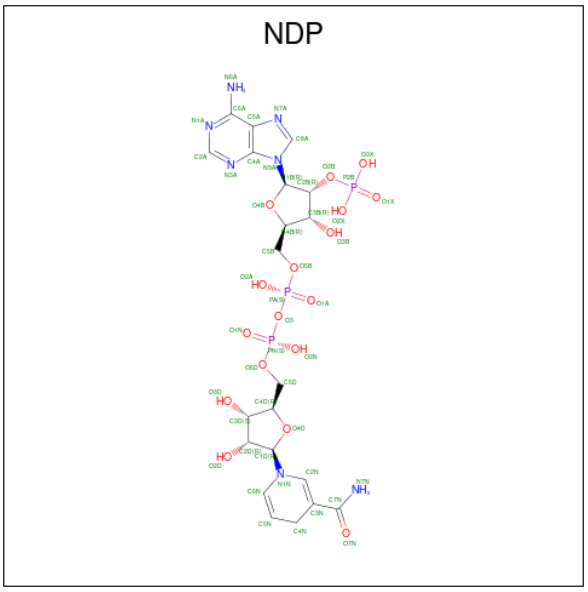
Mol	Chain	Residues	Atoms	AltConf
82	G	1	Total Fe S 8 4 4	0
82	G	1	Total Fe S 8 4 4	0

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



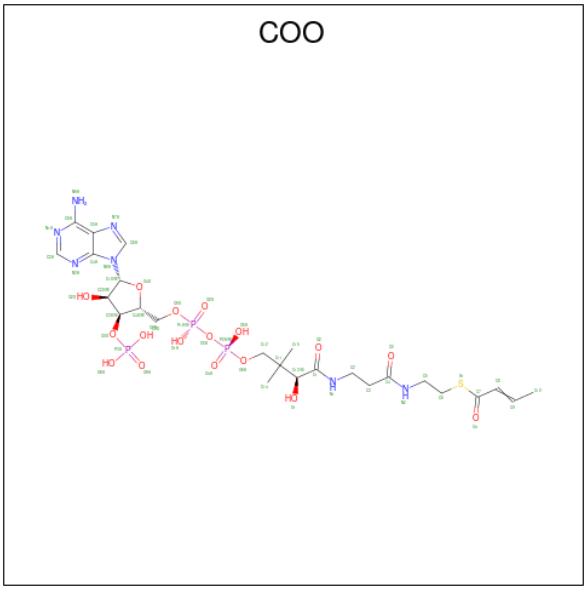
Mol	Chain	Residues	Atoms	AltConf
83	5J	1	Total C N O P S 35 23 2 8 1 1	0
83	5k	1	Total C N O P S 35 23 2 8 1 1	0
83	J	1	Total C N O P S 35 23 2 8 1 1	0
83	k	1	Total C N O P S 35 23 2 8 1 1	0

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



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

- Molecule 85 is CROTONYL COENZYME A (three-letter code: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$).



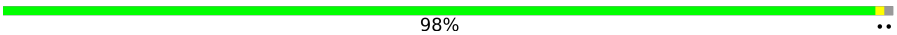
Mol	Chain	Residues	Atoms						AltConf
85	5s	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	
85	s	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

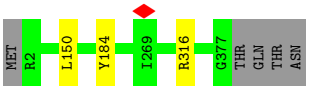
3 Residue-property plots

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

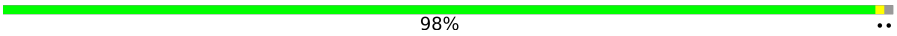
Chain 1A:





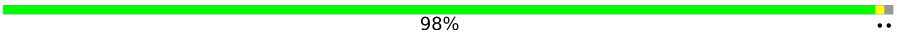
• Molecule 1: Cytochrome b

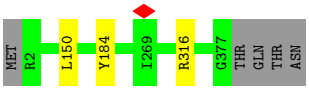
Chain 1B:



• Molecule 1: Cytochrome b

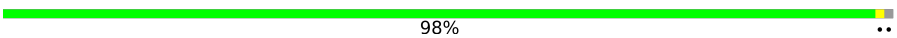
Chain 6A:





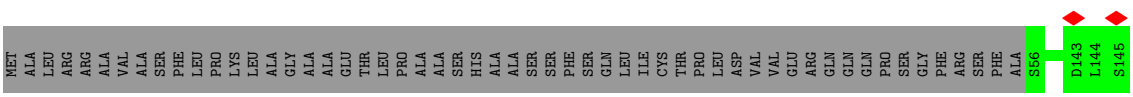
• Molecule 1: Cytochrome b

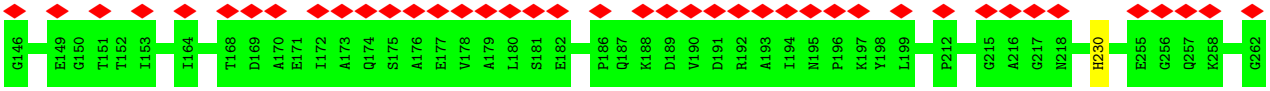
Chain 6B:



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

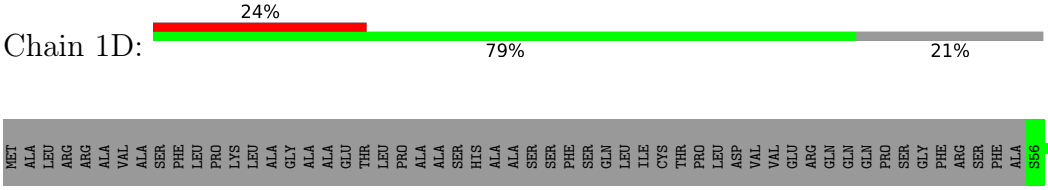
Chain 1C:





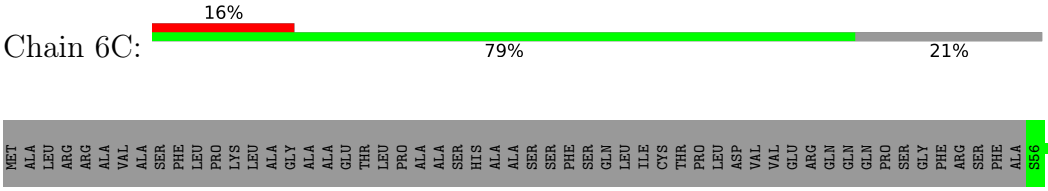
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

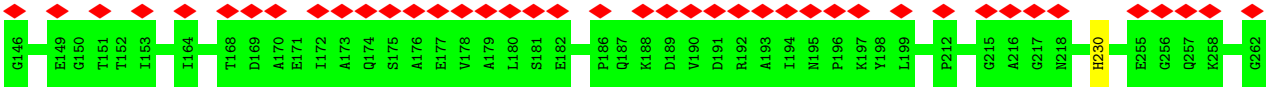
Chain 1D:



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

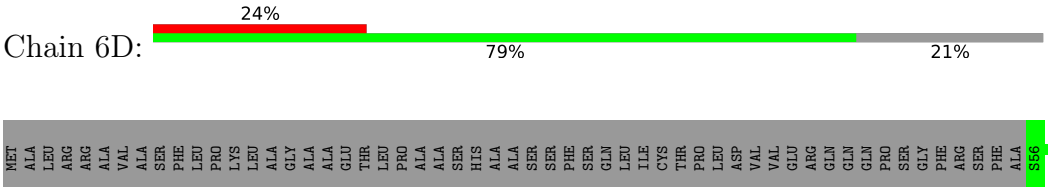
Chain 6C:

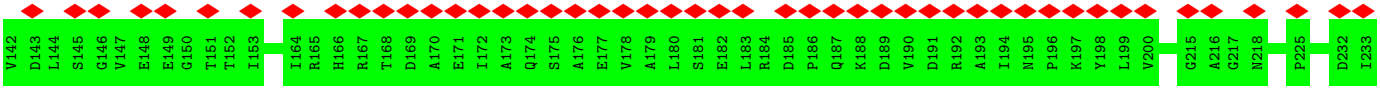




• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

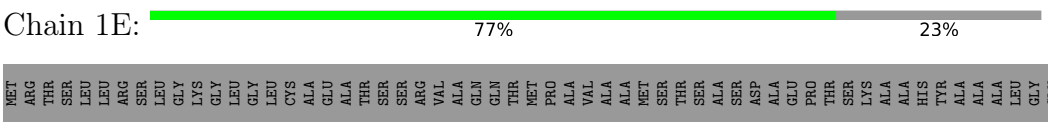
Chain 6D:

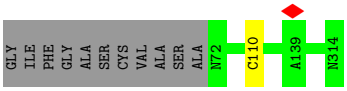




• Molecule 3: Cytochrome c1

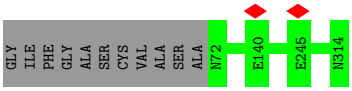
Chain 1E:





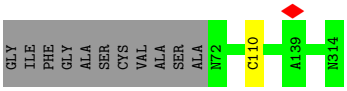
• Molecule 3: Cytochrome c1

Chain 1F:



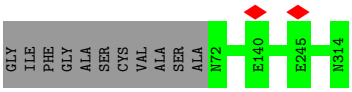
• Molecule 3: Cytochrome c1

Chain 6E:



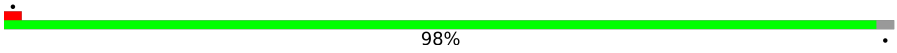
• Molecule 3: Cytochrome c1

Chain 6F:



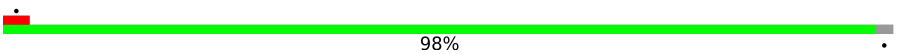
• Molecule 4: Complex III subunit 9

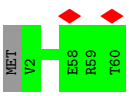
Chain 1G:



• Molecule 4: Complex III subunit 9

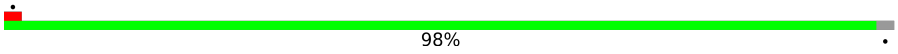
Chain 1H:





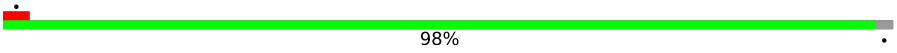
• Molecule 4: Complex III subunit 9

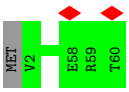
Chain 6G:



• Molecule 4: Complex III subunit 9

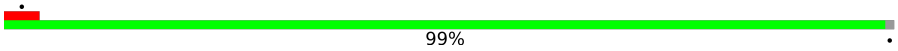
Chain 6H:

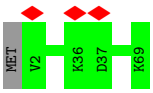




• Molecule 5: Cytochrome b-c1 complex subunit 6

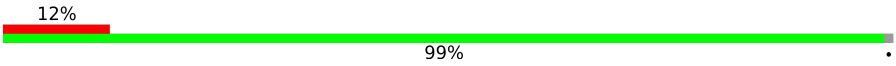
Chain 1I:

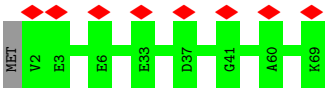




• Molecule 5: Cytochrome b-c1 complex subunit 6

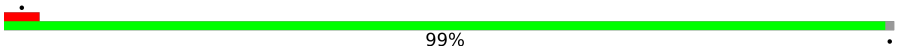
Chain 1J:

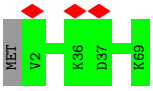




• Molecule 5: Cytochrome b-c1 complex subunit 6

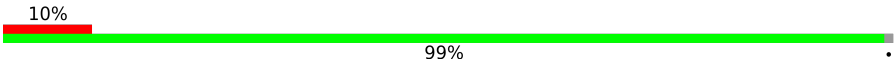
Chain 6I:

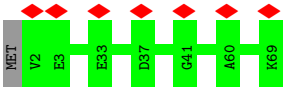




• Molecule 5: Cytochrome b-c1 complex subunit 6

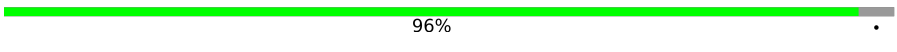
Chain 6J:

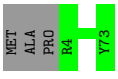




• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

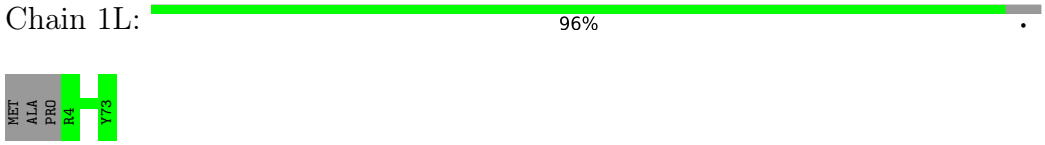
Chain 1K:





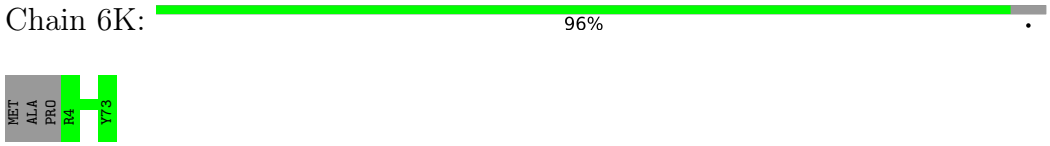
• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1L:



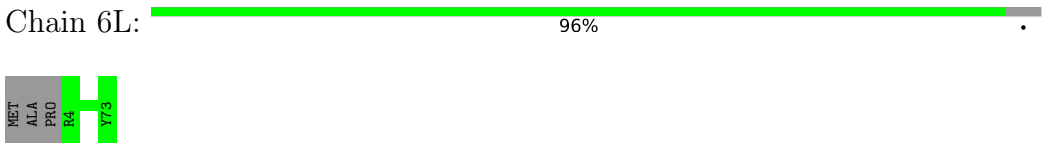
• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 6K:



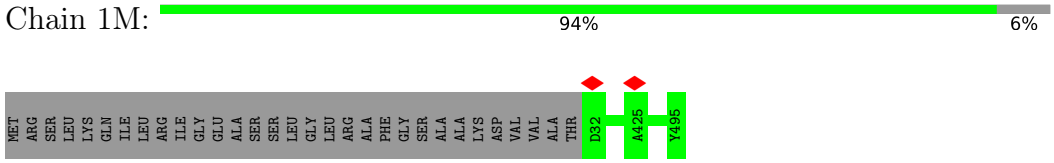
• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 6L:



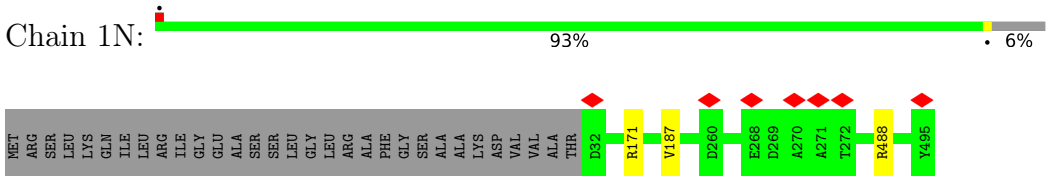
• Molecule 7: MPP-Beta

Chain 1M:



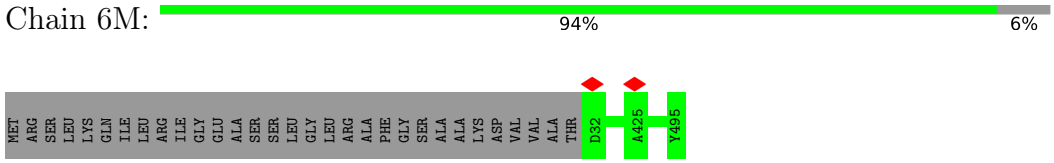
• Molecule 7: MPP-Beta

Chain 1N:



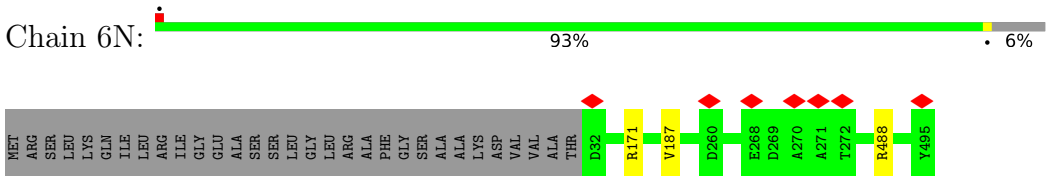
• Molecule 7: MPP-Beta

Chain 6M:



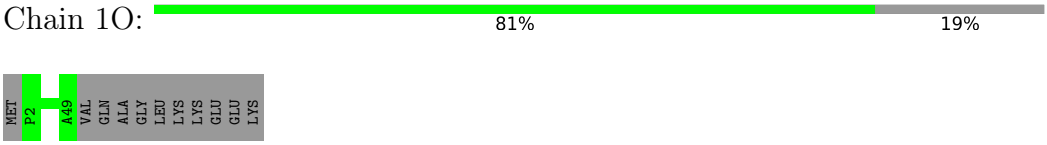
• Molecule 7: MPP-Beta

Chain 6N:



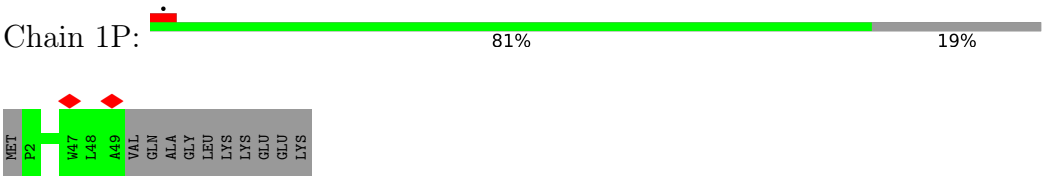
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 1O:



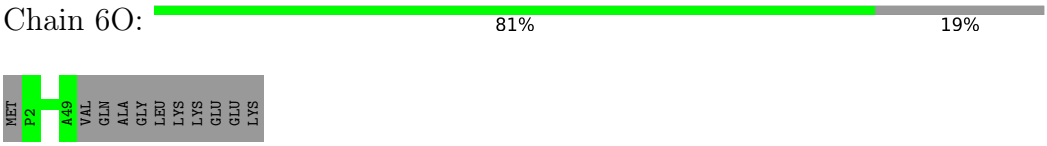
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 1P:



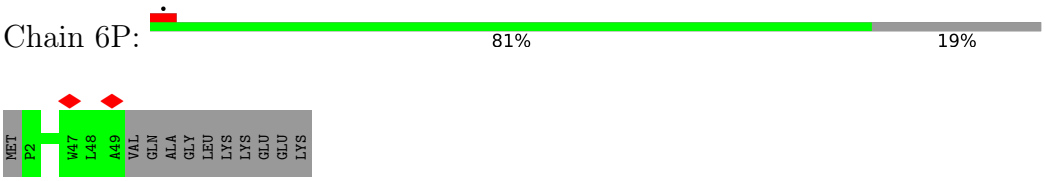
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 6O:



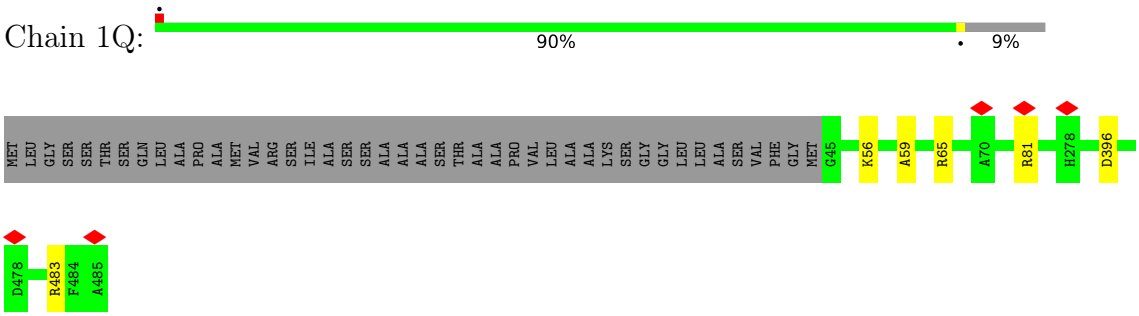
• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 6P:



• Molecule 9: Alpha-MPP

Chain 1Q:



• Molecule 9: Alpha-MPP

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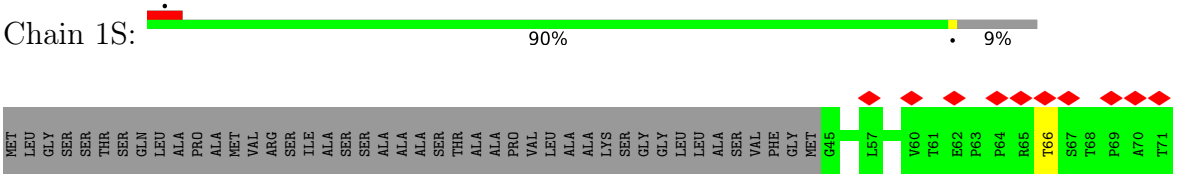

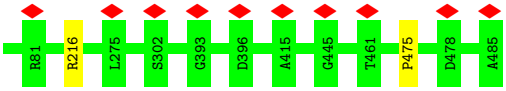

• Molecule 9: Alpha-MPP

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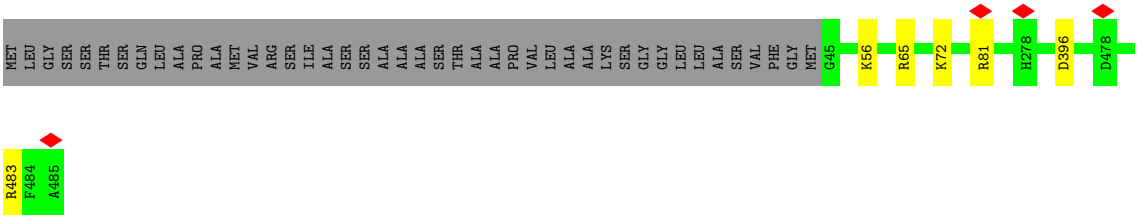
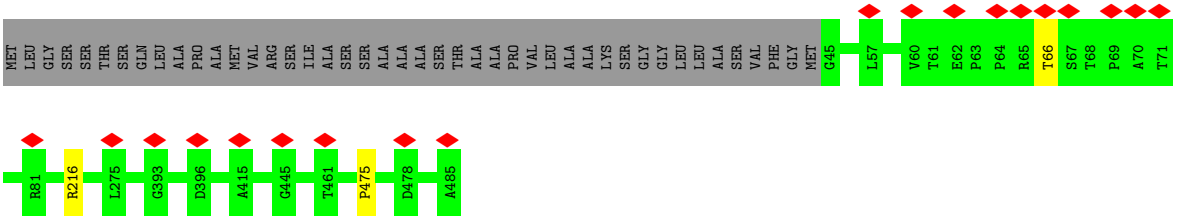


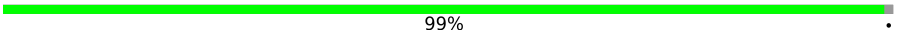
• Molecule 9: Alpha-MPP

Chain 6S:



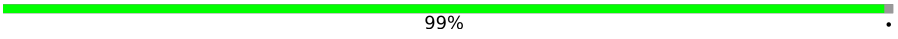
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1R:



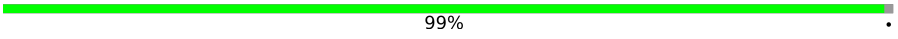
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1T:



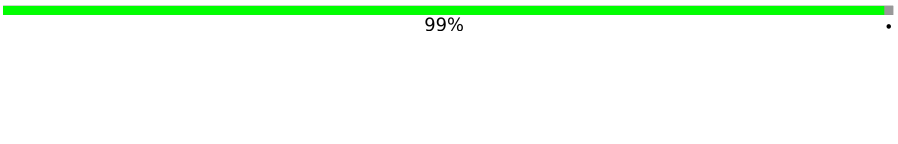
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 6R:



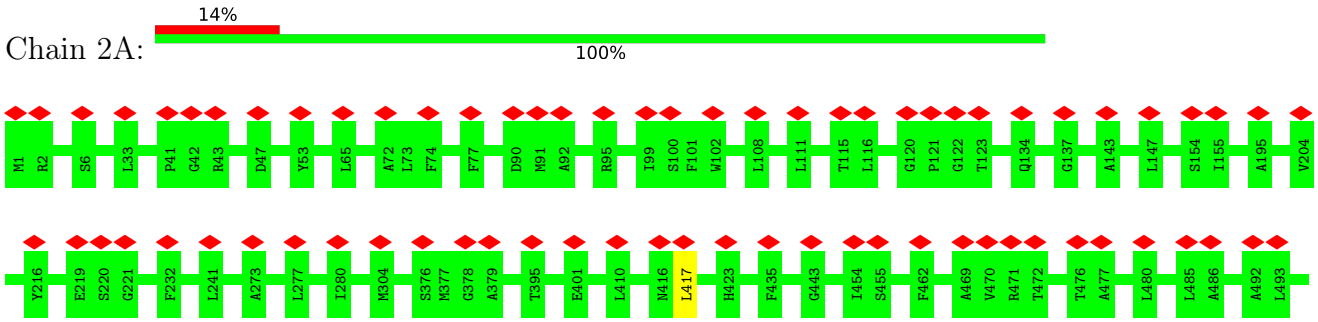
• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 6T:



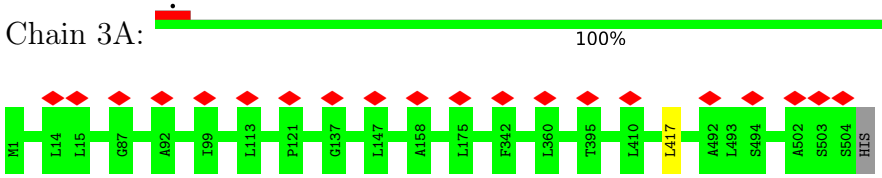
• Molecule 11: Cytochrome c oxidase subunit 1

Chain 2A:



• Molecule 11: Cytochrome c oxidase subunit 1

Chain 3A:

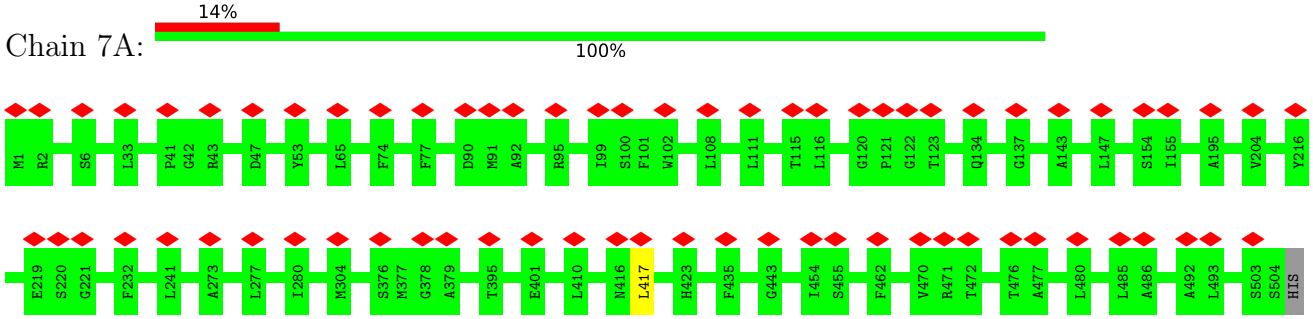


• Molecule 11: Cytochrome c oxidase subunit 1

Chain 4A:

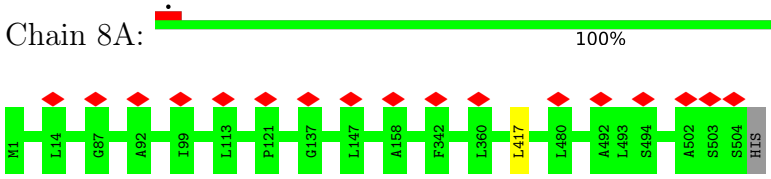
• Molecule 11: Cytochrome c oxidase subunit 1

Chain 7A:



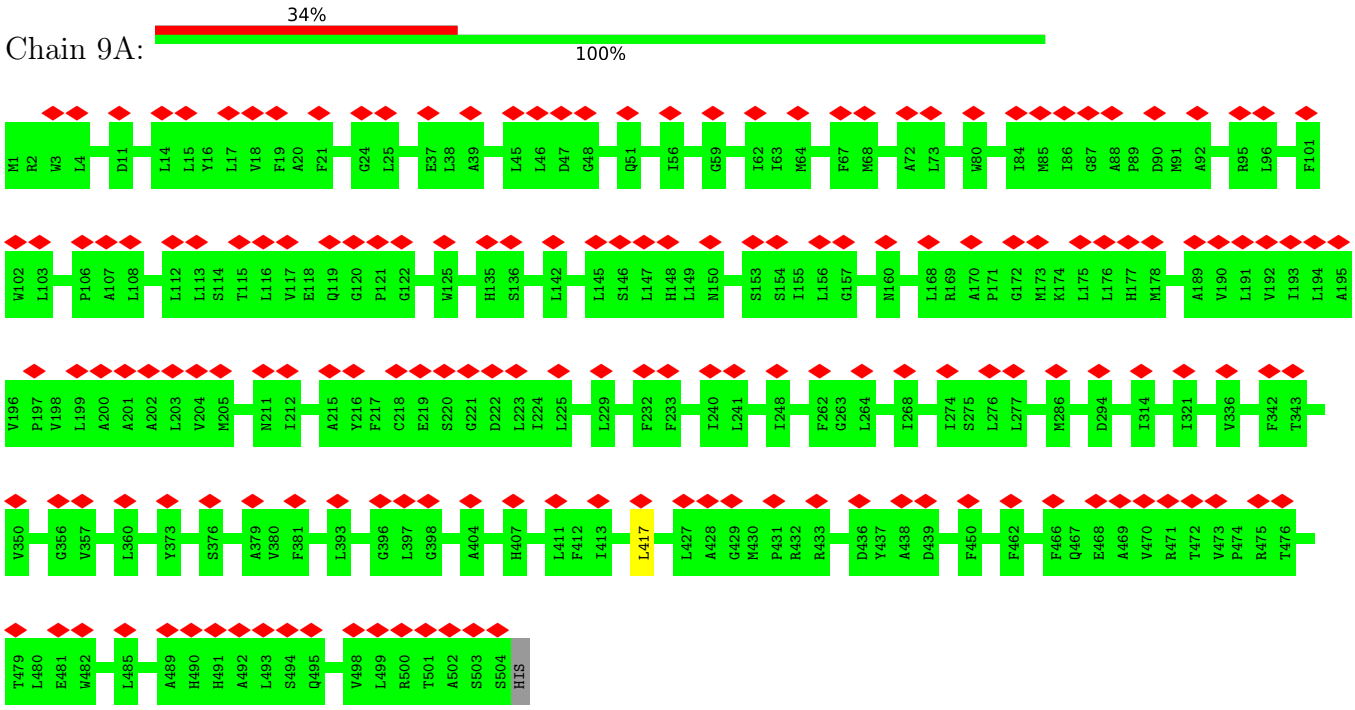
• Molecule 11: Cytochrome c oxidase subunit 1

Chain 8A:



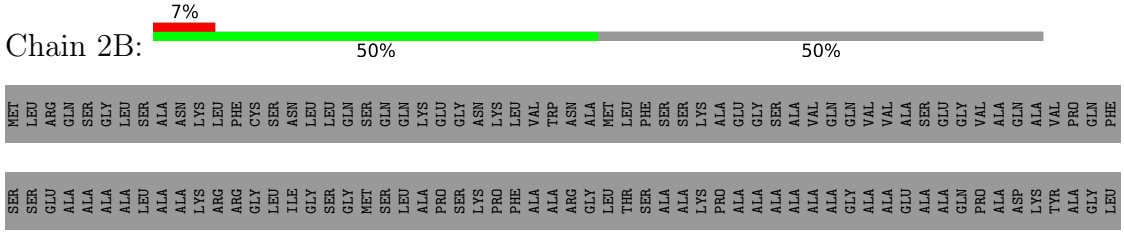
• Molecule 11: Cytochrome c oxidase subunit 1

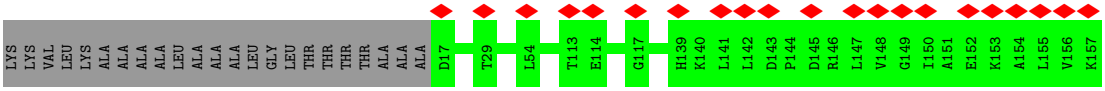
Chain 9A:



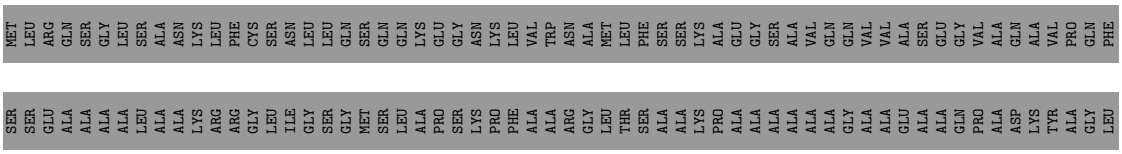
• Molecule 12: Cytochrome c oxidase polypeptide II

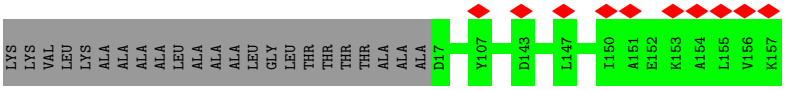
Chain 2B:



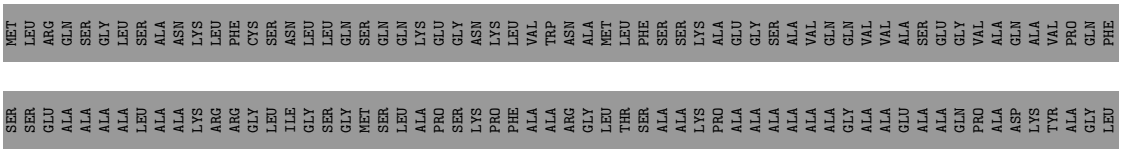


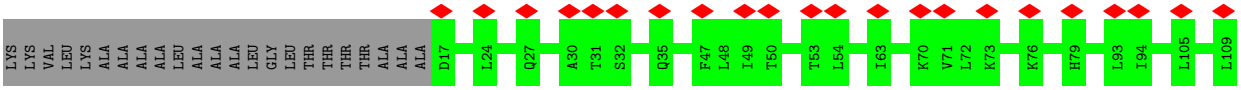
• Molecule 12: Cytochrome c oxidase polypeptide II

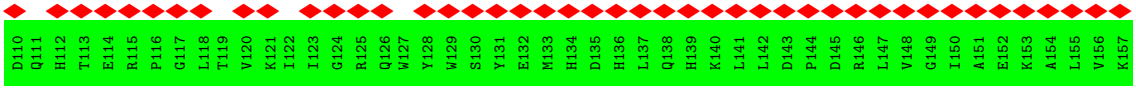




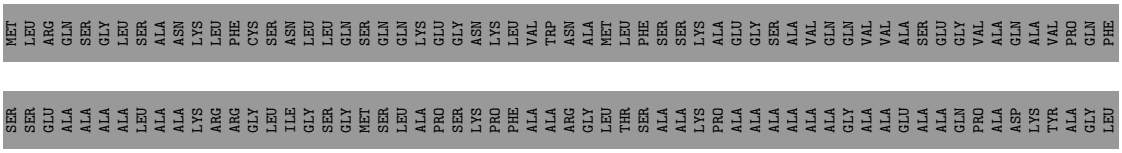
• Molecule 12: Cytochrome c oxidase polypeptide II

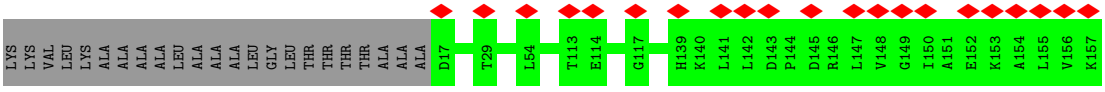




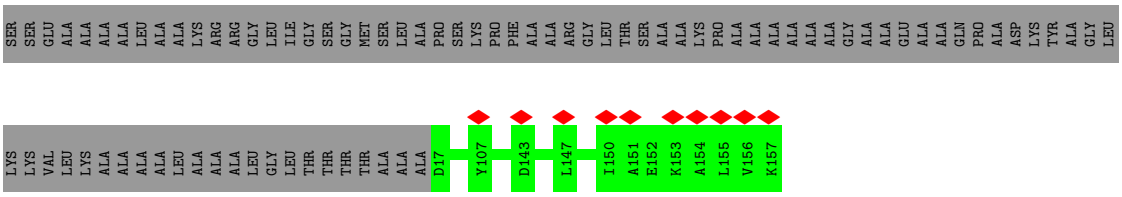


• Molecule 12: Cytochrome c oxidase polypeptide II

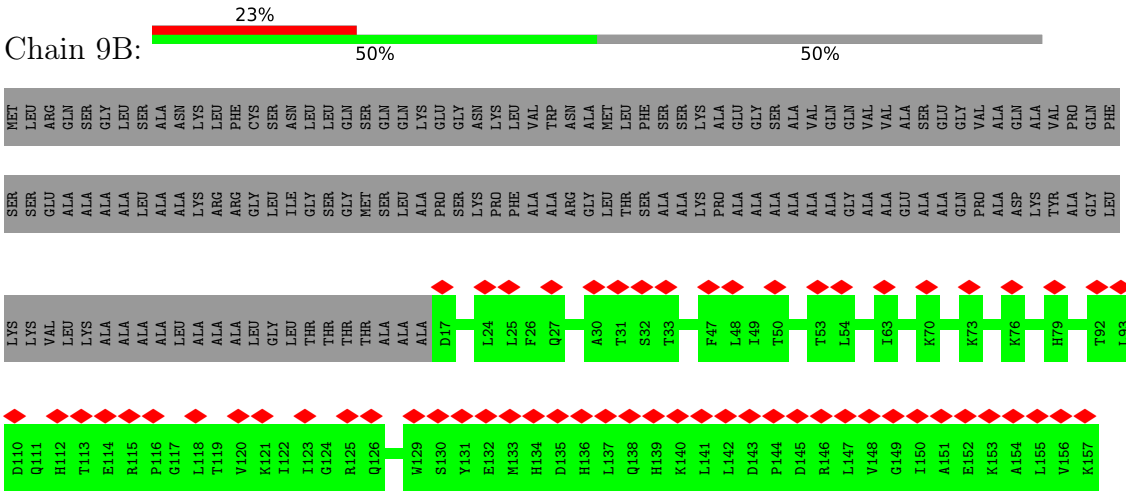




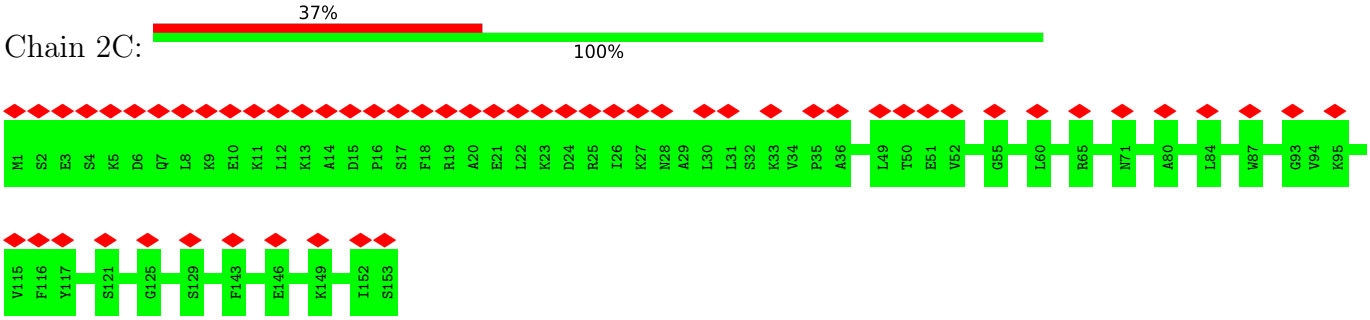
• Molecule 12: Cytochrome c oxidase polypeptide II



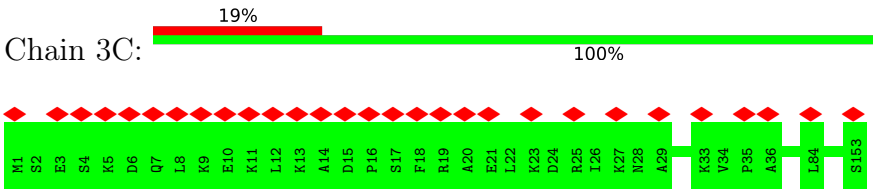
• Molecule 12: Cytochrome c oxidase polypeptide II



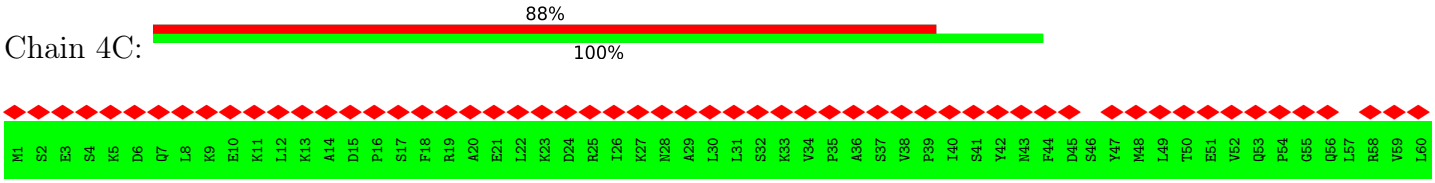
• Molecule 13: cytochrome-c oxidase

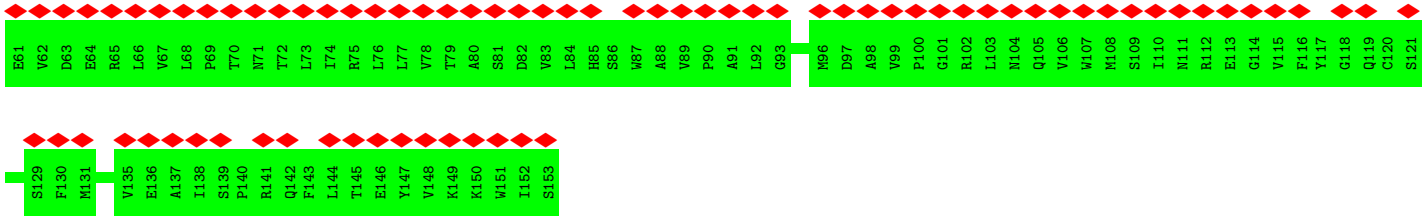


• Molecule 13: cytochrome-c oxidase

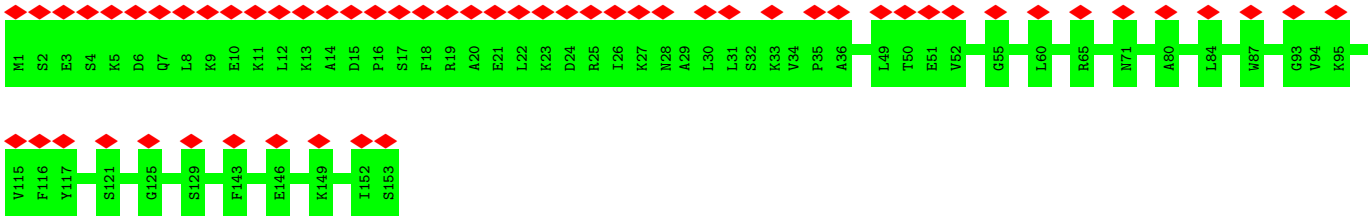


• Molecule 13: cytochrome-c oxidase

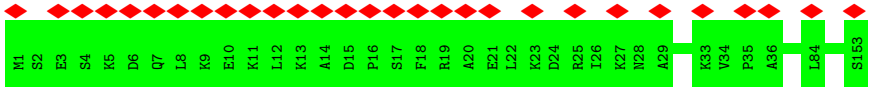




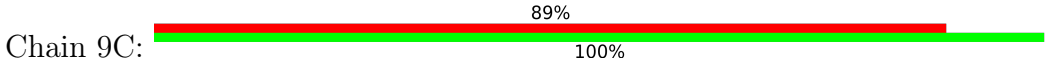
• Molecule 13: cytochrome-c oxidase

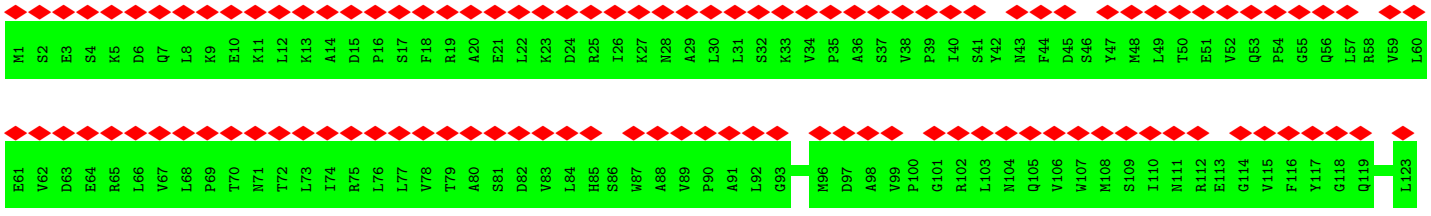


• Molecule 13: cytochrome-c oxidase

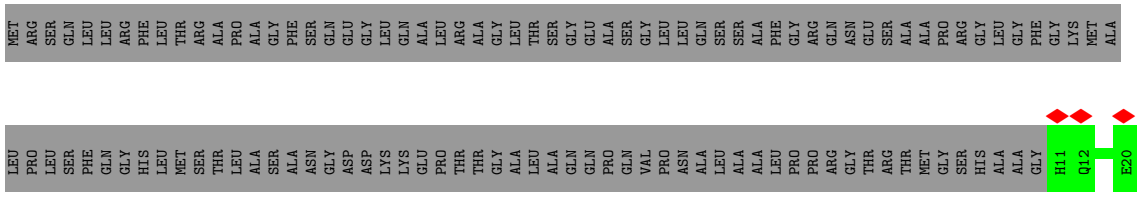


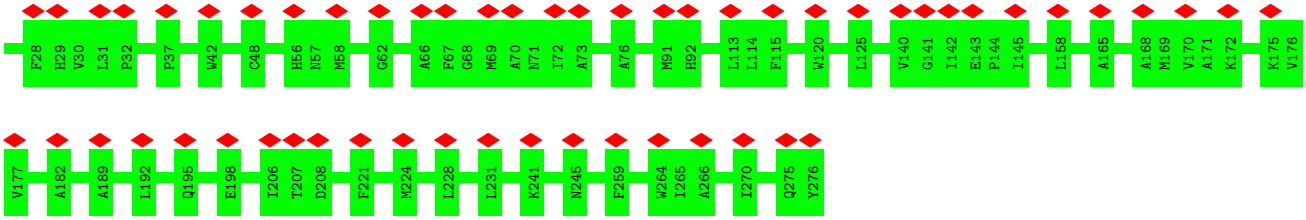
• Molecule 13: cytochrome-c oxidase



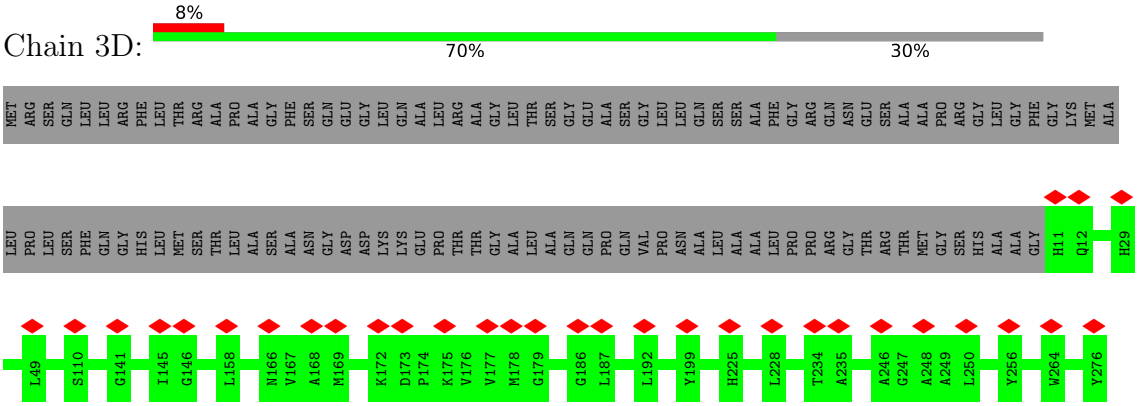


• Molecule 14: Cytochrome c oxidase subunit 3

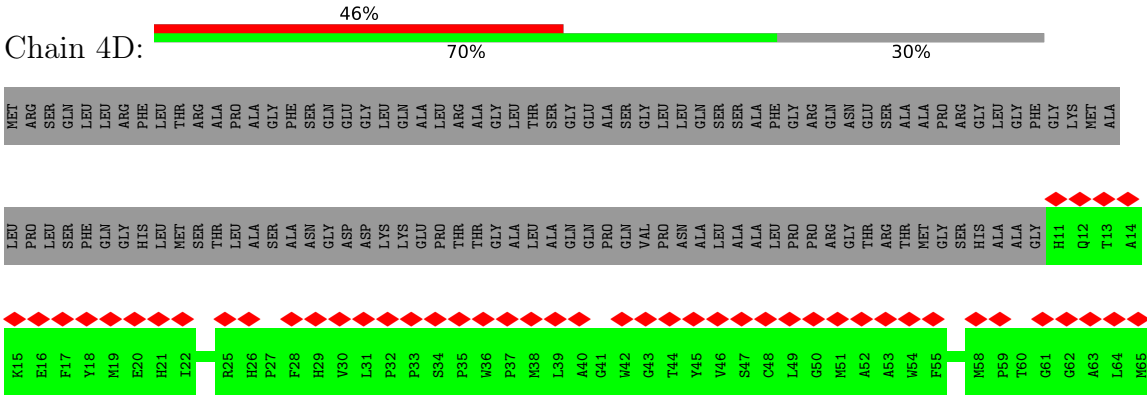




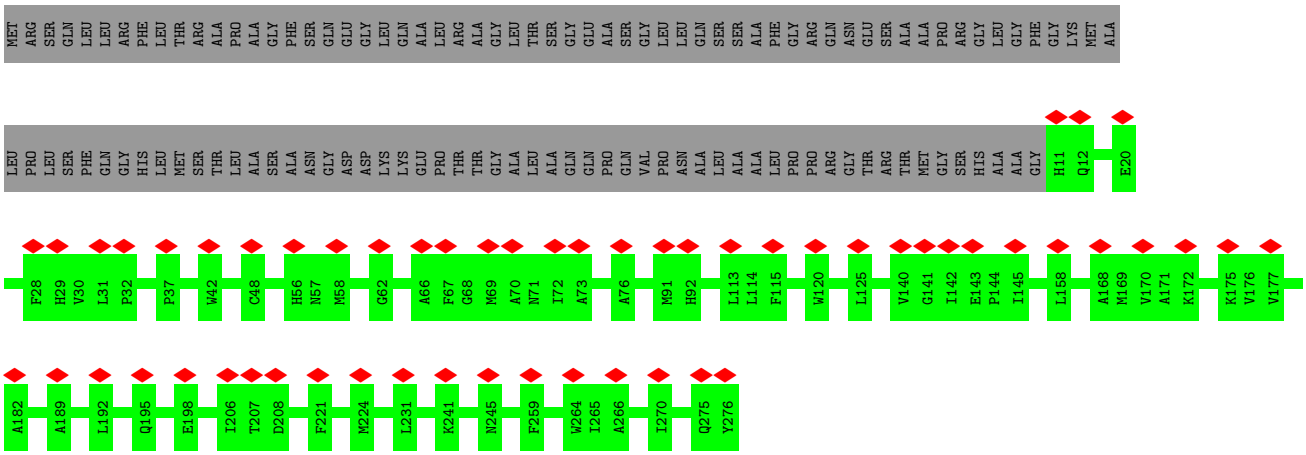
• Molecule 14: Cytochrome c oxidase subunit 3



