



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 12:46 AM JST

PDB ID : 5GPN / pdb_00005gpn
EMDB ID : EMD-9534
Title : Architecture of mammalian respirasome
Authors : Gu, J.; Wu, M.; Guo, R.; Yang, M.
Deposited on : 2016-08-03
Resolution : 5.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

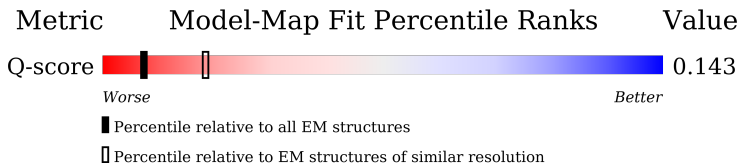
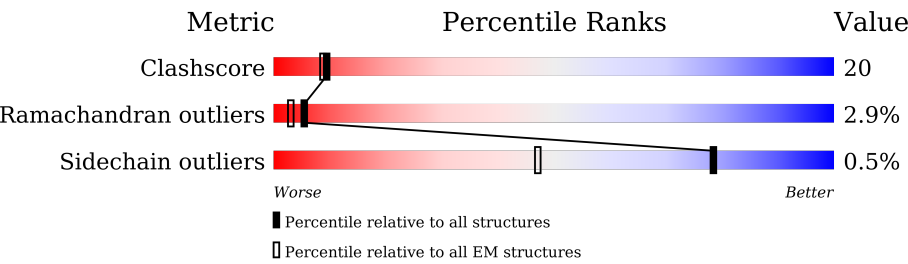
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	538 (4.90 - 5.90)

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

Mol	Chain	Length	Quality of chain
1	A	446	16% 57% 35% 8%
1	M	446	15% 58% 35% 7%
2	B	439	22% 63% 28% 5%
2	N	439	8% 61% 32% 5%

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Mol	Chain	Length	Quality of chain
3	C	379	
3	O	379	
4	D	241	
4	P	241	
5	E	274	
5	Q	274	
6	F	110	
6	R	110	
7	G	81	
7	S	81	
8	H	78	
8	T	78	
9	I	78	
9	U	78	
10	J	62	
10	L	62	
11	K	56	
11	V	56	
12	W	264	
13	Y	727	
14	Z	463	
15	a	216	
16	b	212	
17	c	464	
18	d	249	

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Mol	Chain	Length	Quality of chain
19	e	318	
20	f	347	
21	g	115	
22	h	459	
23	i	98	
24	j	606	
25	k	175	
25	l	175	
26	m	84	
27	n	99	
28	o	106	
29	p	377	
30	q	357	
30	v	357	
31	r	144	
32	Aa	156	
32	t	156	
33	Ai	189	
33	u	189	
34	w	175	
35	x	123	
36	0	261	
37	1	147	
38	2	109	
39	3	98	

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Mol	Chain	Length	Quality of chain
40	4	84	
41	5	85	
42	6	73	
43	7	59	
44	8	56	
45	9	47	
46	s	46	
47	y	514	
48	z	227	
49	Ab	134	
49	Ah	134	
50	Ac	70	
51	Ad	43	
51	Ao	43	
51	Ap	43	
51	Av	43	
52	Ae	116	
53	Af	128	
54	Ag	141	
55	Aj	176	
56	Ak	178	
57	Al	122	
58	Am	76	
59	An	172	
60	Aq	76	

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Mol	Chain	Length	Quality of chain
60	As	76	
60	Aw	76	
61	Ar	34	
62	At	17	
63	Au	13	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
64	HEM	C	402	-	-	X	-
67	SF4	Y	801	-	-	X	-
67	SF4	b	301	-	-	X	-
67	SF4	c	501	-	-	X	-
68	FMN	c	502	-	-	X	-
69	NDP	p	401	-	-	X	-

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 75545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	446	Total	C	N	O	0	0
			2198	1306	446	446		
1	M	446	Total	C	N	O	0	0
			2198	1306	446	446		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	419	Total	C	N	O	0	0
			2061	1223	419	419		
2	N	419	Total	C	N	O	0	0
			2061	1223	419	419		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	379	Total	C	N	O	0	0
			1870	1112	379	379		
3	O	379	Total	C	N	O	0	0
			1870	1112	379	379		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	241	Total	C	N	O	0	0
			1188	706	241	241		
4	P	241	Total	C	N	O	0	0
			1188	706	241	241		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	196	Total	C	N	O	0	0
			967	575	196	196		
5	Q	196	Total	C	N	O	0	0
			966	574	196	196		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	106	Total	C	N	O	0	0
			527	315	106	106		
6	R	106	Total	C	N	O	0	0
			527	315	106	106		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	81	Total	C	N	O	0	0
			401	239	81	81		
7	S	78	Total	C	N	O	0	0
			386	230	78	78		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	64	Total	C	N	O	0	0
			320	192	64	64		
8	T	64	Total	C	N	O	0	0
			320	192	64	64		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	33	Total	C	N	O	0	0
			163	97	33	33		
9	U	33	Total	C	N	O	0	0
			163	97	33	33		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	62	Total	C	N	O	0	0
			307	183	62	62		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	62	Total	C	N	O	0	0
			307	183	62	62		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	43	Total	C	N	O	0	0
			211	125	43	43		
11	V	37	Total	C	N	O	0	0
			182	108	37	37		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	169	Total	C	N	O	S	0	0
			1366	884	234	246	2		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	672	Total	C	N	O	S	0	0
			4998	3128	874	958	38		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	375	Total	C	N	O	S	0	0
			3003	1917	515	548	23		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	a	147	Total	C	N	O	S	0	0
			1146	730	204	198	14		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	149	Total	C	N	O	S	0	0
			1189	746	205	228	10		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	410	Total	C	N	O	S	0	0
			3125	1974	558	573	20		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	169	Total	C	N	O	S	0	0
			1324	852	218	245	9		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	315	Total	C	N	O	S	0	0
			2486	1665	381	419	21		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	346	Total	C	N	O	S	0	0
			2698	1774	418	461	45		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	106	Total	C	N	O	S	0	0
			829	559	120	144	6		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	457	Total	C	N	O	S	0	0
			3610	2396	570	606	38		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	90	Total	C	N	O	S	0	0
			677	448	101	115	13		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	594	Total	C	N	O	S	0	0
			4705	3120	729	807	49		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	142	Total	C	N	O	S	0	0
			1059	712	152	183	12		
25	l	15	Total	C	N	O		0	0
			73	43	15	15			

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	m	53	Total	C	N	O	0	0
			263	157	53	53		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	n	83	Total	C	N	O	0	0
			411	245	83	83		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	o	51	Total	C	N	O	0	0
			251	149	51	51		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	p	314	Total	C	N	O	0	0
			1546	918	314	314		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	q	196	Total	C	N	O	0	0
			967	575	196	196		
30	v	51	Total	C	N	O	0	0
			252	150	51	51		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	r	63	Total	C	N	O	0	0
			311	185	63	63		

- Molecule 32 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	t	81	Total	C	N	O	0	0
			403	241	81	81		
32	Aa	81	Total	C	N	O	0	0
			403	241	81	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
33	u	54	Total	C	N	O	0	0
			267	159	54	54		
33	Ai	34	Total	C	N	O	0	0
			167	99	34	34		

- Molecule 34 is a protein called Mitochondrial NADH dehydrogenase Fe-S protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	w	107	Total	C	N	O	0	0
			530	316	107	107		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	x	46	Total	C	N	O	0	0
			221	129	46	46		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	0	261	Total	C	N	O	0	0
			1284	762	261	261		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	1	144	Total	C	N	O	0	0
			716	428	144	144		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2	109	Total	C	N	O	0	0
			539	321	109	109		

- Molecule 39 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	3	98	Total	C	N	O	0	0
			481	285	98	98		

- Molecule 40 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	4	84	Total	C	N	O	0	0
			411	243	84	84		

- Molecule 41 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	5	75	Total	C	N	O	0	0
			371	221	75	75		

- Molecule 42 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	6	73	Total	C	N	O	0	0
			361	215	73	73		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	7	56	Total	C	N	O	0	0
			274	162	56	56		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	8	49	Total	C	N	O	0	0
			241	143	49	49		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	9	47	Total	C	N	O	0	0
			231	137	47	47		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	s	43	Total	C	N	O	0	0
			213	127	43	43		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	y	514	Total	C	N	O	0	0
			2523	1495	514	514		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	z	227	Total	C	N	O	0	0
			1127	673	227	227		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	Ab	129	Total	C	N	O	0	0
			637	379	129	129		
49	Ah	106	Total	C	N	O	0	0
			526	314	106	106		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Ac	55	Total	C	N	O	0	0
			271	161	55	55		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ad	43	Total	C	N	O	0	0
			211	125	43	43		
51	Ao	41	Total	C	N	O	0	0
			205	123	41	41		
51	Ap	35	Total	C	N	O	0	0
			173	103	35	35		
51	Av	39	Total	C	N	O	0	0
			193	115	39	39		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Ae	88	Total	C	N	O	0	0
			435	259	88	88		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Af	90	Total	C	N	O	0	0
			448	268	90	90		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Ag	131	Total	C	N	O	0	0
			637	375	131	131		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Aj	133	Total	C	N	O	0	0
			663	397	133	133		

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Ak	151	Total	C	N	O	0	0
			750	448	151	151		

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Al	96	Total	C	N	O	0	0
			473	281	96	96		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Am	27	Total	C	N	O	0	0
			134	80	27	27		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	An	97	Total	C	N	O	0	0
			482	288	97	97		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	Aq	67	Total	C	N	O	0	0
			335	201	67	67		
60	As	65	Total	C	N	O	0	0
			322	192	65	65		
60	Aw	76	Total	C	N	O	0	0
			376	224	76	76		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	Ar	34	Total	C	N	O	0	0
			169	101	34	34		

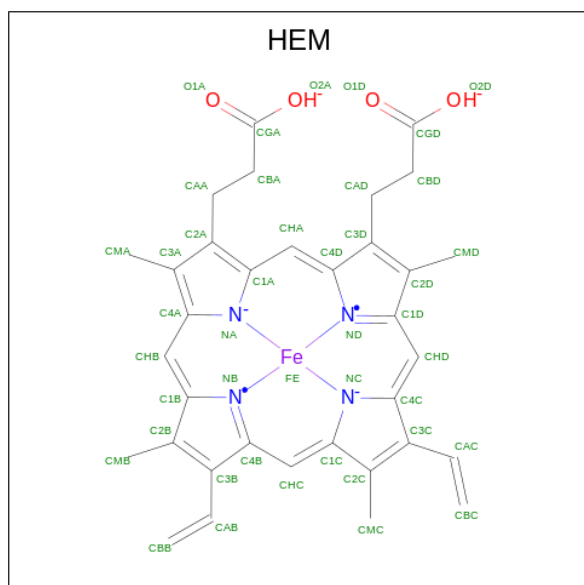
- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	At	17	Total	C	N	O	0	0
			84	50	17	17		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	Au	13	Total	C	N	O	0	0
			62	36	13	13		

- Molecule 64 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



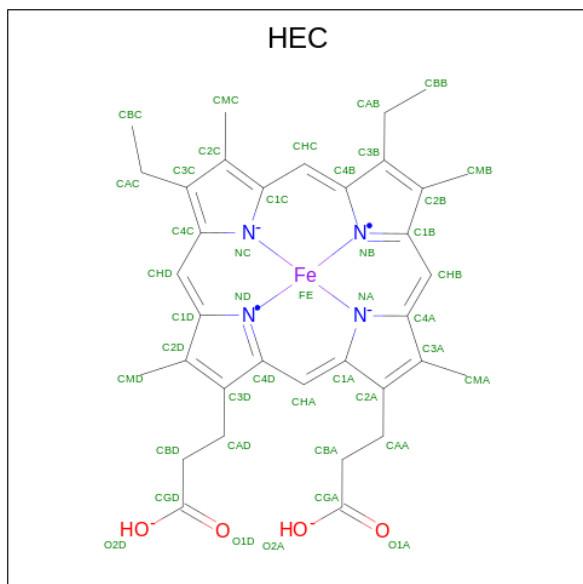
Mol	Chain	Residues	Atoms					AltConf
64	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
64	O	1	Total 43	C 34	Fe 1	N 4	O 4	0

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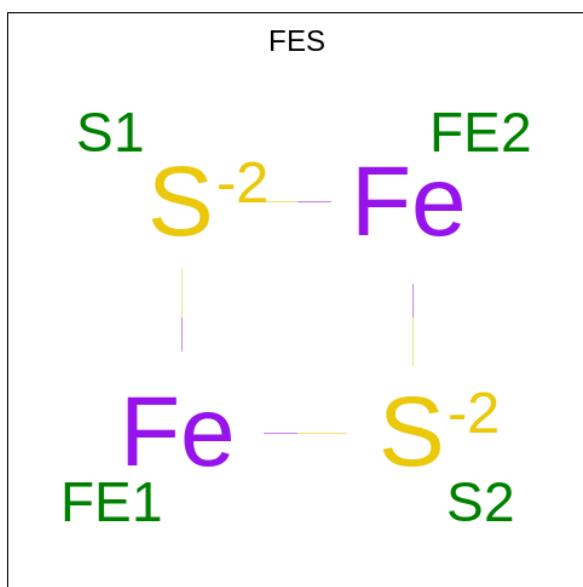
Mol	Chain	Residues	Atoms					AltConf
64	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 65 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



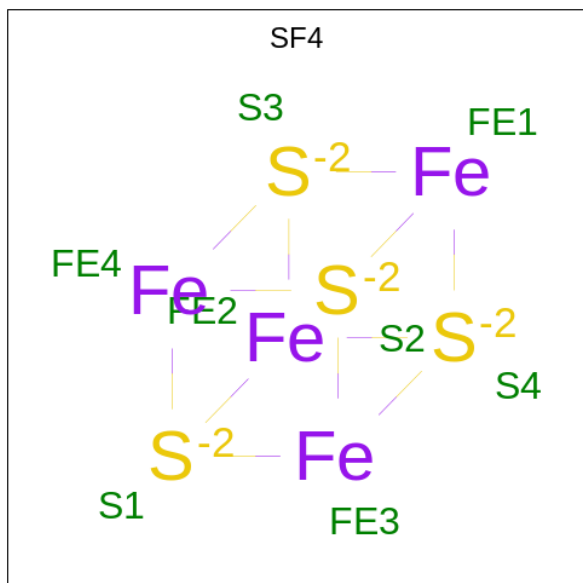
Mol	Chain	Residues	Atoms					AltConf
65	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
65	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 66 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



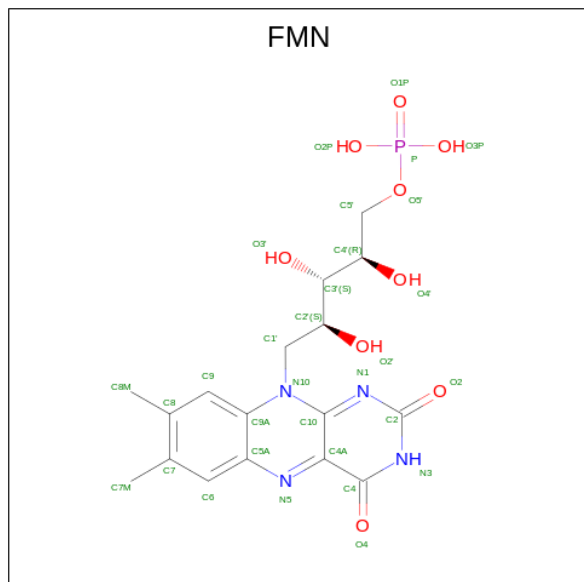
Mol	Chain	Residues	Atoms			AltConf
66	E	1	Total	Fe	S	0
			4	2	2	
66	Q	1	Total	Fe	S	0
			4	2	2	
66	Y	1	Total	Fe	S	0
			4	2	2	
66	d	1	Total	Fe	S	0
			4	2	2	

- Molecule 67 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



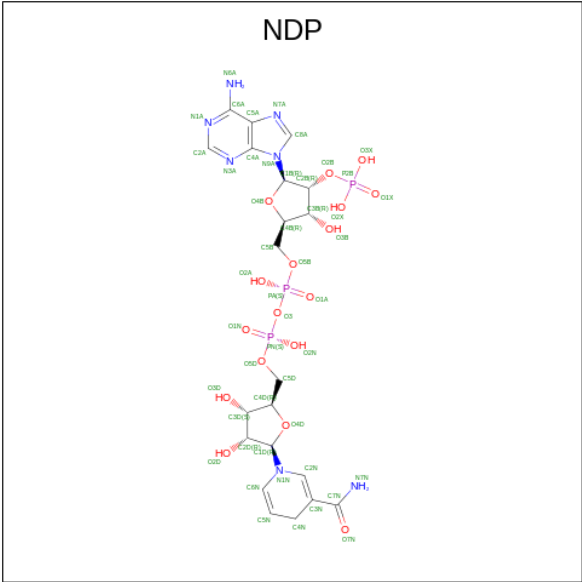
Mol	Chain	Residues	Atoms			AltConf
67	Y	1	Total	Fe	S	0
			8	4	4	
67	Y	1	Total	Fe	S	0
			8	4	4	
67	a	1	Total	Fe	S	0
			8	4	4	
67	b	1	Total	Fe	S	0
			8	4	4	
67	b	1	Total	Fe	S	0
			8	4	4	
67	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 68 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 69 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

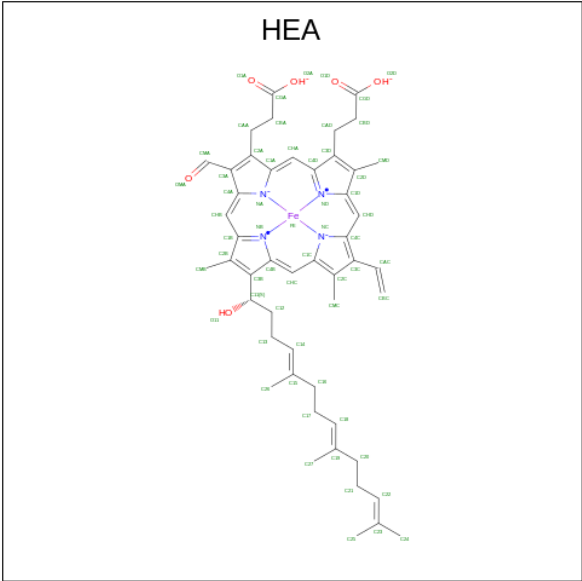


Mol	Chain	Residues	Atoms					AltConf
69	p	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
70	3	1	Total	Zn	0
			1	1	

- Molecule 71 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
71	y	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
71	y	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 72 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
72	y	1	Total	Cu	0
			1	1	
72	z	2	Total	Cu	0
			2	2	

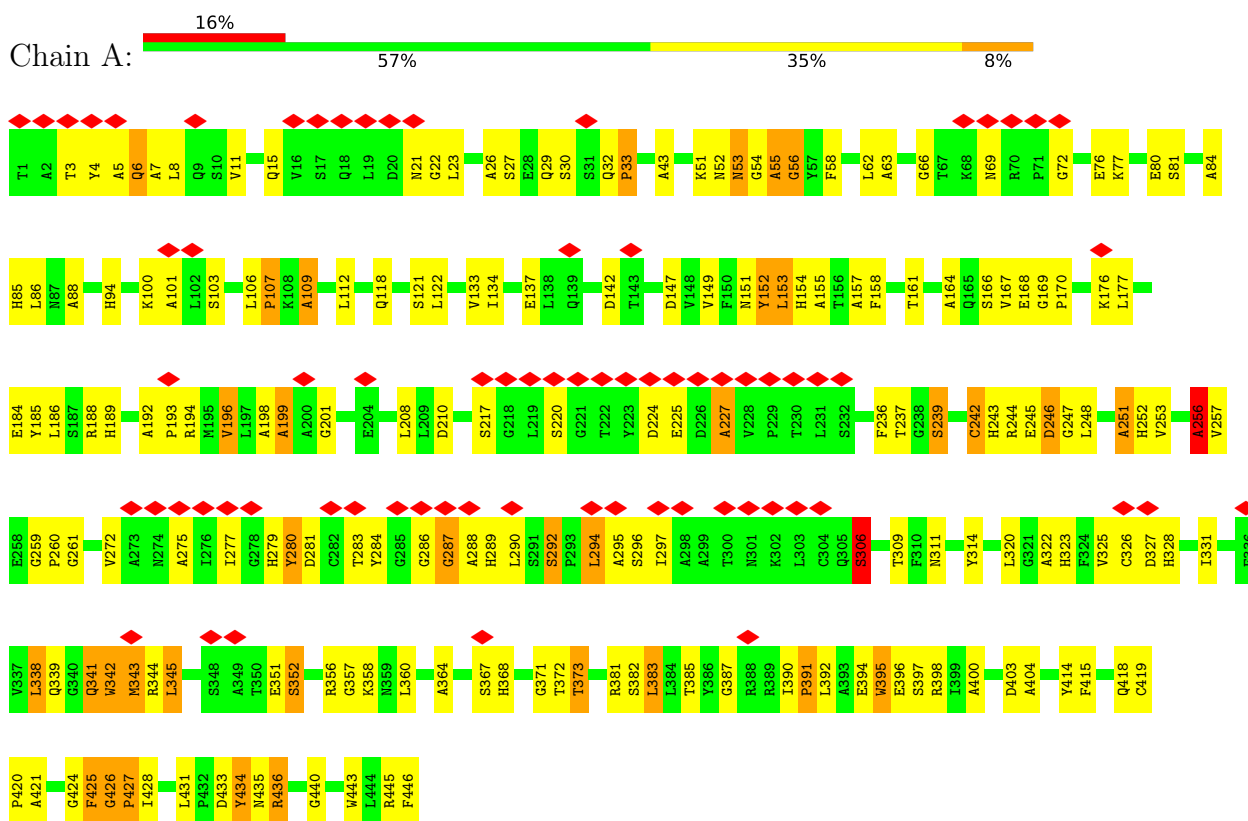
- Molecule 73 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
73	y	1	Total	Mg	0
			1	1	

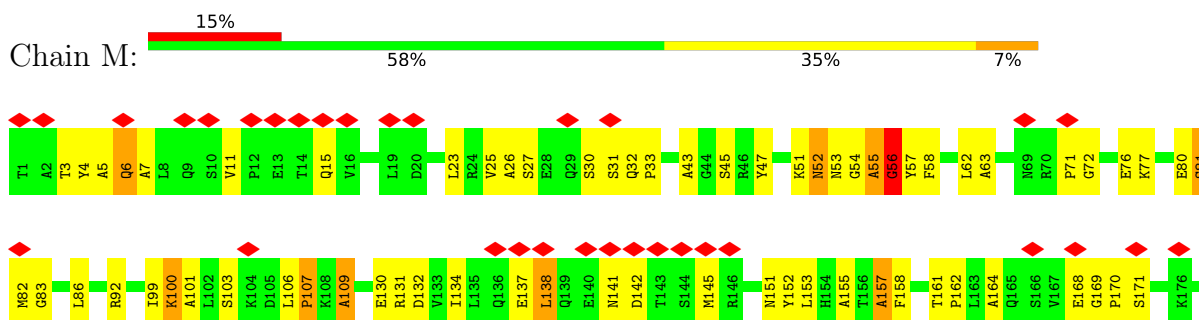
3 Residue-property plots

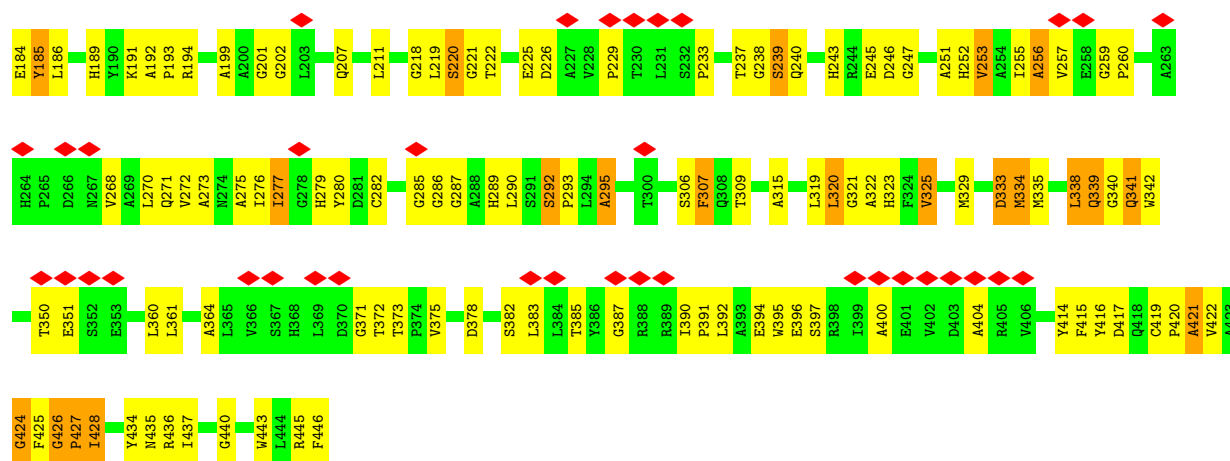
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

