



wwPDB EM Validation Summary Report ⓘ

Jan 11, 2025 – 01:06 PM EST

PDB ID : 8UCA
EMDB ID : EMD-42122
Title : Formation of I2+III2 supercomplex rescues respiratory chain defects
Authors : Letts, J.A.; Padavannil, A.
Deposited on : 2023-09-26
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

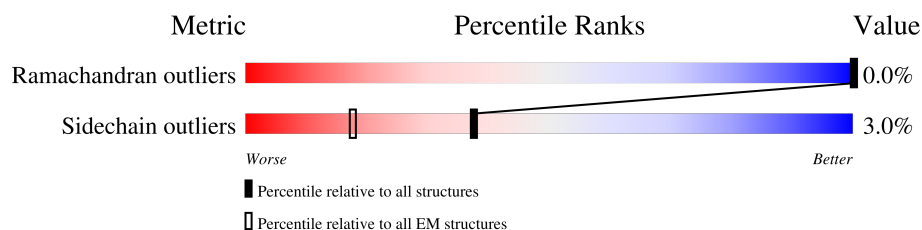
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.70 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	115	
1	3a	115	
2	S3	263	
2	s3	263	
3	S2	463	
3	s2	463	
4	1	318	
4	1a	318	
5	6	172	

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Mol	Chain	Length	Quality of chain
5	6a	172	
6	4L	98	
6	4l	98	
7	5	607	
7	5a	607	
8	4	459	
8	4a	459	
9	2	345	
9	2a	345	
10	AL	355	
10	al	355	
11	A9	377	
11	a9	377	
12	S4	175	
12	s4	175	
13	S6	116	
13	s6	116	
14	A2	99	
14	a2	99	
15	AB	156	
15	AC	156	
15	ab	156	
15	ac	156	
16	A5	116	
16	a5	116	

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Mol	Chain	Length	Quality of chain
17	A6	131	
17	a6	131	
18	A8	172	
18	a8	172	
19	AM	142	
19	am	142	
20	AO	144	
20	ao	144	
21	A1	70	
21	a1	70	
22	A3	84	
22	a3	84	
23	C1	76	
23	c1	76	
24	C2	120	
24	c2	120	
25	S5	106	
25	s5	106	
26	B1	57	
26	b1	57	
27	BM	151	
27	bm	151	
28	B5	189	
28	b5	189	
29	B6	127	

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Mol	Chain	Length	Quality of chain
29	b6	127	
30	B2	105	
30	b2	105	
31	B3	104	
31	b3	104	
32	B8	186	
32	b8	186	
33	B4	129	
33	b4	129	
34	B9	179	
34	b9	179	
35	B7	136	
35	b7	136	
36	BL	176	
36	bl	176	
37	AN	145	
37	an	145	
38	A7	112	
38	a7	112	
39	V3	104	
39	v3	104	
40	3A	446	
40	3L	446	
41	3B	439	
41	3M	439	

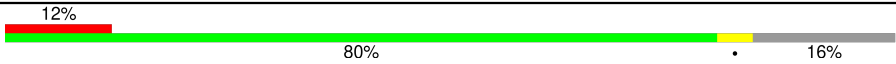

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Mol	Chain	Length	Quality of chain
42	3C	380	
42	3N	380	
43	3D	241	
43	3O	241	
44	3E	196	
44	3P	196	
45	3F	110	
45	3Q	110	
46	3G	81	
46	3R	81	
47	3H	76	
47	3S	76	
48	3J	63	
48	3U	63	
49	3K	56	
49	3V	56	
50	3T	78	
51	V1	457	
51	v1	457	
52	V2	244	
52	v2	244	
53	S1	716	
53	s1	716	
54	S7	224	
54	s7	224	

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Mol	Chain	Length	Quality of chain
55	S8	212	
55	s8	212	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 162102 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	113	Total	C	N	O	S	0	0
			914	622	131	155	6		
1	3a	111	Total	C	N	O	S	0	0
			893	607	128	152	6		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S3	206	Total	C	N	O	S	0	0
			1712	1105	294	310	3		
2	s3	205	Total	C	N	O	S	0	0
			1701	1099	290	309	3		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S2	423	Total	C	N	O	S	0	0
			3410	2180	586	620	24		
3	s2	421	Total	C	N	O	S	0	0
			3386	2165	581	616	24		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	317	Total	C	N	O	S	0	0
			2530	1700	383	426	21		
4	1a	316	Total	C	N	O	S	0	0
			2522	1695	382	425	20		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	170	Total	C	N	O	S	0	0
			1290	868	184	224	14		
5	6a	171	Total	C	N	O	S	0	0
			1298	873	185	225	15		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4L	97	Total	C	N	O	S	0	0
			729	473	111	135	10		
6	4l	97	Total	C	N	O	S	0	0
			727	471	111	135	10		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	605	Total	C	N	O	S	0	0
			4790	3175	745	825	45		
7	5a	605	Total	C	N	O	S	0	0
			4790	3175	745	825	45		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		
8	4a	459	Total	C	N	O	S	0	0
			3630	2407	567	616	40		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		
9	2a	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	al	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		
11	a9	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S4	126	Total	C	N	O	S	0	0
			1021	646	179	192	4		
12	s4	126	Total	C	N	O	S	0	0
			1021	646	179	192	4		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S6	95	Total	C	N	O	S	0	0
			748	464	138	143	3		
13	s6	95	Total	C	N	O	S	0	0
			748	464	138	143	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	84	Total	C	N	O	S	0	0
			671	421	127	120	3		
14	a2	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 15 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AB	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
15	AC	88	Total	C	N	O	S	0	0
			706	453	104	144	5		
15	ab	78	Total	C	N	O	S	0	0
			628	404	93	126	5		
15	ac	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A5	114	Total	C	N	O	S	0	0
			927	604	154	166	3		
16	a5	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A6	112	Total	C	N	O	S	0	0
			957	612	178	161	6		
17	a6	111	Total	C	N	O	S	0	0
			950	607	177	160	6		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A8	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		
18	a8	170	Total	C	N	O	S	0	0
			1389	884	249	246	10		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AM	141	Total	C	N	O	S	0	0
			1045	667	176	193	9		
19	am	141	Total	C	N	O	S	0	0
			1045	667	176	193	9		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AO	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		
20	ao	140	Total	C	N	O	S	0	0
			1161	747	206	200	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A1	69	Total	C	N	O	S	0	0
			564	366	100	94	4		
21	a1	69	Total	C	N	O	S	0	0
			564	366	100	94	4		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A3	83	Total	C	N	O	S	0	0
			648	425	105	114	4		
22	a3	83	Total	C	N	O	S	0	0
			648	425	105	114	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C1	49	Total	C	N	O	S	0	0
			407	266	70	70	1		
23	c1	45	Total	C	N	O	S	0	0
			377	247	65	64	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C2	120	Total	C	N	O	S	0	0
			996	651	171	165	9		
24	c2	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S5	105	Total	C	N	O	S	0	0
			877	555	162	152	8		
25	s5	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	56	Total	C	N	O	S	0	0
			482	314	85	81	2		
26	b1	56	Total	C	N	O	S	0	0
			482	314	85	81	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BM	98	Total	C	N	O	S	0	0
			826	536	133	153	4		
27	bm	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		
28	b5	138	Total	C	N	O	S	0	0
			1158	760	193	202	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	94	Total	C	N	O	S	0	0
			783	511	137	132	3		
29	b6	90	Total	C	N	O	S	0	0
			761	495	133	130	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B2	64	Total	C	N	O	S	0	0
			555	365	92	97	1		
30	b2	63	Total	C	N	O	S	0	0
			545	359	89	96	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B3	70	Total	C	N	O	S	0	0
			569	376	99	92	2		
31	b3	71	Total	C	N	O	S	0	0
			573	378	100	93	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B8	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		
32	b8	155	Total	C	N	O	S	0	0
			1302	840	216	235	11		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B4	125	Total	C	N	O		0	0
			1044	673	188	183			
33	b4	125	Total	C	N	O		0	0
			1044	673	188	183			

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B9	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		
34	b9	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B7	114	Total	C	N	O	S	0	0
			984	620	185	171	8		
35	b7	117	Total	C	N	O	S	0	0
			1005	634	189	174	8		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	167	Total	C	N	O	S	0	0
			1410	888	251	263	8		
36	bl	169	Total	C	N	O	S	0	0
			1430	899	257	266	8		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AN	144	Total	C	N	O	S	0	0
			1201	772	214	211	4		
37	an	144	Total	C	N	O	S	0	0
			1201	772	214	211	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A7	92	Total	C	N	O	S	0	0
			741	469	139	130	3		
38	a7	70	Total	C	N	O	S	0	0
			560	350	108	100	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	V3	40	Total	C	N	O	0	0
			339	213	62	64		
39	v3	36	Total	C	N	O	0	0
			303	190	56	57		

- Molecule 40 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
40	3L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 41 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
41	3M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 42 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
42	3N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 43 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
43	3O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 44 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3E	80	Total	C	N	O	S	0	0
			602	374	100	126	2		
44	3P	81	Total	C	N	O	S	0	0
			610	380	101	127	2		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3F	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	3Q	99	Total	C	N	O	S	0	0
			879	563	156	157	3		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3G	79	Total	C	N	O	S	0	0
			670	432	123	114	1		
46	3R	71	Total	C	N	O		0	0
			600	389	112	99			

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
47	3S	66	Total	C	N	O	S	0	0
			545	333	101	106	5		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	3J	56	Total	C	N	O	0	0
			460	302	81	77		
48	3U	59	Total	C	N	O	0	0
			489	320	85	84		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3K	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
49	3V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3T	56	Total	C	N	O	S	0	0
			397	250	76	69	2		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondr-

drial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	V1	428	Total	C	N	O	S	0	0
			3301	2080	590	609	22		
51	v1	422	Total	C	N	O	S	0	0
			3259	2053	584	600	22		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V2	209	Total	C	N	O	S	0	0
			1630	1038	273	308	11		
52	v2	192	Total	C	N	O	S	0	0
			1517	965	255	286	11		

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S1	687	Total	C	N	O	S	0	0
			5290	3318	918	1013	41		
53	s1	687	Total	C	N	O	S	0	0
			5290	3318	918	1013	41		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S7	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		
54	s7	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

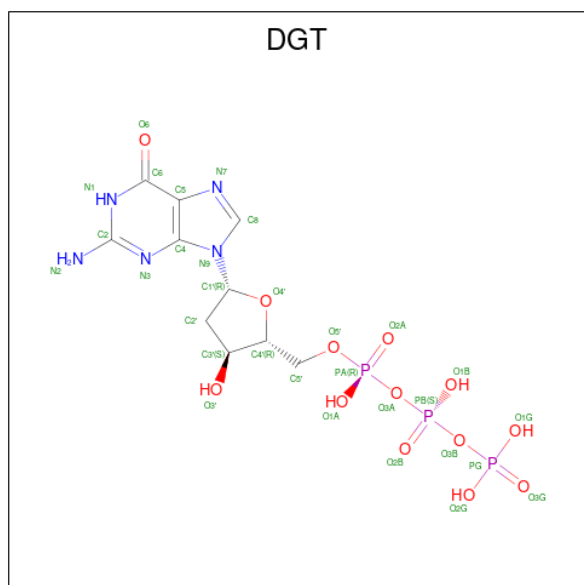
- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

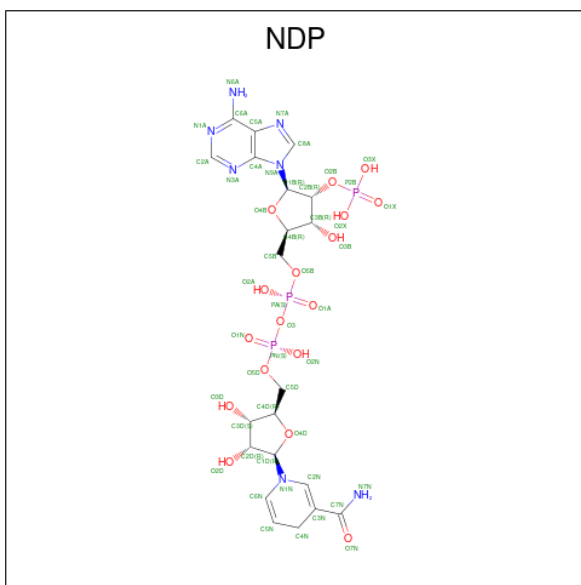
Mol	Chain	Residues	Atoms					AltConf	Trace
55	S8	178	Total	C	N	O	S	0	0
			1408	885	243	268	12		
55	s8	164	Total	C	N	O	S	0	0
			1309	821	226	250	12		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AL	1	Total	Mg	0
			1	1	
56	al	1	Total	Mg	0
			1	1	

- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



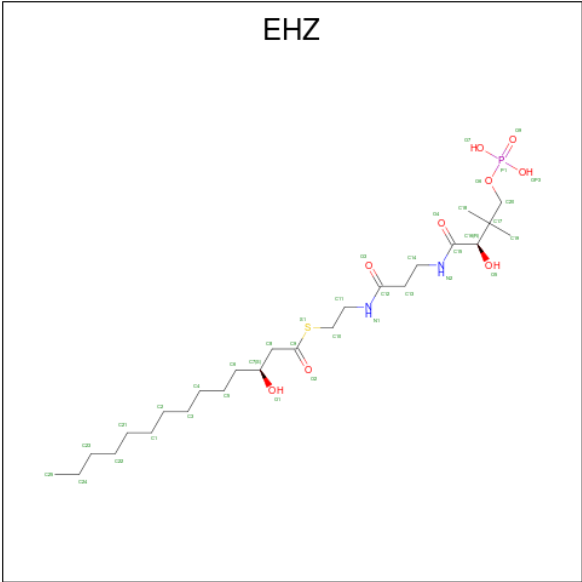


Mol	Chain	Residues	Atoms					AltConf
58	A9	1	Total 48	C 21	N 7	O 17	P 3	0
58	a9	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

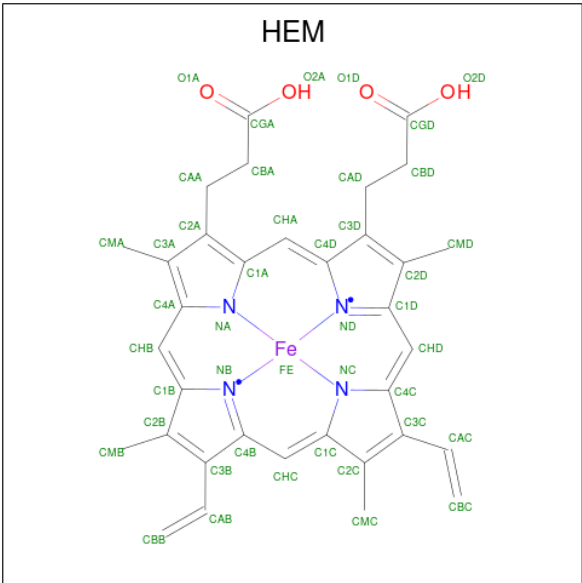
Mol	Chain	Residues	Atoms	AltConf
59	S6	1	Total Zn 1 1	0
59	s6	1	Total Zn 1 1	0

- Molecule 60 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



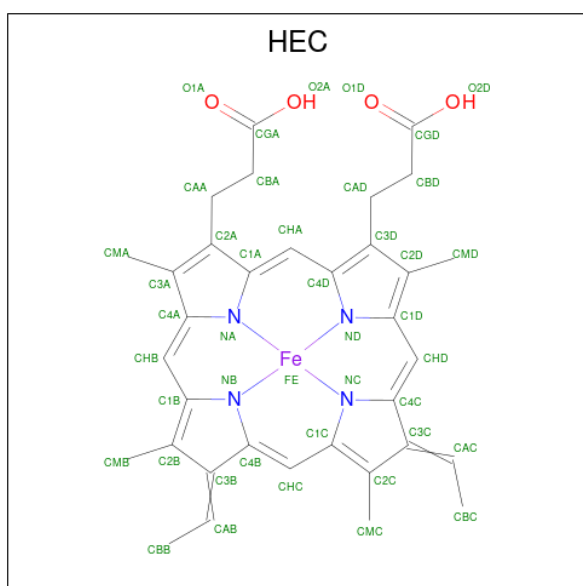
Mol	Chain	Residues	Atoms						AltConf
60	A6	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
60	B9	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
60	5a	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
60	a6	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 61 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



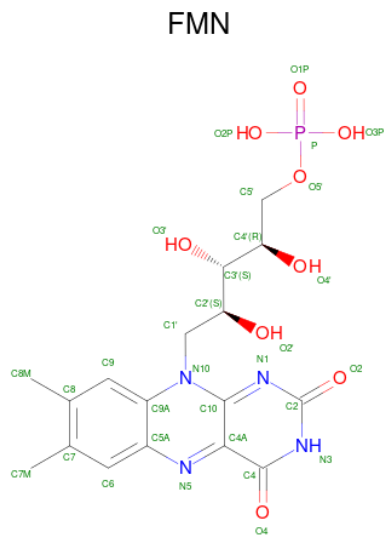
Mol	Chain	Residues	Atoms					AltConf
61	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
61	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
61	3N	1	Total 43	C 34	Fe 1	N 4	O 4	0
61	3N	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 62 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



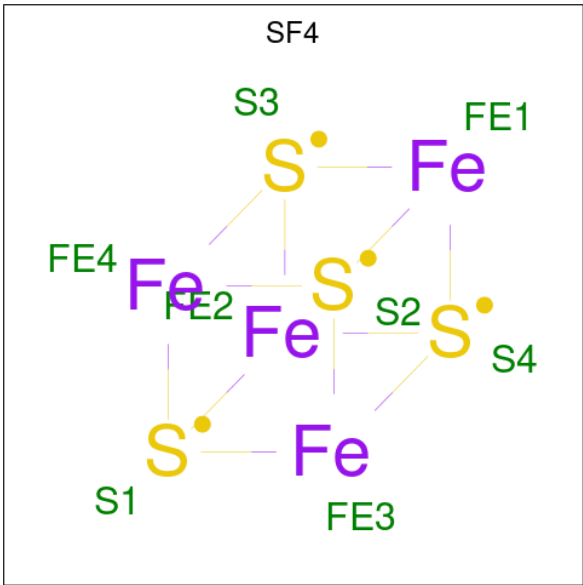
Mol	Chain	Residues	Atoms					AltConf
62	3D	1	Total 43	C 34	Fe 1	N 4	O 4	0
62	3O	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 63 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
63	V1	1	Total 31	C 17	N 4	O 9	P 1	0
63	v1	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 64 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



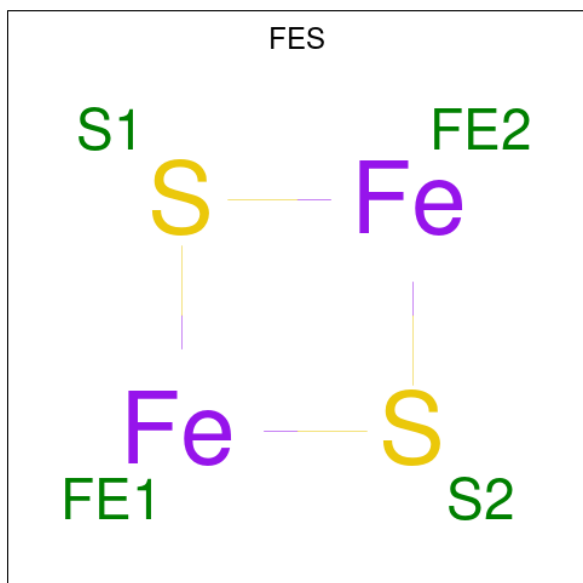
Mol	Chain	Residues	Atoms			AltConf
64	V1	1	Total 8	Fe 4	S 4	0
64	S1	1	Total 8	Fe 4	S 4	0

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Mol	Chain	Residues	Atoms			AltConf
64	S1	1	Total 8	Fe 4	S 4	0
64	S7	1	Total 8	Fe 4	S 4	0
64	S8	1	Total 8	Fe 4	S 4	0
64	S8	1	Total 8	Fe 4	S 4	0
64	v1	1	Total 8	Fe 4	S 4	0
64	s1	1	Total 8	Fe 4	S 4	0
64	s1	1	Total 8	Fe 4	S 4	0
64	s7	1	Total 8	Fe 4	S 4	0
64	s8	1	Total 8	Fe 4	S 4	0
64	s8	1	Total 8	Fe 4	S 4	0

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
65	V2	1	Total 4	Fe 2	S 2	0

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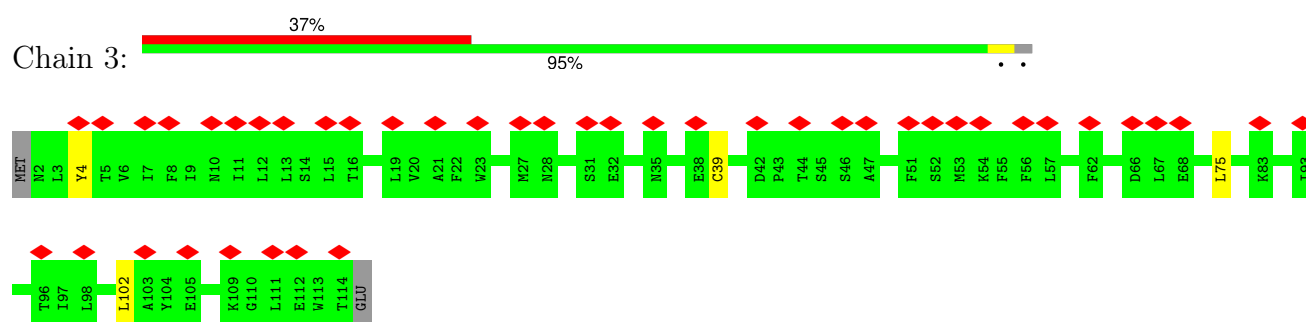
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Mol	Chain	Residues	Atoms			AltConf
65	S1	1	Total 4	Fe 2	S 2	0
65	v2	1	Total 4	Fe 2	S 2	0
65	s1	1	Total 4	Fe 2	S 2	0

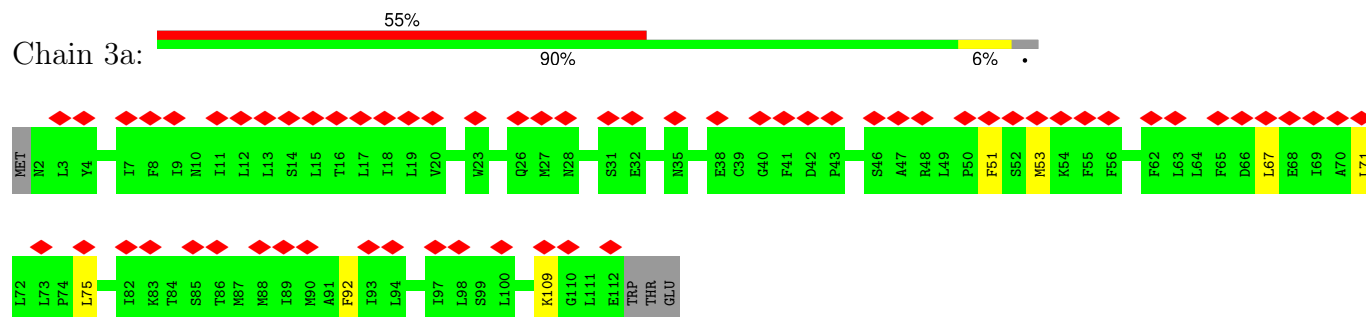
3 Residue-property plots [i](#)

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

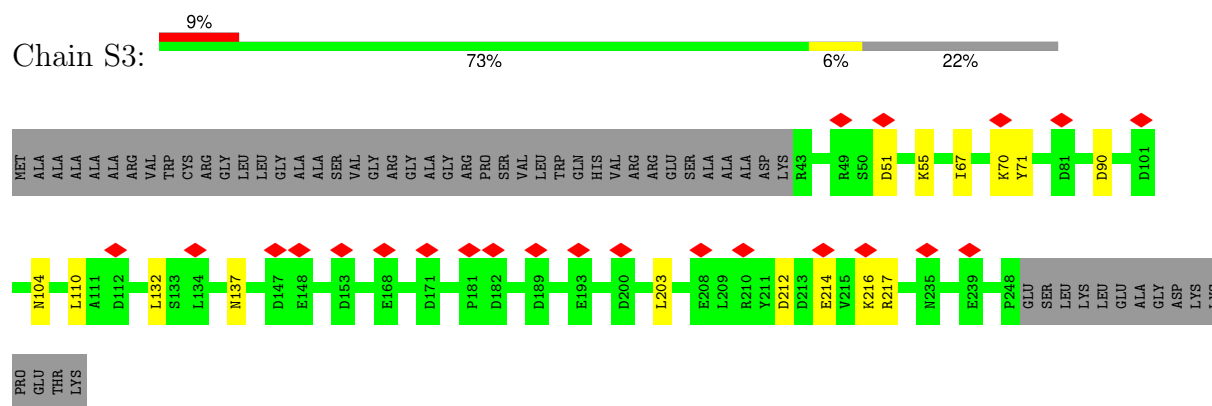
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



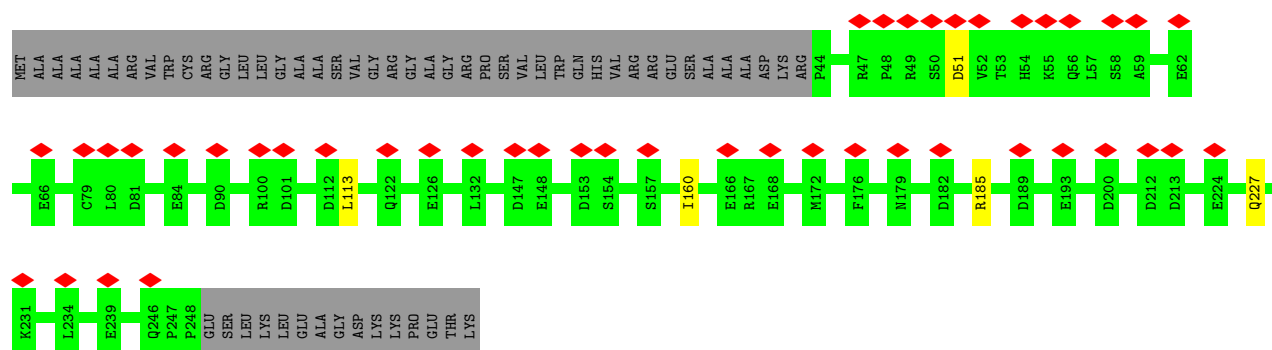
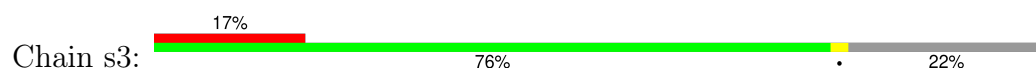
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



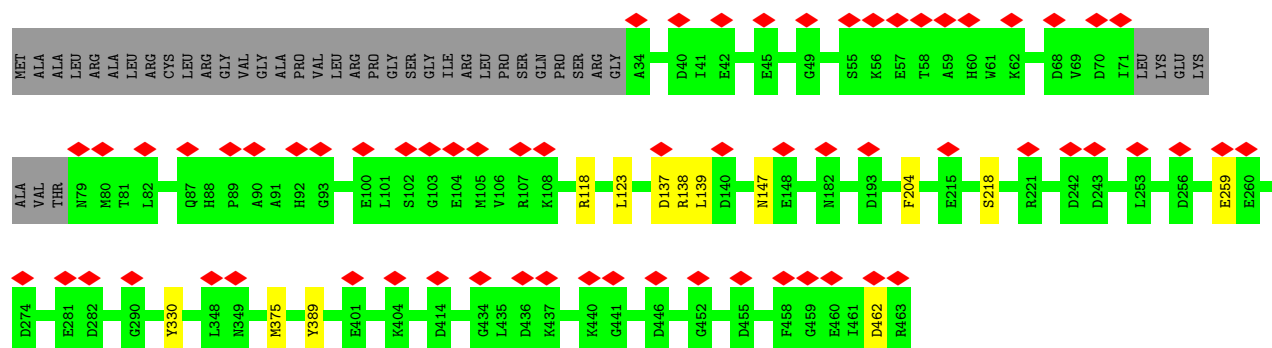
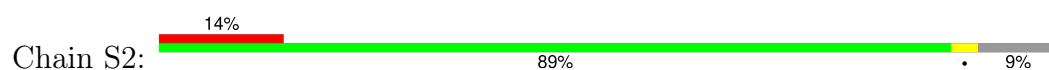
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



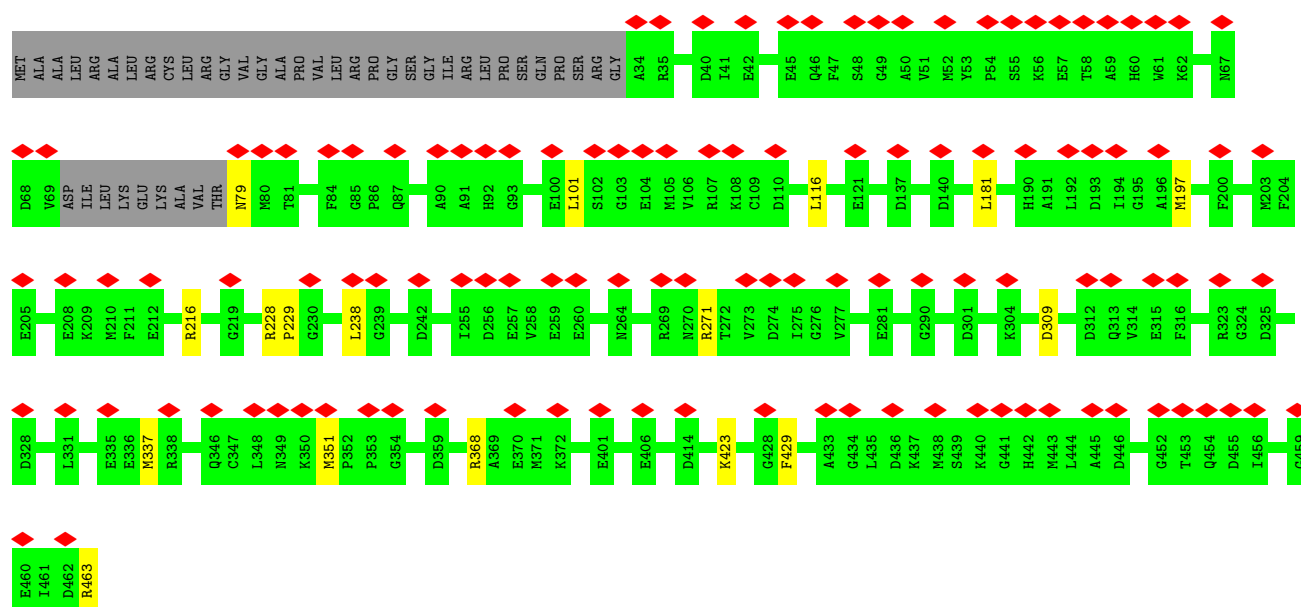
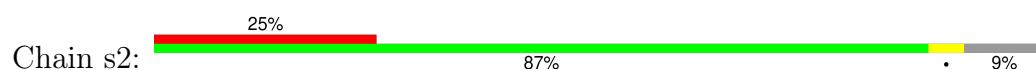
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