• Molecule 14: Cytochrome c oxidase subunit 3

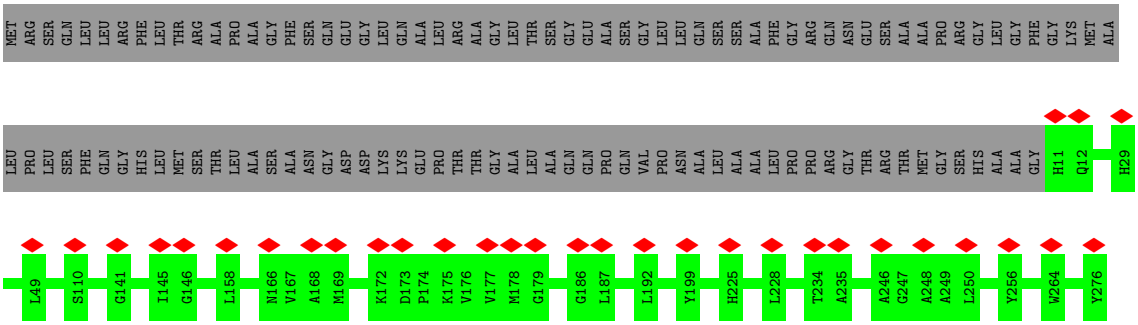


• Molecule 14: Cytochrome c oxidase subunit 3



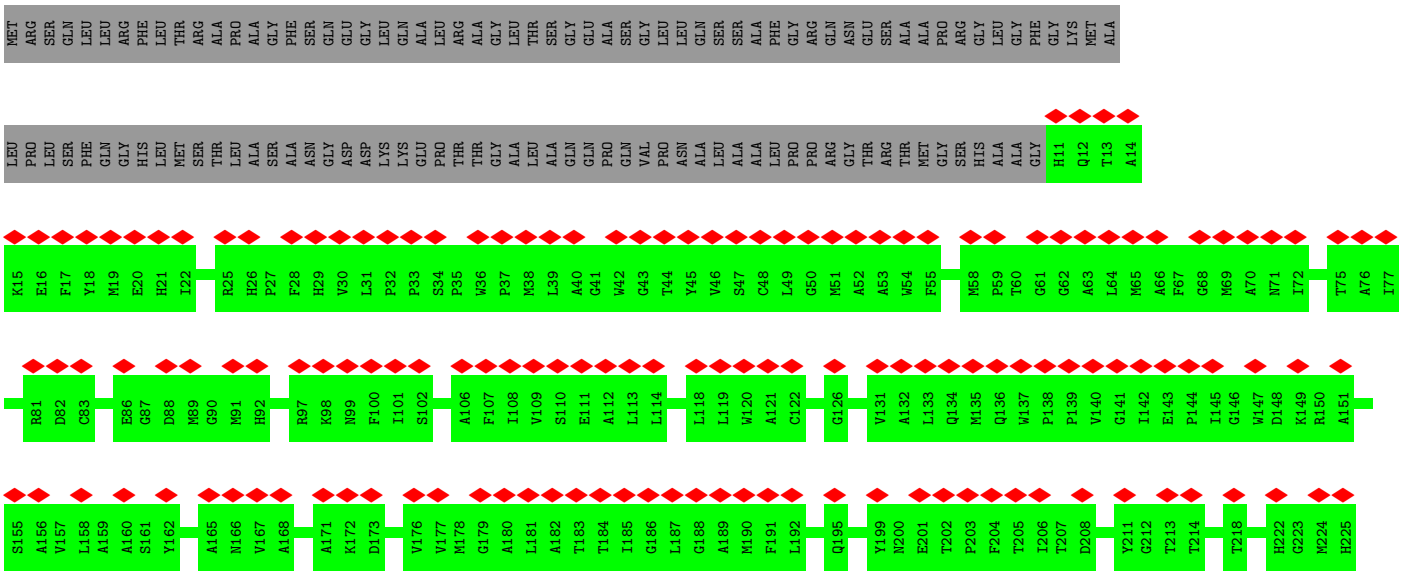
• Molecule 14: Cytochrome c oxidase subunit 3

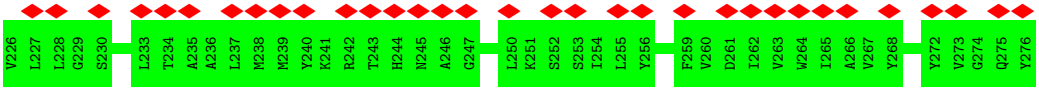
Chain 8D:



• Molecule 14: Cytochrome c oxidase subunit 3

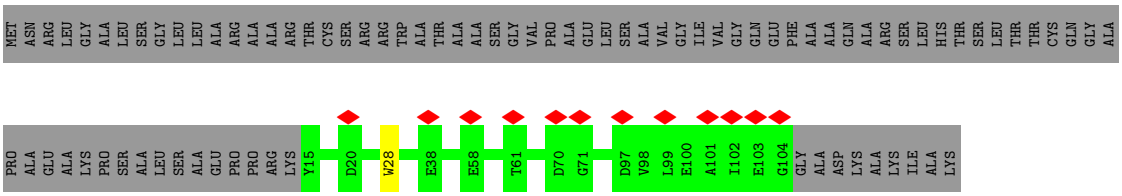
Chain 9D:





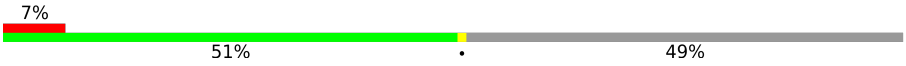
• Molecule 15: Cox5b

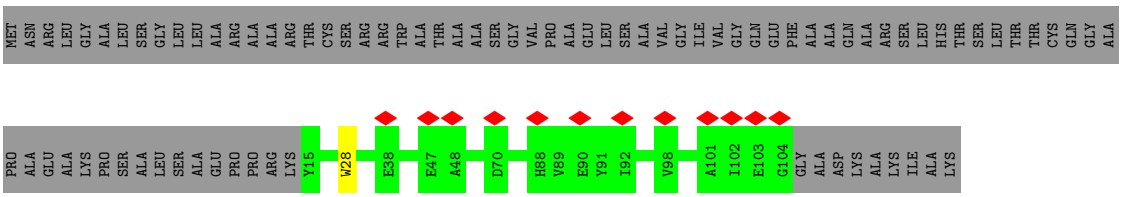
Chain 2E:



• Molecule 15: Cox5b

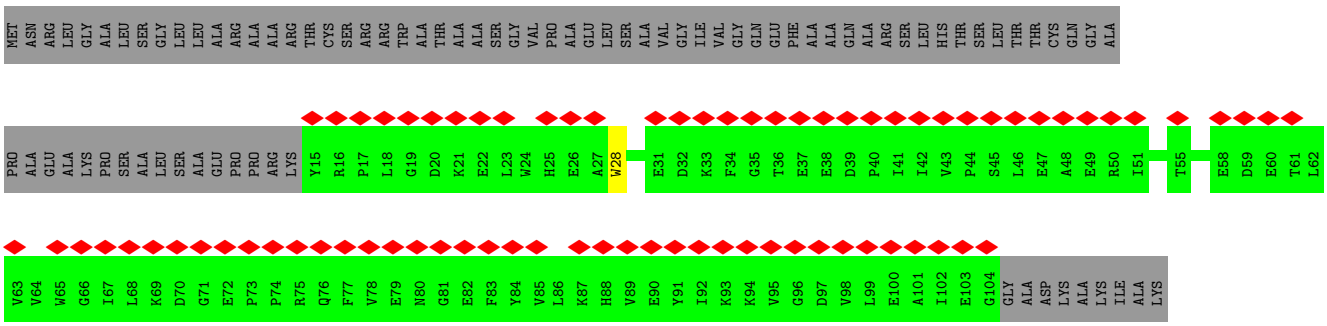
Chain 3E:





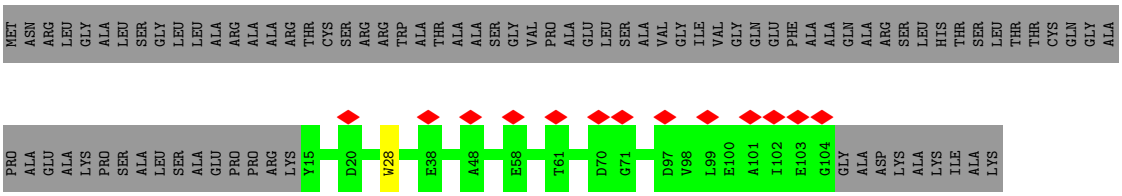
• Molecule 15: Cox5b

Chain 4E:



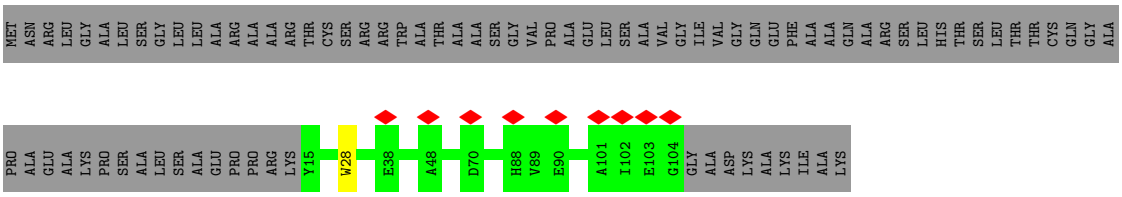
• Molecule 15: Cox5b

Chain 7E:

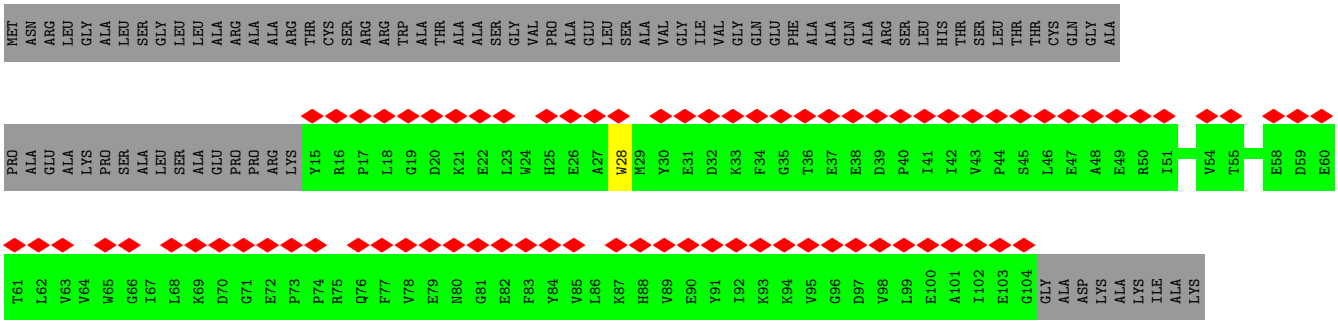


• Molecule 15: Cox5b

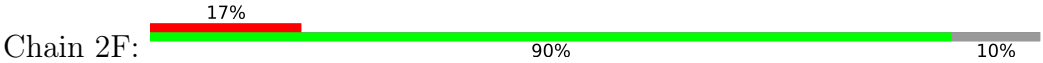
Chain 8E:

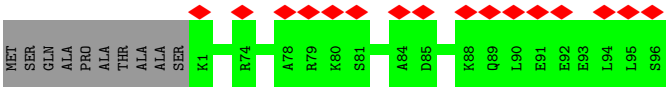


• Molecule 15: Cox5b

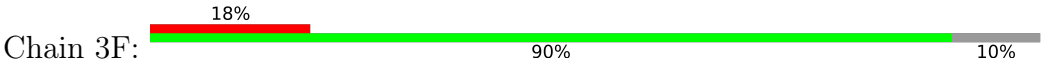


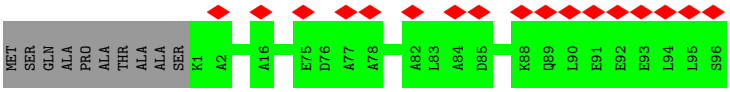
• Molecule 16: Cox5c



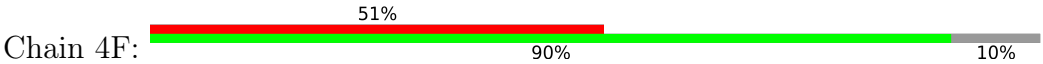


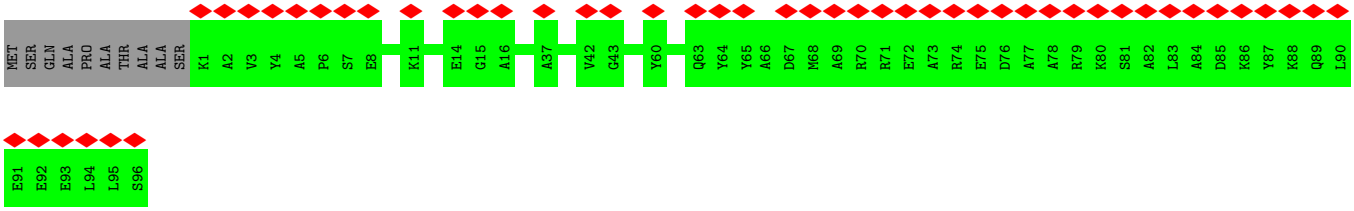
• Molecule 16: Cox5c



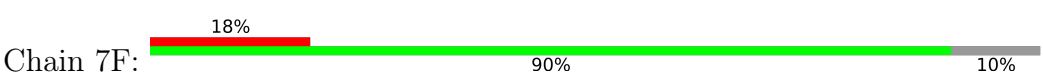


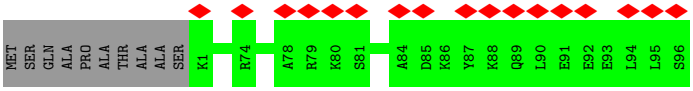
• Molecule 16: Cox5c





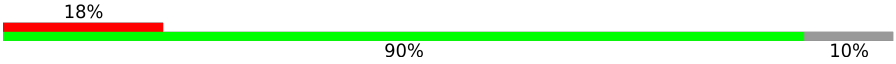
• Molecule 16: Cox5c

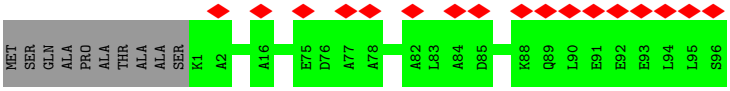




• Molecule 16: Cox5c

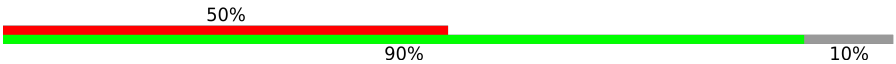
Chain 8F:

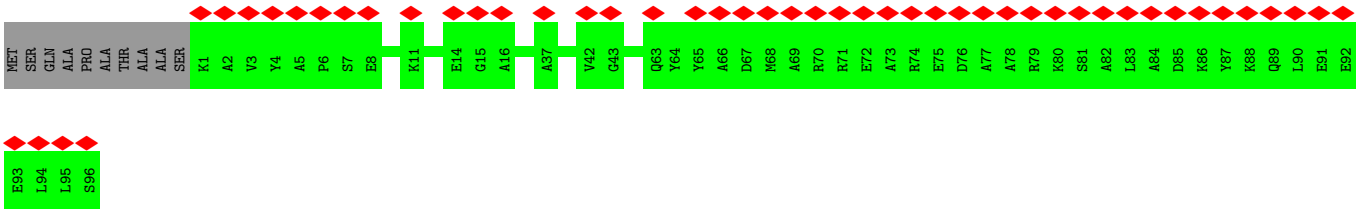




• Molecule 16: Cox5c

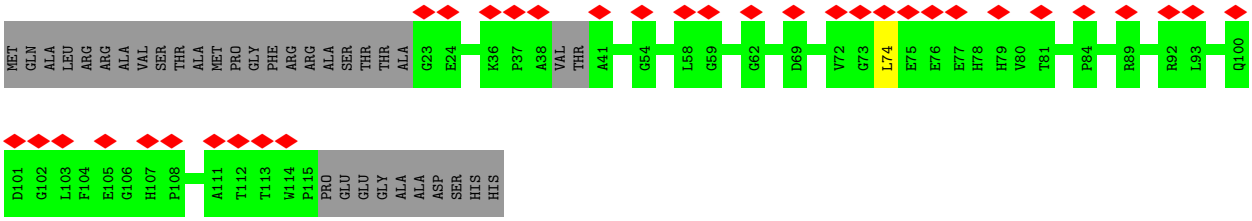
Chain 9F:





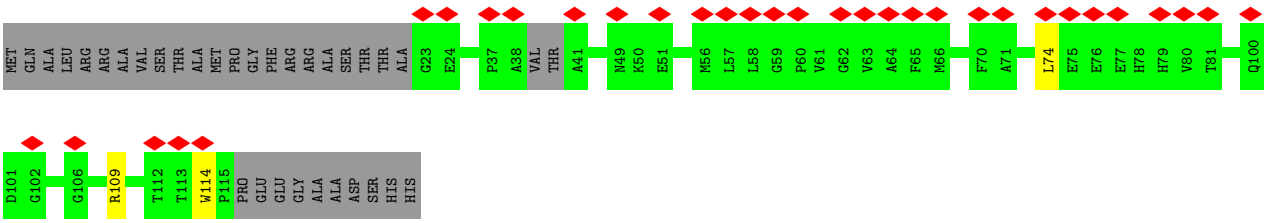
• Molecule 17: Cox6a

Chain 2G:



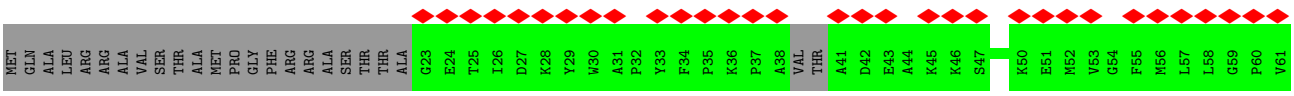
• Molecule 17: Cox6a

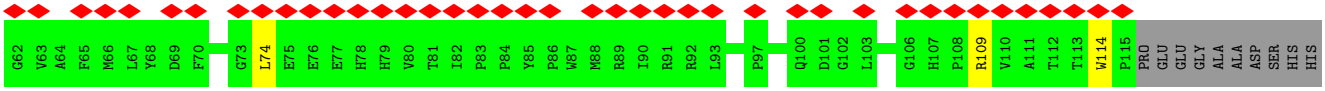
Chain 3G:



• Molecule 17: Cox6a

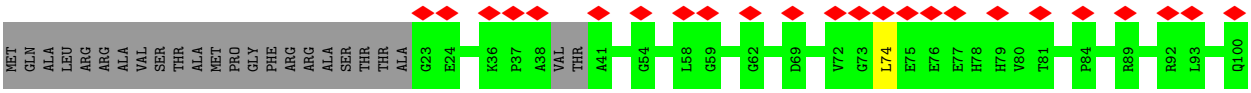
Chain 4G:

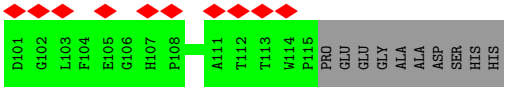




• Molecule 17: Cox6a

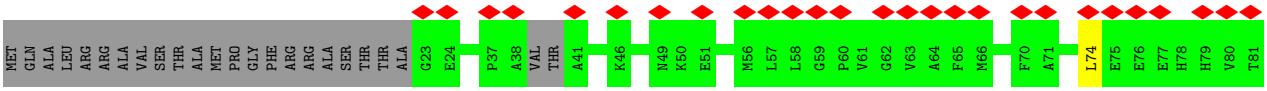
Chain 7G:





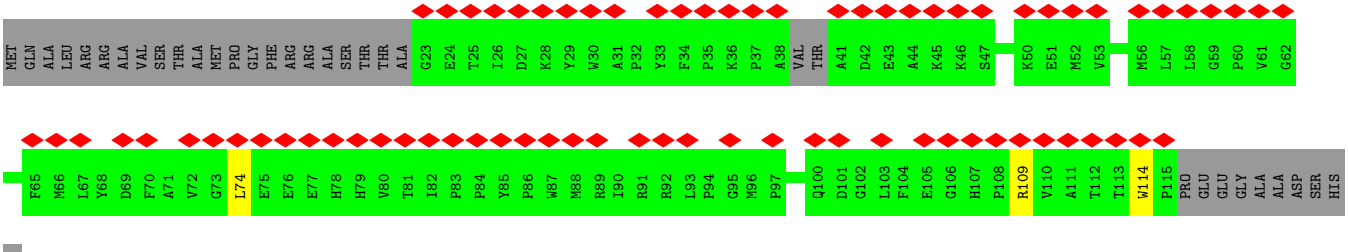
• Molecule 17: Cox6a

Chain 8G:



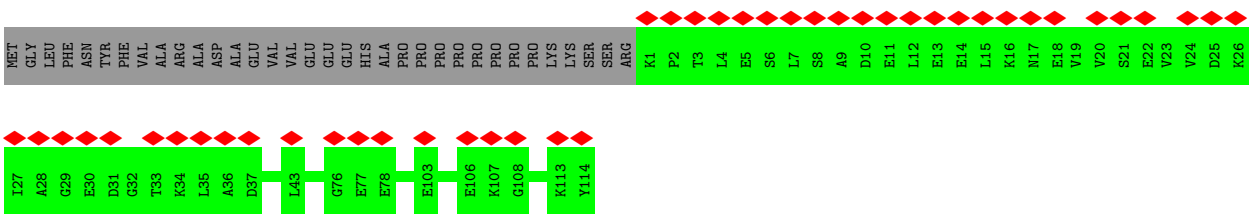
• Molecule 17: Cox6a

Chain 9G:



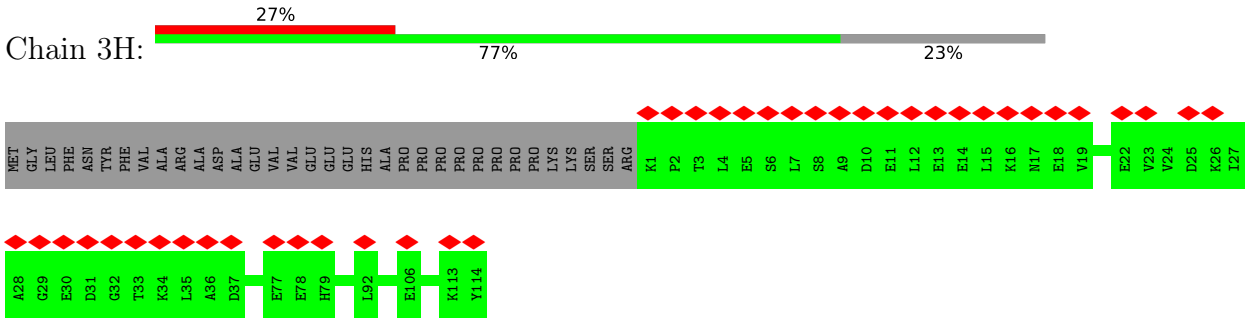
• Molecule 18: Cox6b

Chain 2H:



- Molecule 18: Cox6b

Chain 3H:



- Molecule 18: Cox6b

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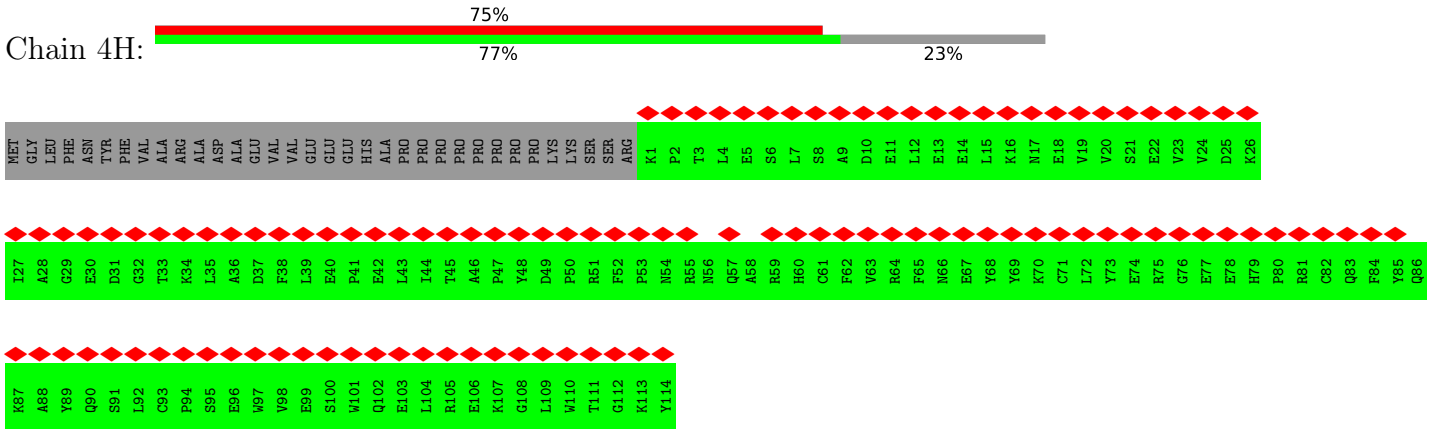
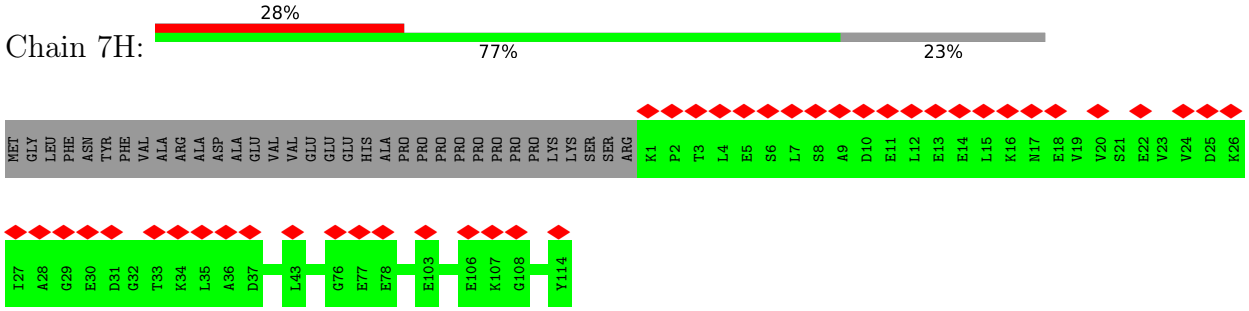


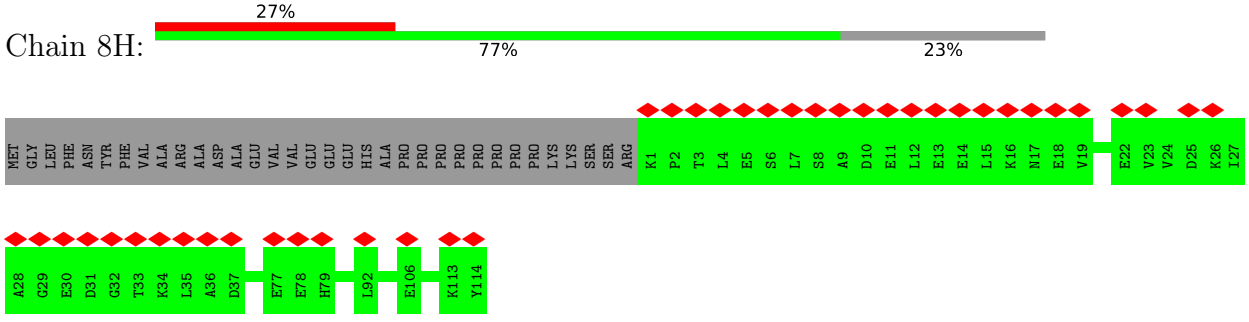
- Molecule 18: Cox6b

Chain 7H:



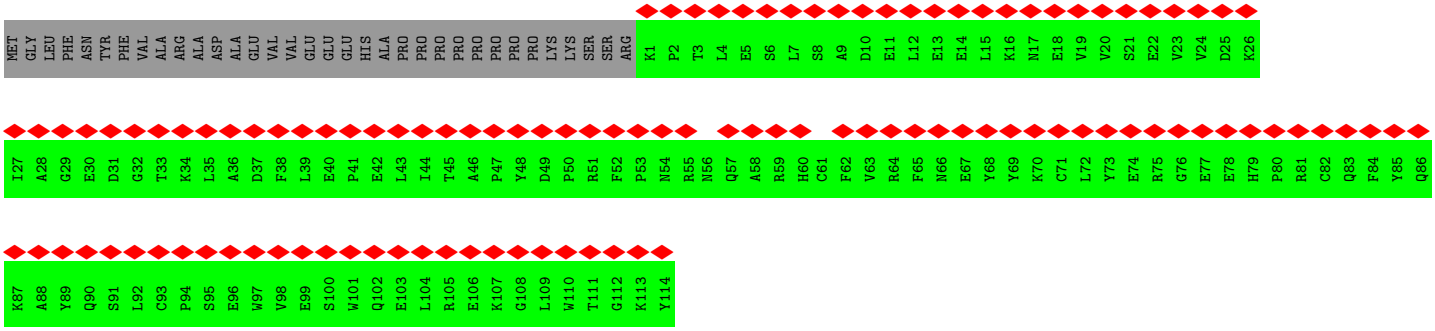
- Molecule 18: Cox6b

Chain 8H:



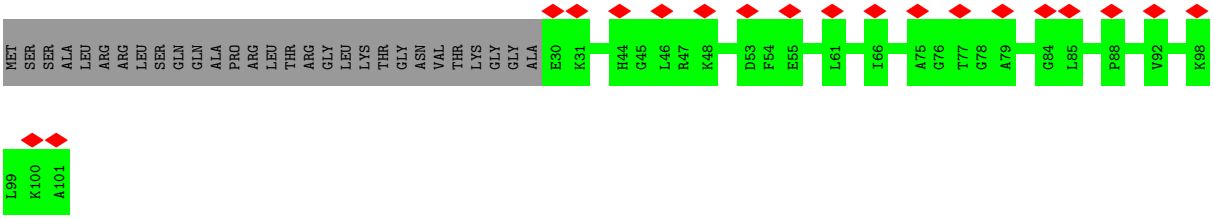
- Molecule 18: Cox6b

Chain 9H:



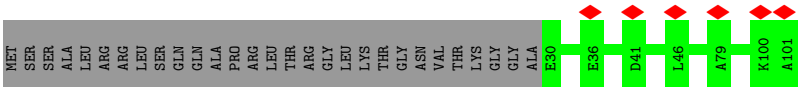
• Molecule 19: Cox7c

Chain 2I:



• Molecule 19: Cox7c

Chain 3I:



• Molecule 19: Cox7c

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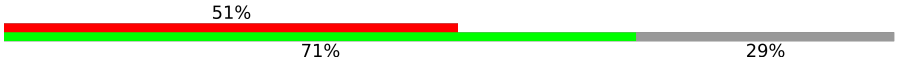

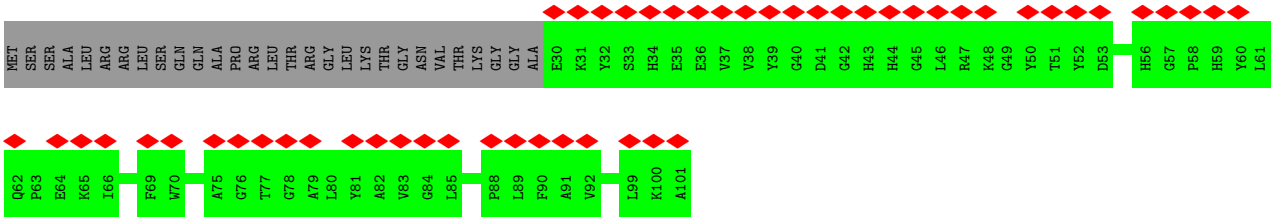

• Molecule 19: Cox7c

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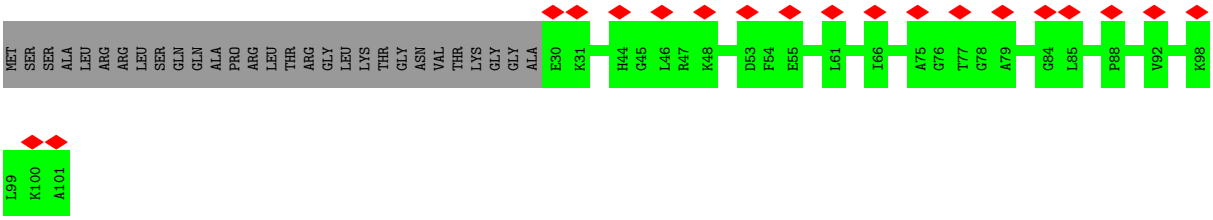
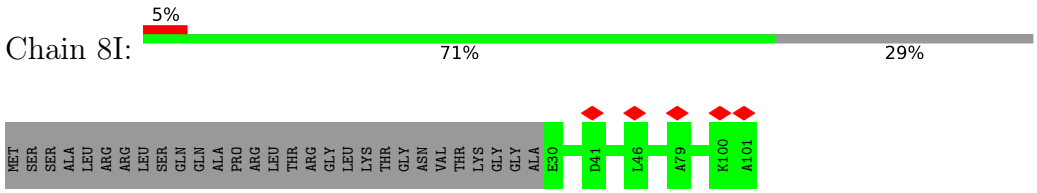


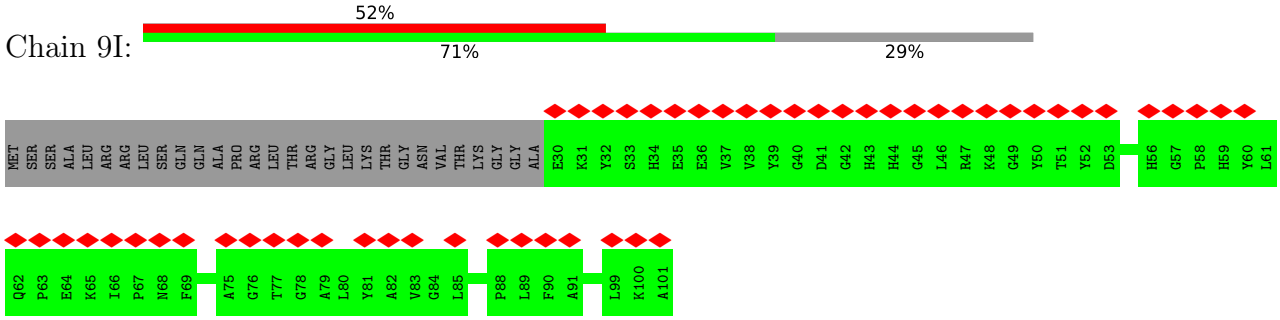
• Molecule 19: Cox7c

Chain 8I:



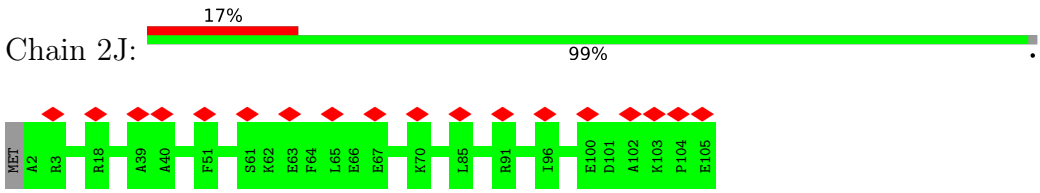
• Molecule 19: Cox7c

Chain 9I:



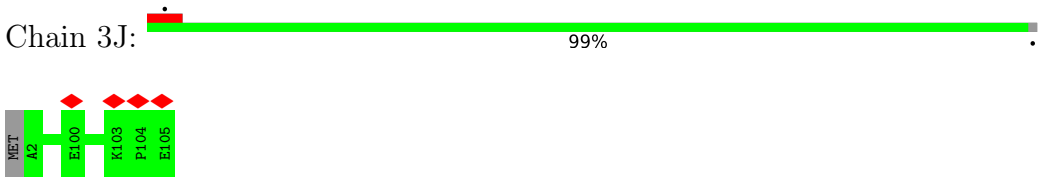
• Molecule 20: Cytochrome c oxidase subunit

Chain 2J:



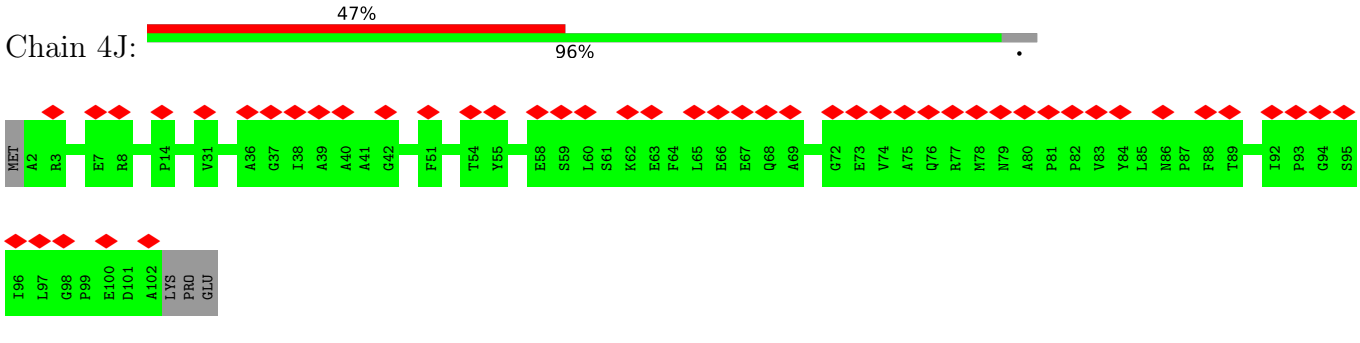
• Molecule 20: Cytochrome c oxidase subunit

Chain 3J:



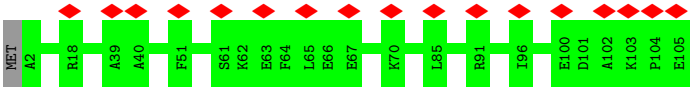
• Molecule 20: Cytochrome c oxidase subunit

Chain 4J:



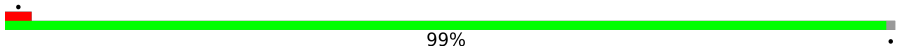
• Molecule 20: Cytochrome c oxidase subunit

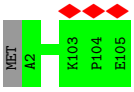
Chain 7J:



• Molecule 20: Cytochrome c oxidase subunit

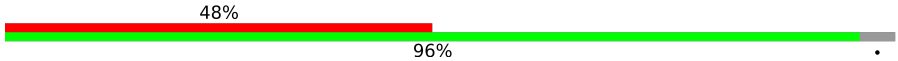
Chain 8J:

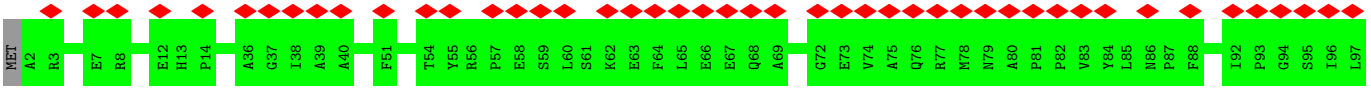


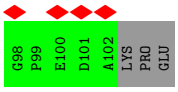


• Molecule 20: Cytochrome c oxidase subunit

Chain 9J:

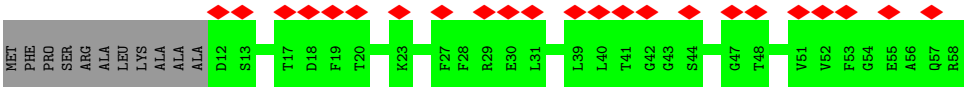






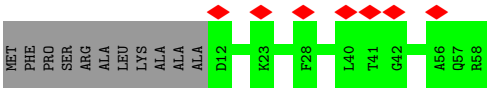
• Molecule 21: Cox7a

Chain 2K:



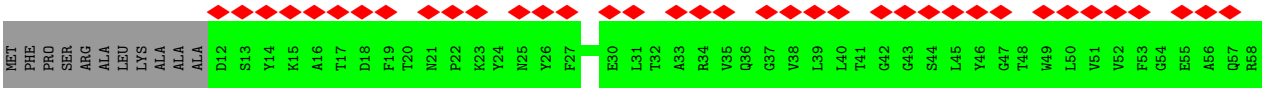
• Molecule 21: Cox7a

Chain 3K:



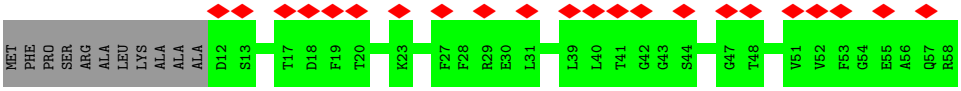
• Molecule 21: Cox7a

Chain 4K:

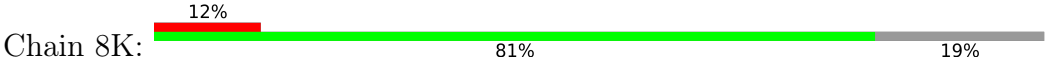


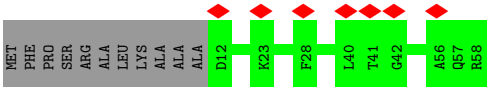
• Molecule 21: Cox7a

Chain 7K:

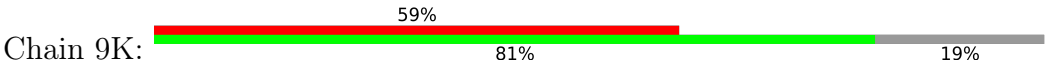


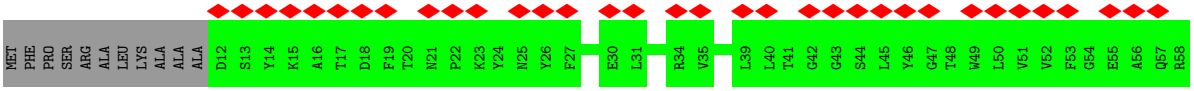
• Molecule 21: Cox7a



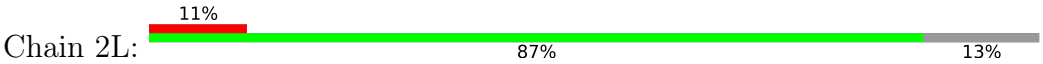


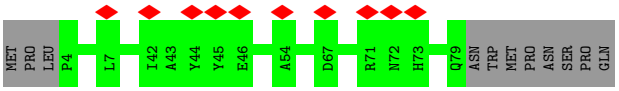
• Molecule 21: Cox7a



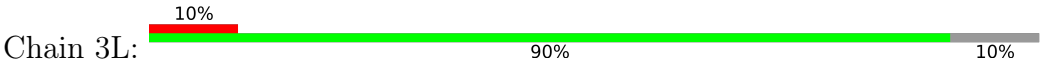


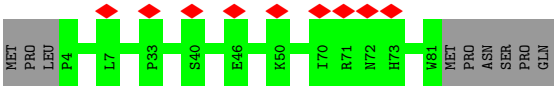
• Molecule 22: CoxIn



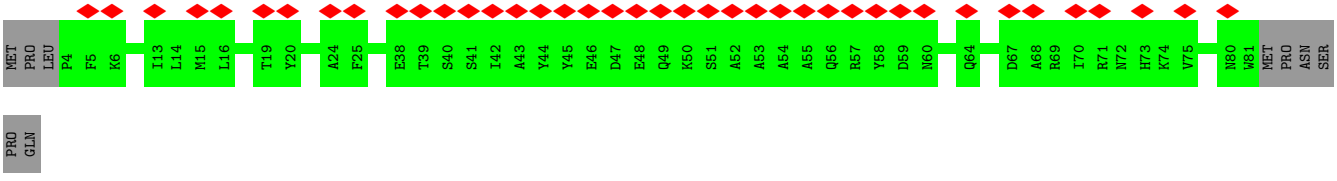


• Molecule 22: CoxIn

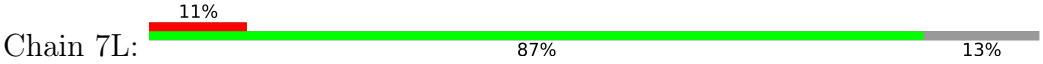


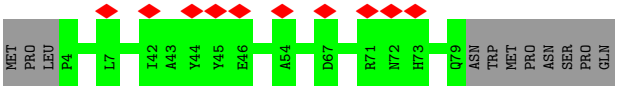


• Molecule 22: CoxIn



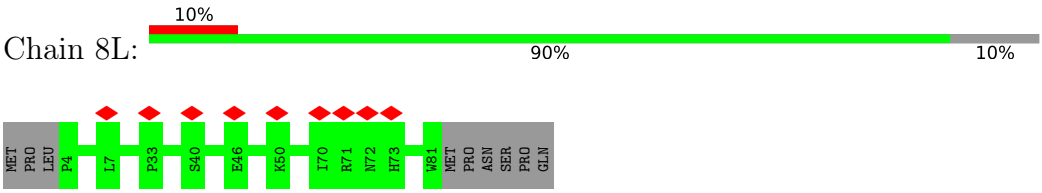
• Molecule 22: CoxIn





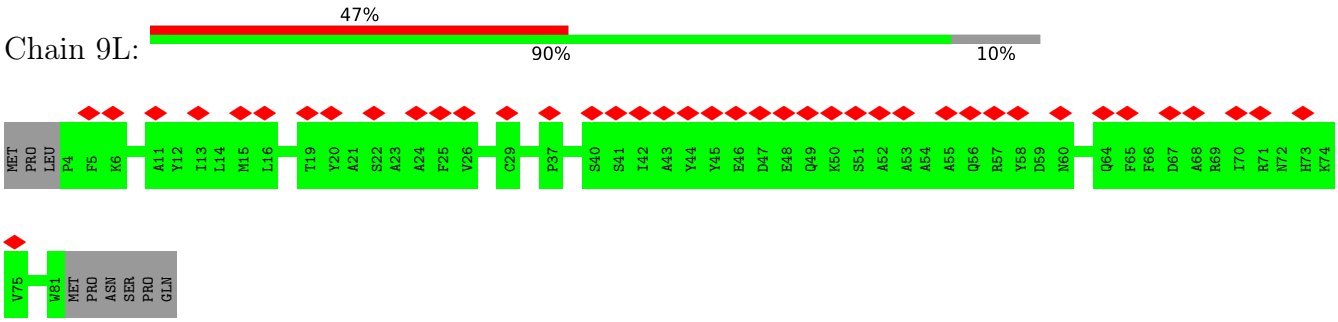
• Molecule 22: CoxIn

Chain 8L:



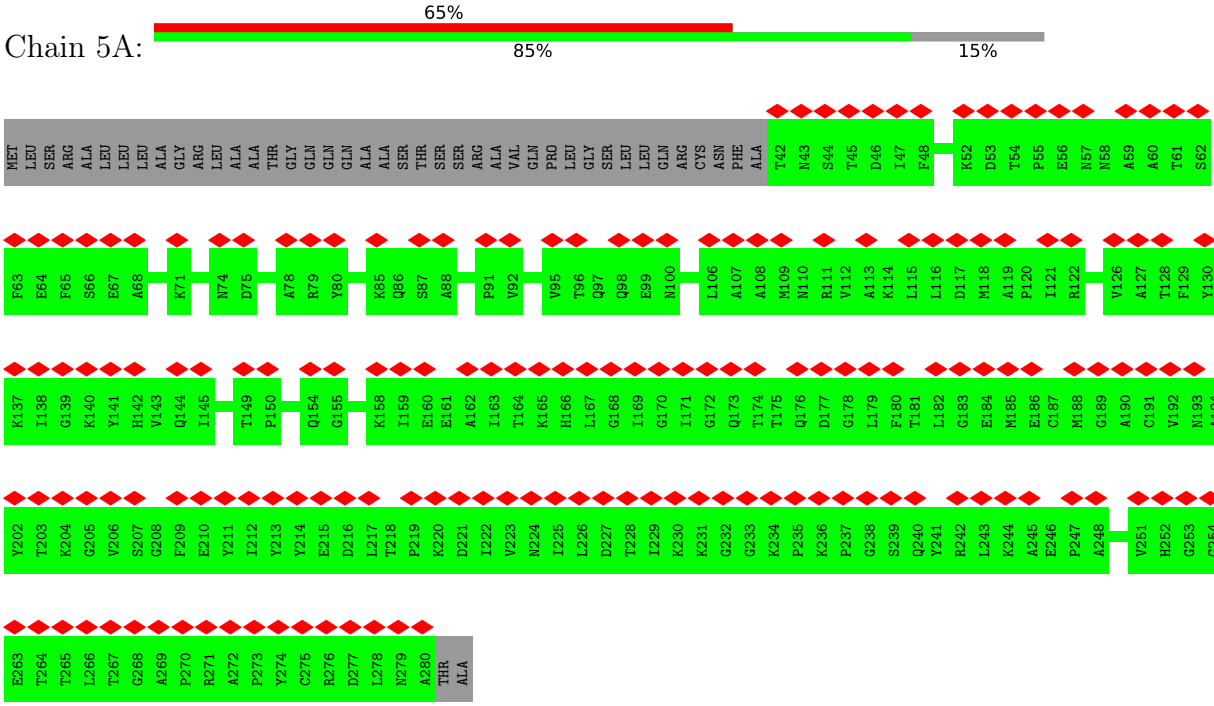
• Molecule 22: CoxIn

Chain 9L:



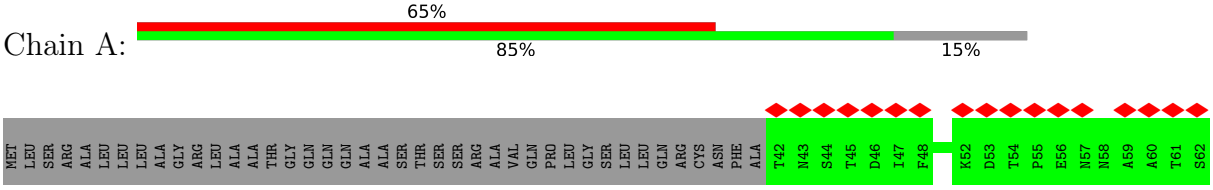
• Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

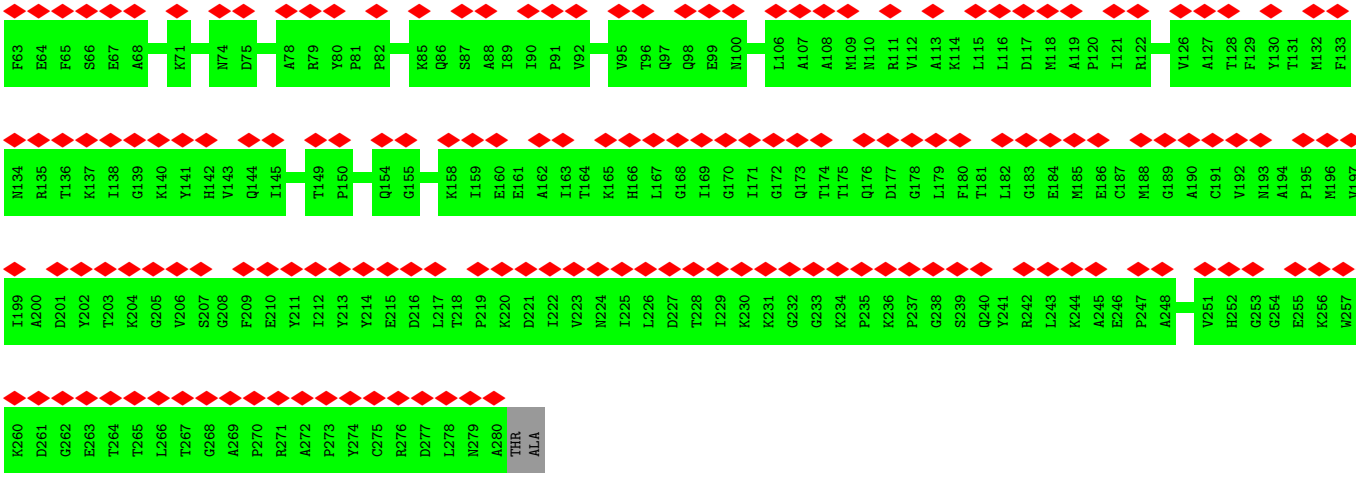
Chain 5A:



• Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

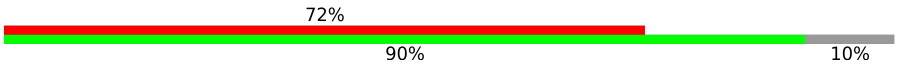
Chain A:

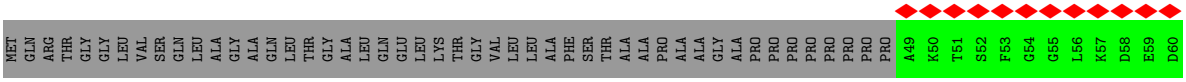


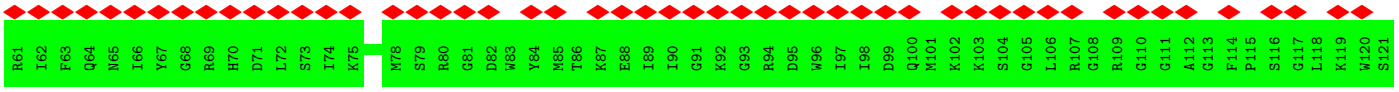


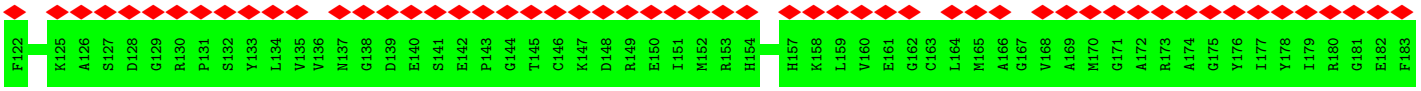
• Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

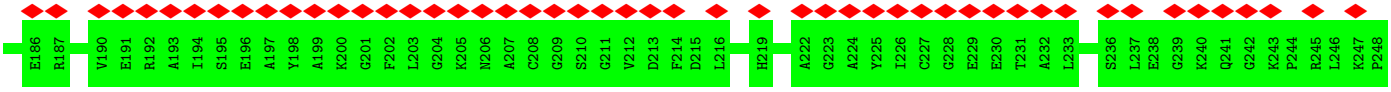
Chain 5B:

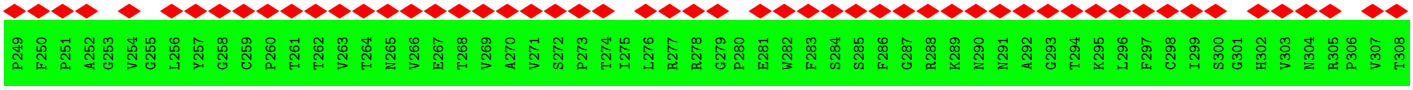


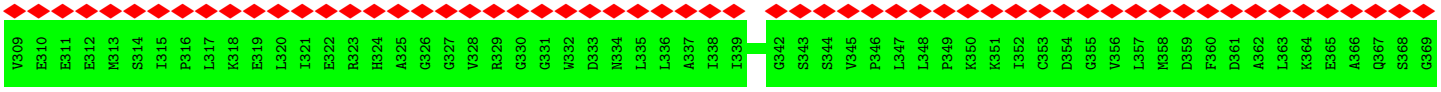


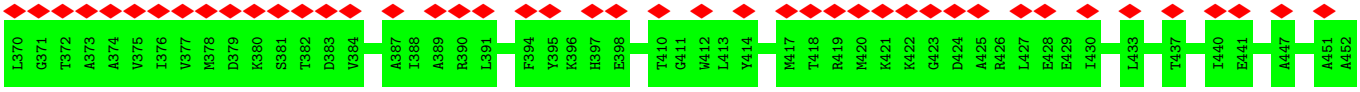






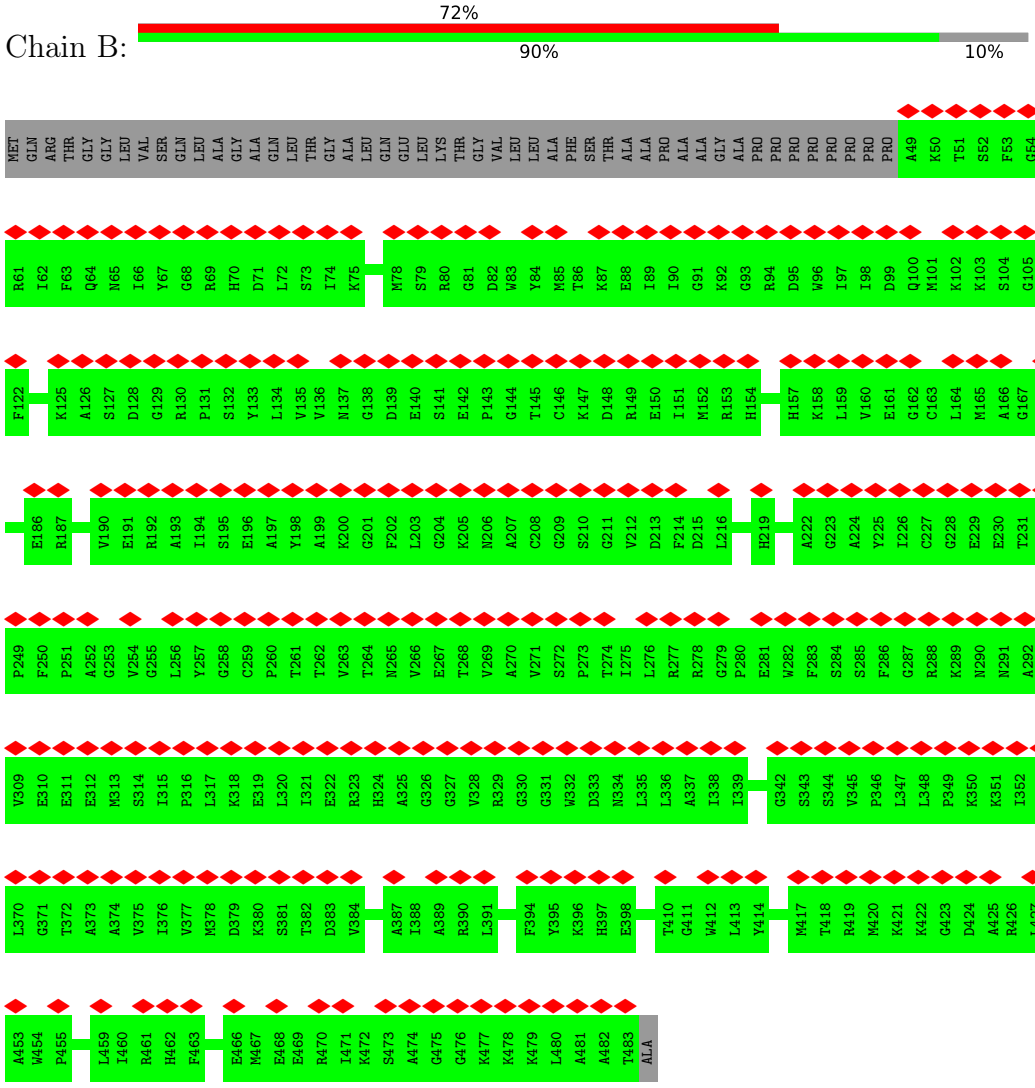






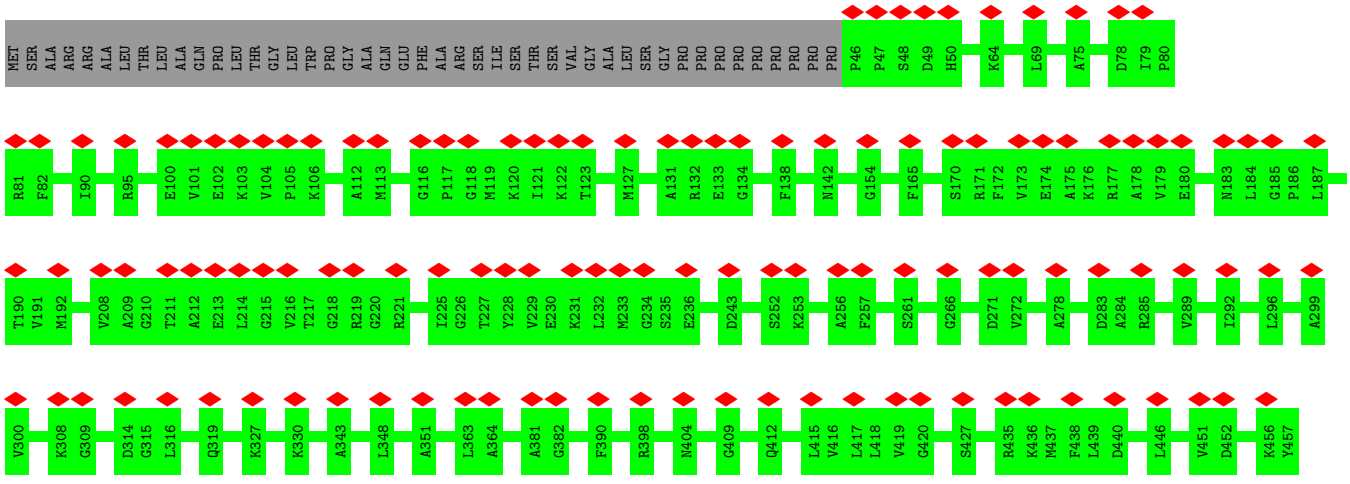
• Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

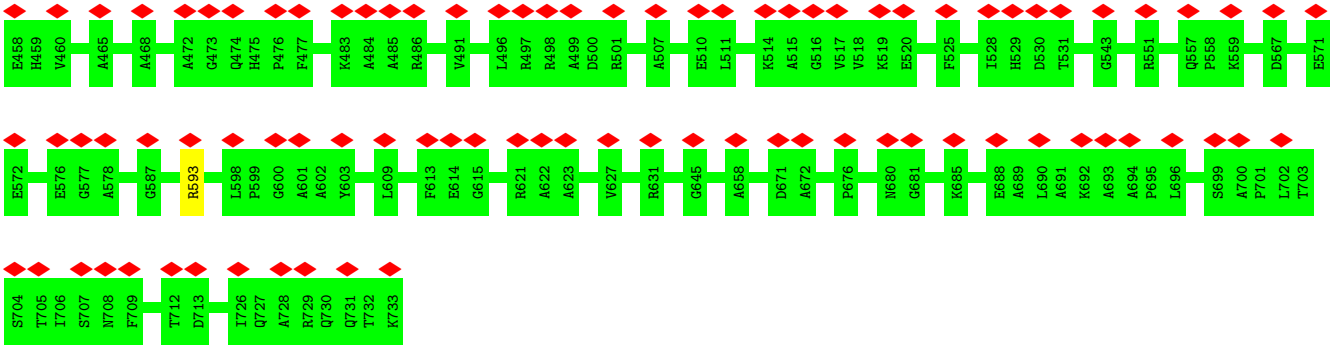
Chain B:



• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

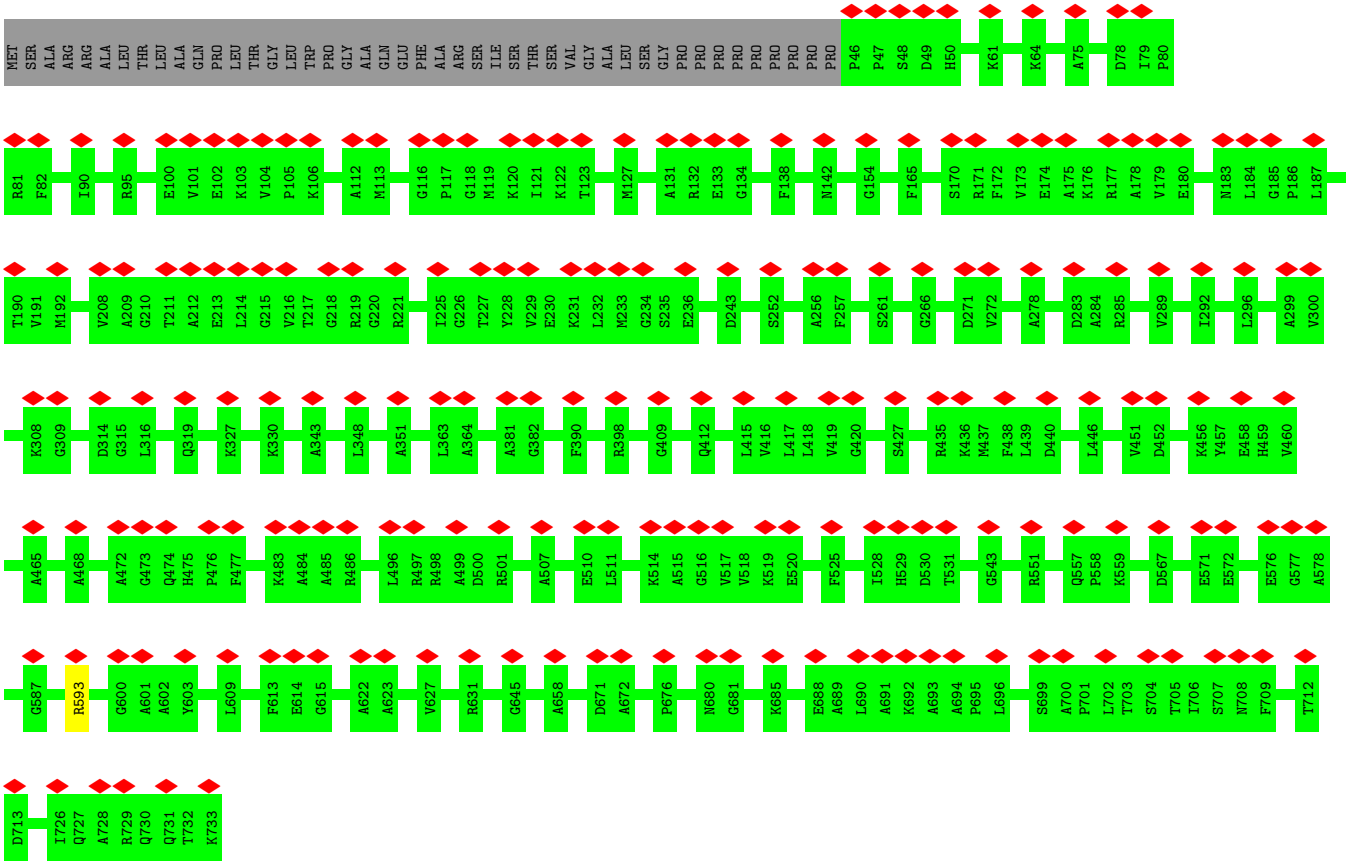
Chain 5C:





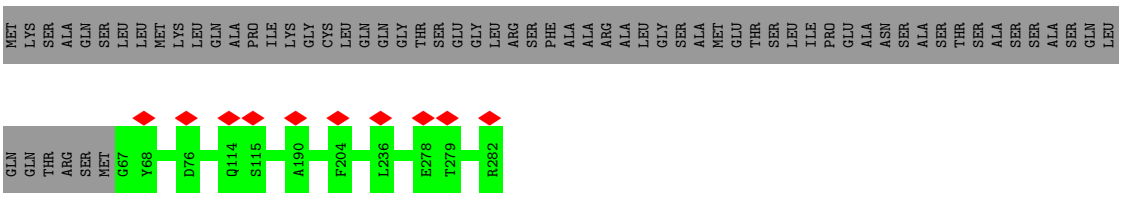
• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

Chain C:



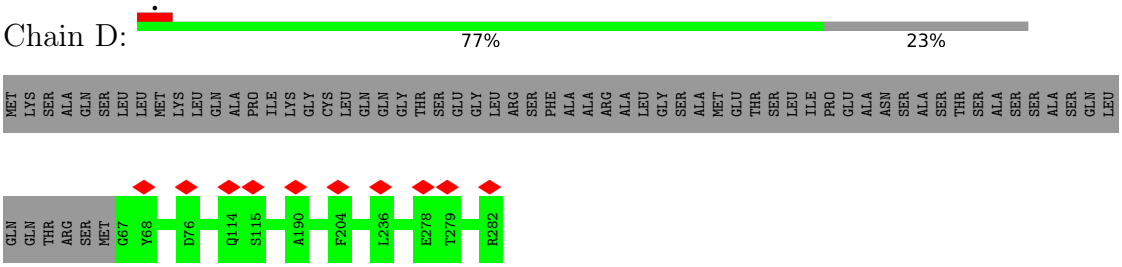
• Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

Chain 5D:



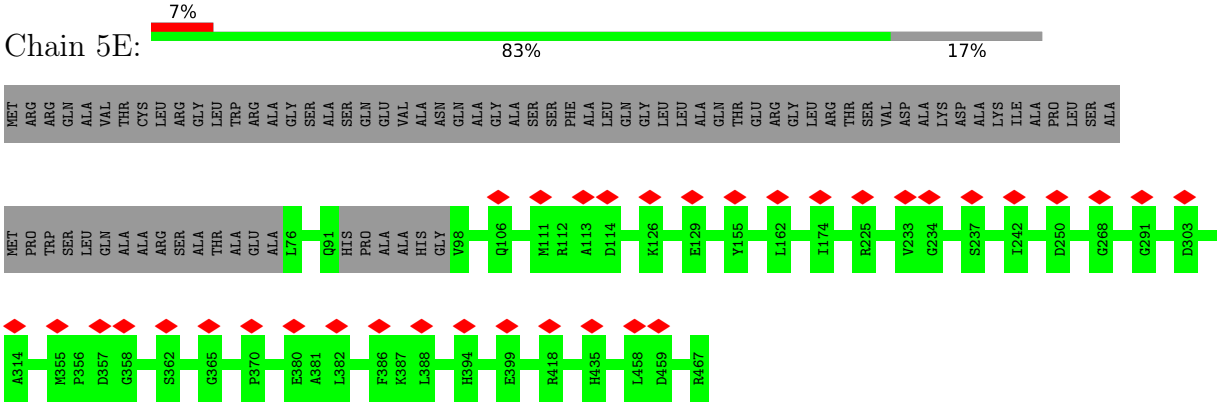
• Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

Chain D:



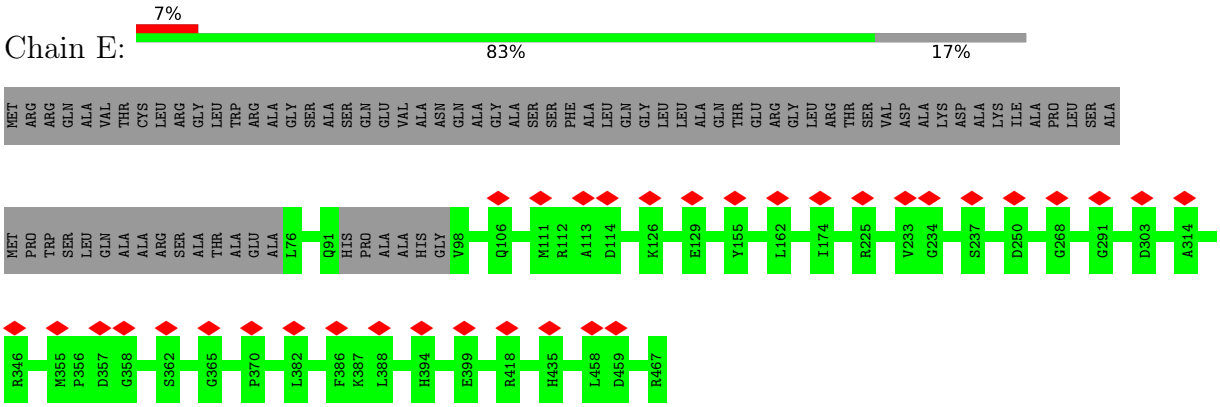
• Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit

Chain 5E:



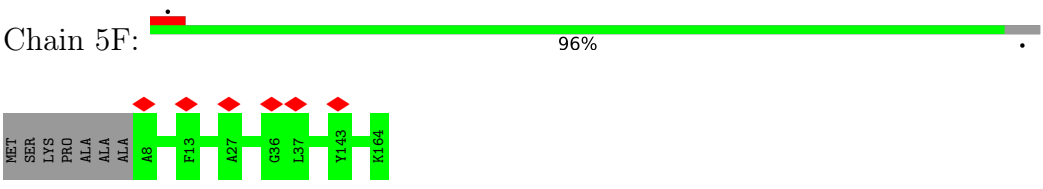
• Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit

Chain E:



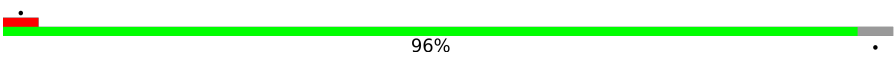
• Molecule 28: NADH:ubiquinone oxidoreductase subunit 10

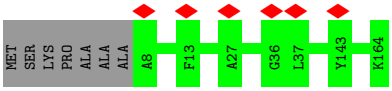
Chain 5F:



• Molecule 28: NADH:ubiquinone oxidoreductase subunit 10

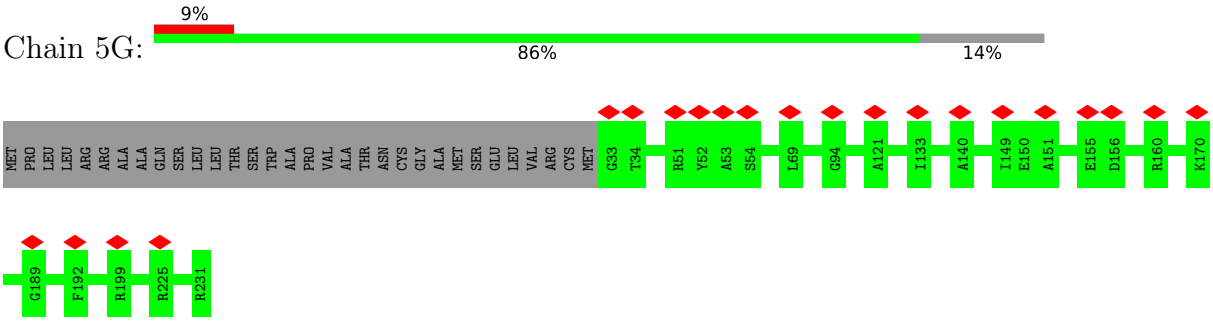
Chain F:





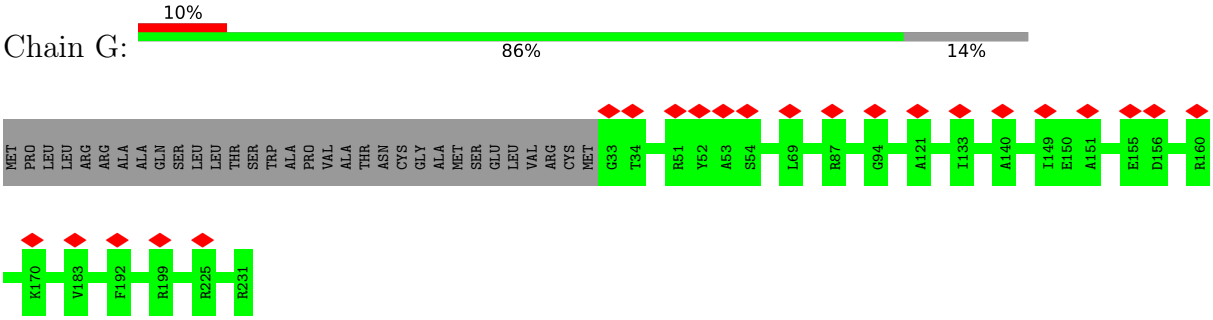
• Molecule 29: NADH:ubiquinone oxidoreductase subunit 8

Chain 5G:



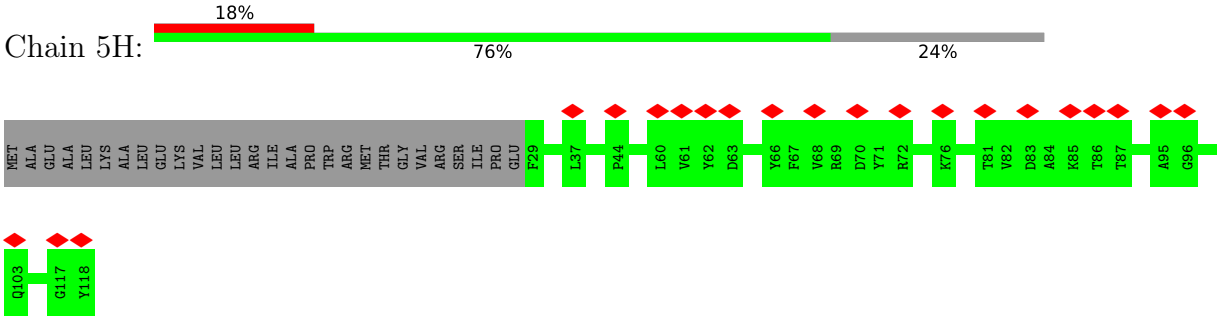
• Molecule 29: NADH:ubiquinone oxidoreductase subunit 8

Chain G:



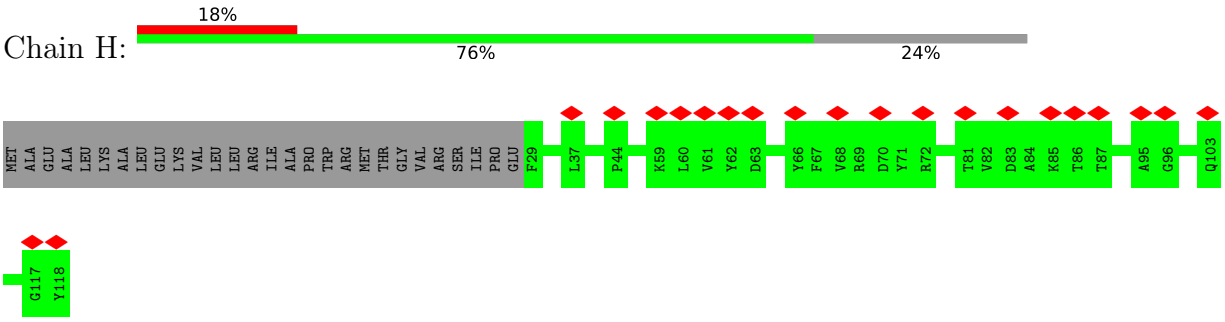
• Molecule 30: B14.5a

Chain 5H:



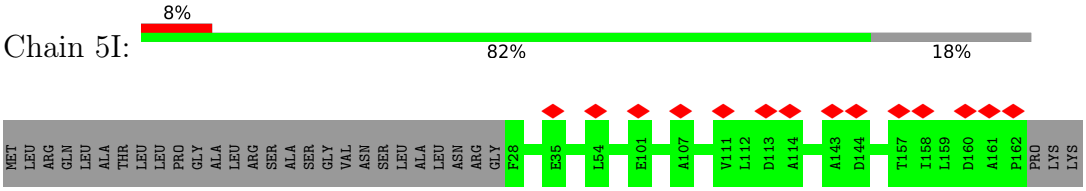
• Molecule 30: B14.5a

Chain H:



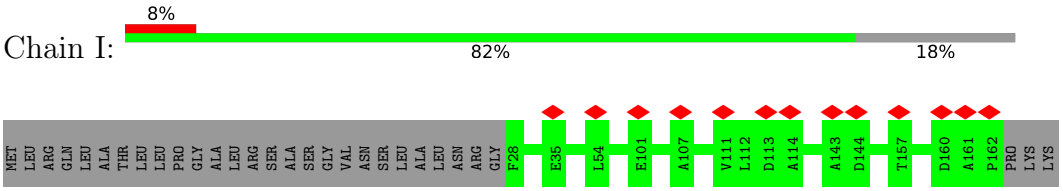
• Molecule 31: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit

Chain 5I:



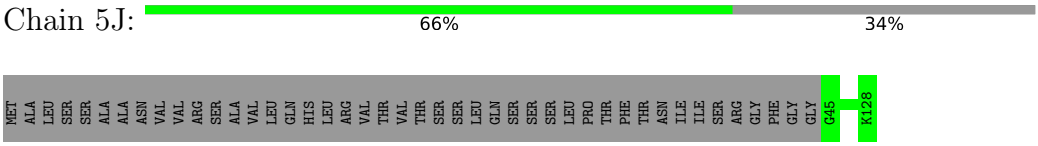
• Molecule 31: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit

Chain I:



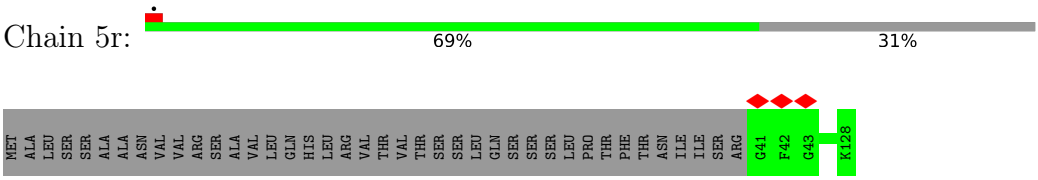
• Molecule 32: Acyl carrier protein

Chain 5J:



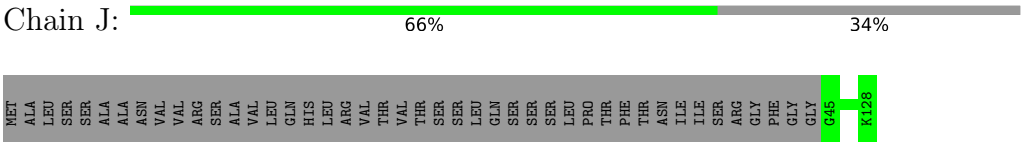
• Molecule 32: Acyl carrier protein

Chain 5r:



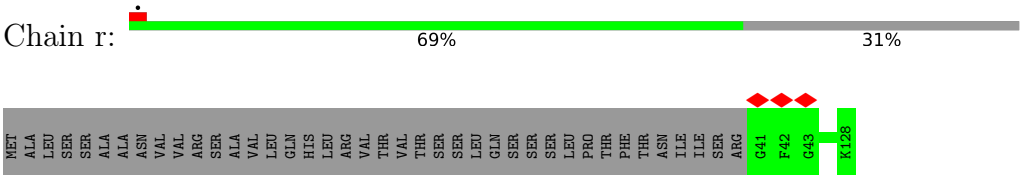
• Molecule 32: Acyl carrier protein

Chain J:



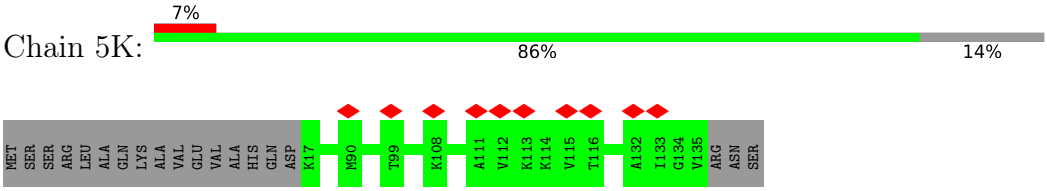
• Molecule 32: Acyl carrier protein

Chain r:



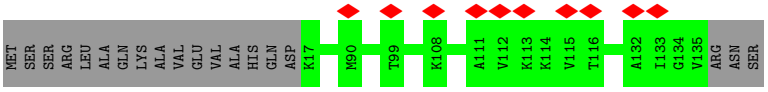
• Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

Chain 5K:



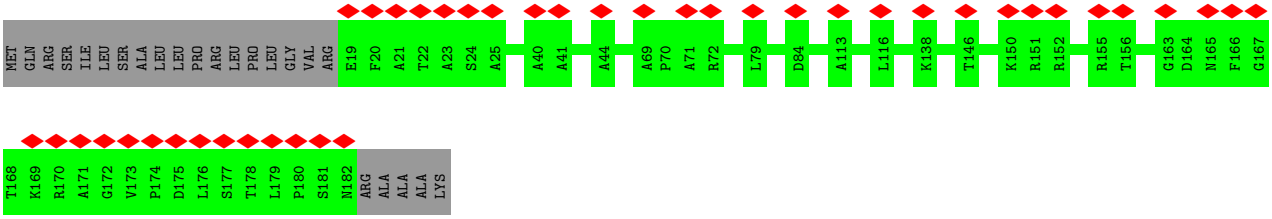
• Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

Chain K:



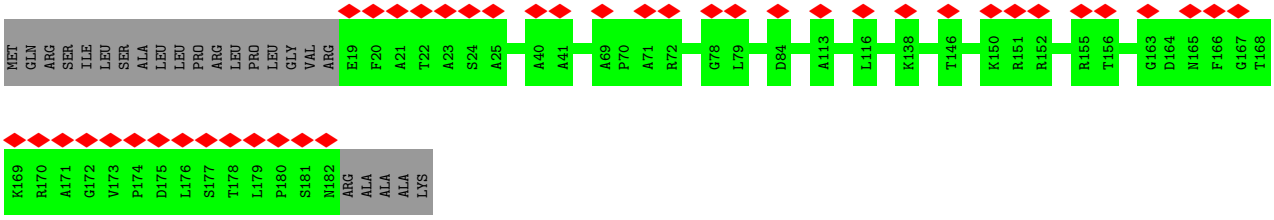
• Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 5L:



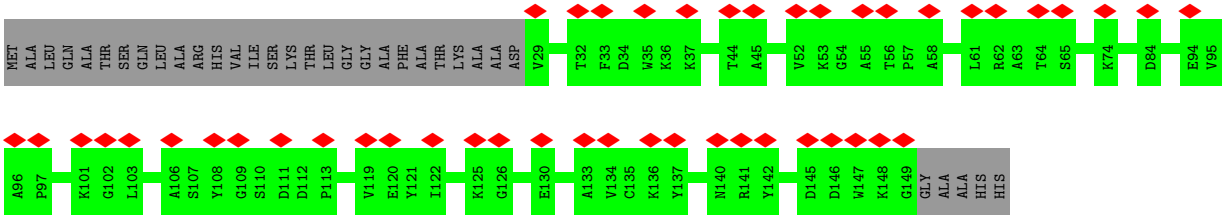
• Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



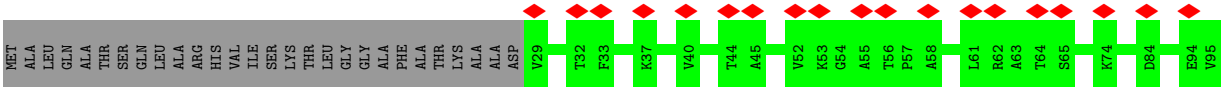
• Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit

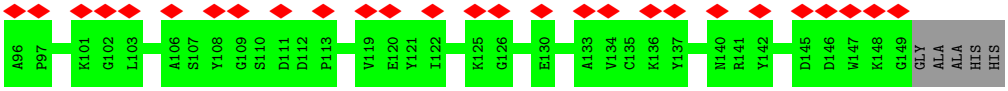
Chain 5M:



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

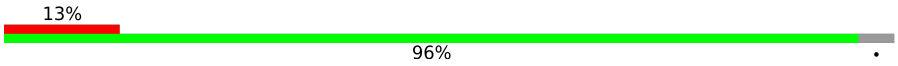
Chain M:

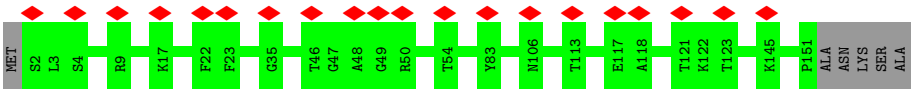




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

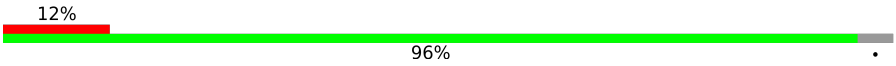
Chain 5N:

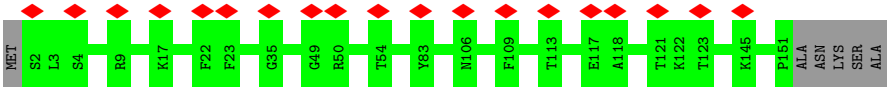




• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

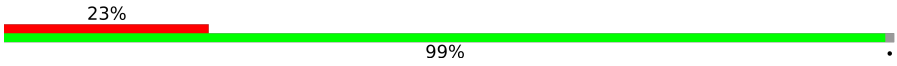
Chain N:

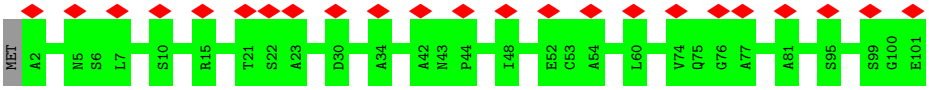




• Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit

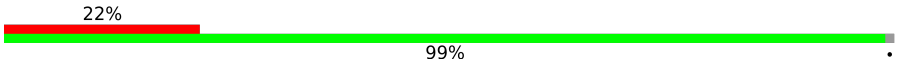
Chain 5O:

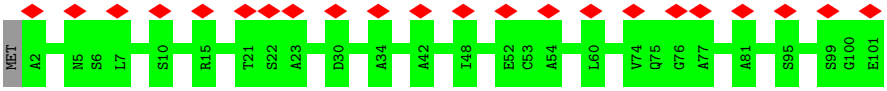




• Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit

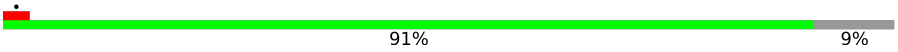
Chain O:

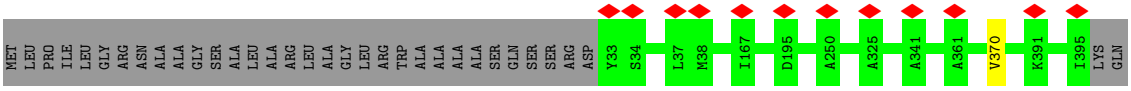




• Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

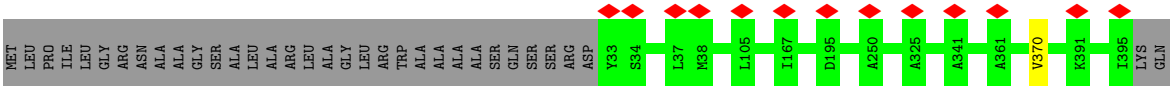
Chain 5P:





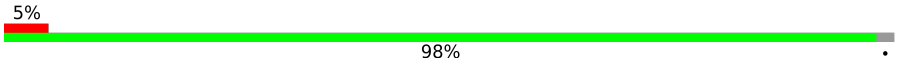
• Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

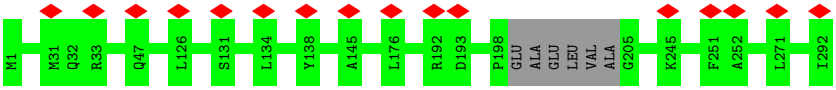
Chain P:



• Molecule 39: NADH-ubiquinone oxidoreductase chain 1

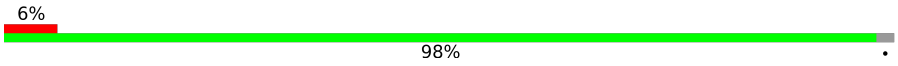
Chain 5Q:

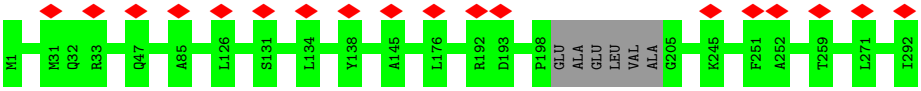




• Molecule 39: NADH-ubiquinone oxidoreductase chain 1

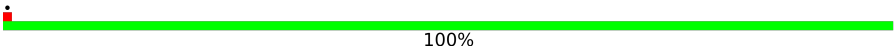
Chain Q:

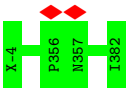




• Molecule 40: NADH-ubiquinone oxidoreductase chain 2

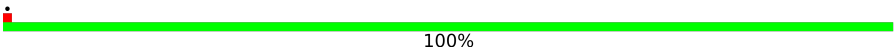
Chain 5R:





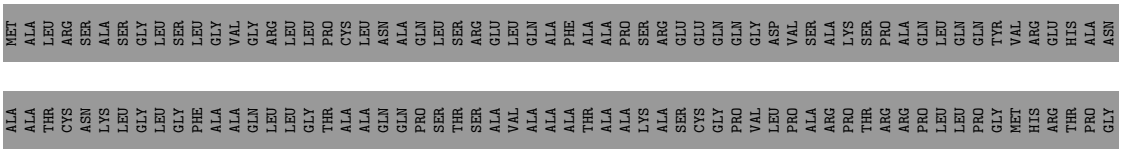
• Molecule 40: NADH-ubiquinone oxidoreductase chain 2

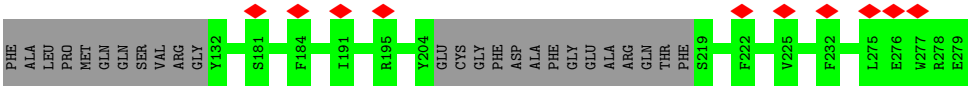
Chain R:



• Molecule 41: NADH-ubiquinone oxidoreductase chain 3

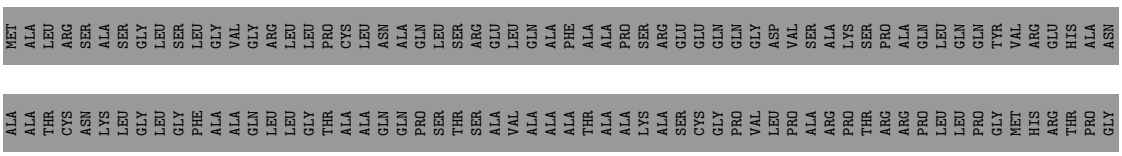
Chain 5S:

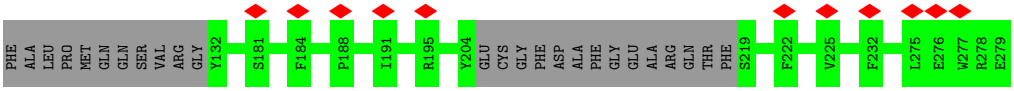




• Molecule 41: NADH-ubiquinone oxidoreductase chain 3

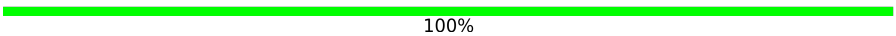
Chain S:





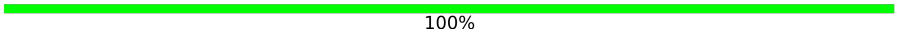
• Molecule 42: NADH-ubiquinone oxidoreductase chain 4

Chain 5T:



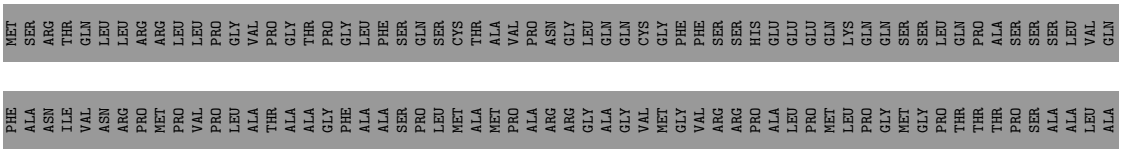
• Molecule 42: NADH-ubiquinone oxidoreductase chain 4

Chain T:



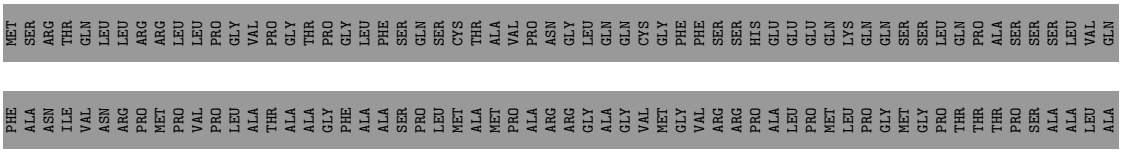
• Molecule 43: NADH dehydrogenase subunit 4L

Chain 5U:



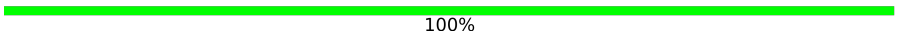
• Molecule 43: NADH dehydrogenase subunit 4L

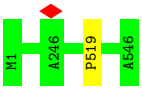
Chain U:



• Molecule 44: NADH-ubiquinone oxidoreductase chain 5

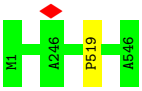
Chain 5V:





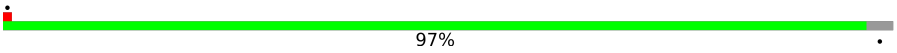
• Molecule 44: NADH-ubiquinone oxidoreductase chain 5

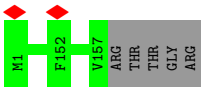
Chain V:



• Molecule 45: NADH-ubiquinone oxidoreductase chain 6

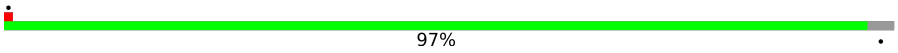
Chain 5W:

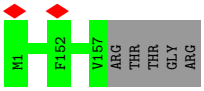




• Molecule 45: NADH-ubiquinone oxidoreductase chain 6

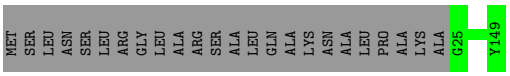
Chain W:





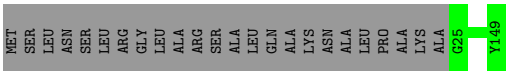
• Molecule 46: ASHI

Chain 5X:



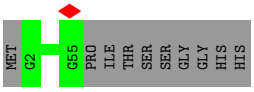
• Molecule 46: ASHI

Chain X:



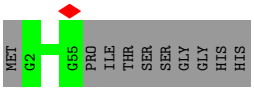
• Molecule 47: P9

Chain 5Y:



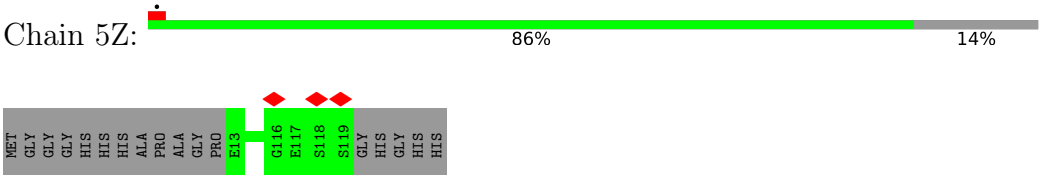
• Molecule 47: P9

Chain Y:



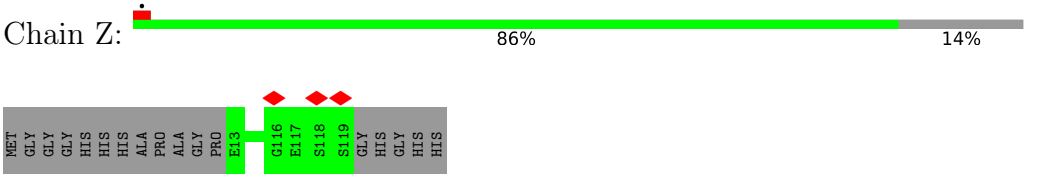
• Molecule 48: KFYI

Chain 5Z:



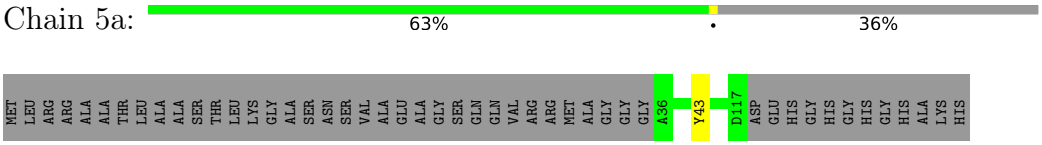
• Molecule 48: KFYI

Chain Z:



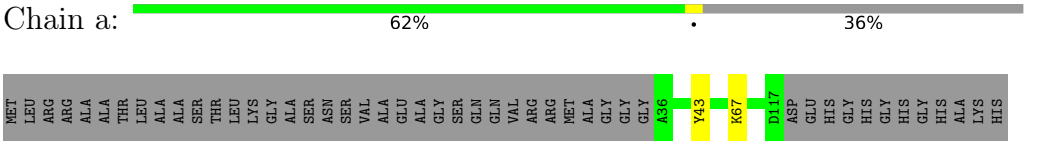
• Molecule 49: AGGG

Chain 5a:



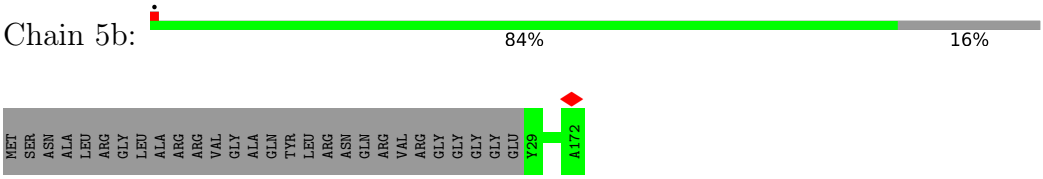
• Molecule 49: AGGG

Chain a:



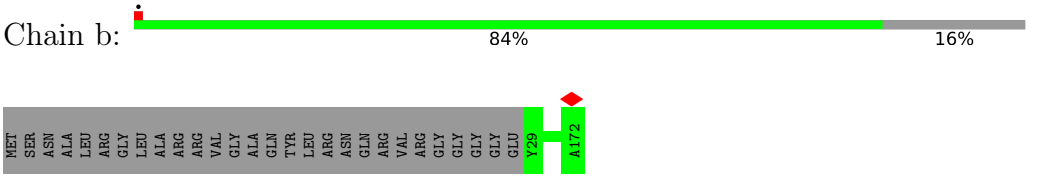
• Molecule 50: ESSS

Chain 5b:



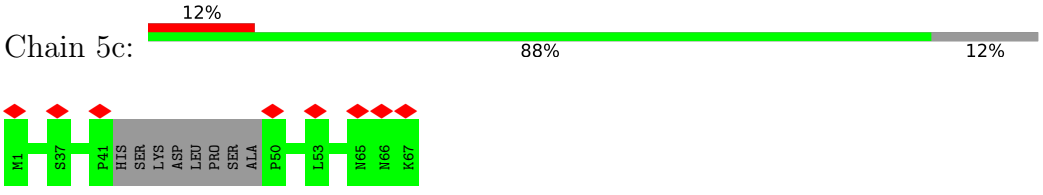
• Molecule 50: ESSS

Chain b:



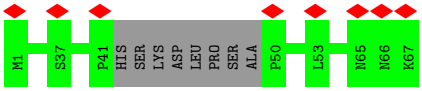
• Molecule 51: B9

Chain 5c:



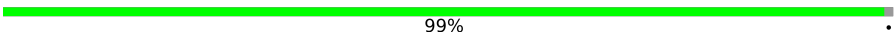
• Molecule 51: B9

Chain c:



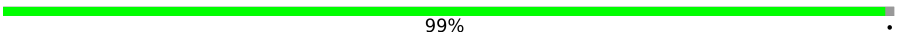
• Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit

Chain 5d:



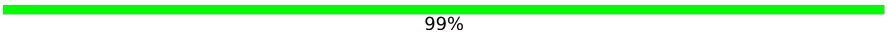
• Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit

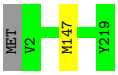
Chain d:



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

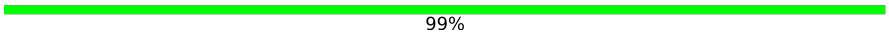
Chain 5e:





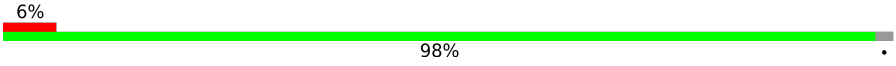
• Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit

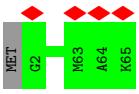
Chain e:



• Molecule 54: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit

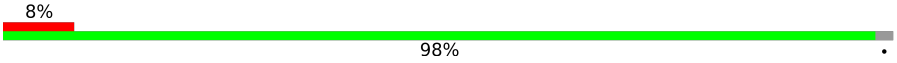
Chain 5f:

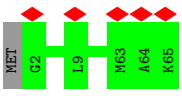




• Molecule 54: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit

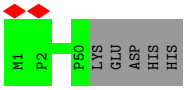
Chain f:





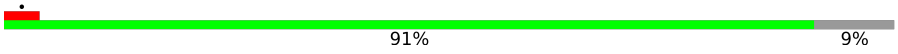
• Molecule 55: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit

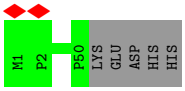
Chain 5g:



• Molecule 55: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit

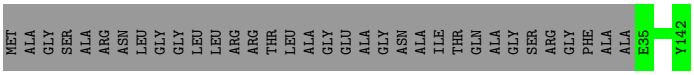
Chain g:





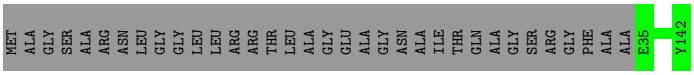
• Molecule 56: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

Chain 5h:



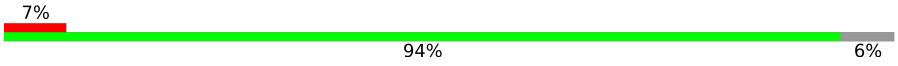
• Molecule 56: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

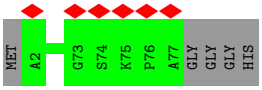
Chain h:



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

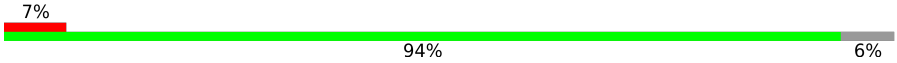
Chain 5i:

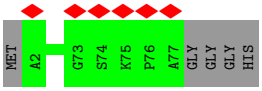




• Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like

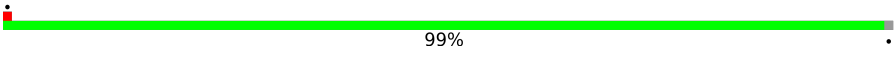
Chain i:





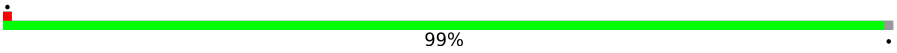
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 5j:



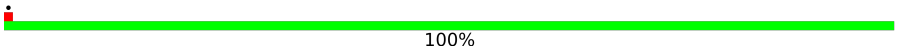
• Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain j:



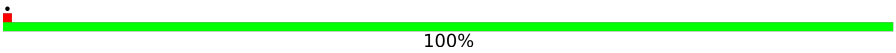
• Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 5k:



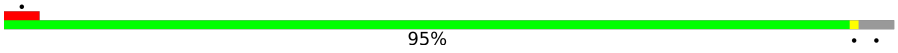
• Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

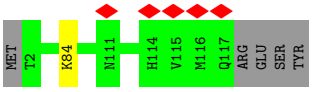
Chain k:



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

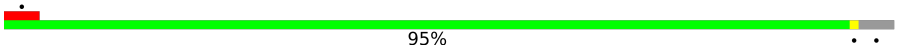
Chain 5l:

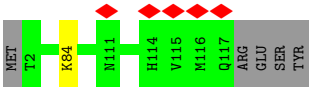




• Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

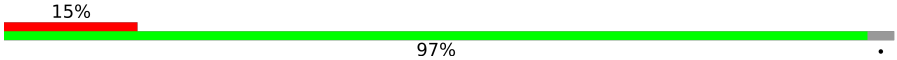
Chain l:

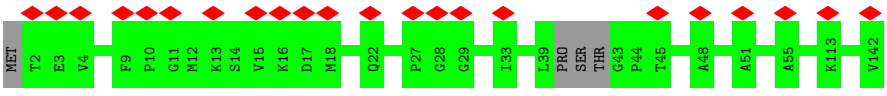




• Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

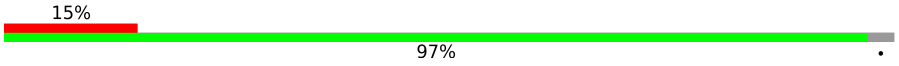
Chain 5m:

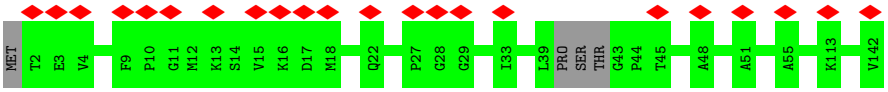




• Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

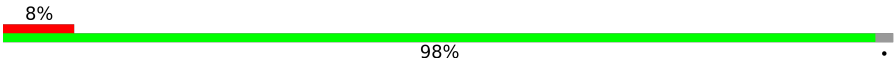
Chain m:

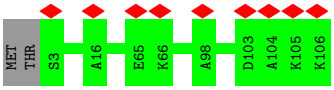




• Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

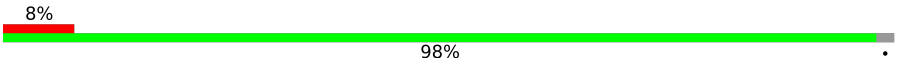
Chain 5n:

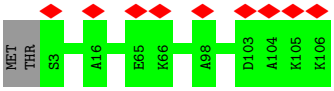




• Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

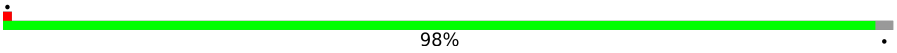
Chain n:

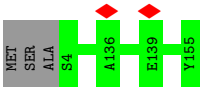




• Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit

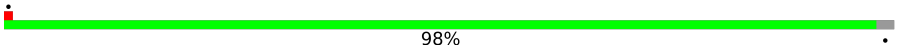
Chain 5o:

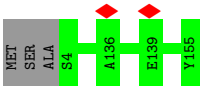




• Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit

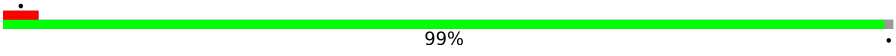
Chain o:

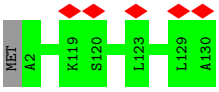




• Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

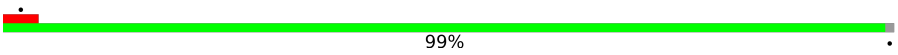
Chain 5p:

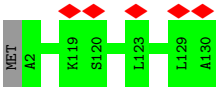




• Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

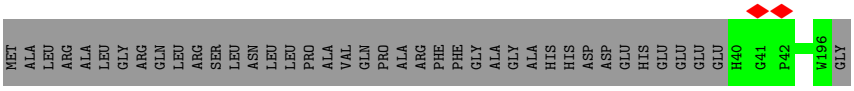
Chain p:





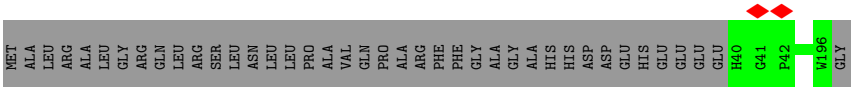
• Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

Chain 5q:



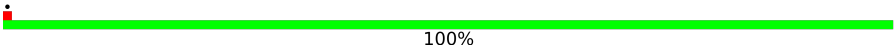
• Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

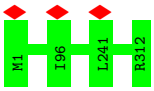
Chain q:



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

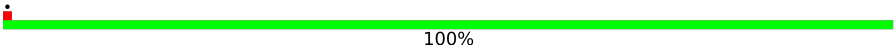
Chain 5s:

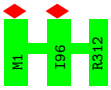




• Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

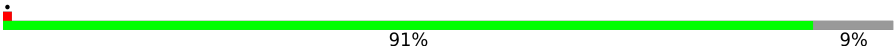
Chain s:

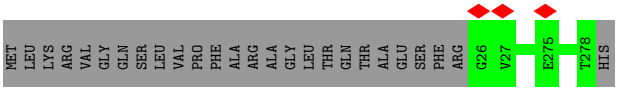




• Molecule 67: CAG2 - CA-like

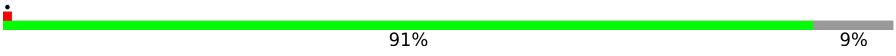
Chain 5t:

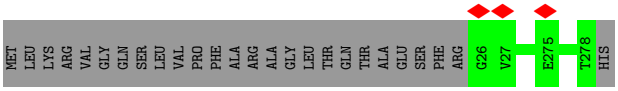




• Molecule 67: CAG2 - CA-like

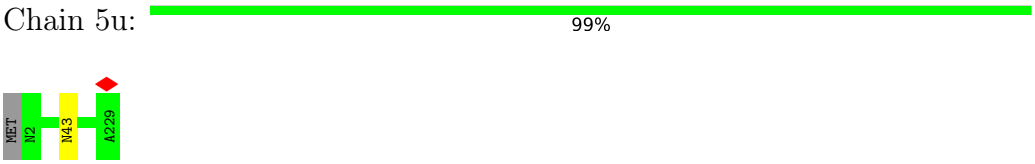
Chain t:





• Molecule 68: CAG1

Chain 5u:

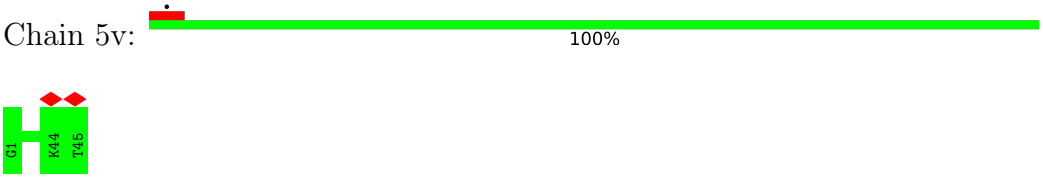


• Molecule 68: CAG1

Chain u:

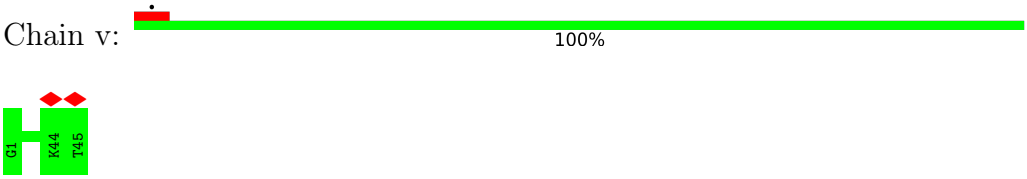
• Molecule 69: P10

Chain 5v:



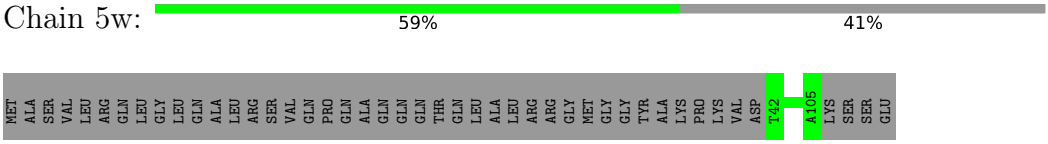
• Molecule 69: P10

Chain v:



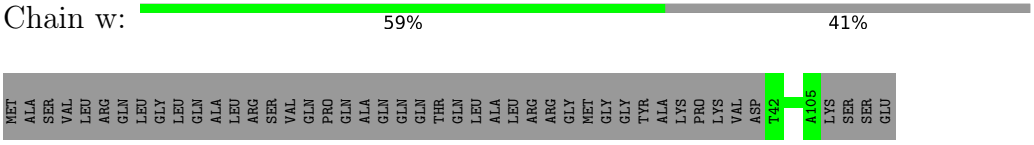
• Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit

Chain 5w:



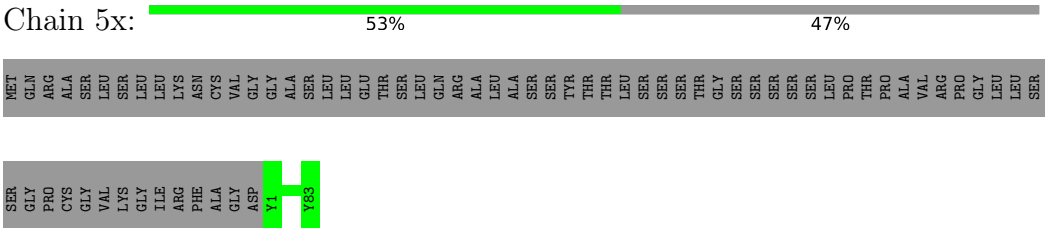
• Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit

Chain w:



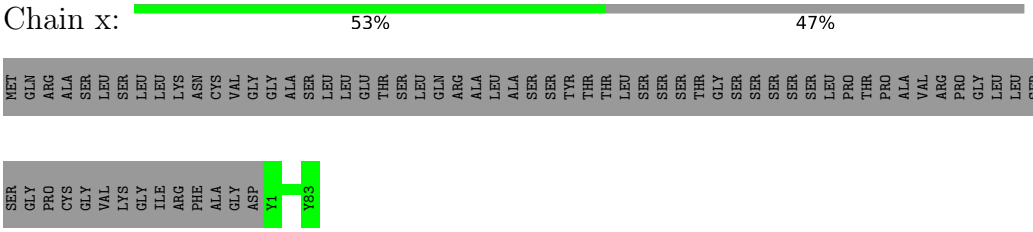
• Molecule 71: NUOP8

Chain 5x:



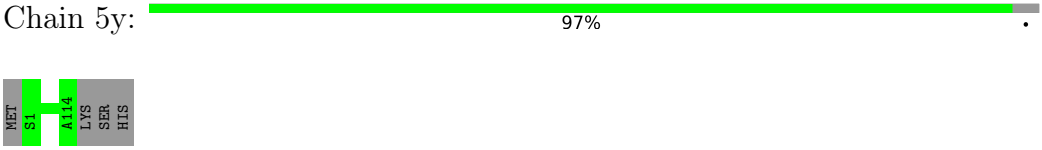
• Molecule 71: NUOP8

Chain x:



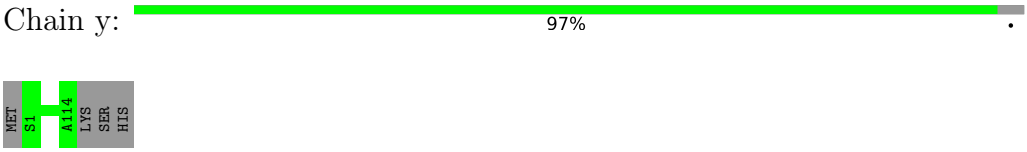
• Molecule 72: NUOP7

Chain 5y:



• Molecule 72: NUOP7

Chain y:



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

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	0.34	0/3060	0.52	1/4187 (0.0%)
1	1B	0.35	0/3060	0.53	0/4187
1	6A	0.34	0/3060	0.52	1/4187 (0.0%)
1	6B	0.35	0/3060	0.53	0/4187
2	1C	0.28	0/1643	0.50	0/2233
2	1D	0.28	0/1643	0.50	0/2233
2	6C	0.28	0/1643	0.50	0/2233
2	6D	0.28	0/1643	0.50	0/2233
3	1E	0.34	0/1953	0.53	1/2654 (0.0%)
3	1F	0.33	0/1953	0.52	0/2654
3	6E	0.34	0/1953	0.53	1/2654 (0.0%)
3	6F	0.33	0/1953	0.52	0/2654
4	1G	0.32	0/496	0.55	0/667
4	1H	0.32	0/496	0.50	0/667
4	6G	0.32	0/496	0.54	0/667
4	6H	0.32	0/496	0.50	0/667
5	1I	0.32	0/567	0.50	0/766
5	1J	0.30	0/567	0.45	0/766
5	6I	0.31	0/567	0.50	0/766
5	6J	0.30	0/567	0.45	0/766
6	1K	0.34	0/609	0.54	0/817
6	1L	0.31	0/609	0.54	0/817
6	6K	0.34	0/609	0.53	0/817
6	6L	0.31	0/609	0.55	0/817
7	1M	0.31	0/3723	0.54	0/5046
7	1N	0.31	0/3723	0.54	0/5046
7	6M	0.31	0/3723	0.54	0/5046
7	6N	0.31	0/3723	0.54	0/5046
8	1O	0.28	0/385	0.53	0/531
8	1P	0.30	0/385	0.59	0/531
8	6O	0.28	0/385	0.53	0/531
8	6P	0.30	0/385	0.59	0/531

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	1Q	0.33	0/3258	0.56	1/4439 (0.0%)
9	1S	0.30	0/3258	0.53	0/4439
9	6Q	0.33	0/3258	0.55	0/4439
9	6S	0.30	0/3258	0.53	0/4439
10	1R	0.32	0/996	0.57	0/1349
10	1T	0.34	0/996	0.58	0/1349
10	6R	0.32	0/996	0.57	0/1349
10	6T	0.34	0/996	0.58	0/1349
11	2A	0.33	0/4011	0.55	1/5484 (0.0%)
11	3A	0.34	0/4011	0.56	1/5484 (0.0%)
11	4A	0.34	0/4011	0.56	1/5484 (0.0%)
11	7A	0.34	0/4011	0.55	1/5484 (0.0%)
11	8A	0.34	0/4011	0.56	1/5484 (0.0%)
11	9A	0.34	0/4011	0.56	1/5484 (0.0%)
12	2B	0.31	0/1204	0.51	0/1641
12	3B	0.30	0/1204	0.52	0/1641
12	4B	0.30	0/1204	0.52	0/1641
12	7B	0.31	0/1204	0.51	0/1641
12	8B	0.30	0/1204	0.52	0/1641
12	9B	0.30	0/1204	0.52	0/1641
13	2C	0.30	0/1237	0.53	0/1676
13	3C	0.32	0/1237	0.54	0/1676
13	4C	0.32	0/1237	0.55	0/1676
13	7C	0.30	0/1237	0.53	0/1676
13	8C	0.32	0/1237	0.55	0/1676
13	9C	0.32	0/1237	0.54	0/1676
14	2D	0.32	0/2152	0.49	0/2937
14	3D	0.32	0/2152	0.50	0/2937
14	4D	0.32	0/2152	0.50	0/2937
14	7D	0.32	0/2152	0.49	0/2937
14	8D	0.32	0/2152	0.50	0/2937
14	9D	0.32	0/2152	0.51	0/2937
15	2E	0.31	0/757	0.63	0/1029
15	3E	0.32	0/757	0.60	0/1029
15	4E	0.32	0/757	0.60	0/1029
15	7E	0.31	0/757	0.63	0/1029
15	8E	0.32	0/757	0.60	0/1029
15	9E	0.32	0/757	0.60	0/1029
16	2F	0.30	0/726	0.46	0/974
16	3F	0.30	0/726	0.46	0/974
16	4F	0.30	0/726	0.46	0/974
16	7F	0.30	0/726	0.46	0/974
16	8F	0.30	0/726	0.46	0/974

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	9F	0.30	0/726	0.46	0/974
17	2G	0.31	0/762	0.58	1/1038 (0.1%)
17	3G	0.30	0/762	0.55	1/1038 (0.1%)
17	4G	0.30	0/762	0.55	1/1038 (0.1%)
17	7G	0.31	0/762	0.58	1/1038 (0.1%)
17	8G	0.30	0/762	0.55	1/1038 (0.1%)
17	9G	0.30	0/762	0.55	1/1038 (0.1%)
18	2H	0.30	0/980	0.51	0/1325
18	3H	0.32	0/980	0.55	0/1325
18	4H	0.32	0/980	0.55	0/1325
18	7H	0.30	0/980	0.51	0/1325
18	8H	0.32	0/980	0.55	0/1325
18	9H	0.33	0/980	0.55	0/1325
19	2I	0.34	0/619	0.51	0/839
19	3I	0.32	0/619	0.50	0/839
19	4I	0.32	0/619	0.50	0/839
19	7I	0.34	0/619	0.51	0/839
19	8I	0.32	0/619	0.50	0/839
19	9I	0.32	0/619	0.50	0/839
20	2J	0.30	0/839	0.51	0/1143
20	3J	0.31	0/839	0.53	0/1143
20	4J	0.31	0/812	0.53	0/1108
20	7J	0.31	0/839	0.51	0/1143
20	8J	0.31	0/839	0.53	0/1143
20	9J	0.31	0/812	0.53	0/1108
21	2K	0.31	0/392	0.50	0/531
21	3K	0.33	0/392	0.51	0/531
21	4K	0.33	0/392	0.51	0/531
21	7K	0.31	0/392	0.51	0/531
21	8K	0.33	0/392	0.51	0/531
21	9K	0.33	0/392	0.51	0/531
22	2L	0.31	0/621	0.56	0/841
22	3L	0.30	0/645	0.55	0/875
22	4L	0.30	0/645	0.55	0/875
22	7L	0.32	0/621	0.56	0/841
22	8L	0.30	0/645	0.56	0/875
22	9L	0.30	0/645	0.55	0/875
23	5A	0.25	0/1878	0.46	0/2549
23	A	0.25	0/1878	0.46	0/2549
24	5B	0.25	0/3400	0.48	0/4573
24	B	0.25	0/3400	0.48	0/4573
25	5C	0.25	0/5272	0.49	0/7143
25	C	0.25	0/5272	0.49	0/7143

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	5D	0.26	0/1843	0.50	0/2506
26	D	0.25	0/1843	0.50	0/2506
27	5E	0.25	0/3181	0.49	0/4303
27	E	0.25	0/3181	0.49	0/4303
28	5F	0.25	0/1258	0.47	0/1706
28	F	0.25	0/1258	0.47	0/1706
29	5G	0.25	0/1648	0.51	0/2222
29	G	0.25	0/1648	0.51	0/2222
30	5H	0.25	0/773	0.51	0/1046
30	H	0.25	0/773	0.51	0/1046
31	5I	0.24	0/1061	0.43	0/1441
31	I	0.24	0/1061	0.43	0/1441
32	5J	0.25	0/649	0.41	0/875
32	5r	0.26	0/673	0.40	0/906
32	J	0.26	0/649	0.41	0/875
32	r	0.26	0/673	0.40	0/906
33	5K	0.26	0/1007	0.47	0/1348
33	K	0.26	0/1007	0.47	0/1348
34	5L	0.26	0/1306	0.50	0/1769
34	L	0.26	0/1306	0.50	0/1769
35	5M	0.24	0/936	0.43	0/1276
35	M	0.24	0/936	0.43	0/1276
36	5N	0.25	0/1277	0.48	0/1735
36	N	0.25	0/1277	0.48	0/1735
37	5O	0.25	0/772	0.51	0/1037
37	O	0.25	0/772	0.51	0/1037
38	5P	0.25	0/2879	0.49	0/3905
38	P	0.25	0/2879	0.49	0/3905
39	5Q	0.27	0/2234	0.45	0/3034
39	Q	0.27	0/2234	0.45	0/3034
40	5R	0.26	0/3075	0.44	0/4191
40	R	0.26	0/3075	0.44	0/4191
41	5S	0.26	0/1106	0.45	0/1512
41	S	0.26	0/1106	0.45	0/1512
42	5T	0.27	0/3533	0.44	0/4825
42	T	0.27	0/3533	0.44	0/4825
43	5U	0.27	0/819	0.45	0/1112
43	U	0.27	0/819	0.45	0/1112
44	5V	0.26	0/4258	0.45	0/5792
44	V	0.26	0/4258	0.44	0/5792
45	5W	0.26	0/1239	0.44	0/1686
45	W	0.26	0/1239	0.43	0/1686
46	5X	0.26	0/1081	0.47	0/1479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
46	X	0.26	0/1081	0.47	0/1479
47	5Y	0.25	0/411	0.45	0/557
47	Y	0.25	0/411	0.45	0/557
48	5Z	0.25	0/894	0.45	0/1218
48	Z	0.25	0/894	0.46	0/1218
49	5a	0.35	0/698	0.47	0/949
49	a	0.36	0/698	0.49	0/949
50	5b	0.25	0/1201	0.46	0/1623
50	b	0.25	0/1201	0.45	0/1623
51	5c	0.25	0/463	0.41	0/623
51	c	0.25	0/463	0.41	0/623
52	5d	0.27	0/721	0.47	0/968
52	d	0.27	0/721	0.47	0/968
53	5e	0.27	0/1688	0.47	0/2301
53	e	0.27	0/1688	0.47	0/2301
54	5f	0.24	0/547	0.42	0/740
54	f	0.24	0/547	0.42	0/740
55	5g	0.33	0/433	0.51	0/587
55	g	0.26	0/433	0.44	0/587
56	5h	0.25	0/948	0.47	0/1285
56	h	0.25	0/948	0.46	0/1285
57	5i	0.23	0/644	0.52	0/860
57	i	0.23	0/644	0.53	0/860
58	5j	0.26	0/732	0.48	0/983
58	j	0.26	0/732	0.48	0/983
59	5k	0.25	0/1011	0.47	0/1361
59	k	0.25	0/1011	0.47	0/1361
60	5l	0.25	0/936	0.41	0/1278
60	l	0.25	0/936	0.41	0/1278
61	5m	0.25	0/1155	0.48	0/1558
61	m	0.25	0/1155	0.48	0/1558
62	5n	0.24	0/886	0.43	0/1188
62	n	0.24	0/886	0.43	0/1188
63	5o	0.25	0/1265	0.49	0/1705
63	o	0.25	0/1265	0.49	0/1705
64	5p	0.25	0/1095	0.50	0/1480
64	p	0.25	0/1095	0.50	0/1480
65	5q	0.26	0/1308	0.46	0/1779
65	q	0.26	0/1308	0.46	0/1779
66	5s	0.26	0/2353	0.47	0/3202
66	s	0.26	0/2353	0.47	0/3202
67	5t	0.25	0/2043	0.51	0/2778
67	t	0.25	0/2043	0.50	0/2778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
68	5u	0.26	0/1730	0.48	0/2341
68	u	0.25	0/1730	0.48	0/2341
69	5v	0.24	0/369	0.45	0/498
69	v	0.24	0/369	0.45	0/498
70	5w	0.27	0/521	0.42	0/702
70	w	0.27	0/521	0.42	0/702
71	5x	0.28	0/727	0.43	0/994
71	x	0.28	0/727	0.43	0/994
72	5y	0.27	0/963	0.46	0/1313
72	y	0.27	0/963	0.46	0/1313
All	All	0.29	0/298402	0.50	17/405254 (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.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2G	74	LEU	CA-CB-CG	6.56	130.38	115.30
17	7G	74	LEU	CA-CB-CG	6.53	130.31	115.30
17	8G	74	LEU	CA-CB-CG	6.45	130.13	115.30
17	9G	74	LEU	CA-CB-CG	6.45	130.13	115.30
17	4G	74	LEU	CA-CB-CG	6.45	130.12	115.30
17	3G	74	LEU	CA-CB-CG	6.44	130.12	115.30
11	3A	417	LEU	CA-CB-CG	6.25	129.69	115.30
11	8A	417	LEU	CA-CB-CG	6.25	129.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	9A	417	LEU	CA-CB-CG	6.25	129.67	115.30
11	4A	417	LEU	CA-CB-CG	6.25	129.67	115.30
9	1Q	59	ALA	N-CA-C	-5.92	95.01	111.00
11	2A	417	LEU	CA-CB-CG	5.63	128.26	115.30
11	7A	417	LEU	CA-CB-CG	5.63	128.24	115.30
3	6E	110	CYS	CA-CB-SG	5.16	123.28	114.00
3	1E	110	CYS	CA-CB-SG	5.14	123.25	114.00
1	1A	150	LEU	CA-CB-CG	5.07	126.95	115.30
1	6A	150	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (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
1	6A	184	TYR	Sidechain
1	6B	184	TYR	Sidechain
17	8G	114	TRP	Peptide
17	9G	114	TRP	Peptide
53	e	147	MET	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
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%)	44	78
7	6M	462/495 (93%)	454 (98%)	8 (2%)	0	100	100
7	6N	462/495 (93%)	456 (99%)	5 (1%)	1 (0%)	44	78
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1Q	439/485 (90%)	419 (95%)	19 (4%)	1 (0%)	44	78
9	1S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	25	64
9	6Q	439/485 (90%)	416 (95%)	22 (5%)	1 (0%)	44	78
9	6S	439/485 (90%)	424 (97%)	13 (3%)	2 (0%)	25	64
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	9D	264/382 (69%)	254 (96%)	10 (4%)	0	100	100
15	2E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	12	46
15	3E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	12	46
15	4E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	12	46
15	7E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	12	46
15	8E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	12	46
15	9E	88/175 (50%)	85 (97%)	2 (2%)	1 (1%)	12	46
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	37	72
38	P	361/397 (91%)	351 (97%)	9 (2%)	1 (0%)	37	72
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	5V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	44	78
44	V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	44	78
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%)	10	41
49	a	80/129 (62%)	78 (98%)	1 (1%)	1 (1%)	10	41
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	50	83

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	1Q	396	ASP

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Mol	Chain	Res	Type
15	2E	28	TRP
15	3E	28	TRP
15	4E	28	TRP
9	6Q	396	ASP
15	7E	28	TRP
15	8E	28	TRP
15	9E	28	TRP
49	5a	43	TYR
49	a	43	TYR
9	1S	66	THR
9	6S	66	THR
38	5P	370	VAL
38	P	370	VAL
7	1N	187	VAL
9	1S	475	PRO
7	6N	187	VAL
9	6S	475	PRO
44	5V	519	PRO
44	V	519	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	312/317 (98%)	311 (100%)	1 (0%)	91 92
1	1B	312/317 (98%)	309 (99%)	3 (1%)	73 82
1	6A	312/317 (98%)	311 (100%)	1 (0%)	91 92
1	6B	312/317 (98%)	309 (99%)	3 (1%)	73 82
2	1C	171/213 (80%)	170 (99%)	1 (1%)	84 88
2	1D	171/213 (80%)	171 (100%)	0	100 100
2	6C	171/213 (80%)	170 (99%)	1 (1%)	84 88
2	6D	171/213 (80%)	171 (100%)	0	100 100
3	1E	191/238 (80%)	191 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	388 (100%)	2 (0%)	86	89
7	6M	390/413 (94%)	390 (100%)	0	100	100
7	6N	390/413 (94%)	388 (100%)	2 (0%)	86	89
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%)	329 (99%)	4 (1%)	67	79
9	1S	333/362 (92%)	332 (100%)	1 (0%)	91	92
9	6Q	333/362 (92%)	328 (98%)	5 (2%)	60	75
9	6S	333/362 (92%)	332 (100%)	1 (0%)	91	92
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	74 (99%)	1 (1%)	65	77
17	4G	75/100 (75%)	74 (99%)	1 (1%)	65	77
17	7G	75/100 (75%)	75 (100%)	0	100	100
17	8G	75/100 (75%)	74 (99%)	1 (1%)	65	77
17	9G	75/100 (75%)	74 (99%)	1 (1%)	65	77
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	536 (100%)	1 (0%)	92	94
25	C	537/572 (94%)	536 (100%)	1 (0%)	92	94
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	68 (100%)	0	100	100
49	a	68/98 (69%)	67 (98%)	1 (2%)	60	75
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%)	93 (99%)	1 (1%)	70	80
60	l	94/99 (95%)	93 (99%)	1 (1%)	70	80
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	84	88
68	u	180/181 (99%)	179 (99%)	1 (1%)	84	88
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%)	30502 (100%)	36 (0%)	92	95

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	316	ARG
1	1B	79	ARG
1	1B	261	ASN
1	1B	316	ARG
2	1C	230	HIS
7	1N	171	ARG
7	1N	488	ARG
9	1Q	56	LYS
9	1Q	65	ARG
9	1Q	81	ARG
9	1Q	483	ARG

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Mol	Chain	Res	Type
9	1S	216	ARG
17	3G	109	ARG
17	4G	109	ARG
25	5C	593	ARG
60	5l	84	LYS
68	5u	43	ASN
1	6A	316	ARG
1	6B	79	ARG
1	6B	261	ASN
1	6B	316	ARG
2	6C	230	HIS
7	6N	171	ARG
7	6N	488	ARG
9	6Q	56	LYS
9	6Q	65	ARG
9	6Q	72	LYS
9	6Q	81	ARG
9	6Q	483	ARG
9	6S	216	ARG
17	8G	109	ARG
17	9G	109	ARG
25	C	593	ARG
49	a	67	LYS
60	l	84	LYS
68	u	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	1B	261	ASN
16	2F	63	GLN
16	3F	56	ASN
30	5H	75	ASN
33	5K	39	GLN
38	5P	93	HIS
39	5Q	267	GLN
44	5V	113	ASN
45	5W	140	ASN
48	5Z	41	HIS
49	5a	44	ASN
49	5a	53	GLN
53	5e	89	GLN

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Mol	Chain	Res	Type
53	5e	149	GLN
53	5e	186	HIS
63	5o	54	ASN
32	5r	62	HIS
66	5s	71	HIS
66	5s	296	GLN
71	5x	12	ASN
1	6B	261	ASN
16	7F	63	GLN
16	8F	56	ASN
30	H	75	ASN
33	K	39	GLN
38	P	93	HIS
39	Q	267	GLN
44	V	113	ASN
45	W	140	ASN
48	Z	41	HIS
49	a	44	ASN
49	a	53	GLN
49	a	70	HIS
53	e	89	GLN
53	e	149	GLN
53	e	186	HIS
63	o	54	ASN
32	r	62	HIS
66	s	71	HIS
66	s	296	GLN
71	x	12	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	$\#\|Z\| > 2$
80	FES	5C	801	25	0,4,4	-	-	-		
82	SF4	G	301	29	0,12,12	-	-	-		
76	HEA	2A	602	11	57,67,67	2.06	17 (29%)	61,103,103	2.43	25 (40%)
82	SF4	F	201	28	0,12,12	-	-	-		
79	CUA	7C	301	-	0,1,1	-	-	-		
84	NDP	P	401	-	45,52,52	2.25	4 (8%)	53,80,80	1.73	11 (20%)
76	HEA	3A	604	11	57,67,67	2.07	15 (26%)	61,103,103	2.47	23 (37%)
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	9A	602	11	57,67,67	2.04	15 (26%)	61,103,103	2.41	25 (40%)
81	FMN	5B	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.16	7 (14%)
74	HEC	6F	501	3	32,50,50	2.09	3 (9%)	24,82,82	1.85	6 (25%)
83	8Q1	5J	200	-	31,34,34	1.72	5 (16%)	40,43,43	1.54	5 (12%)
76	HEA	4A	604	11	57,67,67	2.04	17 (29%)	61,103,103	2.41	25 (40%)
83	8Q1	k	200	-	31,34,34	1.74	5 (16%)	40,43,43	1.68	7 (17%)
82	SF4	C	801	25	0,12,12	-	-	-		
82	SF4	5G	301	29	0,12,12	-	-	-		
73	HEM	1B	401	1	41,50,50	1.54	4 (9%)	45,82,82	1.50	7 (15%)
79	CUA	2C	301	-	0,1,1	-	-	-		
76	HEA	8A	604	11	57,67,67	2.05	15 (26%)	61,103,103	2.42	25 (40%)
84	NDP	5P	401	-	45,52,52	2.26	5 (11%)	53,80,80	1.73	11 (20%)
85	COO	s	401	-	45,55,55	0.82	1 (2%)	55,81,81	4.26	10 (18%)
82	SF4	5B	502	24	0,12,12	-	-	-		
82	SF4	5C	802	25	0,12,12	-	-	-		
76	HEA	7A	602	11	57,67,67	2.08	16 (28%)	61,103,103	2.42	22 (36%)
73	HEM	6B	402	1	41,50,50	1.45	3 (7%)	45,82,82	1.38	8 (17%)
82	SF4	C	802	25	0,12,12	-	-	-		
73	HEM	1A	401	1	41,50,50	1.42	4 (9%)	45,82,82	1.76	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
74	HEC	1F	501	3	32,50,50	2.09	3 (9%)	24,82,82	1.86	6 (25%)
73	HEM	6B	401	1	41,50,50	1.54	4 (9%)	45,82,82	1.50	8 (17%)
79	CUA	3C	301	-	0,1,1	-	-	-		
79	CUA	4C	301	-	0,1,1	-	-	-		
82	SF4	G	302	29	0,12,12	-	-	-		
83	8Q1	J	200	-	31,34,34	1.72	6 (19%)	40,43,43	1.55	5 (12%)
73	HEM	6A	401	1	41,50,50	1.40	3 (7%)	45,82,82	1.52	7 (15%)
74	HEC	6E	401	3	32,50,50	2.18	3 (9%)	24,82,82	1.80	5 (20%)
73	HEM	1A	402	1	41,50,50	1.40	3 (7%)	45,82,82	1.52	7 (15%)
76	HEA	7A	601	11	57,67,67	2.06	17 (29%)	61,103,103	2.43	24 (39%)
73	HEM	1B	402	1	41,50,50	1.44	3 (7%)	45,82,82	1.39	9 (20%)
83	8Q1	5k	200	-	31,34,34	1.75	6 (19%)	40,43,43	1.68	7 (17%)
79	CUA	8C	301	-	0,1,1	-	-	-		
76	HEA	3A	601	11	57,67,67	2.05	16 (28%)	61,103,103	2.42	25 (40%)
76	HEA	2A	601	11	57,67,67	2.09	16 (28%)	61,103,103	2.42	22 (36%)
80	FES	C	803	25	0,4,4	-	-	-		
76	HEA	4A	602	11	57,67,67	2.06	15 (26%)	61,103,103	2.45	23 (37%)
80	FES	5A	301	23	0,4,4	-	-	-		
73	HEM	6A	402	1	41,50,50	1.43	4 (9%)	45,82,82	1.76	11 (24%)
82	SF4	5C	803	25	0,12,12	-	-	-		
82	SF4	5F	201	28	0,12,12	-	-	-		
74	HEC	1E	401	3	32,50,50	2.18	3 (9%)	24,82,82	1.80	5 (20%)
80	FES	A	301	23	0,4,4	-	-	-		
76	HEA	9A	603	11	57,67,67	2.06	15 (26%)	61,103,103	2.46	23 (37%)
85	COO	5s	401	-	45,55,55	0.82	1 (2%)	55,81,81	4.25	10 (18%)
79	CUA	9C	301	-	0,1,1	-	-	-		
76	HEA	8A	601	11	57,67,67	2.07	15 (26%)	61,103,103	2.46	23 (37%)
82	SF4	B	501	24	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	FES	5C	801	25	-	-	0/1/1/1
82	SF4	G	301	29	-	-	0/6/5/5
76	HEA	2A	602	11	-	7/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	SF4	F	201	28	-	-	0/6/5/5
84	NDP	P	401	-	-	8/30/77/77	0/5/5/5
76	HEA	3A	604	11	-	4/32/76/76	-
81	FMN	B	502	-	-	5/18/18/18	0/3/3/3
82	SF4	5G	302	29	-	-	0/6/5/5
76	HEA	9A	602	11	-	7/32/76/76	-
81	FMN	5B	501	-	-	5/18/18/18	0/3/3/3
74	HEC	6F	501	3	-	0/10/54/54	-
83	8Q1	5J	200	-	-	7/41/41/41	-
76	HEA	4A	604	11	-	7/32/76/76	-
83	8Q1	k	200	-	-	21/41/41/41	-
82	SF4	C	801	25	-	-	0/6/5/5
82	SF4	5G	301	29	-	-	0/6/5/5
73	HEM	1B	401	1	-	3/12/54/54	-
76	HEA	8A	604	11	-	7/32/76/76	-
84	NDP	5P	401	-	-	8/30/77/77	0/5/5/5
85	COO	s	401	-	-	22/50/70/70	0/3/3/3
82	SF4	5B	502	24	-	-	0/6/5/5
82	SF4	5C	802	25	-	-	0/6/5/5
76	HEA	7A	602	11	-	5/32/76/76	-
73	HEM	6B	402	1	-	4/12/54/54	-
82	SF4	C	802	25	-	-	0/6/5/5
73	HEM	1A	401	1	-	3/12/54/54	-
74	HEC	1F	501	3	-	0/10/54/54	-
73	HEM	6B	401	1	-	3/12/54/54	-
83	8Q1	J	200	-	-	7/41/41/41	-
82	SF4	G	302	29	-	-	0/6/5/5
73	HEM	6A	401	1	-	4/12/54/54	-
74	HEC	6E	401	3	-	0/10/54/54	-
73	HEM	1A	402	1	-	4/12/54/54	-
76	HEA	7A	601	11	-	7/32/76/76	-
73	HEM	1B	402	1	-	4/12/54/54	-
83	8Q1	5k	200	-	-	21/41/41/41	-
76	HEA	3A	601	11	-	7/32/76/76	-
76	HEA	2A	601	11	-	5/32/76/76	-
80	FES	C	803	25	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	HEA	4A	602	11	-	4/32/76/76	-
80	FES	5A	301	23	-	-	0/1/1/1
73	HEM	6A	402	1	-	3/12/54/54	-
82	SF4	5C	803	25	-	-	0/6/5/5
82	SF4	5F	201	28	-	-	0/6/5/5
74	HEC	1E	401	3	-	0/10/54/54	-
80	FES	A	301	23	-	-	0/1/1/1
76	HEA	9A	603	11	-	4/32/76/76	-
85	COO	5s	401	-	-	22/50/70/70	0/3/3/3
76	HEA	8A	601	11	-	4/32/76/76	-
82	SF4	B	501	24	-	-	0/6/5/5

All (266) 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
84	5P	401	NDP	P2B-O2B	12.47	1.82	1.59
74	1E	401	HEC	C3C-C2C	-6.89	1.33	1.40
74	6E	401	HEC	C3C-C2C	-6.81	1.33	1.40
74	6F	501	HEC	C3C-C2C	-6.36	1.34	1.40
74	1F	501	HEC	C3C-C2C	-6.34	1.34	1.40
74	6E	401	HEC	C2B-C3B	-6.08	1.34	1.40
74	1E	401	HEC	C2B-C3B	-5.98	1.34	1.40
74	6F	501	HEC	C2B-C3B	-5.86	1.34	1.40
83	5k	200	8Q1	C34-N36	5.85	1.46	1.33
83	k	200	8Q1	C34-N36	5.81	1.46	1.33
74	1F	501	HEC	C2B-C3B	-5.81	1.34	1.40
76	7A	602	HEA	C3B-C2B	5.67	1.47	1.34
76	2A	601	HEA	C3B-C2B	5.67	1.47	1.34
83	J	200	8Q1	C34-N36	5.61	1.45	1.33
83	5J	200	8Q1	C34-N36	5.60	1.45	1.33
76	3A	604	HEA	C3B-C2B	5.49	1.47	1.34
76	9A	603	HEA	C3B-C2B	5.46	1.47	1.34
76	8A	601	HEA	C3B-C2B	5.45	1.47	1.34
76	4A	602	HEA	C3B-C2B	5.41	1.46	1.34
76	2A	602	HEA	C3A-C2A	5.39	1.47	1.40
76	7A	601	HEA	C3A-C2A	5.36	1.47	1.40
83	5k	200	8Q1	C39-N41	5.33	1.45	1.33
76	3A	601	HEA	C3B-C2B	5.33	1.46	1.34
83	k	200	8Q1	C39-N41	5.32	1.45	1.33
83	5J	200	8Q1	C39-N41	5.32	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	8A	604	HEA	C3B-C2B	5.32	1.46	1.34
76	9A	602	HEA	C3B-C2B	5.31	1.46	1.34
74	1E	401	HEC	C3D-C2D	5.31	1.53	1.37
74	6E	401	HEC	C3D-C2D	5.31	1.53	1.37
83	J	200	8Q1	C39-N41	5.30	1.45	1.33
76	4A	604	HEA	C3B-C2B	5.29	1.46	1.34
73	6B	401	HEM	C3C-C2C	-5.28	1.33	1.40
74	1F	501	HEC	C3D-C2D	5.25	1.53	1.37
74	6F	501	HEC	C3D-C2D	5.22	1.53	1.37
73	1B	401	HEM	C3C-C2C	-5.19	1.33	1.40
76	3A	604	HEA	C3C-C2C	5.17	1.47	1.40
76	7A	601	HEA	C3B-C2B	5.16	1.46	1.34
76	9A	603	HEA	C3C-C2C	5.14	1.47	1.40
76	2A	602	HEA	C3B-C2B	5.12	1.46	1.34
76	4A	602	HEA	C3C-C2C	5.11	1.47	1.40
76	8A	601	HEA	C3C-C2C	5.10	1.47	1.40
76	3A	601	HEA	C3C-C2C	4.99	1.47	1.40
76	2A	601	HEA	CHC-C4B	4.96	1.47	1.35
76	7A	602	HEA	CHC-C4B	4.96	1.47	1.35
76	8A	604	HEA	C3C-C2C	4.96	1.47	1.40
76	2A	601	HEA	C3D-C2D	4.94	1.47	1.36
76	9A	602	HEA	C3C-C2C	4.94	1.47	1.40
76	7A	602	HEA	C3D-C2D	4.94	1.47	1.36
76	8A	601	HEA	CHC-C4B	4.93	1.47	1.35
76	8A	604	HEA	C3A-C2A	4.92	1.47	1.40
76	7A	601	HEA	C3D-C2D	4.91	1.47	1.36
76	3A	604	HEA	CHC-C4B	4.91	1.47	1.35
76	9A	603	HEA	CHC-C4B	4.91	1.47	1.35
76	8A	604	HEA	CHC-C4B	4.90	1.47	1.35
76	4A	604	HEA	CHC-C4B	4.89	1.47	1.35
76	3A	601	HEA	CHC-C4B	4.89	1.47	1.35
76	4A	602	HEA	CHC-C4B	4.89	1.47	1.35
76	9A	602	HEA	CHC-C4B	4.88	1.47	1.35
76	2A	602	HEA	C3D-C2D	4.86	1.47	1.36
76	2A	602	HEA	CHD-C1D	4.83	1.47	1.35
76	7A	601	HEA	CHD-C1D	4.83	1.47	1.35
76	3A	601	HEA	C3A-C2A	4.83	1.47	1.40
76	8A	601	HEA	C3A-C2A	4.81	1.47	1.40
76	4A	604	HEA	C3C-C2C	4.81	1.47	1.40
76	8A	604	HEA	C3D-C2D	4.80	1.46	1.36
76	3A	604	HEA	C3A-C2A	4.80	1.47	1.40
76	2A	601	HEA	C3A-C2A	4.80	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	2A	601	HEA	C3C-C2C	4.79	1.47	1.40
76	9A	602	HEA	C3A-C2A	4.79	1.47	1.40
76	7A	602	HEA	C3A-C2A	4.78	1.47	1.40
76	9A	602	HEA	C3D-C2D	4.77	1.46	1.36
76	3A	601	HEA	C3D-C2D	4.77	1.46	1.36
76	4A	604	HEA	C3D-C2D	4.76	1.46	1.36
76	4A	602	HEA	C3A-C2A	4.75	1.47	1.40
76	4A	604	HEA	C3A-C2A	4.75	1.47	1.40
76	9A	603	HEA	C3A-C2A	4.74	1.46	1.40
76	7A	601	HEA	C3C-C2C	4.74	1.46	1.40
76	4A	604	HEA	CHD-C1D	4.74	1.47	1.35
76	9A	603	HEA	C3D-C2D	4.73	1.46	1.36
76	2A	601	HEA	CHD-C1D	4.73	1.47	1.35
76	7A	602	HEA	C3C-C2C	4.72	1.46	1.40
76	3A	601	HEA	CHD-C1D	4.72	1.47	1.35
76	8A	604	HEA	CHD-C1D	4.72	1.47	1.35
76	7A	602	HEA	CHD-C1D	4.72	1.47	1.35
76	3A	604	HEA	C3D-C2D	4.70	1.46	1.36
76	7A	601	HEA	CHC-C4B	4.69	1.47	1.35
76	9A	602	HEA	CHD-C1D	4.69	1.47	1.35
76	2A	602	HEA	CHC-C4B	4.68	1.47	1.35
76	8A	601	HEA	CHD-C1D	4.68	1.47	1.35
76	4A	602	HEA	C3D-C2D	4.67	1.46	1.36
76	2A	602	HEA	C3C-C2C	4.67	1.46	1.40
76	8A	601	HEA	C3D-C2D	4.66	1.46	1.36
76	9A	603	HEA	CHD-C1D	4.65	1.46	1.35
76	3A	604	HEA	CHD-C1D	4.63	1.46	1.35
76	4A	602	HEA	CHD-C1D	4.63	1.46	1.35
84	5P	401	NDP	PN-O5D	4.07	1.75	1.59
84	P	401	NDP	PN-O5D	4.06	1.75	1.59
81	5B	501	FMN	C4A-N5	3.86	1.38	1.30
81	B	502	FMN	C4A-N5	3.86	1.38	1.30
73	1B	402	HEM	C3C-CAC	3.76	1.55	1.47
73	6B	402	HEM	C3C-CAC	3.74	1.55	1.47
73	1A	401	HEM	C3C-C2C	-3.71	1.35	1.40
73	6B	401	HEM	C3C-CAC	3.71	1.55	1.47
73	6A	401	HEM	C3C-CAC	3.70	1.55	1.47
73	1B	401	HEM	C3C-CAC	3.70	1.55	1.47
73	6A	402	HEM	C3C-CAC	3.69	1.55	1.47
73	6B	402	HEM	C3C-C2C	-3.69	1.35	1.40
73	1A	402	HEM	C3C-CAC	3.68	1.55	1.47
73	1A	401	HEM	C3C-CAC	3.67	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	6A	402	HEM	C3C-C2C	-3.66	1.35	1.40
73	1B	402	HEM	C3C-C2C	-3.63	1.35	1.40
73	1A	402	HEM	C3C-C2C	-3.57	1.35	1.40
73	6A	401	HEM	C3C-C2C	-3.54	1.35	1.40
73	1B	401	HEM	CAB-C3B	3.27	1.56	1.47
73	6B	401	HEM	CAB-C3B	3.23	1.56	1.47
76	7A	602	HEA	C4B-C3B	3.12	1.49	1.44
76	2A	602	HEA	FE-NB	3.10	2.12	1.96
76	7A	602	HEA	FE-ND	3.10	2.12	1.96
76	7A	601	HEA	FE-NB	3.10	2.12	1.96
73	6B	402	HEM	CAB-C3B	3.09	1.55	1.47
76	8A	601	HEA	C1D-ND	-3.09	1.35	1.40
76	2A	601	HEA	FE-ND	3.08	2.12	1.96
76	7A	602	HEA	C1D-ND	-3.07	1.35	1.40
76	2A	601	HEA	C1D-ND	-3.07	1.35	1.40
73	6A	402	HEM	CAB-C3B	3.06	1.55	1.47
76	4A	602	HEA	FE-ND	3.06	2.12	1.96
84	5P	401	NDP	O2B-C2B	-3.06	1.33	1.44
73	1B	402	HEM	CAB-C3B	3.06	1.55	1.47
76	2A	601	HEA	C4B-C3B	3.06	1.49	1.44
76	4A	602	HEA	C1D-ND	-3.06	1.35	1.40
84	P	401	NDP	O2B-C2B	-3.06	1.33	1.44
76	9A	603	HEA	FE-ND	3.05	2.12	1.96
76	9A	603	HEA	C1D-ND	-3.05	1.35	1.40
76	7A	601	HEA	FE-ND	3.05	2.11	1.96
76	2A	602	HEA	FE-ND	3.04	2.11	1.96
76	8A	601	HEA	FE-ND	3.04	2.11	1.96
76	4A	604	HEA	FE-NB	3.03	2.11	1.96
76	3A	604	HEA	FE-ND	3.03	2.11	1.96
73	1A	401	HEM	CAB-C3B	3.02	1.55	1.47
76	3A	601	HEA	FE-NB	3.02	2.11	1.96
76	9A	602	HEA	FE-NB	3.01	2.11	1.96
76	8A	604	HEA	FE-NB	3.01	2.11	1.96
76	8A	601	HEA	C4B-C3B	3.00	1.49	1.44
73	1A	402	HEM	CAB-C3B	2.99	1.55	1.47
76	4A	602	HEA	C4B-C3B	2.99	1.49	1.44
73	6A	401	HEM	CAB-C3B	2.98	1.55	1.47
76	3A	604	HEA	C4B-C3B	2.98	1.49	1.44
76	3A	604	HEA	C1D-ND	-2.98	1.35	1.40
76	8A	601	HEA	FE-NB	2.98	2.11	1.96
76	2A	601	HEA	FE-NB	2.97	2.11	1.96
76	3A	604	HEA	FE-NB	2.97	2.11	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	7A	602	HEA	FE-NB	2.96	2.11	1.96
76	4A	602	HEA	FE-NB	2.96	2.11	1.96
76	3A	601	HEA	FE-ND	2.96	2.11	1.96
76	9A	603	HEA	C4B-C3B	2.96	1.49	1.44
76	9A	603	HEA	FE-NB	2.96	2.11	1.96
76	8A	604	HEA	FE-ND	2.95	2.11	1.96
76	9A	602	HEA	FE-ND	2.95	2.11	1.96
76	4A	604	HEA	FE-ND	2.95	2.11	1.96
76	9A	602	HEA	C4B-C3B	2.90	1.49	1.44
76	8A	604	HEA	C1D-ND	-2.88	1.35	1.40
76	9A	602	HEA	C1D-ND	-2.87	1.35	1.40
76	3A	601	HEA	C1D-ND	-2.86	1.35	1.40
76	4A	604	HEA	C4B-C3B	2.85	1.49	1.44
76	4A	604	HEA	C1D-ND	-2.83	1.35	1.40
76	8A	601	HEA	C4B-NB	-2.81	1.35	1.40
76	2A	602	HEA	C2A-C1A	2.81	1.48	1.42
76	3A	601	HEA	C4B-C3B	2.80	1.49	1.44
76	7A	601	HEA	C2A-C1A	2.80	1.48	1.42
76	8A	604	HEA	C4B-C3B	2.79	1.49	1.44
76	3A	604	HEA	C4B-NB	-2.78	1.35	1.40
76	7A	601	HEA	C1D-ND	-2.77	1.35	1.40
76	2A	602	HEA	C4B-NB	-2.74	1.35	1.40
76	4A	602	HEA	C4B-NB	-2.73	1.35	1.40
76	9A	603	HEA	C4B-NB	-2.73	1.35	1.40
76	2A	602	HEA	C1D-ND	-2.73	1.35	1.40
76	7A	601	HEA	C4B-NB	-2.73	1.35	1.40
76	8A	604	HEA	C4B-NB	-2.72	1.35	1.40
76	9A	602	HEA	C4B-NB	-2.71	1.35	1.40
76	3A	601	HEA	C4B-NB	-2.68	1.35	1.40
76	4A	604	HEA	C4B-NB	-2.68	1.35	1.40
76	2A	601	HEA	C2A-C1A	2.66	1.48	1.42
76	7A	602	HEA	C2A-C1A	2.59	1.48	1.42
83	5k	200	8Q1	C6-C1	2.53	1.53	1.50
83	k	200	8Q1	C1-S44	2.53	1.82	1.76
83	J	200	8Q1	C6-C1	2.52	1.53	1.50
83	5k	200	8Q1	C1-S44	2.52	1.82	1.76
76	9A	602	HEA	C2A-C1A	2.51	1.48	1.42
83	5J	200	8Q1	C6-C1	2.51	1.53	1.50
83	k	200	8Q1	C6-C1	2.51	1.53	1.50
83	J	200	8Q1	C1-S44	2.50	1.82	1.76
76	4A	604	HEA	C2A-C1A	2.50	1.48	1.42
76	8A	604	HEA	C2A-C1A	2.50	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	5J	200	8Q1	C1-S44	2.50	1.82	1.76
76	3A	601	HEA	C2A-C1A	2.49	1.48	1.42
76	7A	602	HEA	C4B-NB	-2.49	1.36	1.40
81	B	502	FMN	C10-N1	2.47	1.38	1.33
81	5B	501	FMN	C10-N1	2.46	1.38	1.33
85	s	401	COO	C5A-C4A	2.45	1.47	1.40
76	7A	602	HEA	C1C-CHC	2.44	1.47	1.41
76	2A	601	HEA	C4D-C3D	2.43	1.49	1.45
76	2A	601	HEA	C4B-NB	-2.41	1.36	1.40
85	5s	401	COO	C5A-C4A	2.41	1.47	1.40
76	2A	601	HEA	C1C-CHC	2.41	1.47	1.41
84	P	401	NDP	C2A-N1A	2.40	1.38	1.33
76	2A	602	HEA	C4B-C3B	2.40	1.48	1.44
84	5P	401	NDP	C2A-N1A	2.40	1.38	1.33
76	4A	602	HEA	C2A-C1A	2.36	1.47	1.42
76	7A	602	HEA	C4D-C3D	2.36	1.49	1.45
76	8A	601	HEA	C1C-CHC	2.36	1.47	1.41
76	2A	602	HEA	C4C-CHD	2.36	1.47	1.41
76	7A	601	HEA	C4C-CHD	2.36	1.47	1.41
76	3A	604	HEA	C1C-CHC	2.35	1.47	1.41
76	3A	604	HEA	C2A-C1A	2.34	1.47	1.42
76	8A	601	HEA	C2A-C1A	2.33	1.47	1.42
76	9A	603	HEA	C2A-C1A	2.32	1.47	1.42
76	9A	603	HEA	C1C-CHC	2.31	1.47	1.41
76	4A	602	HEA	C1C-CHC	2.28	1.47	1.41
76	9A	603	HEA	C4D-C3D	2.28	1.49	1.45
76	7A	601	HEA	C4B-C3B	2.27	1.48	1.44
76	3A	604	HEA	C4D-C3D	2.24	1.48	1.45
76	8A	601	HEA	C4D-C3D	2.24	1.48	1.45
76	4A	602	HEA	C4D-C3D	2.22	1.48	1.45
76	9A	603	HEA	C4C-CHD	2.21	1.47	1.41
76	3A	604	HEA	C4C-CHD	2.21	1.47	1.41
76	9A	602	HEA	C4C-CHD	2.19	1.47	1.41
76	4A	604	HEA	C4C-CHD	2.19	1.47	1.41
76	4A	602	HEA	C4C-CHD	2.19	1.47	1.41
83	k	200	8Q1	O40-C39	-2.18	1.18	1.23
76	8A	601	HEA	C4C-CHD	2.18	1.47	1.41
76	8A	604	HEA	C1D-C2D	2.18	1.48	1.44
76	9A	602	HEA	C1C-CHC	2.17	1.47	1.41
76	3A	601	HEA	C1D-C2D	2.17	1.48	1.44
76	7A	602	HEA	C4C-CHD	2.17	1.47	1.41
76	2A	601	HEA	C4C-CHD	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	2A	602	HEA	C1D-C2D	2.16	1.48	1.44
76	4A	604	HEA	C1C-CHC	2.16	1.47	1.41
76	4A	604	HEA	C1D-C2D	2.15	1.48	1.44
83	5k	200	8Q1	O40-C39	-2.14	1.18	1.23
76	3A	601	HEA	C4C-CHD	2.13	1.46	1.41
76	8A	604	HEA	C4C-CHD	2.13	1.46	1.41
76	8A	604	HEA	C1C-CHC	2.13	1.46	1.41
76	7A	601	HEA	C1D-C2D	2.12	1.48	1.44
76	3A	601	HEA	C1C-CHC	2.12	1.46	1.41
83	5J	200	8Q1	O40-C39	-2.11	1.19	1.23
83	J	200	8Q1	O40-C39	-2.11	1.19	1.23
73	6B	401	HEM	CAA-C2A	2.10	1.55	1.52
73	1B	401	HEM	CAA-C2A	2.10	1.55	1.52
73	6A	402	HEM	CAA-C2A	2.10	1.55	1.52
76	9A	602	HEA	C1D-C2D	2.09	1.48	1.44
76	7A	601	HEA	C1C-CHC	2.09	1.46	1.41
76	4A	604	HEA	C4D-ND	-2.08	1.34	1.38
76	7A	601	HEA	CHB-C1B	2.06	1.47	1.41
76	2A	602	HEA	C1C-CHC	2.06	1.46	1.41
76	2A	602	HEA	C1B-C2B	2.05	1.48	1.44
76	3A	601	HEA	C4D-ND	-2.05	1.34	1.38
76	7A	601	HEA	C1B-C2B	2.04	1.48	1.44
76	2A	601	HEA	C1D-C2D	2.03	1.48	1.44
83	5k	200	8Q1	O35-C34	-2.03	1.19	1.23
76	7A	602	HEA	C1D-C2D	2.03	1.48	1.44
76	2A	602	HEA	CHB-C1B	2.03	1.46	1.41
73	1A	401	HEM	CAA-C2A	2.03	1.55	1.52
84	5P	401	NDP	O5D-C5D	-2.02	1.37	1.44
76	4A	604	HEA	C1B-NB	-2.01	1.34	1.38
83	J	200	8Q1	O35-C34	-2.00	1.19	1.23