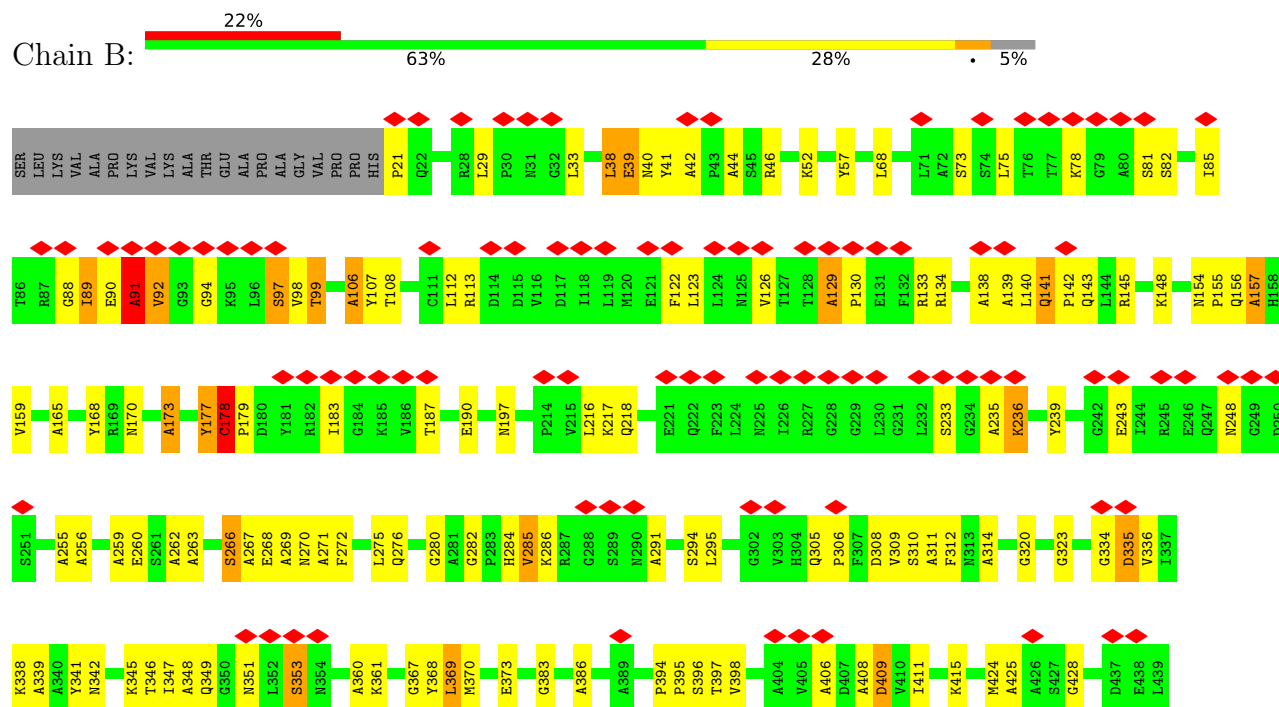


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

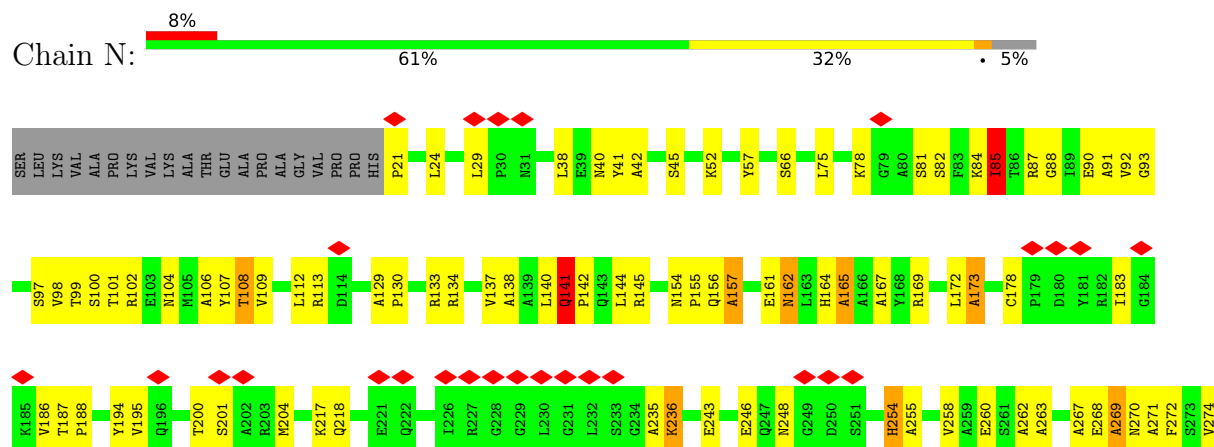


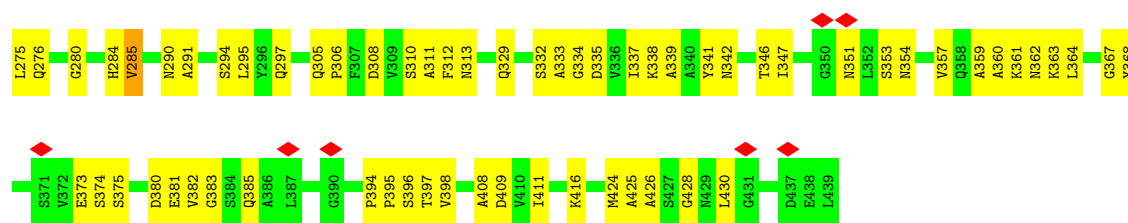


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

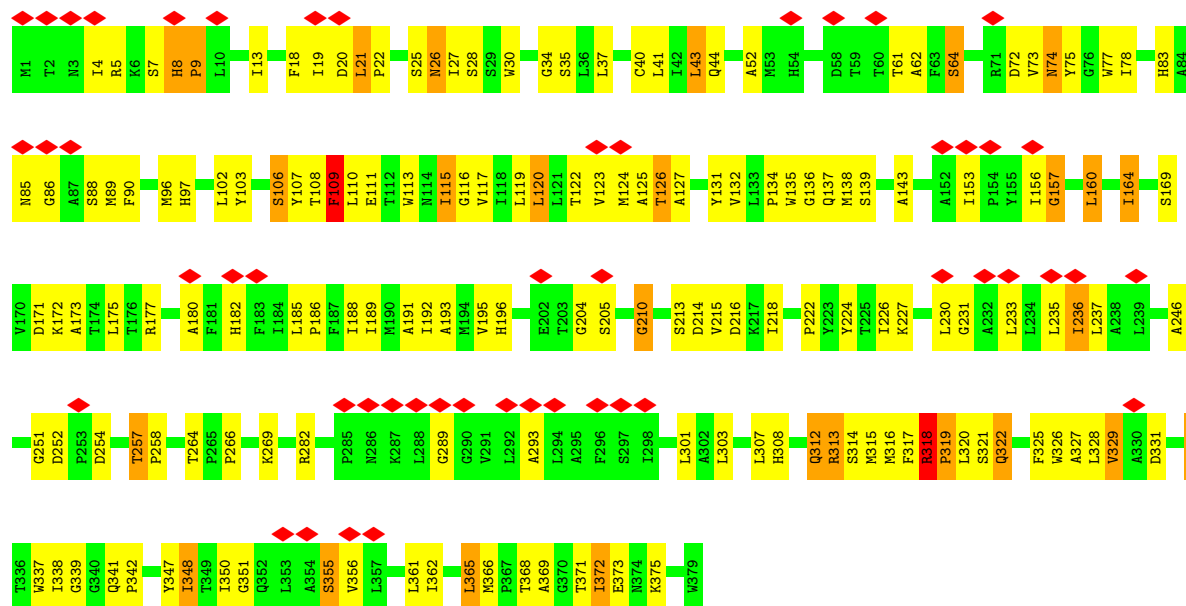


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

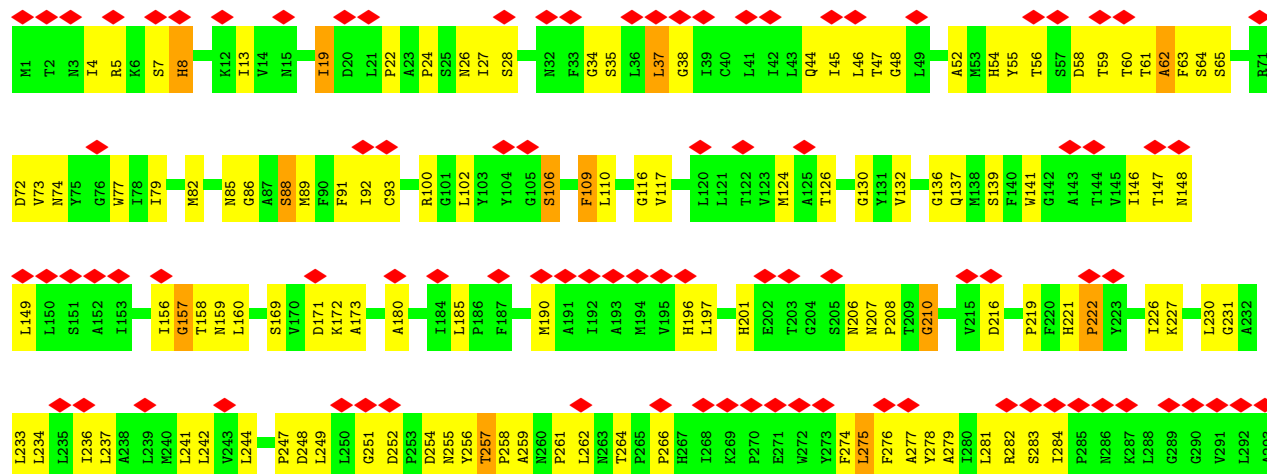




• Molecule 3: Cytochrome b

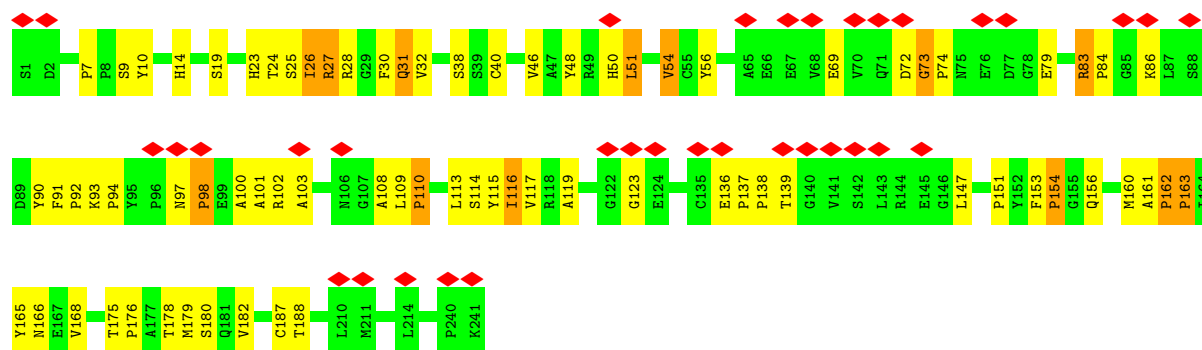


• Molecule 3: Cytochrome b

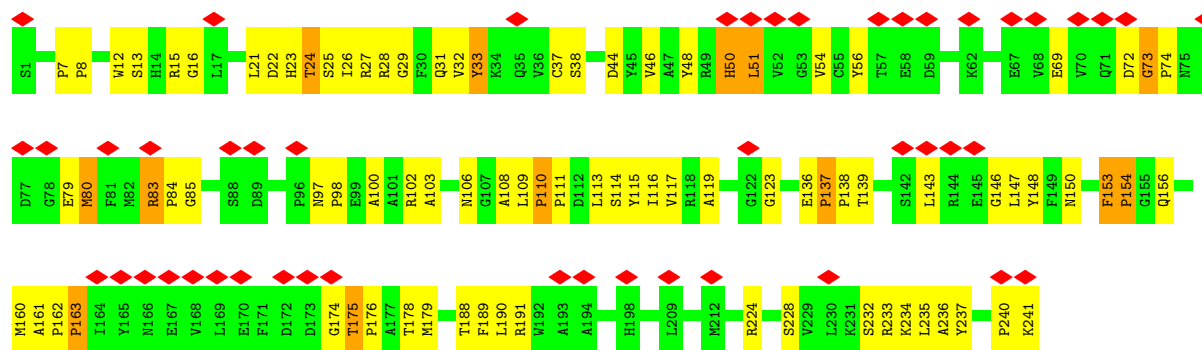




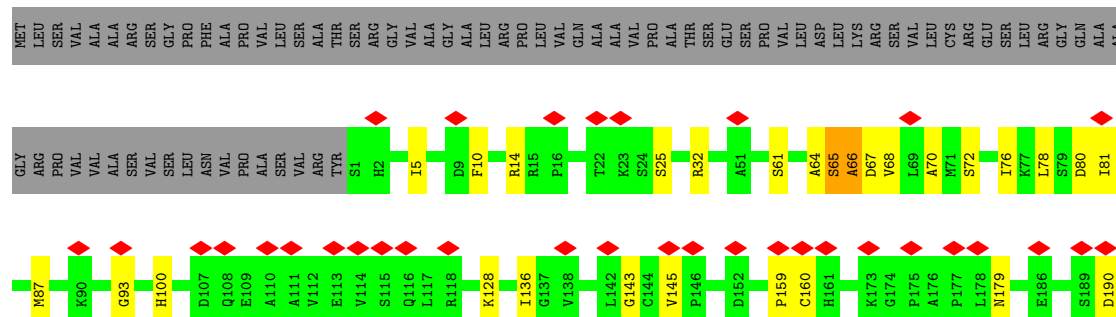
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

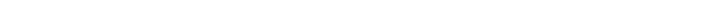


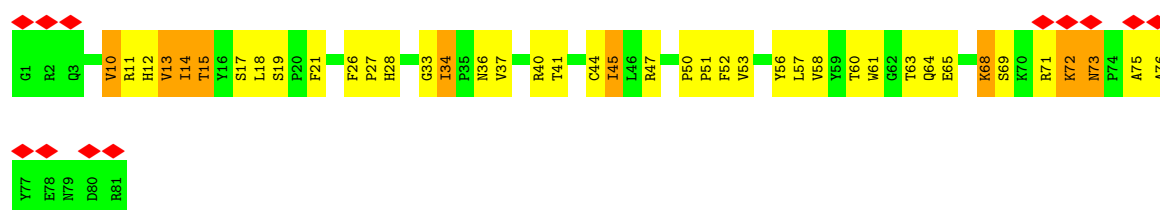
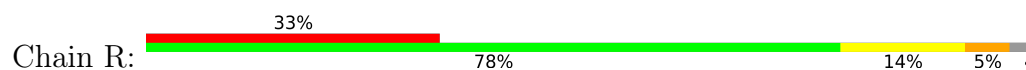
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



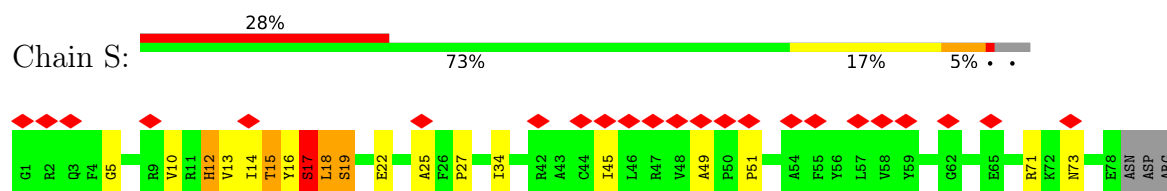
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



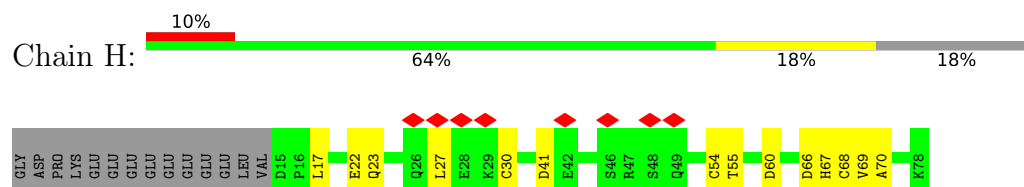
- Chain Q: 



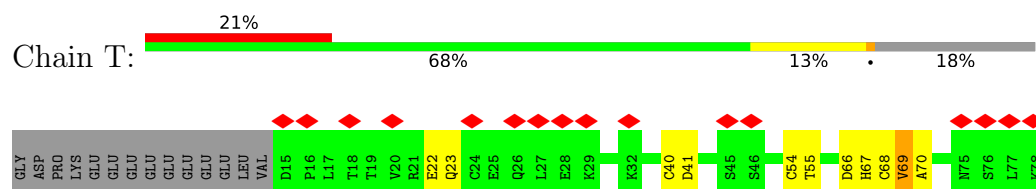
- Molecule 7: Cytochrome b-c1 complex subunit 8



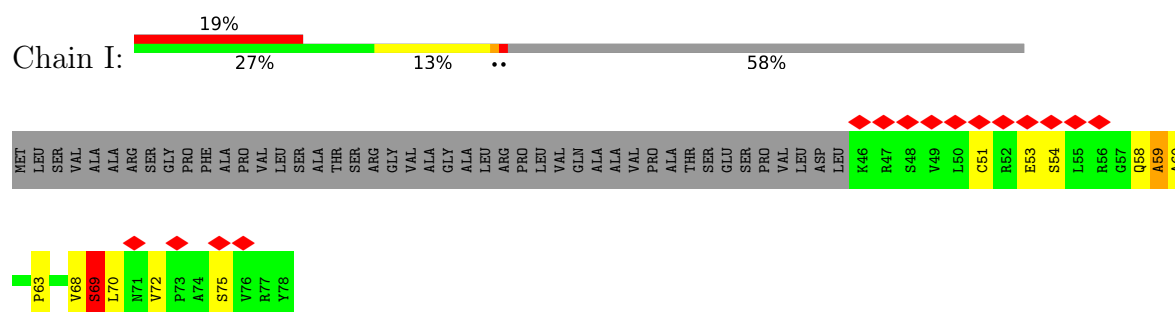
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



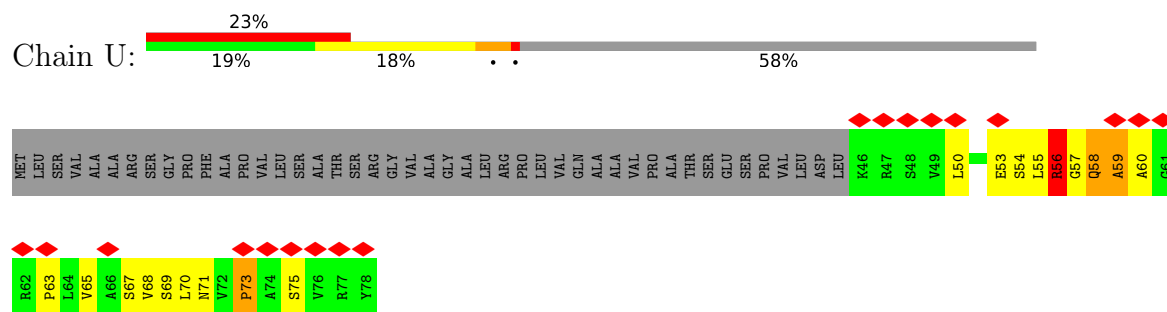
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

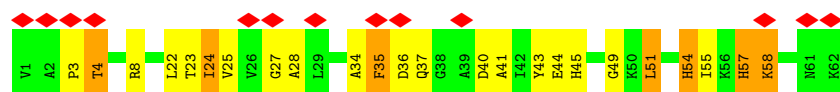


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

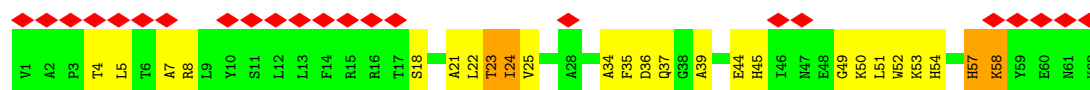


- Molecule 10: Cytochrome b-c1 complex subunit 9





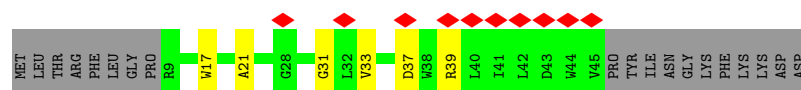
- Molecule 10: Cytochrome b-c1 complex subunit 9



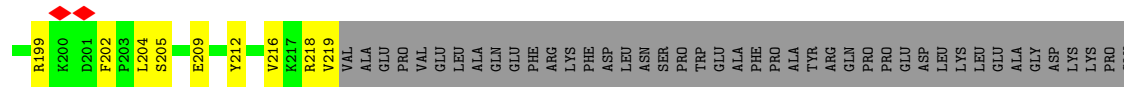
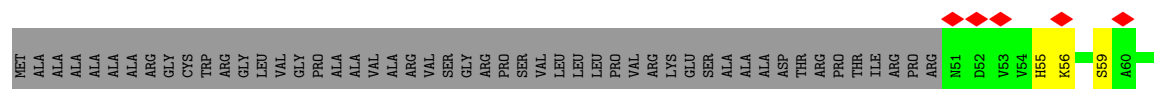
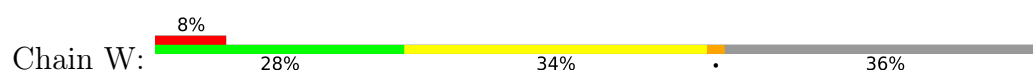
- Molecule 11: Cytochrome b-c1 complex subunit 10