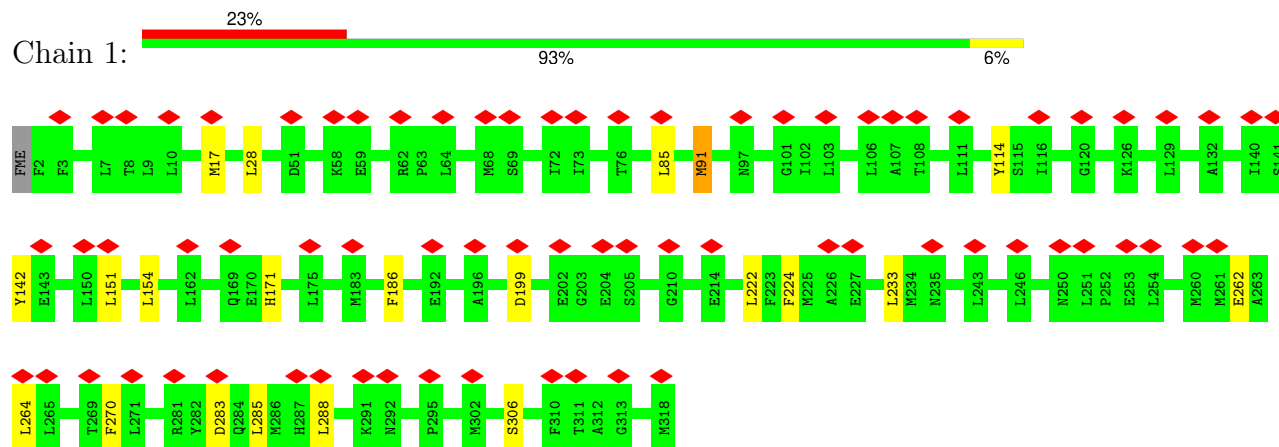
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



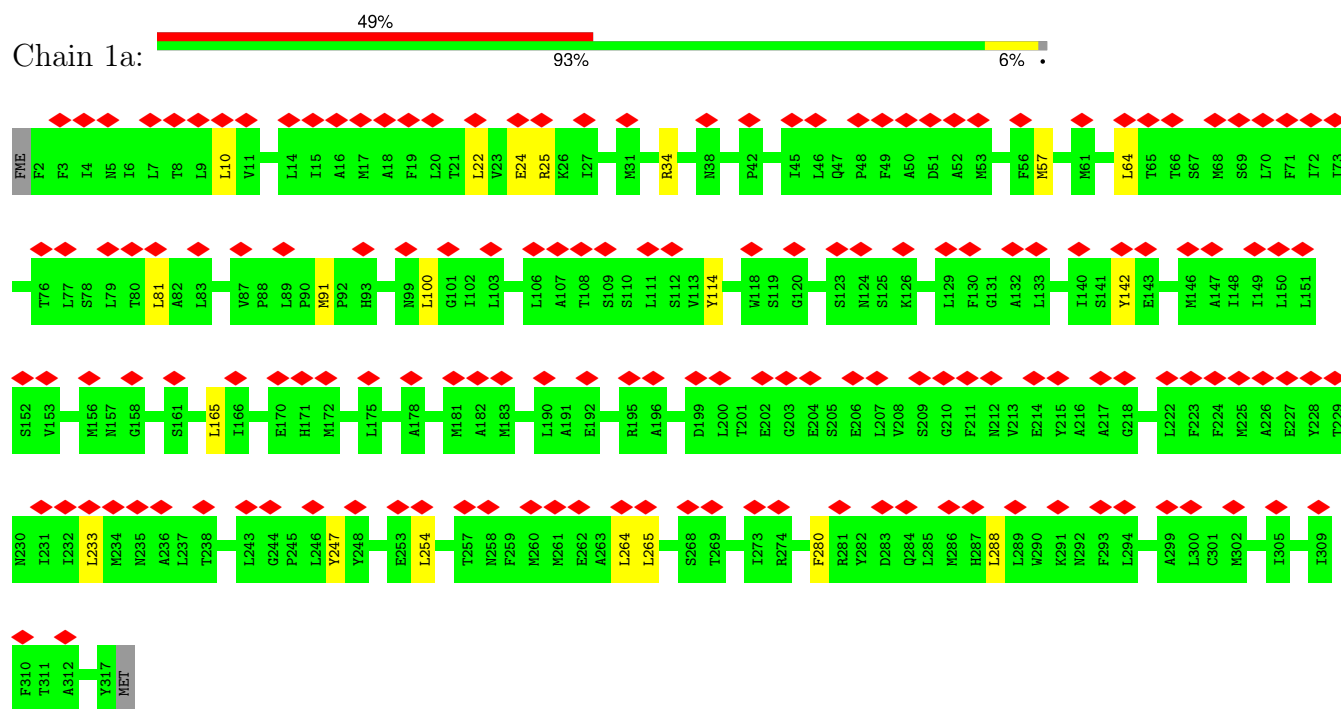
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



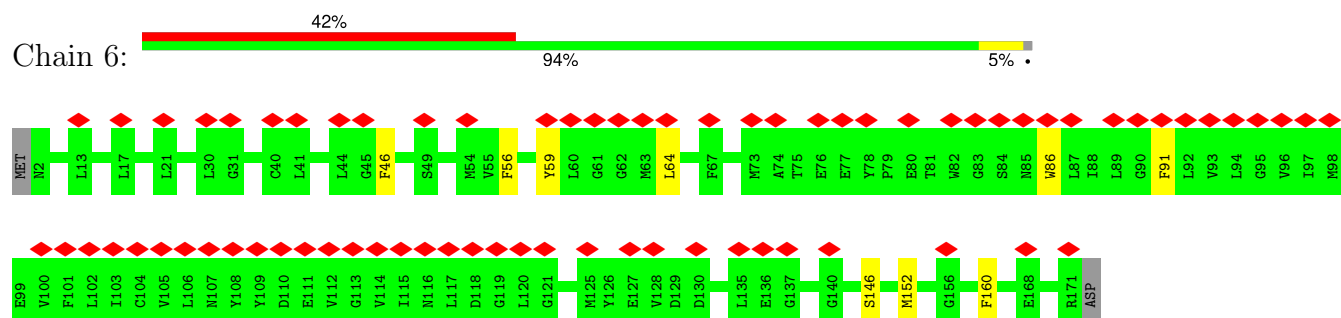
- Molecule 4: NADH-ubiquinone oxidoreductase chain 1



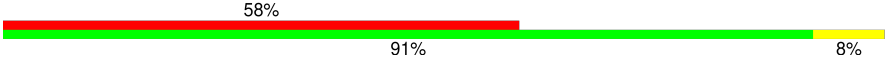
- Molecule 4: NADH-ubiquinone oxidoreductase chain 1

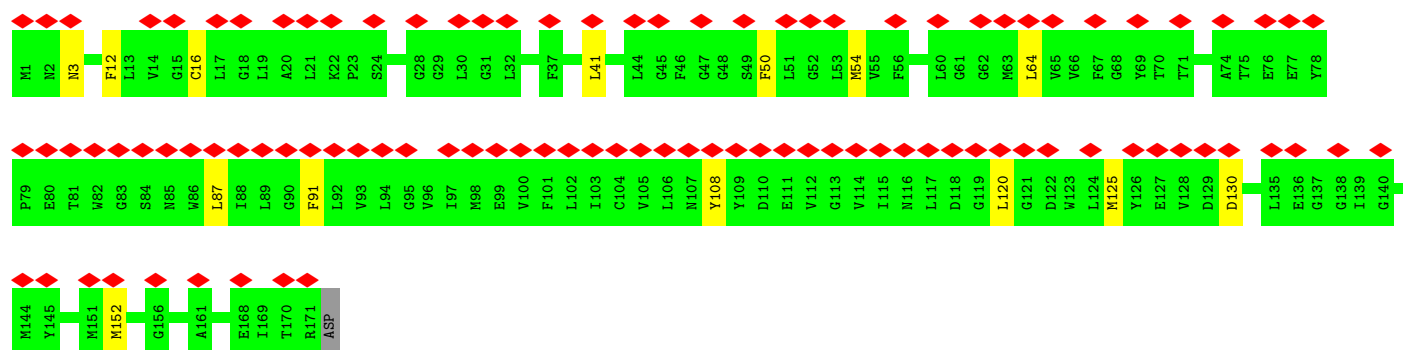


- Molecule 5: NADH-ubiquinone oxidoreductase chain 6



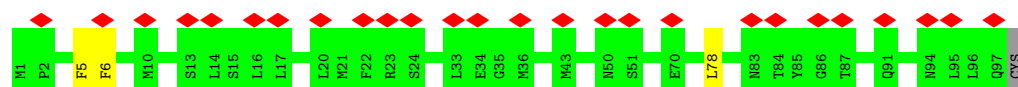
- Molecule 5: NADH-ubiquinone oxidoreductase chain 6

Chain 6a: 



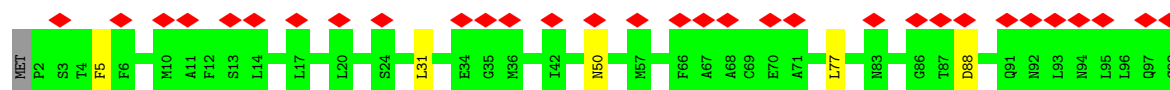
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L: 



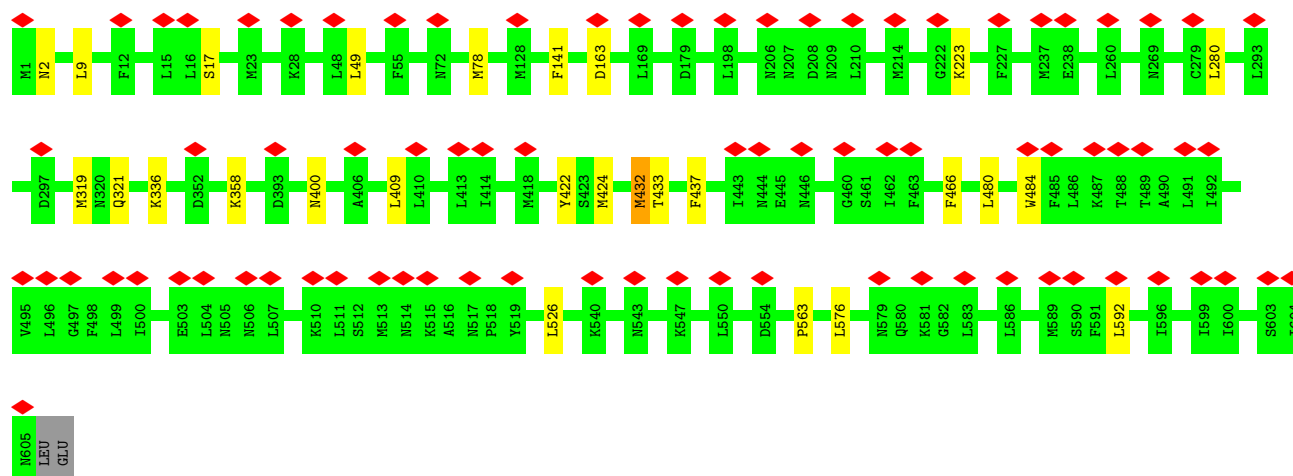
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L: 



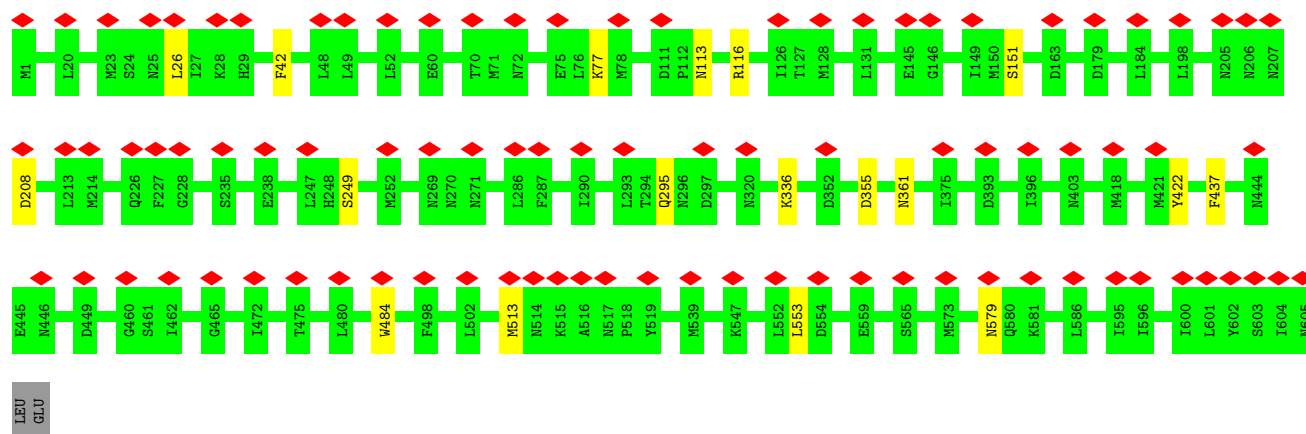
- Molecule 7: NADH-ubiquinone oxidoreductase chain 5

Chain 5: 

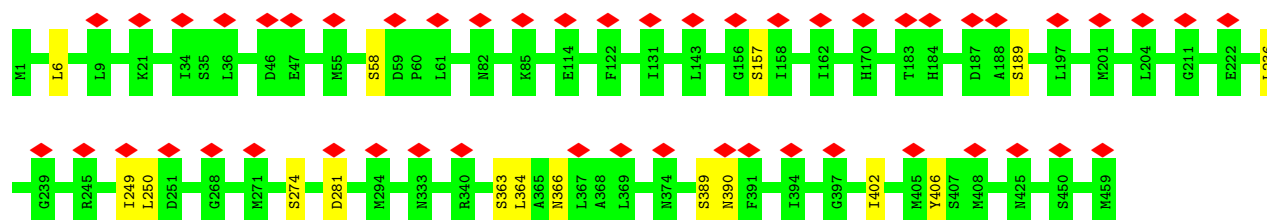


- Molecule 7: NADH-ubiquinone oxidoreductase chain 5

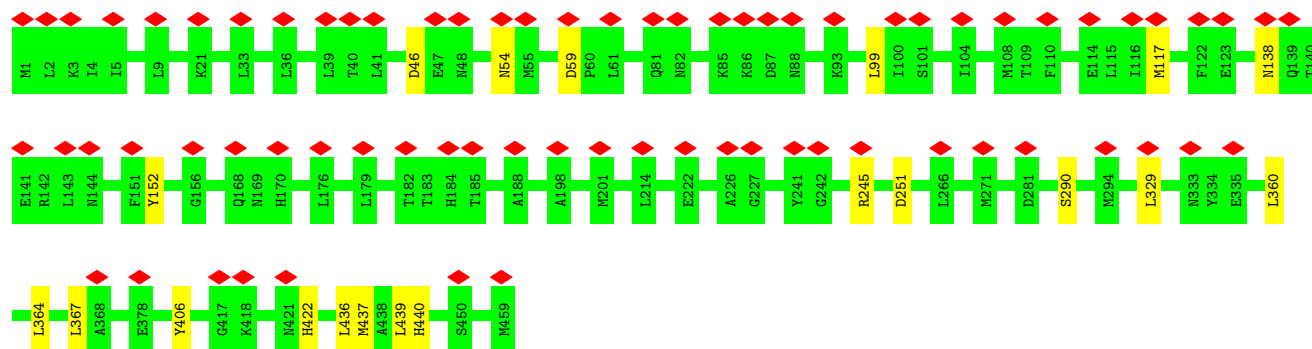
Chain 5a: 



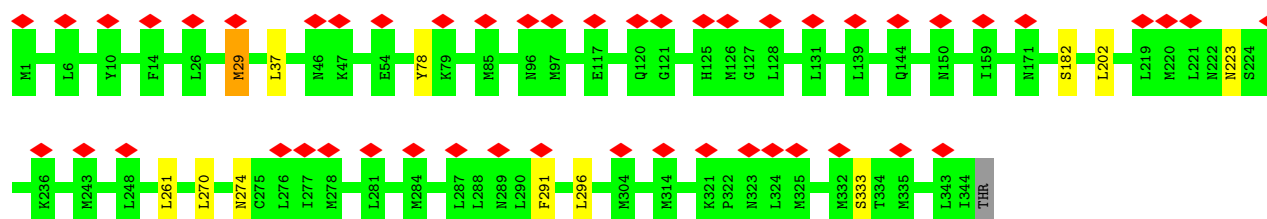
• Molecule 8: NADH-ubiquinone oxidoreductase chain 4



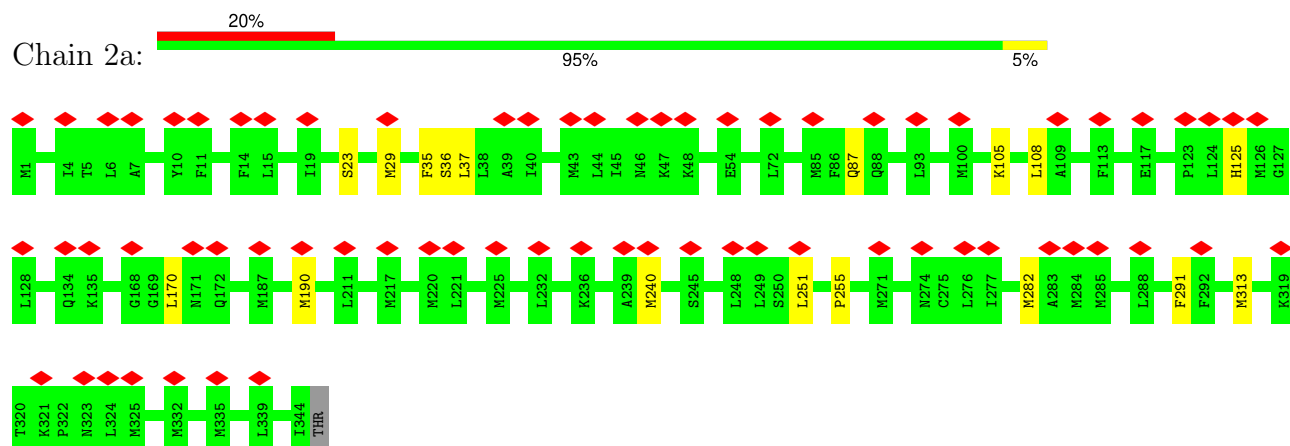
• Molecule 8: NADH-ubiquinone oxidoreductase chain 4



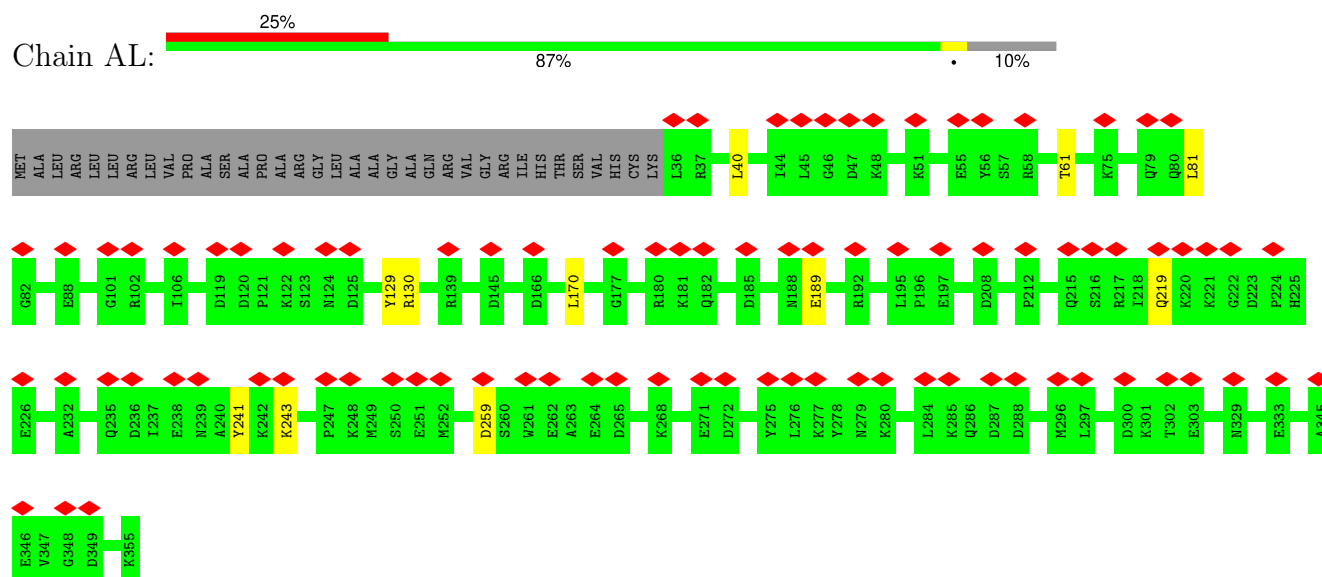
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2



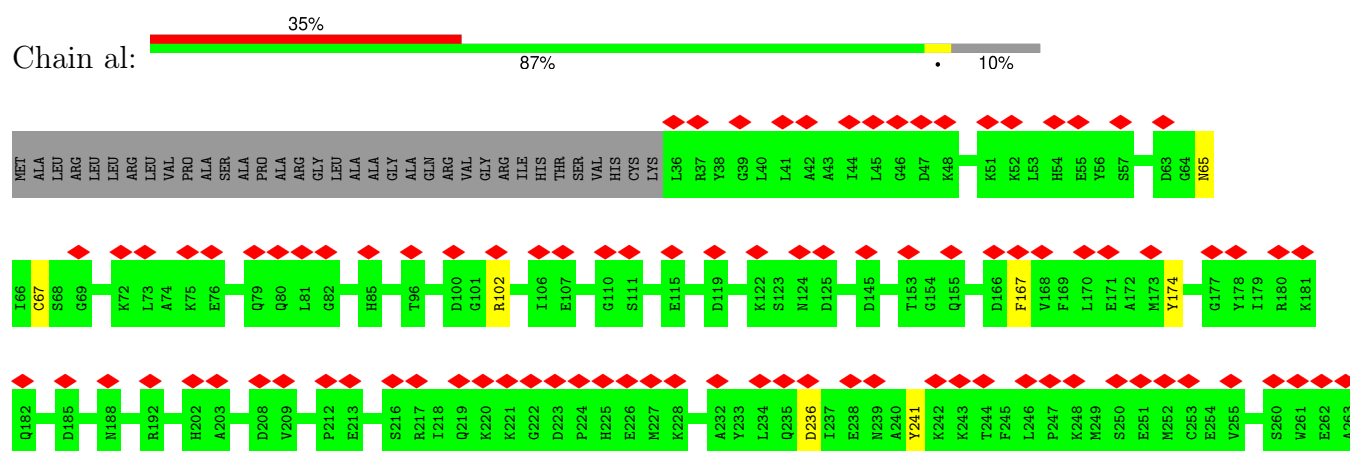
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

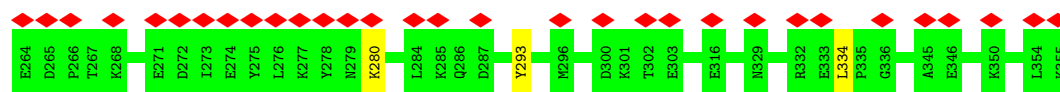


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

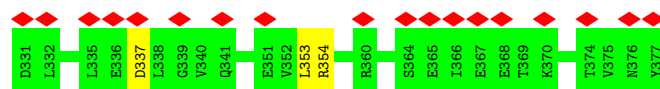
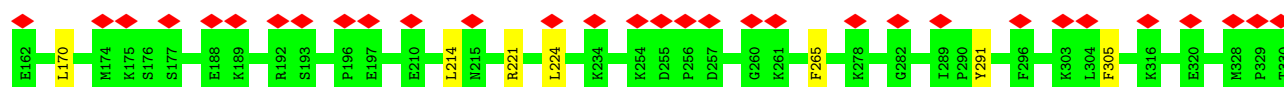
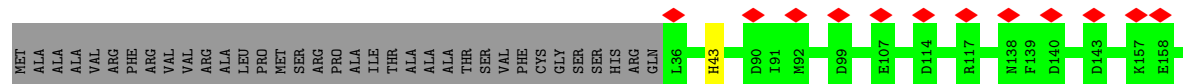


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

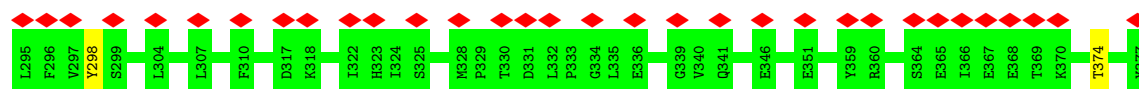
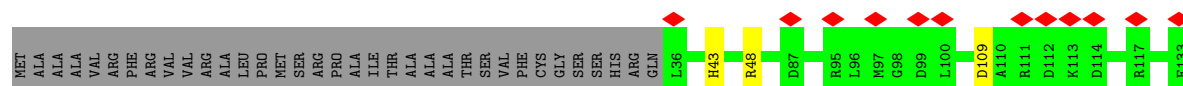
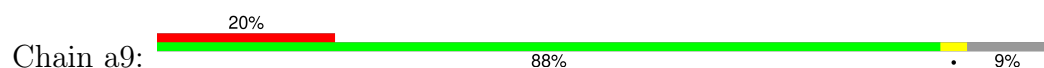




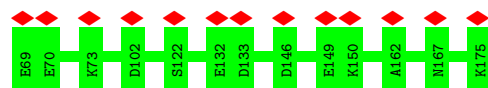
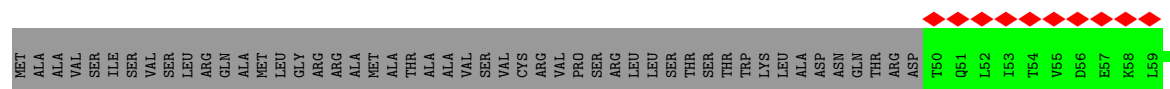
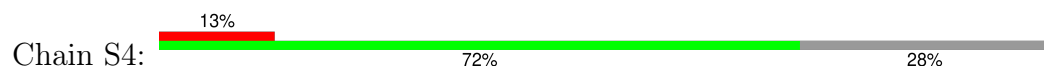
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

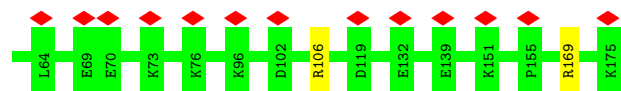
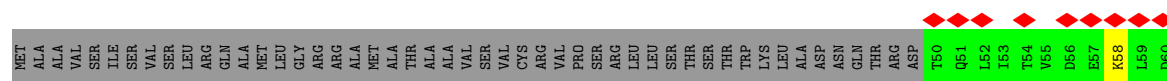


- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

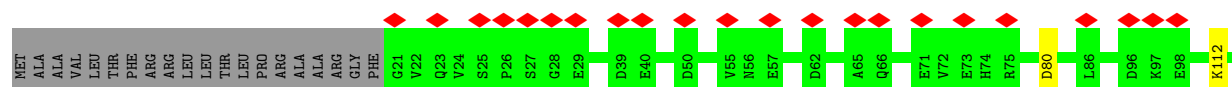
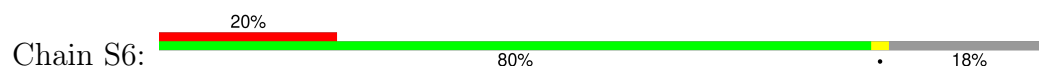


- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

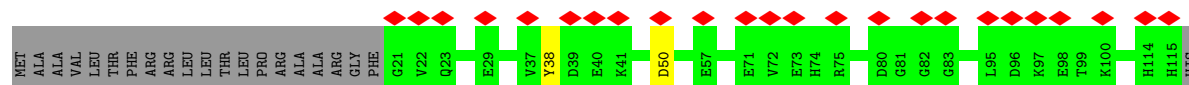
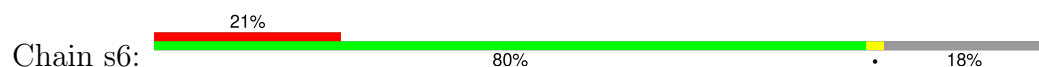




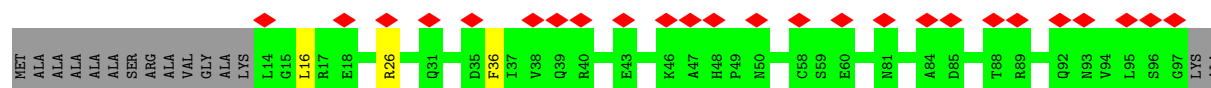
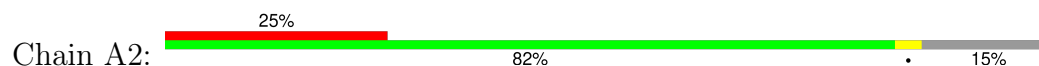
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



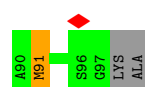
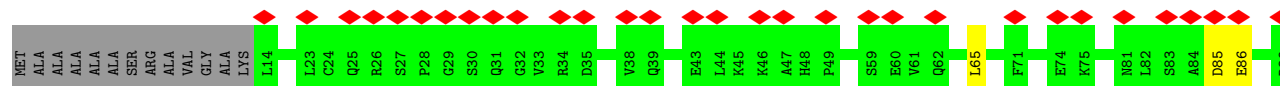
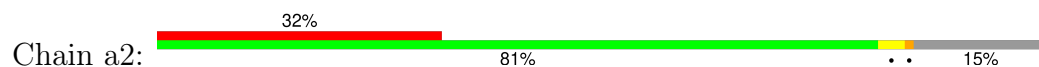
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

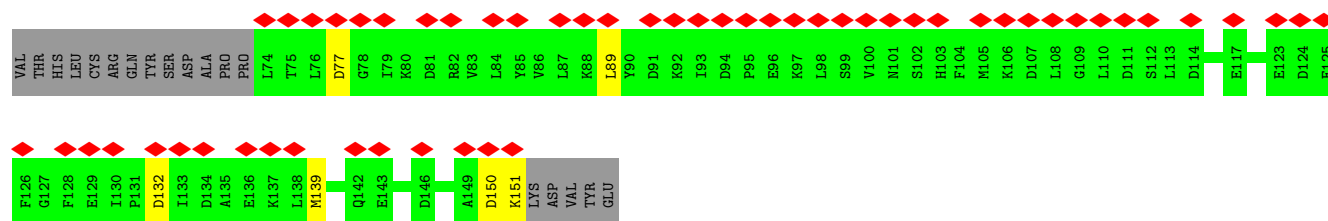


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

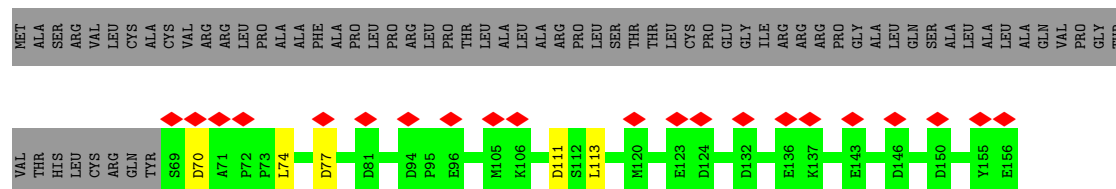


- Molecule 15: Acyl carrier protein, mitochondrial

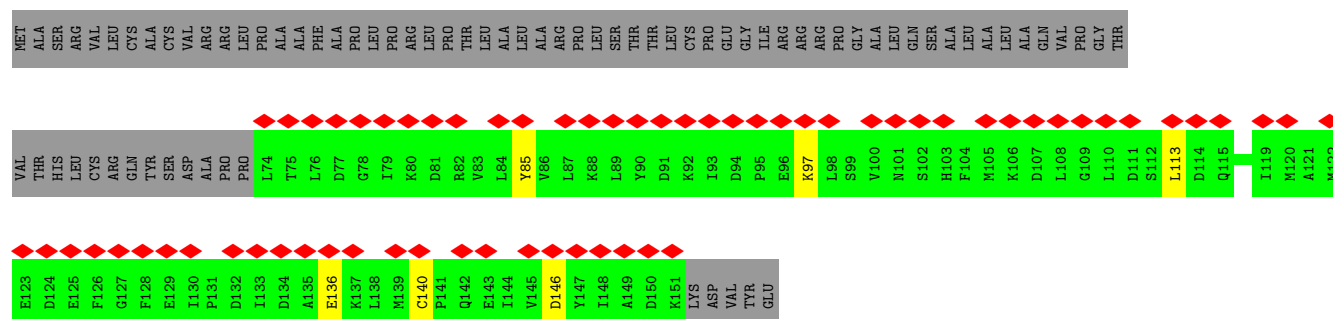
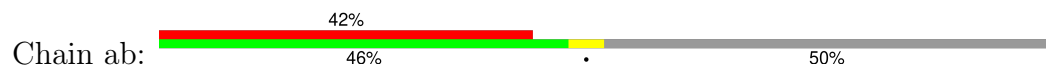




