



wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 12:31 AM JST

PDB ID : 5GPN
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

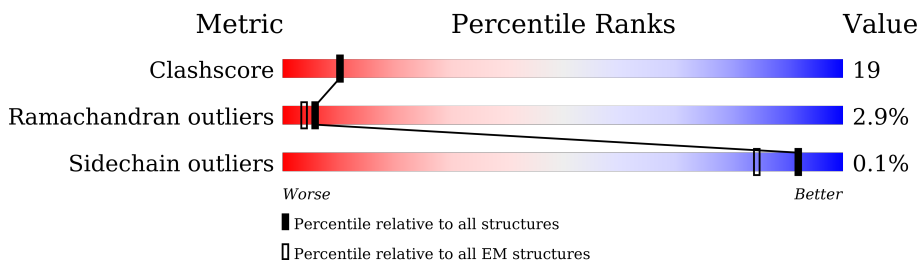
1 Overall quality at a glance i

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)
Clashscore	210492	15764
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	A	446	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">16%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">70%</div> <div style="text-align: center;">24%</div> <div style="text-align: center;">6%</div> </div>
1	M	446	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">68%</div> <div style="text-align: center;">28%</div> <div style="text-align: center;">•</div> </div>
2	B	439	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">22%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">73%</div> <div style="text-align: center;">20%</div> <div style="text-align: center;">• 5%</div> </div>
2	N	439	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">8%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">73%</div> <div style="text-align: center;">21%</div> <div style="text-align: center;">• 5%</div> </div>
3	C	379	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">72%</div> <div style="text-align: center;">25%</div> <div style="text-align: center;">• •</div> </div>
3	O	379	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">33%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">76%</div> <div style="text-align: center;">22%</div> <div style="text-align: center;">•</div> </div>
4	D	241	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">79%</div> <div style="text-align: center;">17%</div> <div style="text-align: center;">•</div> </div>
4	P	241	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">20%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="text-align: center;">73%</div> <div style="text-align: center;">24%</div> <div style="text-align: center;">•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	274	13% 63% 8% 28%
5	Q	274	24% 50% 19% 28%
6	F	110	10% 75% 17% ..
6	R	110	33% 83% 12% ..
7	G	81	15% 62% 32% 6%
7	S	81	28% 78% 16% ..
8	H	78	10% 68% 14% 18%
8	T	78	21% 72% 9% 18%
9	I	78	19% 29% 10% 58%
9	U	78	23% 22% 17% 58%
10	J	62	21% 74% 21% 5%
10	L	62	37% 66% 26% 8%
11	K	56	25% 62% 14% 23%
11	V	56	18% 57% 9% 34%
12	W	264	8% 31% 31% 36%
13	Y	727	9% 44% 46% 8%
14	Z	463	. 42% 38% 19%
15	a	216	. 64% 32%
16	b	212	. 70% 30%
17	c	464	8% 86% 12%
18	d	249	9% 66% 32%
19	e	318	23% 98% ..
20	f	347	18% 99% .
21	g	115	27% 91% 8%
22	h	459	20% 97% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	i	98	9% 90% 8%
24	j	606	27% 95% ..
25	k	175	19% 79% 19%
25	l	175	8% 91%
26	m	84	11% 62% 37%
27	n	99	13% 83% 16%
28	o	106	44% 52%
29	p	377	8% 80% 17%
30	q	357	53% 45%
30	v	357	14% 86%
31	r	144	7% 44% 56%
32	Aa	156	21% 50% 48%
32	t	156	9% 51% 48%
33	Ai	189	18% 82%
33	u	189	29% 71%
34	w	175	9% 60% 39%
35	x	123	8% 36% 63%
36	0	261	78% 100%
37	1	147	67% 96% ..
38	2	109	80% 100%
39	3	98	74% 92% 7%
40	4	84	96% 88% 10%
41	5	85	71% 87% 12%
42	6	73	100% 100%
43	7	59	92% 92% 5%

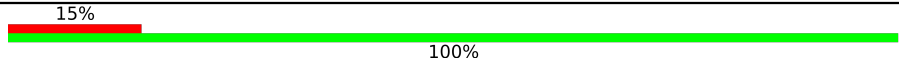
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
44	8	56	75% 88% 12%
45	9	47	91% 100%
46	s	46	74% 93% 7%
47	y	514	59% 99%
48	z	227	57% 99%
49	Ab	134	13% 96%
49	Ah	134	10% 79% 21%
50	Ac	70	13% 76% 21%
51	Ad	43	16% 100%
51	Ao	43	23% 95% 5%
51	Ap	43	9% 81% 19%
51	Av	43	19% 91% 9%
52	Ae	116	19% 74% 24%
53	Af	128	68% 30%
54	Ag	141	28% 87% 6% 7%
55	Aj	176	72% 24%
56	Ak	178	13% 80% 15%
57	Al	122	6% 75% 21%
58	Am	76	36% 64%
59	An	172	9% 55% 44%
60	Aq	76	20% 88% 12%
60	As	76	24% 86% 14%
60	Aw	76	5% 100%
61	Ar	34	12% 100%
62	At	17	47% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
63	Au	13	 15% 100%

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	-

2 Entry composition [i](#)

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
			Total	C	N	O		
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
			Total	C	N	O		
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
			Total	C	N	O		
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
			Total	C	N	O		
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		

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O		
36	0	261	1284	762	261	261	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O		
50	Ac	55	271	161	55	55	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

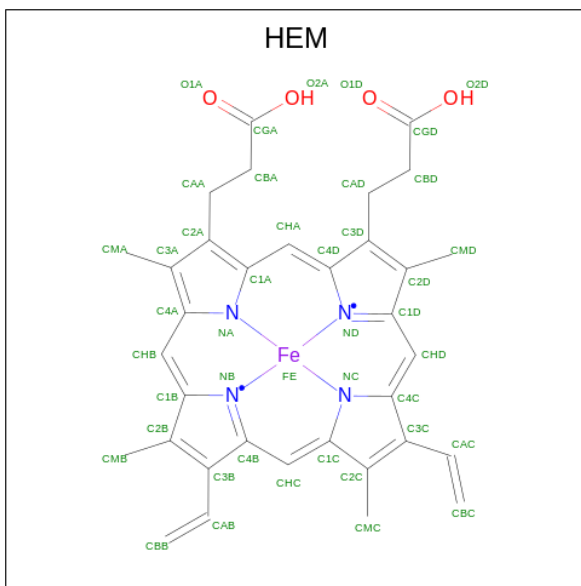
- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

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.

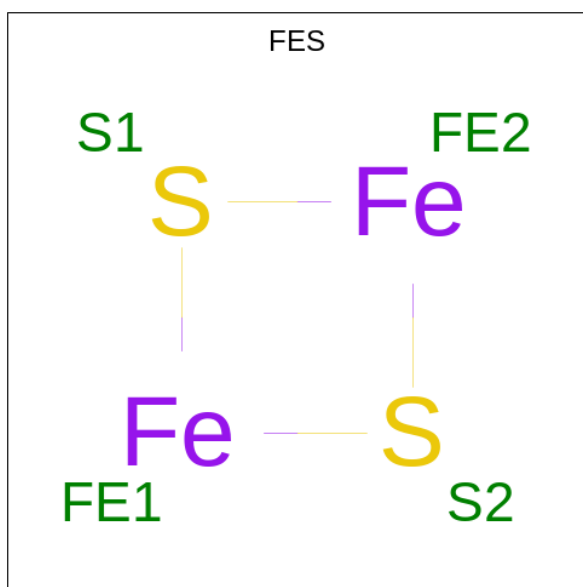
Mol	Chain	Residues	Atoms				AltConf	Trace
63	Au	13	Total	C	N	O	0	0
			62	36	13	13		

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



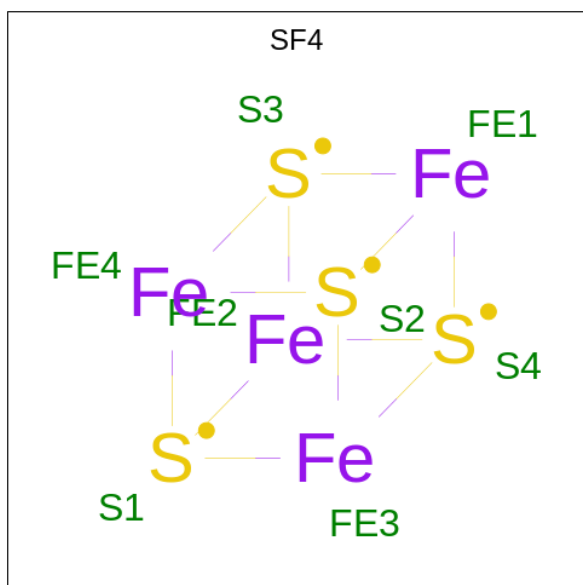
Mol	Chain	Residues	Atoms					AltConf
64	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
64	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
64	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...



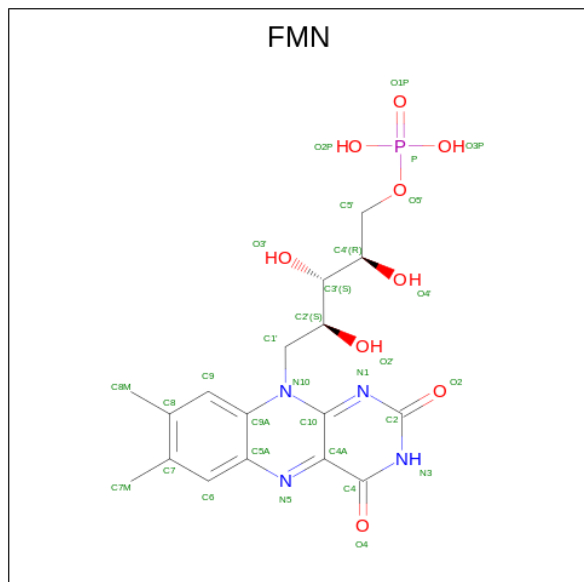
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
66	E	1	4	2	2	0
66	Q	1	4	2	2	0
66	Y	1	4	2	2	0
66	d	1	4	2	2	0

- Molecule 67 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



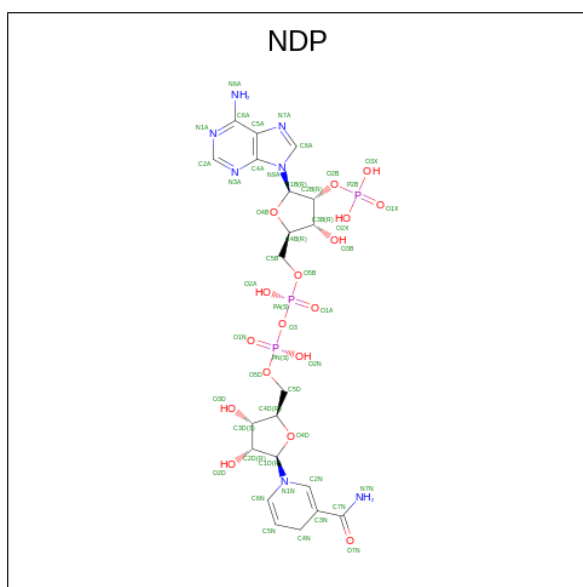
Mol	Chain	Residues	Atoms			AltConf
67	Y	1	Total	Fe	S	0
			8	4	4	
67	Y	1	Total	Fe	S	0
			8	4	4	
67	a	1	Total	Fe	S	0
			8	4	4	
67	b	1	Total	Fe	S	0
			8	4	4	
67	b	1	Total	Fe	S	0
			8	4	4	
67	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 68 is FLAVIN MONONUCLEOTIDE (three-letter code: 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 (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

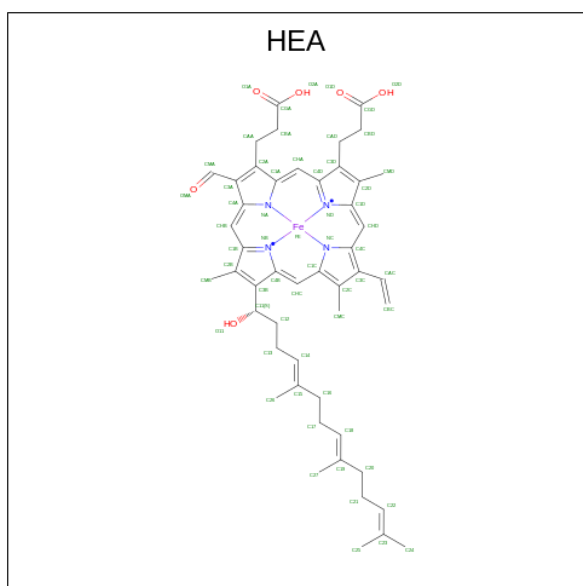


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	p	1	48	21	7	17	3	0

- Molecule 70 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 71 is HEME-A (three-letter code: 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 (three-letter code: CU) (formula: Cu).