- Molecule 11: Cytochrome b-c1 complex subunit 10

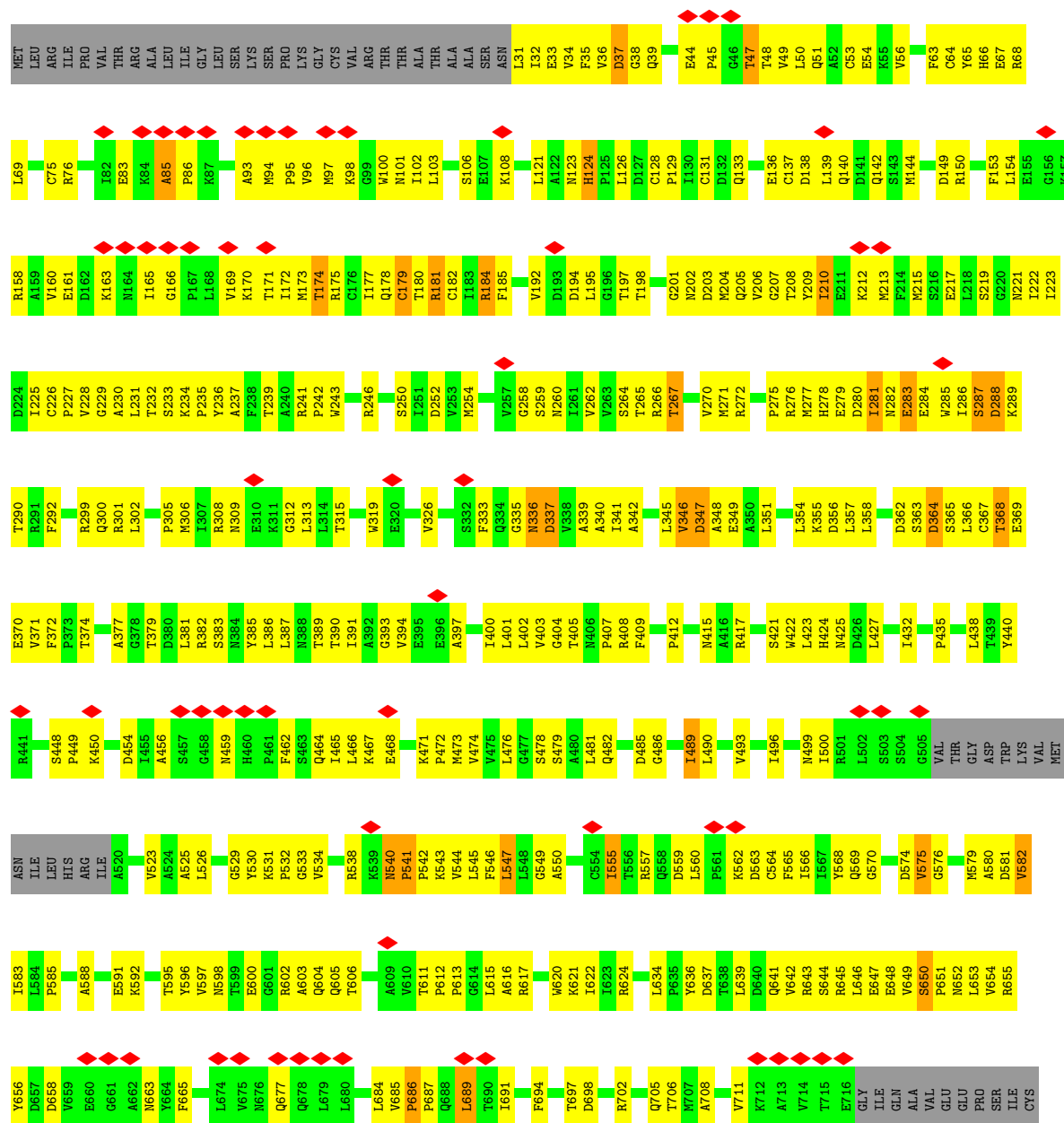


- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

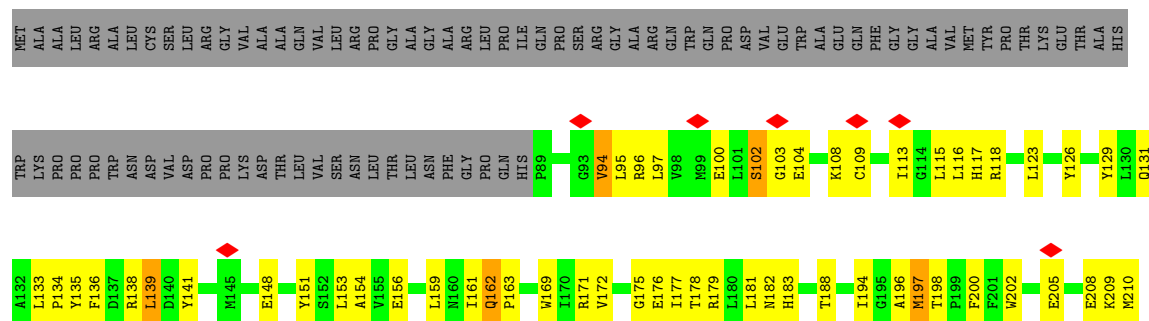


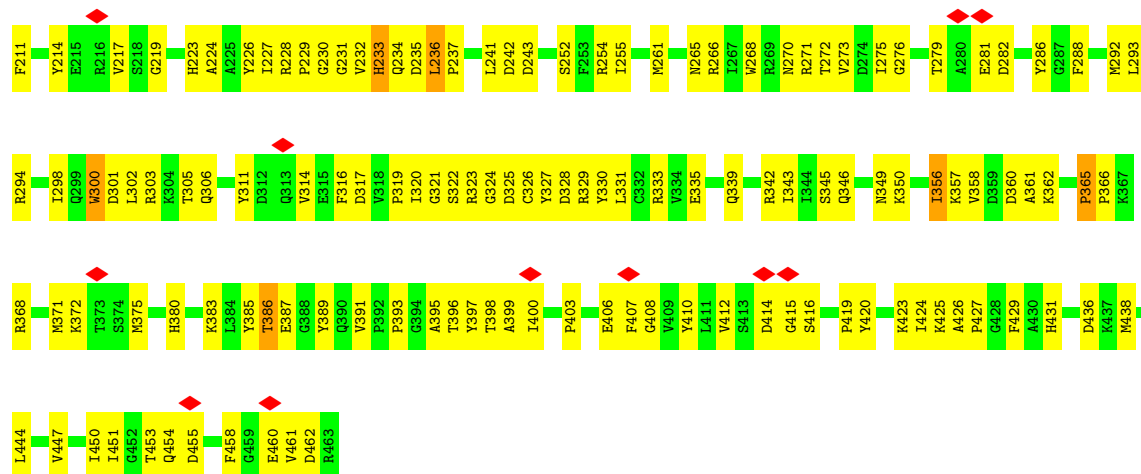
- Molecule 13: NADH-ubiquinone oxidoreductase 75 kDa subunit





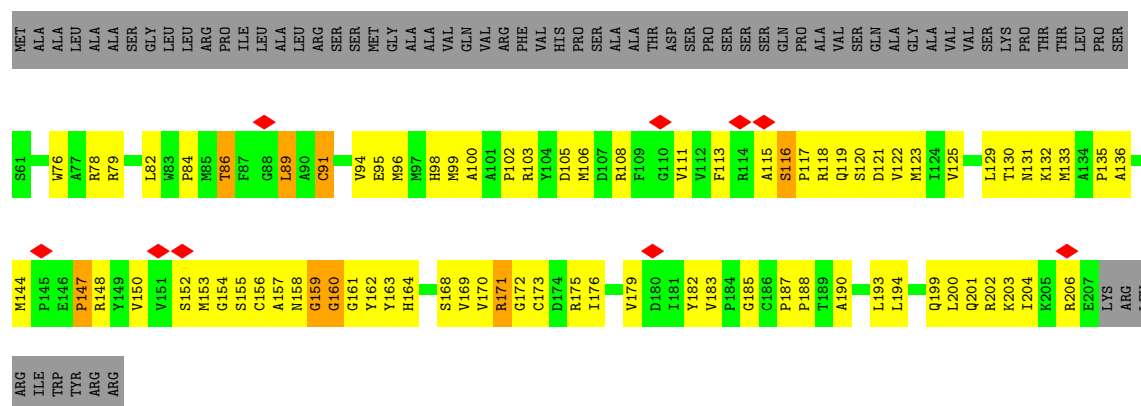
• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2





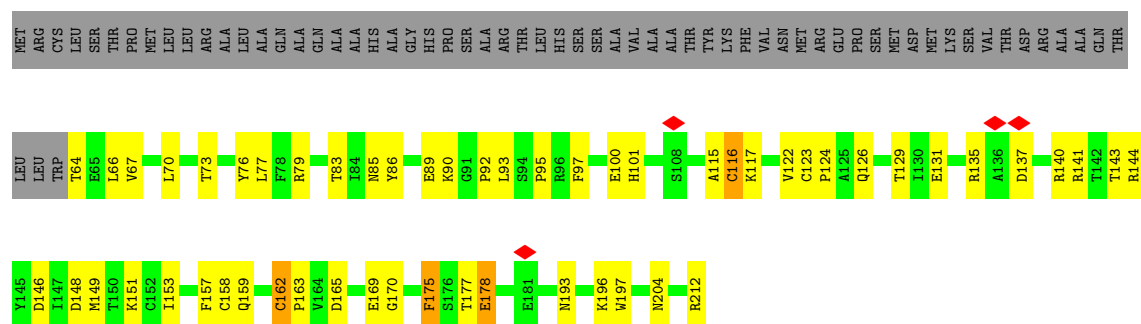
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7

Chain a: 31% 33% 32%



• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8

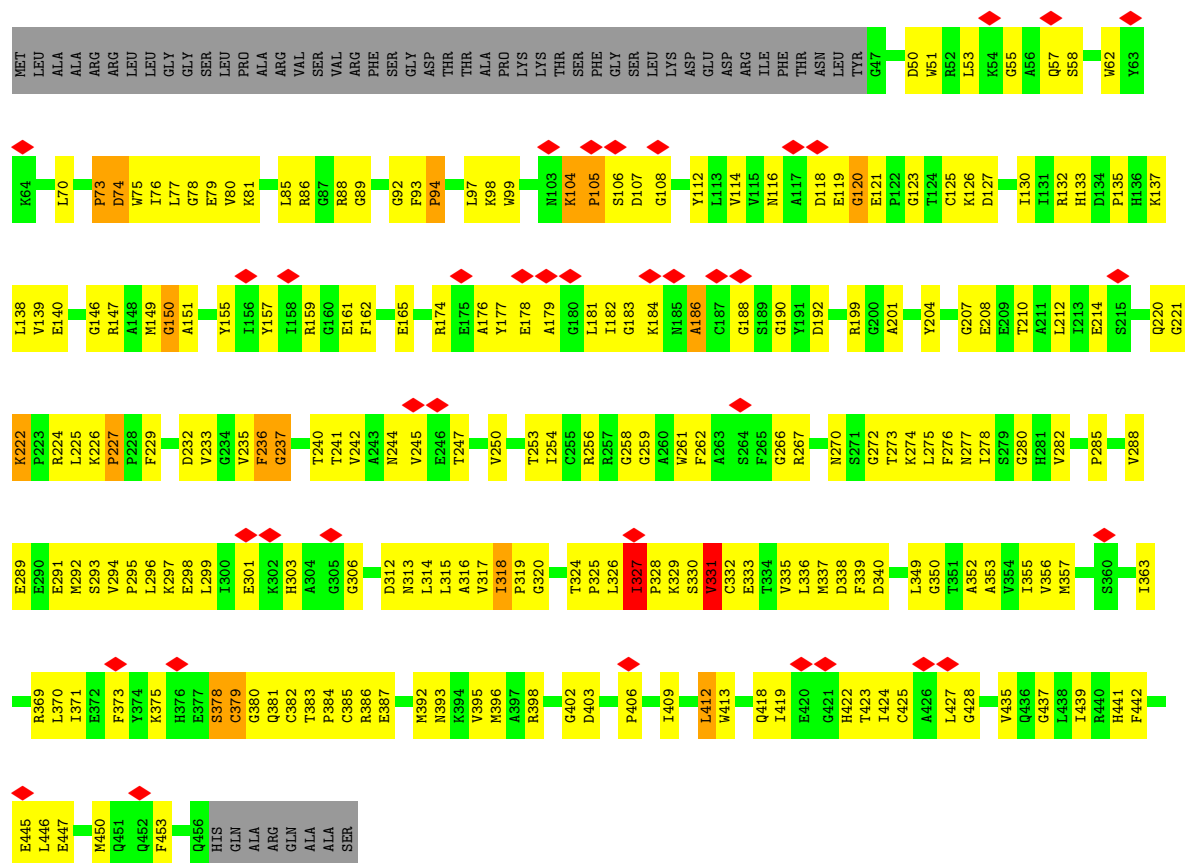
Chain b: 44% 24% 30%



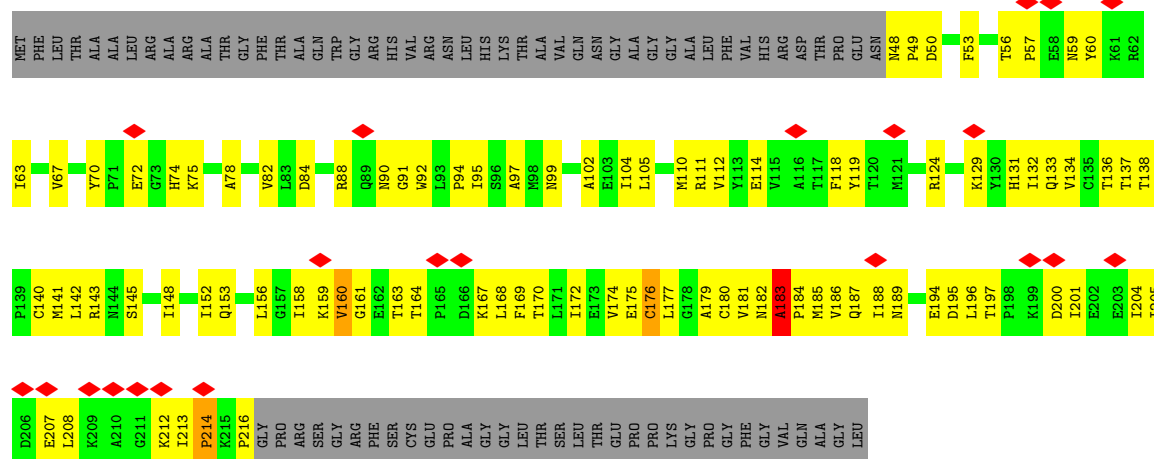
• Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain c: 8% 42% 12%



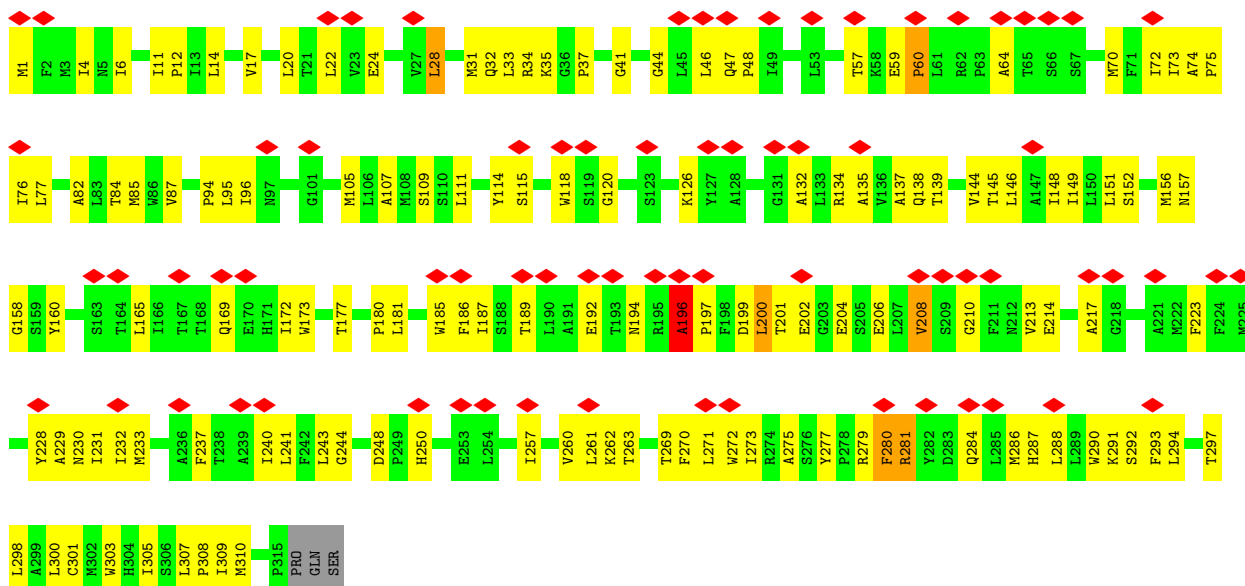


- Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

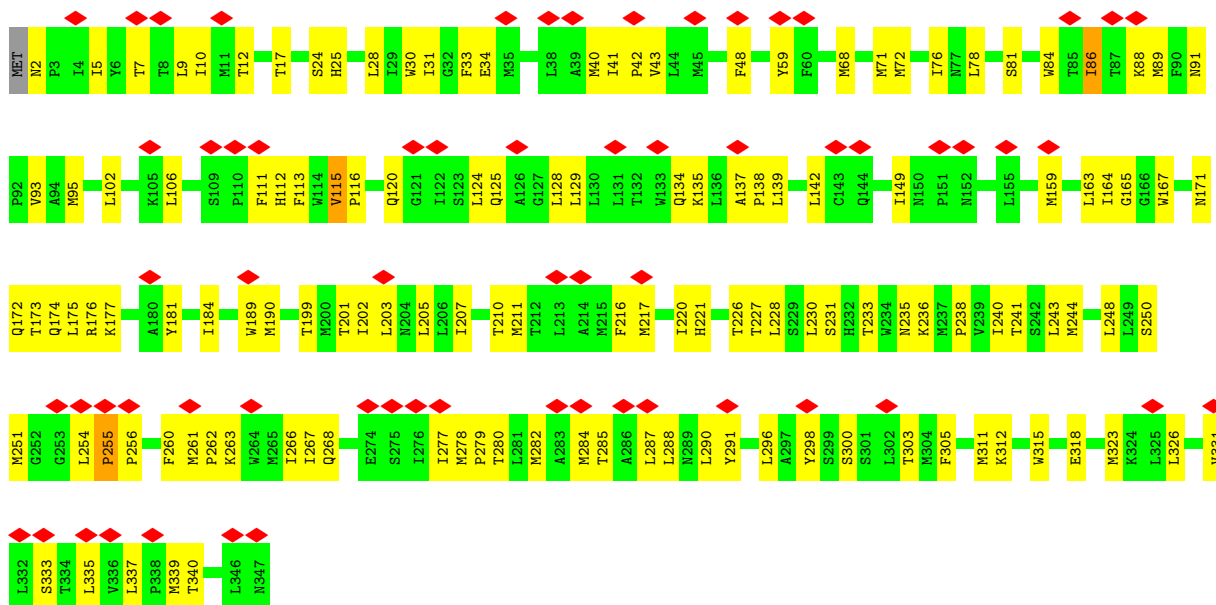


- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

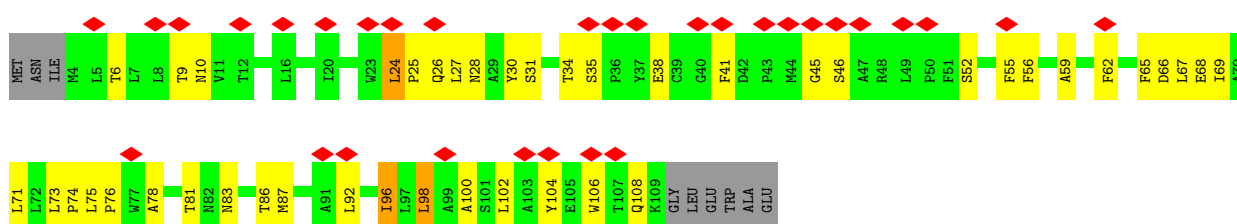




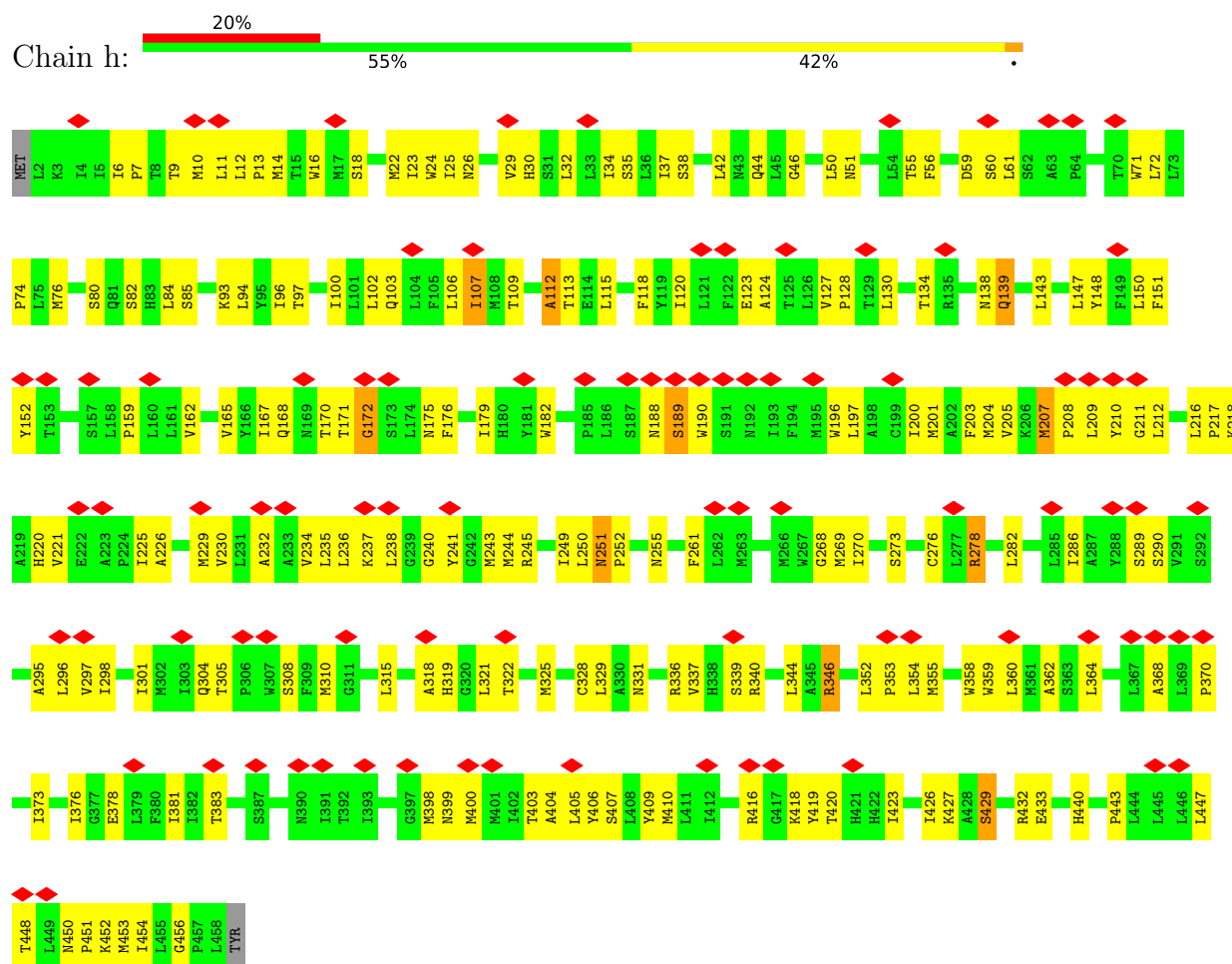
• Molecule 20: NADH-ubiquinone oxidoreductase chain 2



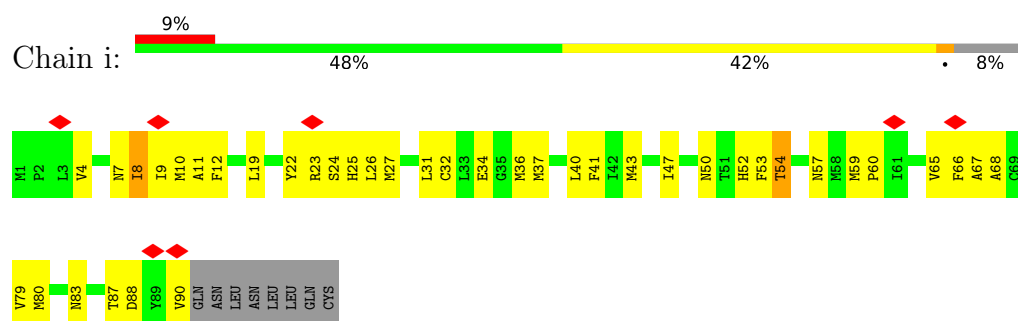
• Molecule 21: NADH-ubiquinone oxidoreductase chain 3