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
85	5s	401	COO	C15-C11-C14	-15.19	78.20	109.17
76	3A	604	HEA	C3D-C4D-ND	6.91	117.05	110.36
84	P	401	NDP	PN-O3-PA	-6.91	109.11	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	5P	401	NDP	PN-O3-PA	-6.89	109.18	132.83
76	8A	601	HEA	C3D-C4D-ND	6.86	117.00	110.36
76	9A	603	HEA	C3D-C4D-ND	6.83	116.97	110.36
76	2A	602	HEA	C3D-C4D-ND	6.79	116.93	110.36
76	4A	602	HEA	C3D-C4D-ND	6.79	116.93	110.36
76	7A	601	HEA	C3D-C4D-ND	6.74	116.88	110.36
76	2A	601	HEA	C3D-C4D-ND	6.72	116.86	110.36
76	7A	602	HEA	C3D-C4D-ND	6.71	116.86	110.36
76	9A	602	HEA	C3D-C4D-ND	6.15	116.32	110.36
76	8A	604	HEA	C3D-C4D-ND	6.13	116.29	110.36
76	3A	601	HEA	C3D-C4D-ND	6.13	116.29	110.36
76	4A	604	HEA	C3D-C4D-ND	6.12	116.29	110.36
83	J	200	8Q1	C6-C1-S44	5.89	120.32	113.46
83	k	200	8Q1	C6-C1-S44	5.83	120.24	113.46
83	5J	200	8Q1	C6-C1-S44	5.81	120.22	113.46
83	5k	200	8Q1	C6-C1-S44	5.79	120.20	113.46
76	4A	602	HEA	C2B-C1B-NB	5.77	116.79	109.88
76	3A	604	HEA	C2B-C1B-NB	5.73	116.74	109.88
76	9A	603	HEA	C2B-C1B-NB	5.73	116.74	109.88
76	8A	604	HEA	C2D-C1D-ND	5.71	116.60	109.84
76	9A	602	HEA	C2D-C1D-ND	5.69	116.58	109.84
76	4A	604	HEA	C2D-C1D-ND	5.67	116.56	109.84
76	3A	601	HEA	C2D-C1D-ND	5.67	116.56	109.84
76	8A	601	HEA	C2B-C1B-NB	5.66	116.66	109.88
76	2A	601	HEA	C2B-C1B-NB	5.65	116.64	109.88
76	7A	602	HEA	C2D-C1D-ND	5.64	116.53	109.84
76	7A	602	HEA	C2B-C1B-NB	5.64	116.64	109.88
76	2A	601	HEA	C2D-C1D-ND	5.64	116.52	109.84
76	7A	601	HEA	C3B-C4B-NB	5.63	116.51	109.84
76	2A	602	HEA	C3B-C4B-NB	5.57	116.44	109.84
76	3A	601	HEA	C2B-C1B-NB	5.49	116.46	109.88
76	4A	604	HEA	C2B-C1B-NB	5.48	116.45	109.88
76	9A	602	HEA	C2B-C1B-NB	5.45	116.41	109.88
76	8A	604	HEA	C2B-C1B-NB	5.44	116.39	109.88
76	9A	603	HEA	C2D-C1D-ND	5.44	116.28	109.84
76	8A	601	HEA	C2D-C1D-ND	5.41	116.24	109.84
76	4A	602	HEA	C2D-C1D-ND	5.37	116.20	109.84
76	3A	604	HEA	C2D-C1D-ND	5.36	116.19	109.84
76	7A	601	HEA	C2D-C1D-ND	5.28	116.09	109.84
76	2A	602	HEA	C2D-C1D-ND	5.26	116.08	109.84
76	8A	604	HEA	C1D-C2D-C3D	-5.14	101.55	106.96
76	4A	604	HEA	C1D-C2D-C3D	-5.12	101.57	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	3A	601	HEA	C1D-C2D-C3D	-5.12	101.57	106.96
76	8A	604	HEA	C3B-C4B-NB	5.09	115.86	109.84
76	3A	601	HEA	C3B-C4B-NB	5.06	115.84	109.84
76	9A	602	HEA	C3B-C4B-NB	5.03	115.81	109.84
76	9A	602	HEA	C1D-C2D-C3D	-5.02	101.68	106.96
76	4A	604	HEA	C3B-C4B-NB	5.00	115.76	109.84
76	7A	601	HEA	C2B-C1B-NB	4.99	115.86	109.88
76	2A	602	HEA	C2B-C1B-NB	4.99	115.85	109.88
76	7A	602	HEA	C3B-C4B-NB	4.98	115.74	109.84
76	2A	601	HEA	C3B-C4B-NB	4.97	115.72	109.84
85	5s	401	COO	C14-C11-C12	4.95	116.30	108.23
85	s	401	COO	C14-C11-C12	4.93	116.28	108.23
76	3A	604	HEA	C3B-C4B-NB	4.88	115.62	109.84
76	8A	601	HEA	C3B-C4B-NB	4.84	115.58	109.84
76	9A	603	HEA	C3B-C4B-NB	4.82	115.55	109.84
76	4A	602	HEA	C3B-C4B-NB	4.79	115.51	109.84
76	2A	602	HEA	C13-C12-C11	-4.45	107.66	114.35
73	1A	401	HEM	C3B-C2B-C1B	4.45	109.78	106.49
73	6A	402	HEM	C3B-C2B-C1B	4.45	109.78	106.49
76	7A	601	HEA	C13-C12-C11	-4.40	107.73	114.35
76	2A	601	HEA	C3C-C4C-NC	4.26	114.72	109.21
76	9A	602	HEA	C3C-C4C-NC	4.21	114.66	109.21
74	1F	501	HEC	CMB-C2B-C1B	-4.21	122.00	128.46
74	6F	501	HEC	CMB-C2B-C1B	-4.20	122.00	128.46
76	4A	604	HEA	C3C-C4C-NC	4.20	114.64	109.21
76	7A	602	HEA	C3C-C4C-NC	4.19	114.62	109.21
76	8A	604	HEA	C3C-C4C-NC	4.14	114.56	109.21
76	3A	604	HEA	C3C-C4C-NC	4.13	114.55	109.21
76	3A	601	HEA	C3C-C4C-NC	4.13	114.54	109.21
76	9A	603	HEA	C3C-C4C-NC	4.12	114.54	109.21
76	8A	601	HEA	C3C-C4C-NC	4.11	114.53	109.21
76	2A	602	HEA	C1D-C2D-C3D	-4.10	102.64	106.96
76	7A	601	HEA	C1D-C2D-C3D	-4.09	102.65	106.96
85	s	401	COO	C14-C11-C13	4.07	115.88	108.82
85	5s	401	COO	C14-C11-C13	4.07	115.88	108.82
76	4A	602	HEA	C3C-C4C-NC	4.06	114.46	109.21
73	1A	401	HEM	CMB-C2B-C1B	-4.05	118.87	125.04
76	9A	603	HEA	CBA-CAA-C2A	-4.04	105.80	112.60
76	8A	601	HEA	CBA-CAA-C2A	-4.03	105.82	112.60
76	3A	604	HEA	CBA-CAA-C2A	-4.02	105.82	112.60
76	4A	602	HEA	CBA-CAA-C2A	-4.02	105.83	112.60
73	6A	402	HEM	CMB-C2B-C1B	-4.02	118.92	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	4A	602	HEA	CMC-C2C-C3C	4.00	132.17	124.68
76	9A	603	HEA	CMC-C2C-C3C	3.99	132.14	124.68
76	8A	601	HEA	CMC-C2C-C3C	3.98	132.13	124.68
76	3A	604	HEA	CMC-C2C-C3C	3.97	132.11	124.68
73	1A	402	HEM	CMC-C2C-C3C	3.95	132.07	124.68
73	6A	401	HEM	CMC-C2C-C3C	3.94	132.06	124.68
76	4A	604	HEA	CMC-C2C-C3C	3.90	131.98	124.68
74	6E	401	HEC	CMB-C2B-C1B	-3.89	122.48	128.46
76	7A	601	HEA	CMC-C2C-C3C	3.89	131.96	124.68
76	8A	604	HEA	CMC-C2C-C3C	3.87	131.92	124.68
74	1E	401	HEC	CMB-C2B-C1B	-3.87	122.52	128.46
76	2A	602	HEA	CMC-C2C-C3C	3.87	131.91	124.68
76	9A	602	HEA	CMC-C2C-C3C	3.86	131.90	124.68
76	3A	601	HEA	CMC-C2C-C3C	3.86	131.89	124.68
76	7A	601	HEA	C3C-C4C-NC	3.85	114.18	109.21
76	7A	602	HEA	C1D-C2D-C3D	-3.85	102.91	106.96
83	5k	200	8Q1	C32-C34-N36	3.83	124.21	116.58
83	k	200	8Q1	C32-C34-N36	3.83	124.20	116.58
76	2A	602	HEA	C3C-C4C-NC	3.82	114.14	109.21
76	2A	601	HEA	C1D-C2D-C3D	-3.80	102.96	106.96
74	6E	401	HEC	CMC-C2C-C1C	-3.76	122.68	128.46
74	1E	401	HEC	CMC-C2C-C1C	-3.74	122.71	128.46
76	3A	604	HEA	CHA-C4D-ND	-3.72	120.39	124.43
76	8A	601	HEA	CHA-C4D-ND	-3.72	120.39	124.43
73	1A	402	HEM	CMA-C3A-C4A	-3.71	122.76	128.46
76	9A	603	HEA	C27-C19-C20	3.71	121.51	115.27
76	3A	604	HEA	C4D-C3D-C2D	-3.69	101.51	106.90
73	6A	401	HEM	CMA-C3A-C4A	-3.69	122.79	128.46
76	8A	601	HEA	C4D-C3D-C2D	-3.69	101.52	106.90
76	9A	603	HEA	C1D-C2D-C3D	-3.69	103.08	106.96
76	8A	604	HEA	CBA-CAA-C2A	-3.68	106.40	112.60
76	4A	602	HEA	CHA-C4D-ND	-3.68	120.43	124.43
76	9A	603	HEA	C4D-C3D-C2D	-3.68	101.54	106.90
76	9A	603	HEA	CHA-C4D-ND	-3.67	120.44	124.43
76	3A	601	HEA	CBA-CAA-C2A	-3.67	106.43	112.60
76	3A	604	HEA	C27-C19-C20	3.66	121.43	115.27
76	2A	601	HEA	C4D-C3D-C2D	-3.65	101.57	106.90
76	4A	602	HEA	C1D-C2D-C3D	-3.65	103.12	106.96
76	8A	601	HEA	C27-C19-C20	3.65	121.40	115.27
76	8A	601	HEA	C1D-C2D-C3D	-3.65	103.12	106.96
76	4A	602	HEA	C4D-C3D-C2D	-3.64	101.59	106.90
76	4A	602	HEA	C27-C19-C20	3.64	121.40	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	3A	604	HEA	C1D-C2D-C3D	-3.64	103.13	106.96
76	4A	604	HEA	CBA-CAA-C2A	-3.63	106.48	112.60
76	7A	602	HEA	C4D-C3D-C2D	-3.62	101.62	106.90
76	9A	602	HEA	CBA-CAA-C2A	-3.61	106.52	112.60
76	4A	602	HEA	C1B-C2B-C3B	-3.59	102.50	106.80
83	J	200	8Q1	O4-C1-C6	-3.59	119.75	123.99
76	3A	604	HEA	C1B-C2B-C3B	-3.55	102.55	106.80
76	4A	604	HEA	CAD-CBD-CGD	-3.55	105.97	113.60
76	3A	601	HEA	CAD-CBD-CGD	-3.54	105.99	113.60
76	9A	602	HEA	CAD-CBD-CGD	-3.54	105.99	113.60
76	8A	604	HEA	CAD-CBD-CGD	-3.53	106.00	113.60
74	6E	401	HEC	CMB-C2B-C3B	3.52	129.96	125.82
76	8A	601	HEA	C1B-C2B-C3B	-3.52	102.59	106.80
76	9A	603	HEA	C1B-C2B-C3B	-3.52	102.59	106.80
83	5J	200	8Q1	O4-C1-C6	-3.51	119.85	123.99
74	1E	401	HEC	CMB-C2B-C3B	3.49	129.92	125.82
73	1B	402	HEM	CMC-C2C-C3C	3.49	131.20	124.68
83	k	200	8Q1	O4-C1-C6	-3.48	119.88	123.99
76	7A	602	HEA	CHA-C4D-ND	-3.48	120.65	124.43
76	2A	601	HEA	CHA-C4D-ND	-3.46	120.67	124.43
73	6B	402	HEM	CMC-C2C-C3C	3.45	131.14	124.68
76	7A	602	HEA	CBA-CAA-C2A	-3.45	106.79	112.60
76	3A	604	HEA	CAD-C3D-C4D	3.45	130.68	124.66
83	5k	200	8Q1	O4-C1-C6	-3.44	119.92	123.99
76	2A	601	HEA	CBA-CAA-C2A	-3.44	106.80	112.60
76	8A	601	HEA	CAD-C3D-C4D	3.43	130.66	124.66
76	4A	602	HEA	CAD-C3D-C4D	3.40	130.60	124.66
76	9A	603	HEA	CAD-C3D-C4D	3.39	130.58	124.66
76	7A	601	HEA	C4D-C3D-C2D	-3.35	102.02	106.90
73	1A	401	HEM	C4C-CHD-C1D	3.34	126.97	122.56
76	2A	601	HEA	C1B-C2B-C3B	-3.33	102.82	106.80
76	2A	602	HEA	C4D-C3D-C2D	-3.33	102.05	106.90
76	7A	602	HEA	C1B-C2B-C3B	-3.33	102.82	106.80
84	5P	401	NDP	O2B-P2B-O1X	-3.32	96.57	109.39
76	4A	604	HEA	C1B-C2B-C3B	-3.32	102.83	106.80
73	6A	402	HEM	C4C-CHD-C1D	3.32	126.94	122.56
84	P	401	NDP	O2B-P2B-O1X	-3.32	96.59	109.39
76	3A	601	HEA	C1B-C2B-C3B	-3.31	102.84	106.80
73	1B	401	HEM	C4C-CHD-C1D	3.29	126.90	122.56
76	8A	604	HEA	C1B-C2B-C3B	-3.29	102.86	106.80
76	9A	602	HEA	C1B-C2B-C3B	-3.28	102.88	106.80
73	6B	401	HEM	C4C-CHD-C1D	3.28	126.89	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	7A	601	HEA	CMB-C2B-C1B	3.27	130.02	125.04
76	2A	602	HEA	CMB-C2B-C1B	3.25	129.98	125.04
76	8A	604	HEA	C13-C12-C11	-3.24	109.47	114.35
76	3A	601	HEA	C13-C12-C11	-3.24	109.49	114.35
76	9A	602	HEA	C13-C12-C11	-3.21	109.53	114.35
73	1A	401	HEM	CHB-C1B-NB	3.19	128.32	124.38
73	6A	402	HEM	CHB-C1B-NB	3.18	128.31	124.38
76	4A	604	HEA	C13-C12-C11	-3.17	109.59	114.35
74	6F	501	HEC	CMC-C2C-C1C	-3.17	123.59	128.46
74	1F	501	HEC	CMC-C2C-C1C	-3.14	123.63	128.46
73	1B	401	HEM	C3B-C2B-C1B	3.14	108.82	106.49
73	6B	401	HEM	C3B-C2B-C1B	3.14	108.81	106.49
76	7A	602	HEA	C4B-C3B-C2B	-3.14	102.05	107.41
85	5s	401	COO	P1A-O3A-P2A	-3.14	122.06	132.83
73	6A	402	HEM	CMC-C2C-C3C	3.14	130.54	124.68
85	s	401	COO	N3A-C2A-N1A	-3.13	123.78	128.68
73	1A	401	HEM	CMC-C2C-C3C	3.13	130.53	124.68
85	s	401	COO	P1A-O3A-P2A	-3.13	122.09	132.83
85	5s	401	COO	N3A-C2A-N1A	-3.13	123.79	128.68
76	2A	601	HEA	C4B-C3B-C2B	-3.12	102.09	107.41
76	2A	602	HEA	C4B-C3B-C2B	-3.11	102.10	107.41
76	7A	601	HEA	C1B-C2B-C3B	-3.10	103.09	106.80
76	7A	601	HEA	C4B-C3B-C2B	-3.08	102.14	107.41
76	3A	601	HEA	C4B-C3B-C2B	-3.06	102.19	107.41
76	2A	602	HEA	C1B-C2B-C3B	-3.06	103.14	106.80
76	8A	604	HEA	C4B-C3B-C2B	-3.06	102.19	107.41
76	9A	602	HEA	C4B-C3B-C2B	-3.05	102.20	107.41
76	4A	604	HEA	C4B-C3B-C2B	-3.04	102.22	107.41
81	5B	501	FMN	C4-N3-C2	-2.99	120.12	125.64
76	2A	602	HEA	CAD-CBD-CGD	-2.98	107.19	113.60
84	5P	401	NDP	PA-O5B-C5B	-2.98	104.20	121.68
74	1F	501	HEC	C1D-C2D-C3D	-2.98	104.92	107.00
74	6F	501	HEC	C1D-C2D-C3D	-2.97	104.93	107.00
84	P	401	NDP	PA-O5B-C5B	-2.97	104.26	121.68
76	7A	602	HEA	C27-C19-C20	2.97	120.27	115.27
76	3A	604	HEA	C4B-C3B-C2B	-2.97	102.34	107.41
76	8A	601	HEA	C4B-C3B-C2B	-2.96	102.35	107.41
73	1A	402	HEM	C4D-ND-C1D	2.96	108.13	105.07
76	2A	601	HEA	CAD-C3D-C4D	2.96	129.83	124.66
76	7A	602	HEA	CAD-C3D-C4D	2.96	129.83	124.66
76	2A	601	HEA	C27-C19-C20	2.95	120.24	115.27
73	6A	401	HEM	C4D-ND-C1D	2.95	108.12	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	1B	401	HEM	C4D-ND-C1D	2.95	108.12	105.07
73	6B	401	HEM	C4D-ND-C1D	2.95	108.12	105.07
76	7A	601	HEA	CAD-CBD-CGD	-2.94	107.27	113.60
81	B	502	FMN	C4-N3-C2	-2.94	120.21	125.64
85	5s	401	COO	C4A-C5A-N7A	-2.93	106.34	109.40
76	9A	603	HEA	C4B-C3B-C2B	-2.93	102.41	107.41
85	s	401	COO	C3X-C2X-C1X	2.92	106.36	99.89
84	P	401	NDP	PN-O5D-C5D	-2.92	104.58	121.68
84	5P	401	NDP	PN-O5D-C5D	-2.91	104.59	121.68
85	5s	401	COO	C3X-C2X-C1X	2.91	106.33	99.89
76	2A	601	HEA	CMC-C2C-C3C	2.90	130.11	124.68
85	s	401	COO	C4A-C5A-N7A	-2.90	106.38	109.40
76	7A	602	HEA	C1D-ND-C4D	-2.90	102.08	105.07
76	2A	601	HEA	C1D-ND-C4D	-2.89	102.08	105.07
76	7A	602	HEA	CMC-C2C-C3C	2.89	130.08	124.68
76	4A	602	HEA	C4B-C3B-C2B	-2.89	102.48	107.41
76	3A	604	HEA	C1D-ND-C4D	-2.87	102.11	105.07
76	8A	601	HEA	C1D-ND-C4D	-2.87	102.11	105.07
85	5s	401	COO	C10-C9-C8	-2.87	119.68	125.34
73	6A	402	HEM	C4D-ND-C1D	2.86	108.03	105.07
85	s	401	COO	C10-C9-C8	-2.86	119.70	125.34
76	9A	603	HEA	C1D-ND-C4D	-2.85	102.12	105.07
73	1A	401	HEM	C4D-ND-C1D	2.85	108.02	105.07
76	2A	602	HEA	C13-C14-C15	-2.82	120.86	127.66
76	4A	602	HEA	C1D-ND-C4D	-2.81	102.17	105.07
76	7A	601	HEA	C13-C14-C15	-2.81	120.90	127.66
76	7A	602	HEA	CAD-CBD-CGD	-2.80	107.59	113.60
76	2A	601	HEA	CAD-CBD-CGD	-2.79	107.60	113.60
76	3A	604	HEA	CHB-C1B-C2B	-2.77	120.66	124.98
73	1B	402	HEM	C4D-ND-C1D	2.75	107.92	105.07
76	4A	602	HEA	CHB-C1B-C2B	-2.75	120.68	124.98
76	8A	604	HEA	CMD-C2D-C1D	2.74	129.21	125.04
76	8A	604	HEA	C27-C19-C20	2.74	119.87	115.27
74	1F	501	HEC	CMB-C2B-C3B	2.73	129.03	125.82
74	6F	501	HEC	CAA-CBA-CGA	-2.73	106.11	113.76
74	1F	501	HEC	CAA-CBA-CGA	-2.72	106.13	113.76
74	6F	501	HEC	CMB-C2B-C3B	2.72	129.01	125.82
76	8A	601	HEA	CHB-C1B-C2B	-2.71	120.74	124.98
73	6B	402	HEM	C4D-ND-C1D	2.71	107.87	105.07
76	3A	601	HEA	CMD-C2D-C1D	2.71	129.16	125.04
73	1B	401	HEM	C4B-CHC-C1C	2.71	126.13	122.56
76	3A	601	HEA	C27-C19-C20	2.71	119.82	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	9A	602	HEA	C27-C19-C20	2.70	119.82	115.27
76	8A	601	HEA	CAD-CBD-CGD	-2.70	107.80	113.60
76	9A	603	HEA	CHB-C1B-C2B	-2.70	120.77	124.98
76	4A	604	HEA	CMD-C2D-C1D	2.69	129.14	125.04
76	4A	604	HEA	CHA-C4D-C3D	-2.69	120.88	124.84
73	6B	401	HEM	C4B-CHC-C1C	2.69	126.10	122.56
76	2A	602	HEA	C1D-ND-C4D	-2.68	102.30	105.07
76	4A	604	HEA	C27-C19-C20	2.68	119.78	115.27
76	8A	601	HEA	C13-C14-C15	-2.68	121.20	127.66
76	3A	601	HEA	CHA-C4D-C3D	-2.68	120.90	124.84
76	9A	602	HEA	CMD-C2D-C1D	2.67	129.11	125.04
76	7A	602	HEA	C13-C14-C15	-2.67	121.24	127.66
76	3A	604	HEA	CAD-CBD-CGD	-2.67	107.87	113.60
76	7A	602	HEA	C26-C15-C16	2.66	119.75	115.27
76	3A	604	HEA	C13-C14-C15	-2.66	121.25	127.66
76	4A	602	HEA	CAD-CBD-CGD	-2.66	107.88	113.60
76	9A	603	HEA	C13-C14-C15	-2.66	121.26	127.66
76	9A	603	HEA	CAD-CBD-CGD	-2.65	107.89	113.60
76	4A	602	HEA	C13-C14-C15	-2.65	121.27	127.66
76	2A	601	HEA	C26-C15-C16	2.64	119.72	115.27
76	9A	602	HEA	CHA-C4D-C3D	-2.64	120.95	124.84
76	9A	602	HEA	C1D-ND-C4D	-2.64	102.34	105.07
76	8A	604	HEA	CHA-C4D-C3D	-2.64	120.95	124.84
76	2A	601	HEA	C13-C14-C15	-2.64	121.31	127.66
76	7A	601	HEA	C1D-ND-C4D	-2.64	102.35	105.07
76	9A	602	HEA	C4D-C3D-C2D	-2.63	103.06	106.90
76	2A	602	HEA	C27-C19-C20	2.63	119.69	115.27
83	k	200	8Q1	C43-S44-C1	2.62	110.04	101.87
76	7A	601	HEA	C27-C19-C20	2.61	119.66	115.27
76	8A	604	HEA	C1D-ND-C4D	-2.61	102.38	105.07
81	5B	501	FMN	C4A-C4-N3	2.61	119.81	113.19
83	5k	200	8Q1	C43-S44-C1	2.60	109.96	101.87
74	1E	401	HEC	C1D-C2D-C3D	-2.59	105.19	107.00
76	7A	601	HEA	C4B-NB-C1B	-2.59	102.40	105.07
81	B	502	FMN	C4A-C4-N3	2.58	119.75	113.19
76	4A	604	HEA	C1D-ND-C4D	-2.58	102.41	105.07
76	3A	601	HEA	C1D-ND-C4D	-2.58	102.41	105.07
76	9A	603	HEA	CMD-C2D-C1D	2.57	128.95	125.04
76	3A	601	HEA	C4D-C3D-C2D	-2.56	103.16	106.90
76	4A	604	HEA	C4D-C3D-C2D	-2.56	103.16	106.90
76	8A	601	HEA	CMD-C2D-C1D	2.56	128.94	125.04
74	6E	401	HEC	C1D-C2D-C3D	-2.56	105.21	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	8A	604	HEA	C4D-C3D-C2D	-2.56	103.17	106.90
84	P	401	NDP	O3X-P2B-O2X	2.55	117.37	107.64
84	5P	401	NDP	O3X-P2B-O2X	2.54	117.36	107.64
83	J	200	8Q1	C43-S44-C1	2.54	109.78	101.87
76	2A	602	HEA	C4B-NB-C1B	-2.53	102.45	105.07
76	4A	602	HEA	CMD-C2D-C1D	2.53	128.89	125.04
76	3A	604	HEA	CMD-C2D-C1D	2.53	128.89	125.04
83	5J	200	8Q1	C43-S44-C1	2.53	109.73	101.87
76	2A	601	HEA	CHB-C1B-C2B	-2.50	121.08	124.98
76	7A	602	HEA	CHB-C1B-C2B	-2.49	121.08	124.98
73	6A	402	HEM	CMA-C3A-C4A	-2.48	124.64	128.46
76	3A	601	HEA	C26-C15-C16	2.48	119.44	115.27
81	B	502	FMN	C4A-C10-N10	2.47	120.09	116.48
81	5B	501	FMN	C4A-C10-N10	2.46	120.08	116.48
76	9A	602	HEA	C26-C15-C16	2.46	119.42	115.27
76	7A	601	HEA	CBA-CAA-C2A	-2.46	108.46	112.60
76	8A	604	HEA	C13-C14-C15	-2.46	121.75	127.66
76	4A	604	HEA	C13-C14-C15	-2.46	121.75	127.66
81	5B	501	FMN	O4-C4-C4A	-2.45	120.10	126.60
76	2A	602	HEA	CHA-C4D-C3D	-2.45	121.24	124.84
76	8A	604	HEA	C26-C15-C16	2.44	119.38	115.27
76	9A	602	HEA	C13-C14-C15	-2.44	121.79	127.66
76	7A	601	HEA	CHA-C4D-C3D	-2.44	121.26	124.84
81	B	502	FMN	O4-C4-C4A	-2.43	120.15	126.60
73	6A	402	HEM	CHD-C1D-ND	2.43	127.07	124.43
73	1A	401	HEM	CMA-C3A-C4A	-2.43	124.73	128.46
76	4A	604	HEA	C26-C15-C16	2.43	119.36	115.27
76	2A	602	HEA	CBA-CAA-C2A	-2.43	108.52	112.60
76	3A	601	HEA	C13-C14-C15	-2.42	121.82	127.66
83	5k	200	8Q1	O35-C34-N36	-2.42	117.80	122.99
73	1A	401	HEM	CHD-C1D-ND	2.42	127.06	124.43
76	2A	602	HEA	CHB-C1B-NB	-2.42	121.80	124.43
83	k	200	8Q1	O35-C34-N36	-2.40	117.83	122.99
84	5P	401	NDP	C2A-N1A-C6A	-2.40	114.65	118.75
76	2A	602	HEA	CHA-C4D-ND	-2.40	121.83	124.43
76	7A	601	HEA	CHB-C1B-NB	-2.38	121.84	124.43
73	6B	402	HEM	C1B-NB-C4B	2.38	107.53	105.07
73	1B	402	HEM	C3D-C4D-ND	-2.38	107.52	110.17
84	P	401	NDP	C2A-N1A-C6A	-2.38	114.69	118.75
73	6A	402	HEM	C1B-NB-C4B	2.37	107.53	105.07
76	3A	601	HEA	CMB-C2B-C1B	2.37	128.65	125.04
76	4A	604	HEA	CMB-C2B-C1B	2.37	128.64	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	7A	601	HEA	CHA-C4D-ND	-2.36	121.86	124.43
73	1B	401	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
73	1A	401	HEM	C1B-NB-C4B	2.36	107.51	105.07
73	1B	402	HEM	C1B-NB-C4B	2.36	107.51	105.07
76	8A	604	HEA	CMB-C2B-C1B	2.36	128.63	125.04
73	6B	402	HEM	C3D-C4D-ND	-2.35	107.55	110.17
73	6B	401	HEM	CMA-C3A-C4A	-2.35	124.85	128.46
76	7A	602	HEA	C25-C23-C24	2.34	119.77	114.60
76	9A	602	HEA	CMB-C2B-C1B	2.33	128.59	125.04
73	6A	401	HEM	C3D-C4D-ND	-2.33	107.57	110.17
76	2A	601	HEA	C25-C23-C24	2.33	119.74	114.60
76	4A	604	HEA	CHB-C1B-C2B	-2.33	121.34	124.98
76	3A	601	HEA	C4B-NB-C1B	-2.32	102.67	105.07
73	1A	402	HEM	C3D-C4D-ND	-2.32	107.58	110.17
76	8A	604	HEA	CHB-C1B-C2B	-2.32	121.36	124.98
84	5P	401	NDP	O5D-PN-O1N	-2.31	100.03	109.07
76	8A	604	HEA	C4B-NB-C1B	-2.31	102.68	105.07
84	P	401	NDP	O5D-PN-O1N	-2.31	100.04	109.07
74	6F	501	HEC	CBD-CAD-C3D	-2.30	108.70	112.62
76	3A	601	HEA	CHB-C1B-C2B	-2.30	121.39	124.98
73	6B	402	HEM	C4B-CHC-C1C	2.29	125.58	122.56
76	9A	603	HEA	C4B-NB-C1B	-2.29	102.71	105.07
73	6A	401	HEM	C4C-CHD-C1D	2.29	125.58	122.56
76	9A	602	HEA	C4B-NB-C1B	-2.29	102.71	105.07
76	4A	602	HEA	C4B-NB-C1B	-2.28	102.71	105.07
73	1A	402	HEM	C4C-CHD-C1D	2.27	125.56	122.56
76	2A	601	HEA	C4B-NB-C1B	-2.27	102.72	105.07
73	1A	402	HEM	CMB-C2B-C1B	-2.27	121.58	125.04
74	1F	501	HEC	CBD-CAD-C3D	-2.27	108.75	112.62
73	6A	401	HEM	CMB-C2B-C1B	-2.27	121.58	125.04
76	7A	602	HEA	CHD-C1D-C2D	-2.27	120.45	126.72
76	4A	604	HEA	C4B-NB-C1B	-2.27	102.73	105.07
76	9A	603	HEA	C25-C23-C24	2.26	119.61	114.60
73	1B	402	HEM	C4B-CHC-C1C	2.26	125.54	122.56
81	B	502	FMN	C10-C4A-N5	-2.26	120.06	124.86
76	3A	604	HEA	C4B-NB-C1B	-2.26	102.74	105.07
83	k	200	8Q1	C38-C39-N41	2.26	120.22	116.42
83	5k	200	8Q1	C38-C39-N41	2.26	120.22	116.42
84	5P	401	NDP	O2N-PN-O1N	2.26	123.39	112.24
76	4A	602	HEA	C25-C23-C24	2.26	119.58	114.60
73	1A	402	HEM	C4A-C3A-C2A	2.26	108.56	107.00
76	9A	602	HEA	CHB-C1B-C2B	-2.26	121.46	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	7A	602	HEA	C4B-NB-C1B	-2.25	102.75	105.07
76	2A	601	HEA	CHD-C1D-C2D	-2.25	120.50	126.72
84	P	401	NDP	O2N-PN-O1N	2.25	123.36	112.24
84	5P	401	NDP	O4B-C4B-C3B	2.24	109.55	105.11
84	P	401	NDP	O4B-C4B-C3B	2.24	109.55	105.11
76	8A	601	HEA	C25-C23-C24	2.24	119.55	114.60
81	5B	501	FMN	C10-C4A-N5	-2.23	120.12	124.86
76	3A	604	HEA	C25-C23-C24	2.23	119.52	114.60
73	1B	401	HEM	CBD-CAD-C3D	-2.21	106.47	112.63
73	6A	401	HEM	C4A-C3A-C2A	2.20	108.52	107.00
73	6B	401	HEM	CBD-CAD-C3D	-2.19	106.55	112.63
76	8A	601	HEA	C4B-NB-C1B	-2.18	102.82	105.07
74	1E	401	HEC	CAA-CBA-CGA	-2.18	107.64	113.76
84	5P	401	NDP	C5B-C4B-C3B	-2.17	107.04	115.18
76	7A	601	HEA	CHD-C1D-C2D	-2.17	120.73	126.72
84	P	401	NDP	C5B-C4B-C3B	-2.16	107.07	115.18
73	1B	401	HEM	C3D-C4D-ND	-2.16	107.76	110.17
76	2A	602	HEA	CHD-C1D-C2D	-2.16	120.74	126.72
73	6B	402	HEM	CBD-CAD-C3D	-2.16	106.62	112.63
74	6E	401	HEC	CAA-CBA-CGA	-2.16	107.71	113.76
76	8A	604	HEA	CHD-C1D-C2D	-2.16	120.76	126.72
73	1B	402	HEM	CBD-CAD-C3D	-2.14	106.67	112.63
76	3A	601	HEA	CHD-C1D-C2D	-2.14	120.80	126.72
73	6B	402	HEM	C4C-CHD-C1D	2.14	125.38	122.56
83	5J	200	8Q1	C38-C39-N41	2.13	120.01	116.42
73	1A	401	HEM	C4B-CHC-C1C	2.13	125.37	122.56
76	3A	604	HEA	C26-C15-C16	2.12	118.84	115.27
76	4A	604	HEA	CHD-C1D-C2D	-2.12	120.86	126.72
76	9A	602	HEA	CHB-C1B-NB	-2.12	122.13	124.43
81	5B	501	FMN	C9A-C5A-N5	-2.12	120.13	122.43
73	6B	401	HEM	C3D-C4D-ND	-2.12	107.81	110.17
83	J	200	8Q1	C38-C39-N41	2.12	119.98	116.42
76	9A	603	HEA	C26-C15-C16	2.11	118.83	115.27
76	4A	602	HEA	C26-C15-C16	2.11	118.82	115.27
76	9A	602	HEA	C25-C23-C24	2.11	119.26	114.60
76	8A	601	HEA	C26-C15-C16	2.11	118.82	115.27
73	6A	402	HEM	C4B-CHC-C1C	2.11	125.34	122.56
76	8A	604	HEA	C25-C23-C24	2.11	119.25	114.60
83	k	200	8Q1	O4-C1-S44	-2.11	119.88	122.61
81	B	502	FMN	C9A-C5A-N5	-2.11	120.14	122.43
76	7A	601	HEA	C26-C15-C16	2.10	118.81	115.27
83	5k	200	8Q1	O4-C1-S44	-2.10	119.88	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	9A	602	HEA	CHD-C1D-C2D	-2.10	120.91	126.72
76	3A	601	HEA	CHB-C1B-NB	-2.10	122.15	124.43
76	4A	604	HEA	C25-C23-C24	2.10	119.24	114.60
76	8A	601	HEA	CHD-C1D-C2D	-2.09	120.95	126.72
76	9A	603	HEA	CHD-C1D-C2D	-2.09	120.95	126.72
76	3A	601	HEA	C25-C23-C24	2.08	119.19	114.60
76	4A	602	HEA	CHD-C1D-C2D	-2.07	120.99	126.72
83	5J	200	8Q1	O4-C1-S44	-2.07	119.93	122.61
73	1B	402	HEM	C4C-CHD-C1D	2.07	125.29	122.56
76	2A	602	HEA	C26-C15-C16	2.07	118.75	115.27
83	J	200	8Q1	O4-C1-S44	-2.07	119.93	122.61
76	3A	604	HEA	CHD-C1D-C2D	-2.06	121.02	126.72
76	4A	604	HEA	CHB-C1B-NB	-2.05	122.20	124.43
84	5P	401	NDP	C3B-C2B-C1B	-2.05	99.04	102.89
81	B	502	FMN	C4A-C10-N1	-2.04	119.99	124.73
81	5B	501	FMN	C4A-C10-N1	-2.04	120.00	124.73
84	P	401	NDP	C3B-C2B-C1B	-2.04	99.06	102.89
76	2A	602	HEA	C25-C23-C24	2.03	119.08	114.60
73	6A	402	HEM	C2D-C1D-ND	-2.02	107.46	109.88
73	1B	402	HEM	CMB-C2B-C1B	-2.01	121.97	125.04
76	8A	604	HEA	CHB-C1B-NB	-2.01	122.24	124.43
73	1B	402	HEM	C3B-C2B-C1B	2.01	107.97	106.49
73	6B	402	HEM	CMB-C2B-C1B	-2.00	121.99	125.04
73	6B	401	HEM	C3C-C4C-NC	-2.00	107.17	110.94
76	7A	601	HEA	C25-C23-C24	2.00	119.02	114.60
76	2A	602	HEA	C17-C18-C19	-2.00	122.84	127.66

There are no chirality outliers.

All (222) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
73	1B	402	HEM	C2A-CAA-CBA-CGA
73	6B	402	HEM	C2A-CAA-CBA-CGA
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	3A	604	HEA	C3B-C11-C12-C13
76	3A	604	HEA	O11-C11-C12-C13
76	3A	604	HEA	C15-C16-C17-C18
76	3A	604	HEA	C19-C20-C21-C22
76	4A	602	HEA	C3B-C11-C12-C13
76	4A	602	HEA	O11-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
76	4A	602	HEA	C15-C16-C17-C18
76	4A	602	HEA	C19-C20-C21-C22
76	7A	602	HEA	C3B-C11-C12-C13
76	7A	602	HEA	O11-C11-C12-C13
76	7A	602	HEA	C15-C16-C17-C18
76	8A	601	HEA	C3B-C11-C12-C13
76	8A	601	HEA	O11-C11-C12-C13
76	8A	601	HEA	C15-C16-C17-C18
76	8A	601	HEA	C19-C20-C21-C22
76	9A	603	HEA	C3B-C11-C12-C13
76	9A	603	HEA	O11-C11-C12-C13
76	9A	603	HEA	C15-C16-C17-C18
76	9A	603	HEA	C19-C20-C21-C22
83	5J	200	8Q1	C1-C6-C7-C8
83	5J	200	8Q1	O27-C28-C29-C32
83	5k	200	8Q1	O4-C1-S44-C43
83	5k	200	8Q1	C6-C1-S44-C43
83	5k	200	8Q1	C28-C29-C32-C34
83	5k	200	8Q1	C28-C29-C32-O33
83	5k	200	8Q1	C30-C29-C32-C34
83	5k	200	8Q1	C30-C29-C32-O33
83	5k	200	8Q1	C31-C29-C32-C34
83	5k	200	8Q1	C31-C29-C32-O33
83	5k	200	8Q1	O33-C32-C34-N36
83	5k	200	8Q1	C32-C34-N36-C37
83	5k	200	8Q1	C28-O27-P24-O1
83	J	200	8Q1	C1-C6-C7-C8
83	J	200	8Q1	O27-C28-C29-C32
83	k	200	8Q1	O4-C1-S44-C43
83	k	200	8Q1	C6-C1-S44-C43
83	k	200	8Q1	C28-C29-C32-C34
83	k	200	8Q1	C28-C29-C32-O33
83	k	200	8Q1	C30-C29-C32-C34
83	k	200	8Q1	C30-C29-C32-O33
83	k	200	8Q1	C31-C29-C32-C34
83	k	200	8Q1	C31-C29-C32-O33
83	k	200	8Q1	O33-C32-C34-N36
83	k	200	8Q1	C32-C34-N36-C37
83	k	200	8Q1	C28-O27-P24-O1
84	5P	401	NDP	C5B-O5B-PA-O1A
84	5P	401	NDP	C5B-O5B-PA-O2A
84	P	401	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
84	P	401	NDP	C5B-O5B-PA-O2A
85	5s	401	COO	C14-C11-C13-O1
85	5s	401	COO	C12-C11-C13-O1
85	5s	401	COO	C14-C11-C13-C1
85	5s	401	COO	C12-C11-C13-C1
85	5s	401	COO	C13-C11-C12-O6A
85	5s	401	COO	C13-C1-N1-C2
85	5s	401	COO	O2-C1-N1-C2
85	5s	401	COO	C3-C4-N2-C5
85	5s	401	COO	O3-C4-N2-C5
85	5s	401	COO	O4-C7-S1-C6
85	5s	401	COO	C8-C7-S1-C6
85	5s	401	COO	S1-C7-C8-C9
85	s	401	COO	C14-C11-C13-O1
85	s	401	COO	C12-C11-C13-O1
85	s	401	COO	C14-C11-C13-C1
85	s	401	COO	C12-C11-C13-C1
85	s	401	COO	C13-C11-C12-O6A
85	s	401	COO	C13-C1-N1-C2
85	s	401	COO	O2-C1-N1-C2
85	s	401	COO	C3-C4-N2-C5
85	s	401	COO	O3-C4-N2-C5
85	s	401	COO	O4-C7-S1-C6
85	s	401	COO	C8-C7-S1-C6
85	s	401	COO	S1-C7-C8-C9
83	5k	200	8Q1	O35-C34-N36-C37
83	k	200	8Q1	O35-C34-N36-C37
84	5P	401	NDP	O4B-C4B-C5B-O5B
84	5P	401	NDP	C3B-C4B-C5B-O5B
84	P	401	NDP	O4B-C4B-C5B-O5B
84	P	401	NDP	C3B-C4B-C5B-O5B
84	5P	401	NDP	O4D-C1D-N1N-C6N
84	P	401	NDP	O4D-C1D-N1N-C6N
73	1B	401	HEM	C2A-CAA-CBA-CGA
73	6B	401	HEM	C2A-CAA-CBA-CGA
76	3A	601	HEA	C2A-CAA-CBA-CGA
76	4A	604	HEA	C2A-CAA-CBA-CGA
76	8A	604	HEA	C2A-CAA-CBA-CGA
76	9A	602	HEA	C2A-CAA-CBA-CGA
84	5P	401	NDP	O4D-C4D-C5D-O5D
84	P	401	NDP	O4D-C4D-C5D-O5D
76	2A	601	HEA	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
76	7A	602	HEA	C19-C20-C21-C22
83	5J	200	8Q1	O27-C28-C29-C30
83	5J	200	8Q1	O27-C28-C29-C31
83	J	200	8Q1	O27-C28-C29-C30
83	J	200	8Q1	O27-C28-C29-C31
85	5s	401	COO	C15-C11-C12-O6A
85	s	401	COO	C15-C11-C12-O6A
85	5s	401	COO	N2-C5-C6-S1
85	s	401	COO	N2-C5-C6-S1
83	5k	200	8Q1	C11-C10-C9-C8
83	k	200	8Q1	C11-C10-C9-C8
83	5k	200	8Q1	C6-C7-C8-C9
83	k	200	8Q1	C6-C7-C8-C9
85	5s	401	COO	O4-C7-C8-C9
85	s	401	COO	O4-C7-C8-C9
84	5P	401	NDP	C3D-C4D-C5D-O5D
84	P	401	NDP	C3D-C4D-C5D-O5D
83	5k	200	8Q1	O33-C32-C34-O35
83	k	200	8Q1	O33-C32-C34-O35
81	5B	501	FMN	C5'-O5'-P-O1P
81	B	502	FMN	C5'-O5'-P-O1P
85	5s	401	COO	P1A-O3A-P2A-O4A
85	s	401	COO	P1A-O3A-P2A-O4A
73	1A	401	HEM	C2A-CAA-CBA-CGA
73	6A	402	HEM	C2A-CAA-CBA-CGA
83	5k	200	8Q1	C28-O27-P24-O2
83	k	200	8Q1	C28-O27-P24-O2
83	5k	200	8Q1	O27-C28-C29-C30
83	5k	200	8Q1	O27-C28-C29-C31
83	k	200	8Q1	O27-C28-C29-C30
83	k	200	8Q1	O27-C28-C29-C31
85	5s	401	COO	C2X-C3X-O3X-P3X
85	s	401	COO	C2X-C3X-O3X-P3X
76	2A	601	HEA	C11-C12-C13-C14
76	7A	602	HEA	C11-C12-C13-C14
83	5k	200	8Q1	C28-O27-P24-O3
83	k	200	8Q1	C28-O27-P24-O3
76	2A	602	HEA	C2A-CAA-CBA-CGA
76	7A	601	HEA	C2A-CAA-CBA-CGA
85	5s	401	COO	P1A-O3A-P2A-O5A
85	s	401	COO	P1A-O3A-P2A-O5A
85	5s	401	COO	O2-C1-C13-C11

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Mol	Chain	Res	Type	Atoms
85	s	401	COO	O2-C1-C13-C11
85	5s	401	COO	N1-C1-C13-C11
85	s	401	COO	N1-C1-C13-C11
73	1A	402	HEM	CAD-CBD-CGD-O1D
73	6A	401	HEM	CAD-CBD-CGD-O1D
83	J	200	8Q1	C7-C8-C9-C10
83	5J	200	8Q1	C7-C8-C9-C10
81	5B	501	FMN	C3'-C4'-C5'-O5'
81	B	502	FMN	C3'-C4'-C5'-O5'
73	6B	402	HEM	CAA-CBA-CGA-O1A
73	1B	402	HEM	CAA-CBA-CGA-O1A
73	1B	402	HEM	CAA-CBA-CGA-O2A
73	6B	402	HEM	CAA-CBA-CGA-O2A
83	J	200	8Q1	C11-C12-C13-C14
83	5J	200	8Q1	C11-C12-C13-C14
76	7A	601	HEA	CAA-CBA-CGA-O2A
83	5J	200	8Q1	O4-C1-S44-C43
83	J	200	8Q1	O4-C1-S44-C43
76	2A	602	HEA	CAA-CBA-CGA-O2A
73	1A	402	HEM	CAA-CBA-CGA-O2A
73	6A	401	HEM	CAA-CBA-CGA-O2A
73	1A	402	HEM	CAA-CBA-CGA-O1A
73	6A	401	HEM	CAA-CBA-CGA-O1A
73	6B	401	HEM	CAD-CBD-CGD-O2D
76	2A	602	HEA	C26-C15-C16-C17
76	7A	601	HEA	C26-C15-C16-C17
73	1B	401	HEM	CAD-CBD-CGD-O2D
73	1B	401	HEM	CAD-CBD-CGD-O1D
73	6B	401	HEM	CAD-CBD-CGD-O1D
81	5B	501	FMN	C5'-O5'-P-O2P
81	B	502	FMN	C5'-O5'-P-O2P
85	5s	401	COO	C3X-O3X-P3X-O9A
85	s	401	COO	C3X-O3X-P3X-O9A
76	3A	601	HEA	C26-C15-C16-C17
76	4A	604	HEA	C26-C15-C16-C17
76	8A	604	HEA	C26-C15-C16-C17
76	9A	602	HEA	C26-C15-C16-C17
73	1A	401	HEM	CAD-CBD-CGD-O2D
73	6A	402	HEM	CAD-CBD-CGD-O2D
81	5B	501	FMN	O4'-C4'-C5'-O5'
81	B	502	FMN	O4'-C4'-C5'-O5'
76	2A	602	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
76	7A	601	HEA	CAD-CBD-CGD-O2D
76	2A	602	HEA	CAA-CBA-CGA-O1A
76	7A	601	HEA	CAA-CBA-CGA-O1A
73	1A	402	HEM	CAD-CBD-CGD-O2D
73	6A	401	HEM	CAD-CBD-CGD-O2D
76	2A	602	HEA	CAD-CBD-CGD-O1D
76	3A	601	HEA	CAD-CBD-CGD-O2D
76	4A	604	HEA	CAD-CBD-CGD-O1D
76	4A	604	HEA	CAD-CBD-CGD-O2D
76	7A	601	HEA	CAD-CBD-CGD-O1D
76	8A	604	HEA	CAD-CBD-CGD-O1D
76	8A	604	HEA	CAD-CBD-CGD-O2D
76	9A	602	HEA	CAD-CBD-CGD-O1D
76	9A	602	HEA	CAD-CBD-CGD-O2D
73	1A	401	HEM	CAD-CBD-CGD-O1D
76	3A	601	HEA	CAD-CBD-CGD-O1D
73	6A	402	HEM	CAD-CBD-CGD-O1D
84	5P	401	NDP	C5B-O5B-PA-O3
84	P	401	NDP	C5B-O5B-PA-O3
85	5s	401	COO	C3X-O3X-P3X-O8A
85	s	401	COO	C3X-O3X-P3X-O8A
76	3A	601	HEA	CAA-CBA-CGA-O2A
76	4A	604	HEA	CAA-CBA-CGA-O2A
76	8A	604	HEA	CAA-CBA-CGA-O2A
76	9A	602	HEA	CAA-CBA-CGA-O2A
76	2A	602	HEA	C19-C20-C21-C22
76	7A	601	HEA	C19-C20-C21-C22
83	5k	200	8Q1	C7-C8-C9-C10
83	k	200	8Q1	C7-C8-C9-C10
76	4A	604	HEA	CAA-CBA-CGA-O1A
76	8A	604	HEA	CAA-CBA-CGA-O1A
76	3A	601	HEA	C3B-C11-C12-C13
76	4A	604	HEA	C3B-C11-C12-C13
76	8A	604	HEA	C3B-C11-C12-C13
76	9A	602	HEA	C3B-C11-C12-C13
76	9A	602	HEA	CAA-CBA-CGA-O1A
76	3A	601	HEA	CAA-CBA-CGA-O1A
73	6B	402	HEM	CAD-CBD-CGD-O1D
83	5k	200	8Q1	C37-C38-C39-O40
83	k	200	8Q1	C37-C38-C39-O40
81	5B	501	FMN	N10-C1'-C2'-O2'
81	B	502	FMN	N10-C1'-C2'-O2'

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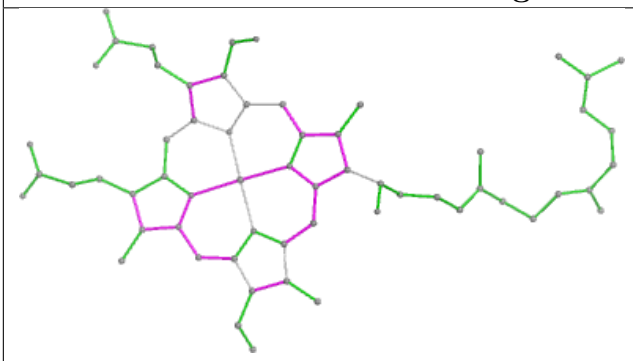
Mol	Chain	Res	Type	Atoms
73	1B	402	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

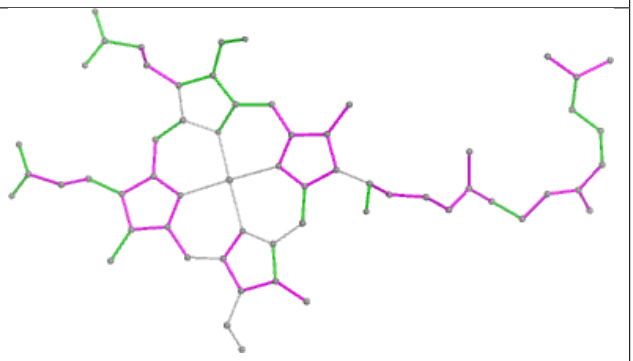
No monomer is involved in short contacts.