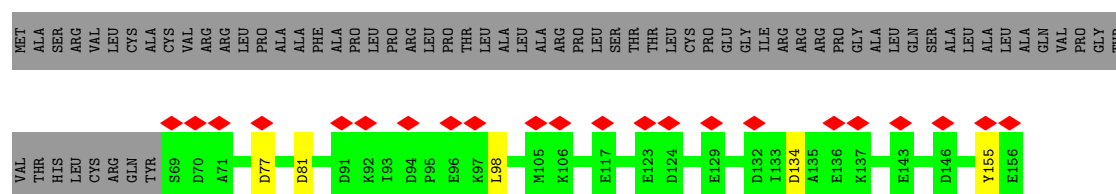
- Molecule 15: Acyl carrier protein, mitochondrial



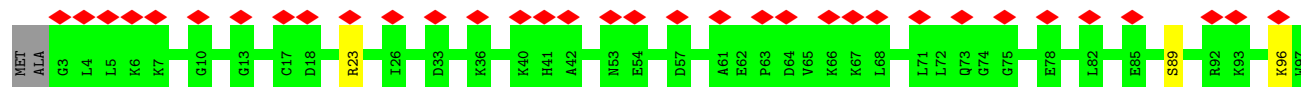
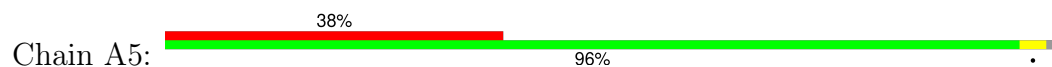
- Molecule 15: Acyl carrier protein, mitochondrial

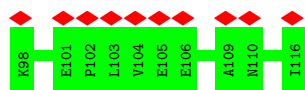


- Molecule 15: Acyl carrier protein, mitochondrial

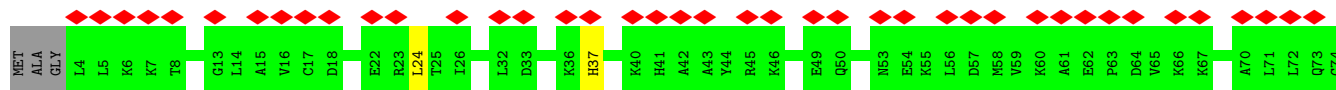


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

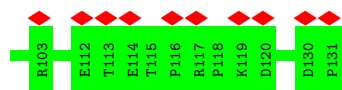
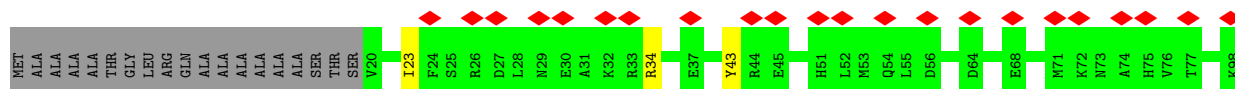
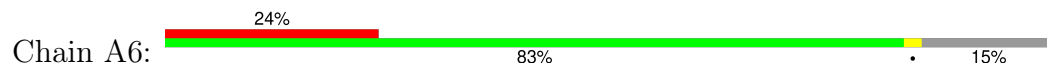




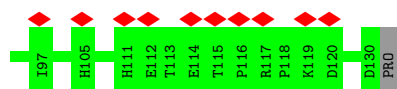
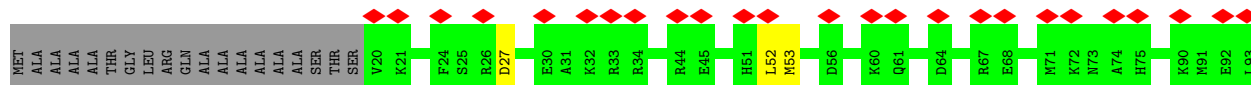
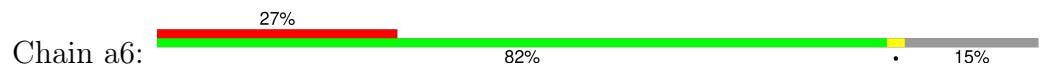
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



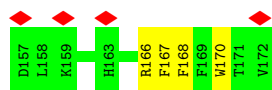
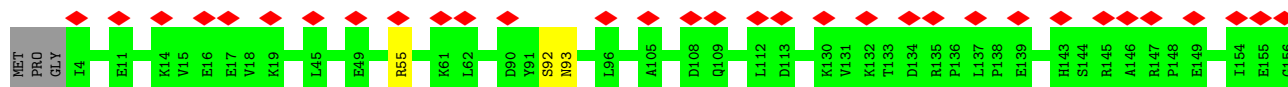
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



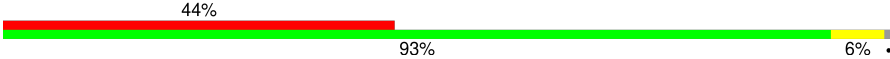
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

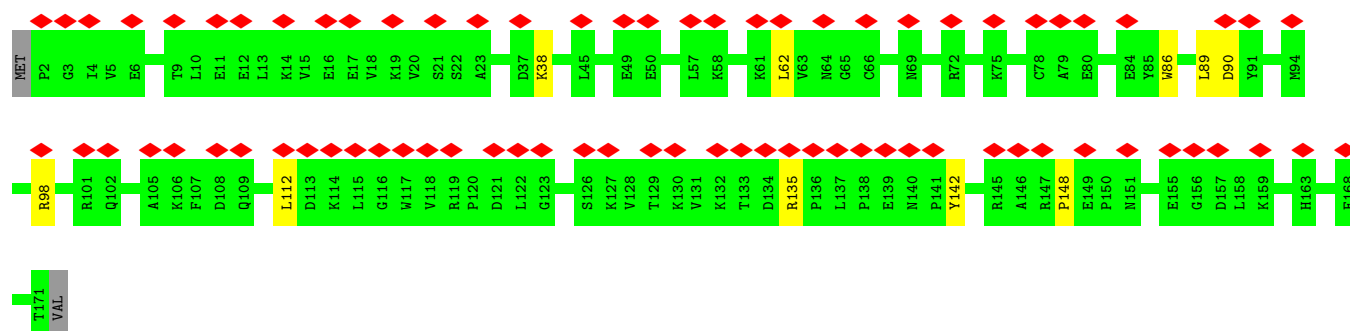


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



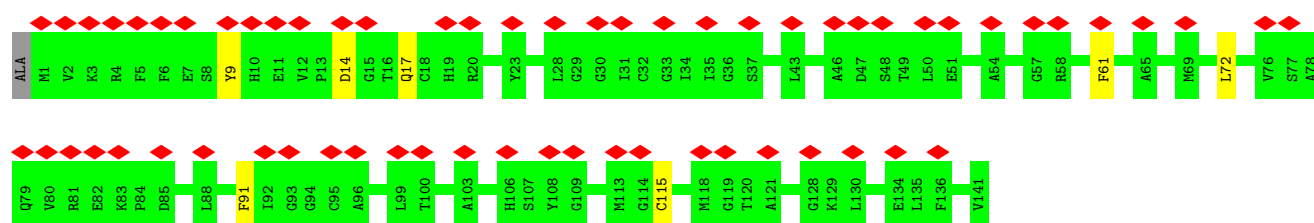
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain a8: 



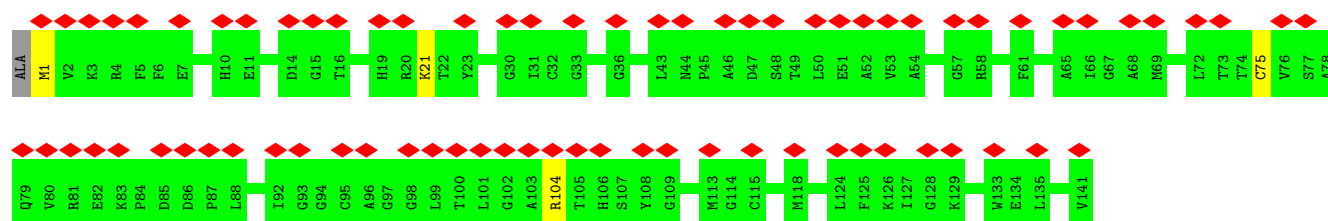
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AM: 



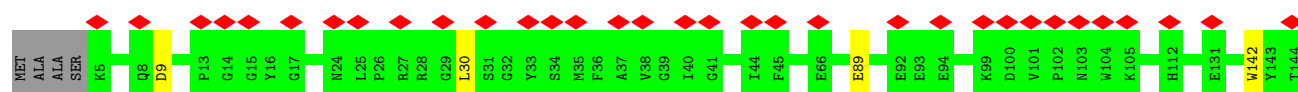
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain am: 

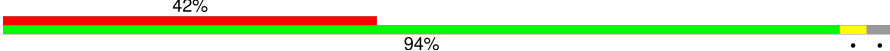


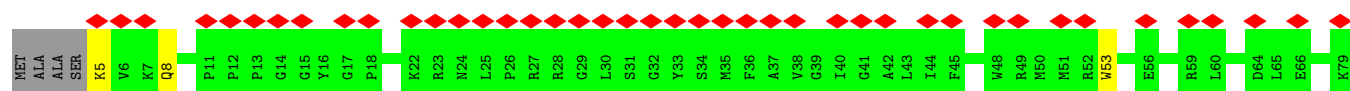
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

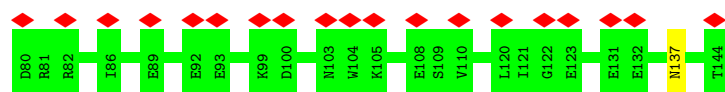
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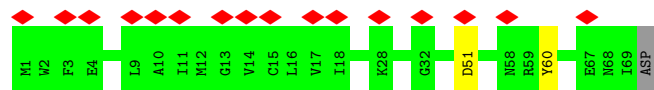
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain ao: 

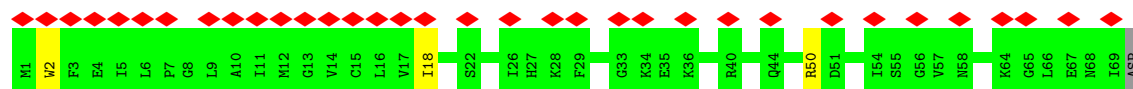




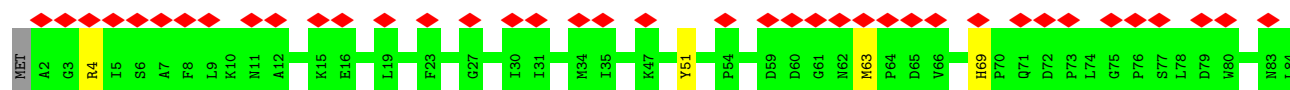
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



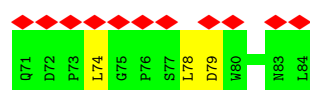
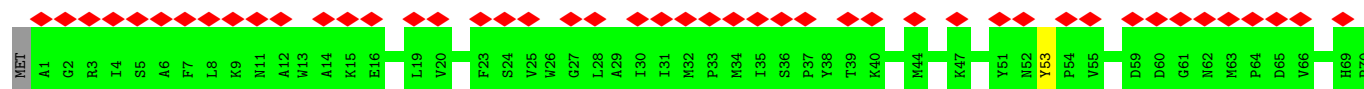
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



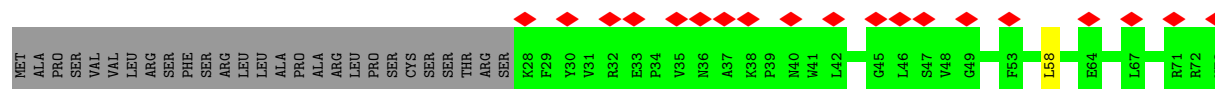
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



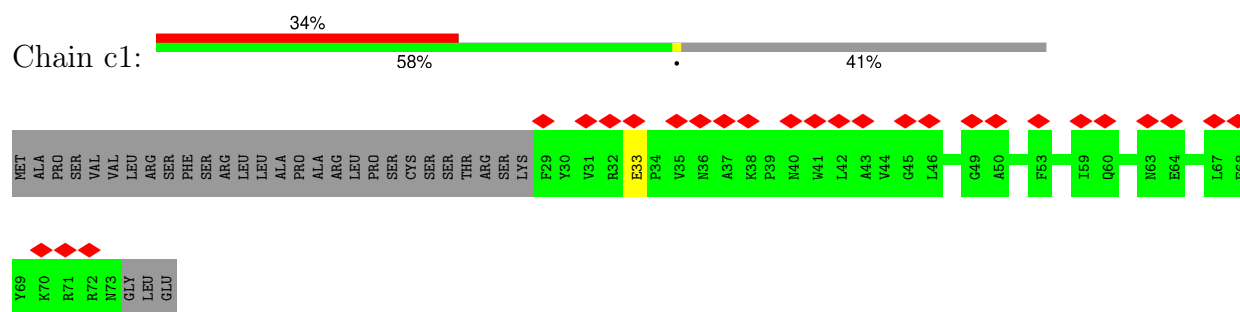
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



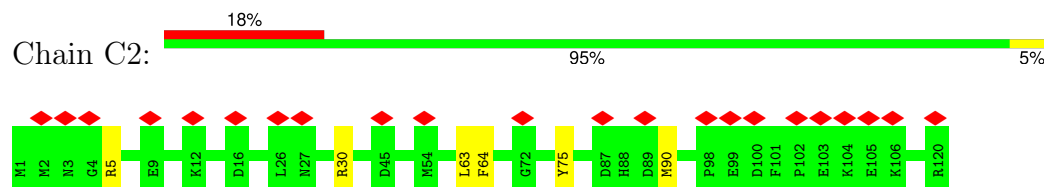
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



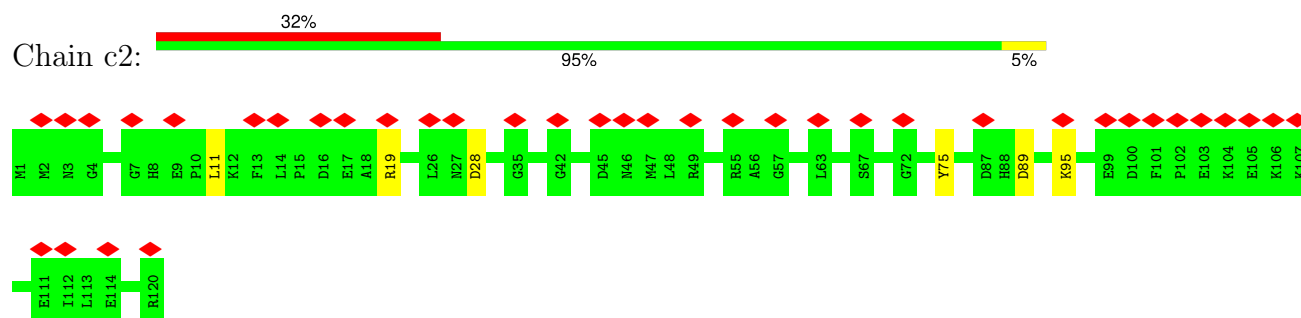
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



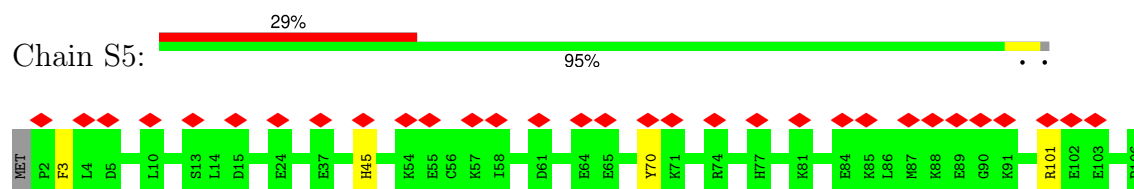
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



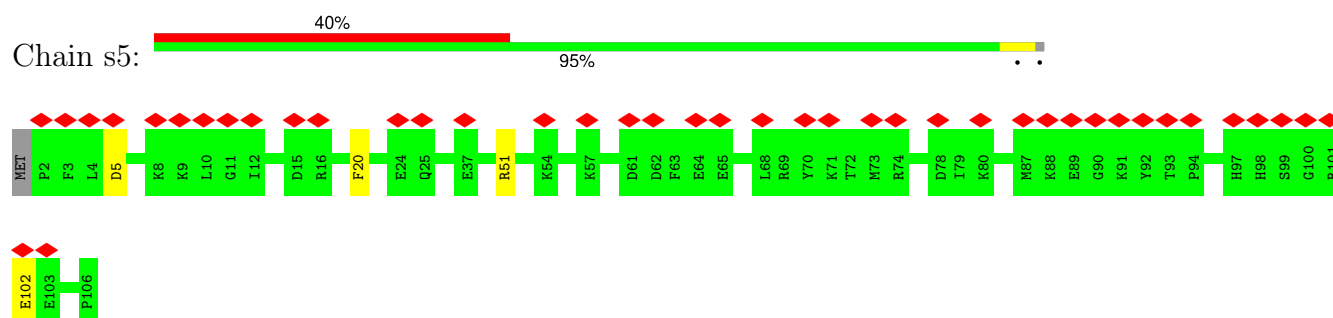
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



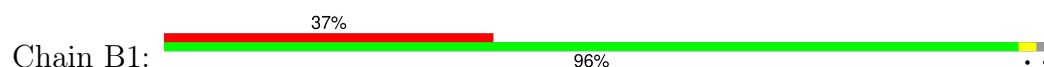
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

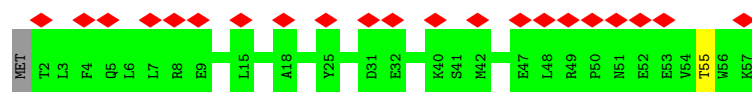


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

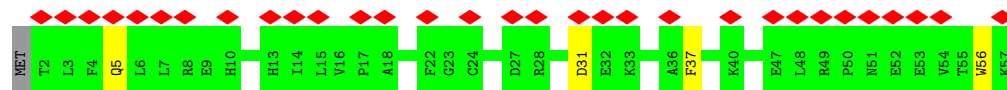
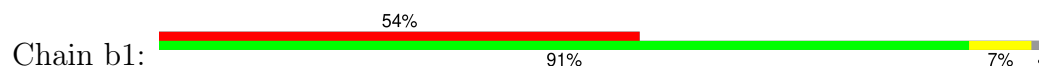


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

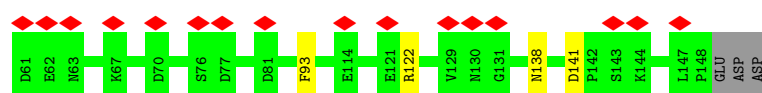
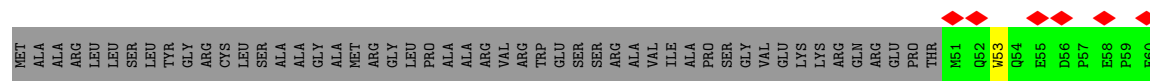




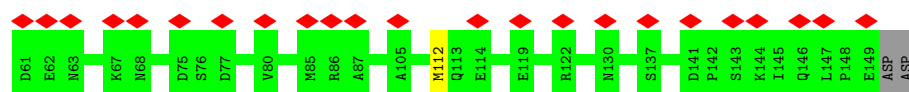
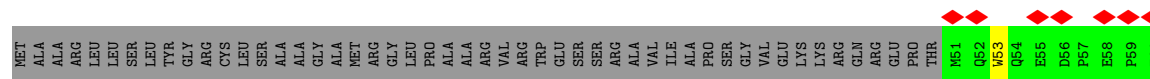
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



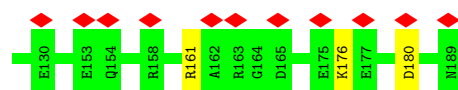
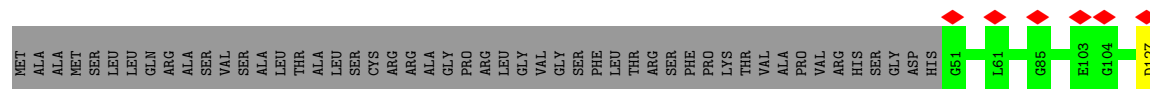
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



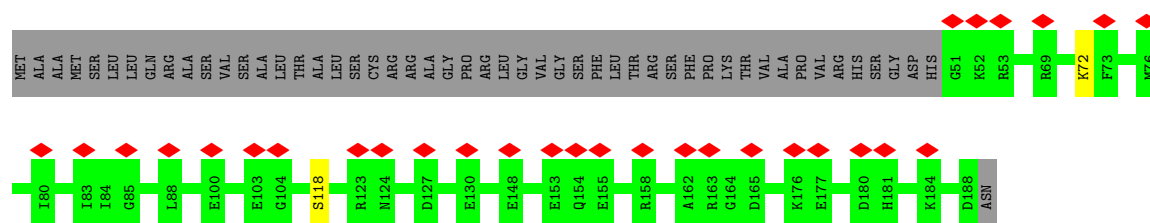
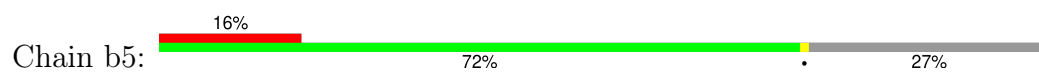
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



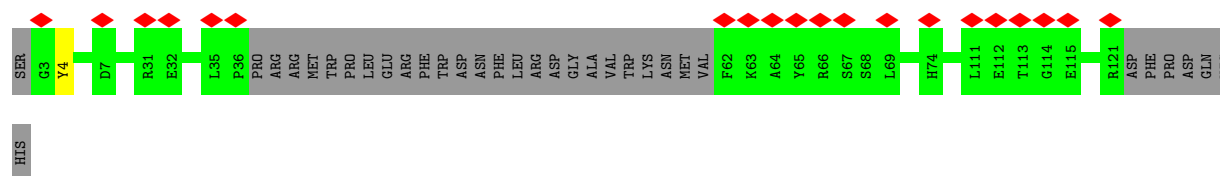
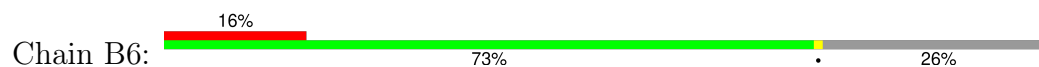
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



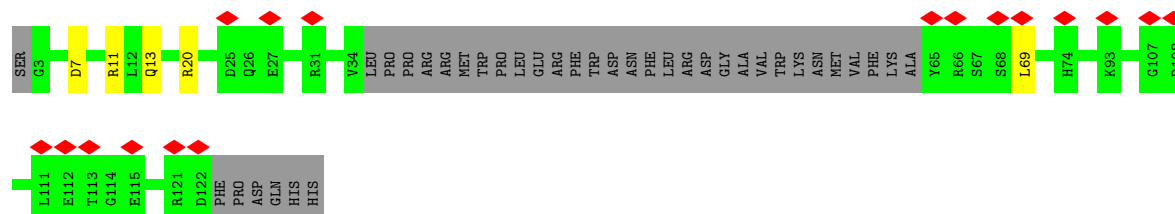
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



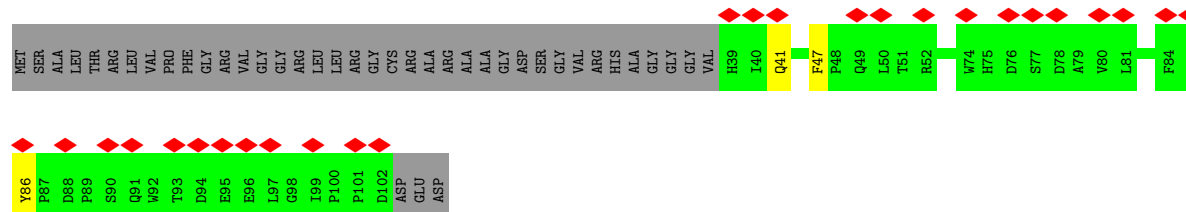
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



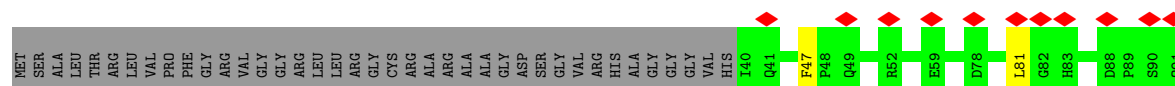
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

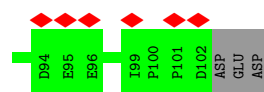


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

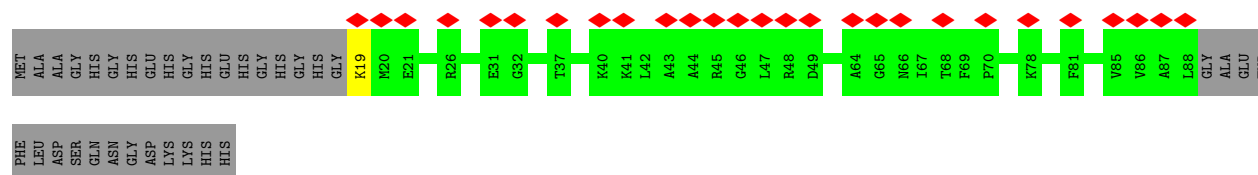


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

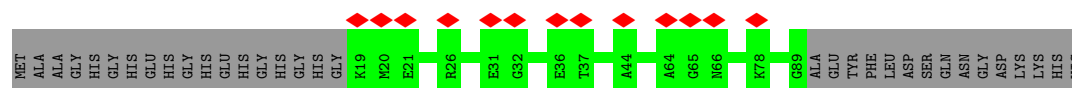




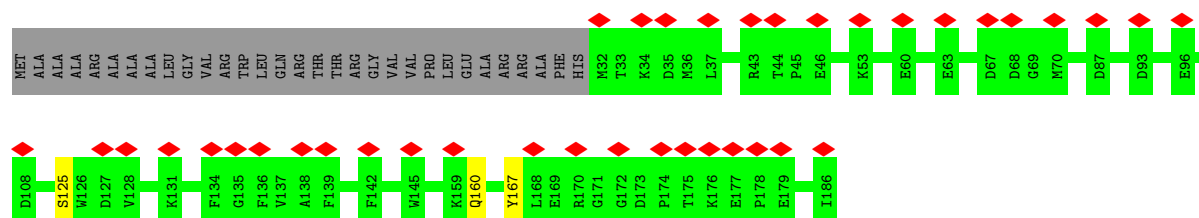
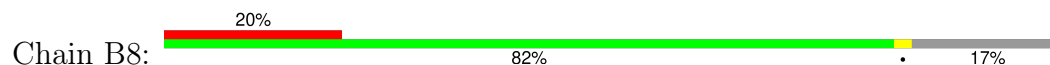
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



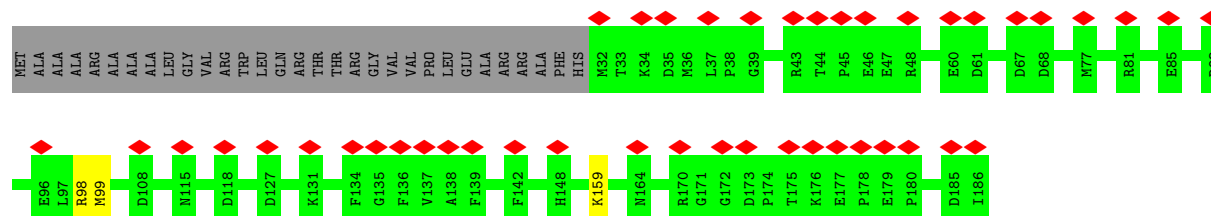
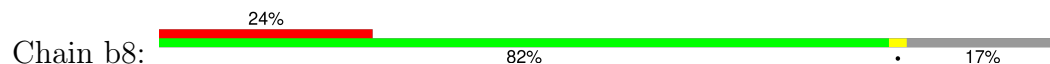
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

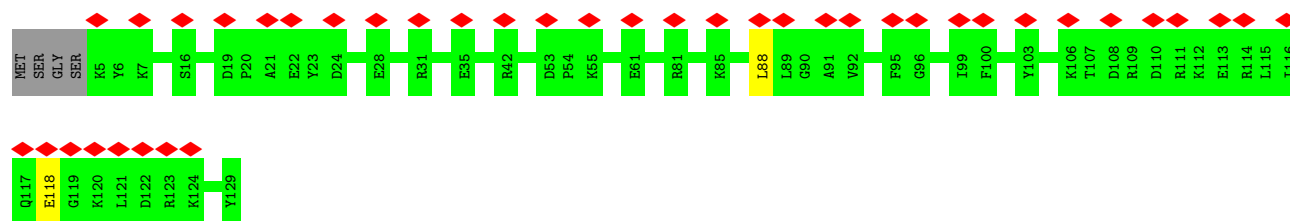


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



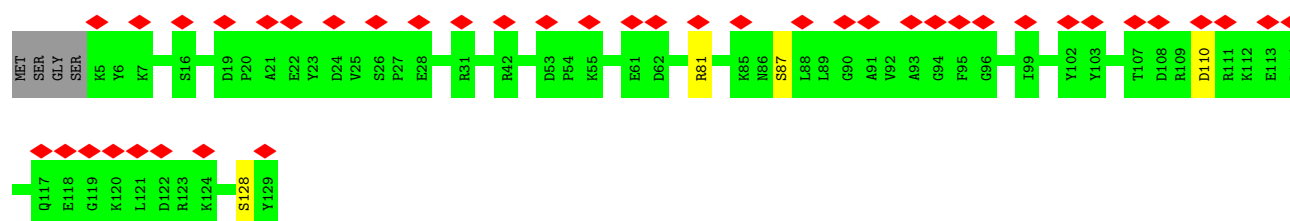
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4





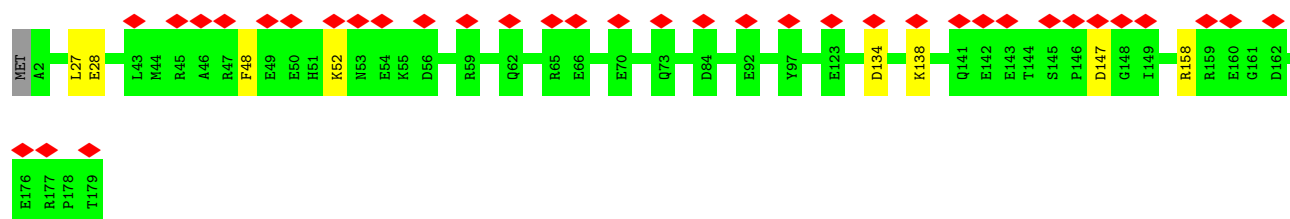
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain b4:



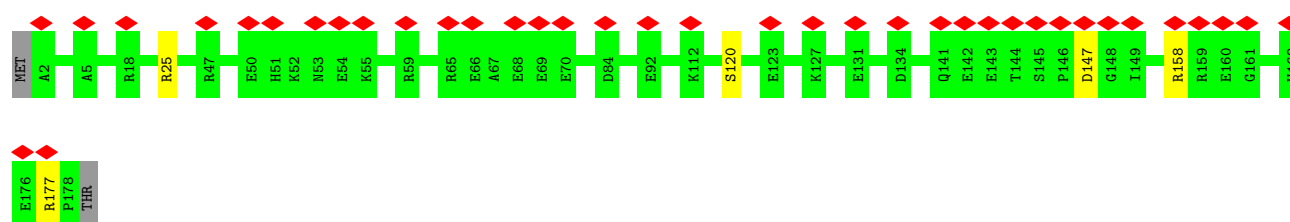
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:



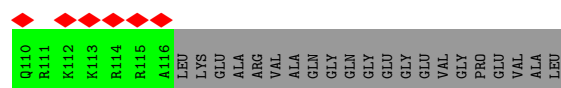
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain b9:

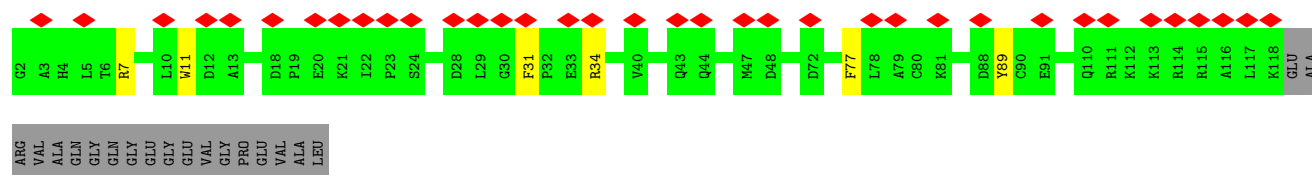
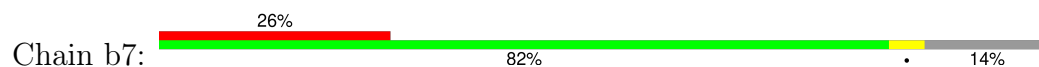


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

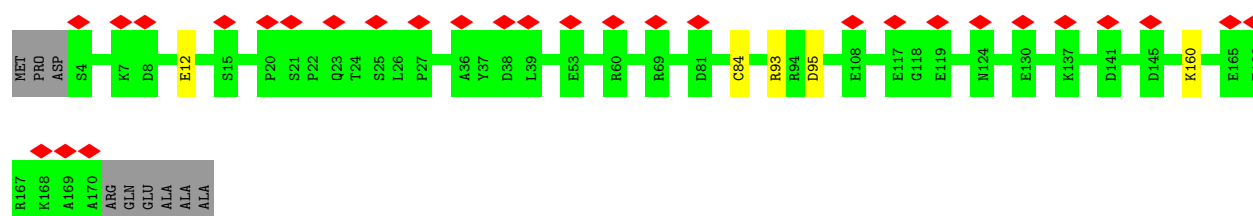
Chain B7:



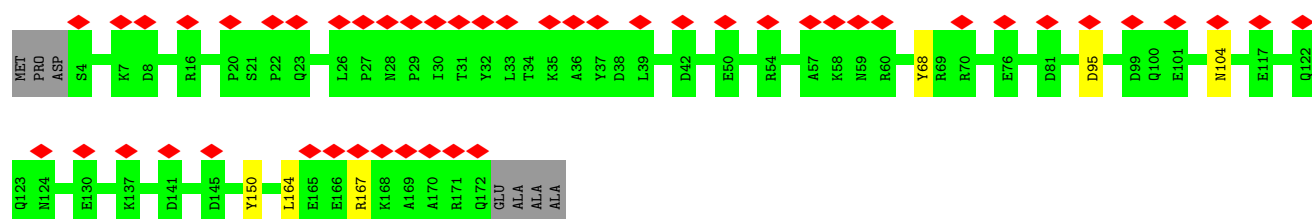
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



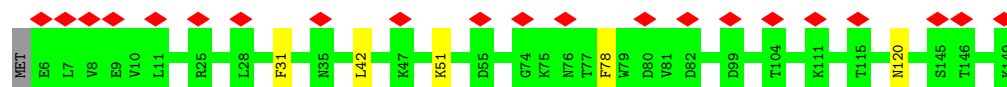
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

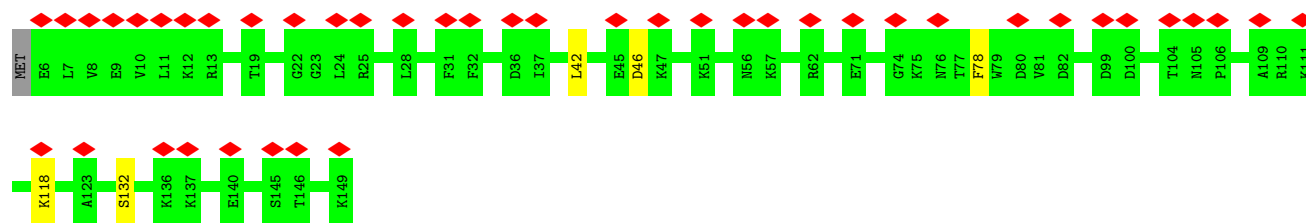


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

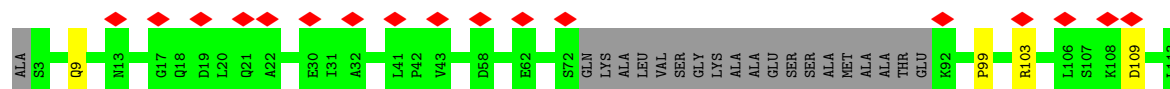
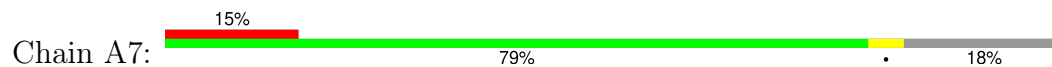


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

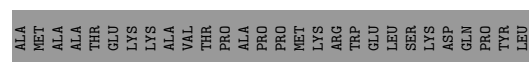
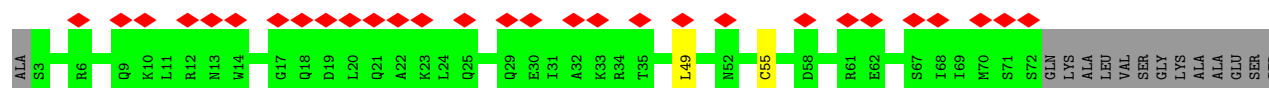




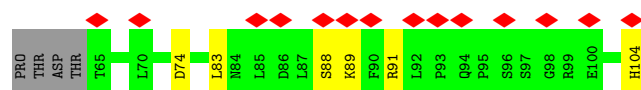
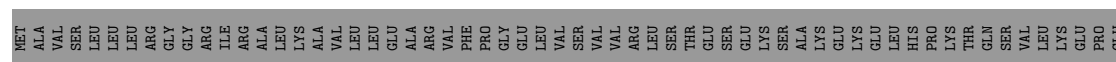
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



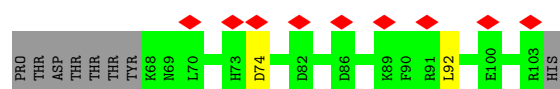
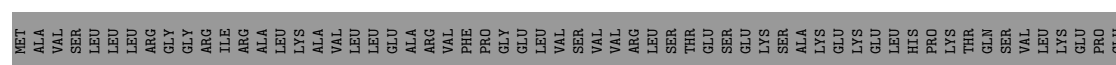
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

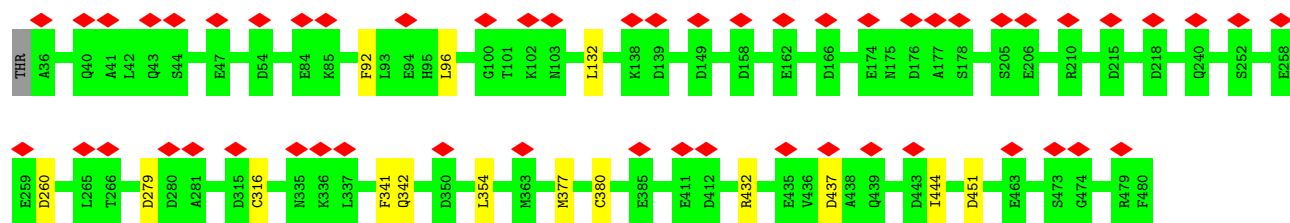


- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

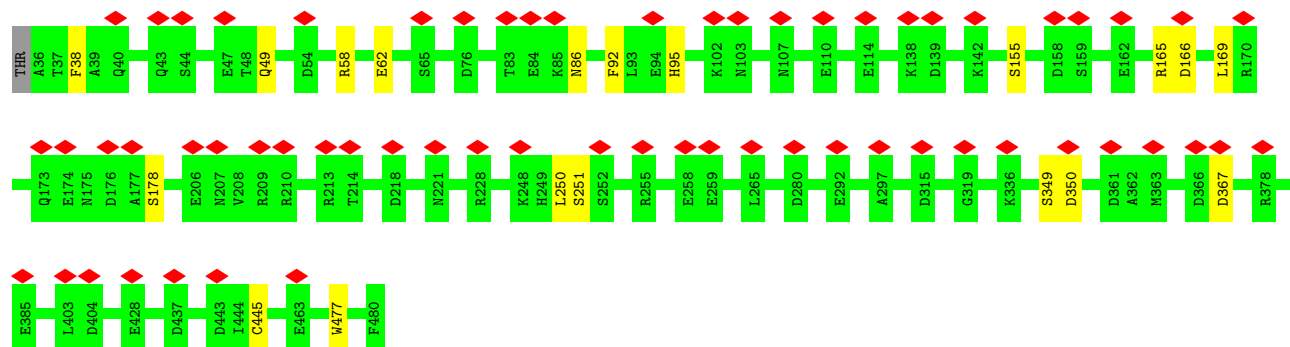


- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial

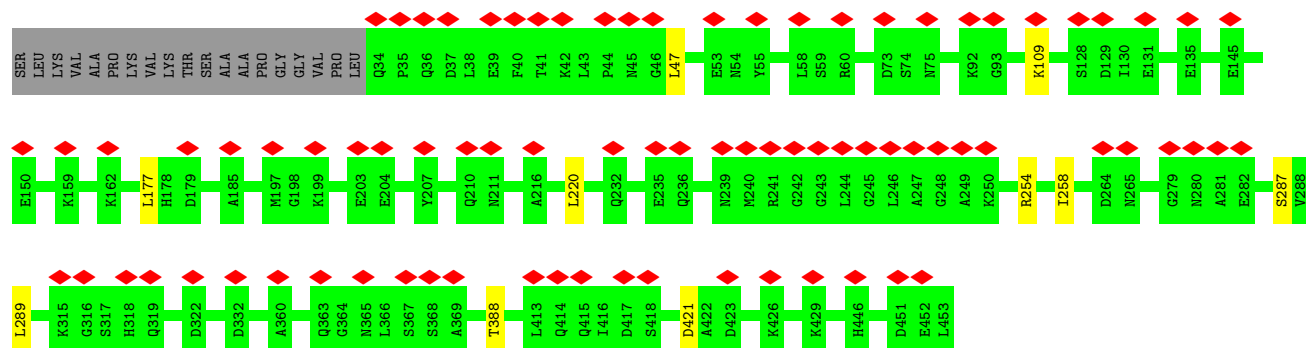




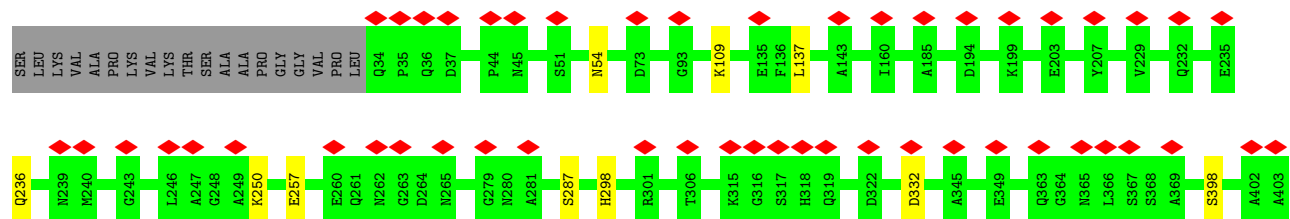
- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial

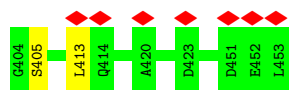


- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial

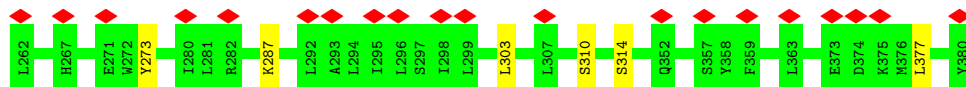


- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial

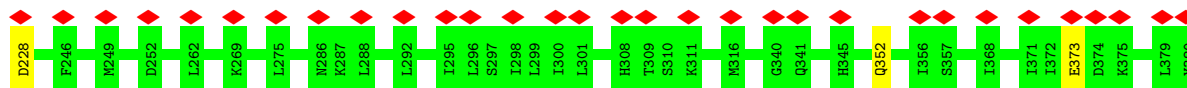
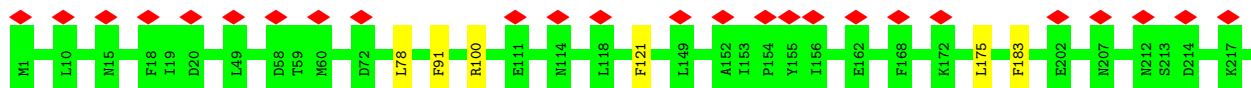




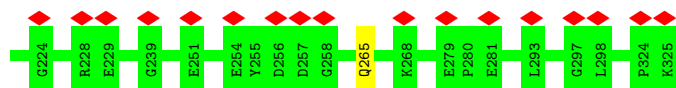
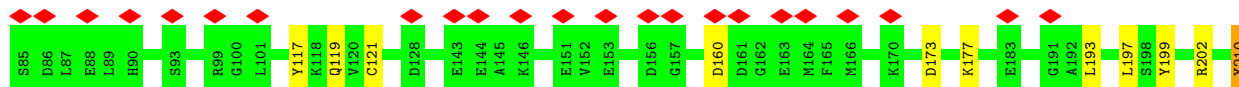
- Molecule 42: Cytochrome b



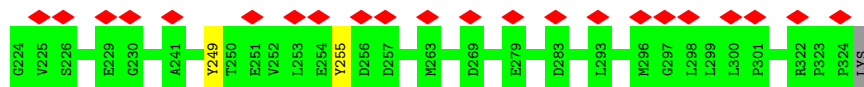
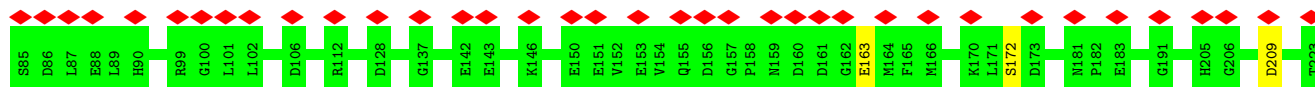
- Molecule 42: Cytochrome b



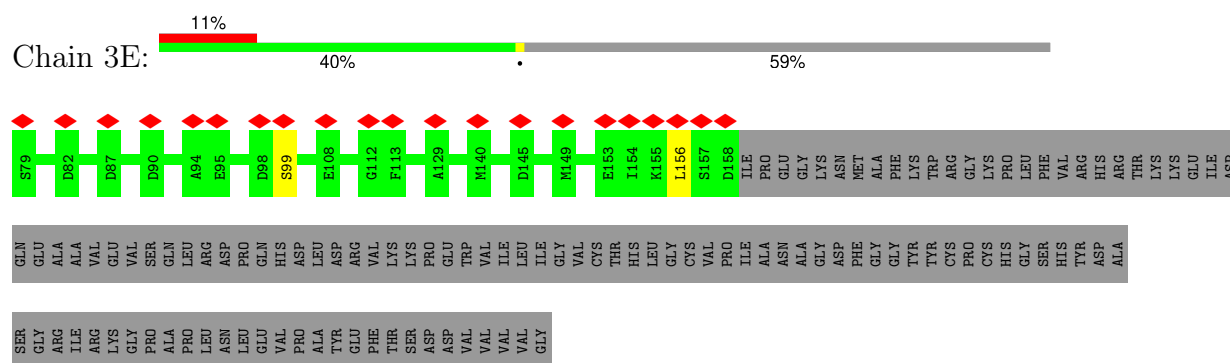
- Molecule 43: Cytochrome c1, heme protein, mitochondrial



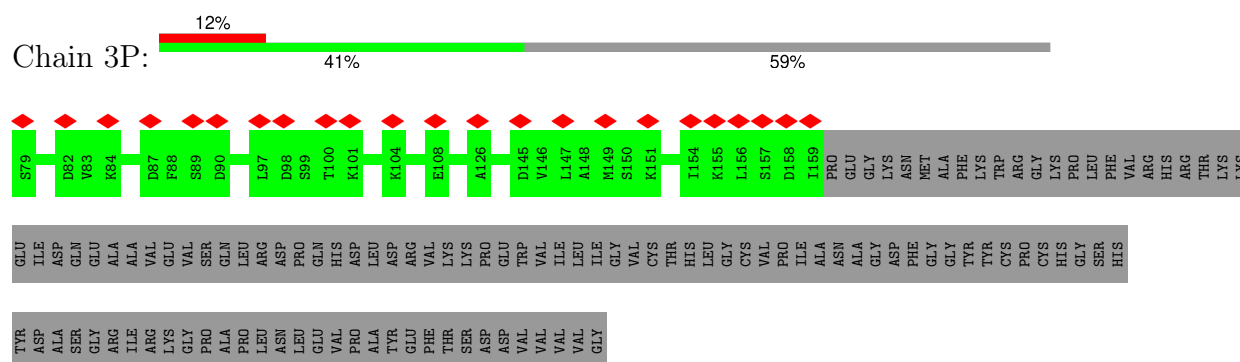
- Molecule 43: Cytochrome c1, heme protein, mitochondrial



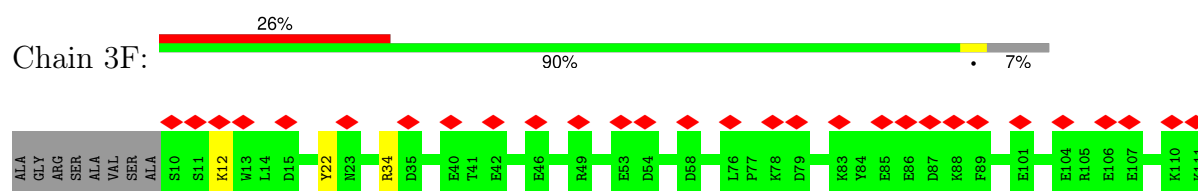
- Molecule 44: Cytochrome b-c1 complex subunit 9



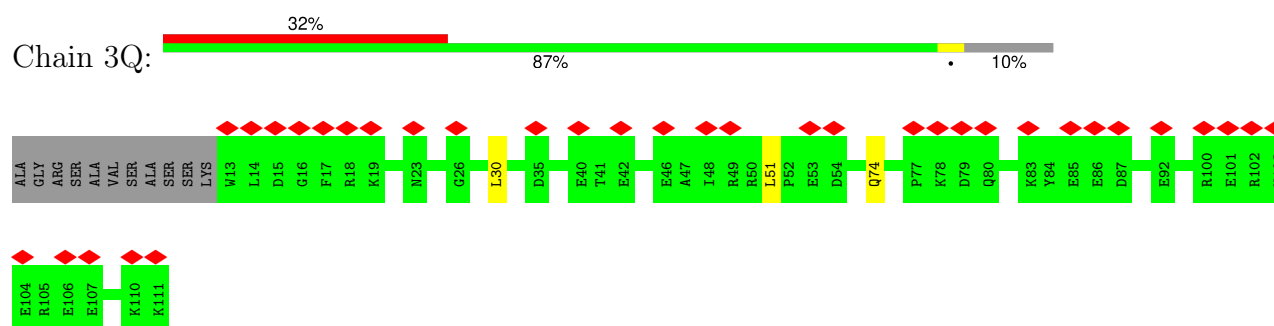
- Molecule 44: Cytochrome b-c1 complex subunit 9



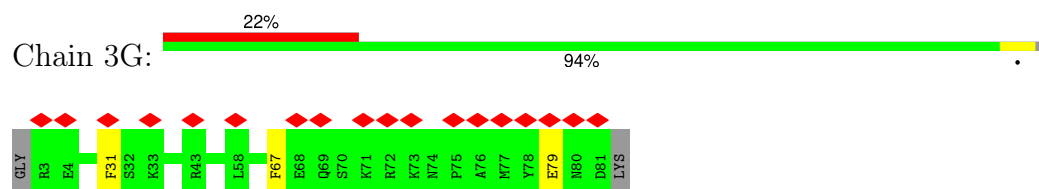
- Molecule 45: Cytochrome b-c1 complex subunit 7



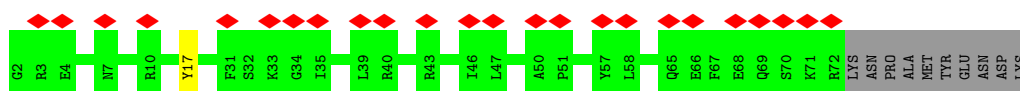
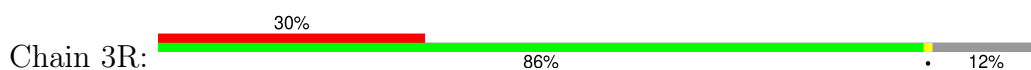
- Molecule 45: Cytochrome b-c1 complex subunit 7



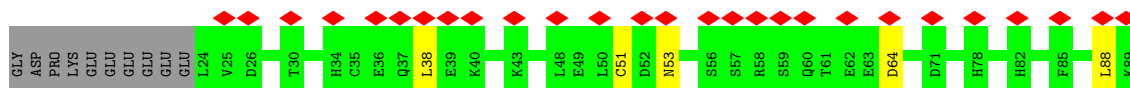
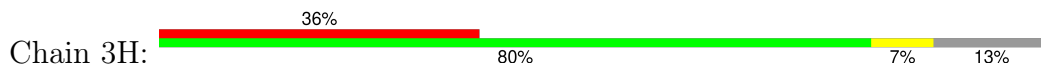
- Molecule 46: Cytochrome b-c1 complex subunit 8



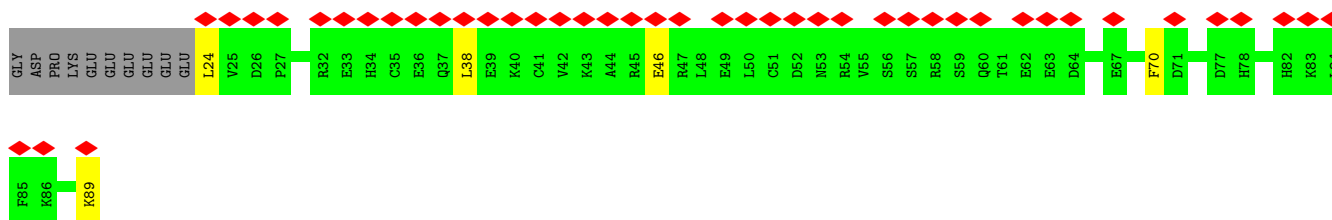
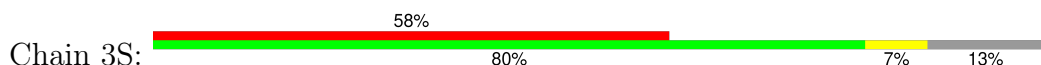
- Molecule 46: Cytochrome b-c1 complex subunit 8



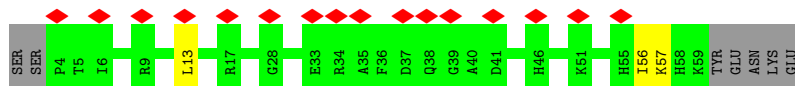
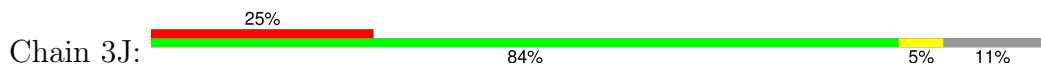
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



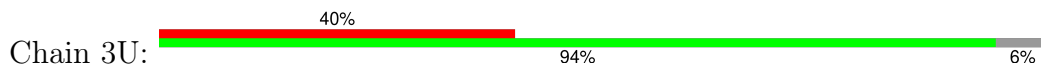
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



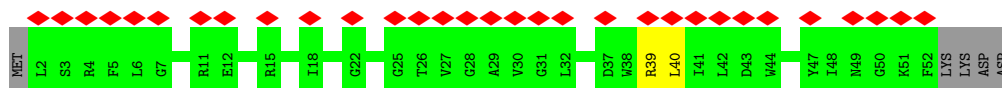
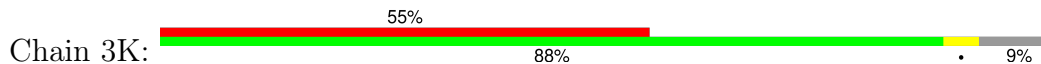
- Molecule 48: Cytochrome b-c1 complex subunit 9



- Molecule 48: Cytochrome b-c1 complex subunit 9

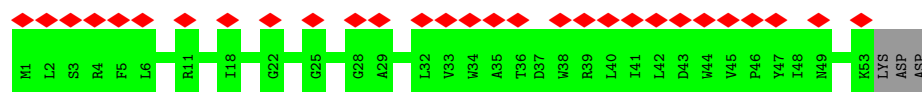


- Molecule 49: Cytochrome b-c1 complex subunit 10

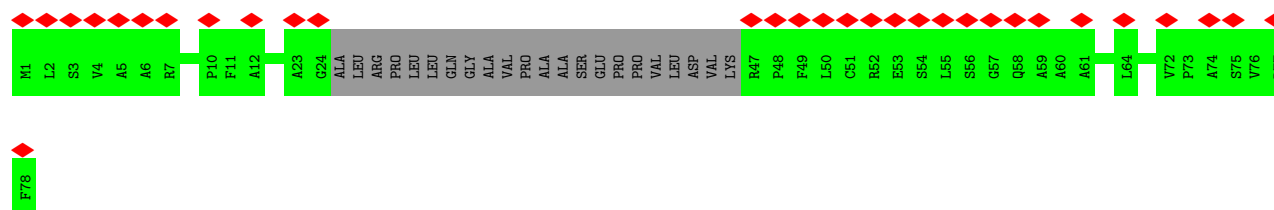
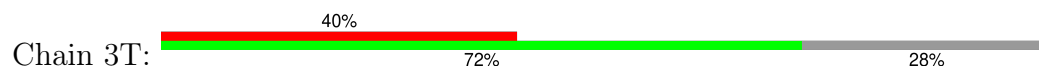


- Molecule 49: Cytochrome b-c1 complex subunit 10

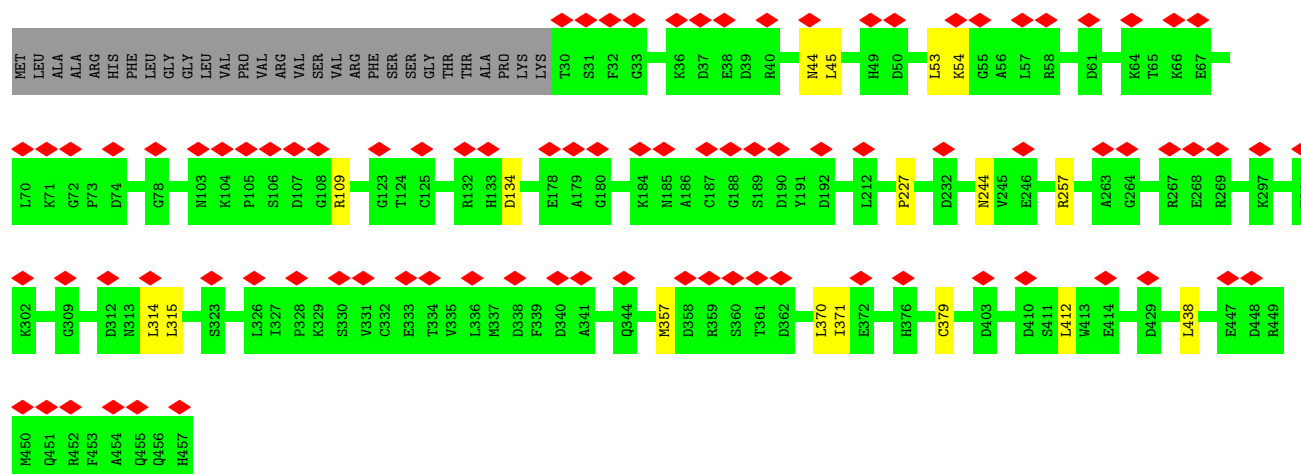
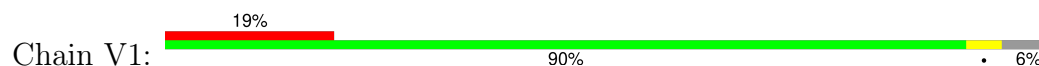




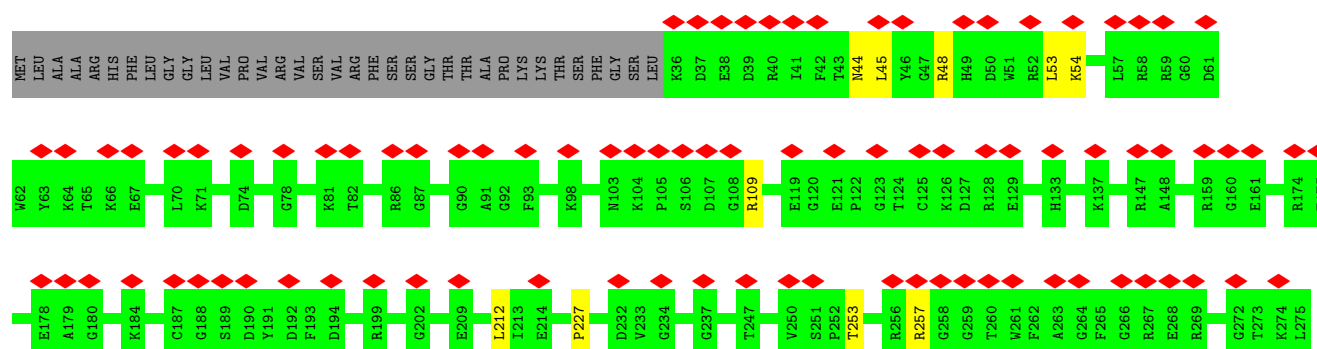
- Molecule 50: Cytochrome b-c1 complex subunit Rieske, mitochondrial

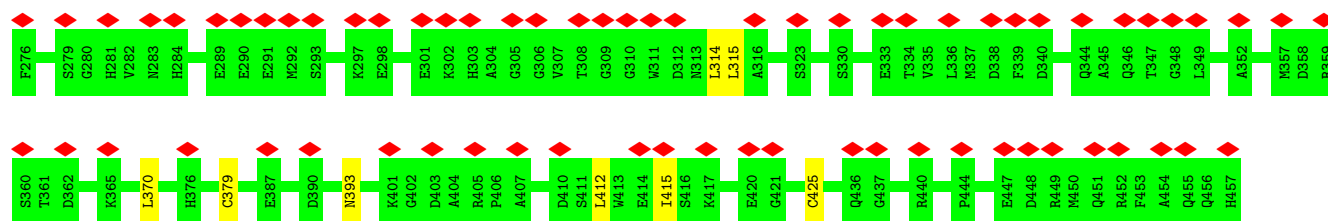


- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

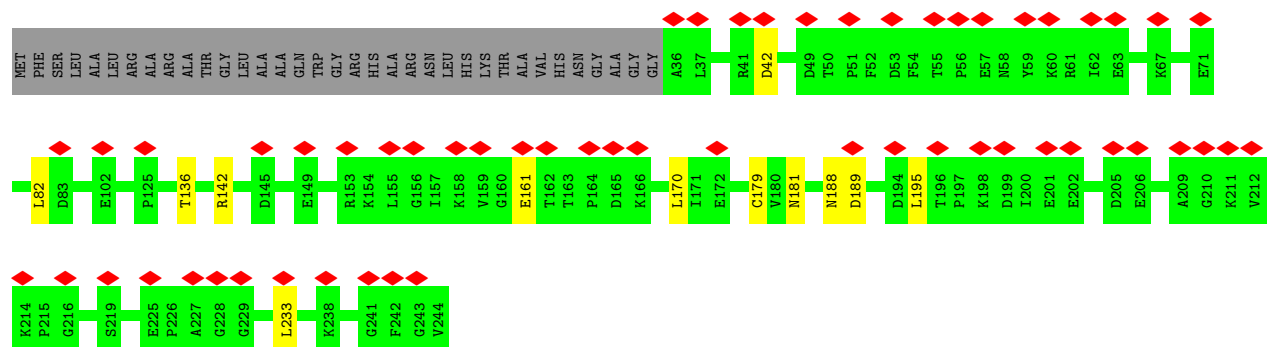
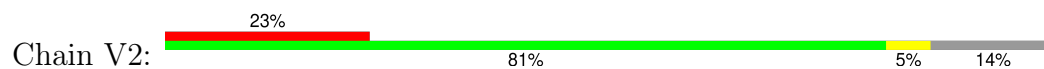


- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

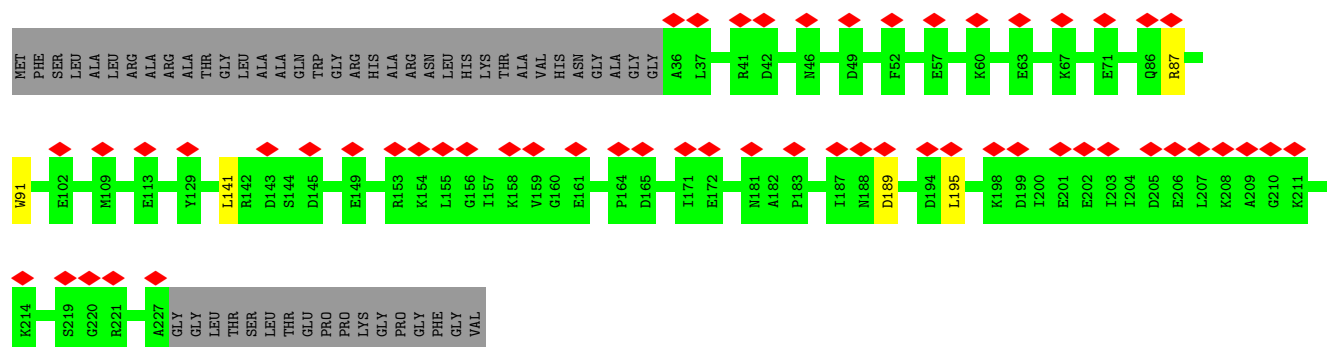
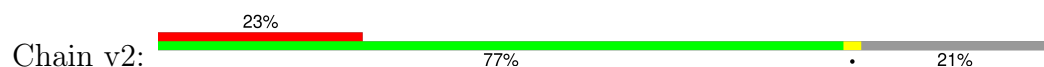




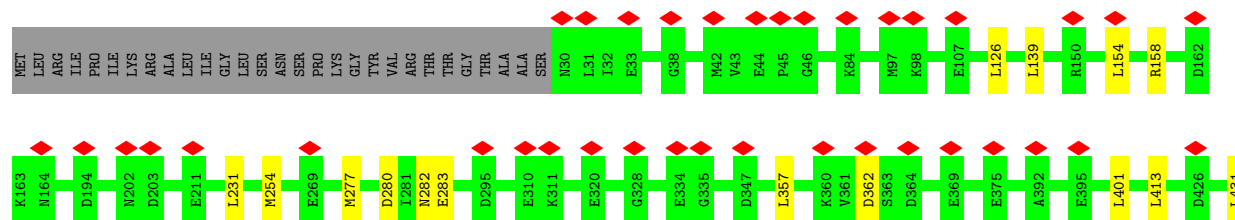
- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

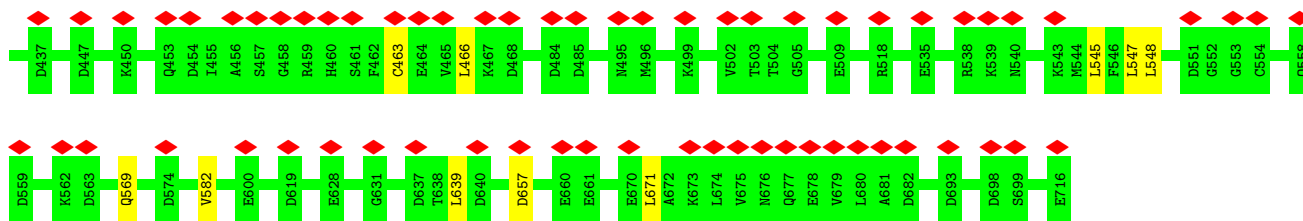


- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



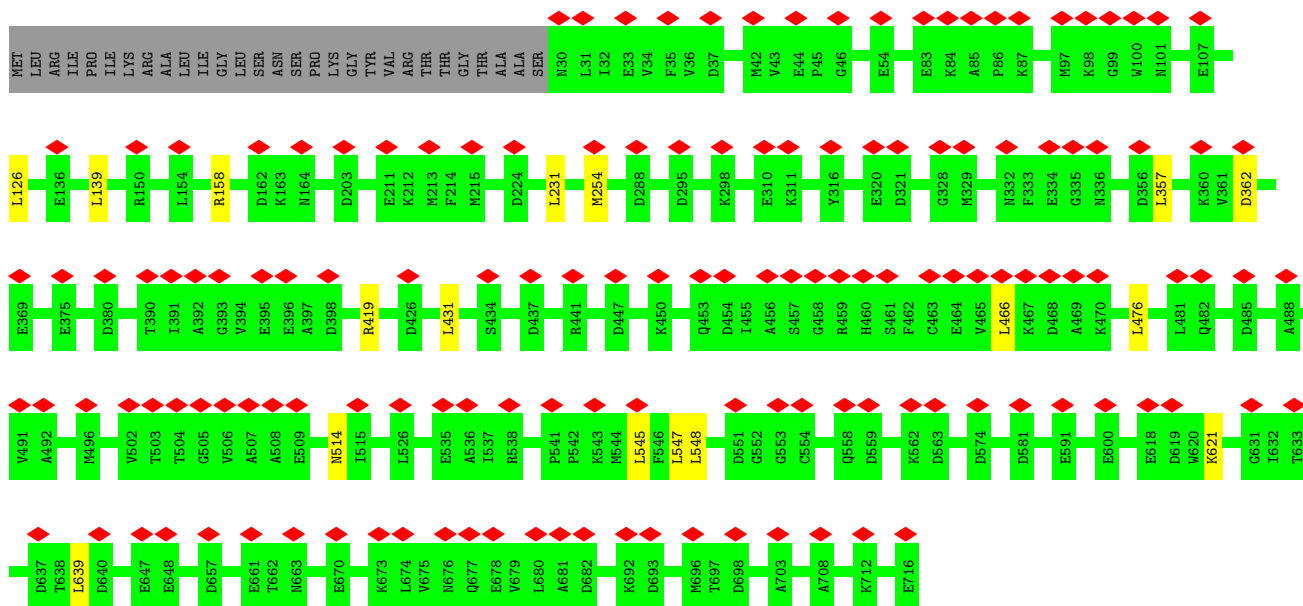
- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





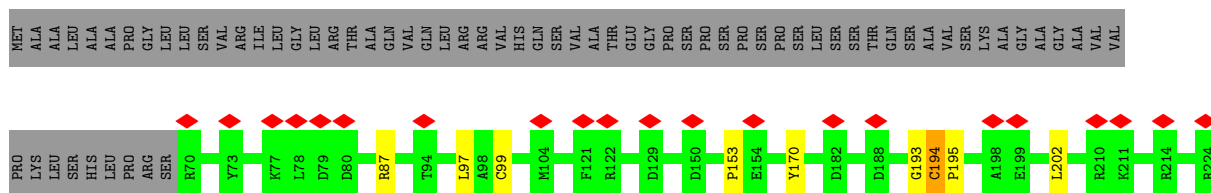
- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain s1: 20% 94%



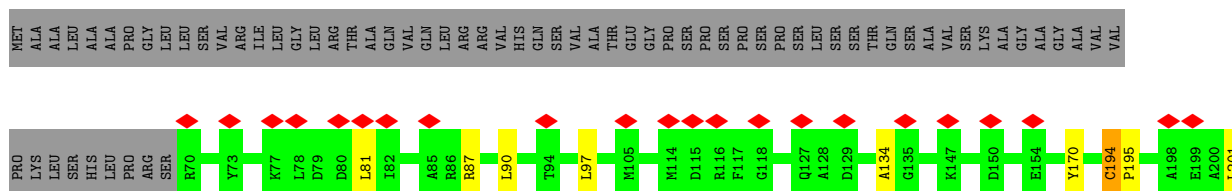
- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

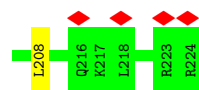
Chain S7: 9% 65% 31%



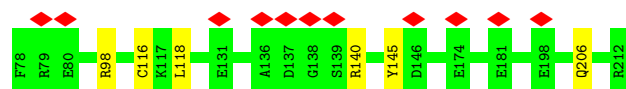
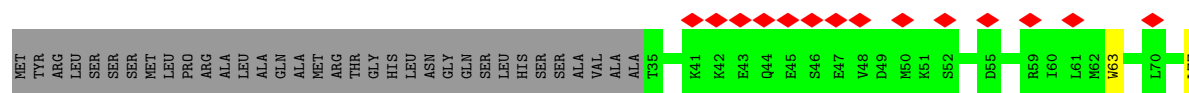
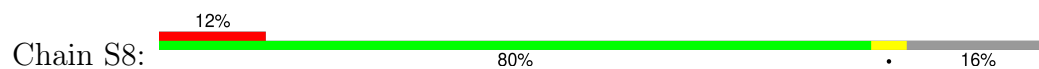
- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain s7: 12% 65% 31%

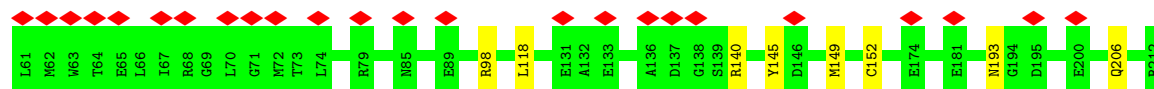
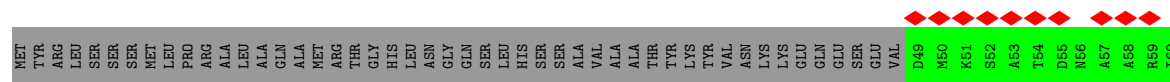
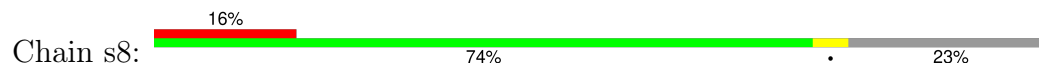




- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.227	Depositor
Minimum map value	-9.364	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.291	Depositor
Recommended contour level	3.4	Depositor
Map size (\AA)	249.92, 338.8, 238.48	wwPDB
Map dimensions	271, 385, 284	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, FES, ZN, MG, NDP, HEM, SF4, DGT, HEC, 2MR, EH2

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	3	0.42	0/940	0.83	1/1285 (0.1%)
1	3a	0.41	0/917	0.78	3/1252 (0.2%)
2	S3	0.38	0/1762	0.74	2/2401 (0.1%)
2	s3	0.37	0/1751	0.73	2/2386 (0.1%)
3	S2	0.38	0/3485	0.71	5/4720 (0.1%)
3	s2	0.38	0/3469	0.71	5/4698 (0.1%)
4	1	0.43	0/2607	0.87	12/3564 (0.3%)
4	1a	0.41	0/2599	0.87	11/3554 (0.3%)
5	6	0.40	0/1322	0.67	1/1799 (0.1%)
5	6a	0.37	0/1330	0.71	3/1809 (0.2%)
6	4L	0.39	0/740	0.72	0/1005
6	4l	0.37	0/738	0.72	1/1002 (0.1%)
7	5	0.39	0/4913	0.77	11/6685 (0.2%)
7	5a	0.39	0/4913	0.71	2/6685 (0.0%)
8	4	0.41	0/3717	0.82	7/5062 (0.1%)
8	4a	0.37	0/3717	0.80	10/5062 (0.2%)
9	2	0.39	0/2756	0.80	5/3751 (0.1%)
9	2a	0.49	3/2756 (0.1%)	0.94	10/3751 (0.3%)
10	AL	0.32	0/2674	0.59	0/3626
10	al	0.32	0/2674	0.63	3/3626 (0.1%)
11	A9	0.36	0/2823	0.68	3/3828 (0.1%)
11	a9	0.33	0/2823	0.66	1/3828 (0.0%)
12	S4	0.30	0/1044	0.61	0/1409
12	s4	0.30	0/1044	0.60	0/1409
13	S6	0.31	0/762	0.59	0/1026
13	s6	0.31	0/762	0.66	1/1026 (0.1%)
14	A2	0.33	0/682	0.75	1/920 (0.1%)
14	a2	0.31	0/682	0.75	2/920 (0.2%)
15	AB	0.33	0/637	0.66	0/858
15	AC	0.33	0/718	0.73	1/970 (0.1%)
15	ab	0.30	0/637	0.62	1/858 (0.1%)
15	ac	0.30	0/718	0.59	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	A5	0.29	0/949	0.64	0/1286
16	a5	0.32	0/945	0.67	2/1281 (0.2%)
17	A6	0.34	0/980	0.71	1/1317 (0.1%)
17	a6	0.34	0/972	0.69	1/1305 (0.1%)
18	A8	0.37	0/1422	0.70	1/1921 (0.1%)
18	a8	0.34	0/1427	0.66	3/1927 (0.2%)
19	AM	0.36	0/1069	0.65	1/1449 (0.1%)
19	am	0.35	0/1069	0.61	0/1449
20	AO	0.33	0/1192	0.62	0/1608
20	ao	0.33	0/1192	0.64	0/1608
21	A1	0.40	0/577	0.71	0/777
21	a1	0.42	1/577 (0.2%)	0.71	0/777
22	A3	0.31	0/671	0.54	0/921
22	a3	0.31	0/671	0.66	2/921 (0.2%)
23	C1	0.31	0/418	0.58	0/567
23	c1	0.32	0/388	0.56	0/528
24	C2	0.34	0/1028	0.63	1/1387 (0.1%)
24	c2	0.34	0/1028	0.64	1/1387 (0.1%)
25	S5	0.33	0/900	0.61	0/1199
25	s5	0.33	0/900	0.61	0/1199
26	B1	0.34	0/495	0.63	0/667
26	b1	0.36	0/495	0.69	1/667 (0.1%)
27	BM	0.35	0/854	0.58	0/1163
27	bm	0.36	0/863	0.69	1/1175 (0.1%)
28	B5	0.34	0/1201	0.64	0/1626
28	b5	0.34	0/1193	0.64	0/1615
29	B6	0.37	0/807	0.70	0/1096
29	b6	0.31	0/784	0.68	1/1063 (0.1%)
30	B2	0.34	0/580	0.65	0/794
30	b2	0.32	0/569	0.59	1/779 (0.1%)
31	B3	0.34	0/587	0.65	0/793
31	b3	0.35	0/591	0.62	0/798
32	B8	0.32	0/1356	0.58	0/1851
32	b8	0.32	0/1356	0.60	0/1851
33	B4	0.34	0/1073	0.64	0/1455
33	b4	0.34	0/1073	0.64	1/1455 (0.1%)
34	B9	0.34	0/1596	0.67	3/2162 (0.1%)
34	b9	0.32	0/1589	0.62	0/2152
35	B7	0.31	0/1009	0.68	2/1355 (0.1%)
35	b7	0.35	0/1030	0.66	0/1382
36	BL	0.32	0/1443	0.60	0/1951
36	bl	0.32	0/1463	0.60	0/1977
37	AN	0.34	0/1243	0.67	1/1692 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	an	0.32	0/1243	0.63	0/1692
38	A7	0.28	0/759	0.60	0/1027
38	a7	0.31	0/572	0.64	0/774
39	V3	0.31	0/349	0.75	1/473 (0.2%)
39	v3	0.34	0/311	0.72	1/420 (0.2%)
40	3A	0.35	1/3529 (0.0%)	0.72	5/4793 (0.1%)
40	3L	0.37	0/3530	0.77	4/4793 (0.1%)
41	3B	0.33	0/3205	0.68	5/4332 (0.1%)
41	3M	0.33	0/3205	0.64	2/4332 (0.0%)
42	3C	0.35	0/3147	0.66	3/4297 (0.1%)
42	3N	0.37	0/3147	0.65	1/4297 (0.0%)
43	3D	0.35	0/1978	0.68	5/2685 (0.2%)
43	3O	0.31	0/1968	0.62	0/2674
44	3E	0.32	0/609	0.62	1/821 (0.1%)
44	3P	0.33	0/617	0.61	0/832
45	3F	0.30	0/922	0.65	0/1234
45	3Q	0.31	0/901	0.69	2/1207 (0.2%)
46	3G	0.39	0/689	0.78	0/931
46	3R	0.39	0/617	0.72	0/833
47	3H	0.36	0/552	0.77	2/739 (0.3%)
47	3S	0.30	0/552	0.69	2/739 (0.3%)
48	3J	0.45	0/473	0.85	2/637 (0.3%)
48	3U	0.36	0/503	0.60	0/678
49	3K	0.36	0/437	0.69	0/598
49	3V	0.36	0/454	0.64	0/619
50	3T	0.33	0/403	0.67	0/546
51	V1	0.38	0/3376	0.78	7/4561 (0.2%)
51	v1	0.39	0/3333	0.77	7/4503 (0.2%)
52	V2	0.43	0/1670	0.81	7/2276 (0.3%)
52	v2	0.40	0/1553	0.80	1/2116 (0.0%)
53	S1	0.35	0/5377	0.77	18/7285 (0.2%)
53	s1	0.35	0/5377	0.74	12/7285 (0.2%)
54	S7	0.47	1/1272 (0.1%)	0.87	3/1722 (0.2%)
54	s7	0.40	0/1272	0.86	6/1722 (0.3%)
55	S8	0.43	1/1438 (0.1%)	0.78	2/1946 (0.1%)
55	s8	0.42	0/1337	0.77	1/1808 (0.1%)
All	All	0.36	7/165414 (0.0%)	0.71	229/224305 (0.1%)

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
2	S3	0	1
4	1	0	2
7	5a	0	1
8	4	0	2
18	A8	0	1
37	AN	0	1
41	3B	0	1
42	3C	0	1
51	V1	0	1
51	v1	0	2
52	V2	0	4
52	v2	0	1
54	S7	0	4
54	s7	0	3
All	All	0	25

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2a	255	PRO	CB-CG	-11.26	0.93	1.50
9	2a	255	PRO	CG-CD	-8.09	1.24	1.50
54	S7	194	CYS	CB-SG	-7.07	1.70	1.82
9	2a	255	PRO	N-CA	6.87	1.58	1.47
55	S8	116	CYS	CB-SG	-6.02	1.72	1.82

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2a	255	PRO	N-CD-CG	-17.40	77.11	103.20
9	2a	255	PRO	CA-CB-CG	-16.51	72.64	104.00
9	2a	255	PRO	CB-CG-CD	14.85	164.40	106.50
7	5	526	LEU	CA-CB-CG	10.95	140.48	115.30
52	V2	189	ASP	CB-CG-OD1	10.38	127.64	118.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1	154	LEU	Peptide
4	1	199	ASP	Peptide
8	4	249	ILE	Peptide
8	4	366	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	S3	70	LYS	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	3	111/115 (96%)	109 (98%)	2 (2%)	0	100	100
1	3a	109/115 (95%)	102 (94%)	7 (6%)	0	100	100
2	S3	204/263 (78%)	197 (97%)	7 (3%)	0	100	100
2	s3	203/263 (77%)	188 (93%)	15 (7%)	0	100	100
3	S2	418/463 (90%)	401 (96%)	17 (4%)	0	100	100
3	s2	416/463 (90%)	400 (96%)	16 (4%)	0	100	100
4	1	315/318 (99%)	294 (93%)	20 (6%)	1 (0%)	37	67
4	1a	314/318 (99%)	293 (93%)	20 (6%)	1 (0%)	37	67
5	6	168/172 (98%)	160 (95%)	8 (5%)	0	100	100
5	6a	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
6	4L	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
6	4l	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
7	5	603/607 (99%)	573 (95%)	28 (5%)	2 (0%)	37	67
7	5a	603/607 (99%)	562 (93%)	41 (7%)	0	100	100
8	4	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
8	4a	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
9	2	342/345 (99%)	331 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2a	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
10	AL	318/355 (90%)	299 (94%)	19 (6%)	0	100	100
10	al	318/355 (90%)	304 (96%)	14 (4%)	0	100	100
11	A9	340/377 (90%)	321 (94%)	19 (6%)	0	100	100
11	a9	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
12	S4	124/175 (71%)	118 (95%)	6 (5%)	0	100	100
12	s4	124/175 (71%)	122 (98%)	2 (2%)	0	100	100
13	S6	93/116 (80%)	93 (100%)	0	0	100	100
13	s6	93/116 (80%)	90 (97%)	3 (3%)	0	100	100
14	A2	82/99 (83%)	78 (95%)	4 (5%)	0	100	100
14	a2	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
15	AB	76/156 (49%)	73 (96%)	3 (4%)	0	100	100
15	AC	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
15	ab	76/156 (49%)	73 (96%)	3 (4%)	0	100	100
15	ac	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
16	A5	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
16	a5	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
17	A6	110/131 (84%)	105 (96%)	5 (4%)	0	100	100
17	a6	109/131 (83%)	103 (94%)	6 (6%)	0	100	100
18	A8	167/172 (97%)	159 (95%)	8 (5%)	0	100	100
18	a8	168/172 (98%)	162 (96%)	6 (4%)	0	100	100
19	AM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
19	am	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
20	AO	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
20	ao	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
21	A1	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
21	a1	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
22	A3	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
22	a3	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
23	C1	47/76 (62%)	47 (100%)	0	0	100	100
23	c1	43/76 (57%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	C2	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
24	c2	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
25	S5	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
25	s5	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
26	B1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
26	b1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
27	BM	96/151 (64%)	93 (97%)	3 (3%)	0	100	100
27	bm	97/151 (64%)	93 (96%)	4 (4%)	0	100	100
28	B5	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
28	b5	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
29	B6	90/127 (71%)	89 (99%)	1 (1%)	0	100	100
29	b6	86/127 (68%)	83 (96%)	3 (4%)	0	100	100
30	B2	62/105 (59%)	57 (92%)	5 (8%)	0	100	100
30	b2	61/105 (58%)	61 (100%)	0	0	100	100
31	B3	68/104 (65%)	65 (96%)	3 (4%)	0	100	100
31	b3	69/104 (66%)	66 (96%)	3 (4%)	0	100	100
32	B8	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
32	b8	153/186 (82%)	149 (97%)	4 (3%)	0	100	100
33	B4	123/129 (95%)	121 (98%)	2 (2%)	0	100	100
33	b4	123/129 (95%)	118 (96%)	5 (4%)	0	100	100
34	B9	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
34	b9	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
35	B7	112/136 (82%)	110 (98%)	2 (2%)	0	100	100
35	b7	115/136 (85%)	109 (95%)	6 (5%)	0	100	100
36	BL	165/176 (94%)	159 (96%)	6 (4%)	0	100	100
36	bl	167/176 (95%)	159 (95%)	8 (5%)	0	100	100
37	AN	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
37	an	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
38	A7	88/112 (79%)	84 (96%)	4 (4%)	0	100	100
38	a7	68/112 (61%)	63 (93%)	5 (7%)	0	100	100
39	V3	38/104 (36%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	v3	34/104 (33%)	34 (100%)	0	0	100	100
40	3A	443/446 (99%)	427 (96%)	16 (4%)	0	100	100
40	3L	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
41	3B	418/439 (95%)	405 (97%)	13 (3%)	0	100	100
41	3M	418/439 (95%)	396 (95%)	22 (5%)	0	100	100
42	3C	378/380 (100%)	366 (97%)	12 (3%)	0	100	100
42	3N	378/380 (100%)	361 (96%)	17 (4%)	0	100	100
43	3D	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
43	3O	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
44	3E	78/196 (40%)	76 (97%)	2 (3%)	0	100	100
44	3P	79/196 (40%)	73 (92%)	6 (8%)	0	100	100
45	3F	100/110 (91%)	97 (97%)	3 (3%)	0	100	100
45	3Q	97/110 (88%)	94 (97%)	3 (3%)	0	100	100
46	3G	77/81 (95%)	70 (91%)	7 (9%)	0	100	100
46	3R	69/81 (85%)	63 (91%)	6 (9%)	0	100	100
47	3H	64/76 (84%)	63 (98%)	1 (2%)	0	100	100
47	3S	64/76 (84%)	63 (98%)	1 (2%)	0	100	100
48	3J	54/63 (86%)	52 (96%)	1 (2%)	1 (2%)	6	35
48	3U	57/63 (90%)	56 (98%)	1 (2%)	0	100	100
49	3K	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
49	3V	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
50	3T	52/78 (67%)	50 (96%)	2 (4%)	0	100	100
51	V1	426/457 (93%)	371 (87%)	55 (13%)	0	100	100
51	v1	420/457 (92%)	375 (89%)	45 (11%)	0	100	100
52	V2	207/244 (85%)	178 (86%)	28 (14%)	1 (0%)	25	57
52	v2	190/244 (78%)	176 (93%)	14 (7%)	0	100	100
53	S1	685/716 (96%)	620 (90%)	65 (10%)	0	100	100
53	s1	685/716 (96%)	619 (90%)	66 (10%)	0	100	100
54	S7	153/224 (68%)	138 (90%)	15 (10%)	0	100	100
54	s7	153/224 (68%)	138 (90%)	15 (10%)	0	100	100
55	S8	176/212 (83%)	158 (90%)	18 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	s8	162/212 (76%)	145 (90%)	16 (10%)	1 (1%)	22	54
All	All	19905/22630 (88%)	18869 (95%)	1029 (5%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1	91	MET
7	5	433	THR
4	1a	91	MET
48	3J	57	LYS
55	s8	152	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	102/104 (98%)	99 (97%)	3 (3%)	37	59
1	3a	100/104 (96%)	96 (96%)	4 (4%)	27	52
2	S3	188/227 (83%)	176 (94%)	12 (6%)	14	42
2	s3	187/227 (82%)	184 (98%)	3 (2%)	58	74
3	S2	364/394 (92%)	355 (98%)	9 (2%)	42	62
3	s2	362/394 (92%)	350 (97%)	12 (3%)	33	57
4	1	279/279 (100%)	270 (97%)	9 (3%)	34	57
4	1a	278/279 (100%)	268 (96%)	10 (4%)	30	55
5	6	136/138 (99%)	128 (94%)	8 (6%)	16	44
5	6a	137/138 (99%)	125 (91%)	12 (9%)	8	32
6	4L	87/88 (99%)	84 (97%)	3 (3%)	32	56
6	4l	87/88 (99%)	83 (95%)	4 (5%)	23	49
7	5	548/550 (100%)	533 (97%)	15 (3%)	40	61
7	5a	548/550 (100%)	533 (97%)	15 (3%)	40	61
8	4	415/415 (100%)	407 (98%)	8 (2%)	52	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	4a	415/415 (100%)	405 (98%)	10 (2%)	44	63
9	2	307/308 (100%)	299 (97%)	8 (3%)	41	61
9	2a	307/308 (100%)	297 (97%)	10 (3%)	33	57
10	AL	284/309 (92%)	273 (96%)	11 (4%)	27	53
10	al	284/309 (92%)	277 (98%)	7 (2%)	42	62
11	A9	299/325 (92%)	291 (97%)	8 (3%)	40	61
11	a9	299/325 (92%)	290 (97%)	9 (3%)	36	58
12	S4	112/153 (73%)	112 (100%)	0	100	100
12	s4	112/153 (73%)	109 (97%)	3 (3%)	40	61
13	S6	80/96 (83%)	78 (98%)	2 (2%)	42	62
13	s6	80/96 (83%)	79 (99%)	1 (1%)	65	77
14	A2	74/80 (92%)	72 (97%)	2 (3%)	40	61
14	a2	74/80 (92%)	71 (96%)	3 (4%)	26	52
15	AB	72/135 (53%)	66 (92%)	6 (8%)	9	34
15	AC	81/135 (60%)	77 (95%)	4 (5%)	21	47
15	ab	72/135 (53%)	67 (93%)	5 (7%)	13	39
15	ac	81/135 (60%)	77 (95%)	4 (5%)	21	47
16	A5	101/102 (99%)	98 (97%)	3 (3%)	36	58
16	a5	101/102 (99%)	100 (99%)	1 (1%)	73	82
17	A6	106/114 (93%)	104 (98%)	2 (2%)	52	70
17	a6	105/114 (92%)	103 (98%)	2 (2%)	52	70
18	A8	152/154 (99%)	147 (97%)	5 (3%)	33	57
18	a8	152/154 (99%)	145 (95%)	7 (5%)	23	49
19	AM	106/106 (100%)	100 (94%)	6 (6%)	17	45
19	am	106/106 (100%)	102 (96%)	4 (4%)	28	53
20	AO	121/123 (98%)	117 (97%)	4 (3%)	33	57
20	ao	121/123 (98%)	117 (97%)	4 (3%)	33	57
21	A1	59/60 (98%)	57 (97%)	2 (3%)	32	56
21	a1	59/60 (98%)	57 (97%)	2 (3%)	32	56
22	A3	72/73 (99%)	68 (94%)	4 (6%)	17	45
22	a3	72/73 (99%)	70 (97%)	2 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	C1	43/67 (64%)	42 (98%)	1 (2%)	45	64
23	c1	40/67 (60%)	39 (98%)	1 (2%)	42	62
24	C2	107/107 (100%)	102 (95%)	5 (5%)	22	48
24	c2	107/107 (100%)	102 (95%)	5 (5%)	22	48
25	S5	93/94 (99%)	89 (96%)	4 (4%)	25	50
25	s5	93/94 (99%)	89 (96%)	4 (4%)	25	50
26	B1	52/53 (98%)	51 (98%)	1 (2%)	52	70
26	b1	52/53 (98%)	49 (94%)	3 (6%)	17	44
27	BM	89/129 (69%)	84 (94%)	5 (6%)	17	45
27	bm	90/129 (70%)	89 (99%)	1 (1%)	70	80
28	B5	123/162 (76%)	119 (97%)	4 (3%)	33	57
28	b5	122/162 (75%)	120 (98%)	2 (2%)	58	74
29	B6	86/119 (72%)	85 (99%)	1 (1%)	67	79
29	b6	85/119 (71%)	81 (95%)	4 (5%)	22	48
30	B2	60/87 (69%)	57 (95%)	3 (5%)	20	47
30	b2	59/87 (68%)	58 (98%)	1 (2%)	56	73
31	B3	55/78 (70%)	54 (98%)	1 (2%)	54	71
31	b3	55/78 (70%)	55 (100%)	0	100	100
32	B8	140/161 (87%)	137 (98%)	3 (2%)	48	67
32	b8	140/161 (87%)	137 (98%)	3 (2%)	48	67
33	B4	111/114 (97%)	109 (98%)	2 (2%)	54	71
33	b4	111/114 (97%)	108 (97%)	3 (3%)	40	61
34	B9	163/164 (99%)	158 (97%)	5 (3%)	35	57
34	b9	162/164 (99%)	157 (97%)	5 (3%)	35	57
35	B7	106/120 (88%)	100 (94%)	6 (6%)	17	45
35	b7	108/120 (90%)	102 (94%)	6 (6%)	17	45
36	BL	152/158 (96%)	147 (97%)	5 (3%)	33	57
36	bl	154/158 (98%)	148 (96%)	6 (4%)	27	53
37	AN	130/131 (99%)	127 (98%)	3 (2%)	45	64
37	an	130/131 (99%)	125 (96%)	5 (4%)	28	53
38	A7	83/95 (87%)	79 (95%)	4 (5%)	21	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	a7	63/95 (66%)	61 (97%)	2 (3%)	34	57
39	V3	39/95 (41%)	34 (87%)	5 (13%)	3	19
39	v3	35/95 (37%)	34 (97%)	1 (3%)	37	59
40	3A	372/373 (100%)	363 (98%)	9 (2%)	44	63
40	3L	372/373 (100%)	357 (96%)	15 (4%)	27	52
41	3B	330/344 (96%)	325 (98%)	5 (2%)	60	75
41	3M	330/344 (96%)	320 (97%)	10 (3%)	36	58
42	3C	332/332 (100%)	321 (97%)	11 (3%)	33	57
42	3N	332/332 (100%)	324 (98%)	8 (2%)	44	63
43	3D	206/206 (100%)	196 (95%)	10 (5%)	21	47
43	3O	205/206 (100%)	200 (98%)	5 (2%)	44	63
44	3E	69/166 (42%)	68 (99%)	1 (1%)	62	76
44	3P	70/166 (42%)	70 (100%)	0	100	100
45	3F	94/98 (96%)	91 (97%)	3 (3%)	34	57
45	3Q	91/98 (93%)	90 (99%)	1 (1%)	70	80
46	3G	72/73 (99%)	69 (96%)	3 (4%)	25	51
46	3R	64/73 (88%)	63 (98%)	1 (2%)	58	74
47	3H	63/72 (88%)	60 (95%)	3 (5%)	21	48
47	3S	63/72 (88%)	60 (95%)	3 (5%)	21	48
48	3J	47/54 (87%)	47 (100%)	0	100	100
48	3U	50/54 (93%)	50 (100%)	0	100	100
49	3K	41/46 (89%)	39 (95%)	2 (5%)	21	47
49	3V	43/46 (94%)	43 (100%)	0	100	100
50	3T	41/58 (71%)	41 (100%)	0	100	100
51	V1	343/366 (94%)	334 (97%)	9 (3%)	41	61
51	v1	338/366 (92%)	329 (97%)	9 (3%)	40	61
52	V2	182/204 (89%)	180 (99%)	2 (1%)	70	80
52	v2	170/204 (83%)	167 (98%)	3 (2%)	54	71
53	S1	579/602 (96%)	571 (99%)	8 (1%)	62	76
53	s1	579/602 (96%)	574 (99%)	5 (1%)	75	84
54	S7	131/185 (71%)	129 (98%)	2 (2%)	60	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	s7	131/185 (71%)	129 (98%)	2 (2%)	60	75
55	S8	145/178 (82%)	140 (97%)	5 (3%)	32	56
55	s8	138/178 (78%)	132 (96%)	6 (4%)	25	50
All	All	17545/19460 (90%)	17026 (97%)	519 (3%)	37	58