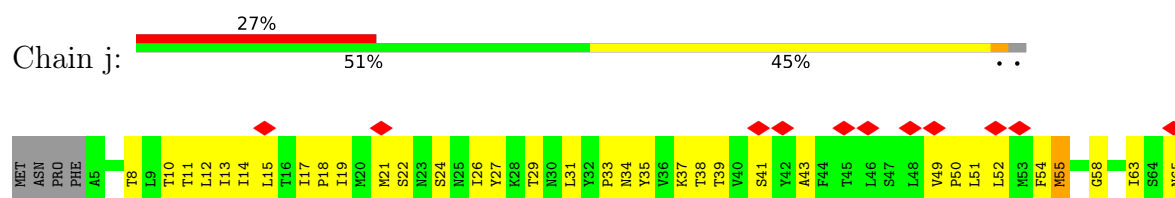
- Molecule 22: NADH-ubiquinone oxidoreductase chain 4

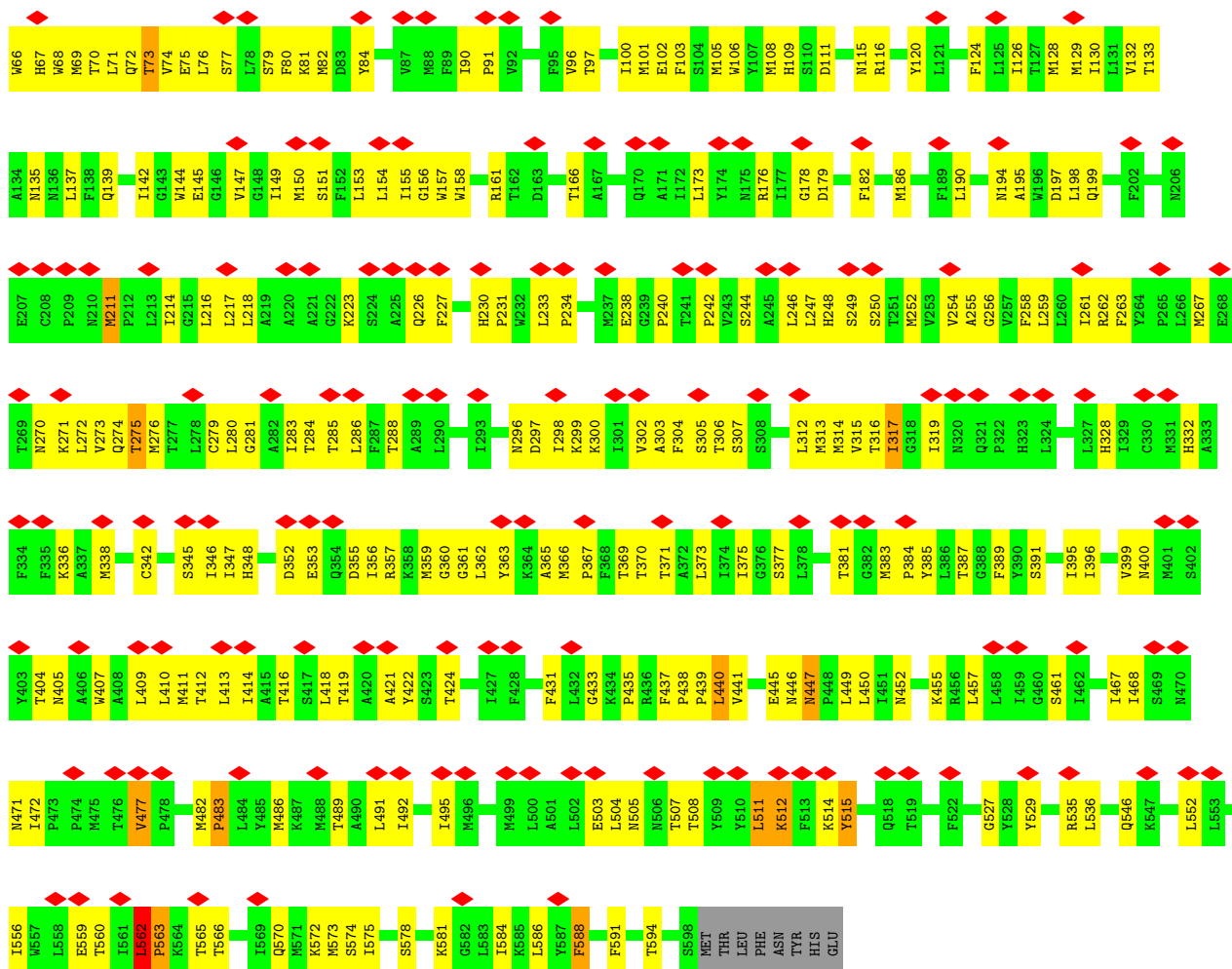


- Molecule 23: NADH-ubiquinone oxidoreductase chain 4L

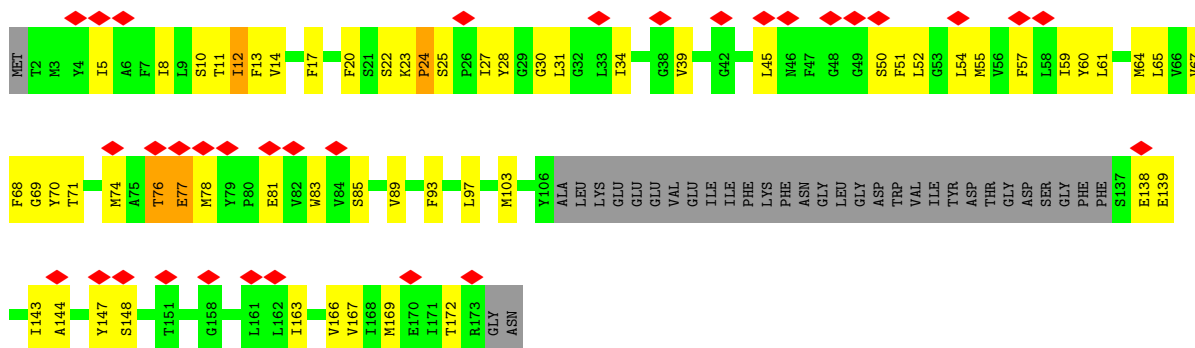


- Molecule 24: NADH-ubiquinone oxidoreductase chain 5

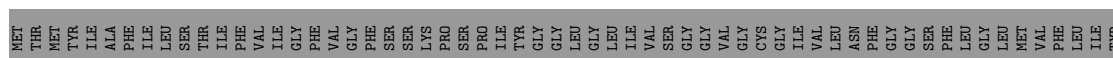


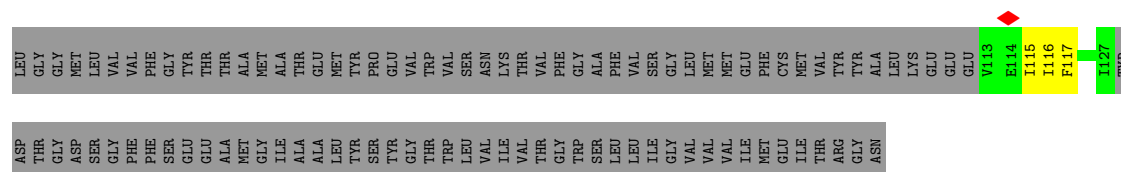


• Molecule 25: NADH-ubiquinone oxidoreductase chain 6



• Molecule 25: NADH-ubiquinone oxidoreductase chain 6

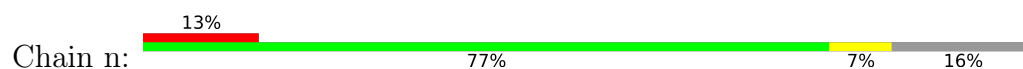




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



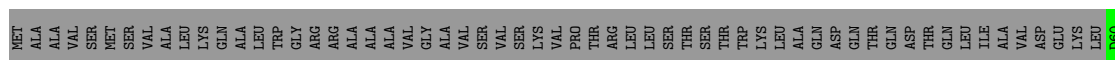
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9

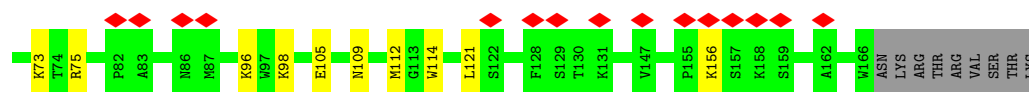


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

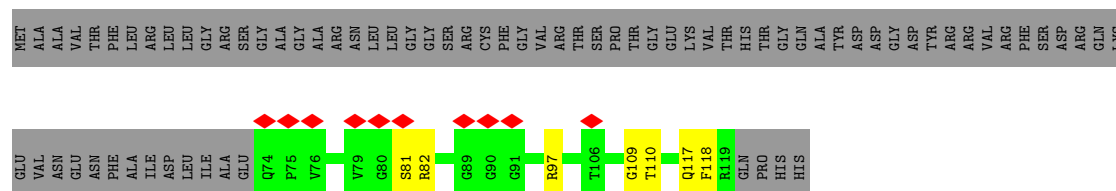




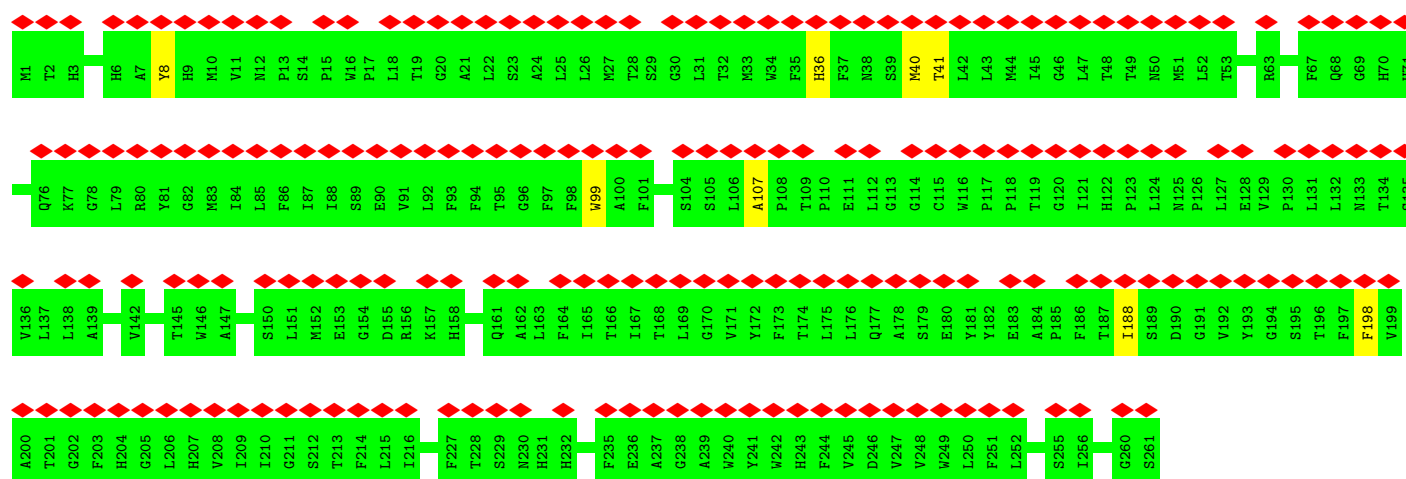
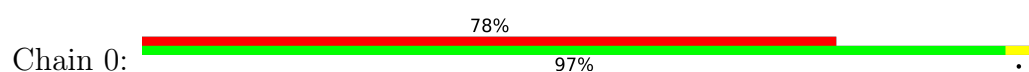




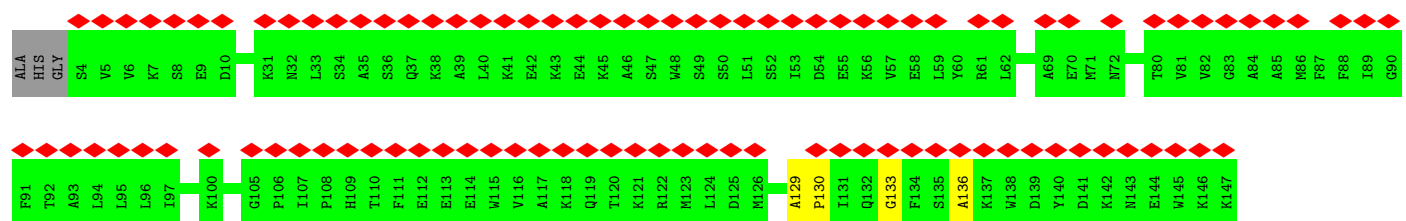
- Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



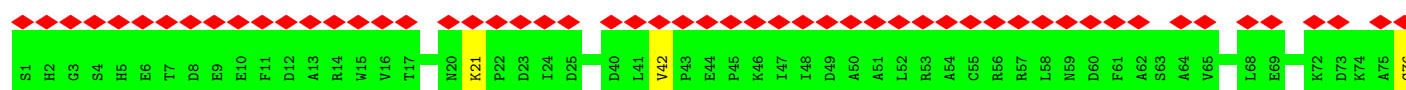
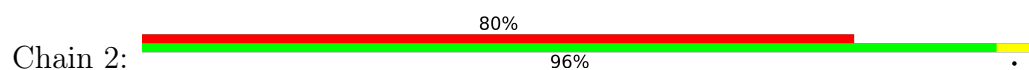
- Molecule 36: Cytochrome c oxidase subunit 3

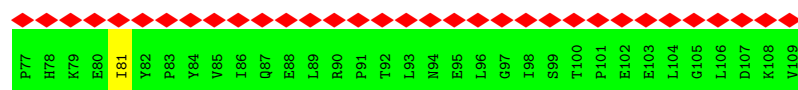


- Molecule 37: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



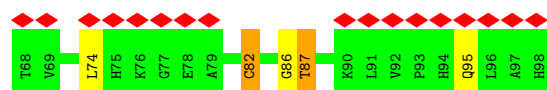
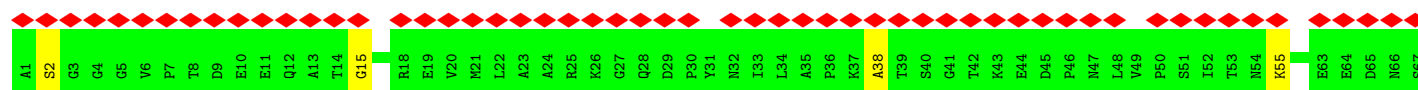
- Molecule 38: Cytochrome c oxidase subunit 5A, mitochondrial





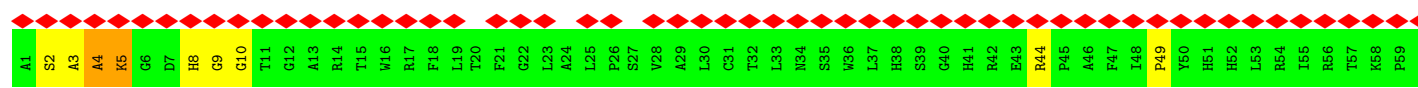
- Molecule 39: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 3:



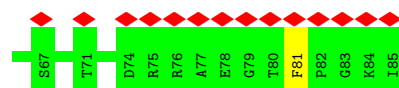
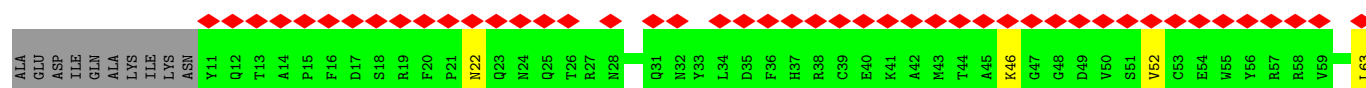
- Molecule 40: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 4:



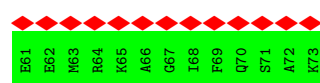
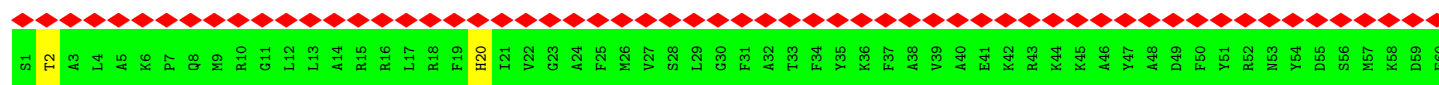
- Molecule 41: Cytochrome c oxidase subunit 6B1

Chain 5:

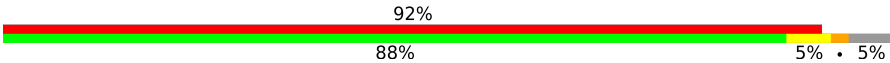


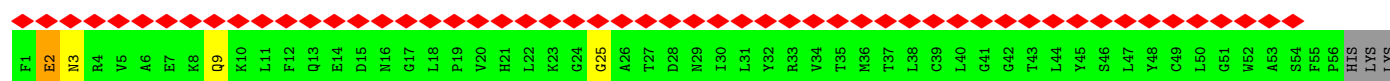
- Molecule 42: Cytochrome c oxidase subunit 6C

Chain 6:



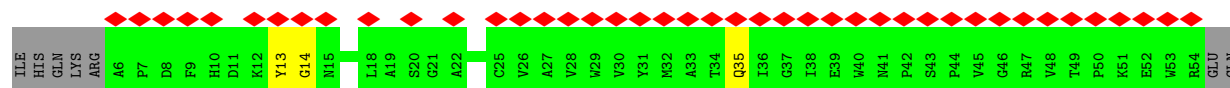
- Molecule 43: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 7: 

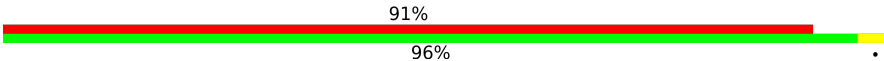


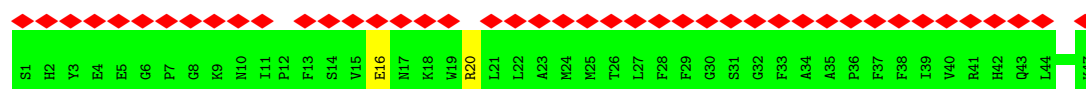
- Molecule 44: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 8: 



- Molecule 45: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 9: 

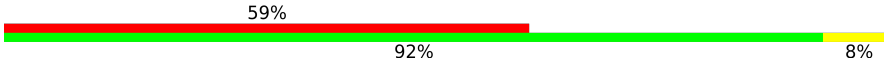


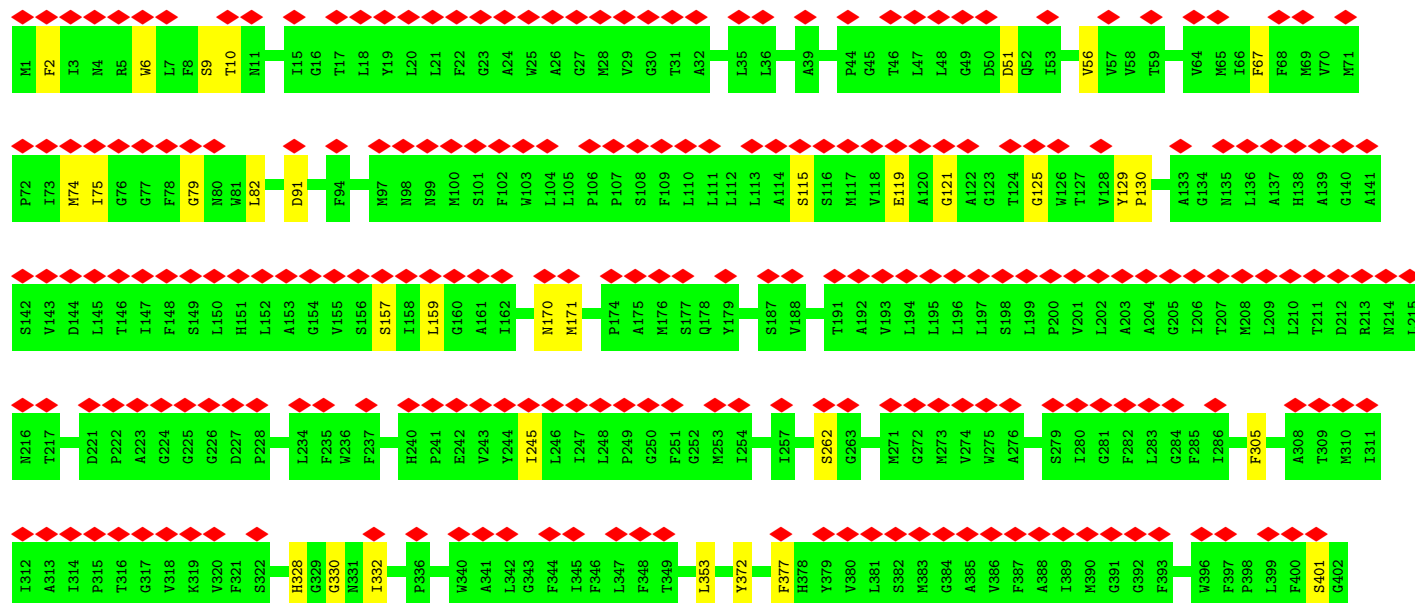
- Molecule 46: Cytochrome c oxidase subunit 8B, mitochondrial

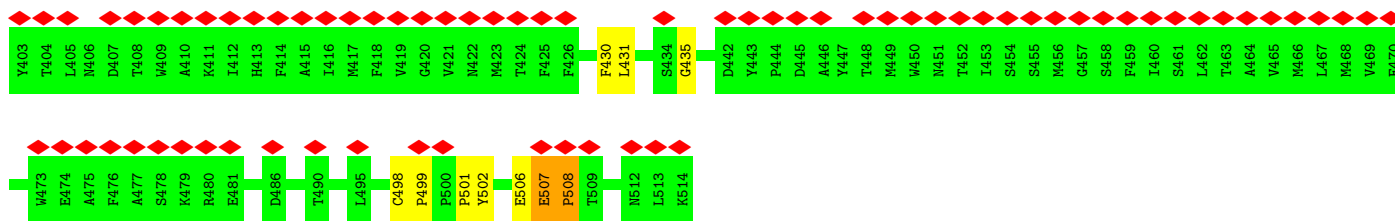
Chain s: 



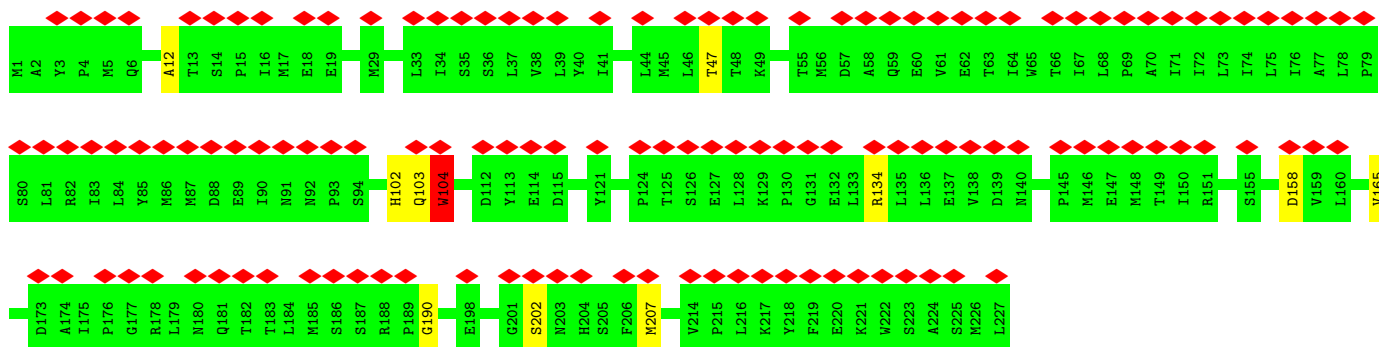
- Molecule 47: Cytochrome c oxidase subunit 1

Chain y: 