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

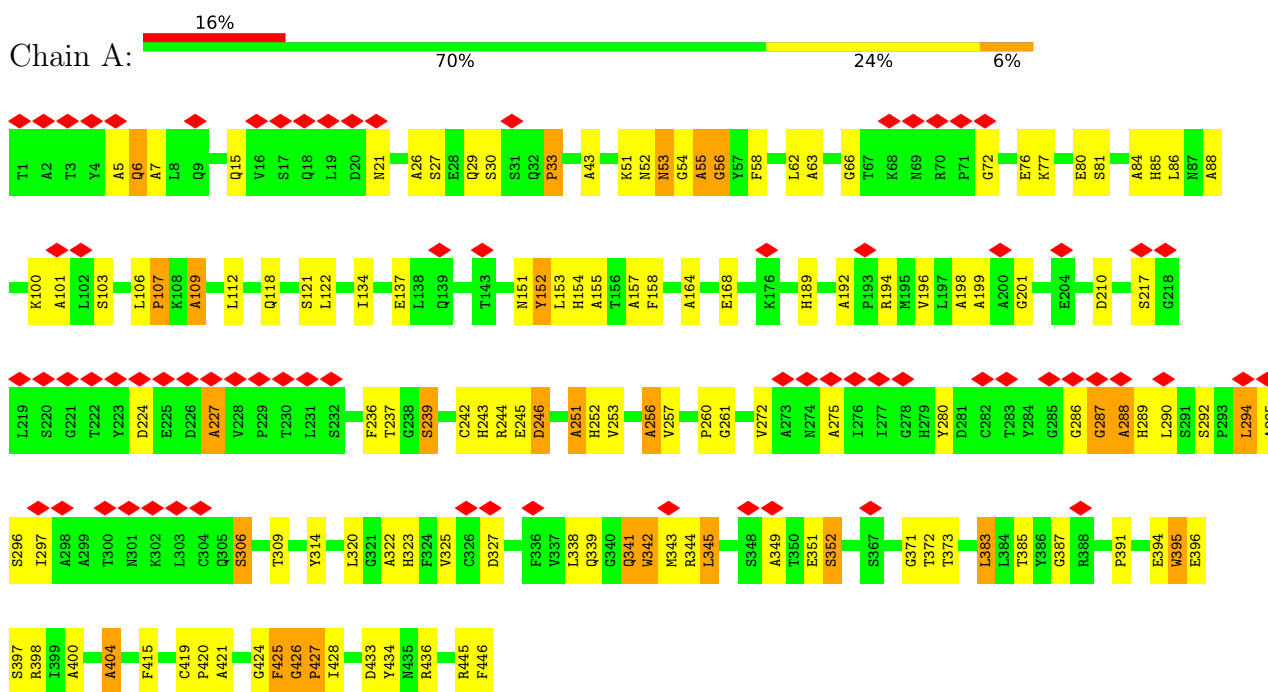
- Molecule 73 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

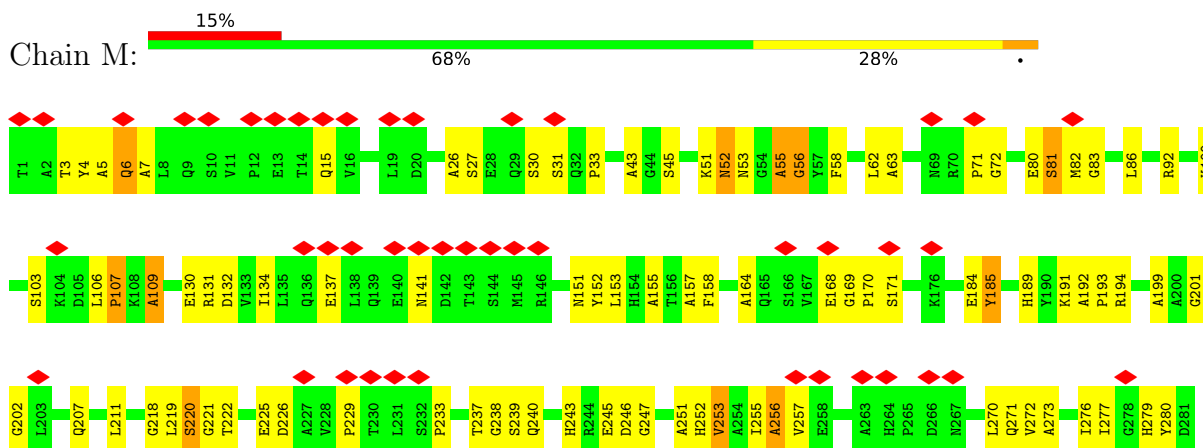
3 Residue-property plots [i](#)

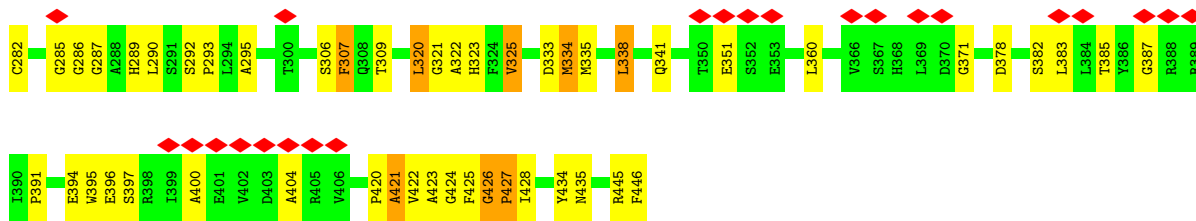
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

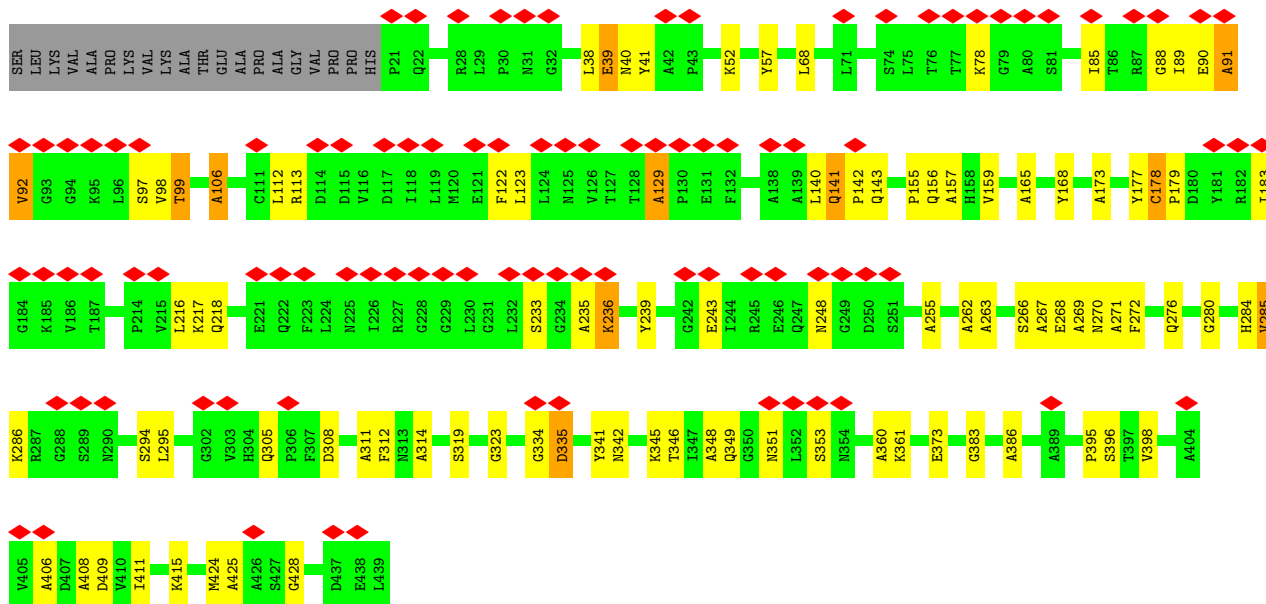


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

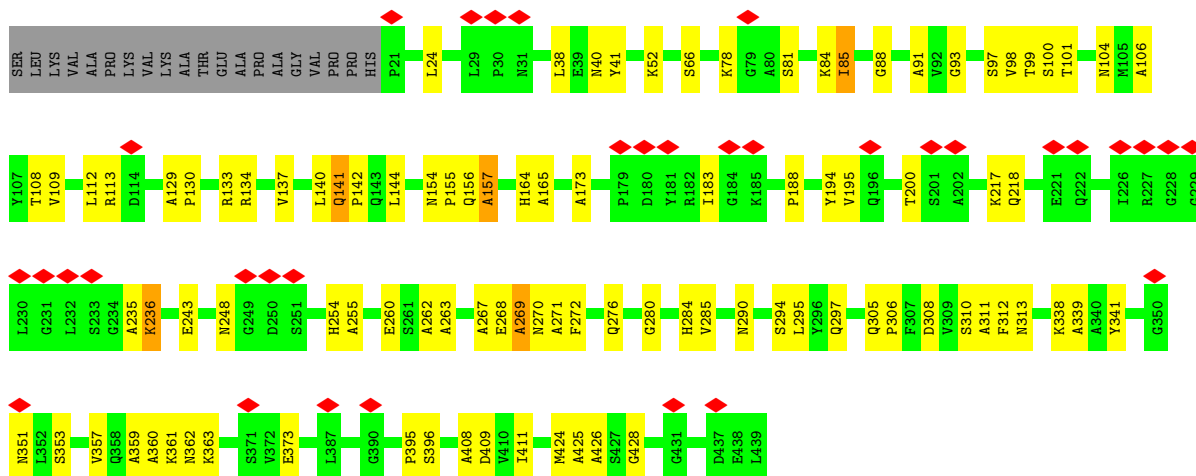




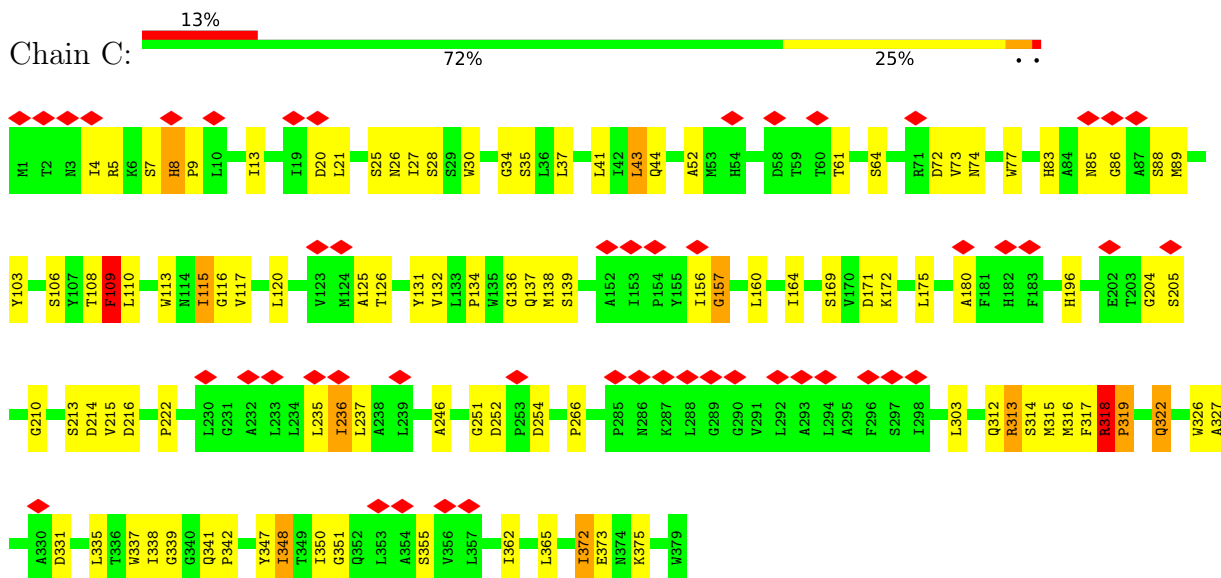
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



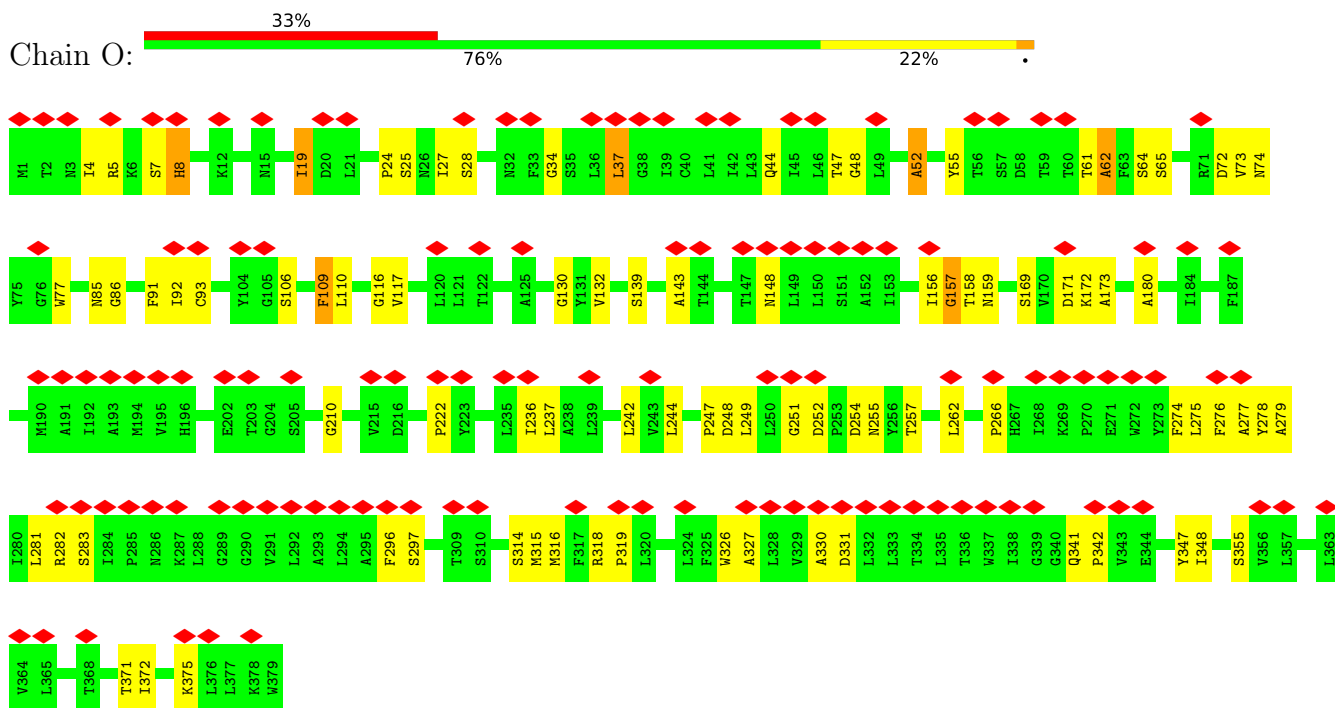
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