5 of 519 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	3Q	74	GLN
51	V1	379	CYS
43	3O	255	TYR
1	3a	92	PHE
39	V3	89	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
38	a7	21	GLN
47	3H	74	HIS
53	s1	514	ASN
40	3L	199	GLN
52	V2	190	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
3	2MR	s2	118	3	3,4,13	0.83	0	2,4,15	1.27	0
3	2MR	S2	118	3	10,12,13	2.72	3 (30%)	5,13,15	7.36	4 (80%)

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
3	2MR	s2	118	3	-	1/1/2/15	-
3	2MR	S2	118	3	-	4/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S2	118	2MR	CZ-NE	5.73	1.46	1.34
3	S2	118	2MR	CZ-NH2	5.42	1.44	1.33
3	S2	118	2MR	CQ1-NH1	-2.49	1.41	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S2	118	2MR	NE-CZ-NH2	12.39	130.84	119.48
3	S2	118	2MR	CD-NE-CZ	10.13	142.39	123.36
3	S2	118	2MR	CQ2-NH2-CZ	3.05	130.19	123.65
3	S2	118	2MR	CG-CD-NE	-2.38	105.52	112.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	s2	118	2MR	O-C-CA-CB
3	S2	118	2MR	CA-CB-CG-CD
3	S2	118	2MR	C-CA-CB-CG
3	S2	118	2MR	N-CA-CB-CG
3	S2	118	2MR	NE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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
62	HEC	3D	401	43	32,50,50	1.98	7 (21%)	30,82,82	3.42	17 (56%)
60	EHZ	5a	701	-	31,36,37	0.25	0	36,44,47	1.14	1 (2%)
61	HEM	3N	402	42	42,50,50	1.30	6 (14%)	46,82,82	1.69	10 (21%)
64	SF4	s8	301	55	0,12,12	-	-	-		
65	FES	S1	803	53	0,4,4	-	-	-		
65	FES	s1	803	53	0,4,4	-	-	-		
64	SF4	s8	302	55	0,12,12	-	-	-		
64	SF4	v1	502	51	0,12,12	-	-	-		
64	SF4	S1	801	53	0,12,12	-	-	-		
58	NDP	A9	501	-	47,52,52	0.53	0	61,80,80	0.60	1 (1%)
64	SF4	V1	502	51	0,12,12	-	-	-		
64	SF4	s7	301	54	0,12,12	-	-	-		
65	FES	v2	301	52	0,4,4	-	-	-		
61	HEM	3C	402	42	42,50,50	1.29	6 (14%)	46,82,82	1.71	11 (23%)
57	DGT	AL	502	56	29,33,33	0.98	2 (6%)	37,52,52	0.77	0
65	FES	V2	301	52	0,4,4	-	-	-		
61	HEM	3N	401	42	42,50,50	1.26	4 (9%)	46,82,82	1.72	9 (19%)
64	SF4	S1	802	53	0,12,12	-	-	-		
64	SF4	s1	801	53	0,12,12	-	-	-		
57	DGT	al	502	-	29,33,33	0.98	2 (6%)	37,52,52	0.77	0
63	FMN	v1	501	-	33,33,33	0.27	0	48,50,50	0.54	1 (2%)
60	EHZ	B9	201	-	31,36,37	0.20	0	36,44,47	1.04	1 (2%)
61	HEM	3C	401	42	42,50,50	1.25	5 (11%)	46,82,82	1.75	10 (21%)
64	SF4	S8	301	55	0,12,12	-	-	-		
64	SF4	s1	802	53	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	EHZ	a6	201	-	31,36,37	0.19	0	36,44,47	1.25	1 (2%)
63	FMN	V1	501	-	33,33,33	0.30	0	48,50,50	0.48	0
62	HEC	3O	401	43	32,50,50	1.76	5 (15%)	30,82,82	3.15	15 (50%)
58	NDP	a9	501	-	47,52,52	0.54	0	61,80,80	0.58	1 (1%)
64	SF4	S7	301	3,54	0,12,12	-	-	-		
64	SF4	S8	302	55	0,12,12	-	-	-		
60	EHZ	A6	201	-	31,36,37	0.20	0	36,44,47	1.26	1 (2%)

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
62	HEC	3D	401	43	-	7/10/54/54	-
60	EHZ	5a	701	-	-	4/42/44/45	-
61	HEM	3N	402	42	-	5/12/54/54	-
64	SF4	s8	301	55	-	-	0/6/5/5
65	FES	S1	803	53	-	-	0/1/1/1
65	FES	s1	803	53	-	-	0/1/1/1
64	SF4	s8	302	55	-	-	0/6/5/5
64	SF4	v1	502	51	-	-	0/6/5/5
64	SF4	S1	801	53	-	-	0/6/5/5
58	NDP	A9	501	-	-	9/30/77/77	0/5/5/5
64	SF4	V1	502	51	-	-	0/6/5/5
64	SF4	s7	301	54	-	-	0/6/5/5
65	FES	v2	301	52	-	-	0/1/1/1
61	HEM	3C	402	42	-	5/12/54/54	-
57	DGT	AL	502	56	-	1/18/34/34	0/3/3/3
65	FES	V2	301	52	-	-	0/1/1/1
61	HEM	3N	401	42	-	7/12/54/54	-
64	SF4	S1	802	53	-	-	0/6/5/5
64	SF4	s1	801	53	-	-	0/6/5/5
57	DGT	al	502	-	-	2/18/34/34	0/3/3/3
63	FMN	v1	501	-	-	4/18/18/18	0/3/3/3
60	EHZ	B9	201	-	-	8/42/44/45	-
61	HEM	3C	401	42	-	7/12/54/54	-
64	SF4	S8	301	55	-	-	0/6/5/5
64	SF4	s1	802	53	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	EHZ	a6	201	-	-	10/42/44/45	-
63	FMN	V1	501	-	-	5/18/18/18	0/3/3/3
62	HEC	3O	401	43	-	5/10/54/54	-
58	NDP	a9	501	-	-	10/30/77/77	0/5/5/5
64	SF4	S7	301	3,54	-	-	0/6/5/5
64	SF4	S8	302	55	-	-	0/6/5/5
60	EHZ	A6	201	-	-	3/42/44/45	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	3D	401	HEC	C3C-C2C	-5.58	1.34	1.40
62	3D	401	HEC	C2B-C3B	-5.02	1.35	1.40
62	3O	401	HEC	C3C-C2C	-5.01	1.35	1.40
62	3O	401	HEC	C2B-C3B	-4.87	1.35	1.40
61	3C	402	HEM	C4D-ND	-3.81	1.33	1.40

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	3D	401	HEC	CBB-CAB-C3B	-7.38	110.23	127.49
60	a6	201	EHZ	C10-S1-C9	7.12	122.89	101.84
60	A6	201	EHZ	C10-S1-C9	6.83	122.02	101.84
62	3O	401	HEC	CBD-CAD-C3D	6.62	123.67	112.54
62	3O	401	HEC	CBB-CAB-C3B	-6.34	112.65	127.49

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

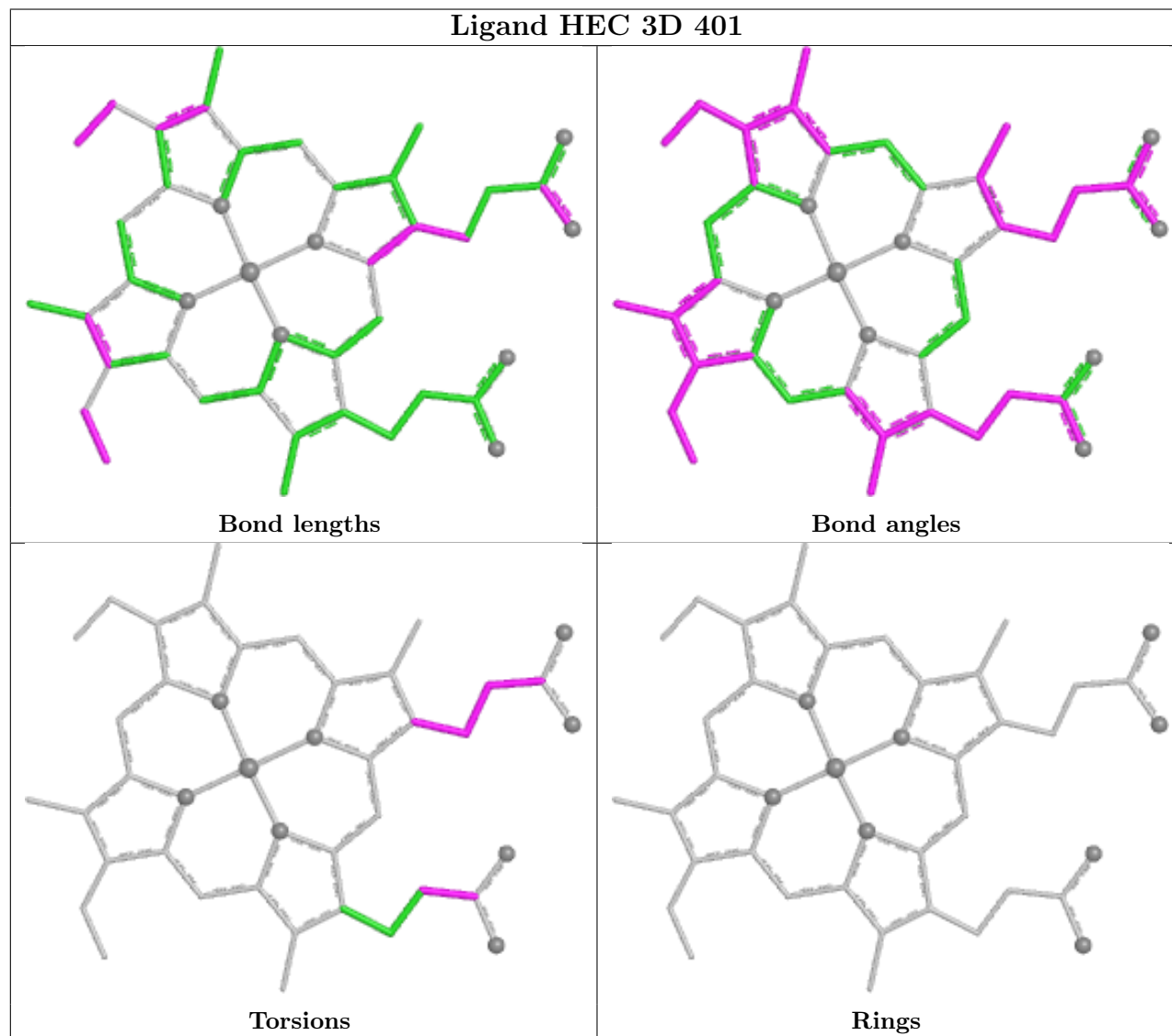
Mol	Chain	Res	Type	Atoms
57	al	502	DGT	PB-O3A-PA-O5'
58	A9	501	NDP	C5B-O5B-PA-O3
58	A9	501	NDP	C2N-C3N-C7N-O7N
58	A9	501	NDP	C2N-C3N-C7N-N7N
58	a9	501	NDP	C5D-O5D-PN-O3

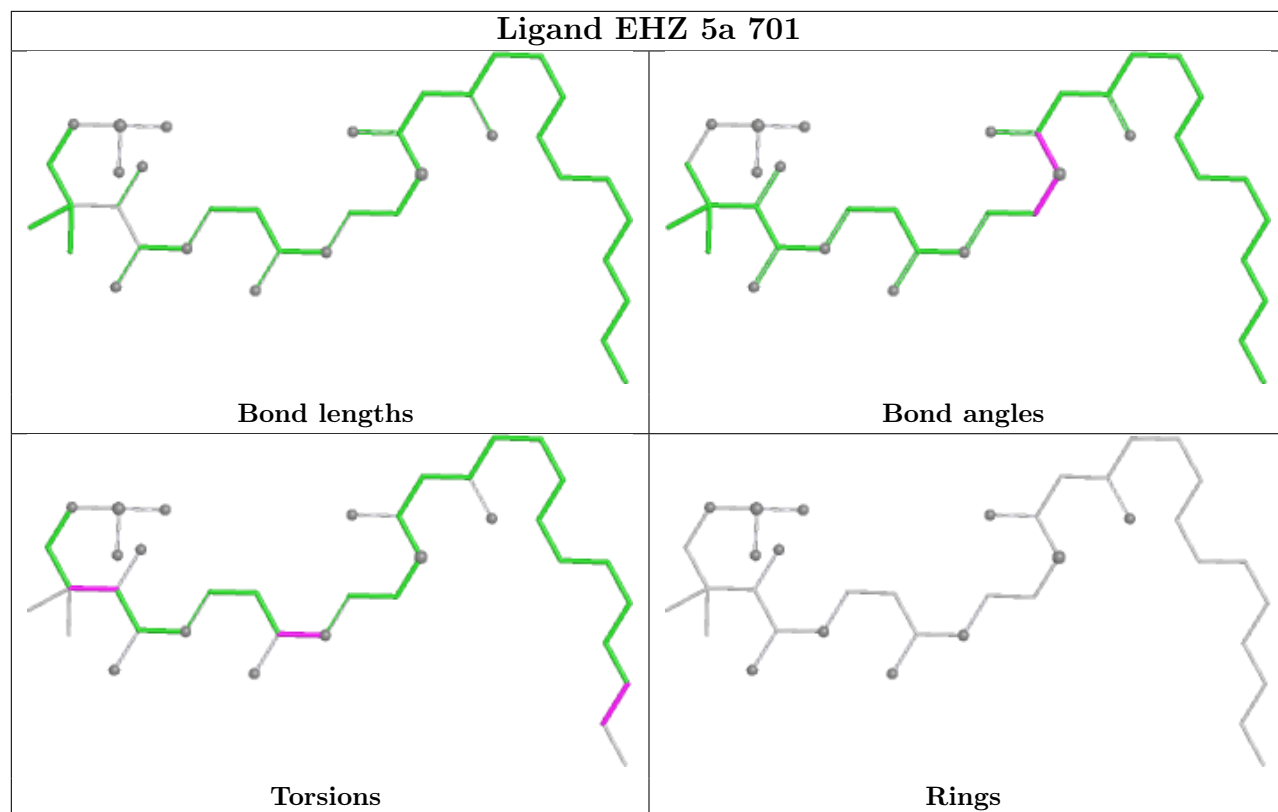
There are no ring outliers.

No monomer is involved in short contacts.

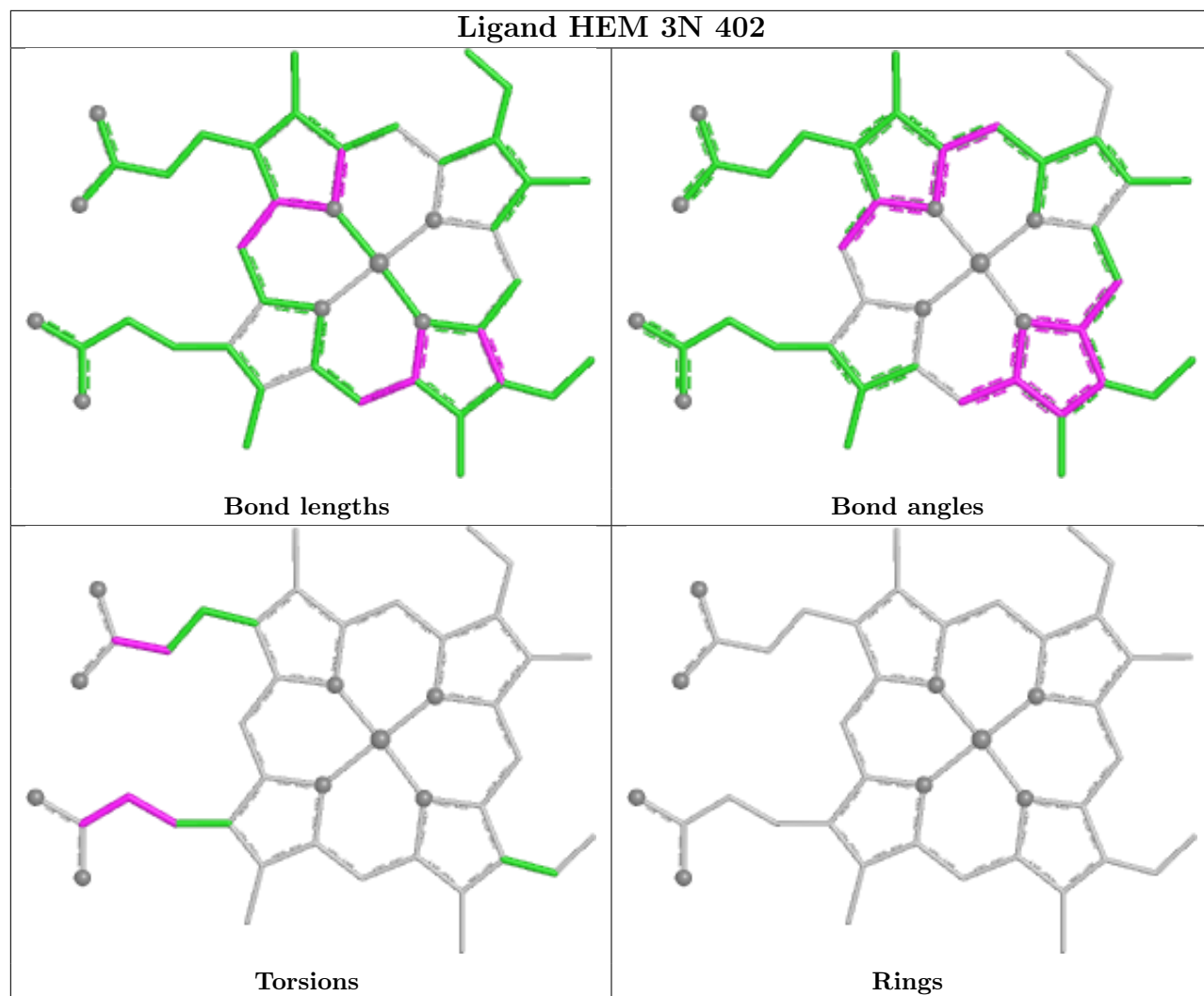
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

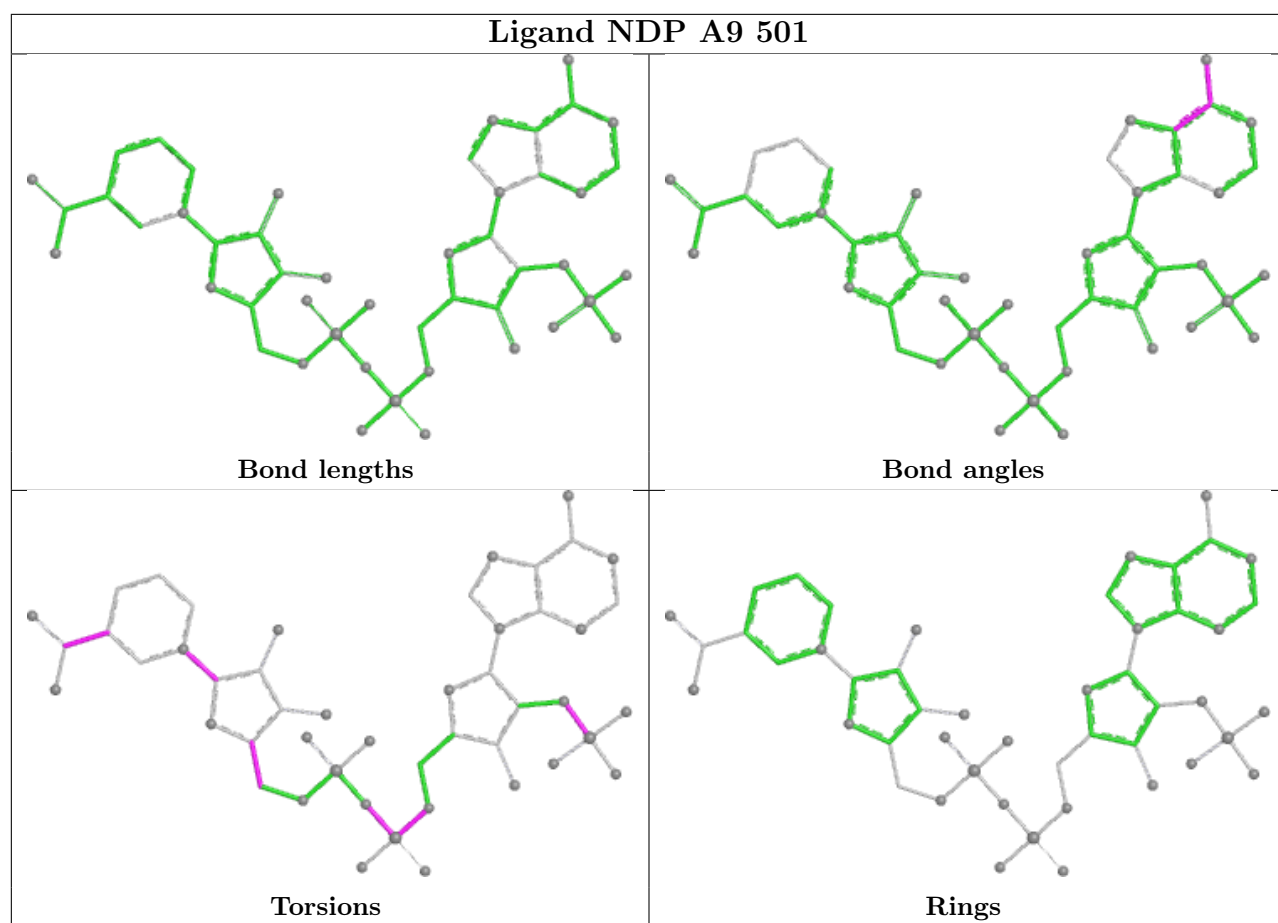
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