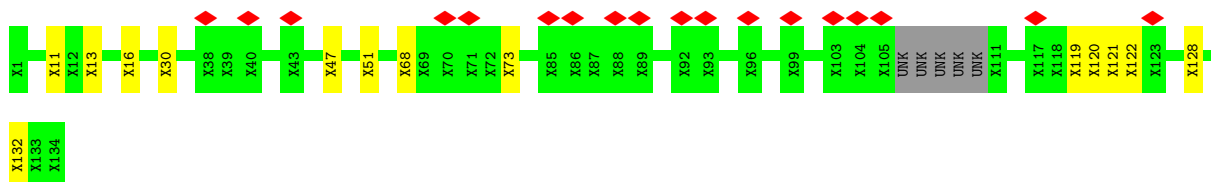
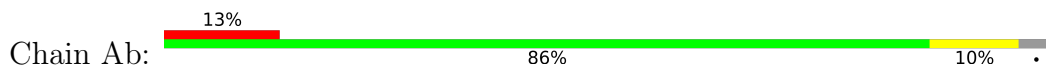




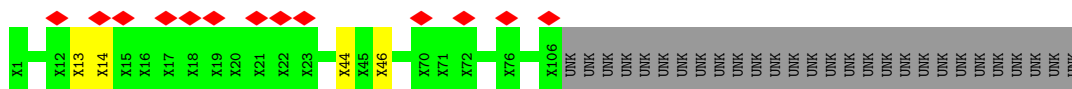
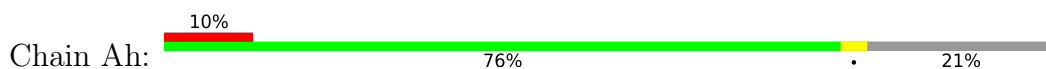
• Molecule 48: Cytochrome c oxidase subunit 2



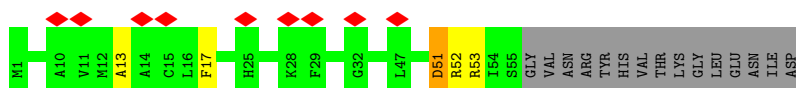
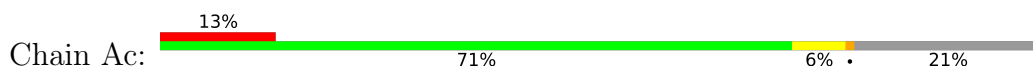
• Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



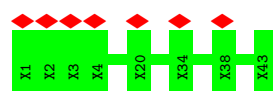
• Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



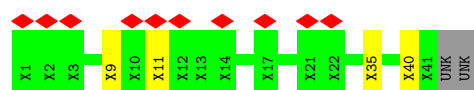
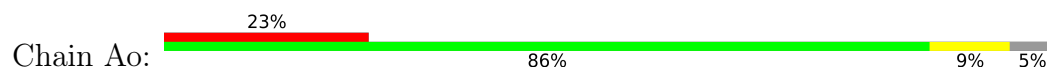
• Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



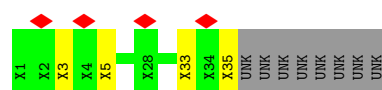
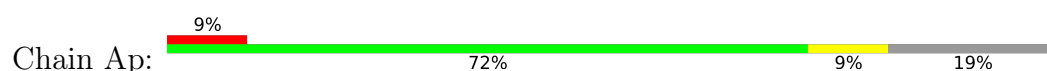
• Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



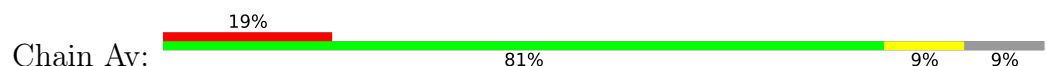
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



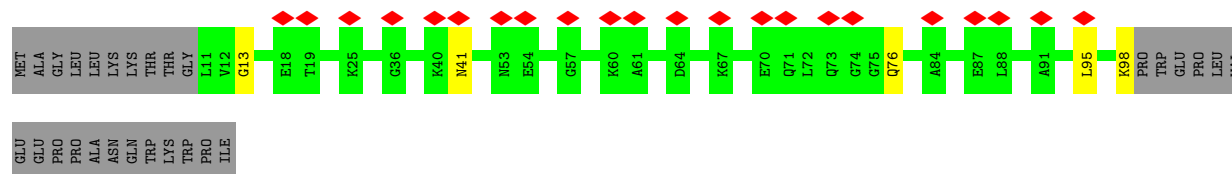
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



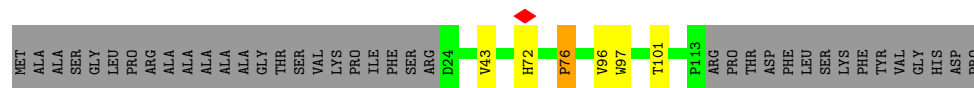
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



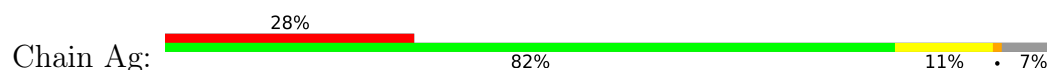
- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

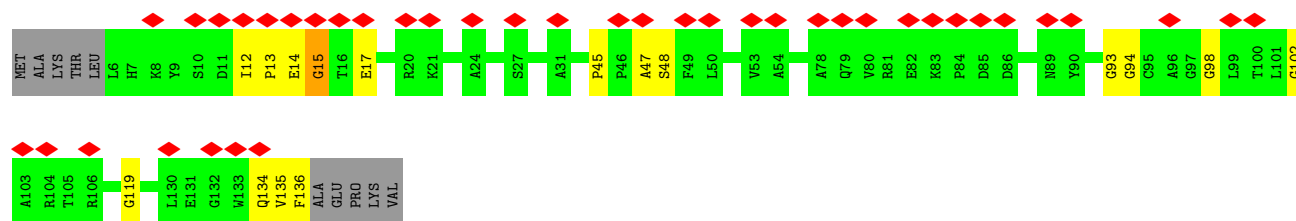


- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

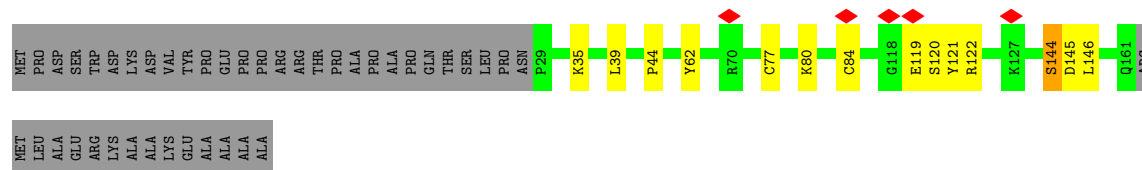


- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

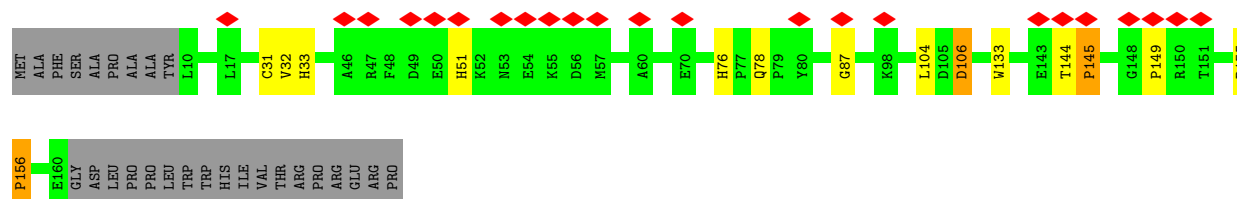
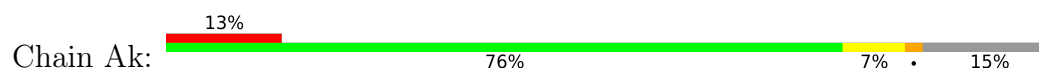




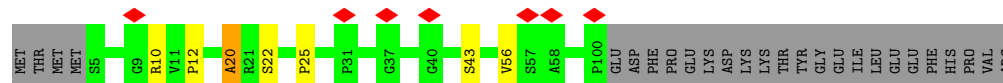
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



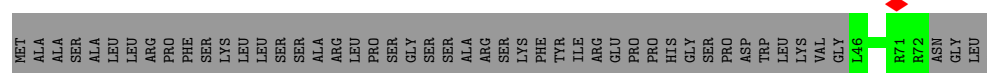
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



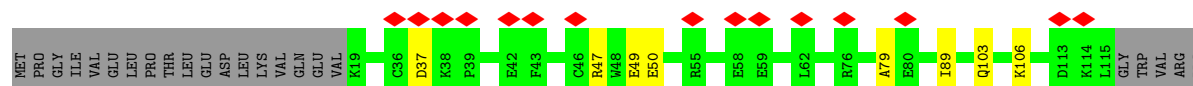
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 58: NADH dehydrogenase [ubiquinone] 1 subunit C1



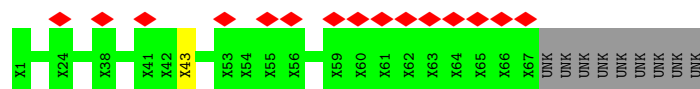
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



ASP LEU GLY LEU SER LYS VAL VAL LYS THR ASP ARG LEU LEU GLU ASN PRO THR HIS SER ARG ALA ARG GLU PRO ASN PRO GLU ALA GLY ASP LEU LYS PRO ALA LYS HIS GLY SER ARG LEU PHE THR MET

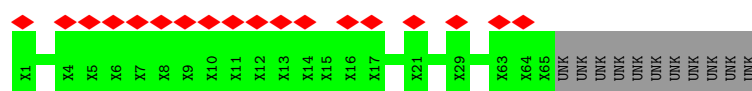
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Aq:  20% 87% 12%



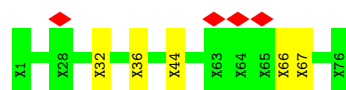
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain As:  24% 86% 14%



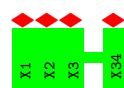
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Aw:  5% 93% 7%



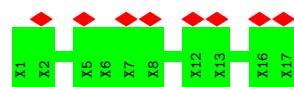
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ar:  12% 100%



- Molecule 62: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain At:  47% 100%



- Molecule 63: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Au:  15% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139996	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	505.4208, 505.4208, 505.4208	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05296, 1.05296, 1.05296	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	2/2197 (0.1%)	2.24	107/3055 (3.5%)
1	M	0.97	4/2197 (0.2%)	2.26	91/3055 (3.0%)
2	B	0.78	2/2060 (0.1%)	2.09	66/2862 (2.3%)
2	N	0.75	0/2060	1.99	59/2862 (2.1%)
3	C	1.06	2/1869 (0.1%)	2.44	108/2600 (4.2%)
3	O	1.08	5/1869 (0.3%)	2.33	90/2600 (3.5%)
4	D	0.71	0/1187	1.84	31/1650 (1.9%)
4	P	0.70	0/1187	1.83	34/1650 (2.1%)
5	E	0.45	0/966	1.26	9/1343 (0.7%)
5	Q	0.76	0/965	2.04	32/1341 (2.4%)
6	F	0.81	1/526 (0.2%)	1.85	13/733 (1.8%)
6	R	0.85	0/526	1.98	12/733 (1.6%)
7	G	0.87	0/400	2.21	22/556 (4.0%)
7	S	0.80	0/385	1.67	11/535 (2.1%)
8	H	0.68	0/319	1.74	5/445 (1.1%)
8	T	0.60	0/319	1.62	1/445 (0.2%)
9	I	0.73	0/162	2.14	4/224 (1.8%)
9	U	0.60	0/162	1.89	5/224 (2.2%)
10	J	0.72	0/306	1.81	7/425 (1.6%)
10	L	0.75	0/306	1.85	4/425 (0.9%)
11	K	0.43	0/210	1.18	1/290 (0.3%)
11	V	0.38	0/181	1.12	1/250 (0.4%)
12	W	0.58	0/1401	1.03	4/1906 (0.2%)
13	Y	0.57	0/5077	0.98	23/6888 (0.3%)
14	Z	0.77	0/3075	0.94	8/4155 (0.2%)
15	a	0.83	0/1174	0.97	1/1591 (0.1%)
16	b	0.81	0/1215	1.05	6/1644 (0.4%)
17	c	0.49	0/3196	0.95	11/4323 (0.3%)
18	d	0.51	0/1353	0.95	4/1841 (0.2%)
19	e	0.76	0/2558	1.01	5/3497 (0.1%)
20	f	0.85	0/2761	0.99	4/3754 (0.1%)
21	g	0.71	0/850	0.87	2/1163 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	h	0.80	0/3700	0.98	12/5045 (0.2%)
23	i	0.87	0/687	1.06	3/931 (0.3%)
24	j	0.67	0/4831	0.95	9/6572 (0.1%)
25	k	0.72	0/1084	0.94	1/1470 (0.1%)
25	l	0.58	0/72	0.88	0/98
26	m	0.75	0/262	1.22	2/364 (0.5%)
27	n	0.51	0/410	1.13	0/570
28	o	0.81	0/250	1.14	1/346 (0.3%)
29	p	0.56	0/1545	1.05	7/2147 (0.3%)
30	q	0.61	0/966	1.24	8/1343 (0.6%)
30	v	0.74	0/251	1.20	2/348 (0.6%)
31	r	0.73	0/310	0.97	0/430
32	Aa	0.52	0/402	1.00	0/560
32	t	0.69	0/402	1.08	1/560 (0.2%)
33	Ai	0.83	0/166	1.02	0/229
33	u	0.86	0/266	1.10	2/369 (0.5%)
34	w	0.63	0/529	1.11	1/736 (0.1%)
35	x	0.63	0/220	0.85	0/301
36	0	0.88	0/1283	1.25	7/1782 (0.4%)
37	1	0.78	0/715	1.17	3/997 (0.3%)
38	2	0.75	0/538	1.22	6/748 (0.8%)
39	3	0.82	0/480	1.33	3/665 (0.5%)
40	4	0.82	0/410	1.34	6/567 (1.1%)
41	5	0.79	0/370	1.46	5/514 (1.0%)
42	6	0.81	0/360	1.12	2/500 (0.4%)
43	7	0.80	0/273	1.27	3/377 (0.8%)
44	8	0.89	0/240	1.23	1/332 (0.3%)
45	9	0.87	0/230	1.19	2/318 (0.6%)
46	s	0.81	0/212	1.15	1/294 (0.3%)
47	y	0.90	0/2522	1.34	28/3501 (0.8%)
48	z	0.88	0/1126	1.33	10/1570 (0.6%)
50	Ac	0.83	0/270	1.01	0/374
52	Ae	0.61	0/434	1.10	0/603
53	Af	0.66	0/447	1.15	3/623 (0.5%)
54	Ag	0.74	0/636	1.06	1/878 (0.1%)
55	Aj	0.78	0/662	1.06	3/924 (0.3%)
56	Ak	0.75	0/749	1.29	10/1044 (1.0%)
57	Al	0.74	0/472	1.15	1/655 (0.2%)
58	Am	0.72	0/133	0.85	0/184
59	An	0.70	0/481	1.10	1/670 (0.1%)
All	All	0.76	16/72415 (0.0%)	1.42	926/99604 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	M	0	3
2	B	0	9
2	N	0	5
3	C	0	14
3	O	0	6
4	D	0	1
4	P	0	2
5	Q	0	5
6	F	0	1
7	G	0	2
7	S	0	2
8	T	0	1
9	I	0	1
10	J	0	1
17	c	0	1
34	w	0	1
54	Ag	0	1
All	All	0	69

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	253	VAL	C-O	11.11	1.36	1.24
3	O	37	LEU	C-N	-8.12	1.24	1.33
3	O	19	ILE	CA-C	-6.33	1.44	1.52
3	O	44	GLN	C-N	-6.31	1.26	1.33
1	M	169	GLY	N-CA	-6.16	1.36	1.44

The worst 5 of 926 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	253	VAL	O-C-N	-23.33	98.92	123.18
1	M	253	VAL	CA-C-O	16.90	137.34	120.27
3	O	44	GLN	CA-C-N	15.27	139.79	120.70
3	O	44	GLN	C-N-CA	15.27	139.79	120.70
56	Ak	155	PRO	N-CA-CB	14.56	110.79	103.22

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLN	Mainchain
1	A	122	LEU	Mainchain
1	A	196	VAL	Mainchain
1	A	210	ASP	Mainchain
1	A	53	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2198	0	1040	107	0
1	M	2198	0	1040	114	0
2	B	2061	0	1028	74	0
2	N	2061	0	1028	104	0
3	C	1870	0	844	114	0
3	O	1870	0	844	72	0
4	D	1188	0	533	39	0
4	P	1188	0	533	67	0
5	E	967	0	441	35	0
5	Q	966	0	440	42	0
6	F	527	0	232	21	0
6	R	527	0	232	9	0
7	G	401	0	180	24	0
7	S	386	0	174	30	0
8	H	320	0	135	7	0
8	T	320	0	135	9	0
9	I	163	0	77	8	0
9	U	163	0	77	28	0
10	J	307	0	149	13	0
10	L	307	0	149	20	0
11	K	211	0	102	9	0
11	V	182	0	90	6	0
12	W	1366	0	1316	85	0
13	Y	4998	0	4891	359	0
14	Z	3003	0	2971	172	0
15	a	1146	0	1143	88	0
16	b	1189	0	1144	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	c	3125	0	3087	198	0
18	d	1324	0	1338	84	0
19	e	2486	0	2587	129	0
20	f	2698	0	2851	123	0
21	g	829	0	863	50	0
22	h	3610	0	3816	160	0
23	i	677	0	726	45	0
24	j	4705	0	4848	205	0
25	k	1059	0	1077	66	0
25	l	73	0	31	1	0
26	m	263	0	125	1	0
27	n	411	0	177	3	0
28	o	251	0	115	4	0
29	p	1546	0	688	41	0
30	q	967	0	431	16	0
30	v	252	0	103	1	0
31	r	311	0	140	1	0
32	Aa	403	0	172	1	0
32	t	403	0	172	0	0
33	Ai	167	0	72	0	0
33	u	267	0	123	1	0
34	w	530	0	230	5	0
35	x	221	0	101	3	0
36	0	1284	0	575	1	0
37	1	716	0	321	1	0
38	2	539	0	243	0	0
39	3	481	0	224	3	0
40	4	411	0	193	3	0
41	5	371	0	161	0	0
42	6	361	0	184	0	0
43	7	274	0	127	0	0
44	8	241	0	115	1	0
45	9	231	0	106	0	0
46	s	213	0	98	8	0
47	y	2523	0	1169	6	0
48	z	1127	0	475	1	0
49	Ab	637	0	132	11	0
49	Ah	526	0	107	5	0
50	Ac	271	0	132	2	0
51	Ad	211	0	42	0	0
51	Ao	205	0	46	4	0
51	Ap	173	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Av	193	0	40	2	0
52	Ae	435	0	195	2	0
53	Af	448	0	190	1	0
54	Ag	637	0	331	4	0
55	Aj	663	0	292	4	0
56	Ak	750	0	321	2	0
57	Al	473	0	204	3	0
58	Am	134	0	54	0	0
59	An	482	0	214	2	0
60	Aq	335	0	69	3	0
60	As	322	0	65	0	0
60	Aw	376	0	76	3	0
61	Ar	169	0	37	0	0
62	At	84	0	18	0	0
63	Au	62	0	12	0	0
64	C	86	0	60	42	0
64	O	86	0	60	9	0
65	D	43	0	32	1	0
65	P	43	0	32	2	0
66	E	4	0	0	0	0
66	Q	4	0	0	0	0
66	Y	4	0	0	0	0
66	d	4	0	0	1	0
67	Y	16	0	0	5	0
67	a	8	0	0	0	0
67	b	16	0	0	3	0
67	c	8	0	0	4	0
68	c	31	0	19	20	0
69	p	48	0	26	26	0
70	3	1	0	0	0	0
71	y	120	0	108	2	0
72	y	1	0	0	0	0
72	z	2	0	0	0	0
73	y	1	0	0	0	0
All	All	75545	0	51782	2557	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 2557 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:85:LEU:CB	30:q:159:VAL:HA	1.13	1.55
1:A:84:ALA:CB	1:A:101:ALA:HB2	1.51	1.41
24:j:507:THR:HG22	46:s:11:SER:CB	1.53	1.37
30:q:85:LEU:CB	30:q:159:VAL:CA	2.02	1.36
3:C:117:VAL:N	64:C:402:HEM:HBC2	1.43	1.34

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	359 (81%)	63 (14%)	22 (5%)	1	15
1	M	444/446 (100%)	377 (85%)	47 (11%)	20 (4%)	2	16
2	B	417/439 (95%)	342 (82%)	66 (16%)	9 (2%)	5	28
2	N	417/439 (95%)	345 (83%)	60 (14%)	12 (3%)	3	23
3	C	377/379 (100%)	307 (81%)	56 (15%)	14 (4%)	2	19
3	O	377/379 (100%)	316 (84%)	50 (13%)	11 (3%)	3	23
4	D	239/241 (99%)	199 (83%)	28 (12%)	12 (5%)	1	15
4	P	239/241 (99%)	201 (84%)	26 (11%)	12 (5%)	1	15
5	E	194/274 (71%)	178 (92%)	12 (6%)	4 (2%)	5	28
5	Q	194/274 (71%)	158 (81%)	28 (14%)	8 (4%)	2	17
6	F	104/110 (94%)	90 (86%)	11 (11%)	3 (3%)	3	23
6	R	104/110 (94%)	89 (86%)	12 (12%)	3 (3%)	3	23
7	G	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	2	18
7	S	76/81 (94%)	72 (95%)	2 (3%)	2 (3%)	4	24
8	H	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	T	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	12
9	U	31/78 (40%)	20 (64%)	7 (23%)	4 (13%)	0	4
10	J	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0	7
10	L	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	11
11	K	41/56 (73%)	40 (98%)	0	1 (2%)	4	26
11	V	35/56 (62%)	33 (94%)	2 (6%)	0	100	100
12	W	167/264 (63%)	136 (81%)	23 (14%)	8 (5%)	2	15
13	Y	668/727 (92%)	575 (86%)	65 (10%)	28 (4%)	2	17
14	Z	373/463 (81%)	343 (92%)	20 (5%)	10 (3%)	4	24
15	a	145/216 (67%)	126 (87%)	11 (8%)	8 (6%)	1	14
16	b	147/212 (69%)	140 (95%)	6 (4%)	1 (1%)	18	55
17	c	408/464 (88%)	369 (90%)	27 (7%)	12 (3%)	3	23
18	d	167/249 (67%)	152 (91%)	11 (7%)	4 (2%)	4	26
19	e	313/318 (98%)	282 (90%)	27 (9%)	4 (1%)	9	40
20	f	344/347 (99%)	324 (94%)	17 (5%)	3 (1%)	14	50
21	g	104/115 (90%)	96 (92%)	7 (7%)	1 (1%)	12	47
22	h	455/459 (99%)	424 (93%)	21 (5%)	10 (2%)	5	28
23	i	88/98 (90%)	82 (93%)	4 (4%)	2 (2%)	5	27
24	j	592/606 (98%)	534 (90%)	40 (7%)	18 (3%)	3	22
25	k	138/175 (79%)	126 (91%)	8 (6%)	4 (3%)	3	23
25	l	13/175 (7%)	11 (85%)	1 (8%)	1 (8%)	1	9
26	m	51/84 (61%)	48 (94%)	2 (4%)	1 (2%)	6	30
27	n	81/99 (82%)	74 (91%)	6 (7%)	1 (1%)	10	43
28	o	49/106 (46%)	42 (86%)	3 (6%)	4 (8%)	0	9
29	p	312/377 (83%)	281 (90%)	19 (6%)	12 (4%)	2	18
30	q	194/357 (54%)	172 (89%)	16 (8%)	6 (3%)	3	21
30	v	49/357 (14%)	46 (94%)	3 (6%)	0	100	100
31	r	61/144 (42%)	60 (98%)	1 (2%)	0	100	100
32	Aa	79/156 (51%)	75 (95%)	1 (1%)	3 (4%)	2	18
32	t	79/156 (51%)	74 (94%)	3 (4%)	2 (2%)	4	25
33	Ai	32/189 (17%)	31 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	u	52/189 (28%)	48 (92%)	4 (8%)	0	100	100
34	w	105/175 (60%)	93 (89%)	11 (10%)	1 (1%)	12	47
35	x	44/123 (36%)	41 (93%)	1 (2%)	2 (4%)	2	16
36	0	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
37	1	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
38	2	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
39	3	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	17
40	4	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	12
41	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	38
42	6	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
43	7	54/59 (92%)	48 (89%)	4 (7%)	2 (4%)	2	19
44	8	47/56 (84%)	41 (87%)	6 (13%)	0	100	100
45	9	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
46	s	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
47	y	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	53
48	z	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	9	40
50	Ac	53/70 (76%)	49 (92%)	2 (4%)	2 (4%)	2	18
52	Ae	86/116 (74%)	82 (95%)	2 (2%)	2 (2%)	5	27
53	Af	88/128 (69%)	81 (92%)	4 (4%)	3 (3%)	3	20
54	Ag	129/141 (92%)	120 (93%)	2 (2%)	7 (5%)	1	14
55	Aj	131/176 (74%)	124 (95%)	2 (2%)	5 (4%)	2	18
56	Ak	149/178 (84%)	131 (88%)	11 (7%)	7 (5%)	2	16
57	Al	94/122 (77%)	83 (88%)	7 (7%)	4 (4%)	2	16
58	Am	25/76 (33%)	23 (92%)	2 (8%)	0	100	100
59	An	95/172 (55%)	87 (92%)	5 (5%)	3 (3%)	3	20
All	All	12001/14873 (81%)	10603 (88%)	1047 (9%)	351 (3%)	5	23