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 then 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.

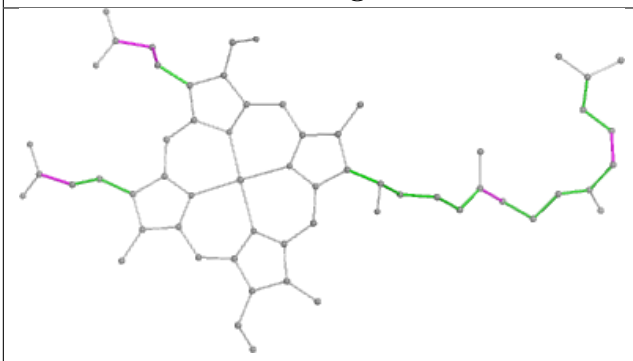
Ligand HEA 2A 602



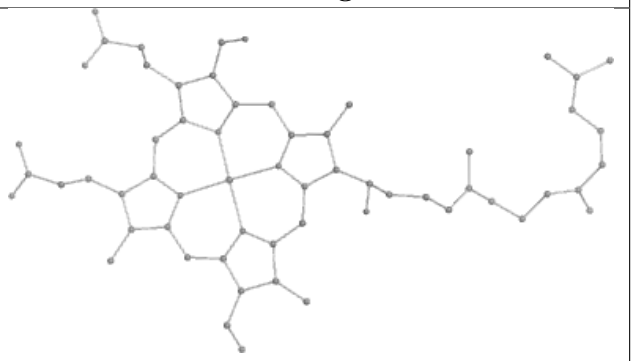
Bond lengths



Bond angles

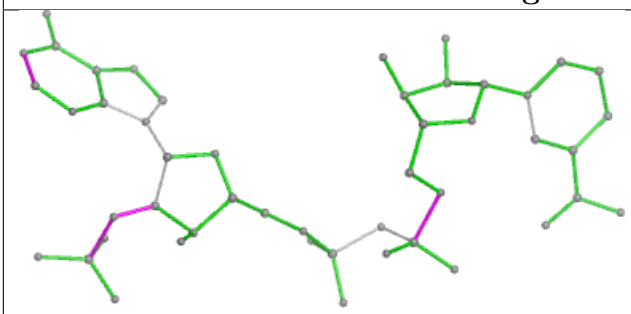


Torsions

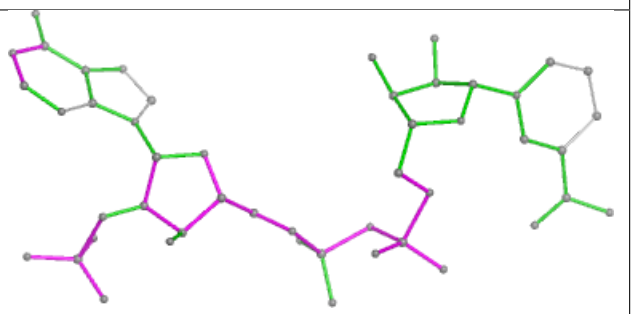


Rings

Ligand NDP P 401



Bond lengths



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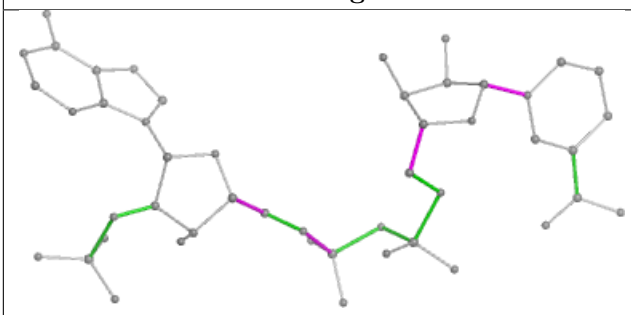

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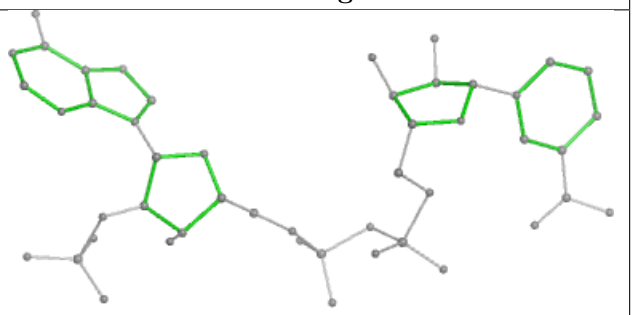
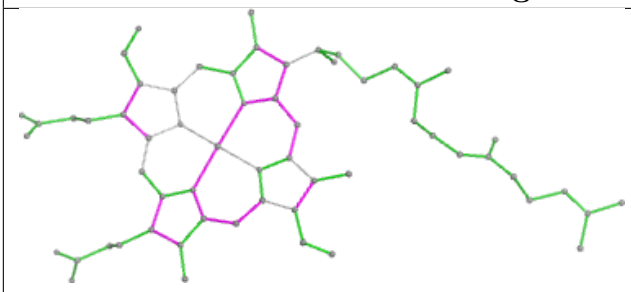


Rings

Ligand HEA 3A 604



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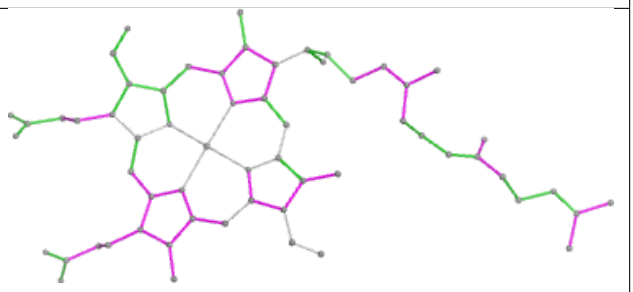
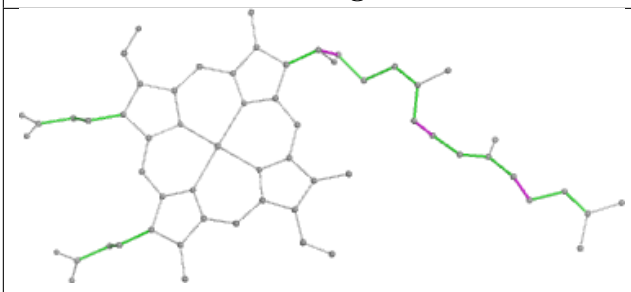


Bond angles



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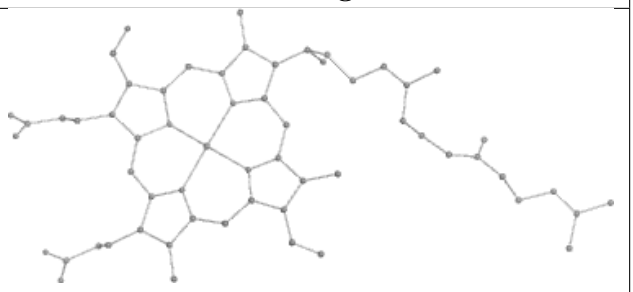
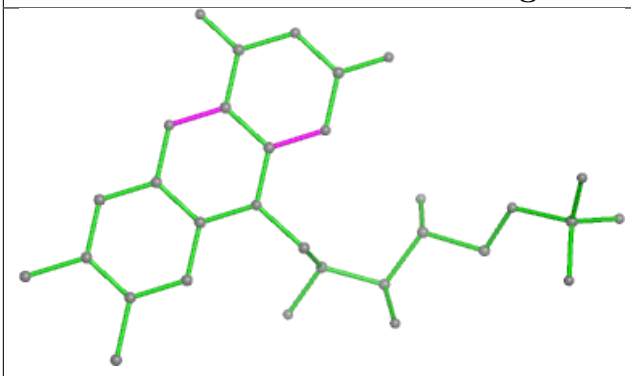
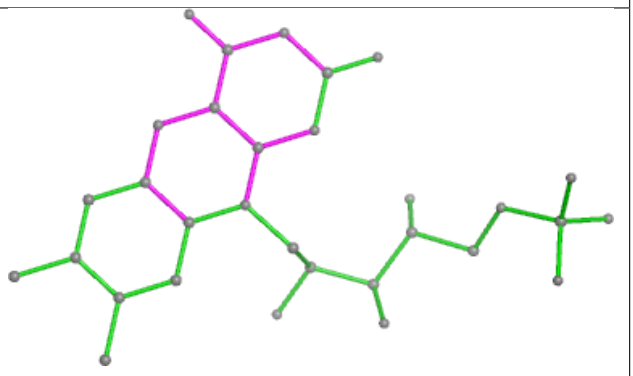


Rings

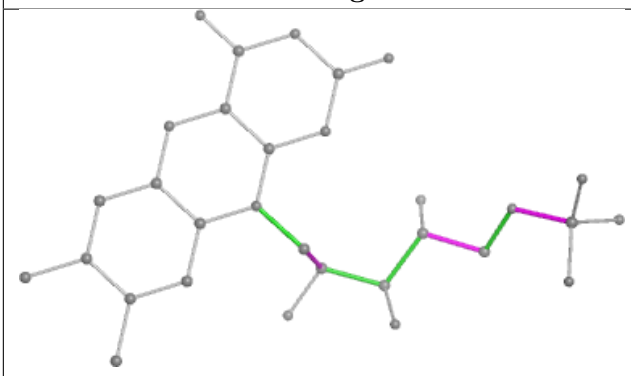
Ligand FMN B 502



Bond lengths



Bond angles



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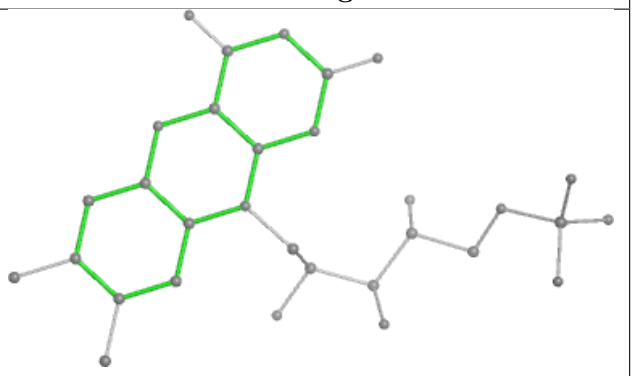
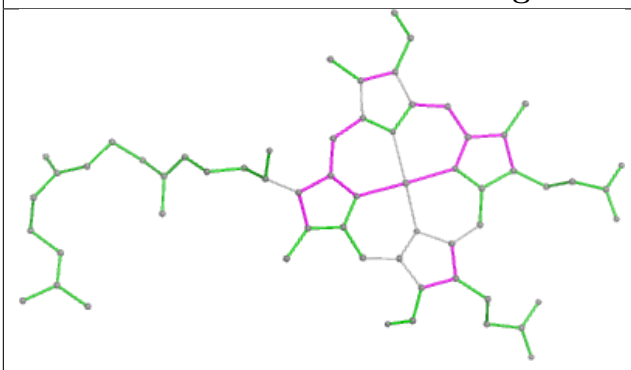


Rings

Ligand HEA 9A 602



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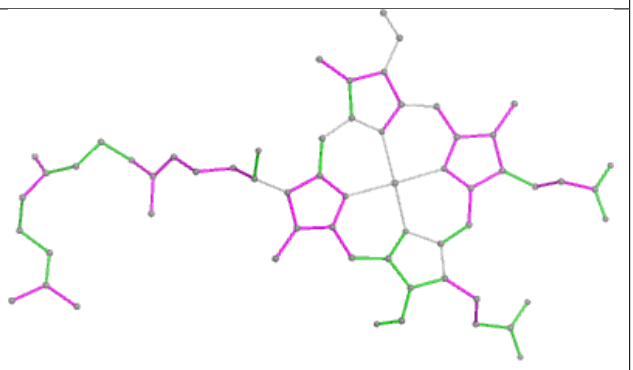
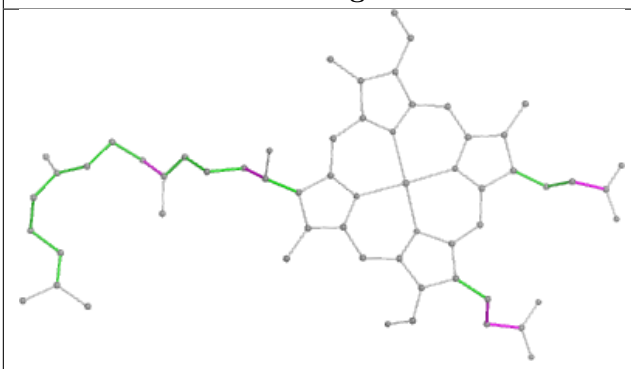


Bond angles



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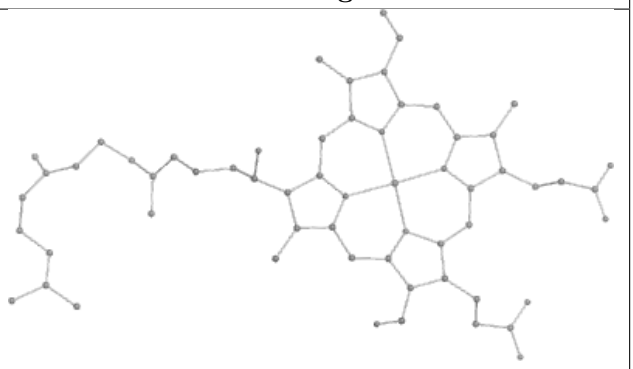
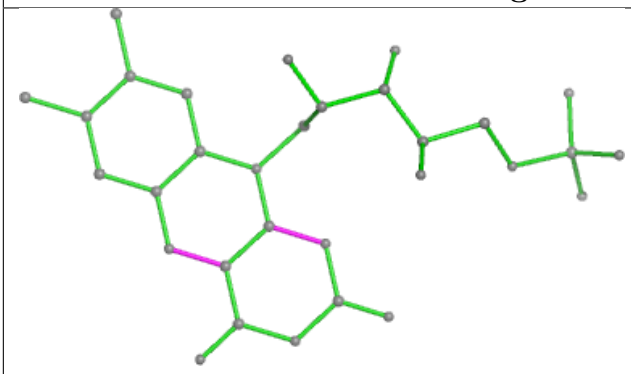


Rings

Ligand FMN 5B 501



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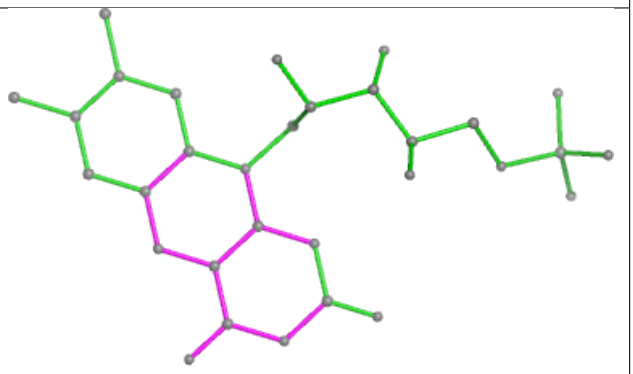
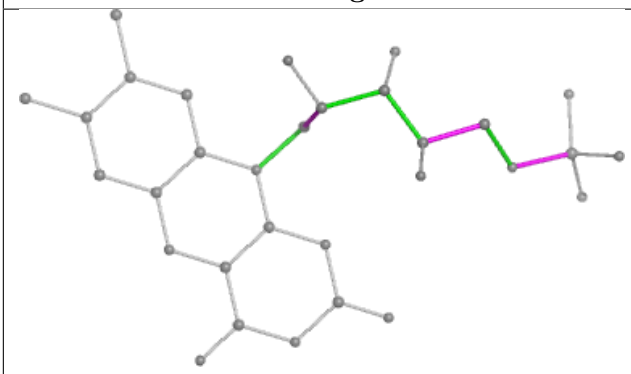
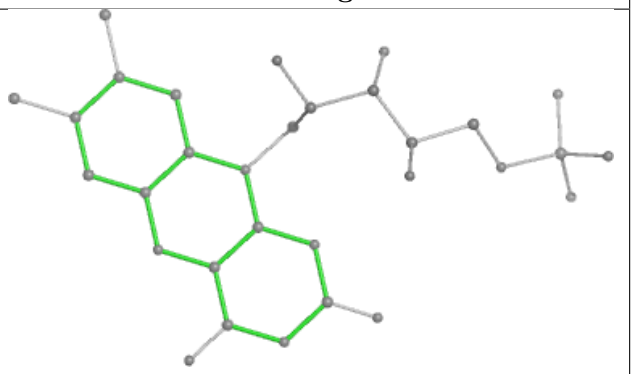


Bond angles

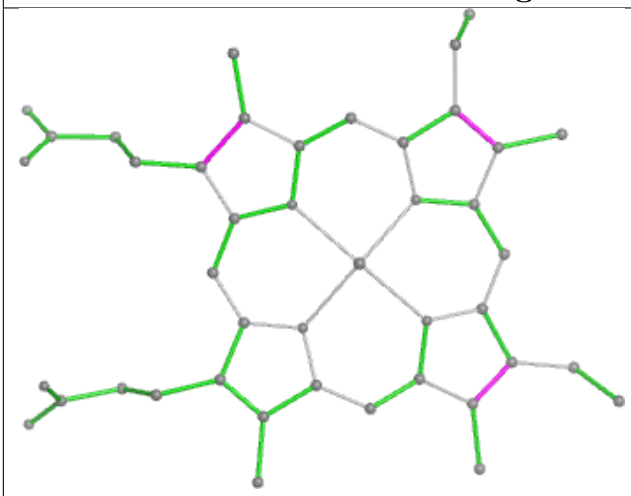


Torsions



Rings

Ligand HEC 6F 501



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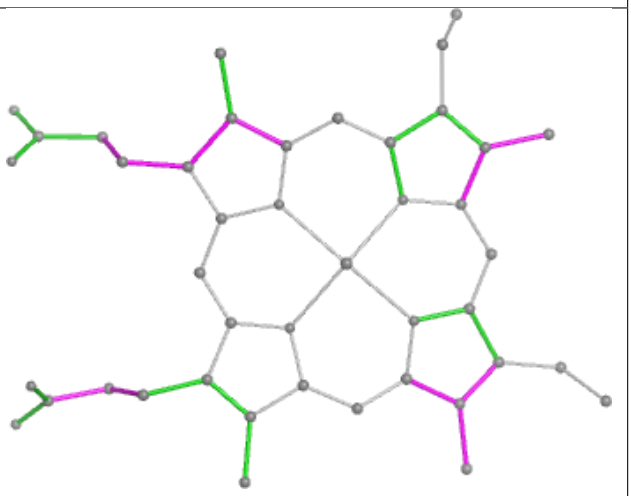
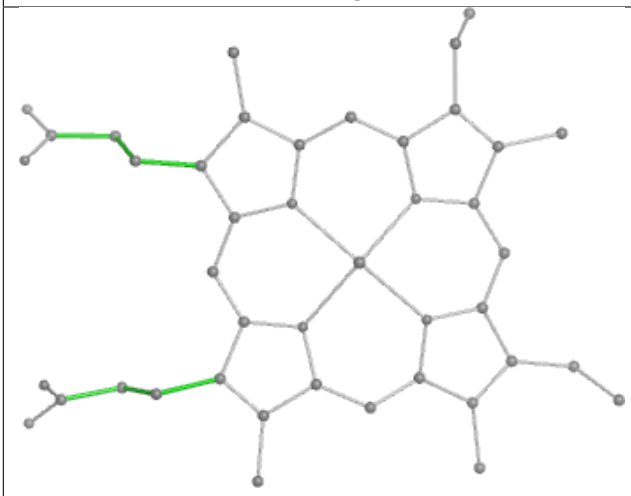
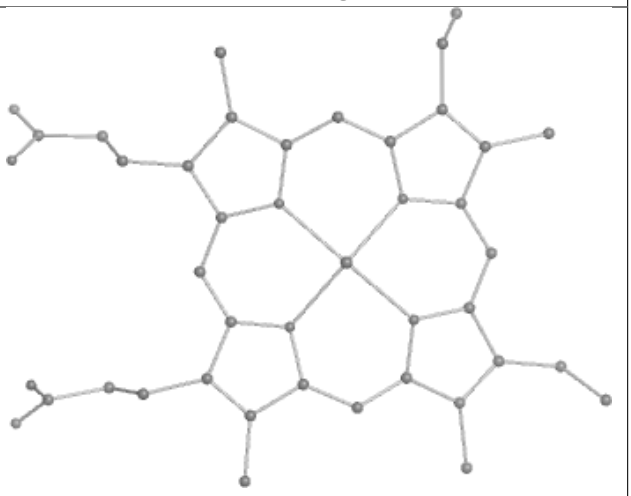


Bond angles

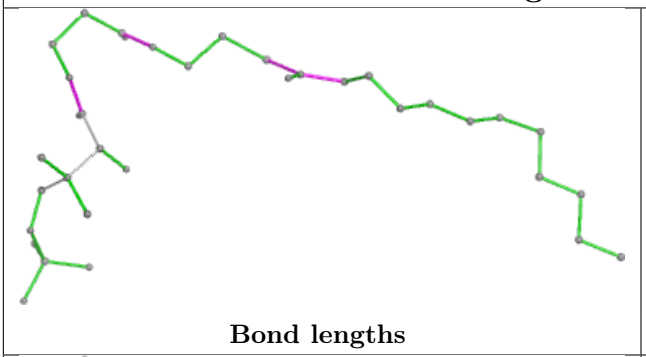


Torsions



Rings

Ligand 8Q1 5J 200



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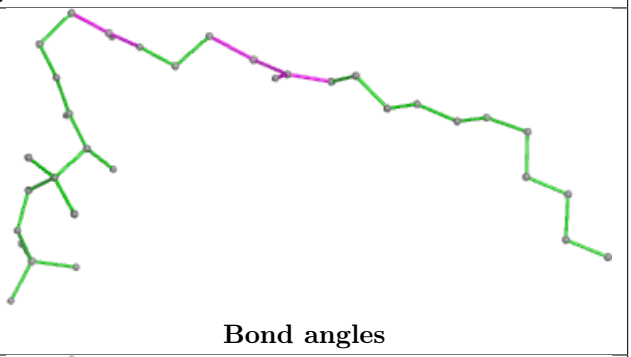

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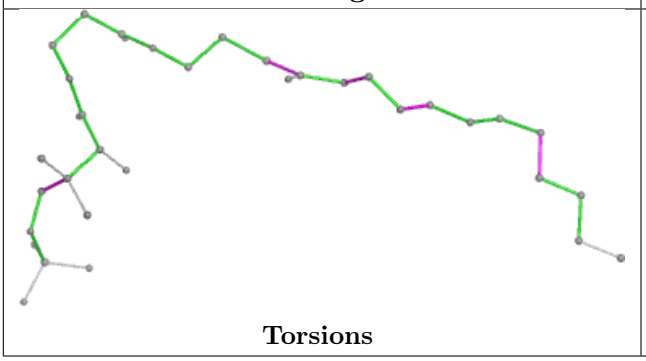

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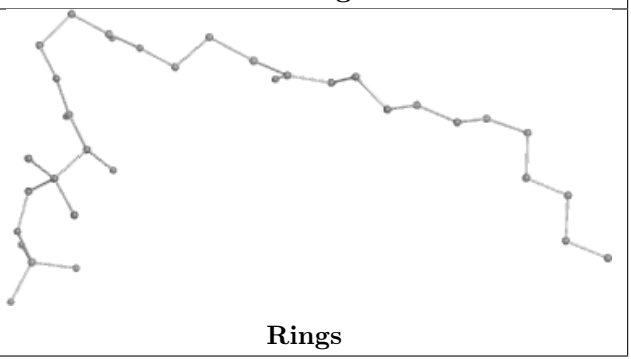
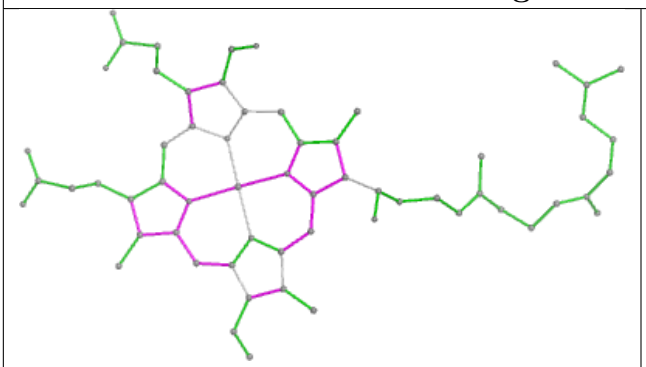


Rings

Ligand HEA 4A 604



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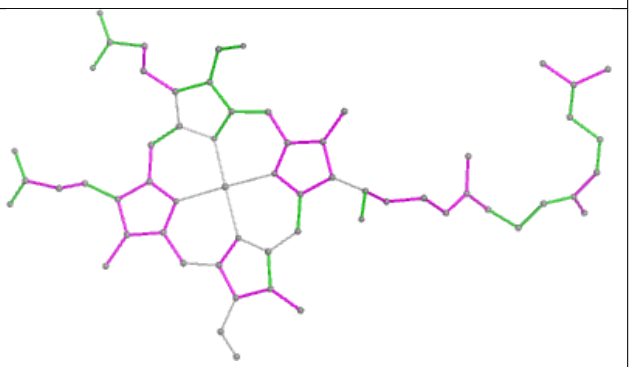

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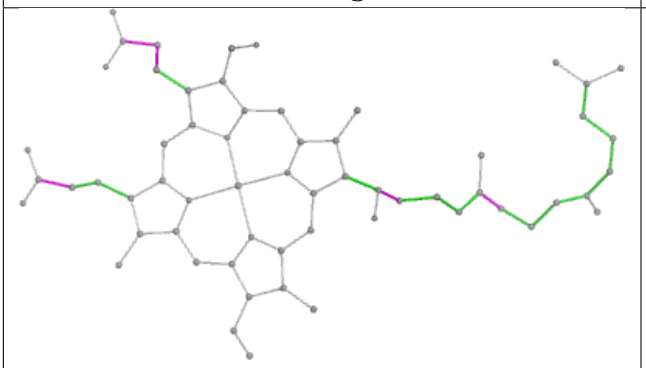

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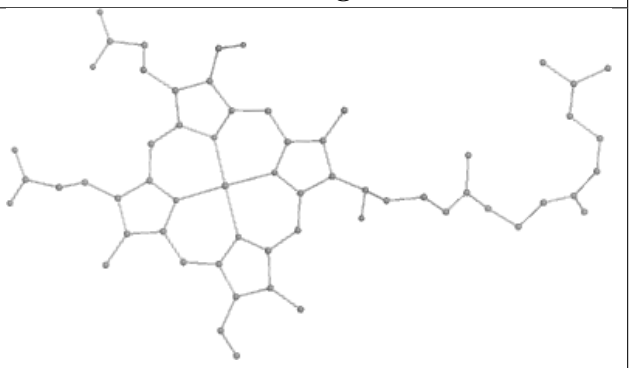
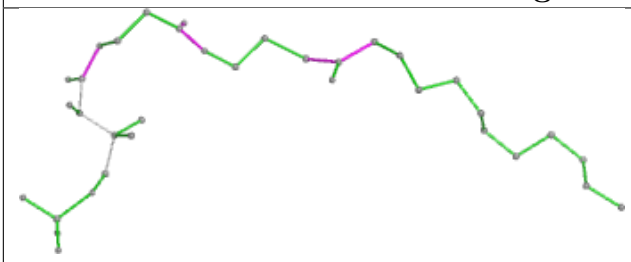


Rings

Ligand 8Q1 k 200



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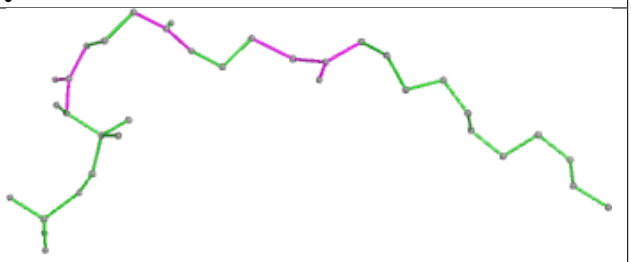
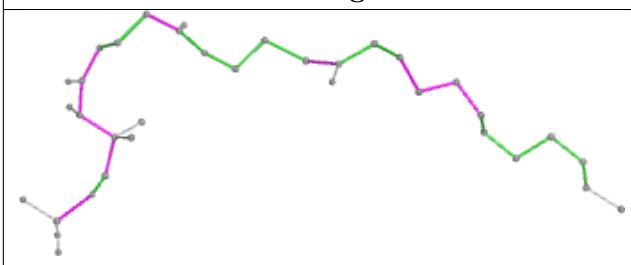


Bond angles



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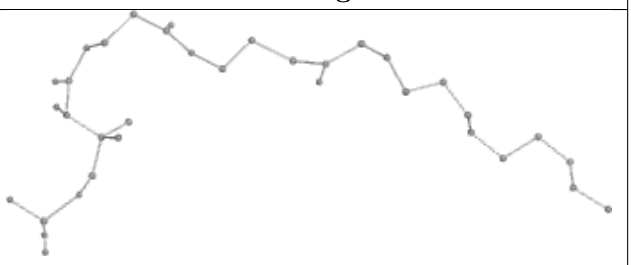
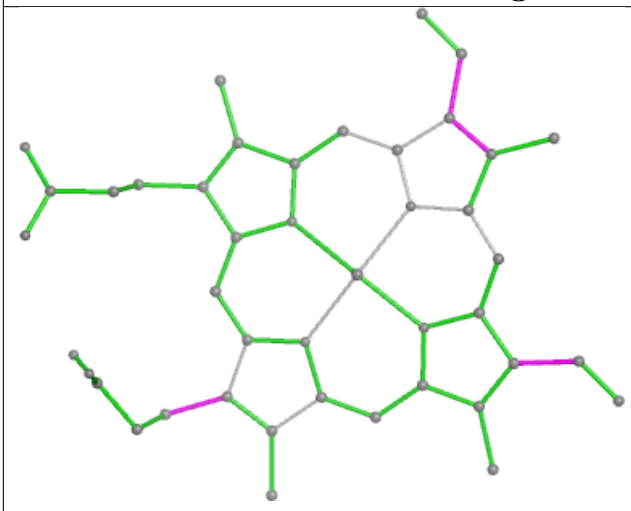


Rings

Ligand HEM 1B 401



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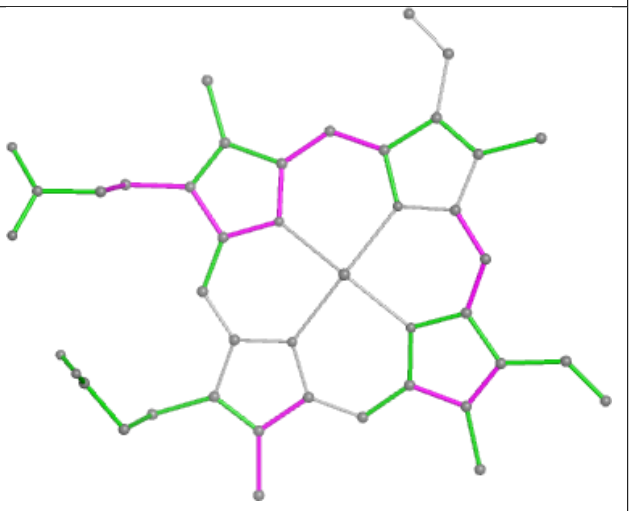

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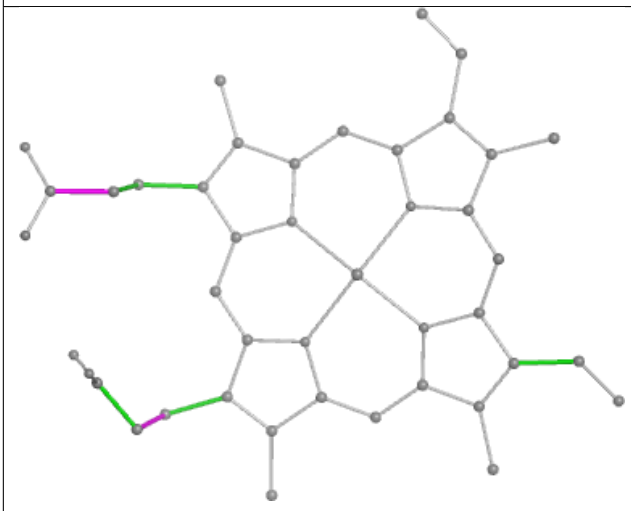

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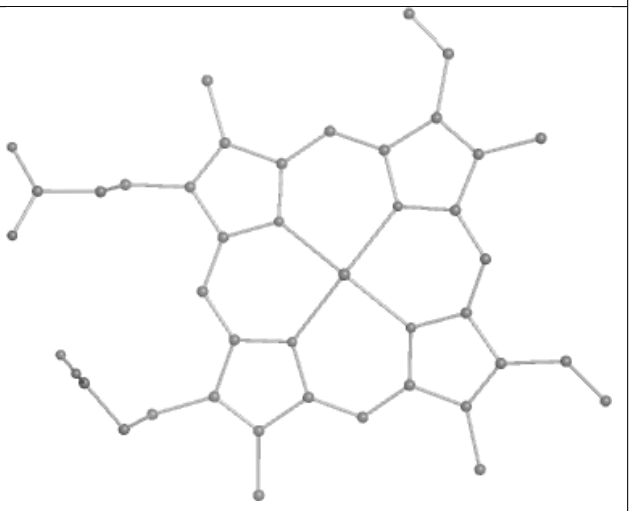
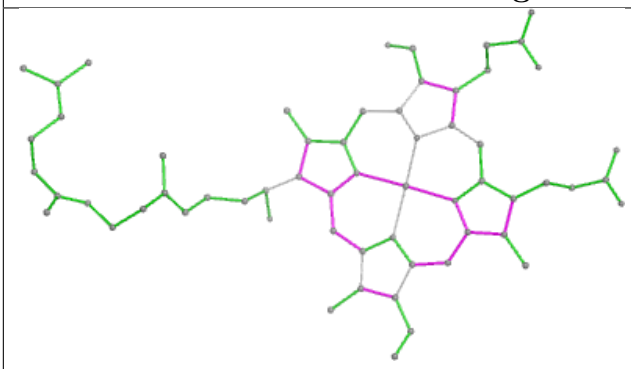


Rings

Ligand HEA 8A 604



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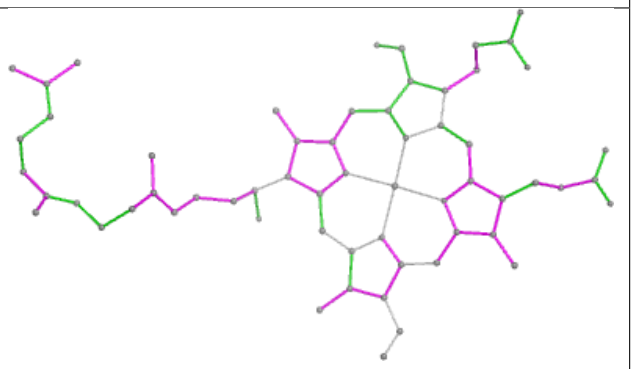

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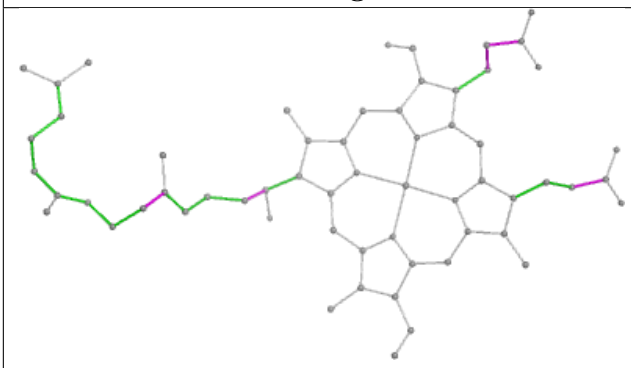

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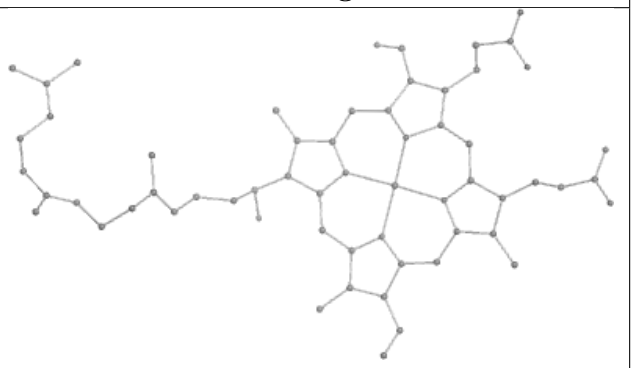
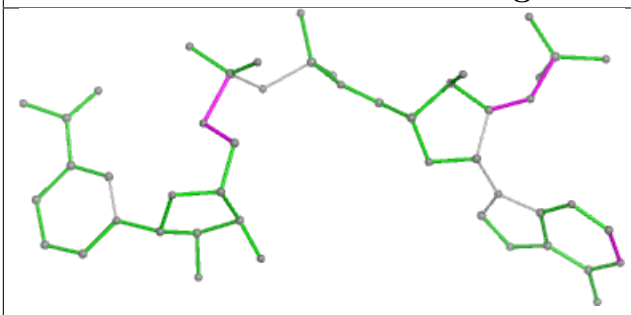


Rings

Ligand NDP 5P 401



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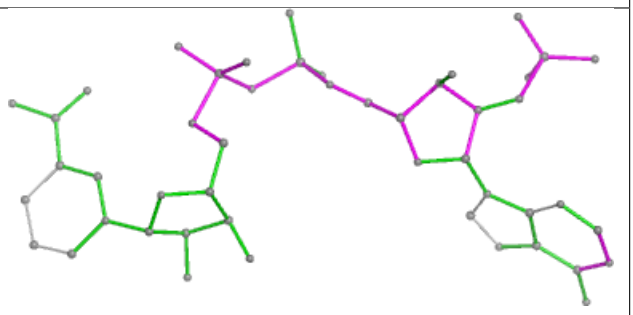

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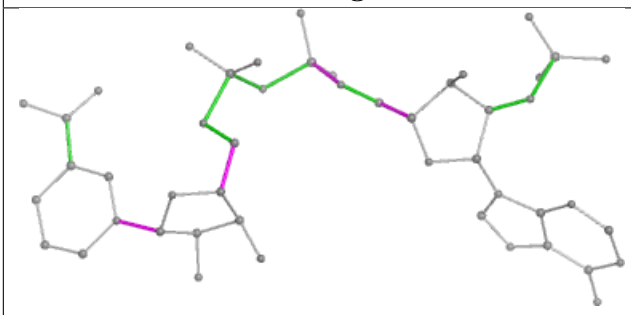

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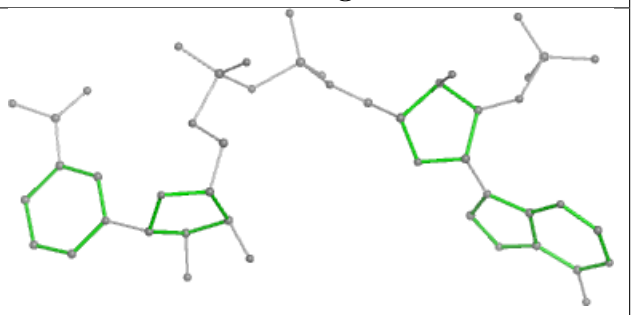
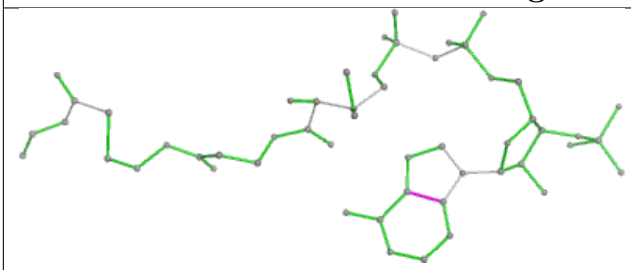


Rings

Ligand COO s 401



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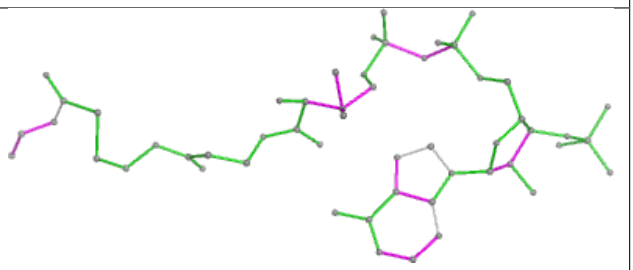

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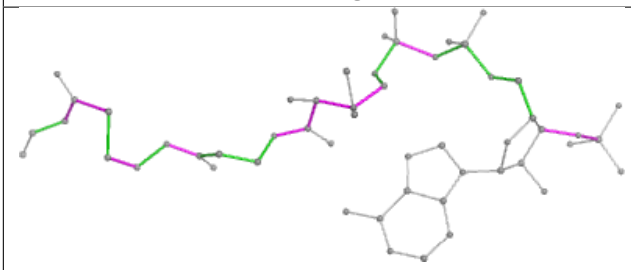

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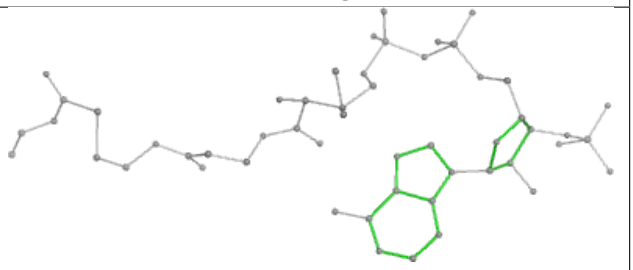
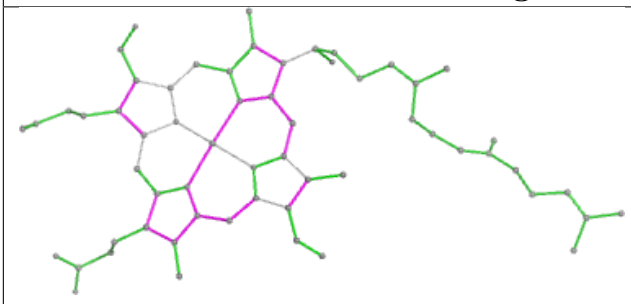


Rings

Ligand HEA 7A 602



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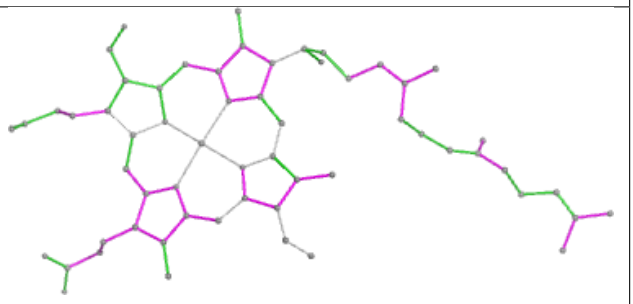

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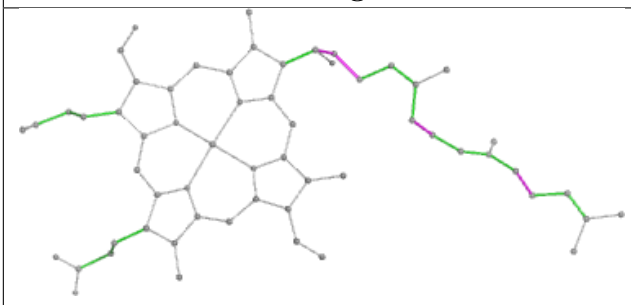

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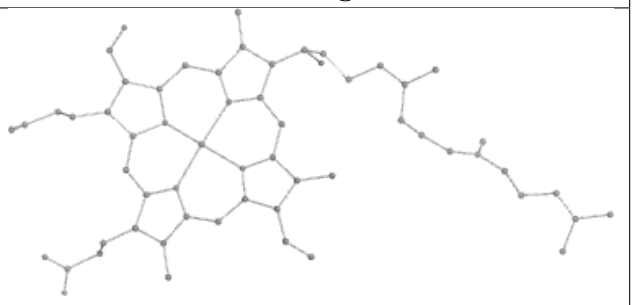
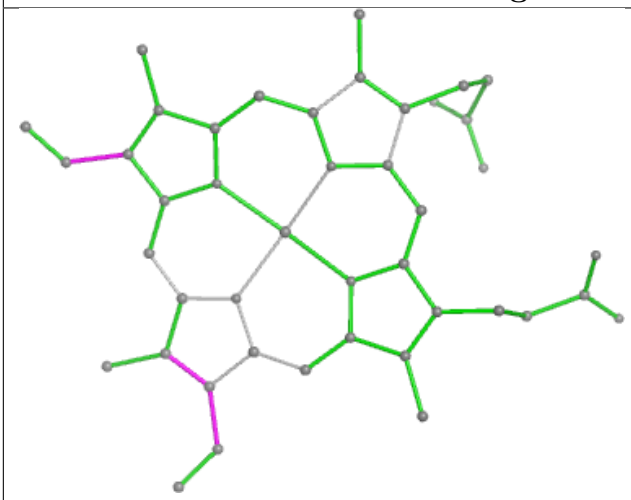