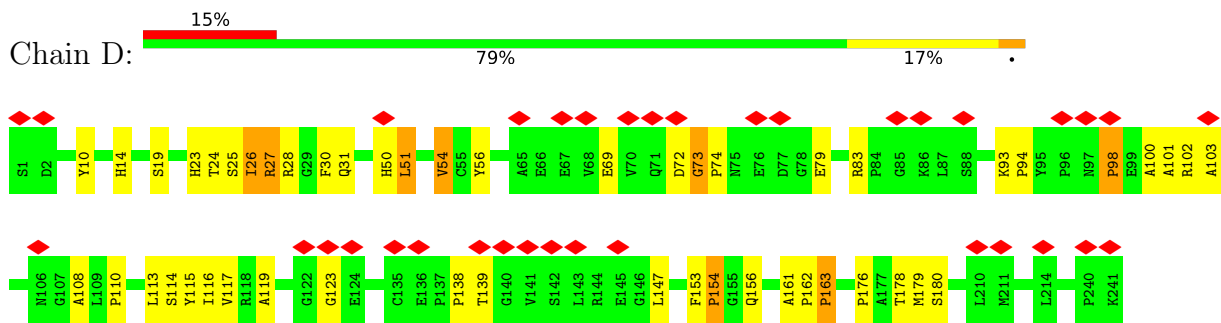
• Molecule 3: Cytochrome b



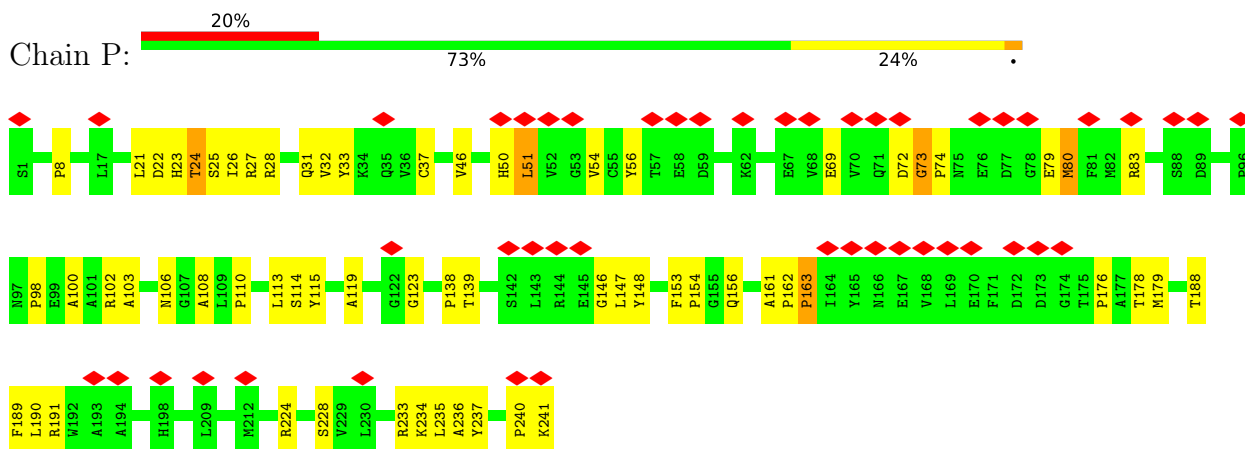
• Molecule 3: Cytochrome b



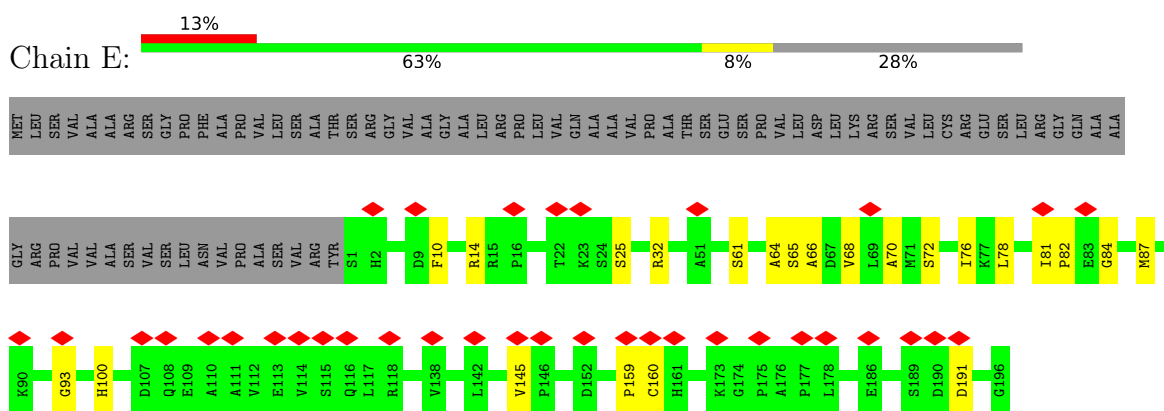
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



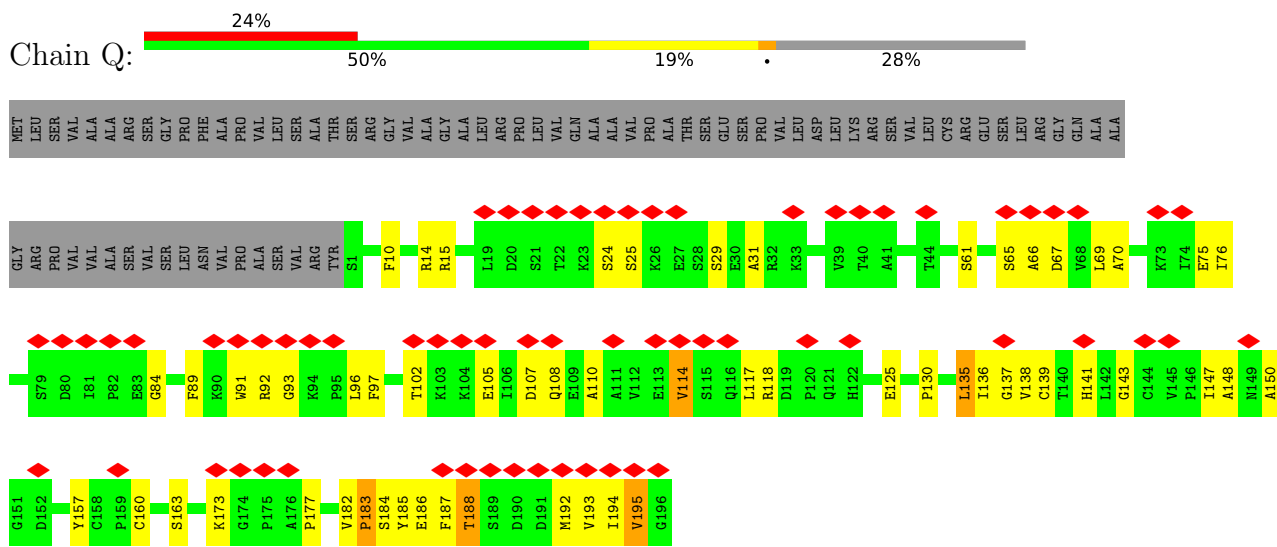
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



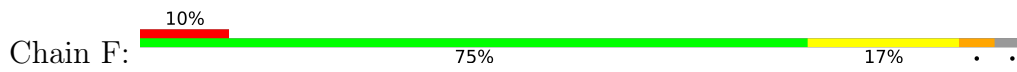
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

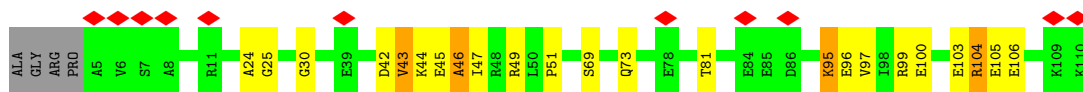


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

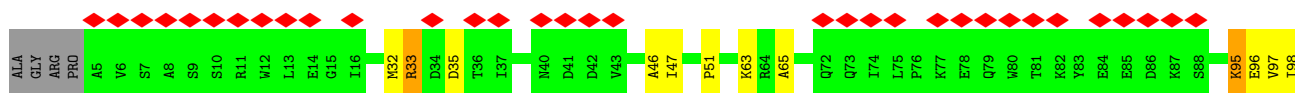
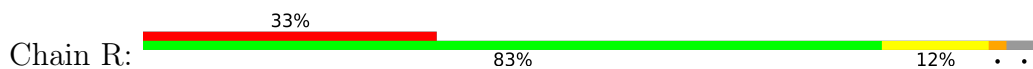


• Molecule 6: Cytochrome b-c1 complex subunit 7

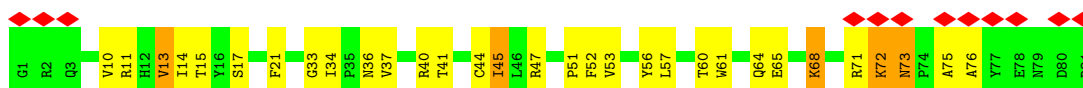




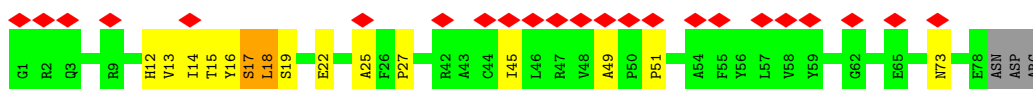
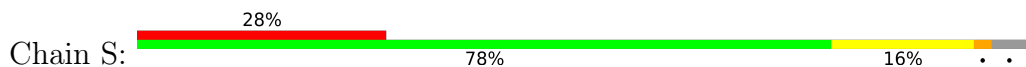
• Molecule 6: Cytochrome b-c1 complex subunit 7



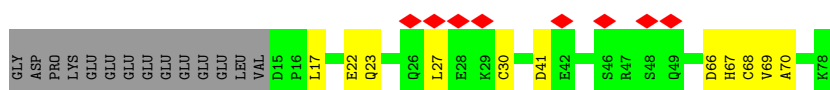
• Molecule 7: Cytochrome b-c1 complex subunit 8



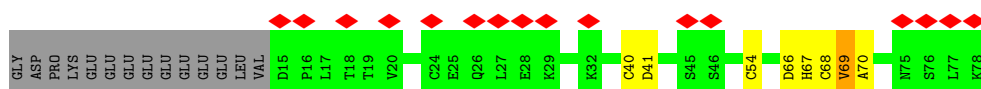
• Molecule 7: Cytochrome b-c1 complex subunit 8



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

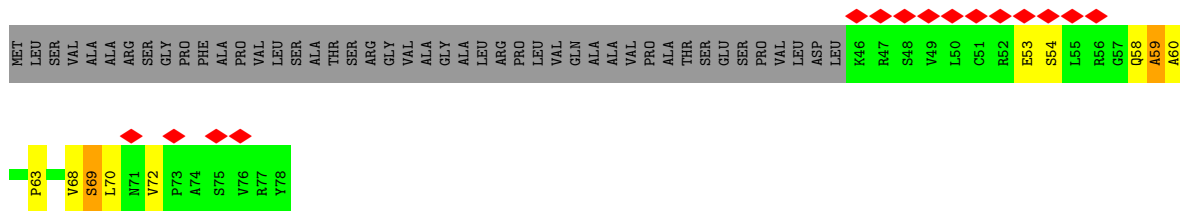


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

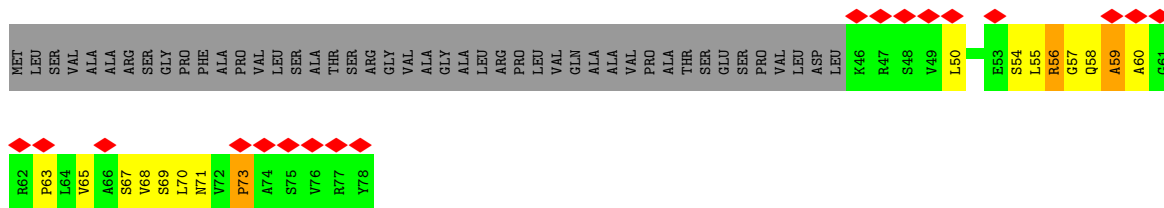


• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

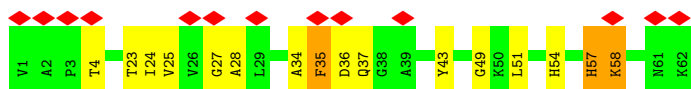
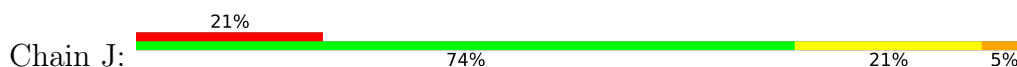




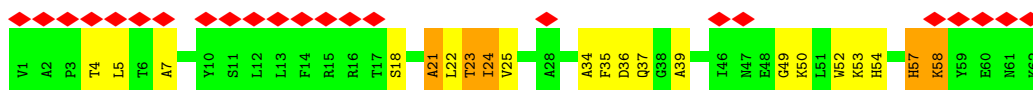
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



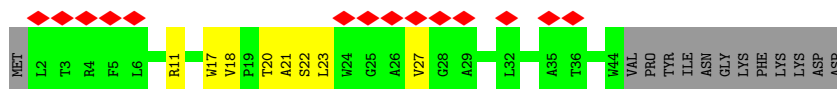
• Molecule 10: Cytochrome b-c1 complex subunit 9



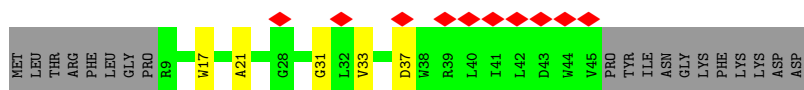
• Molecule 10: Cytochrome b-c1 complex subunit 9



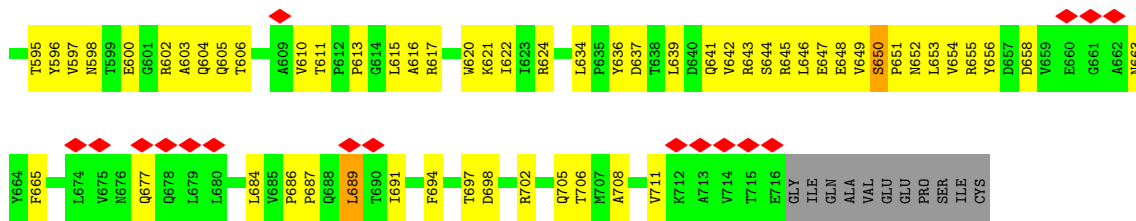
• Molecule 11: Cytochrome b-c1 complex subunit 10