5 of 351 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	A	426	GLY
1	A	427	PRO

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Mol	Chain	Res	Type
2	B	141	GLN
2	B	183	ILE

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	
12	W	145/228 (64%)	144 (99%)	1 (1%)	76	80
13	Y	517/610 (85%)	515 (100%)	2 (0%)	84	83
14	Z	322/393 (82%)	321 (100%)	1 (0%)	86	84
15	a	120/177 (68%)	119 (99%)	1 (1%)	73	78
16	b	126/176 (72%)	126 (100%)	0	100	100
17	c	321/368 (87%)	320 (100%)	1 (0%)	86	84
18	d	145/207 (70%)	145 (100%)	0	100	100
19	e	272/275 (99%)	270 (99%)	2 (1%)	76	80
20	f	309/311 (99%)	309 (100%)	0	100	100
21	g	91/100 (91%)	90 (99%)	1 (1%)	65	74
22	h	407/409 (100%)	404 (99%)	3 (1%)	76	80
23	i	76/85 (89%)	75 (99%)	1 (1%)	61	72
24	j	527/540 (98%)	523 (99%)	4 (1%)	73	78
25	k	112/141 (79%)	111 (99%)	1 (1%)	70	77
All	All	3490/4020 (87%)	3472 (100%)	18 (0%)	78	82

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	j	283	ILE
25	k	12	ILE
24	j	468	ILE
21	g	96	ILE
24	j	63	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
24	j	192	HIS
24	j	328	HIS
25	k	46	ASN
17	c	441	HIS
17	c	418	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
66	FES	d	301	-	0,4,4	-	-	-		
66	FES	E	201	-	0,4,4	-	-	-		
64	HEM	O	402	-	50,50,50	1.34	7 (14%)	66,82,82	1.77	15 (22%)
64	HEM	C	402	-	50,50,50	1.25	6 (12%)	66,82,82	1.84	18 (27%)
67	SF4	Y	802	13	0,12,12	-	-	-		
66	FES	Y	803	13	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	NDP	p	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.76	11 (16%)
71	HEA	y	602	-	66,67,67	1.22	7 (10%)	78,103,103	1.37	12 (15%)
67	SF4	Y	801	13	0,12,12	-	-	-	-	-
68	FMN	c	502	-	33,33,33	1.42	6 (18%)	48,50,50	1.30	8 (16%)
65	HEC	P	301	-	50,50,50	1.30	5 (10%)	68,82,82	1.04	4 (5%)
67	SF4	a	301	15	0,12,12	-	-	-	-	-
71	HEA	y	601	-	66,67,67	1.10	3 (4%)	78,103,103	1.37	11 (14%)
65	HEC	D	301	-	50,50,50	1.28	3 (6%)	68,82,82	1.14	5 (7%)
67	SF4	c	501	17	0,12,12	-	-	-	-	-
64	HEM	C	401	-	50,50,50	1.30	6 (12%)	66,82,82	1.55	9 (13%)
67	SF4	b	302	16	0,12,12	-	-	-	-	-
66	FES	Q	201	-	0,4,4	-	-	-	-	-
64	HEM	O	401	-	50,50,50	1.39	7 (14%)	66,82,82	1.91	18 (27%)
67	SF4	b	301	16	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	FES	d	301	-	-	-	0/1/1/1
66	FES	E	201	-	-	-	0/1/1/1
64	HEM	O	402	-	-	4/14/54/54	-
64	HEM	C	402	-	-	6/14/54/54	-
67	SF4	Y	802	13	-	-	0/6/5/5
66	FES	Y	803	13	-	-	0/1/1/1
69	NDP	p	401	-	-	15/34/77/77	0/5/5/5
71	HEA	y	602	-	-	7/36/76/76	-
67	SF4	Y	801	13	-	-	0/6/5/5
68	FMN	c	502	-	-	4/18/18/18	0/3/3/3
65	HEC	P	301	-	-	8/14/54/54	-
67	SF4	a	301	15	-	-	0/6/5/5
71	HEA	y	601	-	-	9/36/76/76	-
65	HEC	D	301	-	-	8/14/54/54	-
67	SF4	c	501	17	-	-	0/6/5/5
64	HEM	C	401	-	-	4/14/54/54	-
67	SF4	b	302	16	-	-	0/6/5/5
66	FES	Q	201	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	HEM	O	401	-	-	6/14/54/54	-
67	SF4	b	301	16	-	-	0/6/5/5

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	c	502	FMN	C9A-C5A	4.56	1.48	1.41
69	p	401	NDP	C5A-C4A	3.96	1.46	1.39
71	y	602	HEA	CMA-C3A	-3.78	1.37	1.45
65	D	301	HEC	CBB-CAB	-3.54	1.35	1.51
65	P	301	HEC	CBC-CAC	-3.47	1.36	1.51

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	p	401	NDP	C5A-C4A-N3A	-6.26	118.59	126.75
64	O	401	HEM	C3B-C2B-C1B	-5.49	102.41	106.49
69	p	401	NDP	PN-O3-PA	-5.22	114.92	132.83
64	O	402	HEM	C3B-C2B-C1B	5.06	110.24	106.49
69	p	401	NDP	N3A-C4A-N9A	5.00	135.32	127.08

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	O	401	HEM	C2B-C3B-CAB-CBB
68	c	502	FMN	C1'-C2'-C3'-C4'
68	c	502	FMN	C3'-C4'-C5'-O5'
68	c	502	FMN	O4'-C4'-C5'-O5'
69	p	401	NDP	C5B-O5B-PA-O1A

There are no ring outliers.

16 monomers are involved in 115 short contacts:

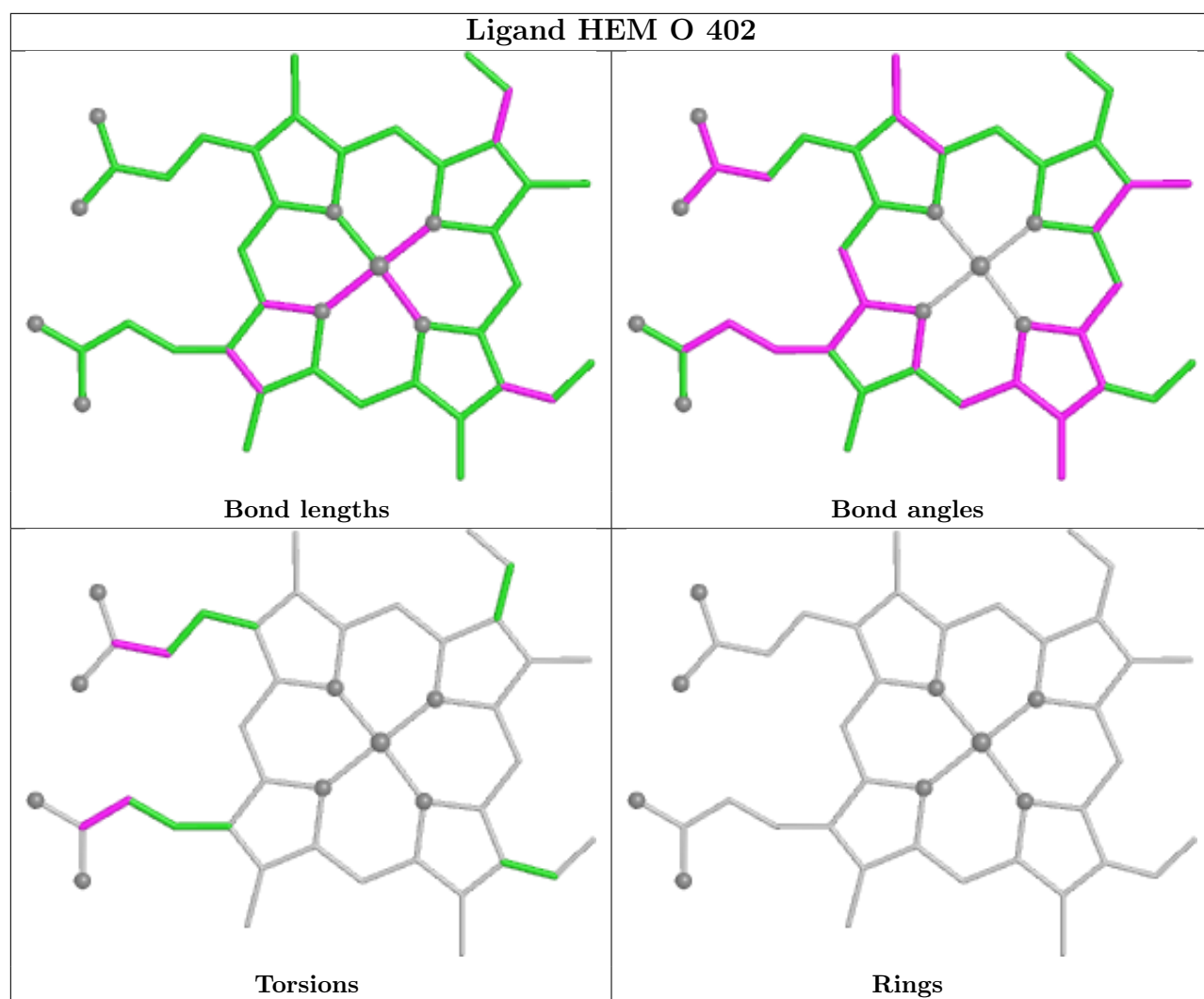
Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	d	301	FES	1	0
64	O	402	HEM	3	0
64	C	402	HEM	39	0
67	Y	802	SF4	1	0
69	p	401	NDP	26	0
71	y	602	HEA	1	0

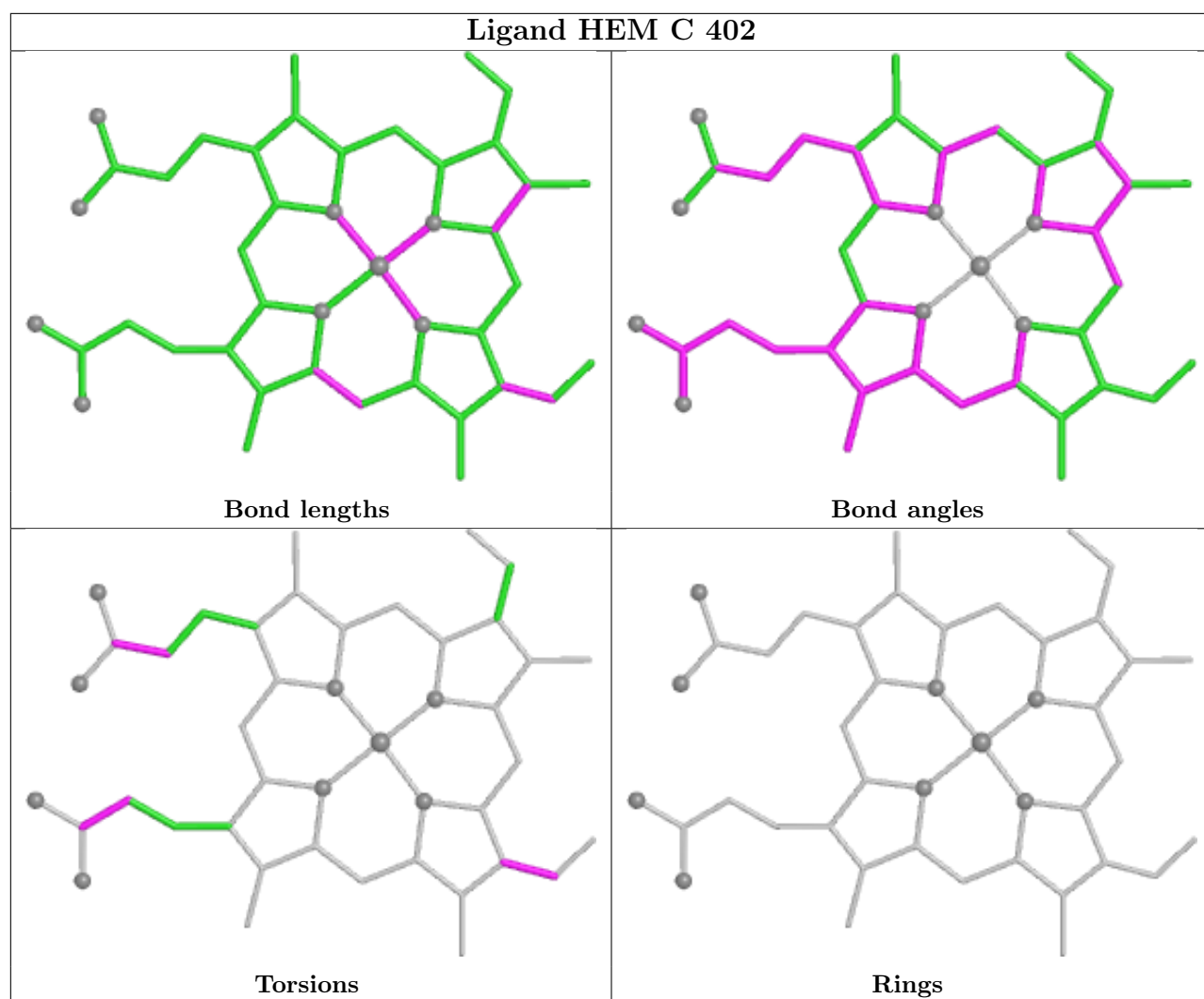
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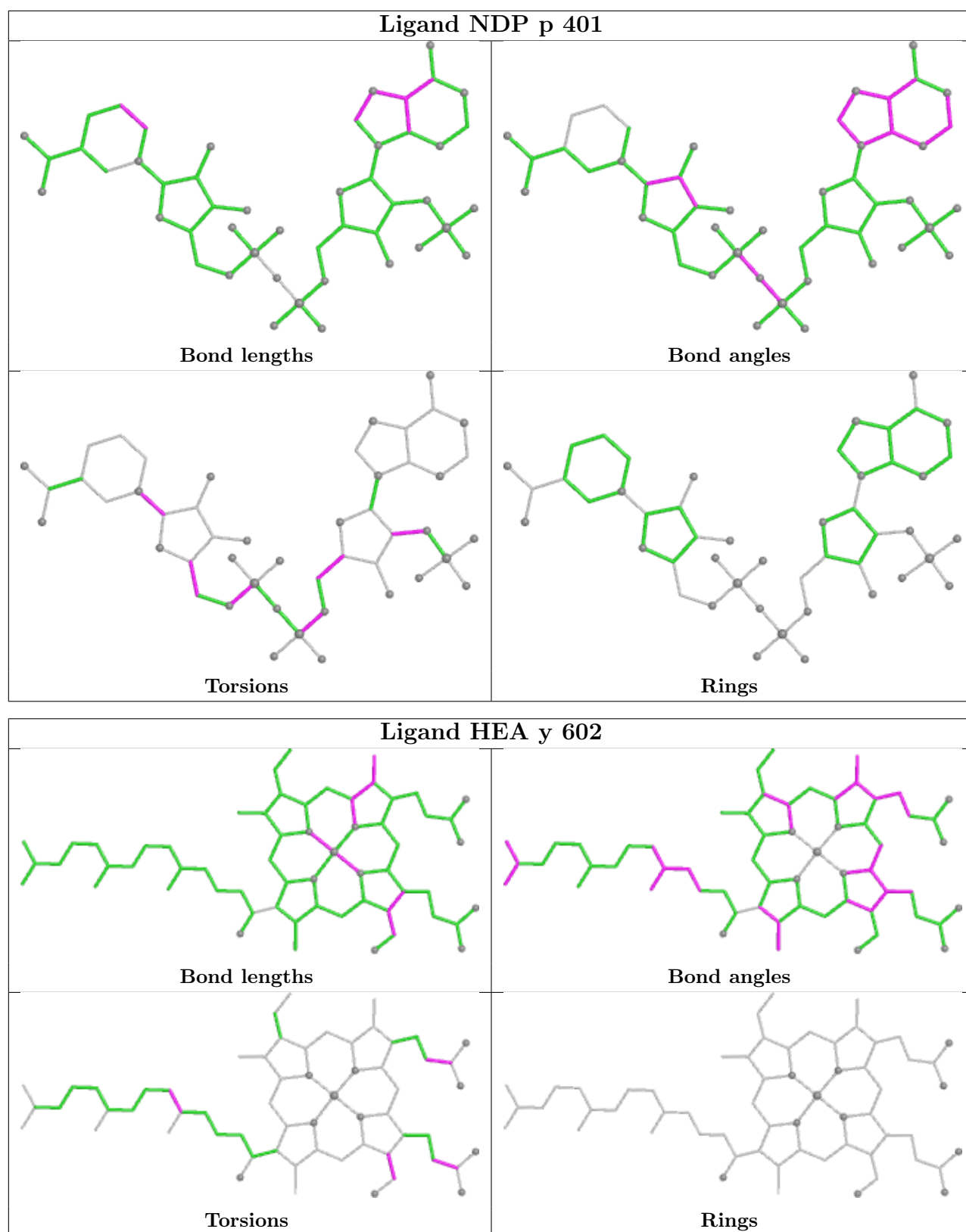
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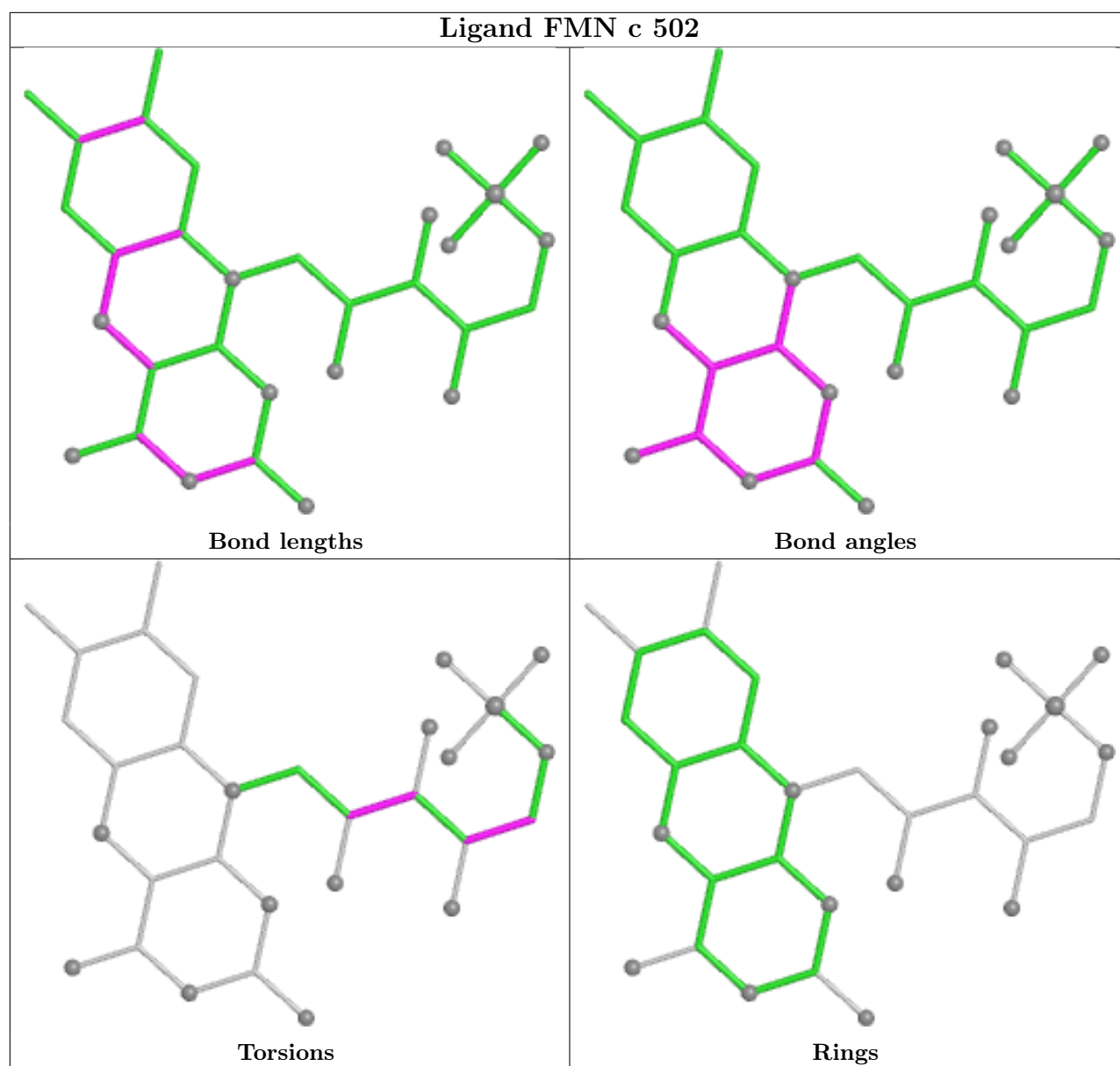
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Y	801	SF4	4	0
68	c	502	FMN	20	0
65	P	301	HEC	2	0
71	y	601	HEA	1	0
65	D	301	HEC	1	0
67	c	501	SF4	4	0
64	C	401	HEM	3	0
67	b	302	SF4	1	0
64	O	401	HEM	6	0
67	b	301	SF4	2	0