Rings

Ligand HEM 6B 402



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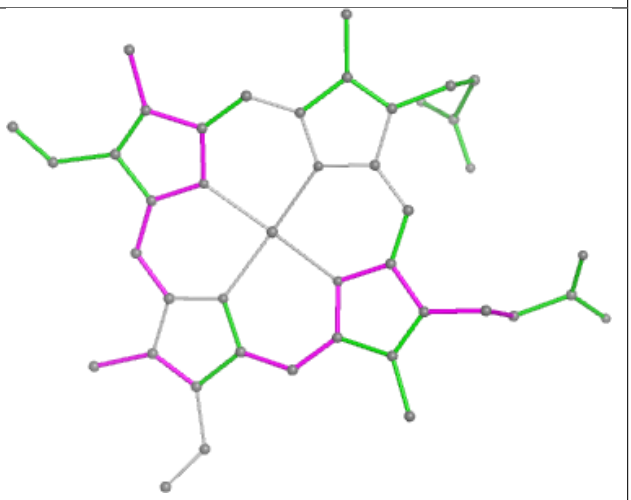

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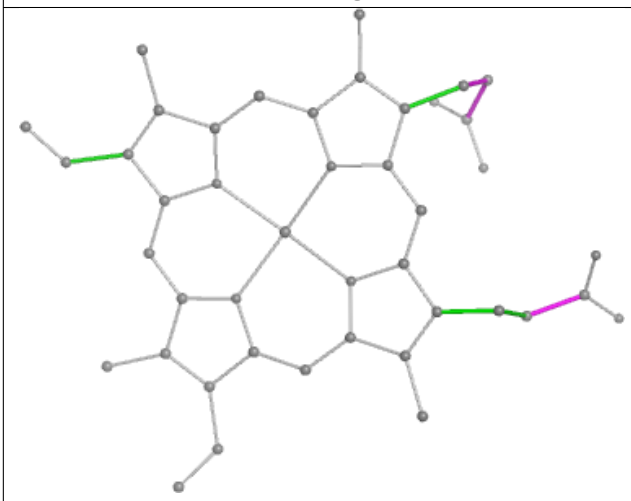

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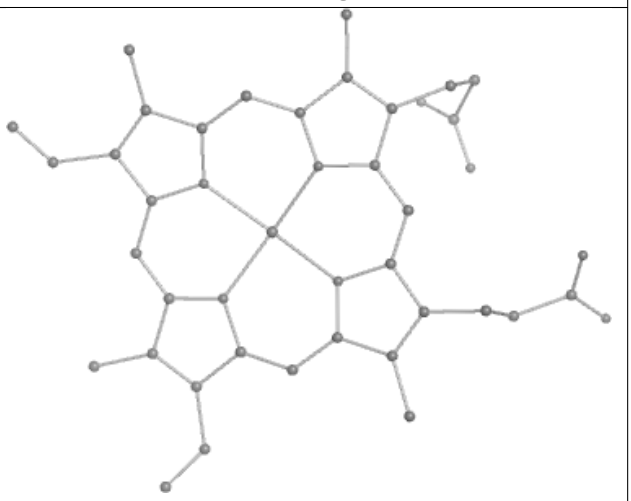
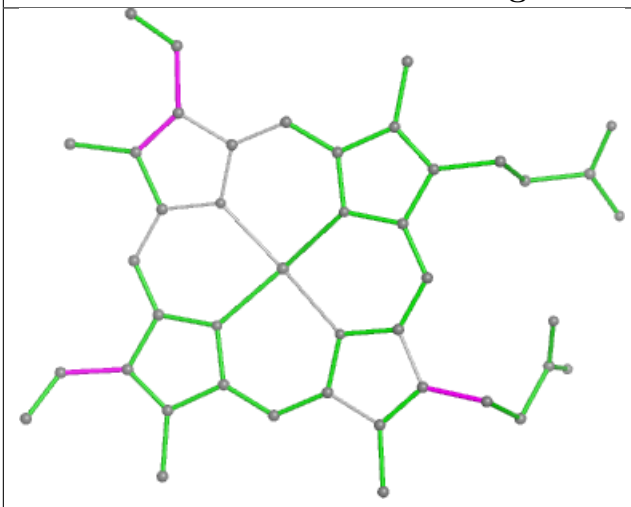


Rings

Ligand HEM 1A 401



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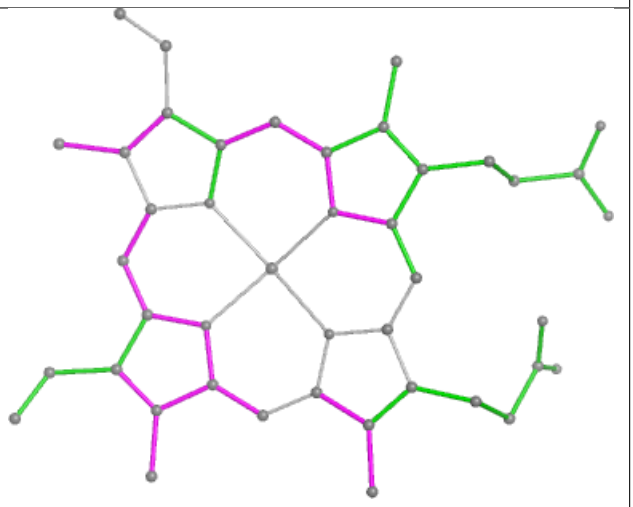

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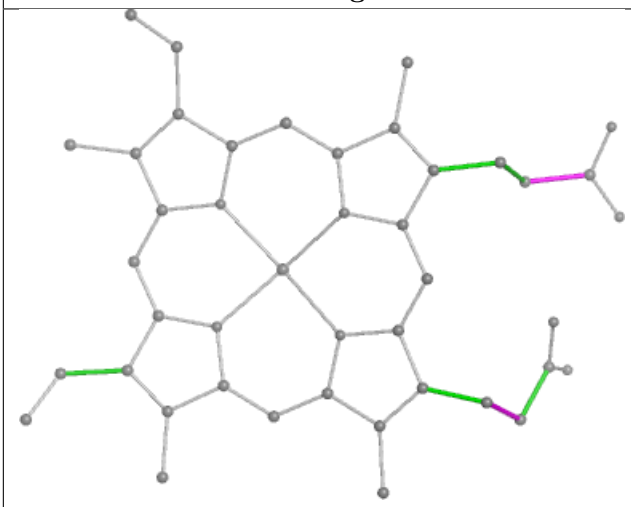

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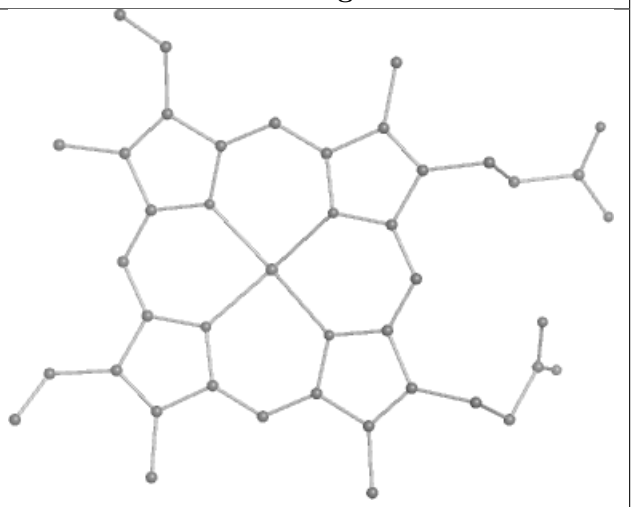
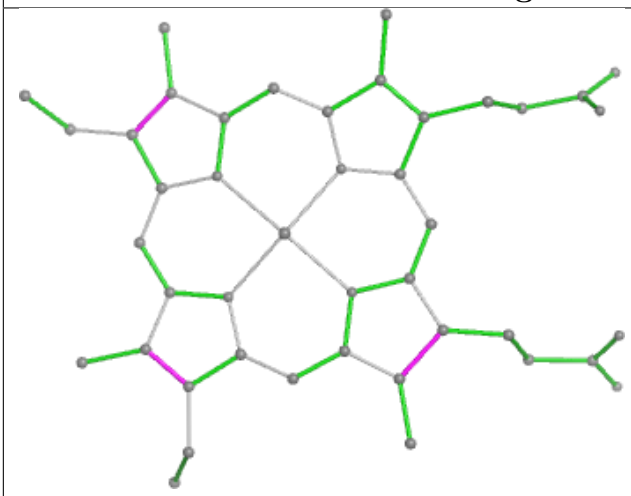


Rings

Ligand HEC 1F 501



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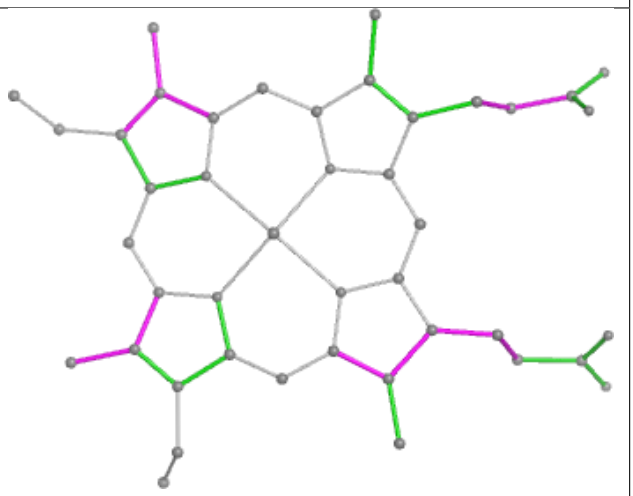
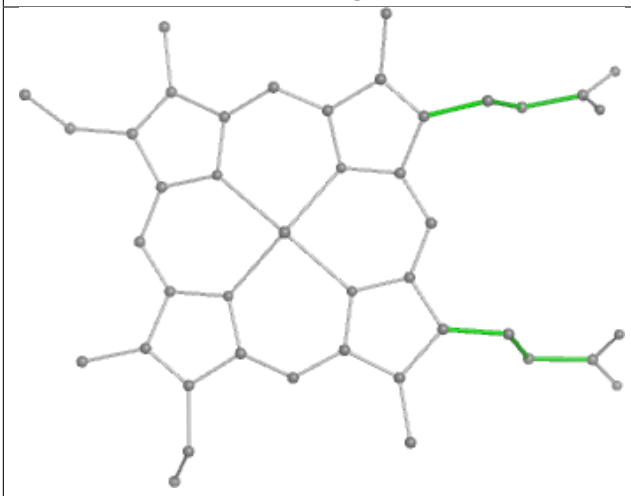


Bond angles



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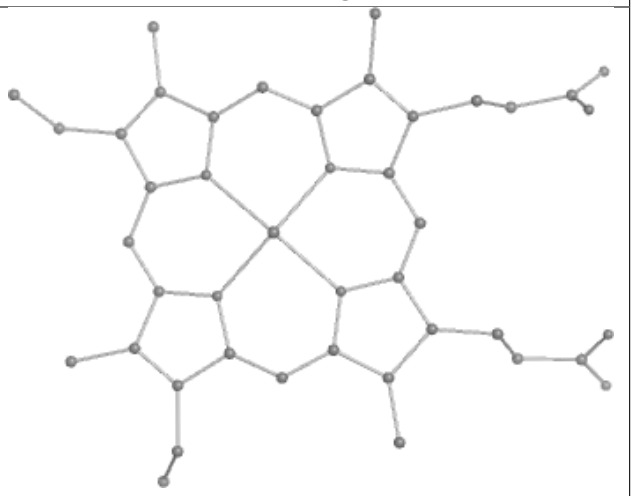
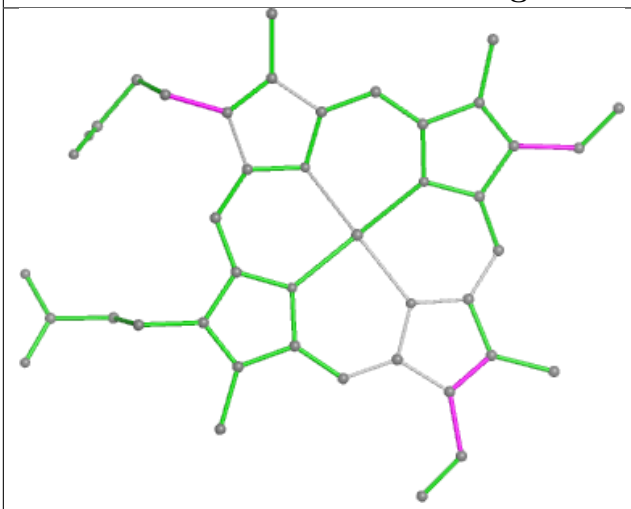


Rings

Ligand HEM 6B 401



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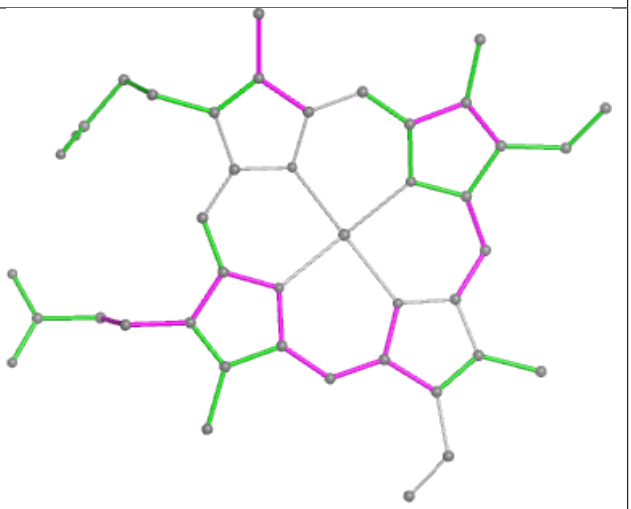
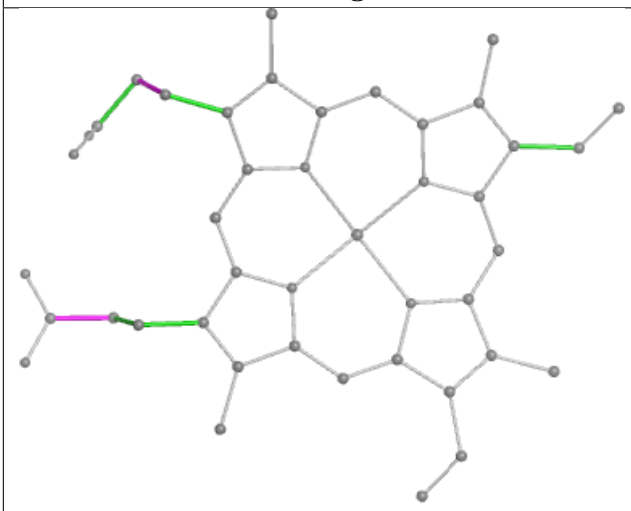
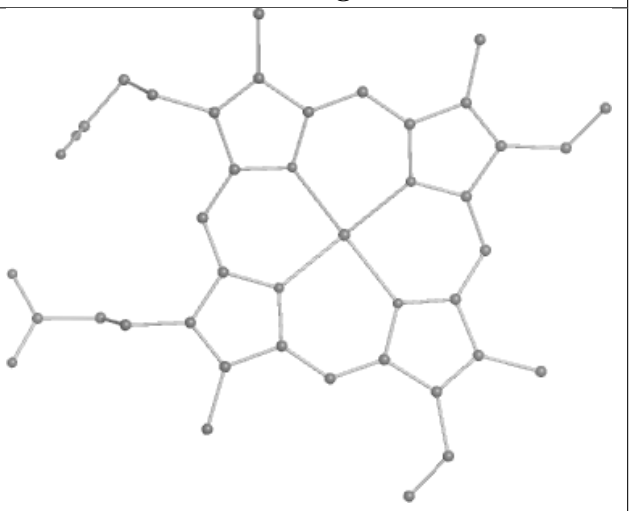


Bond angles

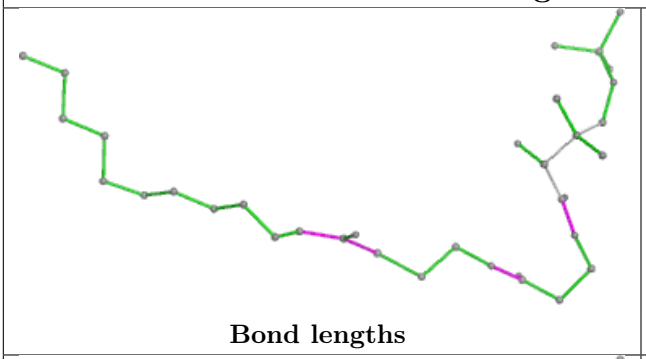


Torsions



Rings

Ligand 8Q1 J 200



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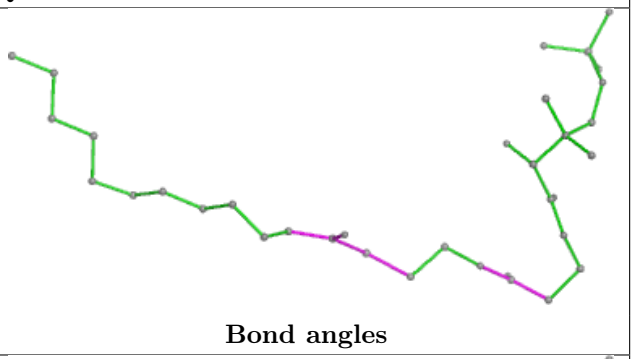
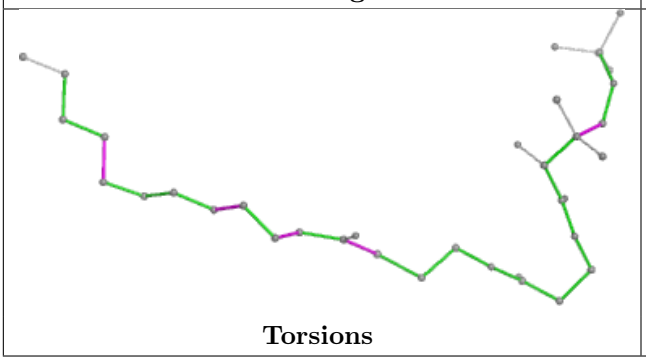
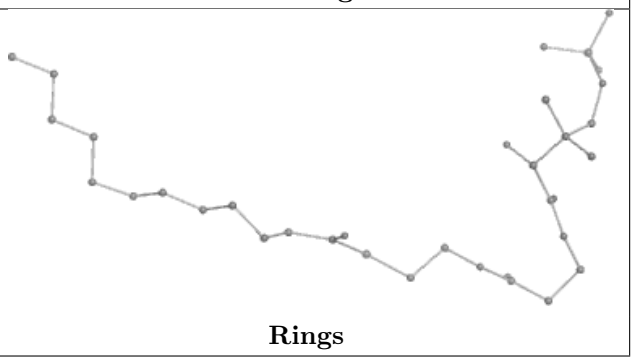


Bond angles

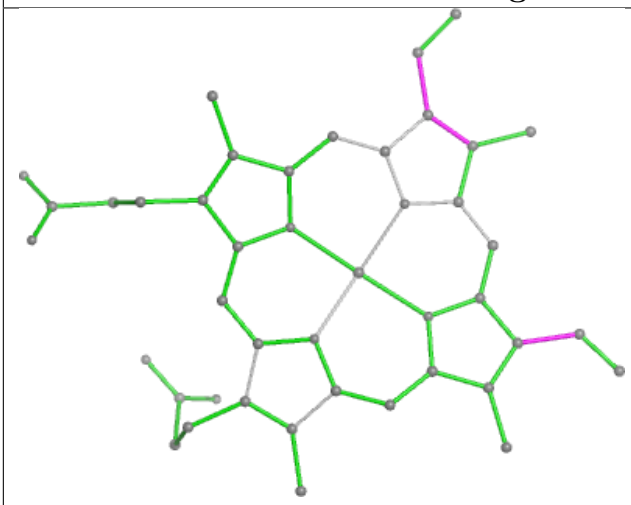


Torsions



Rings

Ligand HEM 6A 401



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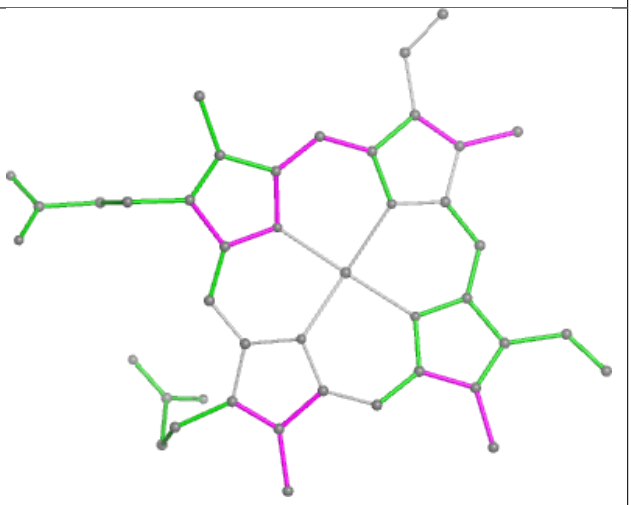

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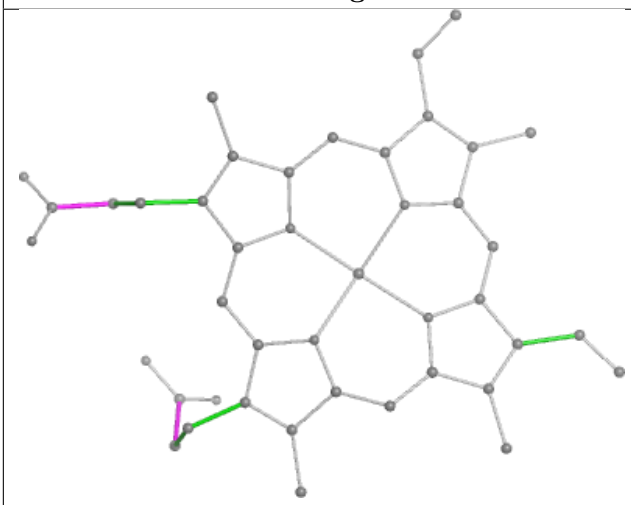

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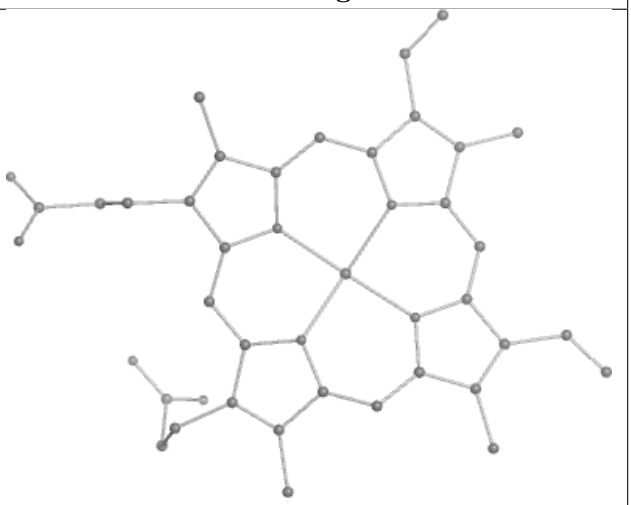
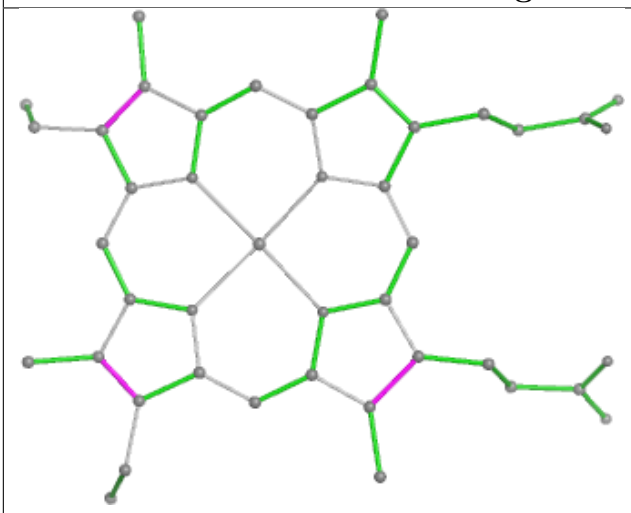


Rings

Ligand HEC 6E 401



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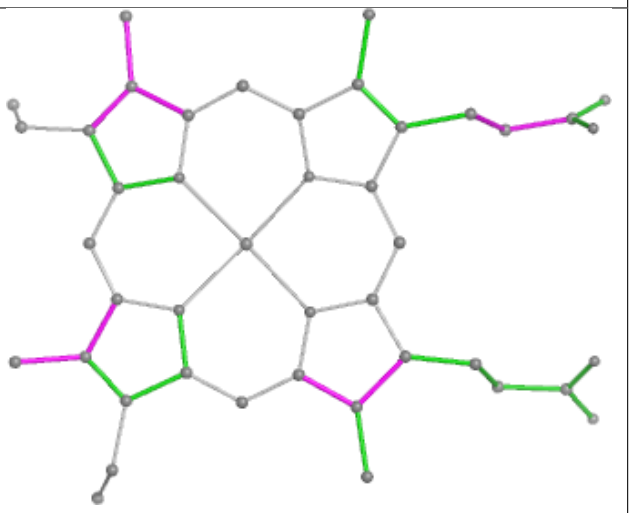

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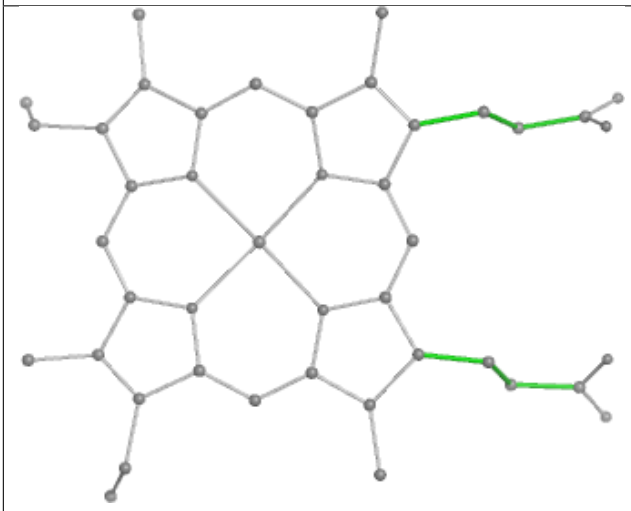

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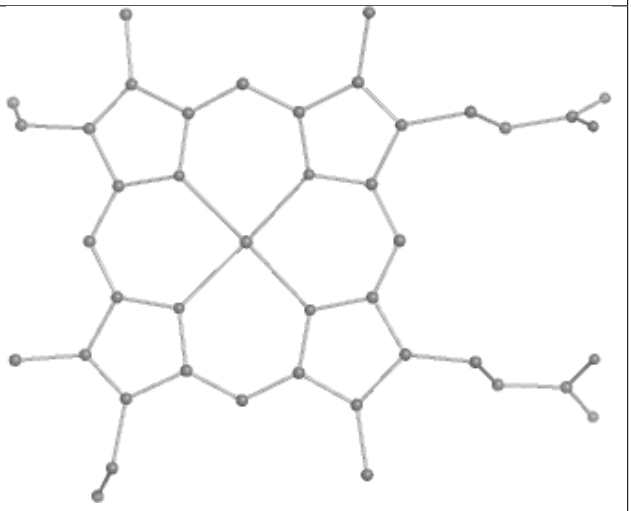
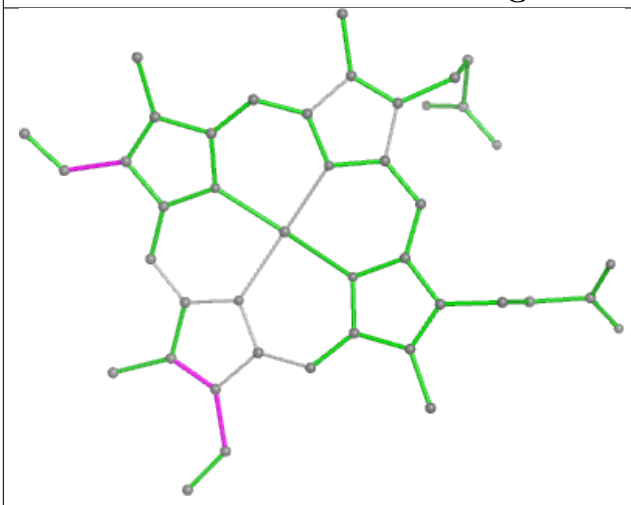


Rings

Ligand HEM 1A 402



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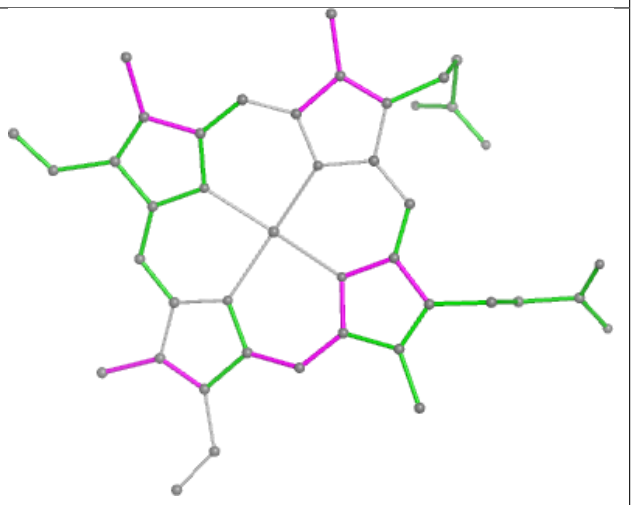

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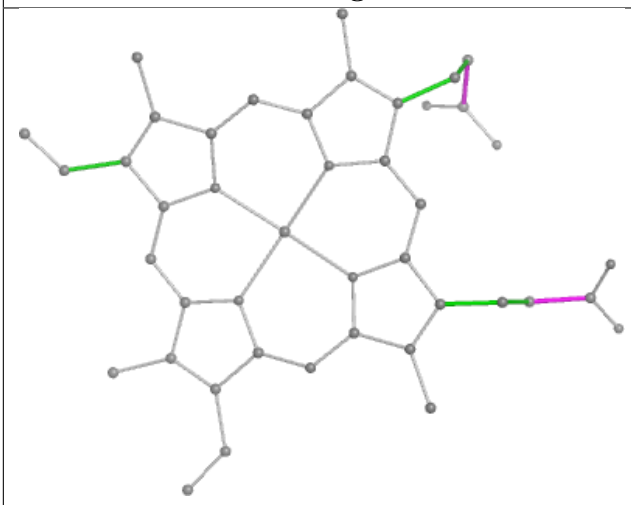

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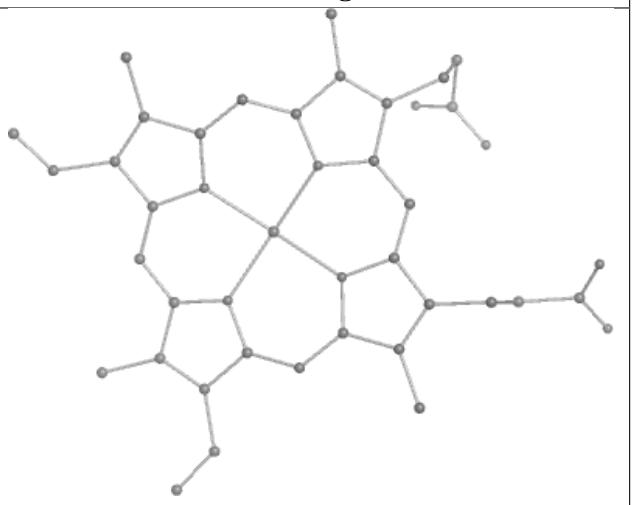
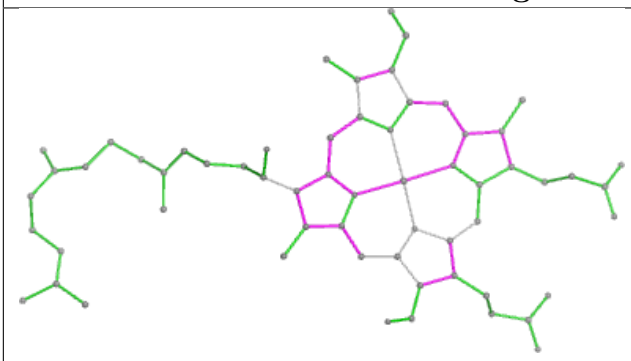


Rings

Ligand HEA 7A 601



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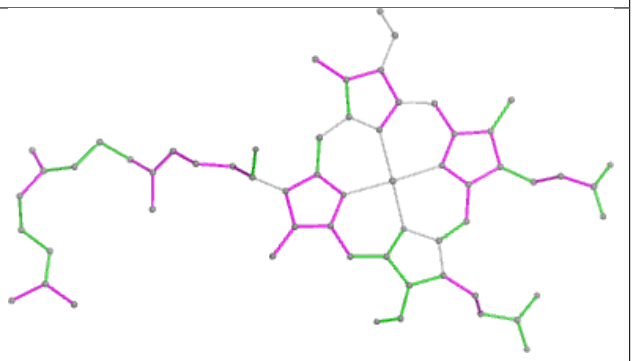

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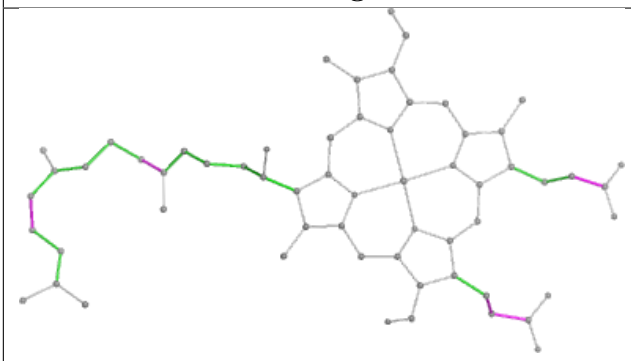

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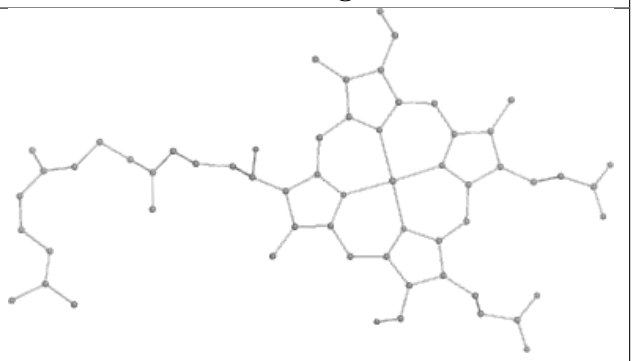
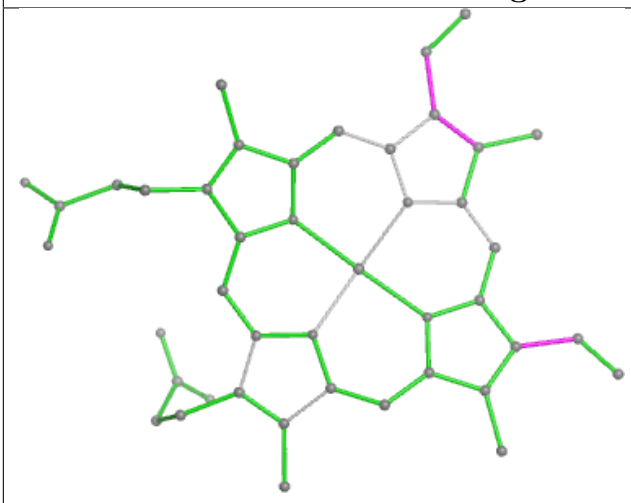


Rings

Ligand HEM 1B 402



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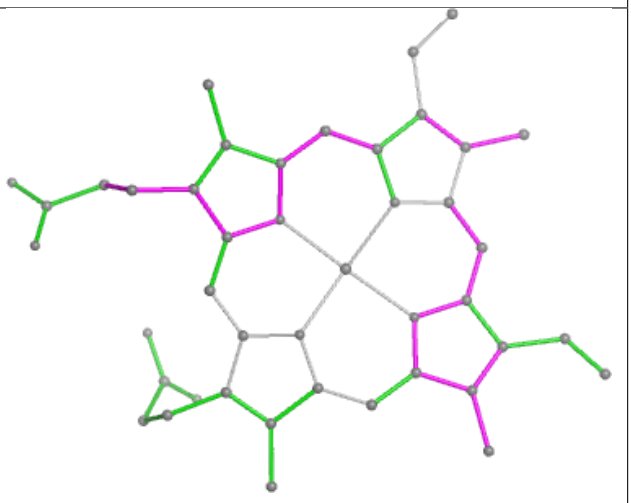

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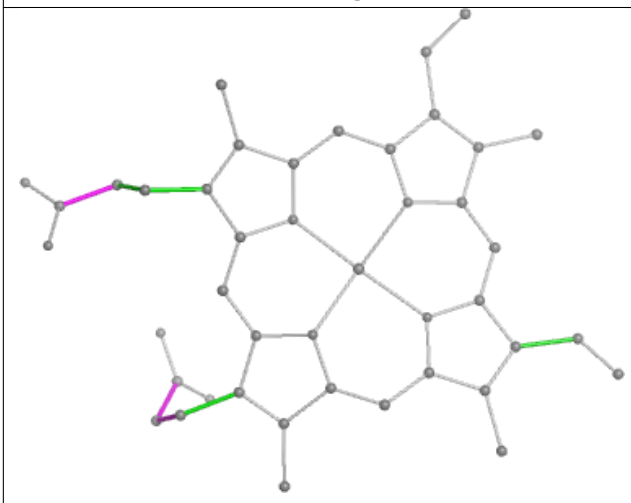

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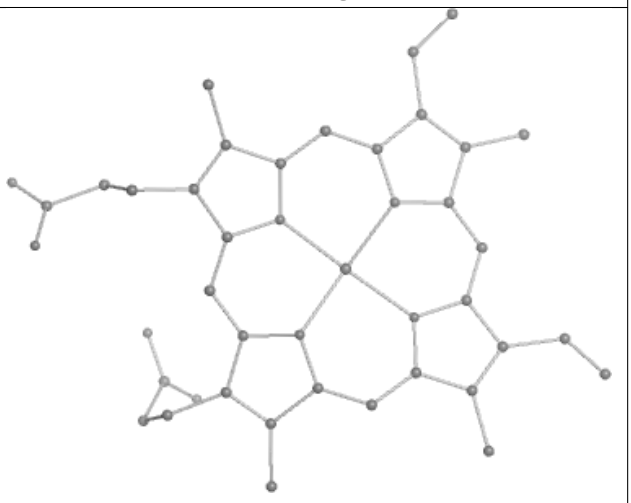
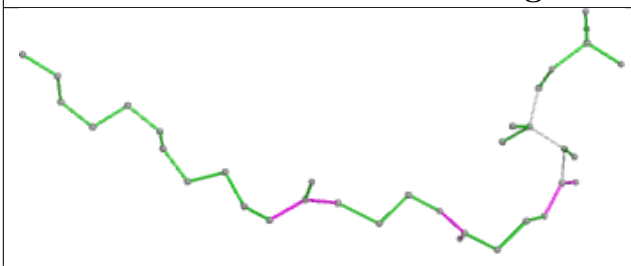


Rings

Ligand 8Q1 5k 200



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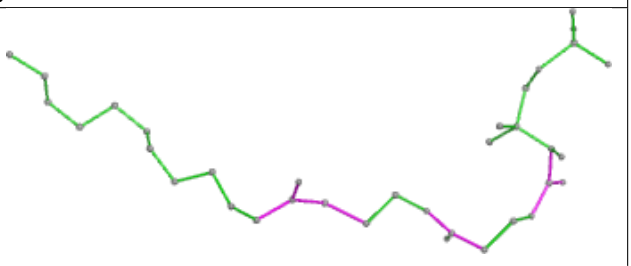

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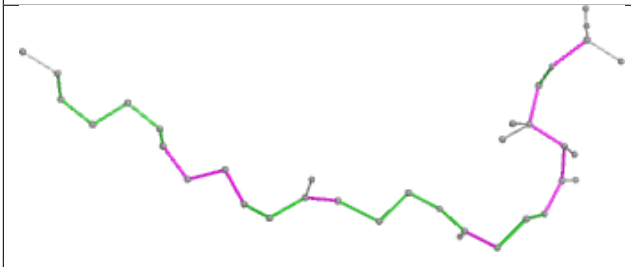
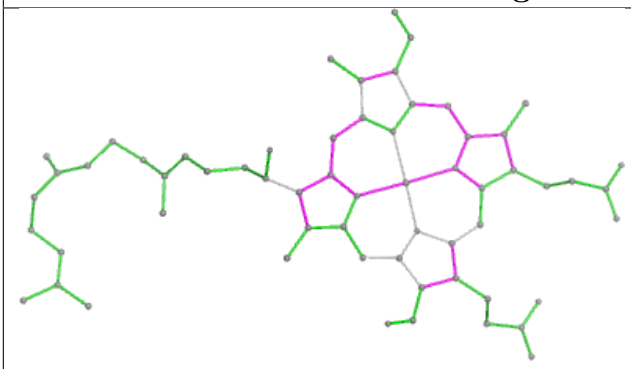


Torsions

Rings

Ligand HEA 3A 601



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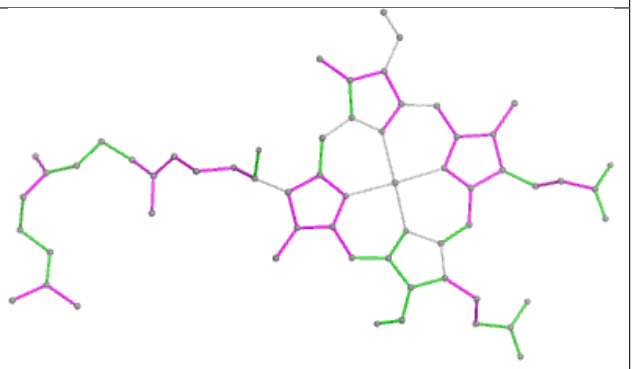

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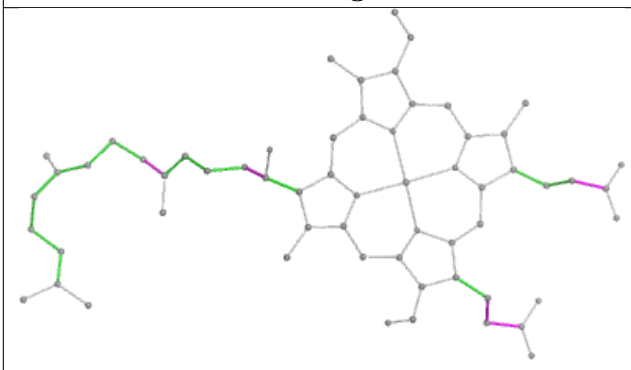

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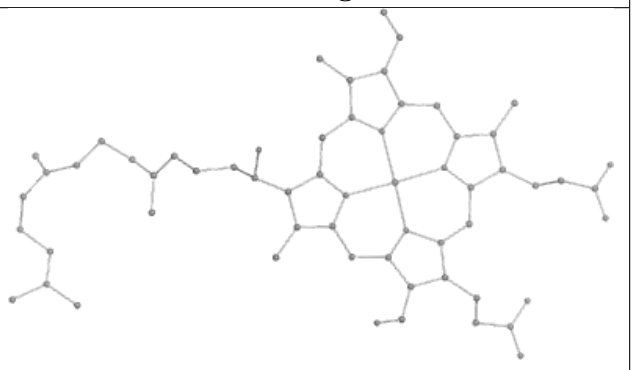
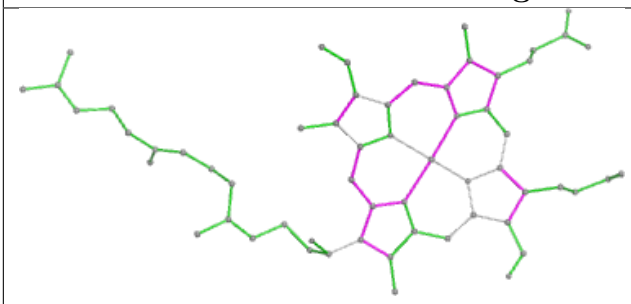


Rings

Ligand HEA 2A 601



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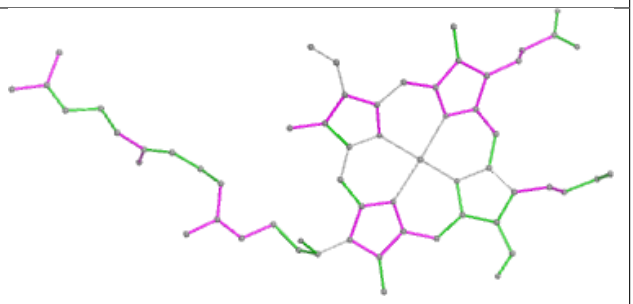

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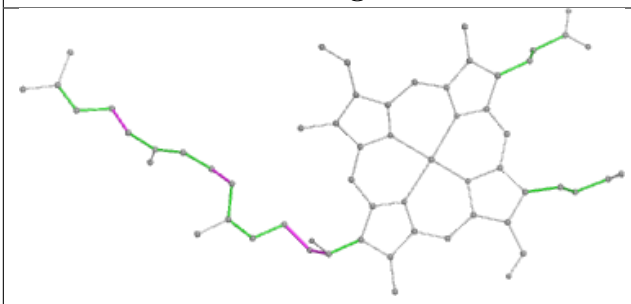

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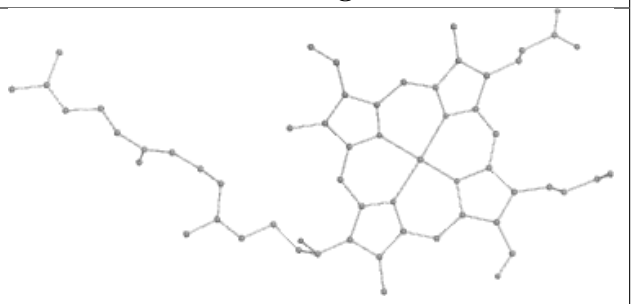
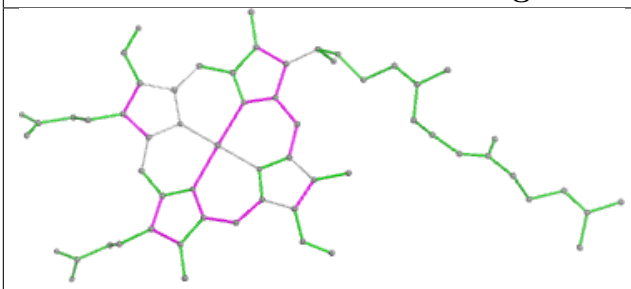


Rings

Ligand HEA 4A 602



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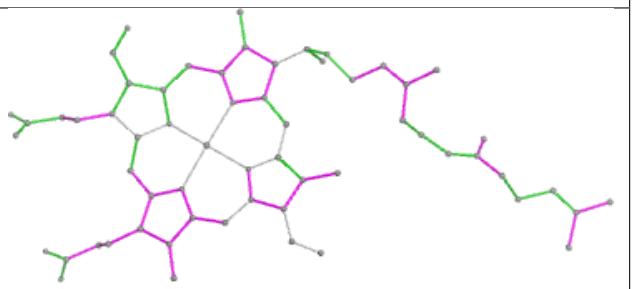
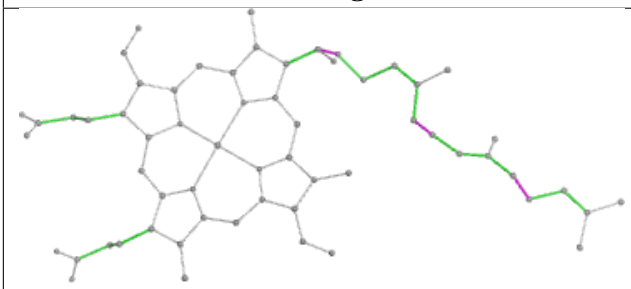


Bond angles



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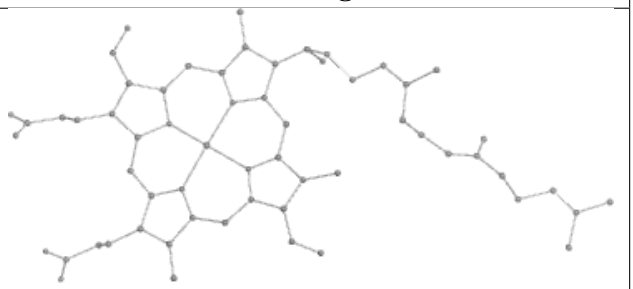
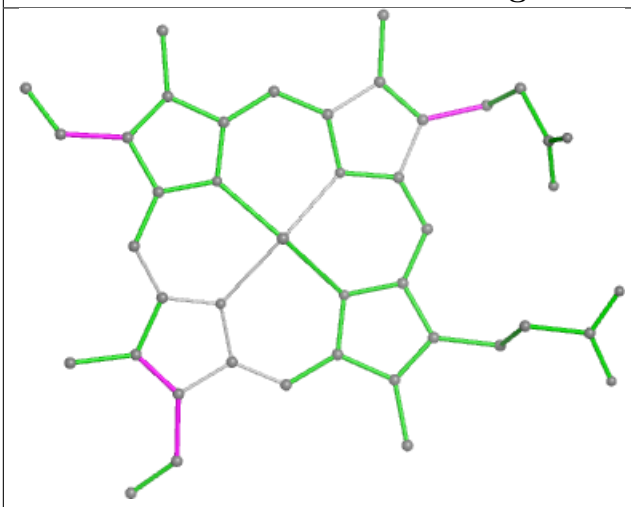


Rings

Ligand HEM 6A 402



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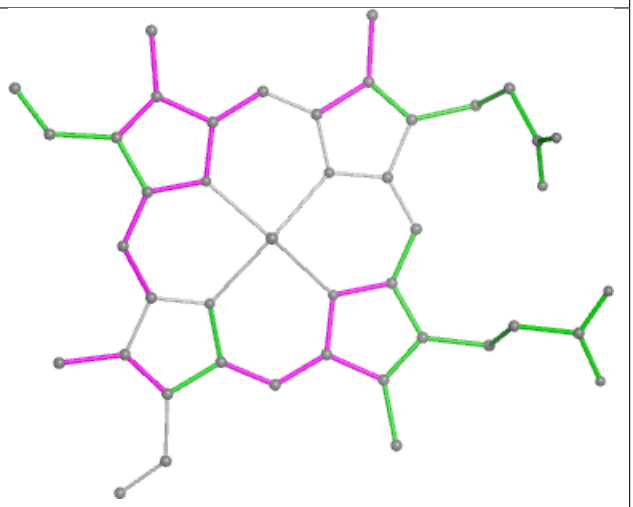

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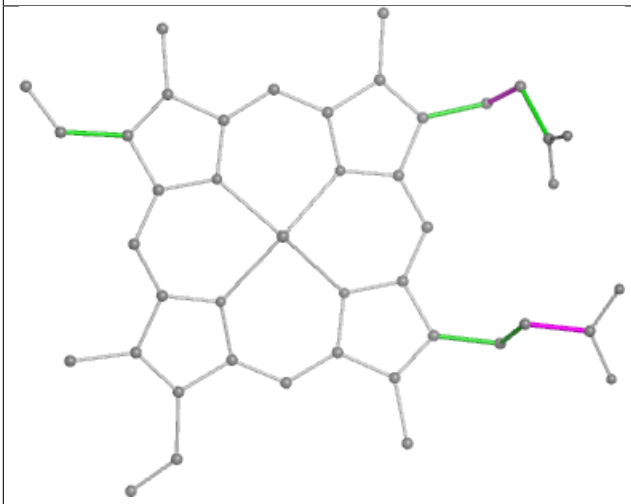