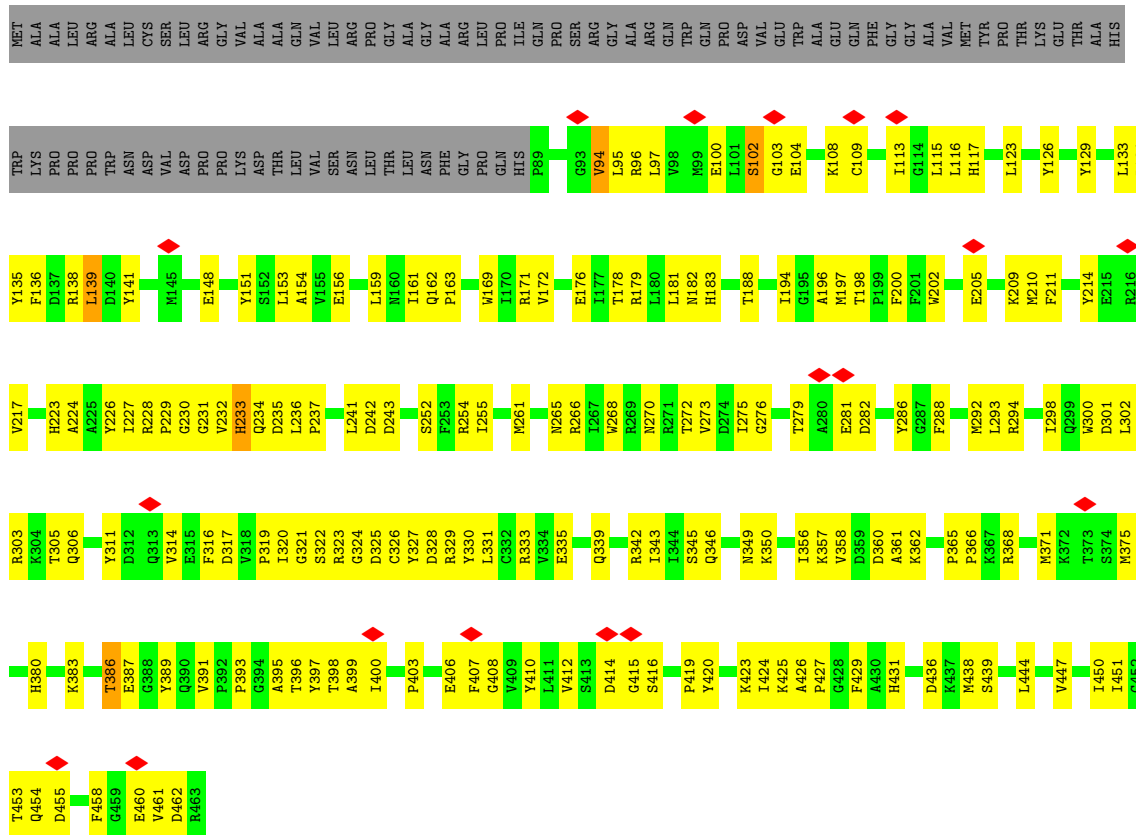
• Molecule 11: Cytochrome b-c1 complex subunit 10



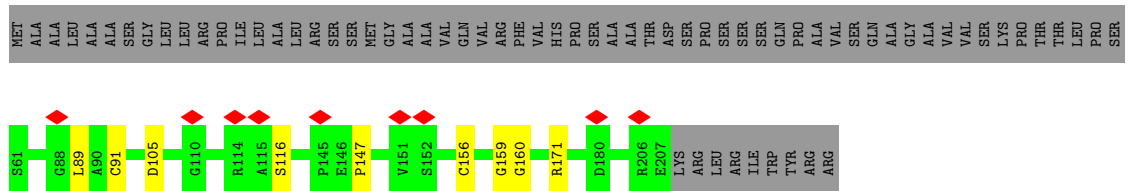
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3



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

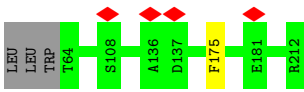
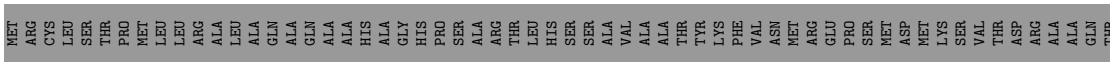


• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7

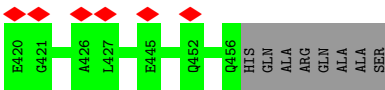
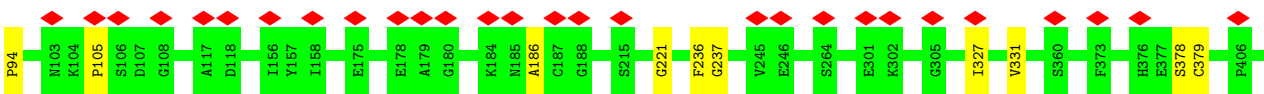
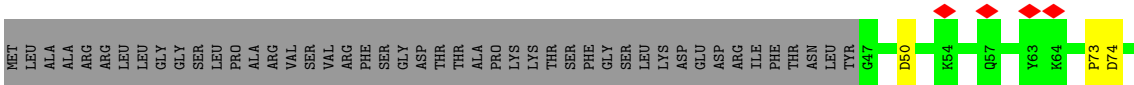
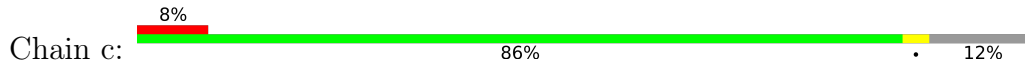


• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8

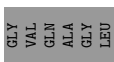
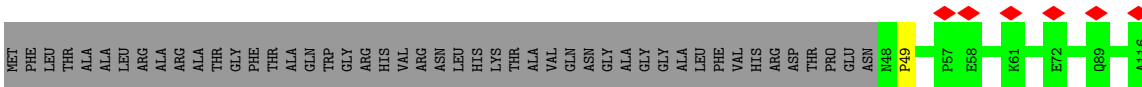




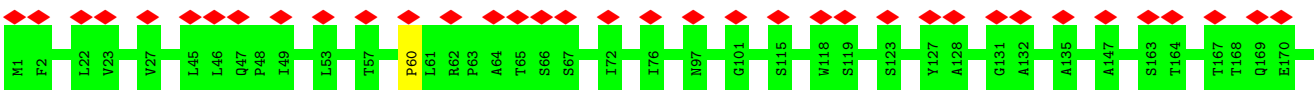
- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



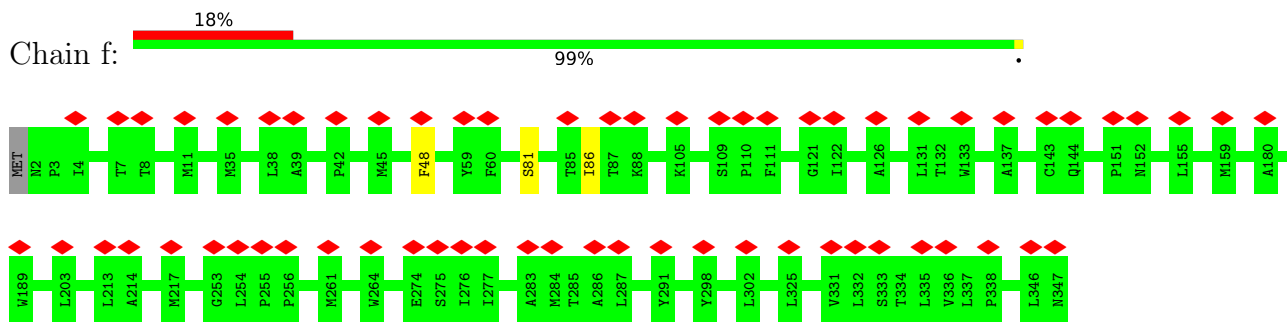
- Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



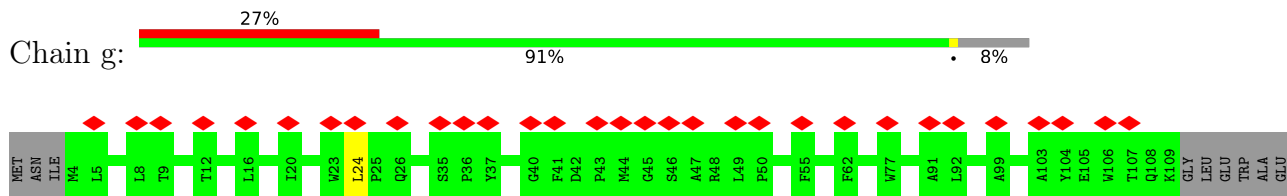
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1



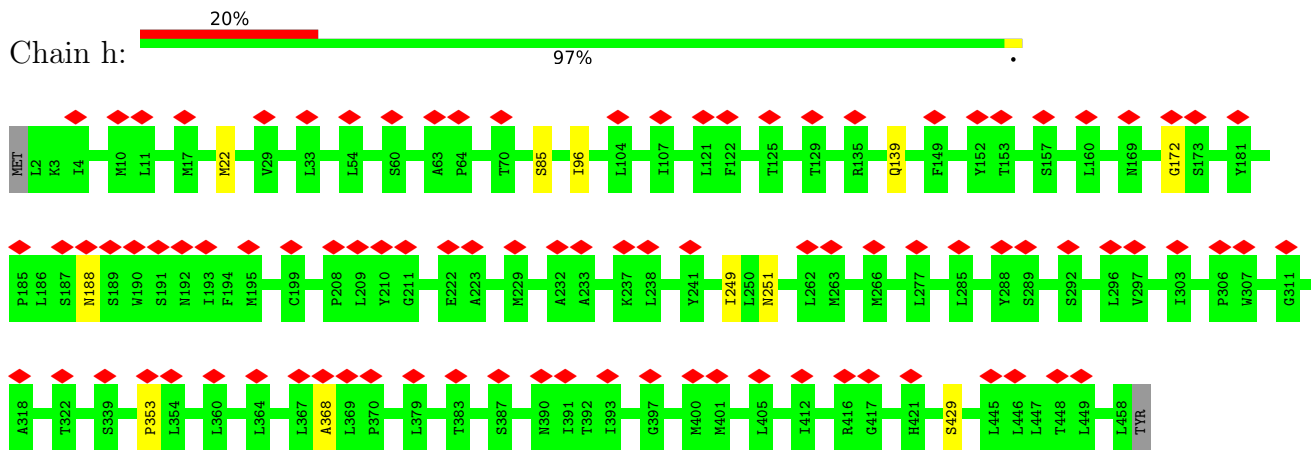
- Molecule 20: NADH-ubiquinone oxidoreductase chain 2



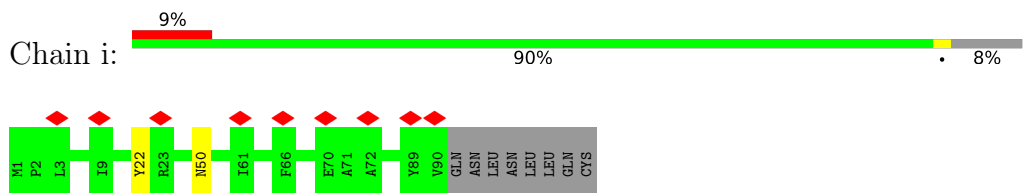
• Molecule 21: NADH-ubiquinone oxidoreductase chain 3



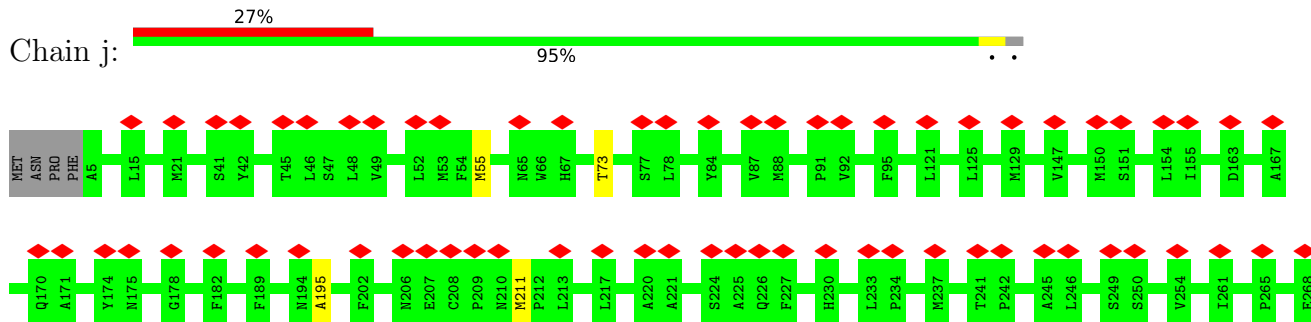
• Molecule 22: NADH-ubiquinone oxidoreductase chain 4

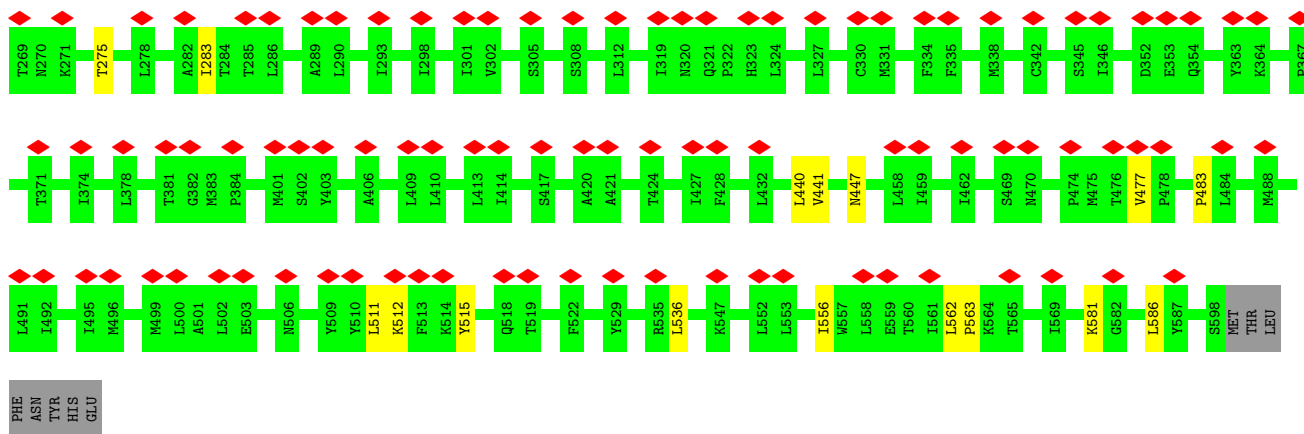


• Molecule 23: NADH-ubiquinone oxidoreductase chain 4L

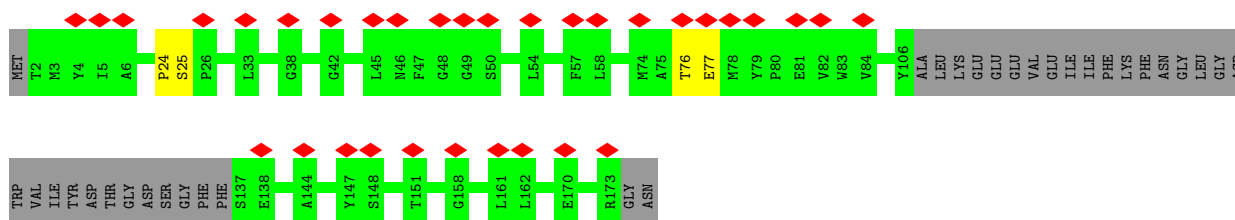
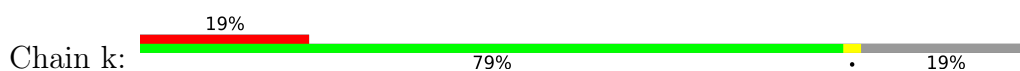