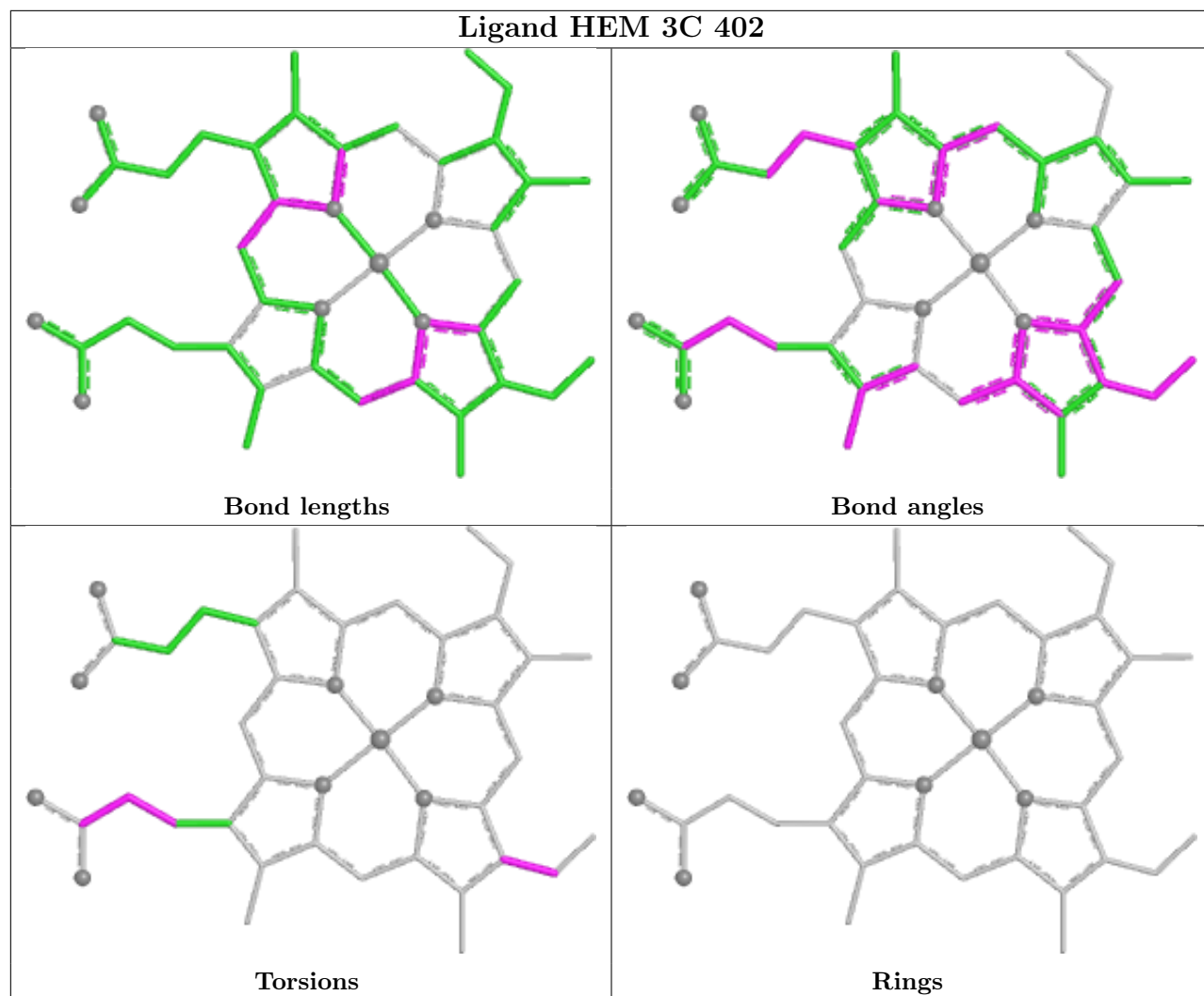


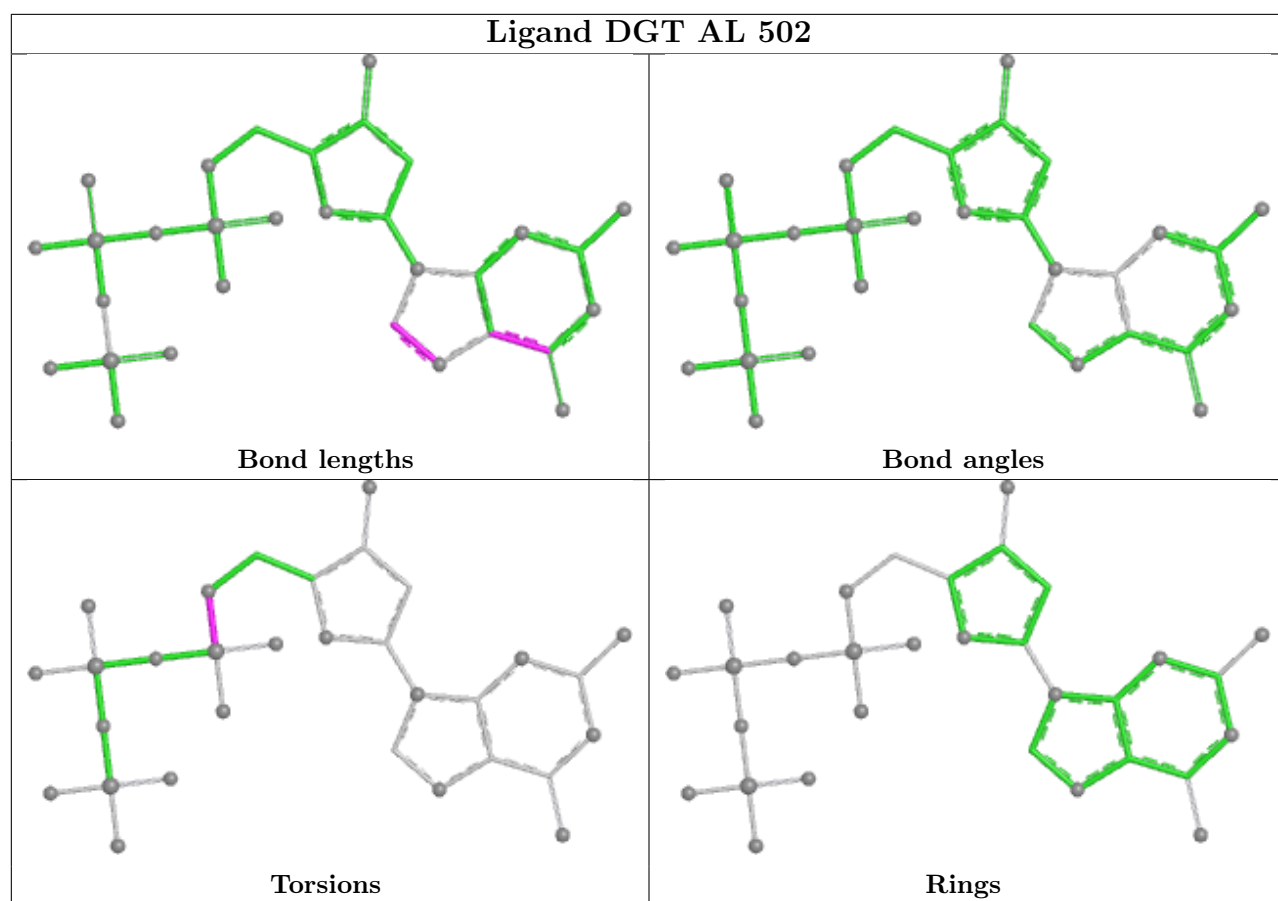
Ligand HEM 3N 402



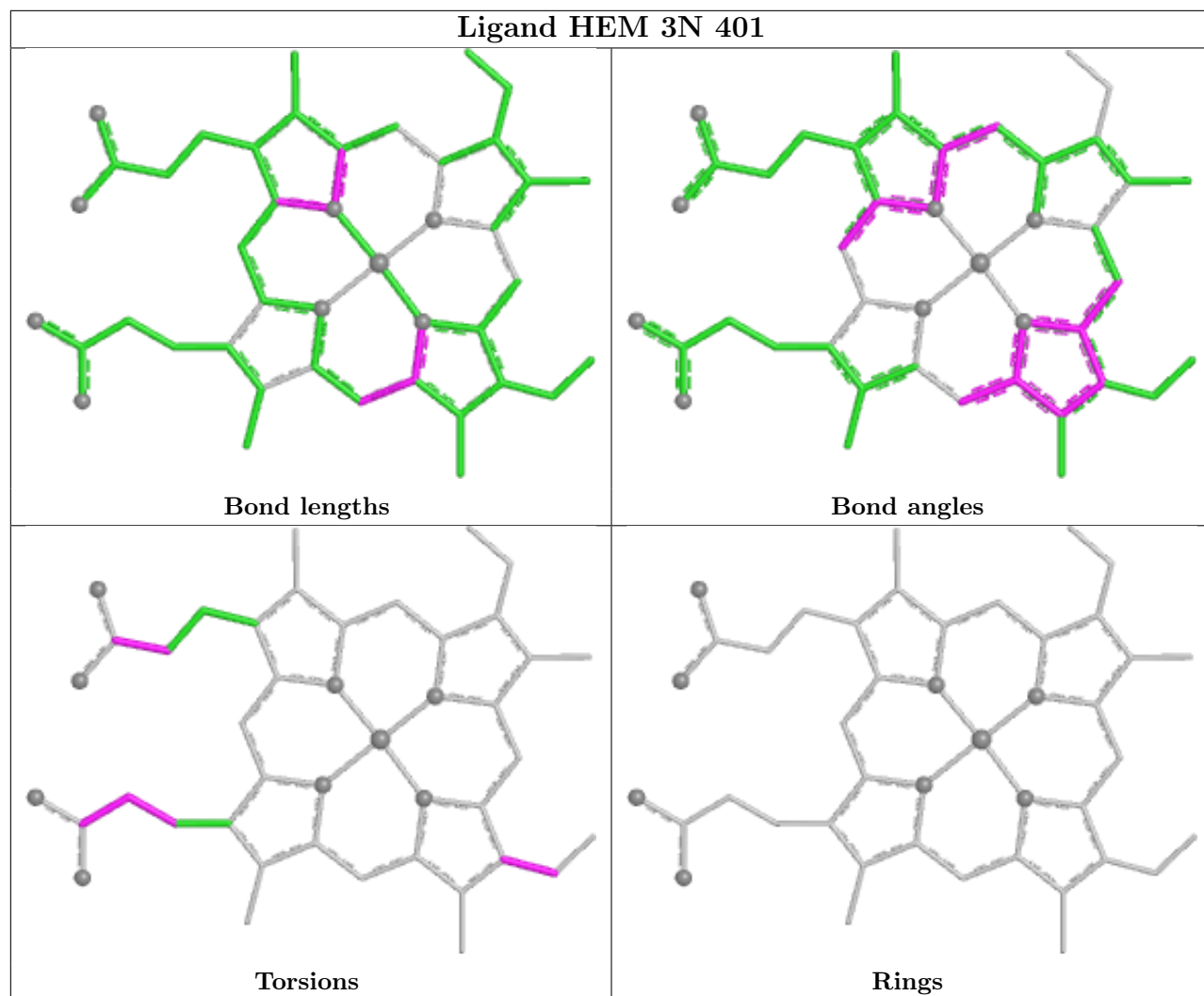


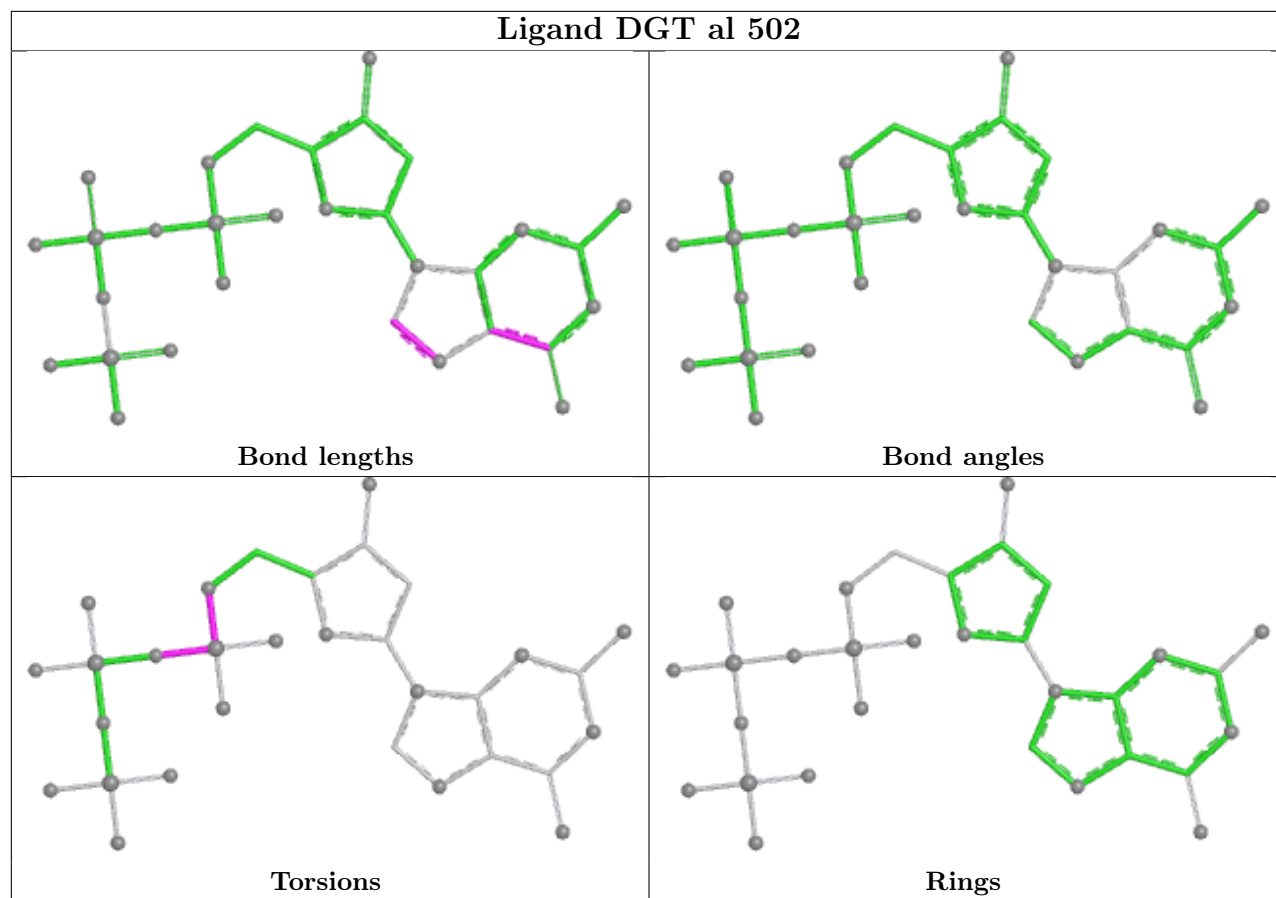
Ligand HEM 3C 402

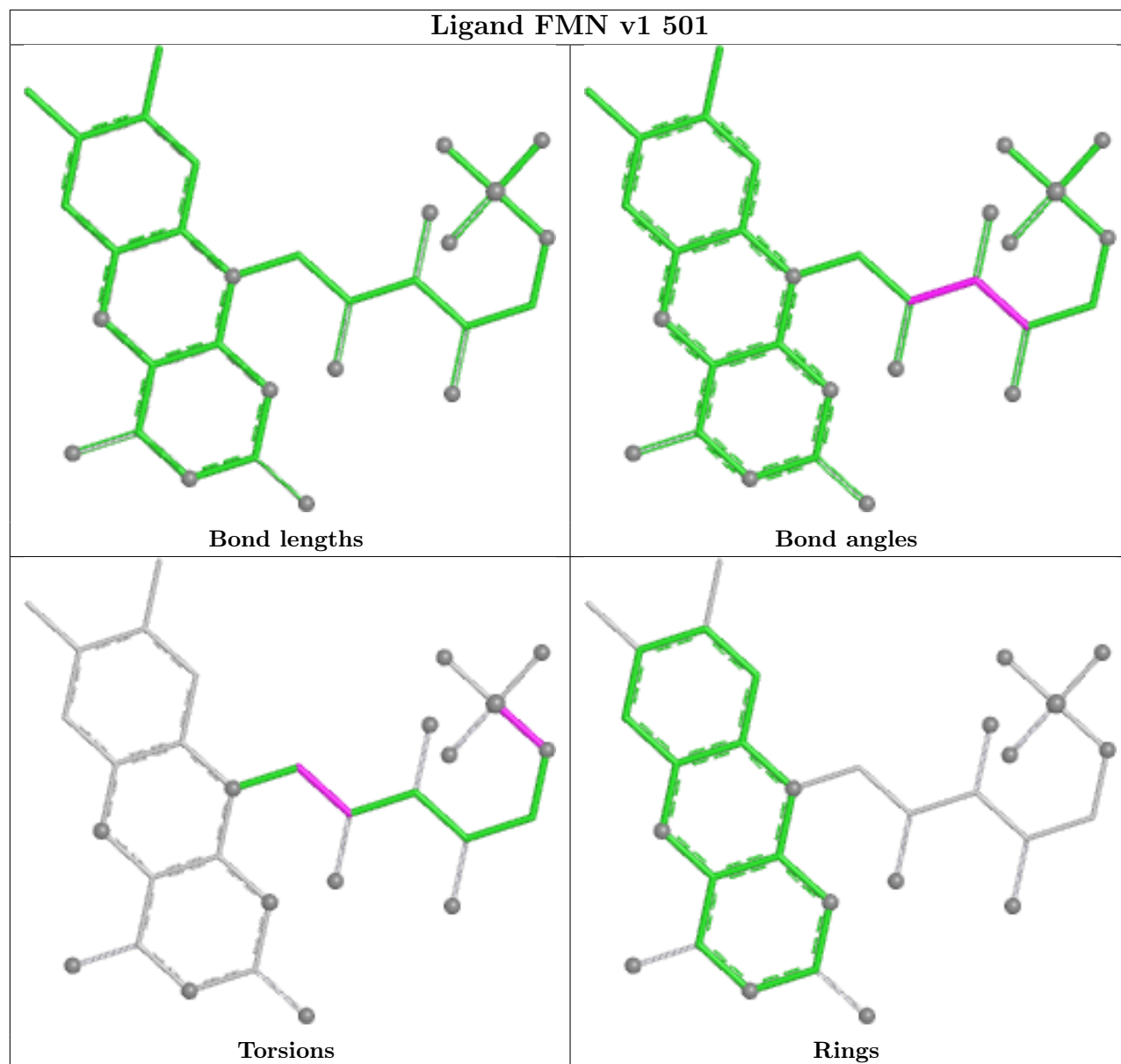


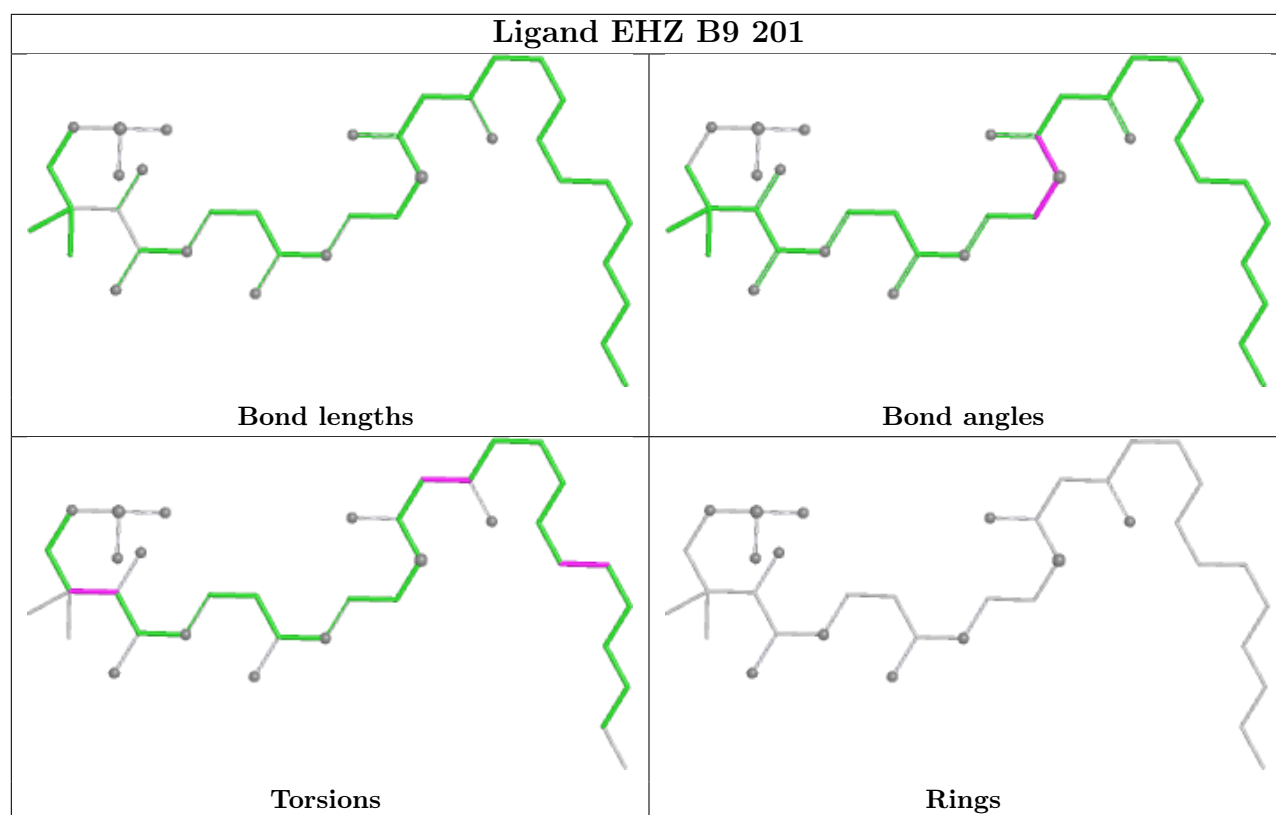


Ligand HEM 3N 401

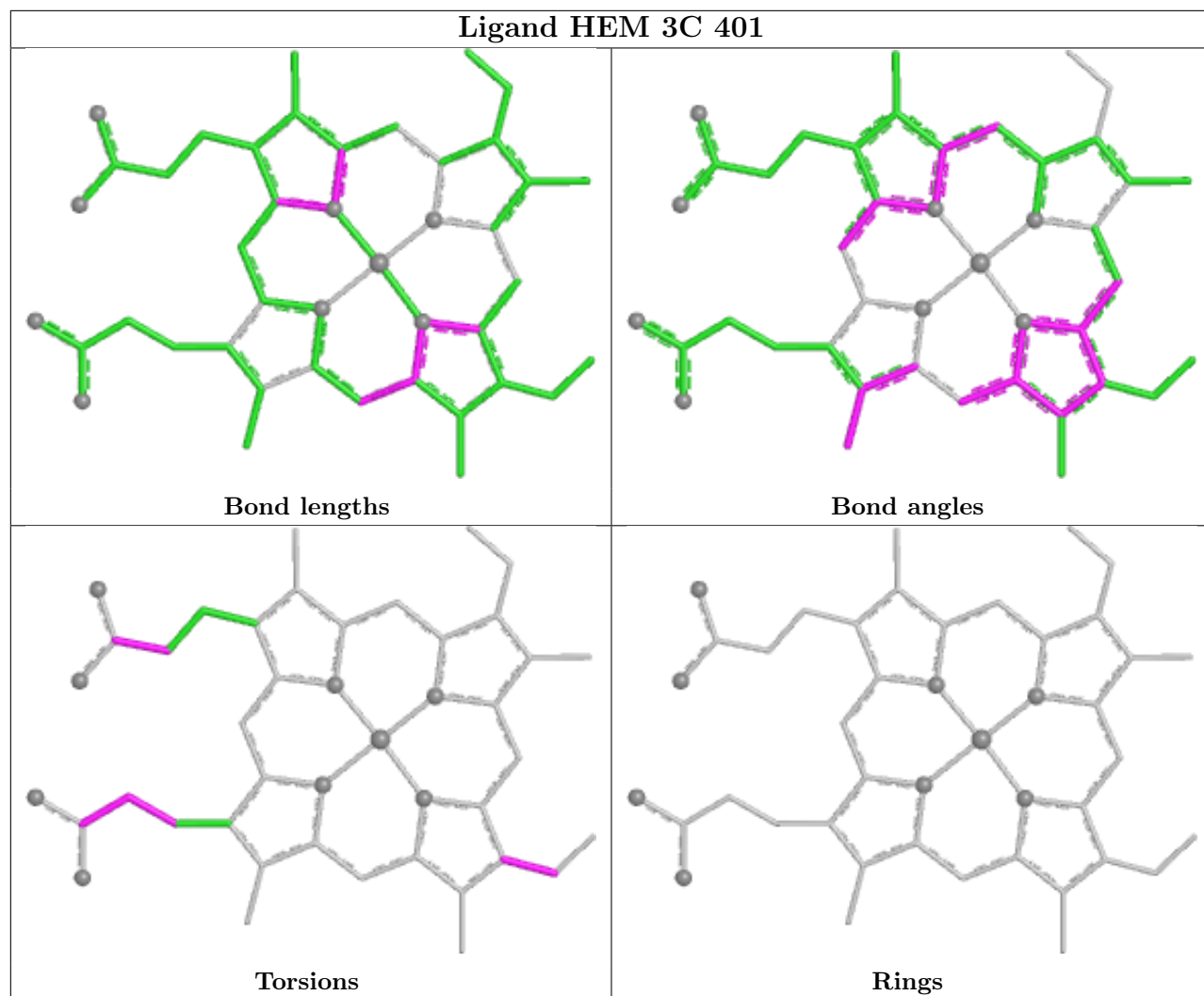


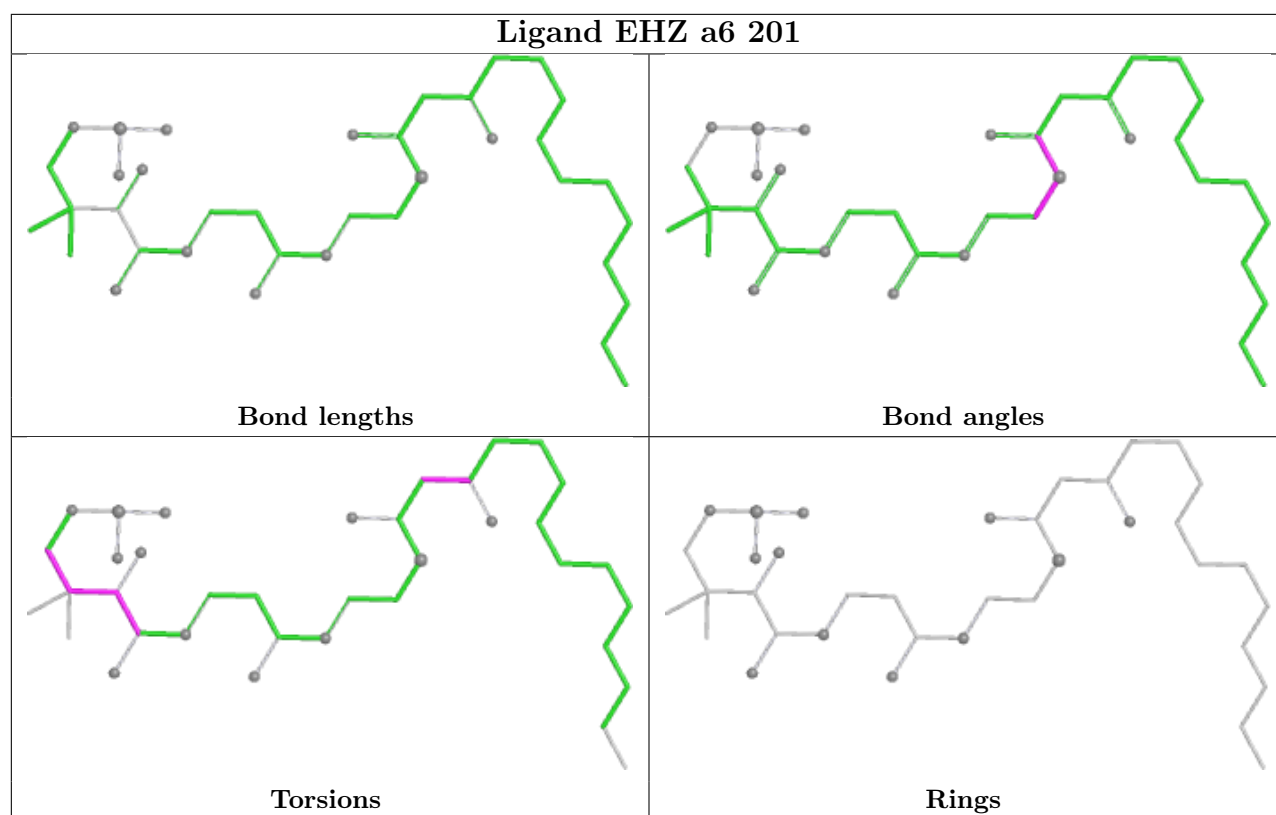




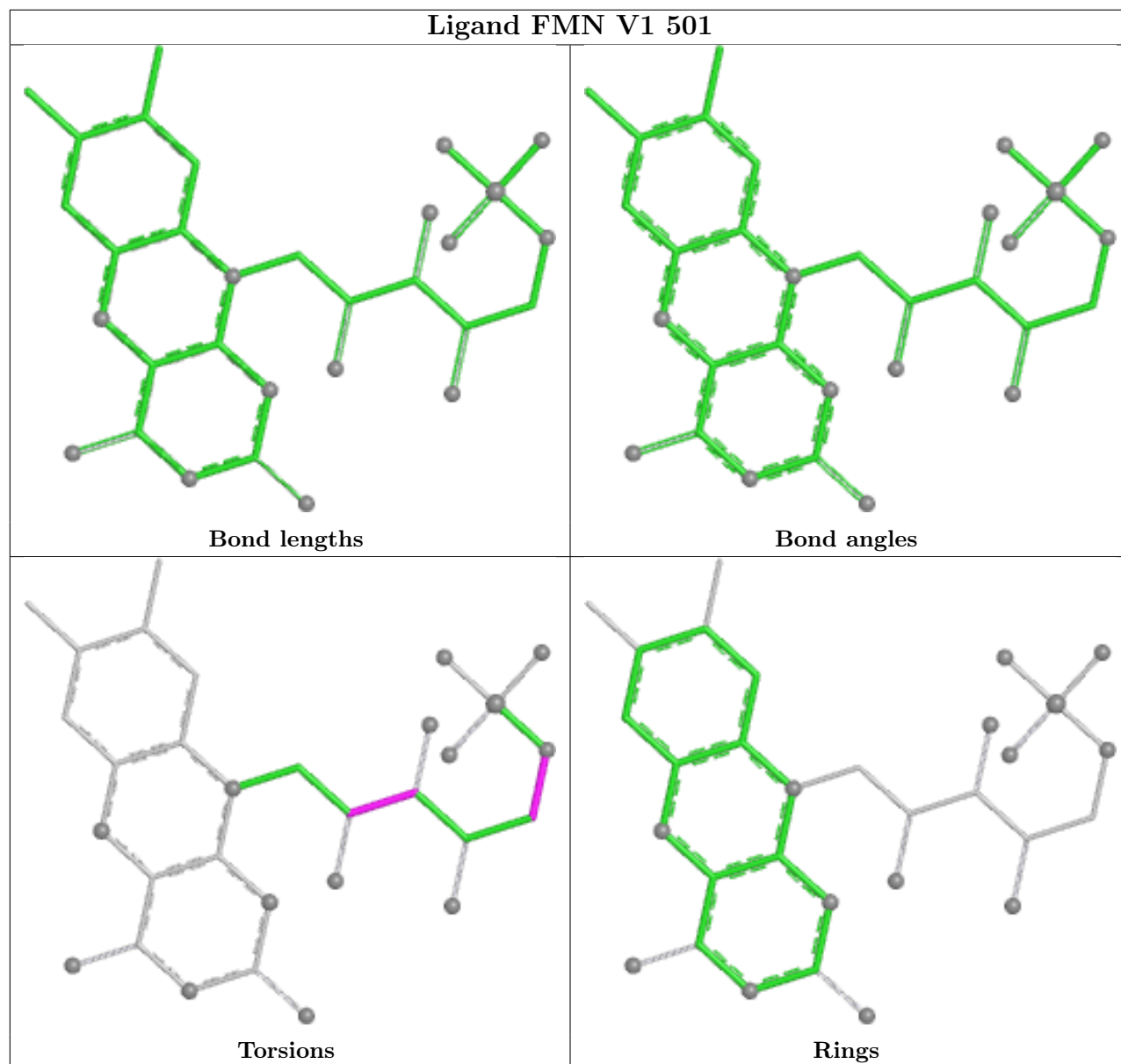


Ligand HEM 3C 401

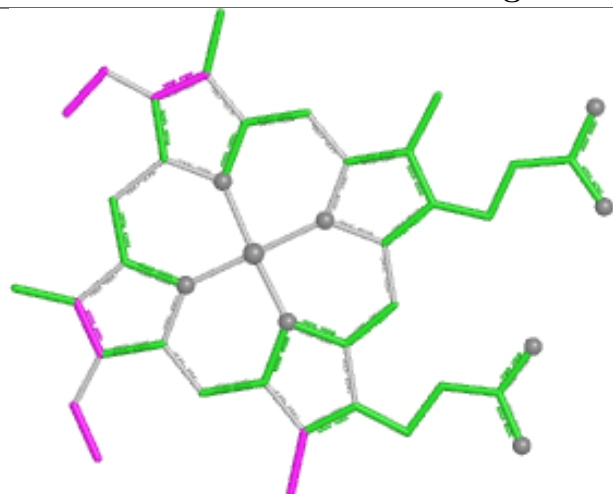




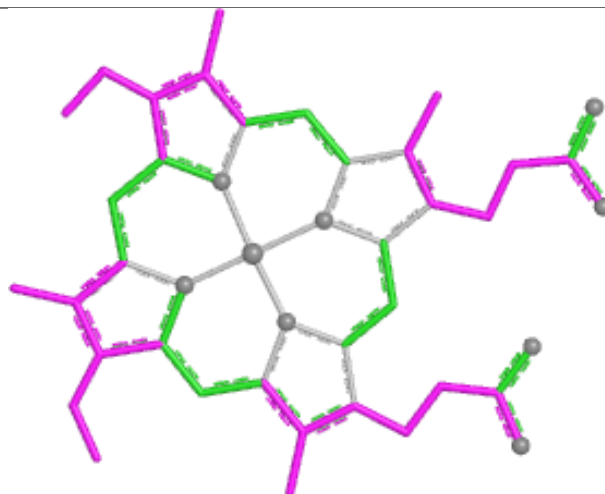
Ligand FMN V1 501



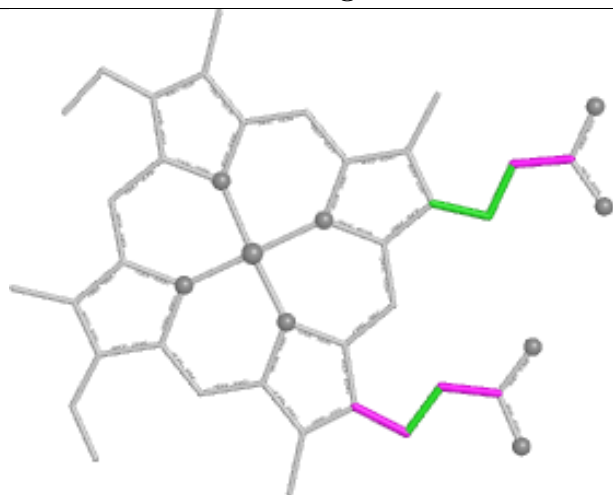
Ligand HEC 3O 401



Bond lengths



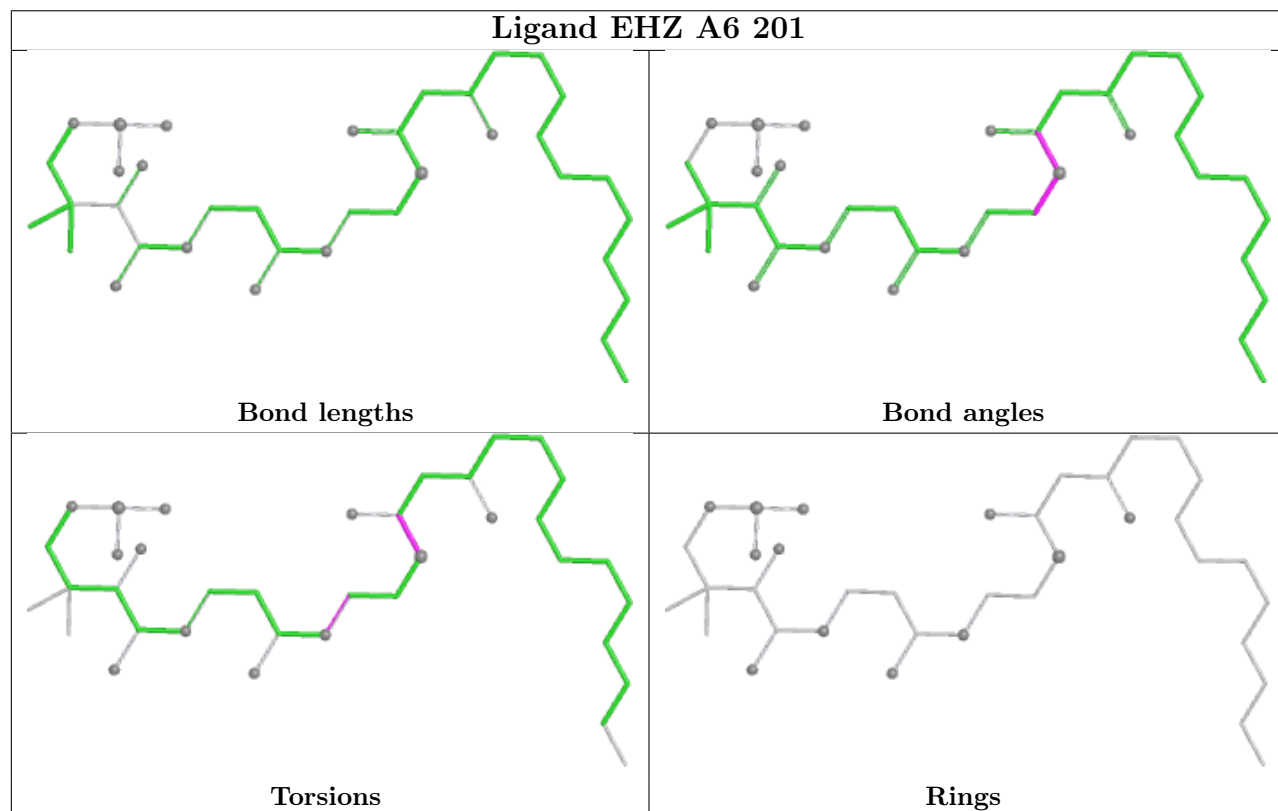
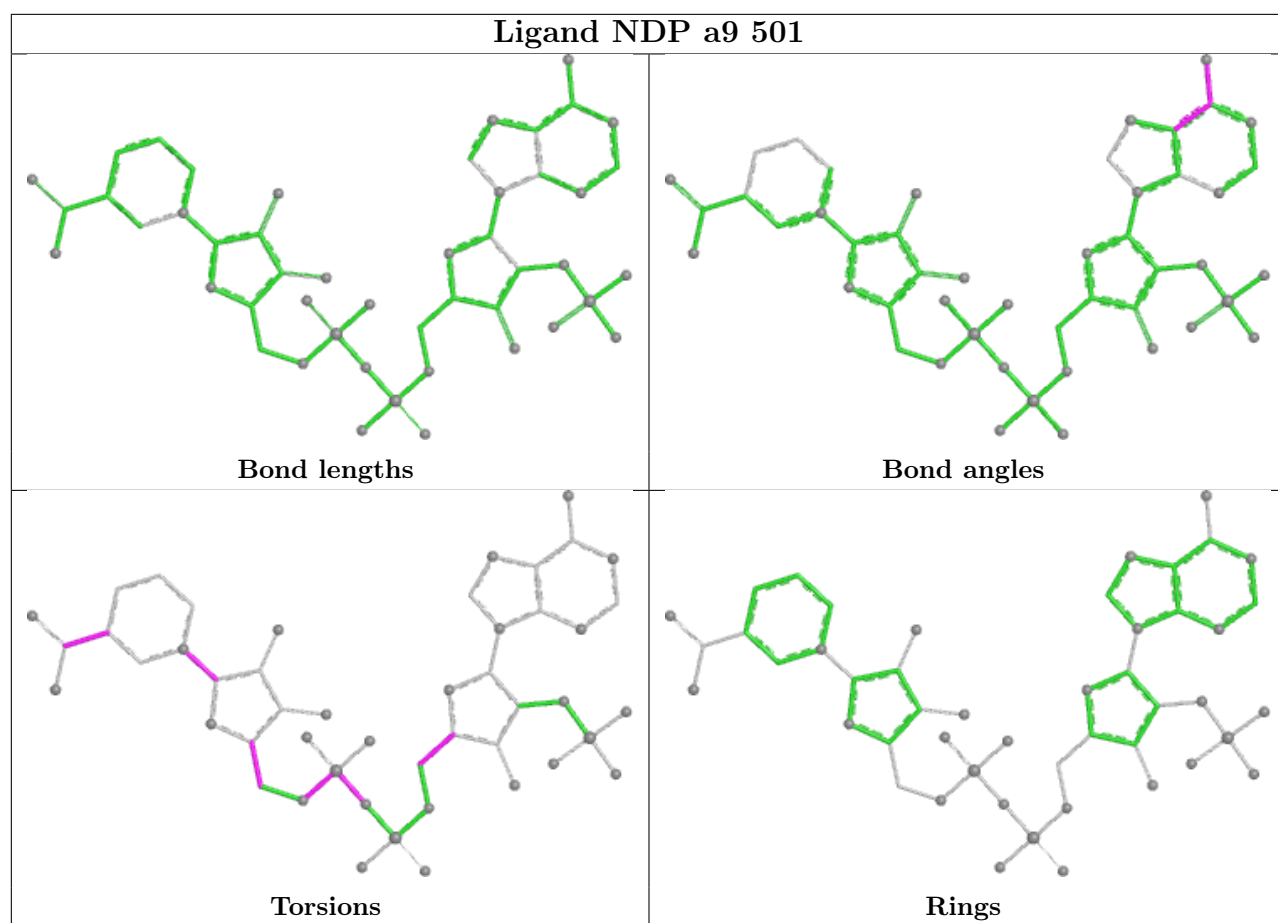
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