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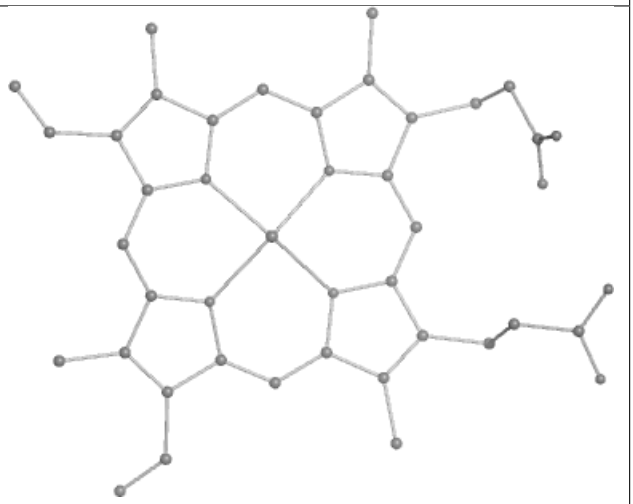
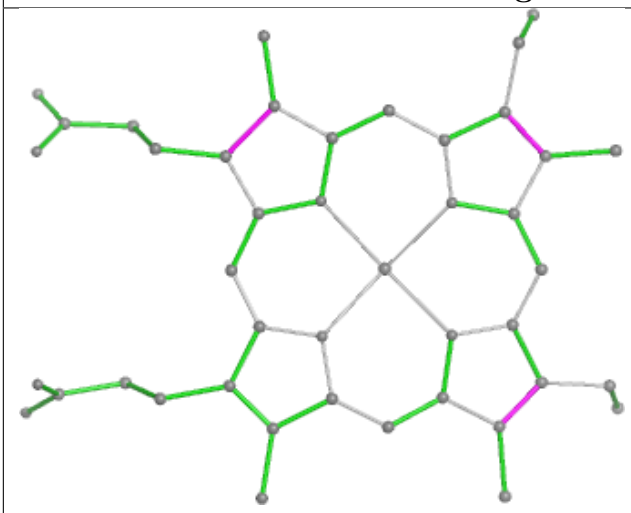


Rings

Ligand HEC 1E 401



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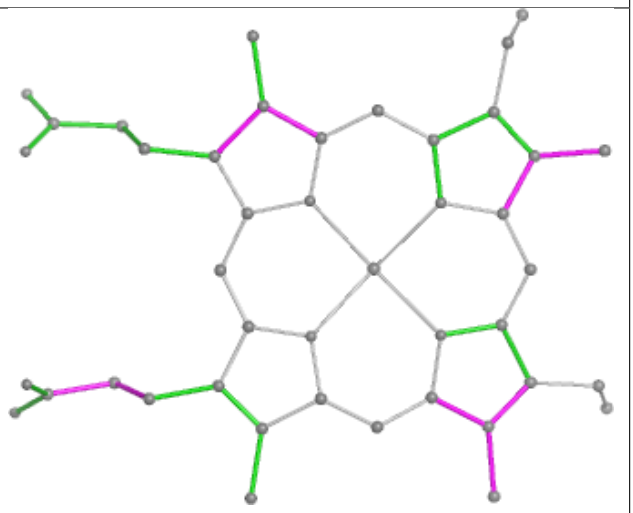
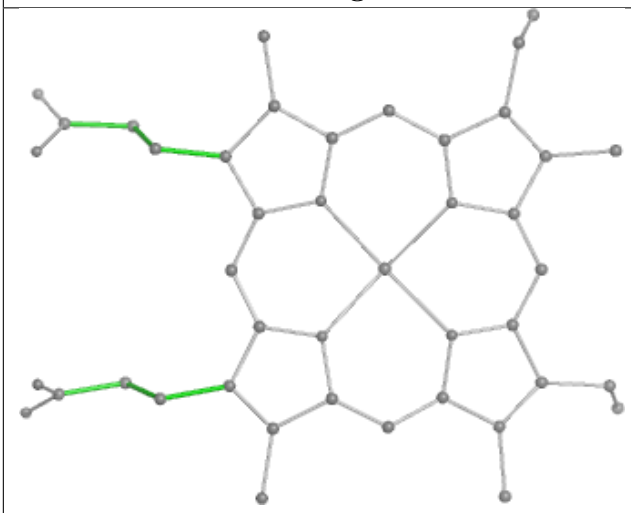


Bond angles



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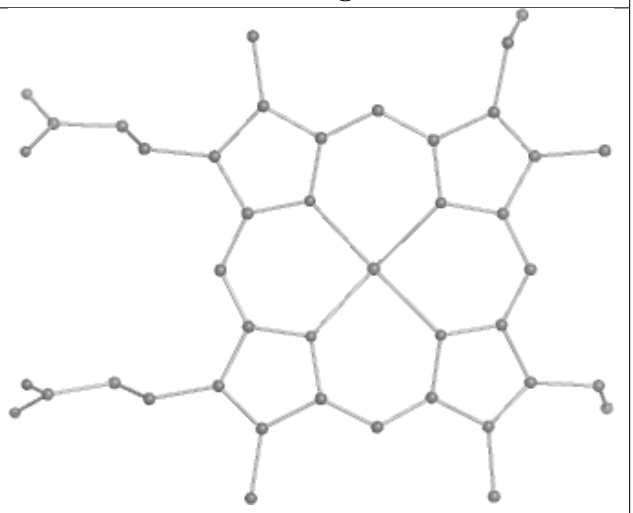
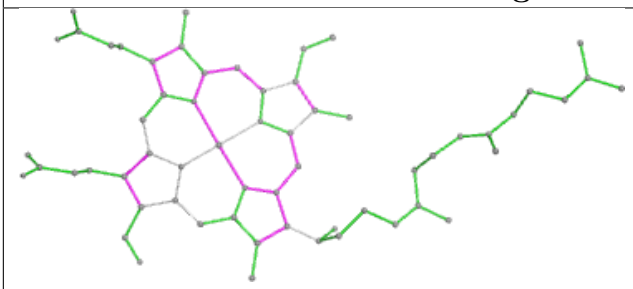


Rings

Ligand HEA 9A 603



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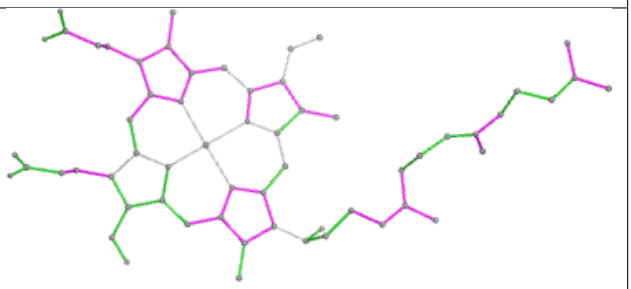
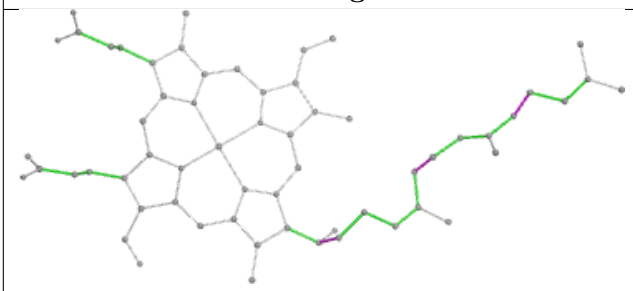


Bond angles



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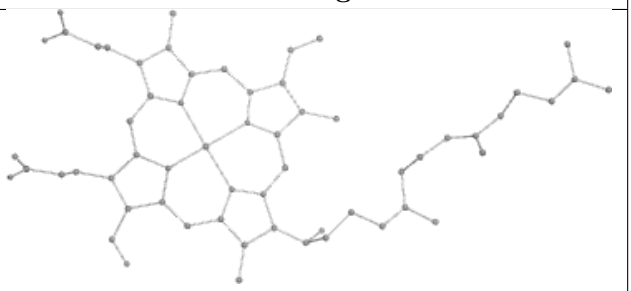
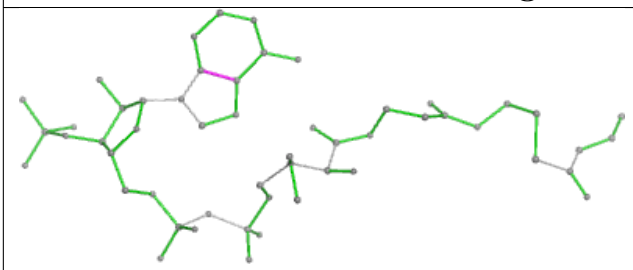


Rings

Ligand COO 5s 401



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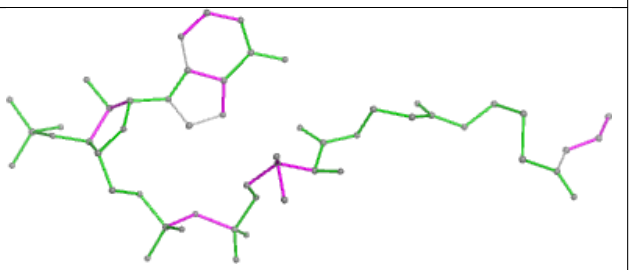
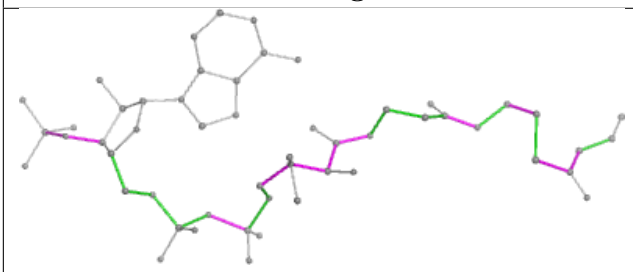


Bond angles



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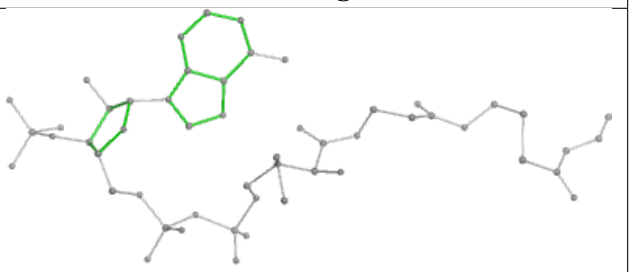
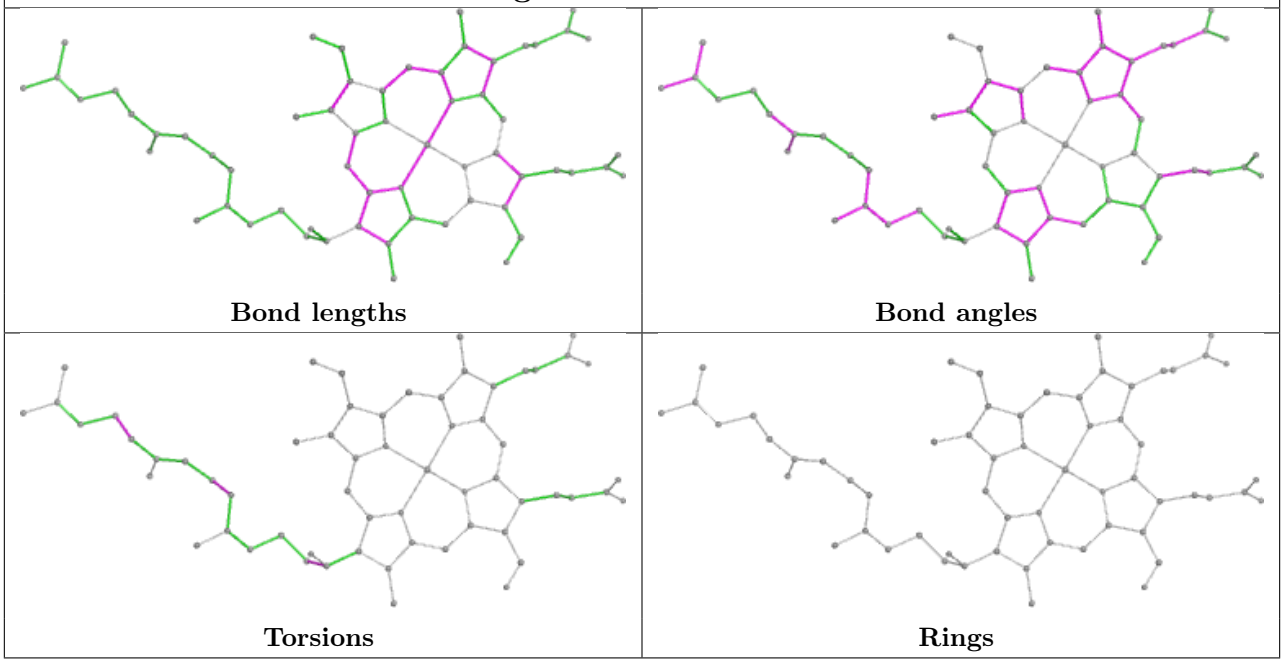


Rings

Ligand HEA 8A 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

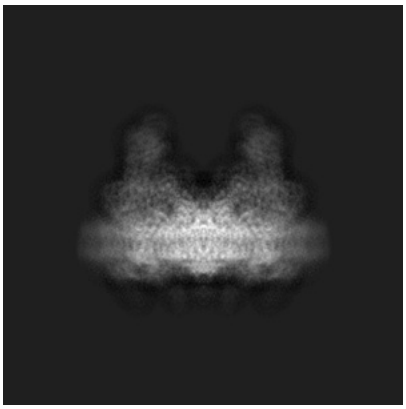
6 Map visualisation

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.

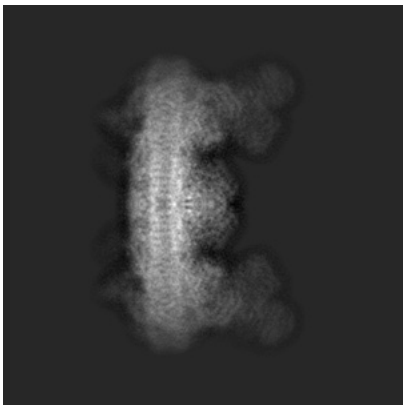
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

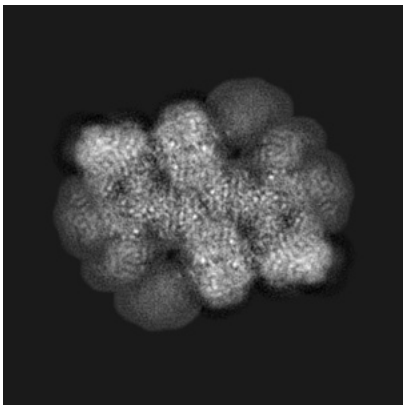
6.1.1 Primary map



X

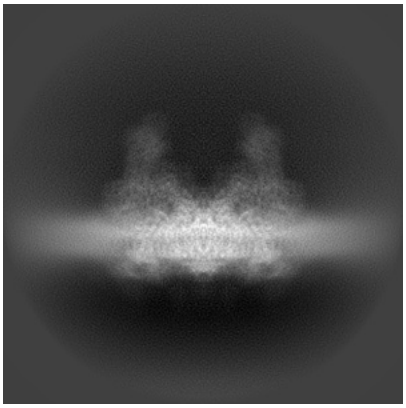


Y

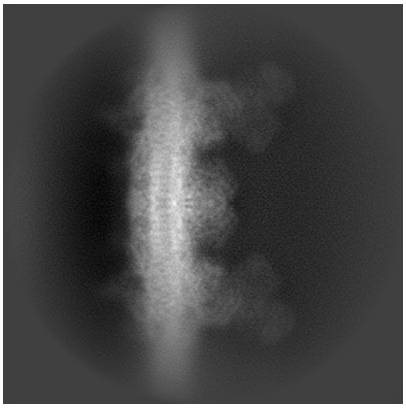


Z

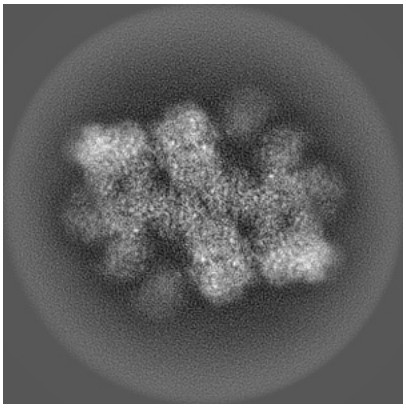
6.1.2 Raw map



X



Y

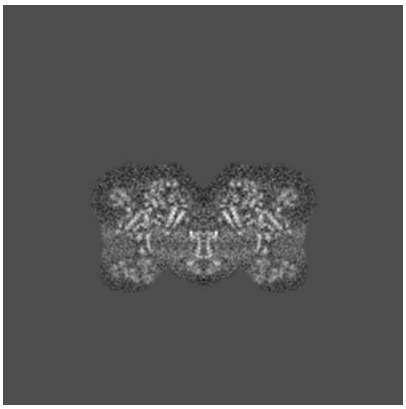


Z

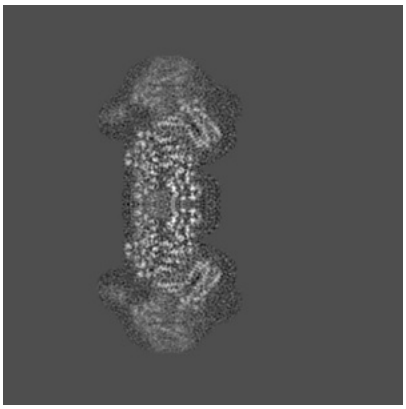
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

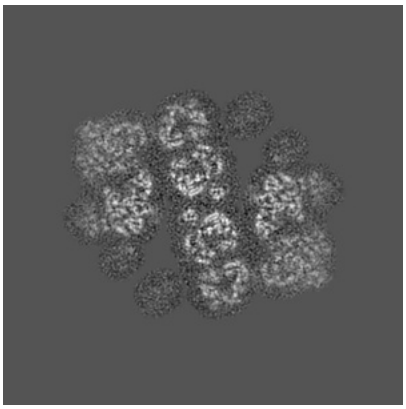
6.2.1 Primary map



X Index: 144

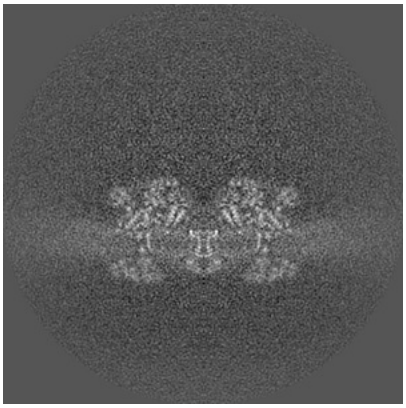


Y Index: 144

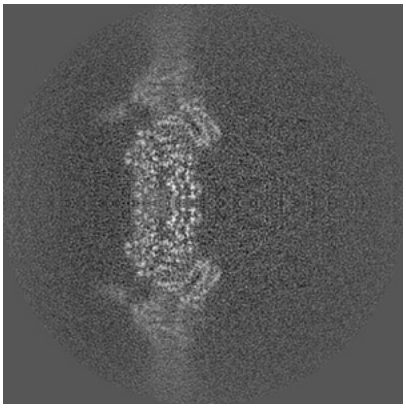


Z Index: 144

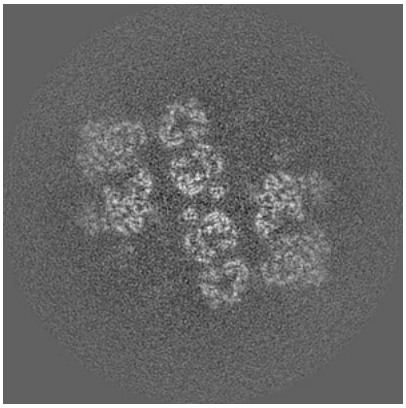
6.2.2 Raw map



X Index: 144



Y Index: 144

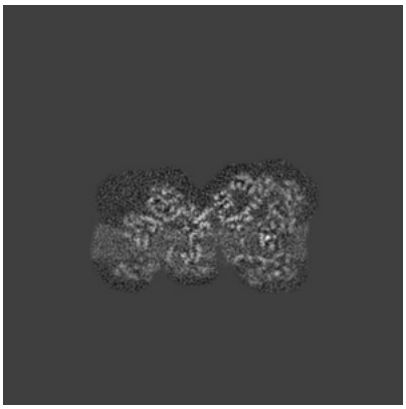


Z Index: 144

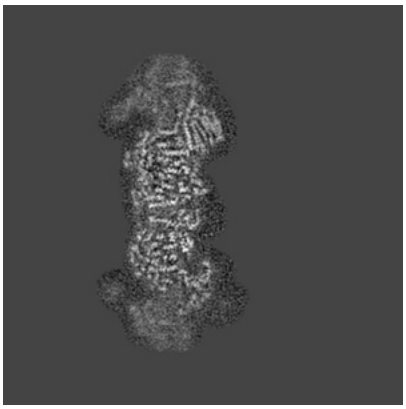
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

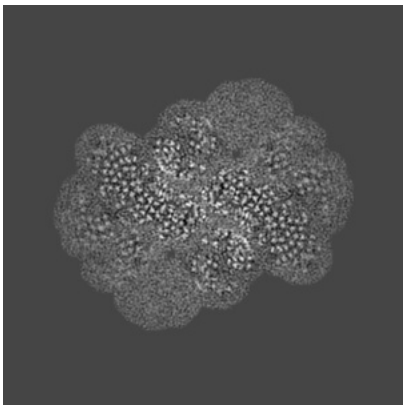
6.3.1 Primary map



X Index: 139

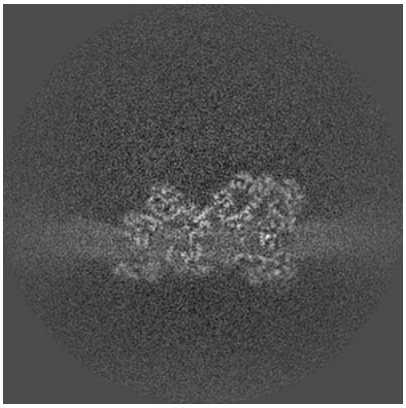


Y Index: 148

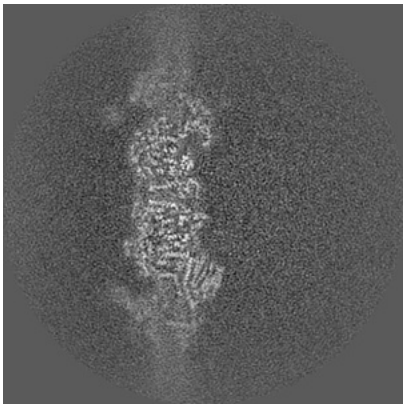


Z Index: 123

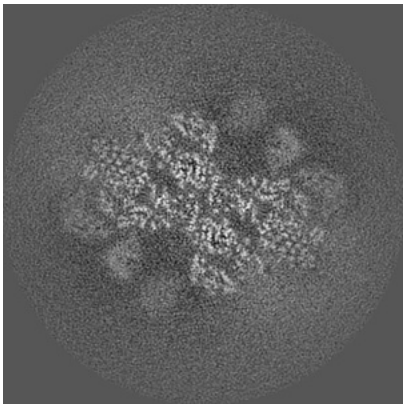
6.3.2 Raw map



X Index: 139



Y Index: 140

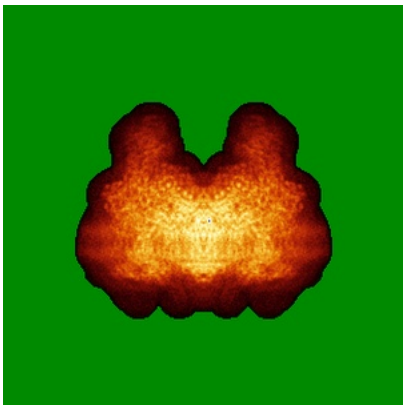


Z Index: 134

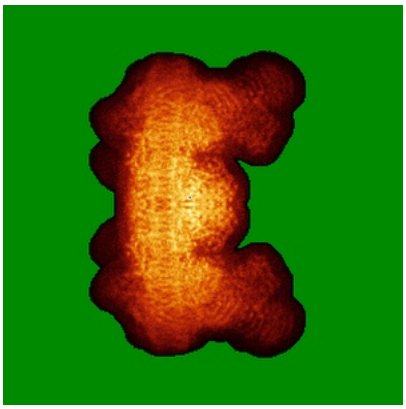
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

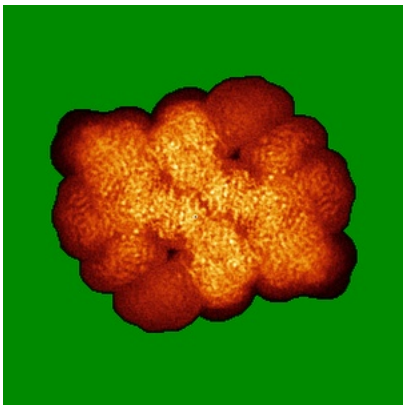
6.4.1 Primary map



X

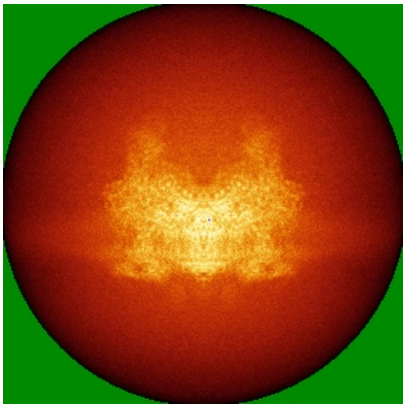


Y

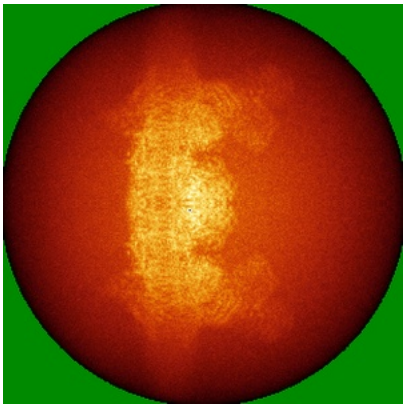


Z

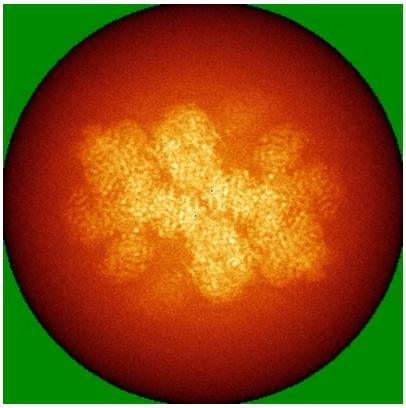
6.4.2 Raw map



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.

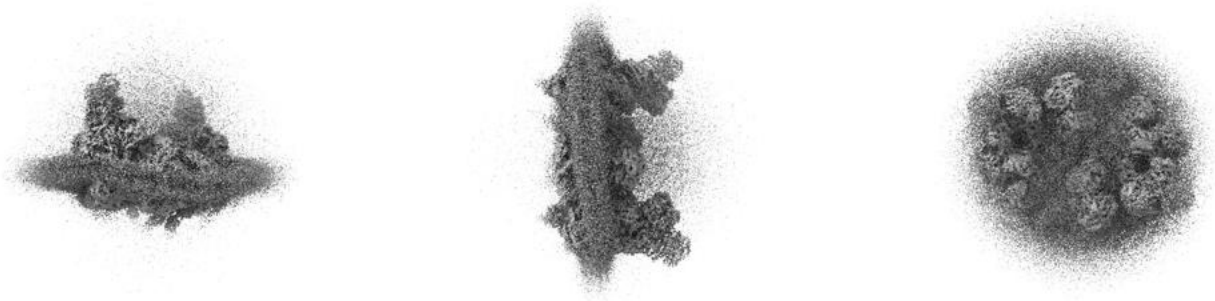
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

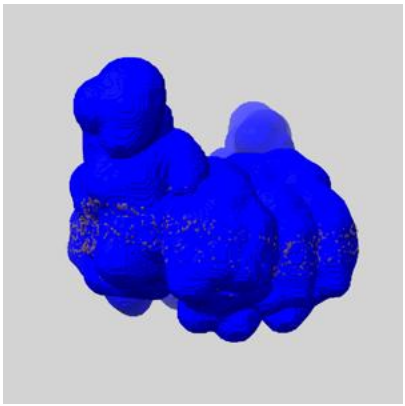
6.6 Mask visualisation (i)

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

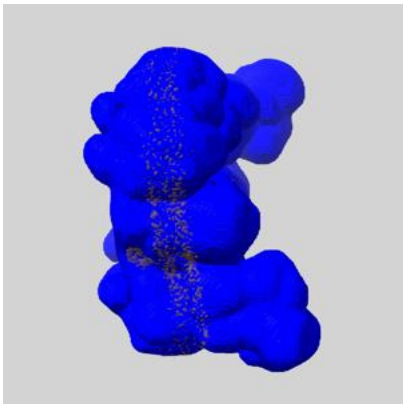
A mask typically either:

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

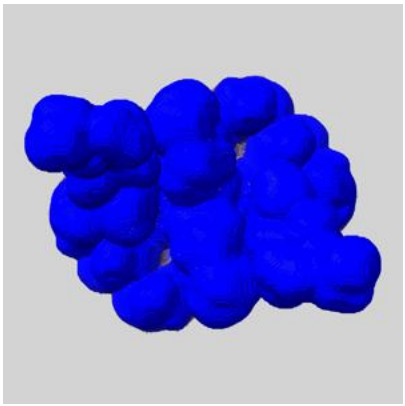
6.6.1 emd_50210_msk_1.map (i)



X



Y

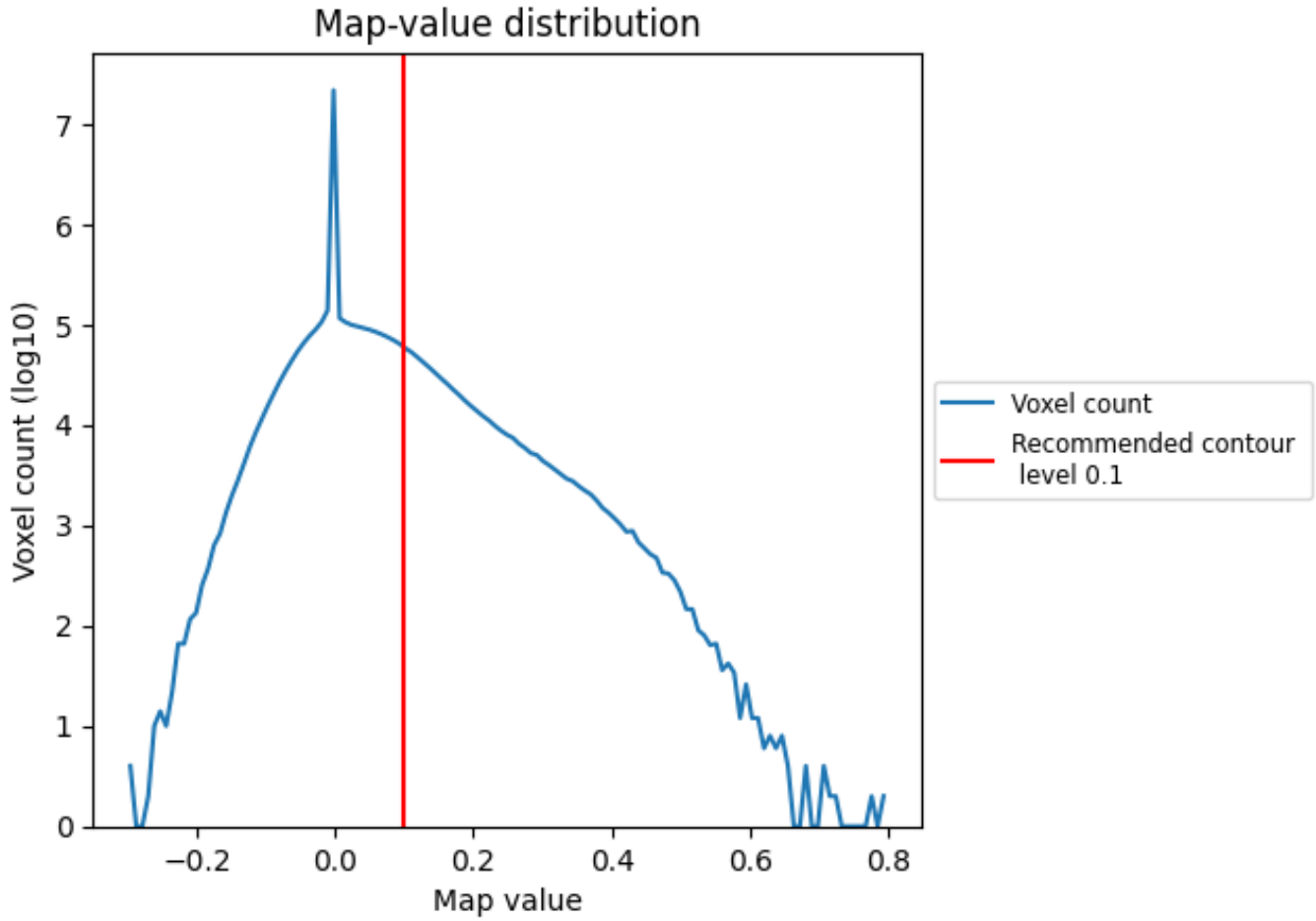


Z

7 Map analysis

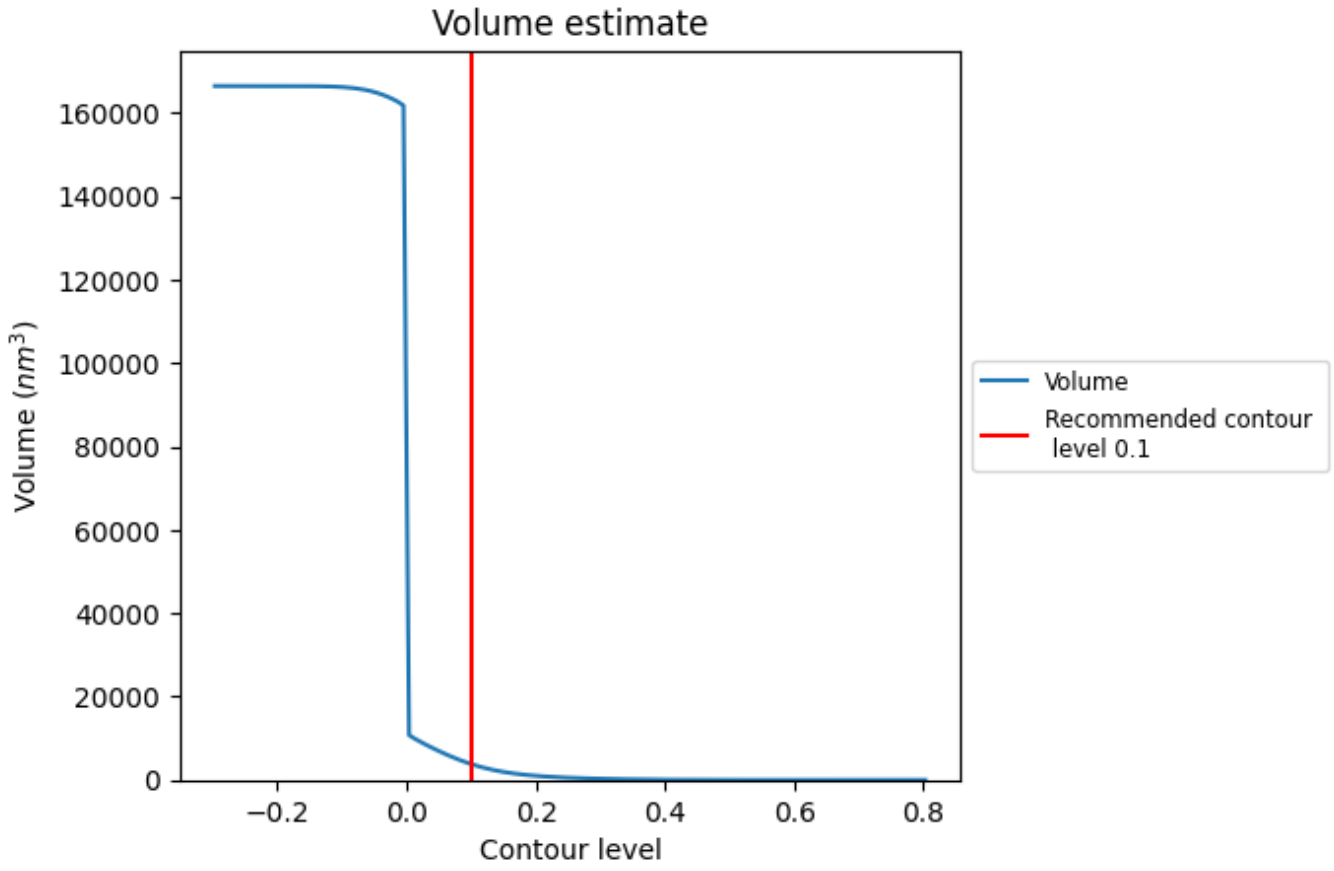
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

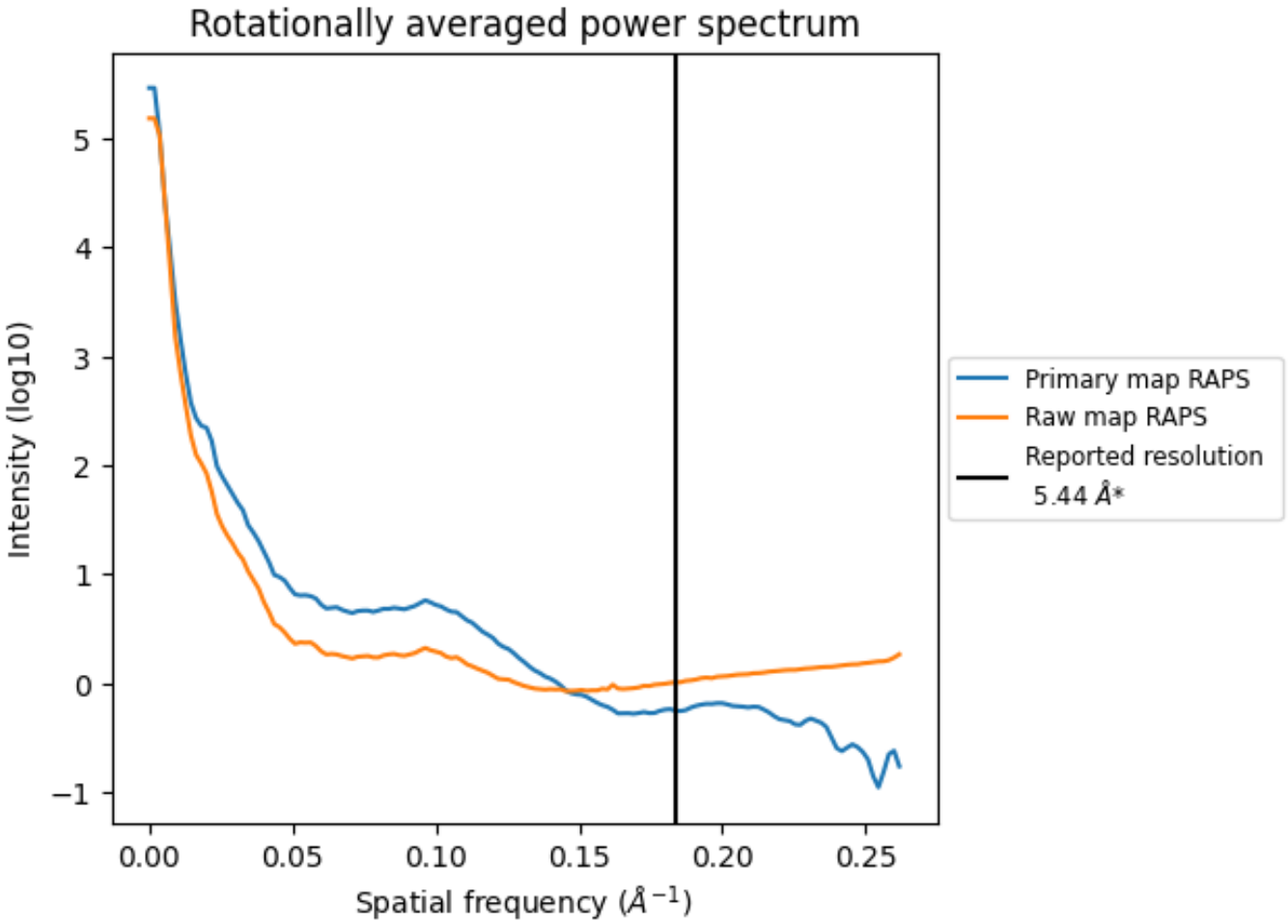
7.2 Volume estimate



The volume at the recommended contour level is 3804 nm^3; 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 (i)

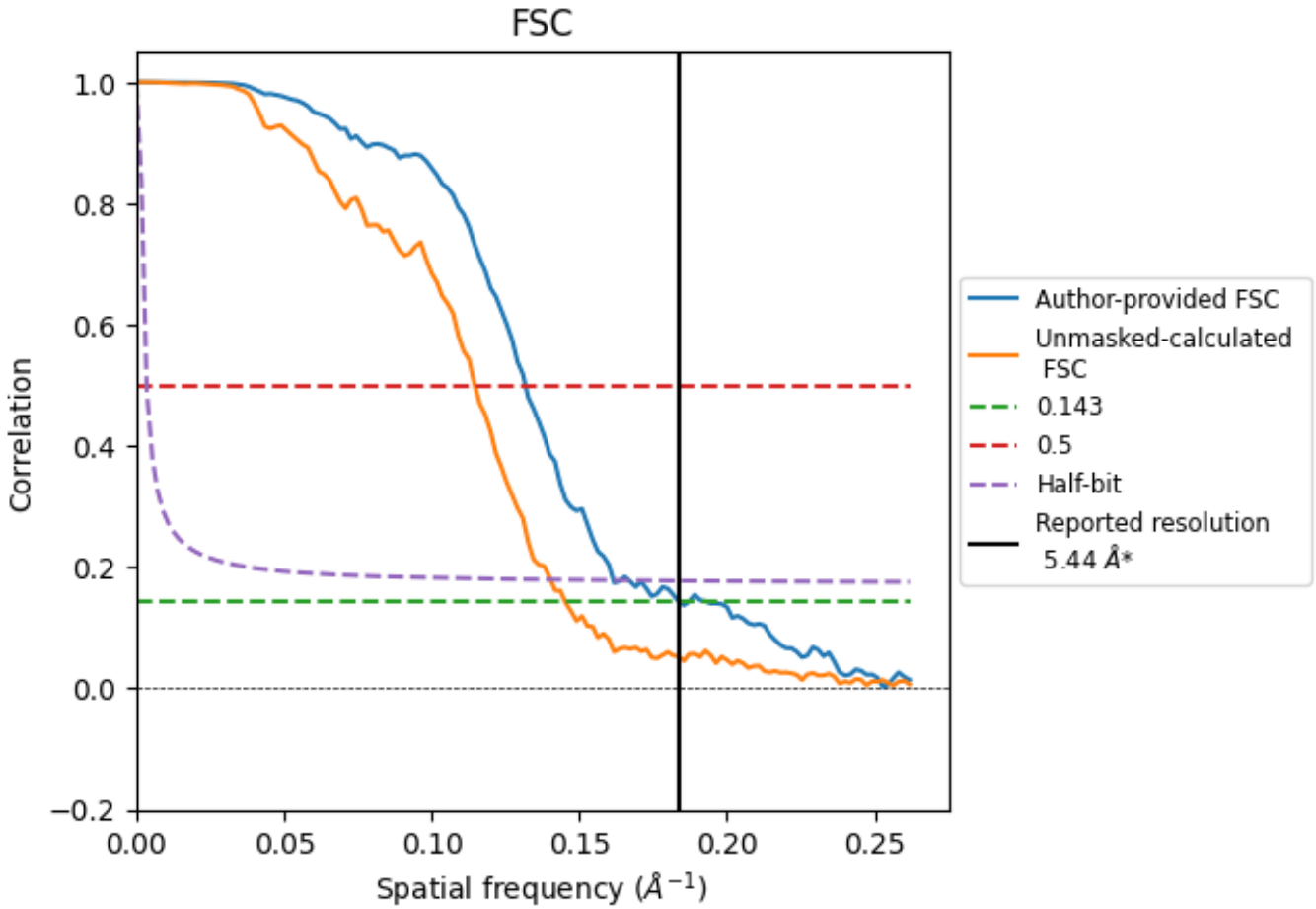


*Reported resolution corresponds to spatial frequency of 0.184 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.184 Å^{-1}

8.2 Resolution estimates (i)

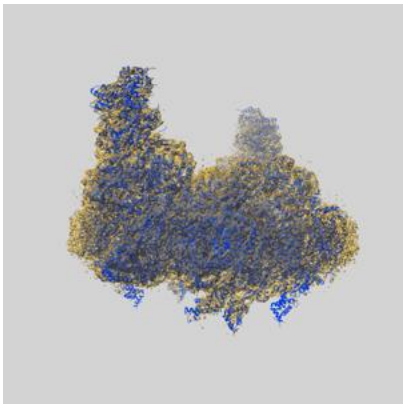
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.44	-	-
Author-provided FSC curve	5.45	7.59	6.19
Unmasked-calculated*	6.88	8.73	7.13

*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 %

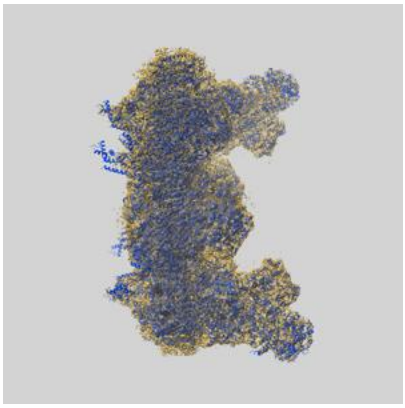
9 Map-model fit

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.

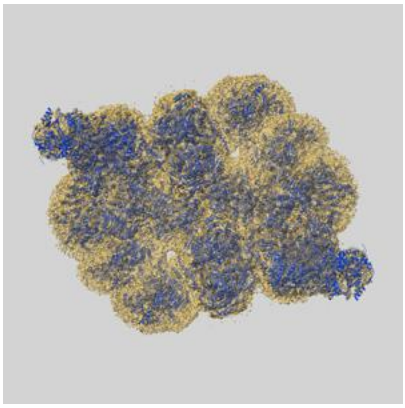
9.1 Map-model overlay



X



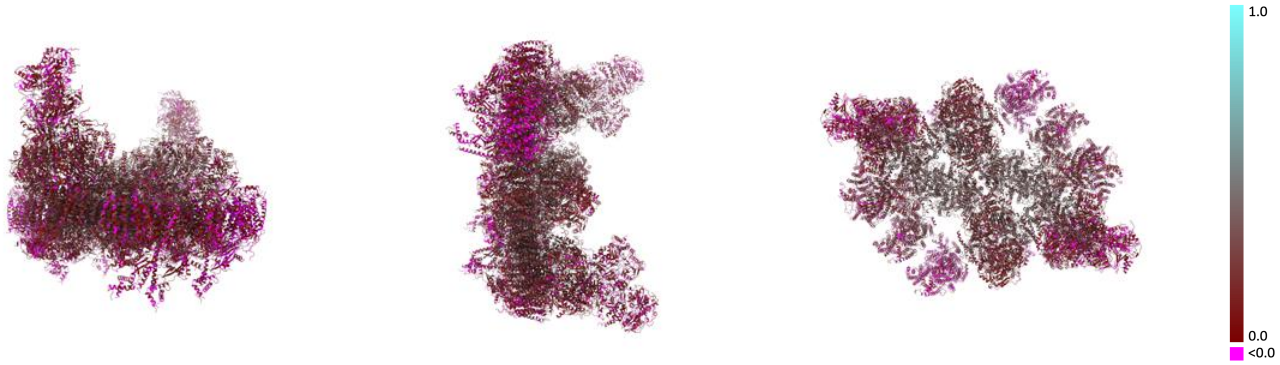
Y



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.

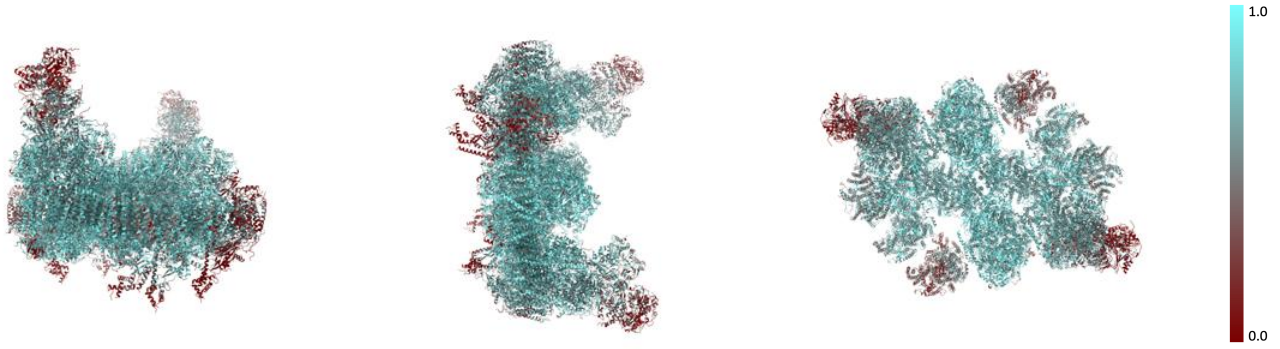
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

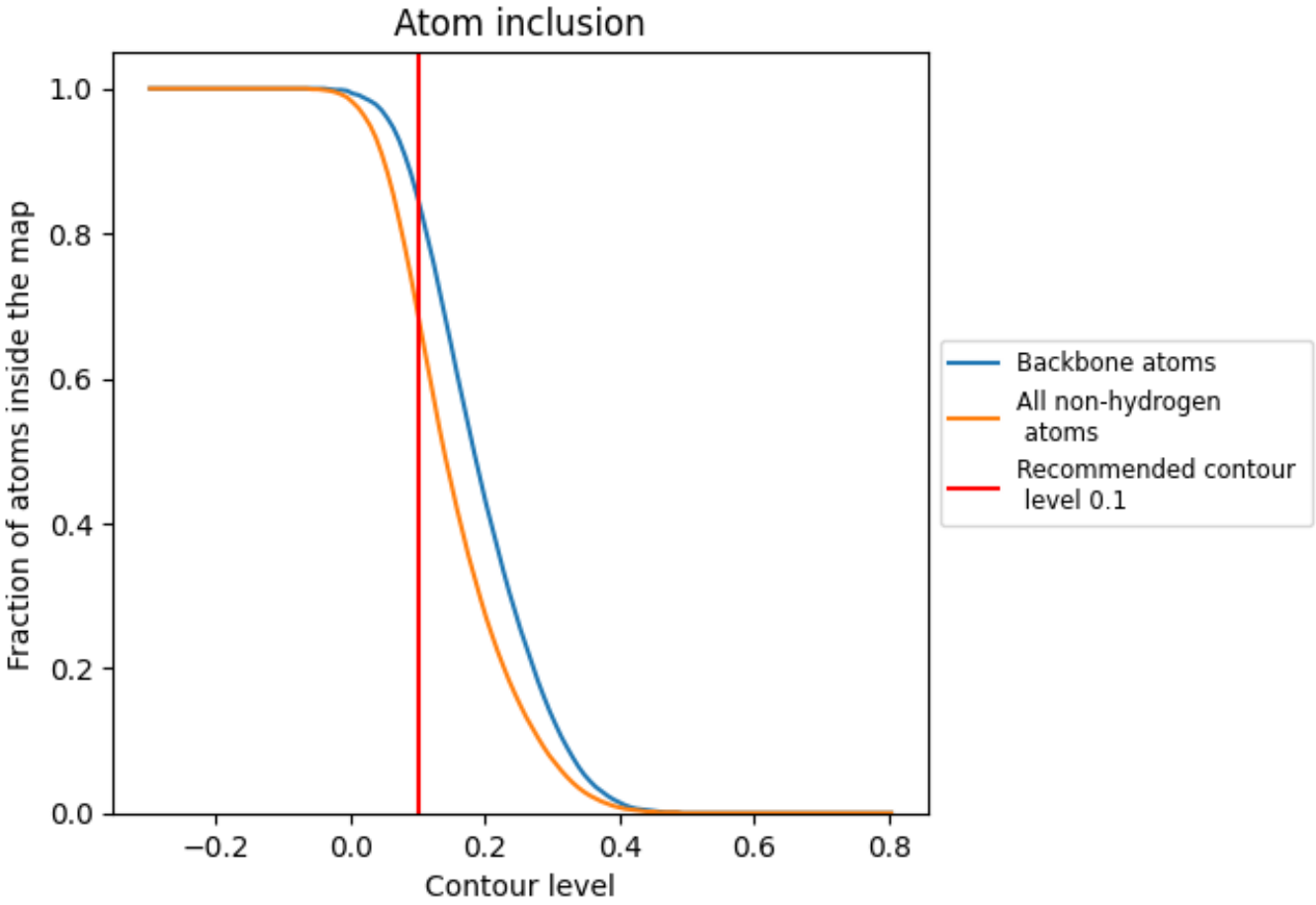
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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