• Molecule 24: NADH-ubiquinone oxidoreductase chain 5

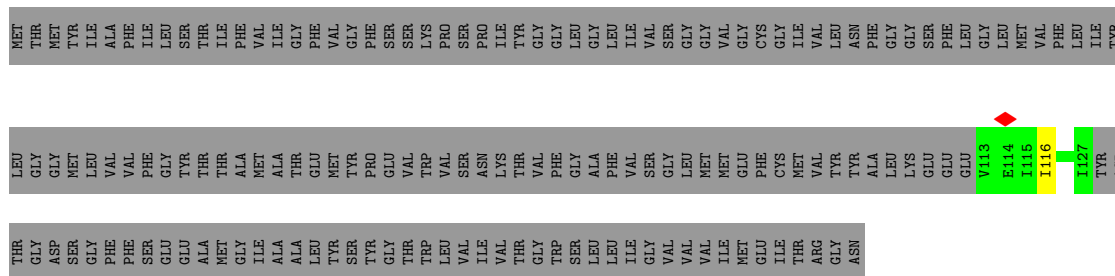




• Molecule 25: NADH-ubiquinone oxidoreductase chain 6



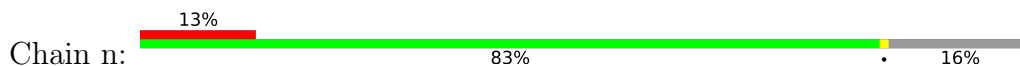
• Molecule 25: NADH-ubiquinone oxidoreductase chain 6

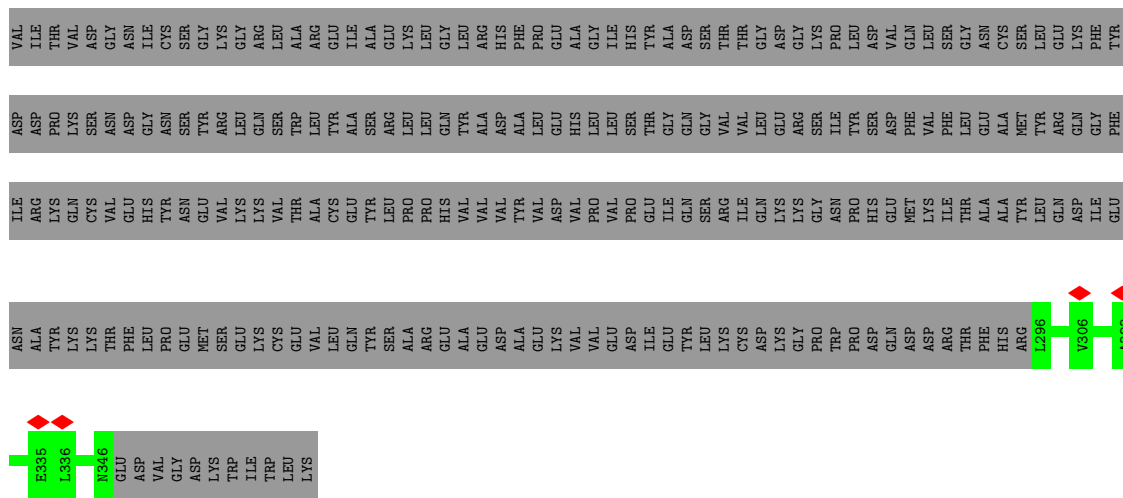


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

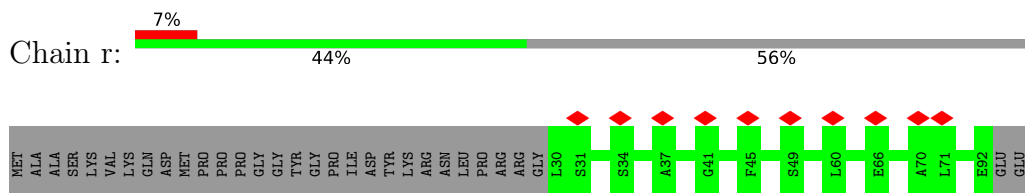


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

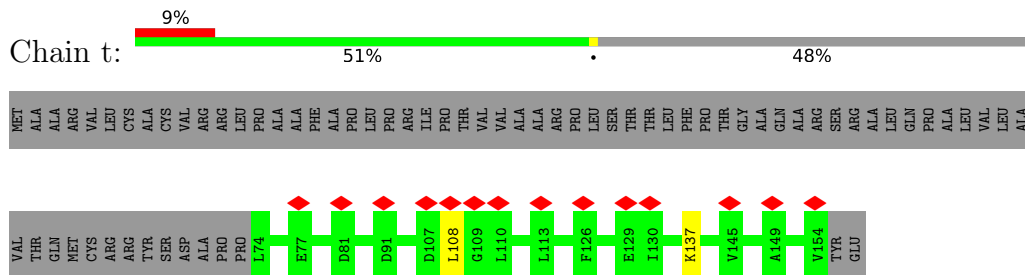




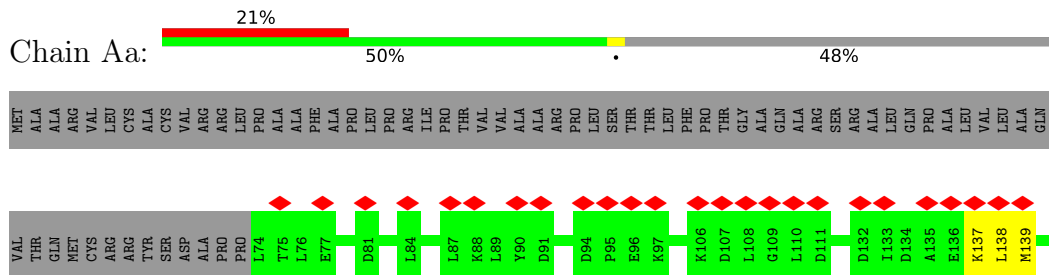
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 32: Acyl carrier protein

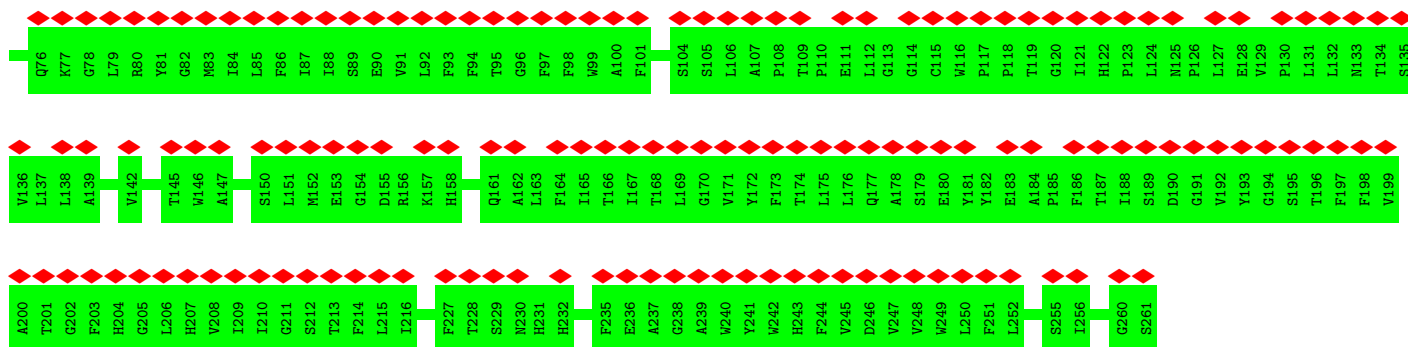


- Molecule 32: Acyl carrier protein

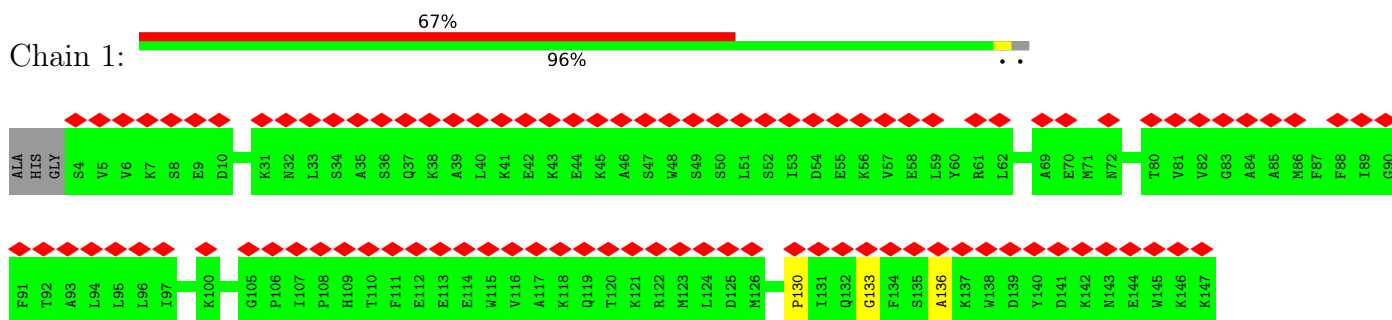


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5

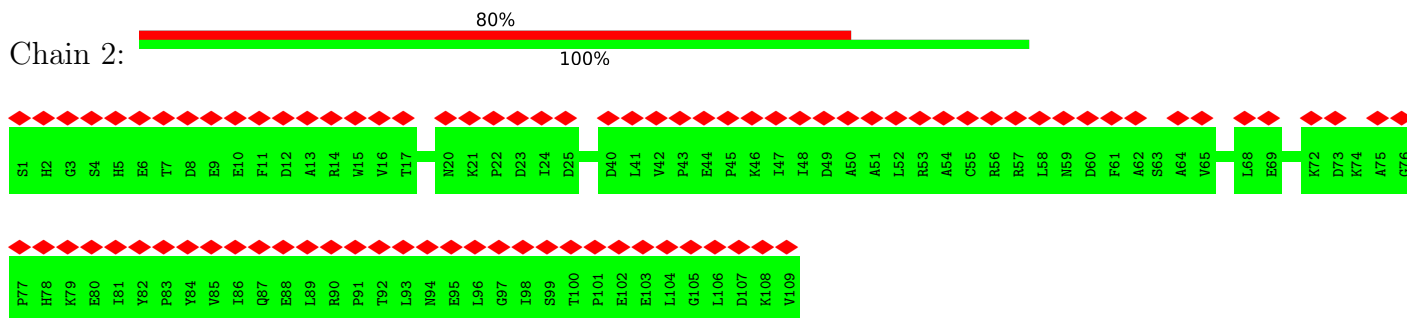




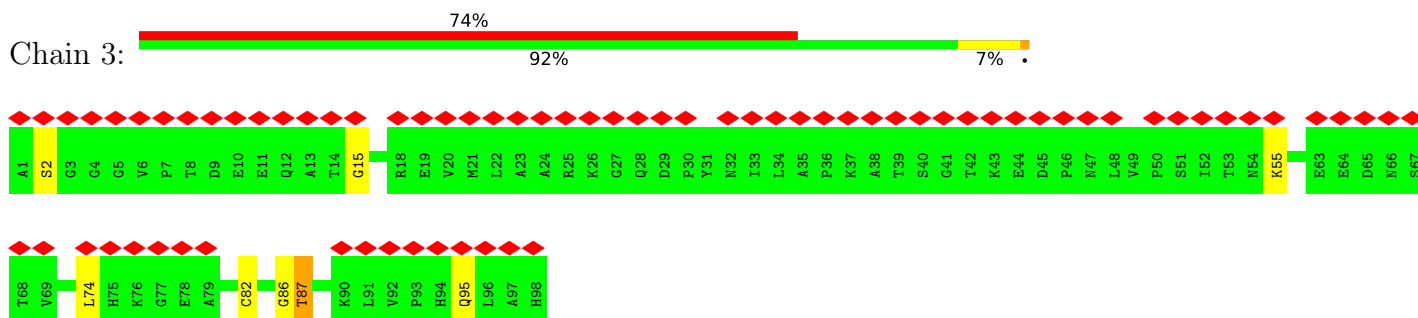
- Molecule 37: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



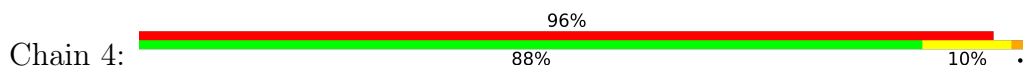
- Molecule 38: Cytochrome c oxidase subunit 5A, mitochondrial