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

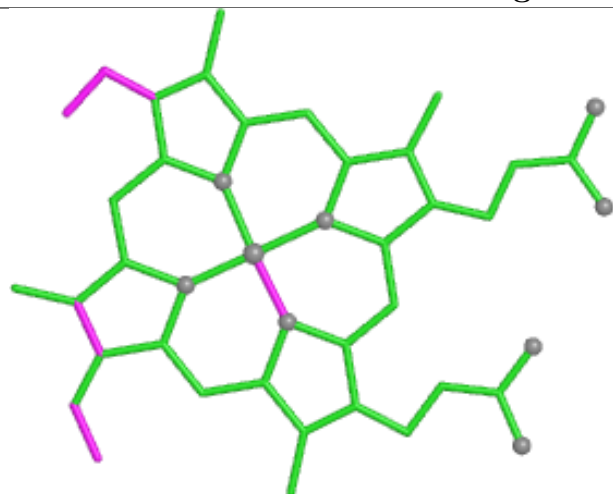




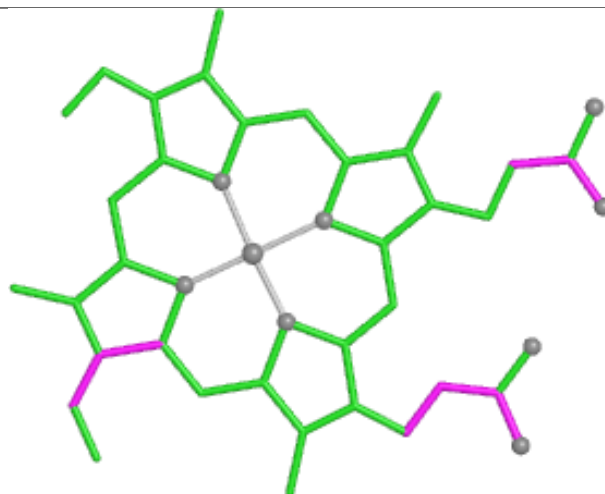




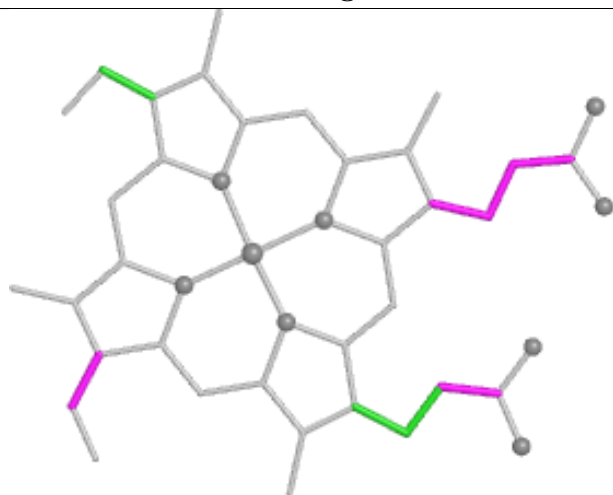
Ligand HEC P 301



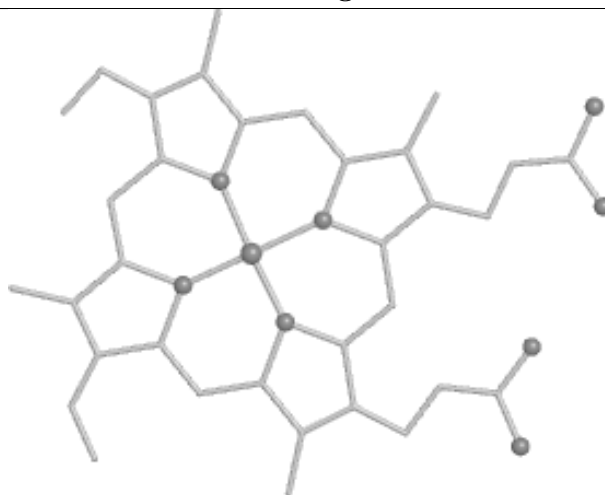
Bond lengths



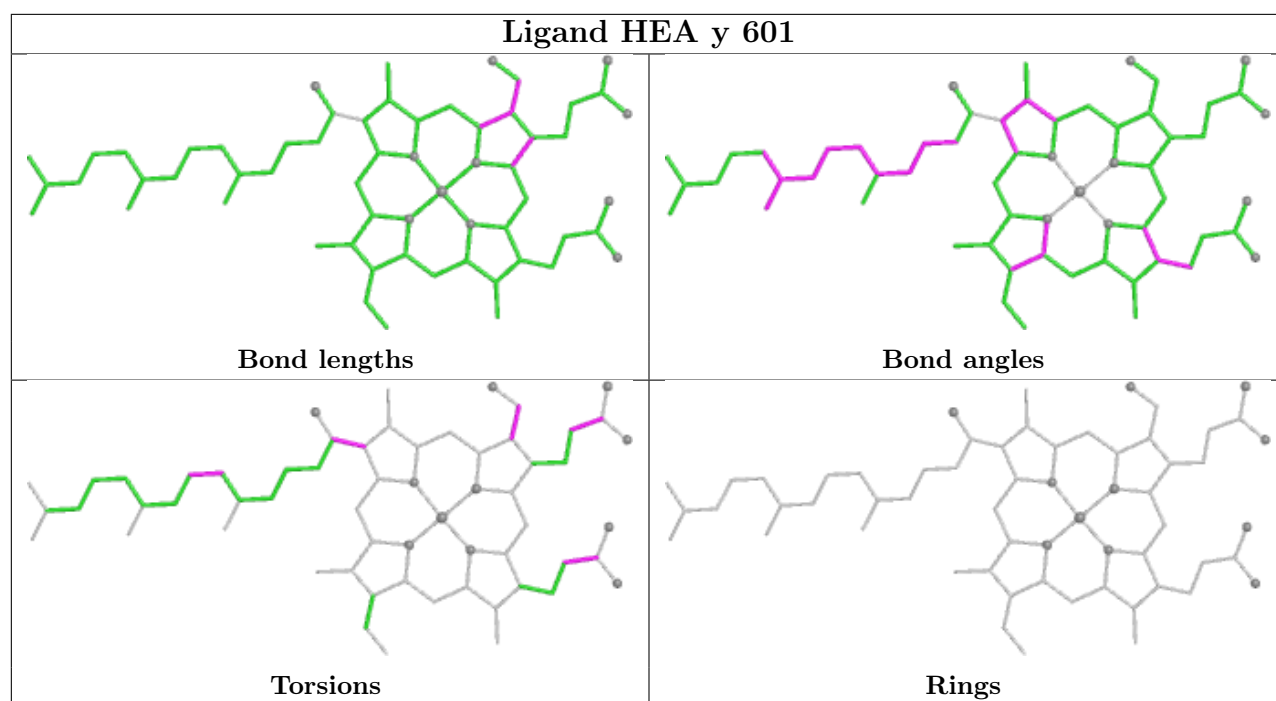
Bond angles

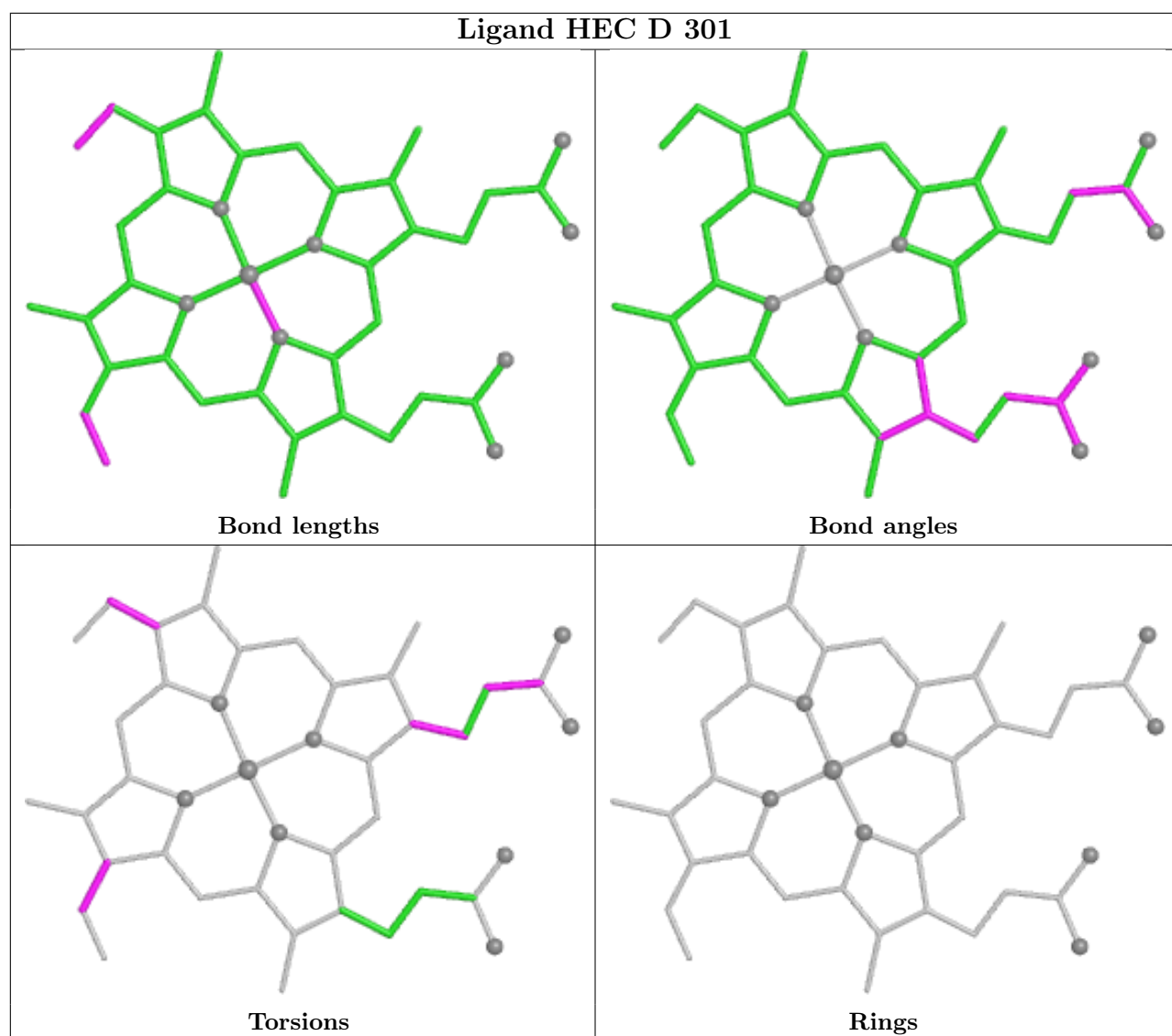


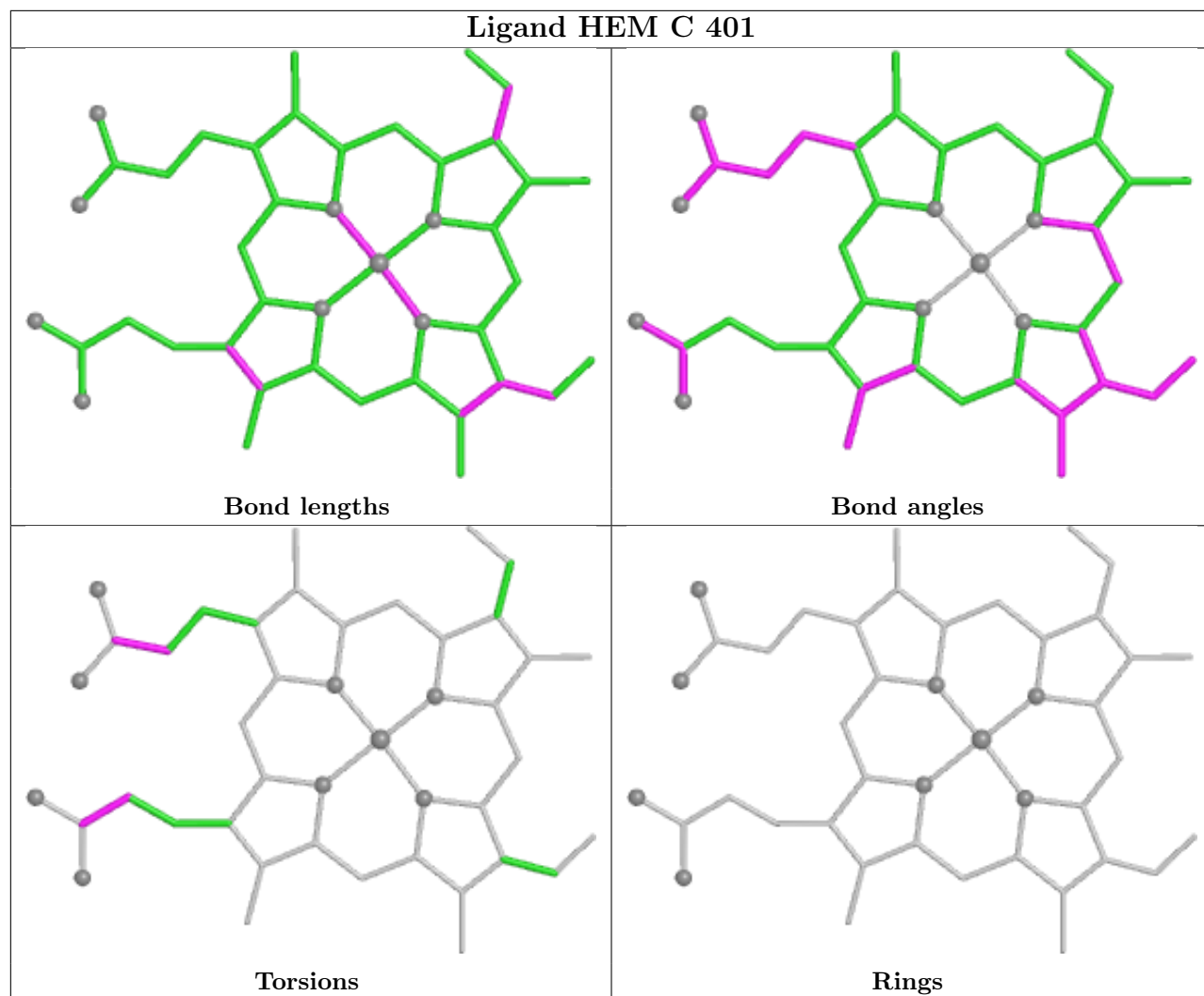
Torsions

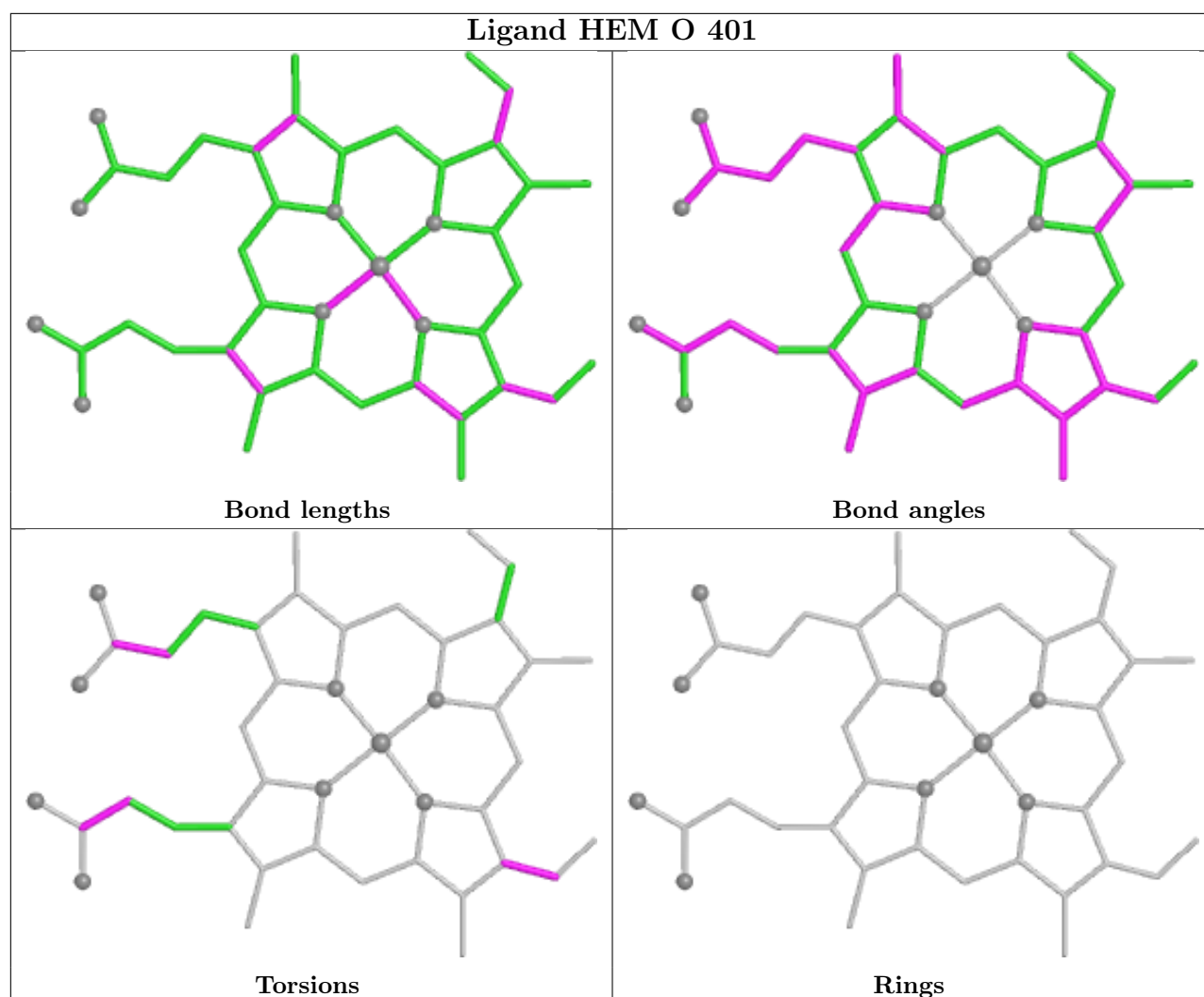


Rings









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.

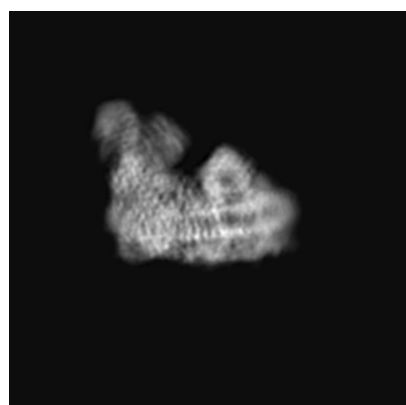
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9534. These allow visual inspection of the internal detail of the map and identification of artifacts.

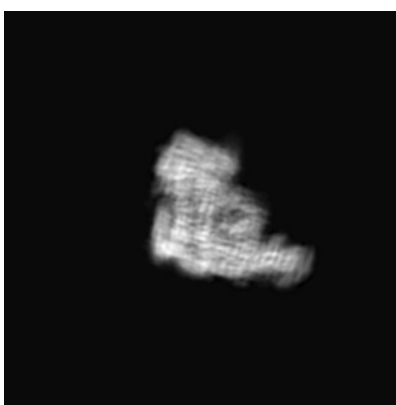
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

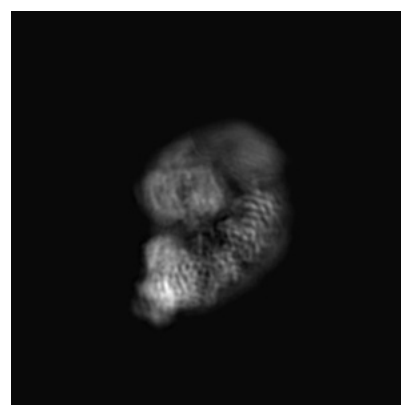
6.1.1 Primary map



X



Y

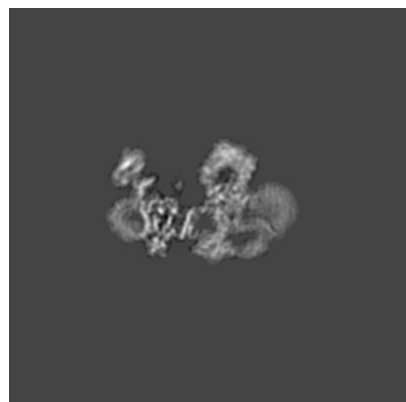


Z

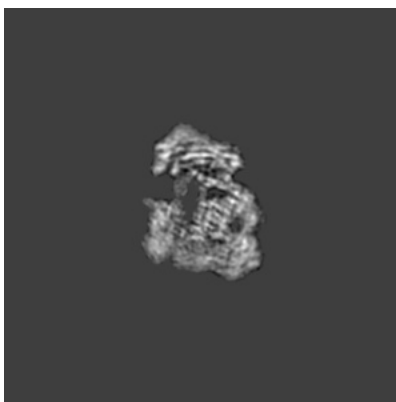
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

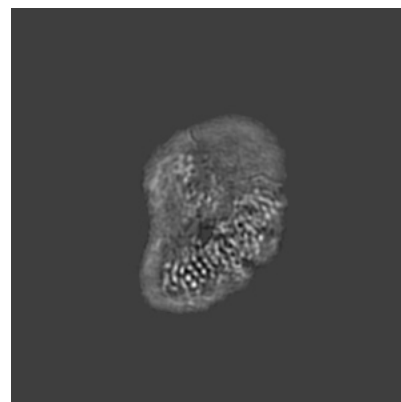
6.2.1 Primary map



X Index: 240



Y Index: 240

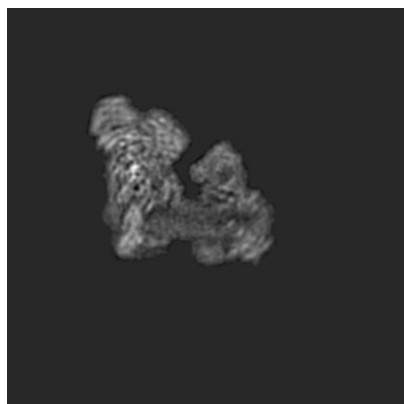


Z Index: 240

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

6.3 Largest variance slices [i](#)

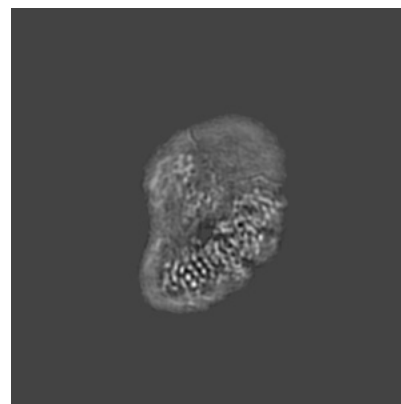
6.3.1 Primary map



X Index: 186



Y Index: 149

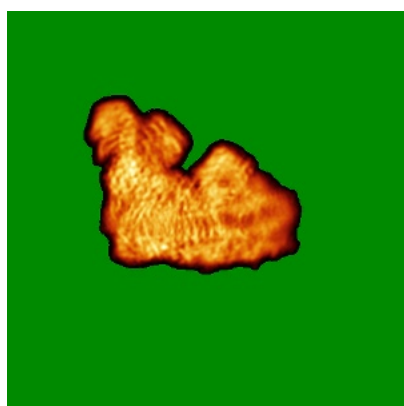


Z Index: 241

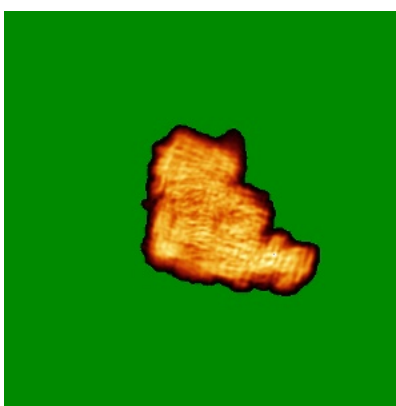
The images above show the largest variance slices of the map in three orthogonal directions.