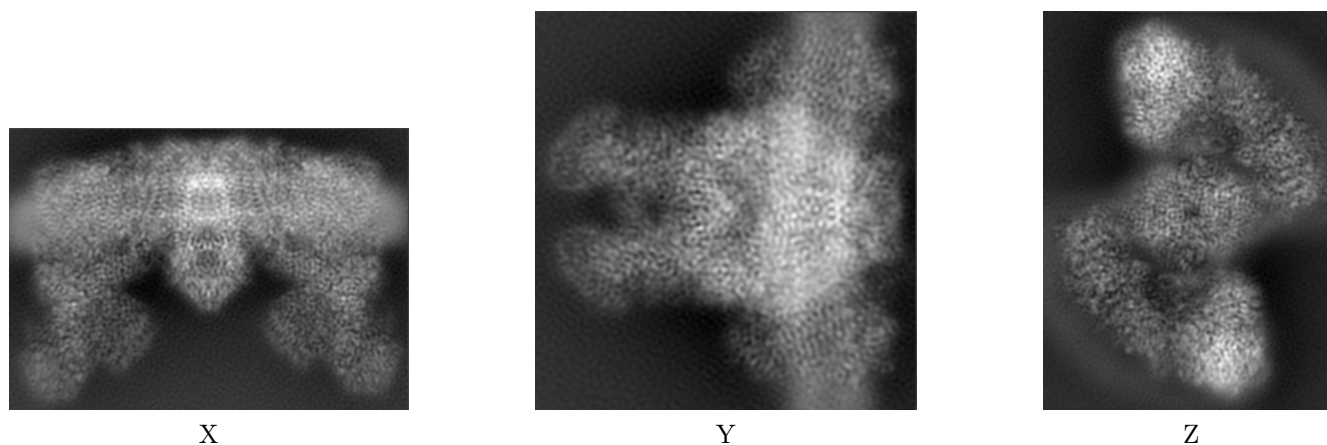
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42122. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

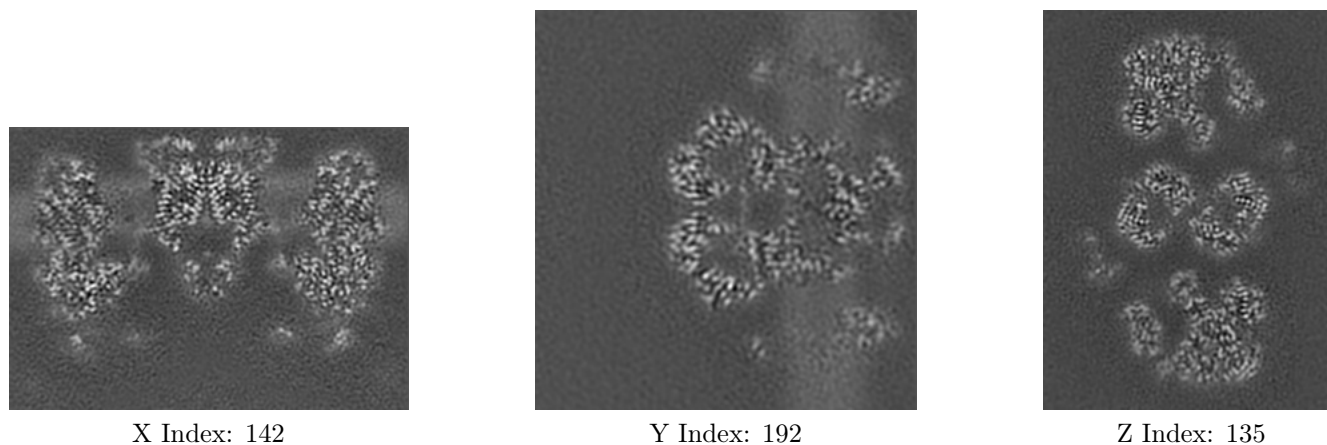
6.1.1 Primary map



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

6.2 Central slices [i](#)

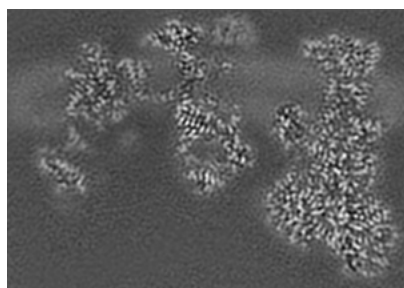
6.2.1 Primary map



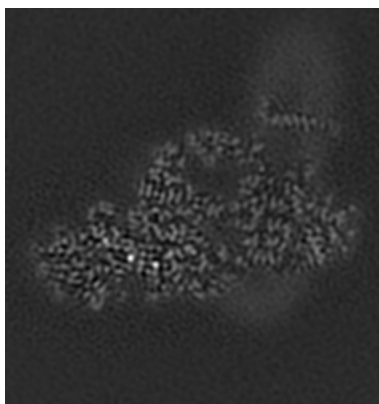
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

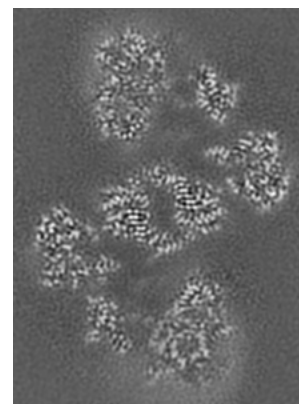
6.3.1 Primary map



X Index: 114



Y Index: 323

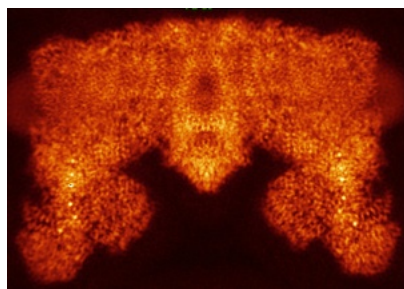


Z Index: 159

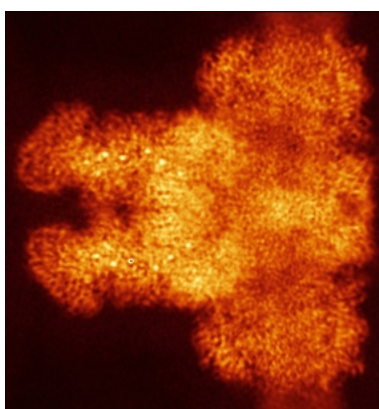
The images above show the largest variance slices of the map in three orthogonal directions.

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

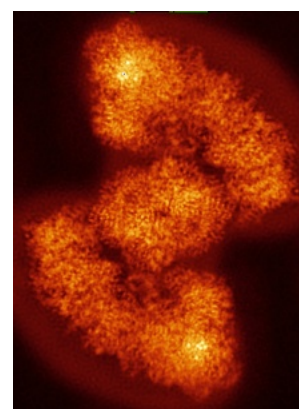
6.4.1 Primary map



X



Y

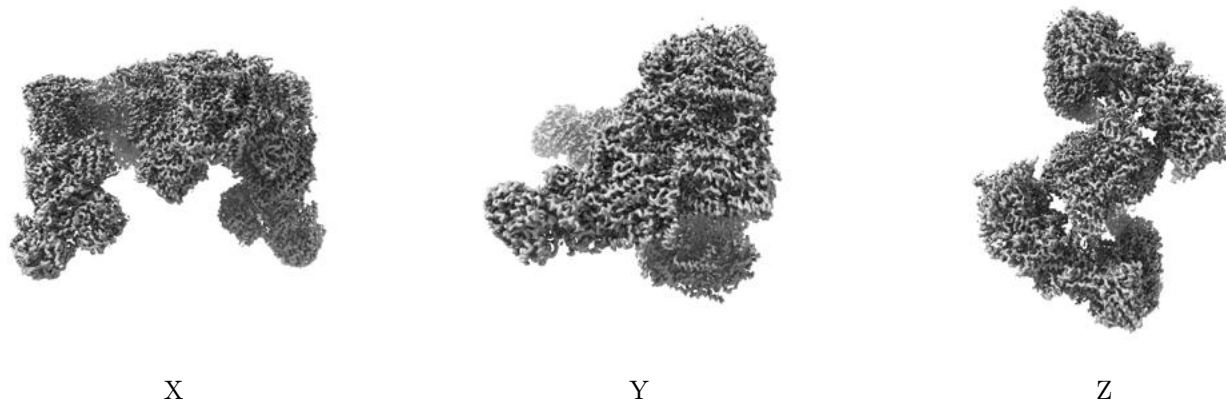


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

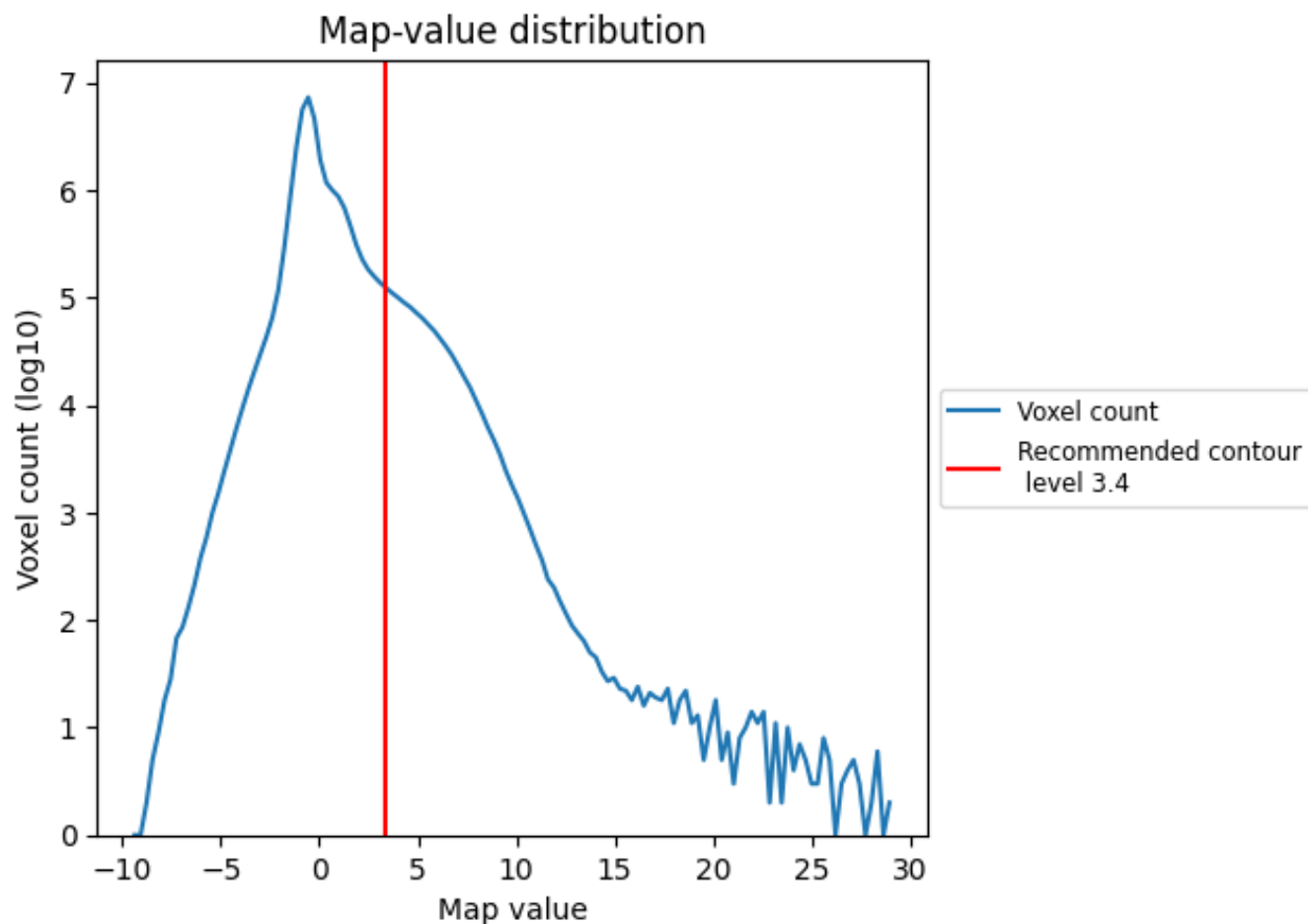
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

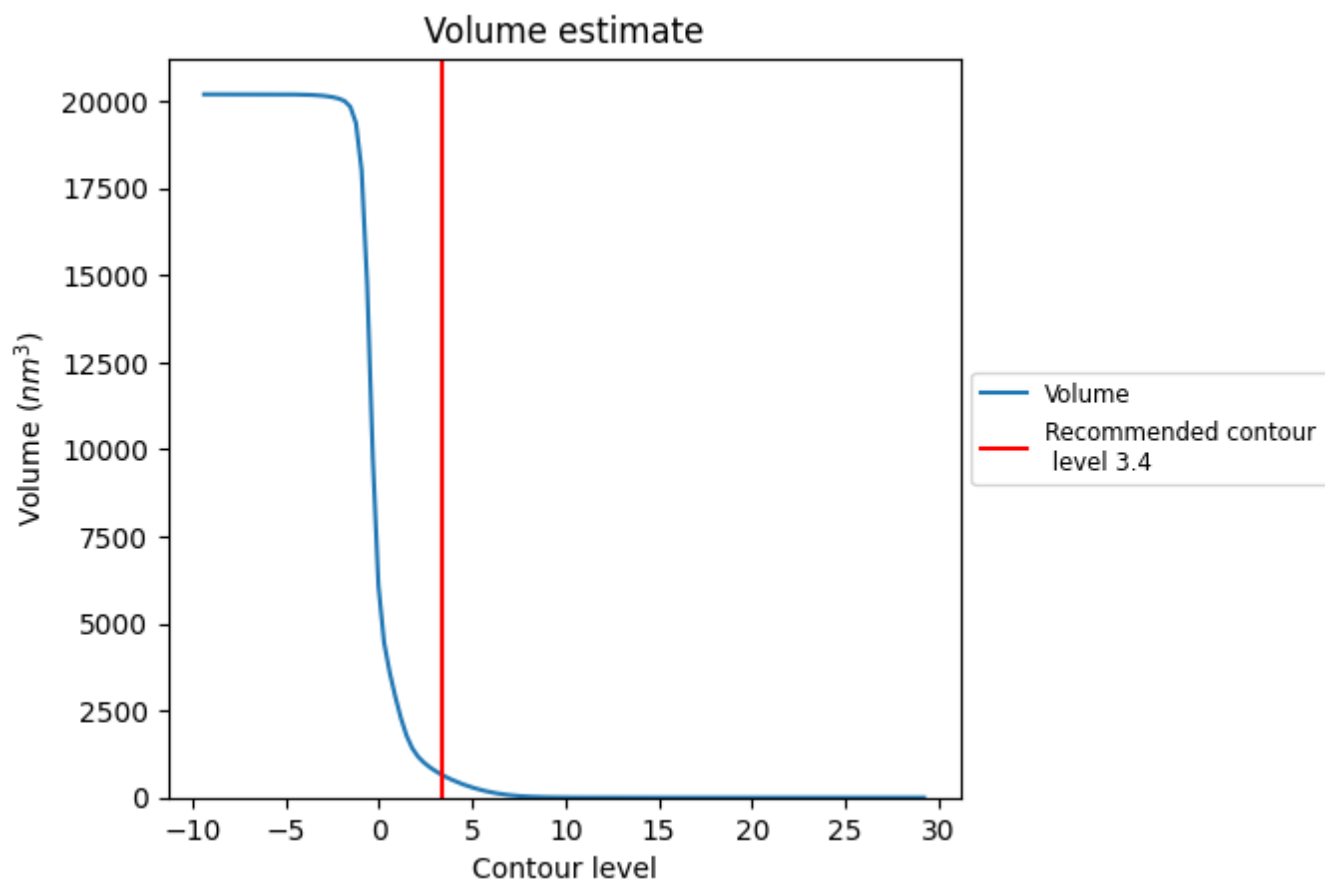
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 650 nm^3 ; this corresponds to an approximate mass of 587 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

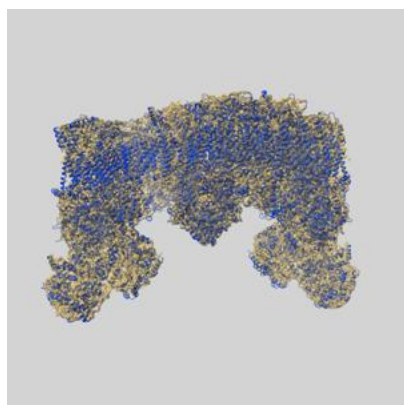
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

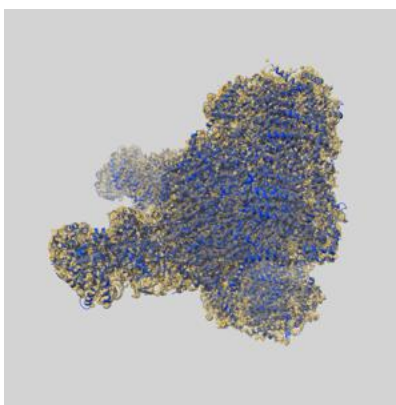
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42122 and PDB model 8UCA. Per-residue inclusion information can be found in section [3](#) on page [26](#).

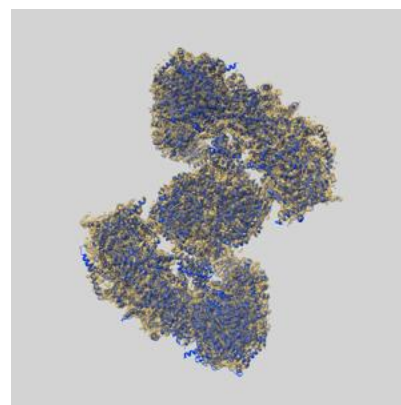
9.1 Map-model overlay [i](#)



X



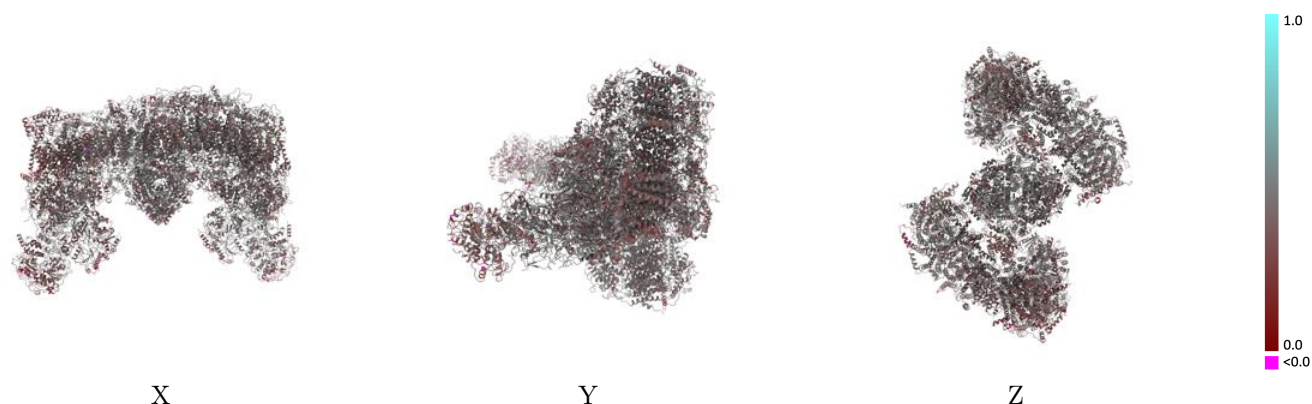
Y



Z

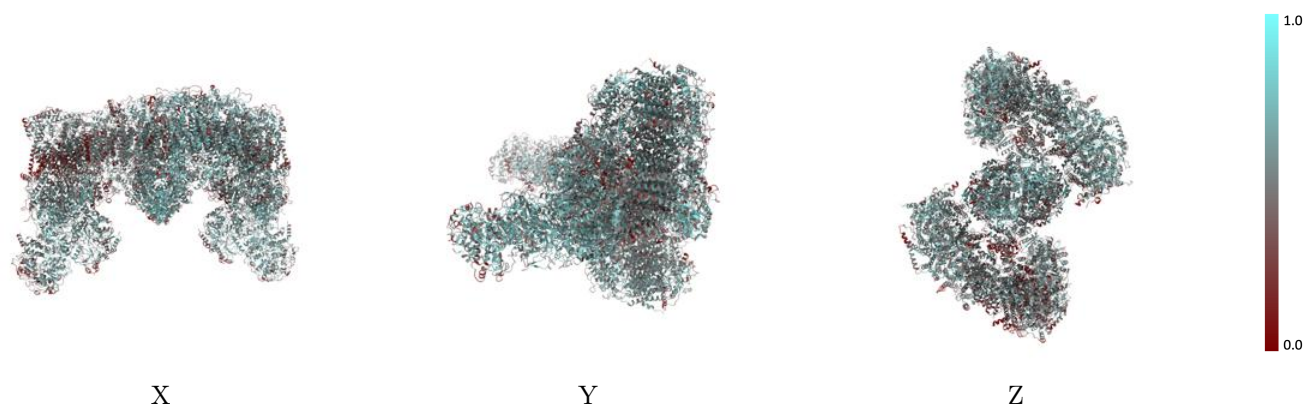
The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



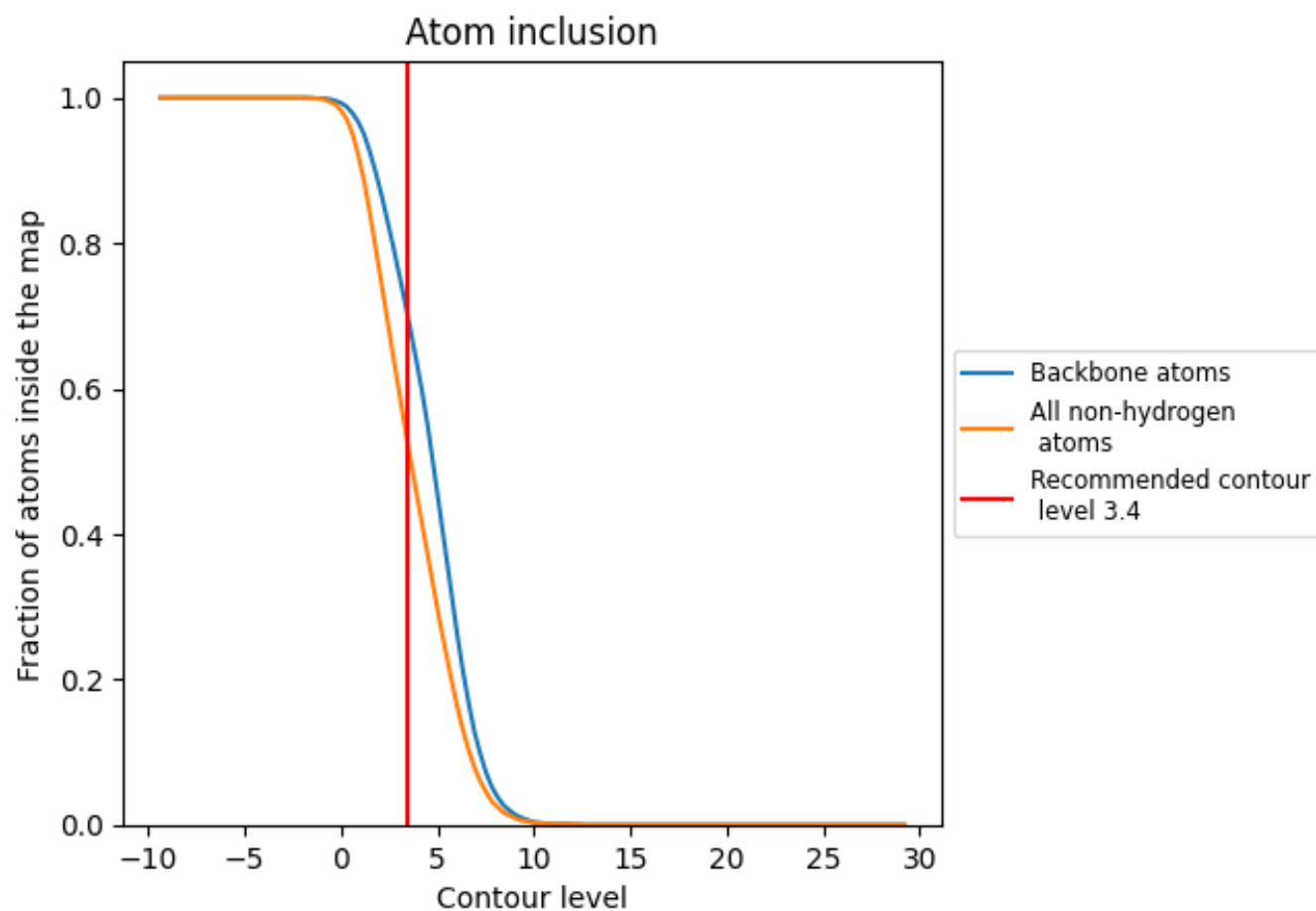
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% 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 (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5330	 0.4110
1	 0.5210	 0.4050
1a	 0.3980	 0.3640
2	 0.5480	 0.4290
2a	 0.5150	 0.4220
3	 0.4490	 0.3920
3A	 0.6140	 0.4350
3B	 0.5740	 0.4260
3C	 0.5920	 0.4440
3D	 0.6190	 0.4400
3E	 0.5060	 0.4320
3F	 0.5480	 0.4460
3G	 0.5250	 0.4390
3H	 0.4370	 0.3540
3J	 0.5230	 0.4200
3K	 0.3370	 0.4010
3L	 0.6100	 0.4420
3M	 0.6080	 0.4430
3N	 0.5740	 0.4400
3O	 0.6000	 0.4380
3P	 0.4920	 0.4320
3Q	 0.4910	 0.4430
3R	 0.4900	 0.4270
3S	 0.2980	 0.3010
3T	 0.3250	 0.3810
3U	 0.4510	 0.3890
3V	 0.3610	 0.3500
3a	 0.3660	 0.3720
4	 0.5710	 0.4400
4L	 0.4940	 0.3990
4a	 0.5440	 0.4360
4l	 0.4650	 0.4130
5	 0.5710	 0.4280
5a	 0.5540	 0.4230
6	 0.4030	 0.3940









































































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Chain	Atom inclusion	Q-score
6a	 0.3330	 0.3610
A1	 0.5710	 0.3930
A2	 0.5350	 0.3830
A3	 0.4360	 0.3900
A5	 0.4740	 0.4070
A6	 0.5330	 0.4290
A7	 0.5730	 0.4530
A8	 0.5680	 0.4150
A9	 0.5830	 0.4350
AB	 0.2790	 0.3290
AC	 0.5610	 0.4100
AL	 0.5300	 0.4090
AM	 0.4050	 0.3950
AN	 0.6070	 0.4500
AO	 0.5450	 0.4120
B1	 0.4540	 0.4070
B2	 0.4670	 0.3660
B3	 0.5120	 0.4090
B4	 0.5100	 0.4150
B5	 0.5930	 0.4440
B6	 0.5750	 0.4330
B7	 0.4950	 0.3860
B8	 0.5450	 0.4300
B9	 0.5830	 0.4230
BL	 0.5800	 0.4180
BM	 0.5440	 0.4290
C1	 0.4070	 0.4080
C2	 0.5450	 0.4330
S1	 0.6080	 0.4110
S2	 0.5980	 0.4350
S3	 0.6310	 0.4510
S4	 0.5670	 0.4530
S5	 0.5270	 0.4110
S6	 0.5800	 0.4490
S7	 0.6000	 0.4040
S8	 0.6340	 0.4100
V1	 0.5730	 0.3660
V2	 0.5350	 0.3580
V3	 0.5210	 0.3920
a1	 0.4350	 0.3780
a2	 0.4740	 0.3900
a3	 0.2510	 0.3150

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Chain	Atom inclusion	Q-score
a5	 0.4020	 0.3610
a6	 0.4820	 0.4280
a7	 0.4450	 0.3780
a8	 0.4440	 0.3740
a9	 0.5320	 0.4220
ab	 0.1850	 0.2990
ac	 0.5540	 0.4370
al	 0.4470	 0.3890
am	 0.3710	 0.3860
an	 0.5170	 0.4170
ao	 0.4310	 0.3790
b1	 0.3650	 0.3860
b2	 0.5240	 0.4110
b3	 0.5820	 0.4150
b4	 0.5010	 0.4210
b5	 0.5430	 0.4240
b6	 0.5630	 0.4360
b7	 0.5070	 0.3960
b8	 0.5220	 0.4340
b9	 0.5740	 0.4340
bl	 0.5090	 0.3970
bm	 0.5130	 0.4180
c1	 0.3390	 0.3770
c2	 0.4940	 0.4180
s1	 0.5610	 0.3800
s2	 0.5210	 0.4040
s3	 0.5670	 0.4270
s4	 0.5520	 0.4300
s5	 0.4720	 0.4000
s6	 0.5510	 0.4290
s7	 0.5790	 0.3810
s8	 0.5730	 0.3740
v1	 0.4820	 0.3250
v2	 0.5020	 0.3540
v3	 0.5320	 0.3610