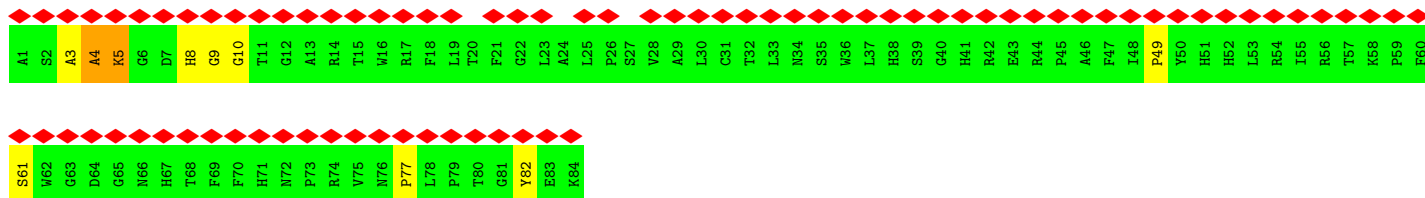


- Molecule 39: Cytochrome c oxidase subunit 5B, mitochondrial

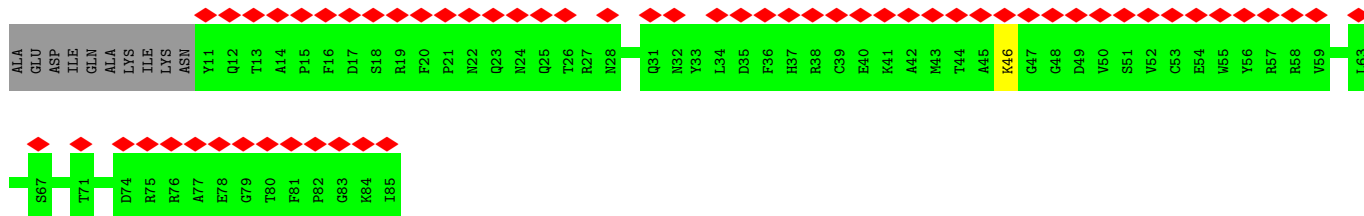
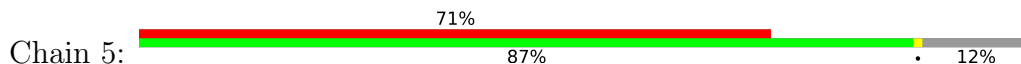


- Molecule 40: Cytochrome c oxidase subunit 6A2, mitochondrial

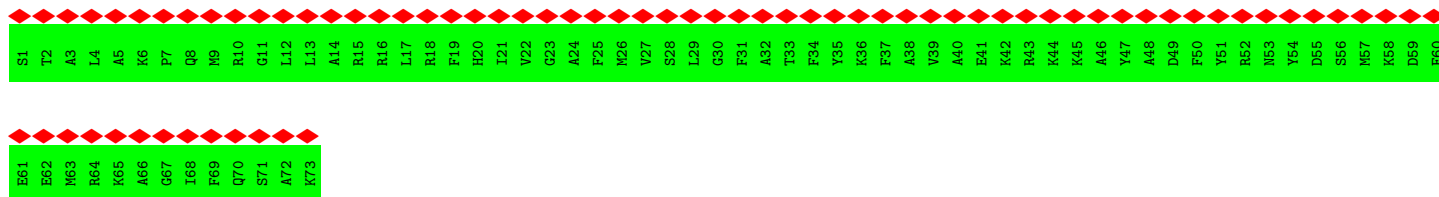




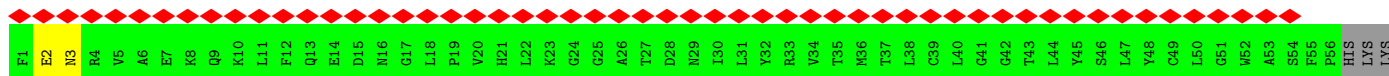
• Molecule 41: Cytochrome c oxidase subunit 6B1



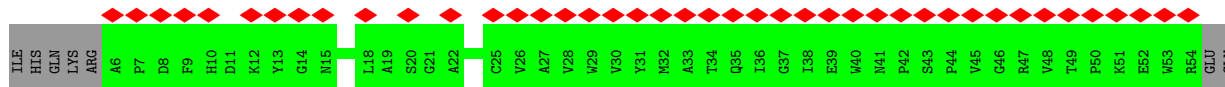
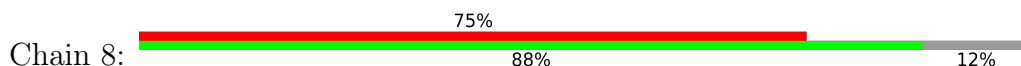
• Molecule 42: Cytochrome c oxidase subunit 6C



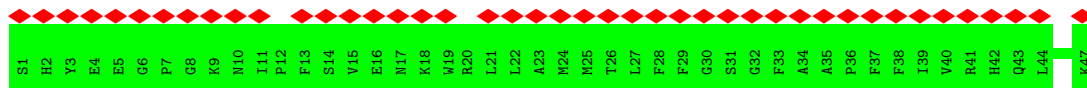
• Molecule 43: Cytochrome c oxidase subunit 7A1, mitochondrial



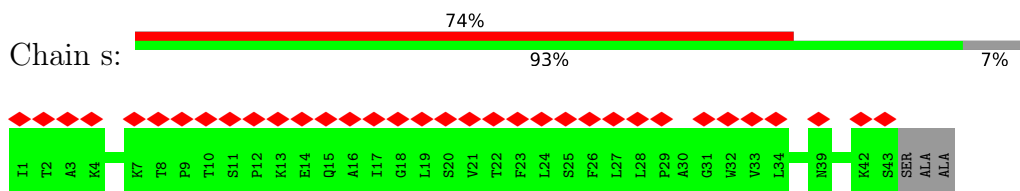
• Molecule 44: Cytochrome c oxidase subunit 7B, mitochondrial



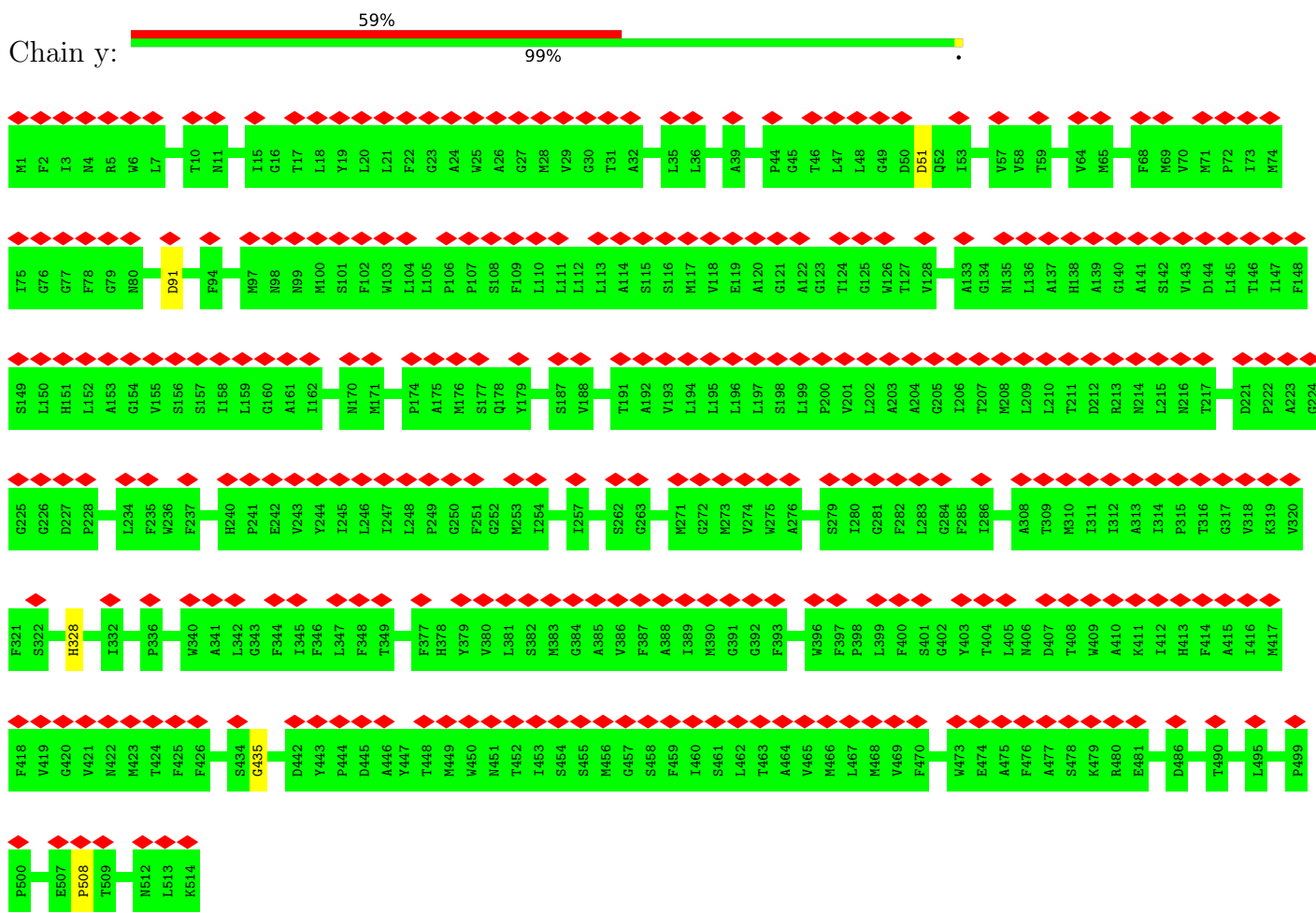
• Molecule 45: Cytochrome c oxidase subunit 7C, mitochondrial



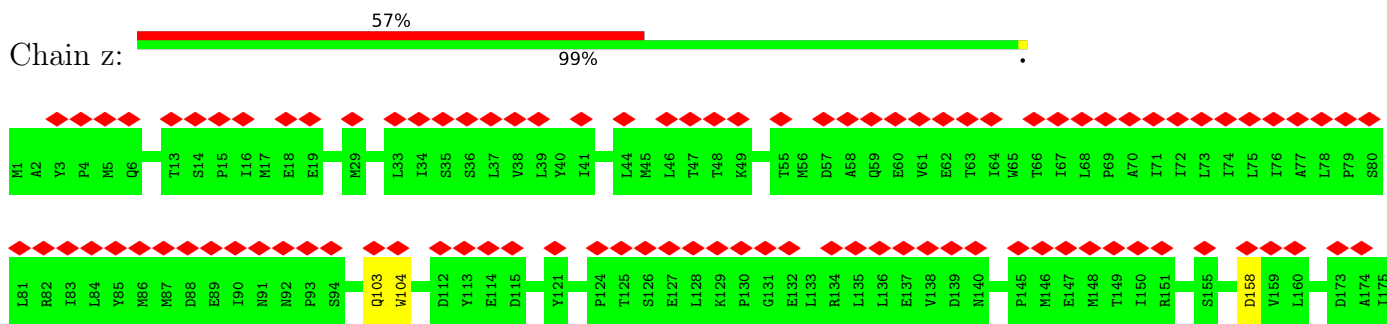
- Molecule 46: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 47: Cytochrome c oxidase subunit 1

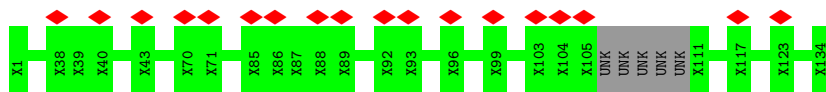


- Molecule 48: Cytochrome c oxidase subunit 2

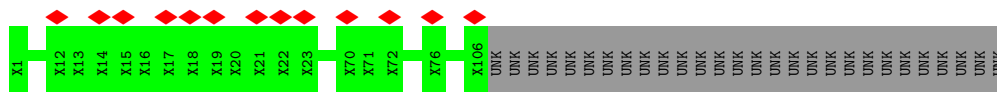
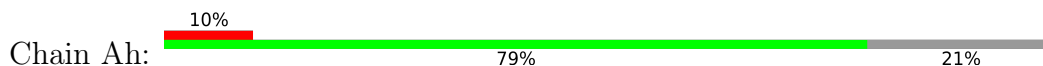




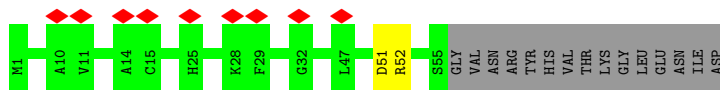
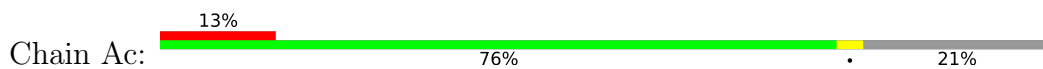
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



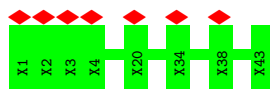
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



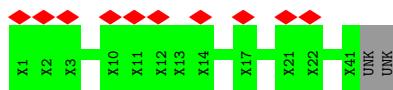
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



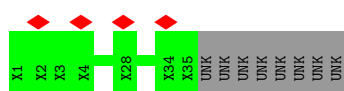
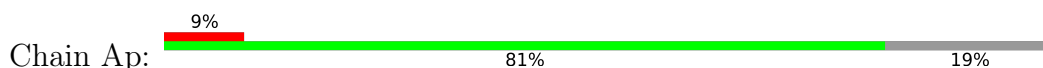
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



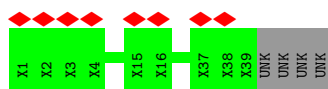
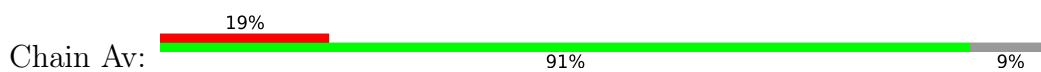
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



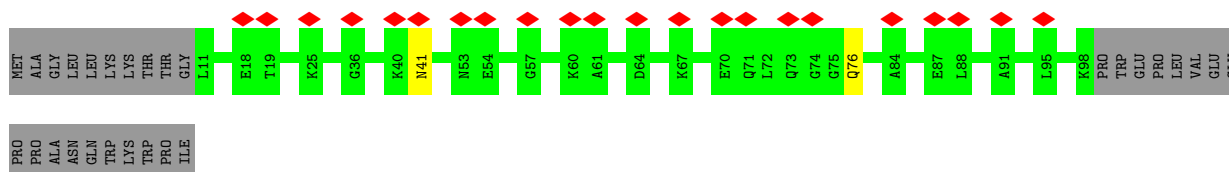
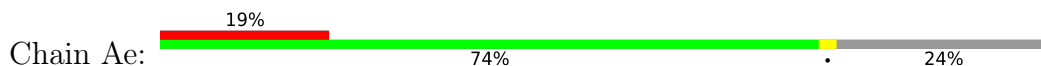
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



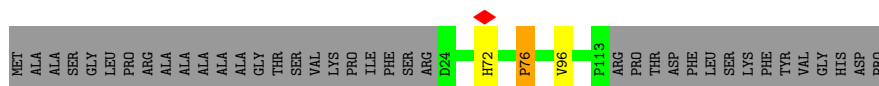
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