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

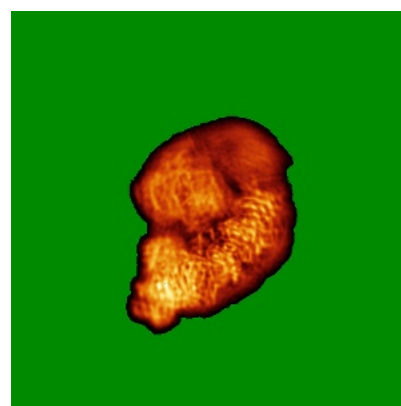
6.4.1 Primary map



X



Y

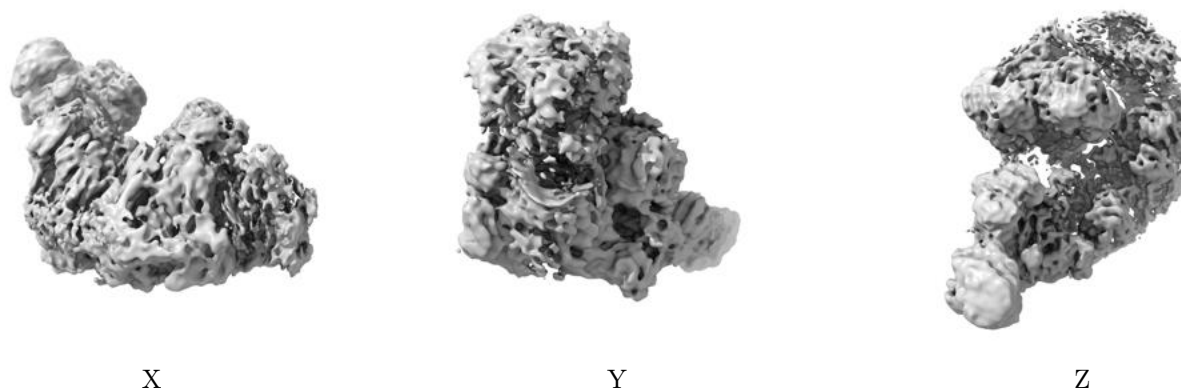


Z

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 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

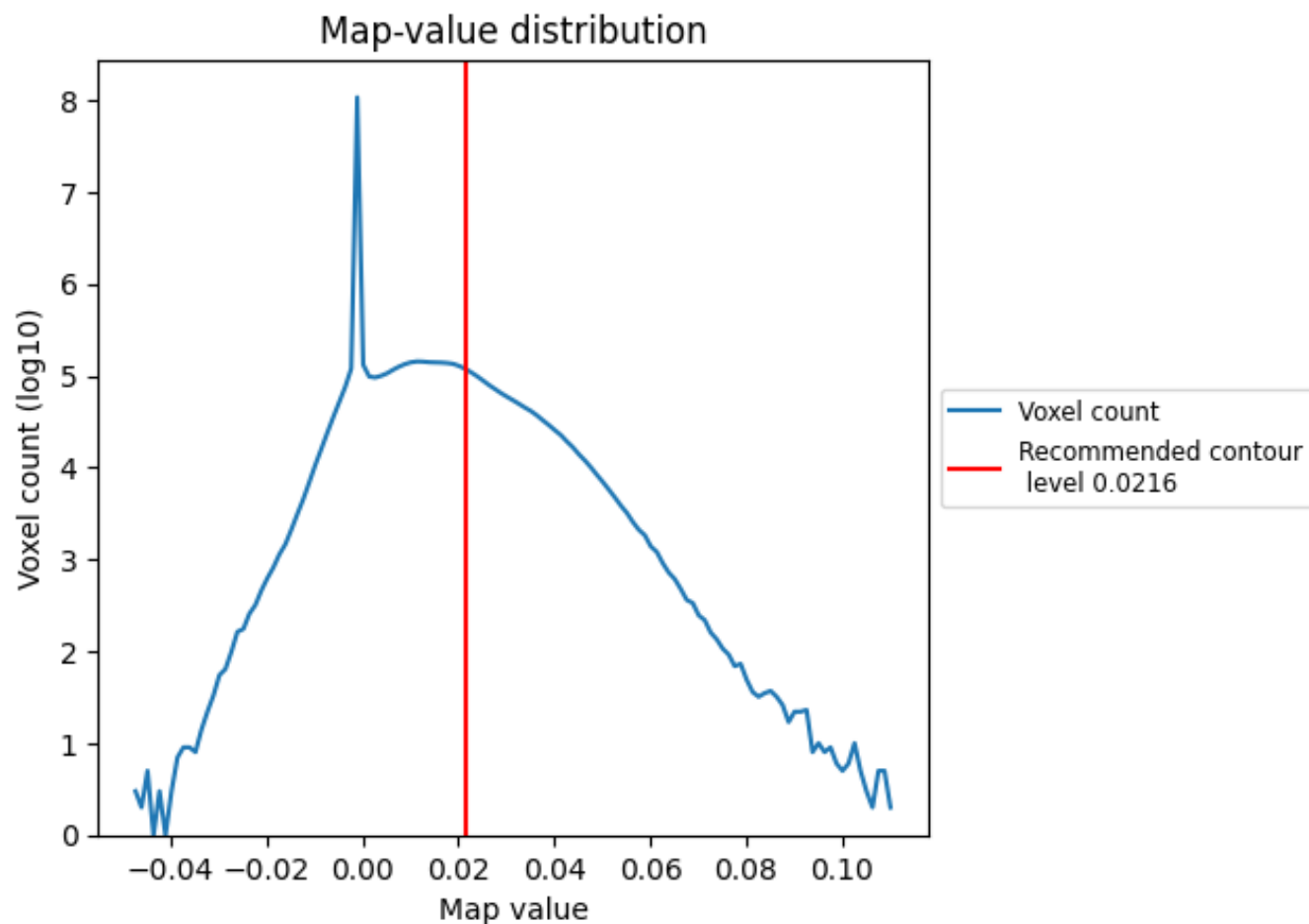
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

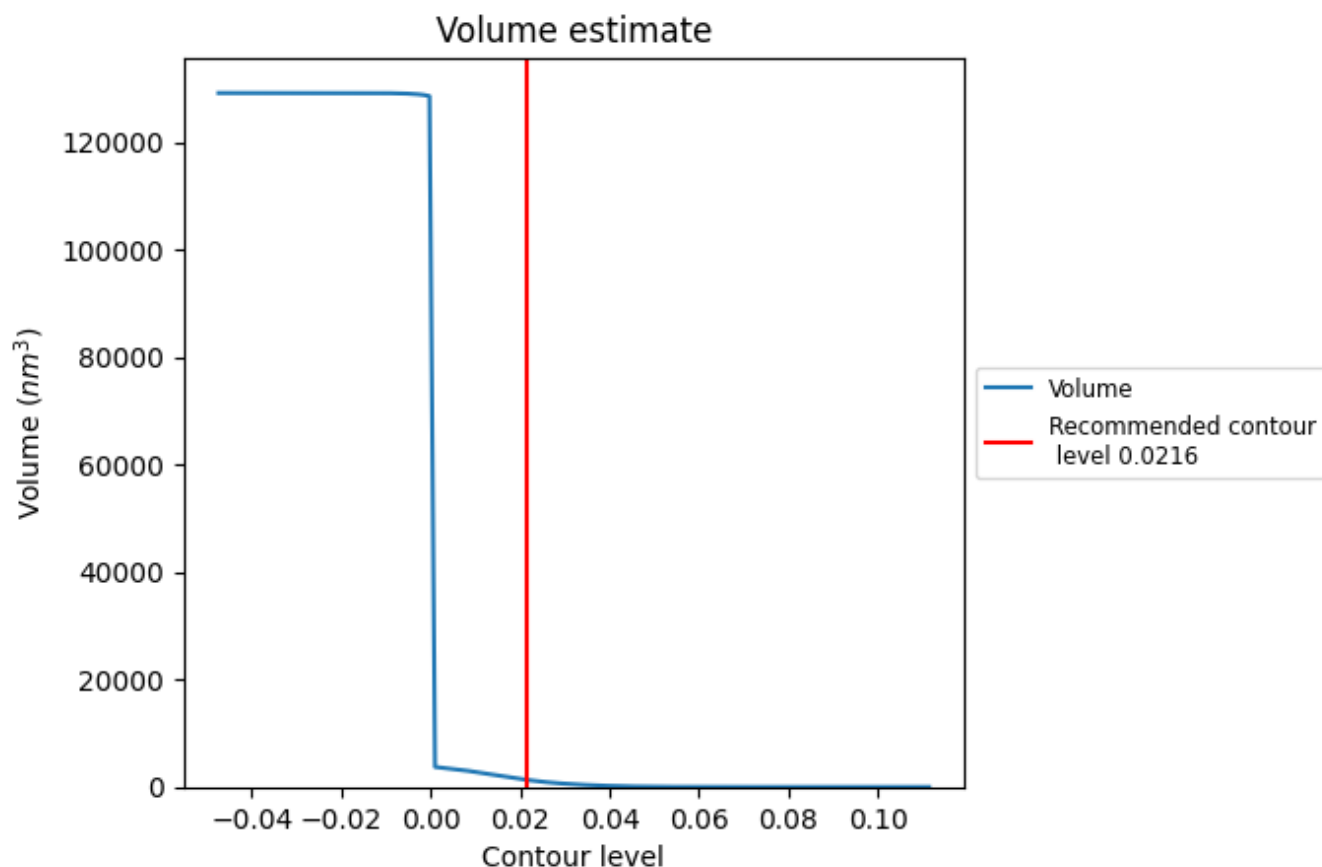
This section contains the results of statistical analysis of the map.

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.

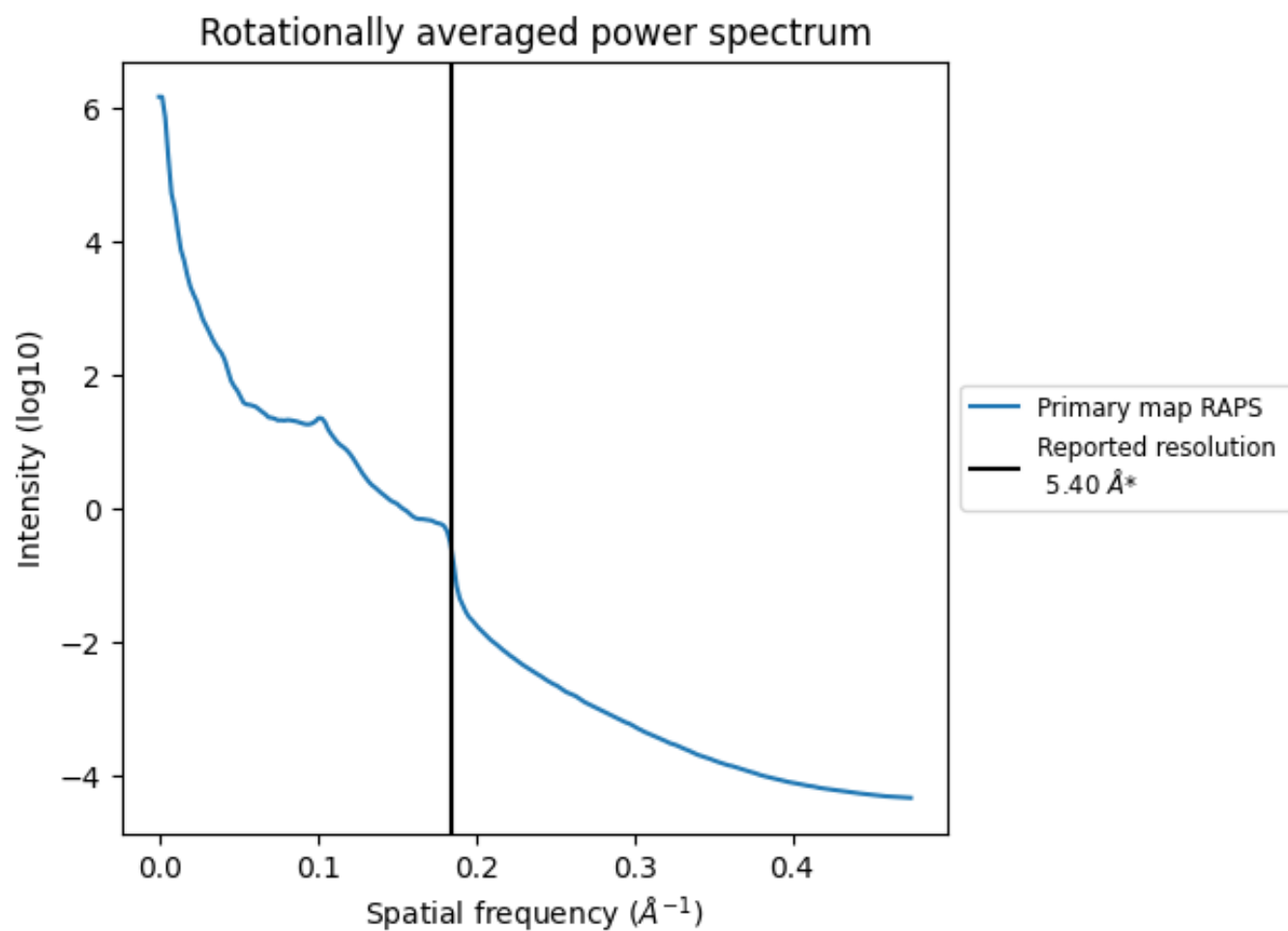
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1312 nm^3 ; this corresponds to an approximate mass of 1185 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

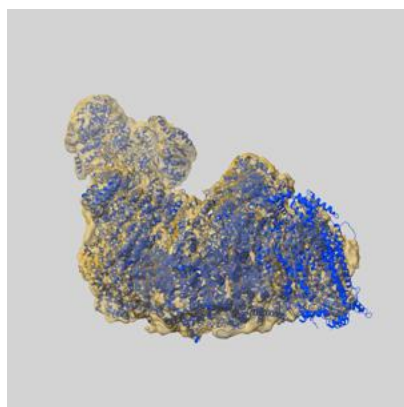
8 Fourier-Shell correlation

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

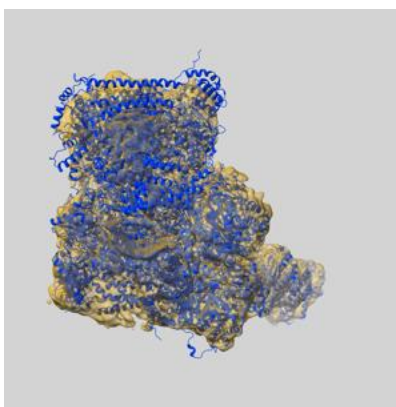
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9534 and PDB model 5GPN. Per-residue inclusion information can be found in section [3](#) on page [23](#).

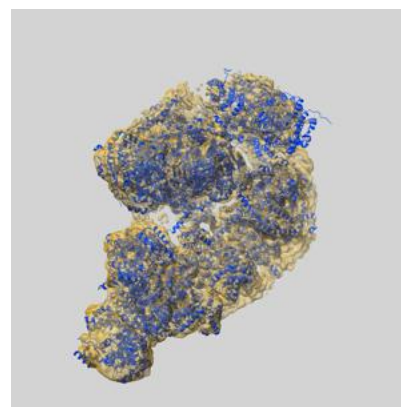
9.1 Map-model overlay [i](#)



X



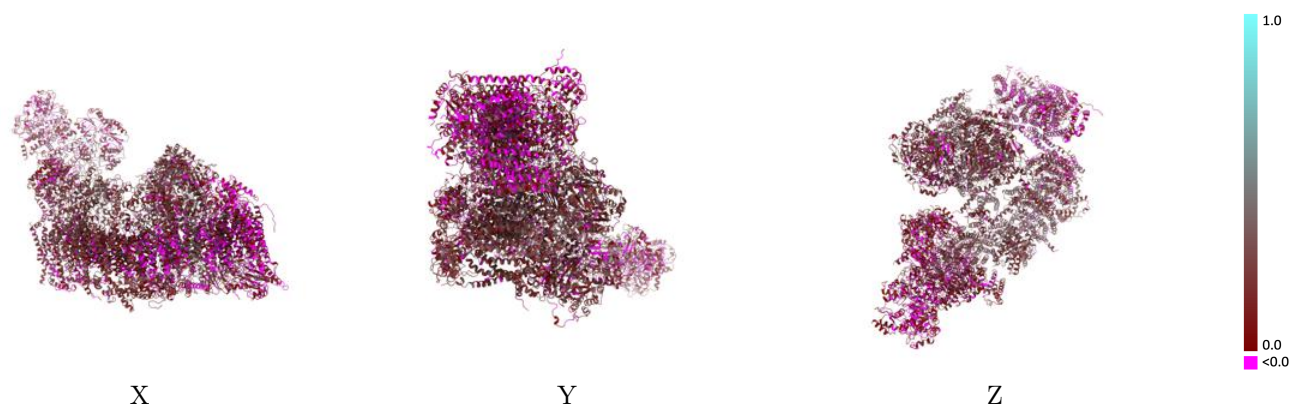
Y



Z

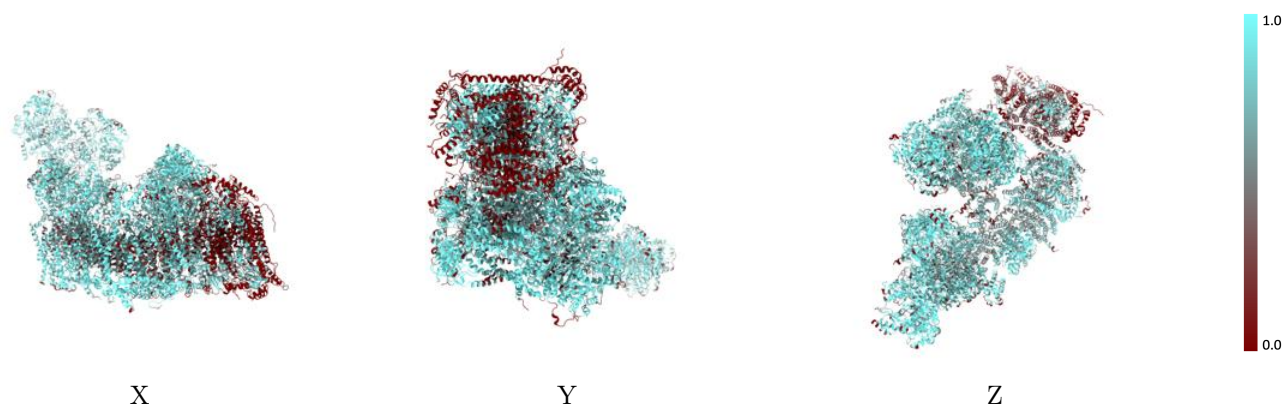
The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



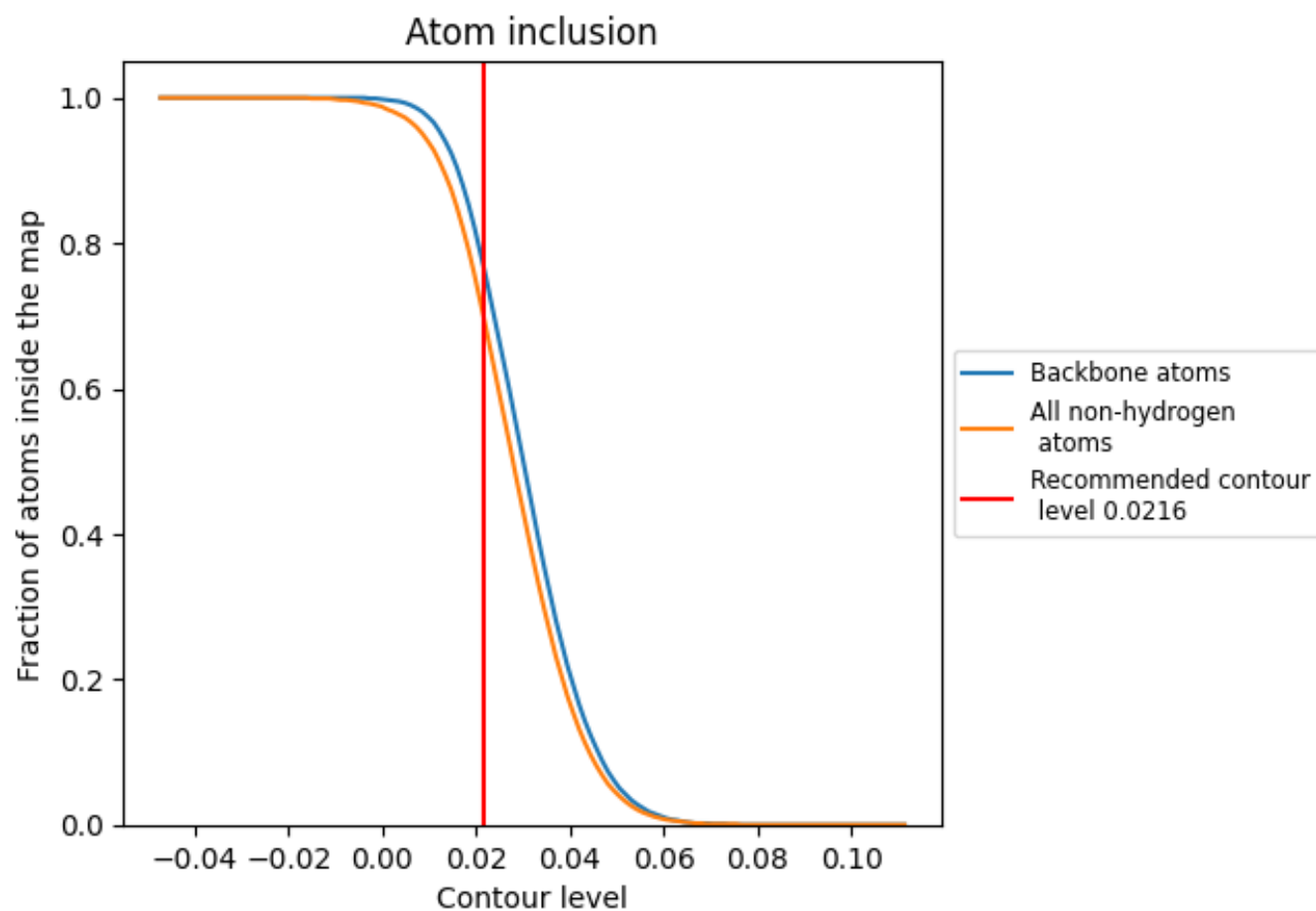
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0216).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.1430
0	 0.2210	 0.0520
1	 0.3110	 0.0940
2	 0.2060	 0.0300
3	 0.2390	 0.0480
4	 0.0530	 0.0860
5	 0.2240	 0.0490
6	 0.0050	 0.0050
7	 0.0470	 0.0620
8	 0.1080	 -0.0160
9	 0.1260	 0.0670
A	 0.8130	 0.1990
Aa	 0.5780	 0.1740
Ab	 0.8100	 0.1770
Ac	 0.7670	 0.1180
Ad	 0.8100	 0.0970
Ae	 0.7820	 0.1690
Af	 0.9550	 0.2780
Ag	 0.6200	 0.2100
Ah	 0.8420	 0.2330
Ai	 0.9700	 0.2580
Aj	 0.9190	 0.2090
Ak	 0.8120	 0.2080
Al	 0.8630	 0.2080
Am	 0.9250	 0.2200
An	 0.8380	 0.0810
Ao	 0.7660	 0.1370
Ap	 0.7800	 0.1640
Aq	 0.7880	 0.0530
Ar	 0.8640	 0.2430
As	 0.7050	 0.1470
At	 0.5950	 0.1800
Au	 0.8060	 0.0730
Av	 0.7620	 0.1860
Aw	 0.8960	 0.2190



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Chain	Atom inclusion	Q-score
B	 0.7550	 0.1650
C	 0.8050	 0.2340
D	 0.8380	 0.1980
E	 0.7900	 0.1510
F	 0.8480	 0.2440
G	 0.8160	 0.2110
H	 0.8380	 0.2320
I	 0.5710	 0.0790
J	 0.7560	 0.2160
K	 0.5690	 0.2490
L	 0.5900	 0.2060
M	 0.8030	 0.2200
N	 0.8930	 0.2260
O	 0.6290	 0.2190
P	 0.7830	 0.1970
Q	 0.6370	 0.1450
R	 0.6410	 0.2130
S	 0.6790	 0.1710
T	 0.7500	 0.1980
U	 0.4780	 0.0850
V	 0.7250	 0.1900
W	 0.7450	 0.1040
Y	 0.8220	 0.1020
Z	 0.8220	 0.1240
a	 0.7940	 0.1260
b	 0.8460	 0.1190
c	 0.8550	 0.0580
d	 0.7930	 0.1080
e	 0.6190	 0.1080
f	 0.6110	 0.1430
g	 0.5360	 0.1410
h	 0.6050	 0.1370
i	 0.6680	 0.1390
j	 0.6030	 0.0970
k	 0.6010	 0.1320
l	 0.8490	 0.1710
m	 0.8330	 0.1610
n	 0.8200	 0.0880
o	 0.9240	 0.1520
p	 0.8530	 0.2180
q	 0.9290	 0.2520
r	 0.8680	 0.0510

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Chain	Atom inclusion	Q-score
s	 0.2350	 0.0630
t	 0.7940	 0.1680
u	 0.9550	 0.2290
v	 0.9170	 0.2780
w	 0.8150	 0.1910
x	 0.7830	 0.1550
y	 0.4080	 0.0650
z	 0.4340	 0.0440