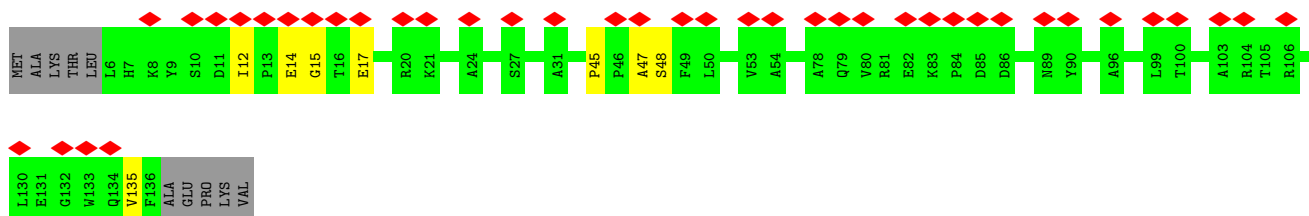
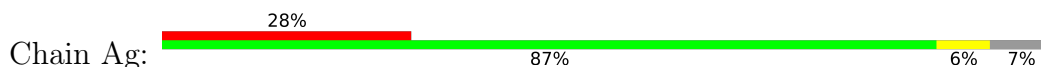
- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



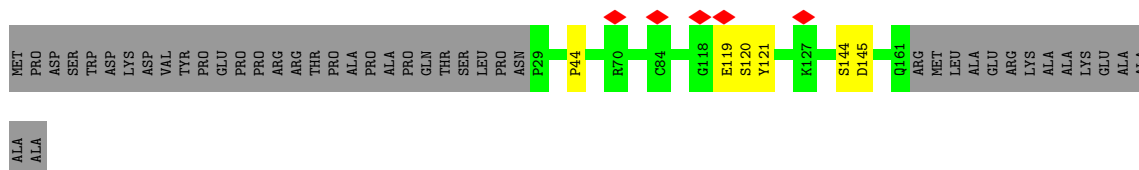
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



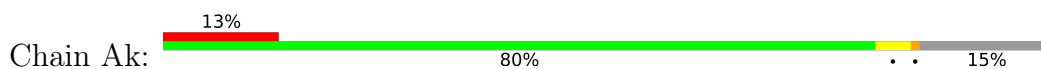
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

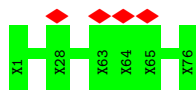


- Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

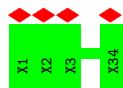


- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

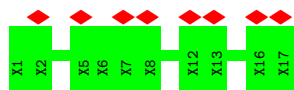




- Molecule 61: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



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



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



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 i

5.1 Standard geometry i

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

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	0.61	0/2197	1.43	13/3055 (0.4%)
1	M	0.66	2/2197 (0.1%)	1.48	17/3055 (0.6%)
2	B	0.53	0/2060	1.33	8/2862 (0.3%)
2	N	0.51	0/2060	1.28	3/2862 (0.1%)
3	C	0.70	1/1869 (0.1%)	1.57	15/2600 (0.6%)
3	O	0.69	1/1869 (0.1%)	1.49	12/2600 (0.5%)
4	D	0.49	0/1187	1.12	0/1650
4	P	0.48	0/1187	1.07	0/1650
5	E	0.27	0/966	0.70	0/1343
5	Q	0.51	0/965	1.27	3/1341 (0.2%)
6	F	0.52	0/526	1.17	2/733 (0.3%)
6	R	0.56	0/526	1.22	3/733 (0.4%)
7	G	0.61	0/400	1.35	2/556 (0.4%)
7	S	0.52	0/385	0.96	0/535
8	H	0.45	0/319	1.04	0/445
8	T	0.42	0/319	0.96	0/445
9	I	0.52	0/162	1.32	1/224 (0.4%)
9	U	0.42	0/162	1.08	0/224
10	J	0.48	0/306	1.18	0/425
10	L	0.50	0/306	1.24	2/425 (0.5%)
11	K	0.23	0/210	0.52	0/290
11	V	0.21	0/181	0.51	0/250
12	W	0.46	0/1401	0.66	0/1906
13	Y	0.43	0/5077	0.61	3/6888 (0.0%)
14	Z	0.61	0/3075	0.64	0/4155
15	a	0.70	0/1174	0.65	0/1591
16	b	0.65	0/1215	0.62	0/1644
17	c	0.37	0/3196	0.56	0/4323
18	d	0.39	0/1353	0.58	1/1841 (0.1%)
19	e	0.57	0/2558	0.68	0/3497
20	f	0.63	0/2761	0.70	0/3754
21	g	0.51	0/850	0.60	0/1163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	h	0.59	0/3700	0.70	0/5045
23	i	0.62	0/687	0.71	0/931
24	j	0.50	0/4831	0.63	1/6572 (0.0%)
25	k	0.59	0/1084	0.64	0/1470
25	l	0.41	0/72	0.59	0/98
26	m	0.44	0/262	0.58	0/364
27	n	0.32	0/410	0.57	0/570
28	o	0.50	0/250	0.63	0/346
29	p	0.34	0/1545	0.55	0/2147
30	q	0.38	0/966	0.61	1/1343 (0.1%)
30	v	0.45	0/251	0.61	0/348
31	r	0.48	0/310	0.62	0/430
32	Aa	0.32	0/402	0.52	0/560
32	t	0.44	0/402	0.57	0/560
33	Ai	0.52	0/166	0.60	0/229
33	u	0.57	0/266	0.60	0/369
34	w	0.39	0/529	0.59	0/736
35	x	0.39	0/220	0.56	0/301
36	0	0.50	0/1283	0.70	0/1782
37	1	0.51	0/715	0.67	1/997 (0.1%)
38	2	0.47	0/538	0.62	0/748
39	3	0.52	0/480	0.80	0/665
40	4	0.50	0/410	0.78	1/567 (0.2%)
41	5	0.49	0/370	0.77	0/514
42	6	0.51	0/360	0.65	0/500
43	7	0.51	0/273	0.78	0/377
44	8	0.51	0/240	0.69	0/332
45	9	0.52	0/230	0.64	0/318
46	s	0.49	0/212	0.61	0/294
47	y	0.52	0/2522	0.76	1/3501 (0.0%)
48	z	0.56	0/1126	0.81	0/1570
50	Ac	0.50	0/270	0.56	0/374
52	Ae	0.38	0/434	0.58	0/603
53	Af	0.40	0/447	0.66	1/623 (0.2%)
54	Ag	0.45	0/636	0.62	0/878
55	Aj	0.51	0/662	0.61	1/924 (0.1%)
56	Ak	0.48	0/749	0.69	3/1044 (0.3%)
57	Al	0.48	0/472	0.65	0/655
58	Am	0.48	0/133	0.54	0/184
59	An	0.44	0/481	0.60	0/670
All	All	0.53	4/72415 (0.0%)	0.89	95/99604 (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
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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	253	VAL	C-O	6.79	1.36	1.23
1	M	169	GLY	N-CA	-6.51	1.36	1.46
3	C	318	ARG	C-N	-5.57	1.23	1.34
3	O	37	LEU	C-N	-5.02	1.24	1.33

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	253	VAL	O-C-N	-14.87	98.92	122.70
1	M	256	ALA	CB-CA-C	-11.05	93.52	110.10
1	M	168	GLU	C-N-CA	10.51	144.36	122.30
1	M	253	VAL	CA-C-O	8.21	137.34	120.10
3	C	204	GLY	C-N-CA	8.16	142.10	121.70

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	96	0
1	M	2198	0	1039	102	0
2	B	2061	0	1028	61	0
2	N	2061	0	1028	90	0
3	C	1870	0	843	101	0
3	O	1870	0	843	63	0
4	D	1188	0	533	33	0
4	P	1188	0	533	59	0
5	E	967	0	441	34	0
5	Q	966	0	440	40	0
6	F	527	0	232	18	0
6	R	527	0	232	7	0
7	G	401	0	180	21	0
7	S	386	0	174	30	0
8	H	320	0	135	7	0
8	T	320	0	135	7	0
9	I	163	0	77	8	0
9	U	163	0	77	28	0
10	J	307	0	149	9	0
10	L	307	0	149	17	0
11	K	211	0	102	9	0
11	V	182	0	90	6	0
12	W	1366	0	1316	79	0
13	Y	4998	0	4891	336	0
14	Z	3003	0	2971	145	0
15	a	1146	0	1143	0	0
16	b	1189	0	1144	0	0
17	c	3125	0	3087	0	0
18	d	1324	0	1338	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	e	2486	0	2587	0	0
20	f	2698	0	2851	0	0
21	g	829	0	863	0	0
22	h	3610	0	3816	0	0
23	i	677	0	726	0	0
24	j	4705	0	4848	0	0
25	k	1059	0	1077	0	0
25	l	73	0	31	0	0
26	m	263	0	125	0	0
27	n	411	0	177	0	0
28	o	251	0	115	0	0
29	p	1546	0	688	0	0
30	q	967	0	431	0	0
30	v	252	0	103	0	0
31	r	311	0	140	0	0
32	Aa	403	0	172	0	0
32	t	403	0	172	0	0
33	Ai	167	0	72	0	0
33	u	267	0	123	0	0
34	w	530	0	230	0	0
35	x	221	0	101	0	0
36	0	1284	0	575	0	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	0	0
45	9	231	0	106	0	0
46	s	213	0	98	0	0
47	y	2523	0	1169	0	0
48	z	1127	0	475	0	0
49	Ab	637	0	132	0	0
49	Ah	526	0	107	0	0
50	Ac	271	0	132	0	0
51	Ad	211	0	42	0	0
51	Ao	205	0	46	0	0
51	Ap	173	0	36	0	0
51	Av	193	0	40	0	0
52	Ae	435	0	195	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	Af	448	0	190	0	0
54	Ag	637	0	331	0	0
55	Aj	663	0	292	0	0
56	Ak	750	0	321	0	0
57	Al	473	0	204	0	0
58	Am	134	0	54	0	0
59	An	482	0	214	0	0
60	Aq	335	0	69	0	0
60	As	322	0	65	0	0
60	Aw	376	0	76	0	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	41	0
64	O	86	0	60	9	0
65	D	43	0	32	3	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	0	0
67	Y	16	0	0	5	0
67	a	8	0	0	0	0
67	b	16	0	0	0	0
67	c	8	0	0	0	0
68	c	31	0	19	0	0
69	p	48	0	26	0	0
70	3	1	0	0	0	0
71	y	120	0	108	0	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	51779	1253	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 19.

The worst 5 of 1253 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)
1:A:84:ALA:CB	1:A:101:ALA:HB2	1.51	1.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:VAL:N	64:C:402:HEM:HBC2	1.43	1.34
1:M:83:GLY:CA	2:N:363:LYS:HA	1.57	1.33
3:C:116:GLY:HA3	64:C:402:HEM:C3C	1.63	1.33
12:W:162:ALA:HB2	14:Z:286:TYR:CA	1.61	1.28

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	29
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	19
7	S	76/81 (94%)	72 (95%)	2 (3%)	2 (3%)	4	25
8	H	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	T	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	8	37

Continued on next page...

Continued from previous page...

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%)	5	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	16
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	25
15	a	145/216 (67%)	126 (87%)	11 (8%)	8 (6%)	1	14
16	b	147/212 (69%)	140 (95%)	6 (4%)	1 (1%)	19	56
17	c	408/464 (88%)	369 (90%)	27 (7%)	12 (3%)	3	23
18	d	167/249 (67%)	152 (91%)	11 (7%)	4 (2%)	5	26
19	e	313/318 (98%)	282 (90%)	27 (9%)	4 (1%)	10	41
20	f	344/347 (99%)	324 (94%)	17 (5%)	3 (1%)	14	51
21	g	104/115 (90%)	96 (92%)	7 (7%)	1 (1%)	13	49
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%)	11	43
28	o	49/106 (46%)	42 (86%)	3 (6%)	4 (8%)	1	9
29	p	312/377 (83%)	281 (90%)	19 (6%)	12 (4%)	2	19
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	19
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

Continued on next page...

Continued from previous page...

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%)	13	49
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	13
41	5	73/85 (86%)	64 (88%)	8 (11%)	1 (1%)	9	39
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	54
48	z	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	10	41
50	Ac	53/70 (76%)	49 (92%)	2 (4%)	2 (4%)	2	19
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	19
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	17
58	Am	25/76 (33%)	23 (92%)	2 (8%)	0	100	100
59	An	95/172 (55%)	87 (92%)	5 (5%)	3 (3%)	3	21
All	All	12001/14873 (81%)	10603 (88%)	1047 (9%)	351 (3%)	6	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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	145/228 (64%)	145 (100%)	0	100	100
13	Y	517/610 (85%)	516 (100%)	1 (0%)	92	94
14	Z	322/393 (82%)	322 (100%)	0	100	100
15	a	120/177 (68%)	119 (99%)	1 (1%)	79	85
16	b	126/176 (72%)	126 (100%)	0	100	100
17	c	321/368 (87%)	321 (100%)	0	100	100
18	d	145/207 (70%)	145 (100%)	0	100	100
19	e	272/275 (99%)	272 (100%)	0	100	100
20	f	309/311 (99%)	309 (100%)	0	100	100
21	g	91/100 (91%)	91 (100%)	0	100	100
22	h	407/409 (100%)	406 (100%)	1 (0%)	92	94
23	i	76/85 (89%)	76 (100%)	0	100	100
24	j	527/540 (98%)	526 (100%)	1 (0%)	92	94
25	k	112/141 (79%)	112 (100%)	0	100	100
All	All	3490/4020 (87%)	3486 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	Y	478	SER
15	a	91	CYS
22	h	96	ILE
24	j	283	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
19	e	235	ASN
20	f	319	HIS
19	e	284	GLN
20	f	134	GLN
22	h	220	HIS

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	$\# Z > 2$
67	SF4	b	302	16	0,12,12	-	-	-		
66	FES	Q	201	-	0,4,4	-	-	-		
67	SF4	a	301	15	0,12,12	-	-	-		
67	SF4	Y	802	13	0,12,12	-	-	-		
68	FMN	c	502	-	33,33,33	1.42	6 (18%)	48,50,50	1.30	8 (16%)
69	NDP	p	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.32	4 (7%)
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
64	HEM	C	401	-	41,50,50	1.49	4 (9%)	45,82,82	1.88	10 (22%)
66	FES	d	301	-	0,4,4	-	-	-	-	-
64	HEM	O	402	-	41,50,50	1.56	4 (9%)	45,82,82	1.95	14 (31%)
64	HEM	O	401	-	41,50,50	1.59	5 (12%)	45,82,82	2.54	19 (42%)
71	HEA	y	602	-	57,67,67	1.47	6 (10%)	61,103,103	1.46	11 (18%)
67	SF4	b	301	16	0,12,12	-	-	-	-	-
67	SF4	c	501	17	0,12,12	-	-	-	-	-
64	HEM	C	402	-	41,50,50	1.37	4 (9%)	45,82,82	2.15	13 (28%)
65	HEC	D	301	-	32,50,50	2.20	4 (12%)	24,82,82	2.09	11 (45%)
65	HEC	P	301	-	32,50,50	2.23	4 (12%)	24,82,82	1.92	9 (37%)
67	SF4	Y	801	13	0,12,12	-	-	-	-	-
71	HEA	y	601	-	57,67,67	1.24	6 (10%)	61,103,103	1.47	11 (18%)
66	FES	E	201	-	0,4,4	-	-	-	-	-

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
67	SF4	b	302	16	-	-	0/6/5/5
66	FES	Q	201	-	-	-	0/1/1/1
67	SF4	a	301	15	-	-	0/6/5/5
67	SF4	Y	802	13	-	-	0/6/5/5
68	FMN	c	502	-	-	4/18/18/18	0/3/3/3
69	NDP	p	401	-	-	15/30/77/77	0/5/5/5
66	FES	Y	803	13	-	-	0/1/1/1
64	HEM	C	401	-	-	4/12/54/54	-
66	FES	d	301	-	-	-	0/1/1/1
64	HEM	O	402	-	-	4/12/54/54	-
64	HEM	O	401	-	-	6/12/54/54	-
71	HEA	y	602	-	-	5/32/76/76	-
67	SF4	b	301	16	-	-	0/6/5/5
64	HEM	C	402	-	-	6/12/54/54	-
67	SF4	c	501	17	-	-	0/6/5/5
65	HEC	D	301	-	-	4/10/54/54	-
65	HEC	P	301	-	-	6/10/54/54	-
67	SF4	Y	801	13	-	-	0/6/5/5
71	HEA	y	601	-	-	7/32/76/76	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	FES	E	201	-	-	-	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	P	301	HEC	C3C-C2C	-7.11	1.33	1.40
65	D	301	HEC	C2B-C3B	-7.03	1.33	1.40
65	P	301	HEC	C2B-C3B	-6.82	1.33	1.40
65	D	301	HEC	C3C-C2C	-6.59	1.33	1.40
71	y	602	HEA	C3A-C2A	-6.35	1.31	1.40

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	O	401	HEM	CMA-C3A-C4A	-6.90	117.87	128.46
64	O	401	HEM	C3B-C2B-C1B	-5.49	102.41	106.49
64	C	402	HEM	CMA-C3A-C4A	-5.39	120.19	128.46
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

There are no chirality outliers.

5 of 61 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.

8 monomers are involved in 60 short contacts:

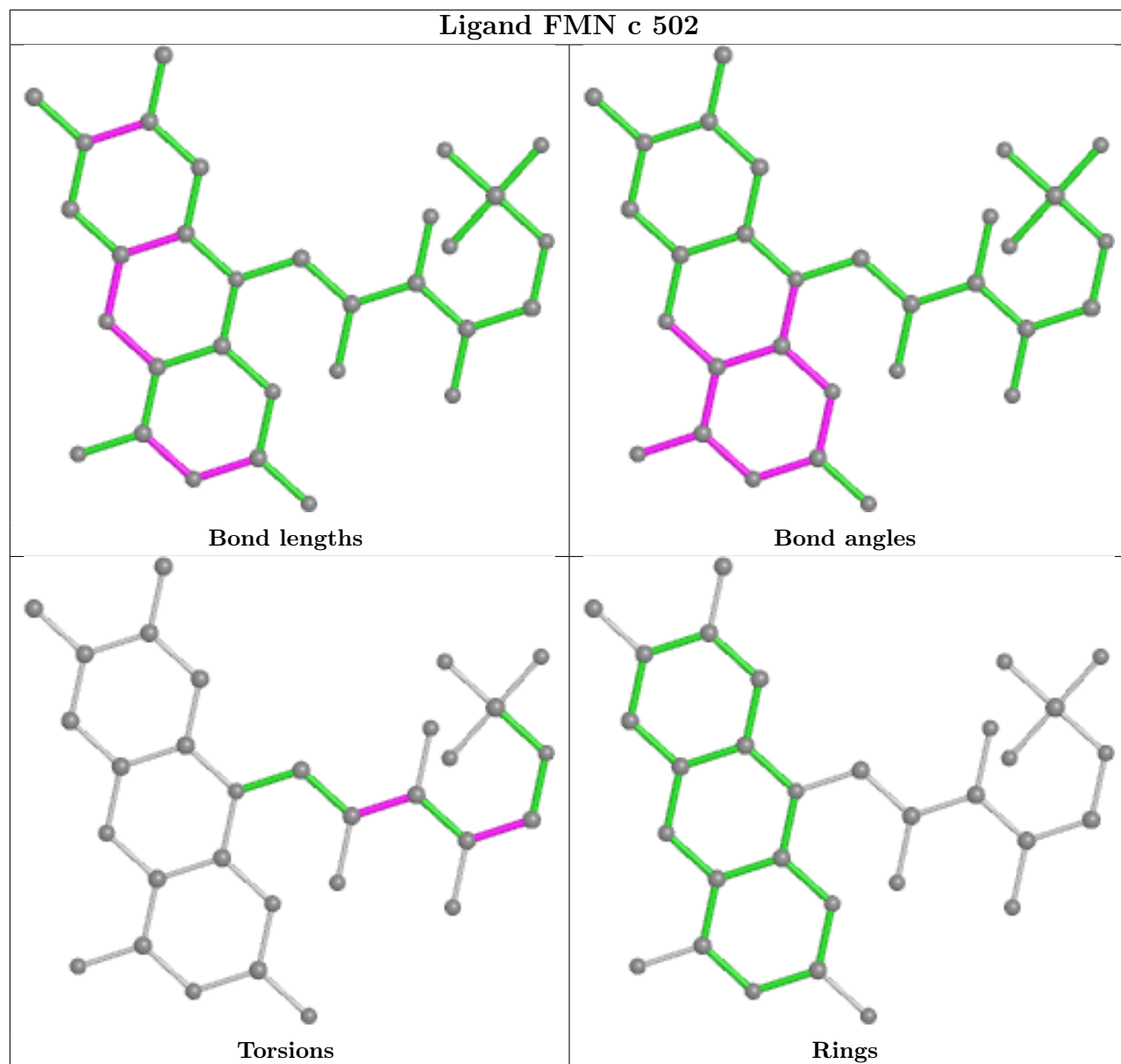
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Y	802	SF4	1	0
64	C	401	HEM	3	0
64	O	402	HEM	3	0
64	O	401	HEM	6	0
64	C	402	HEM	38	0
65	D	301	HEC	3	0
65	P	301	HEC	2	0

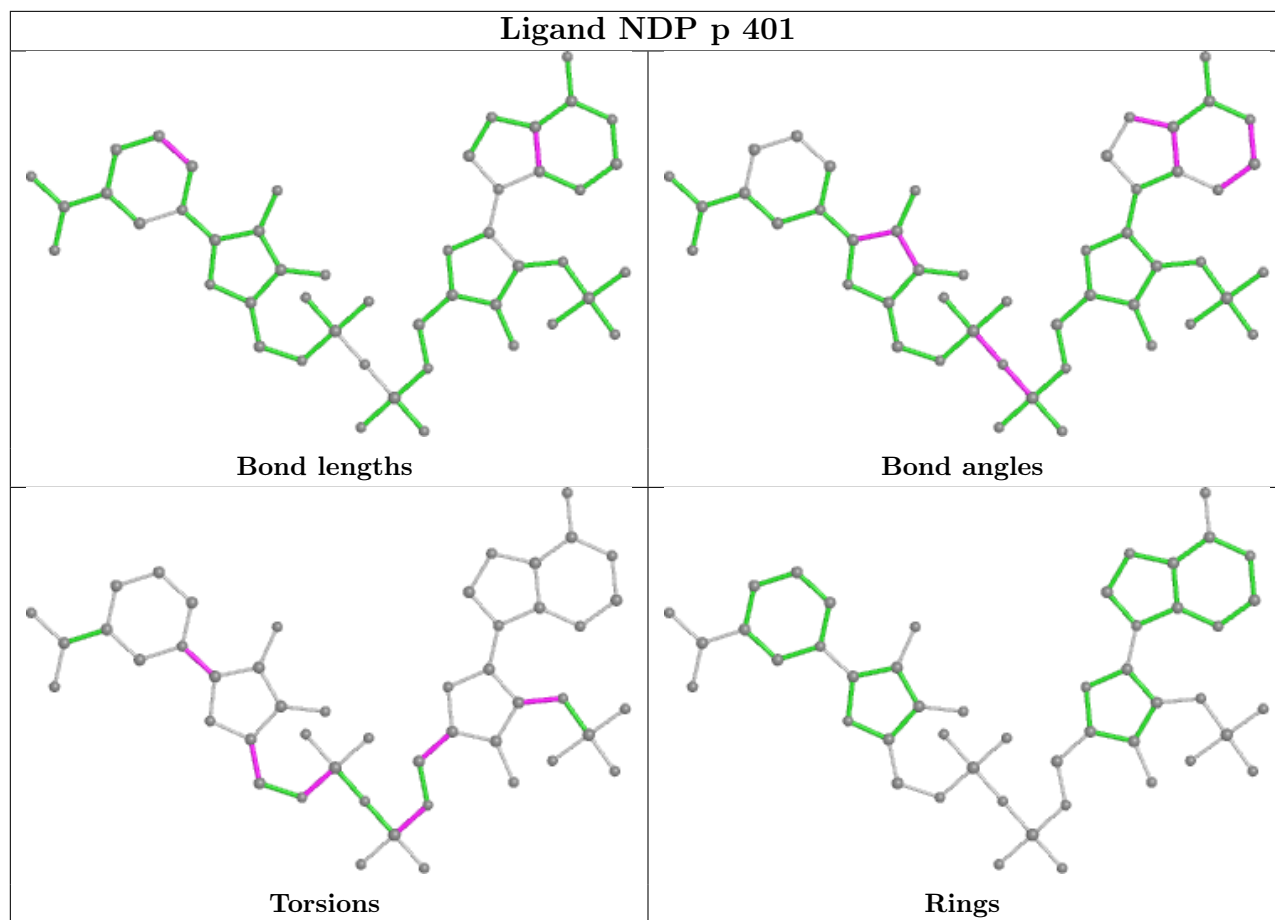
Continued on next page...

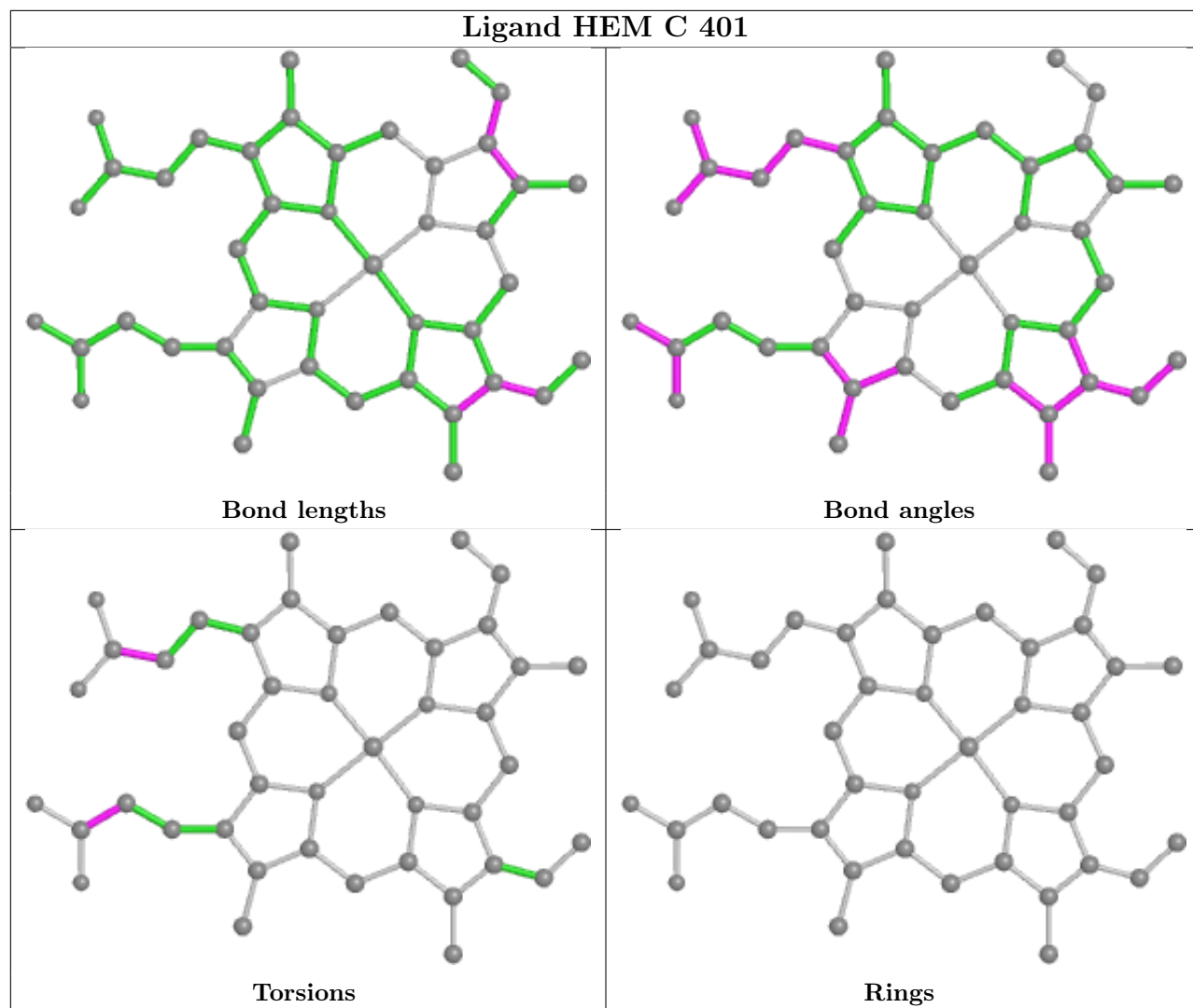
Continued from previous page...

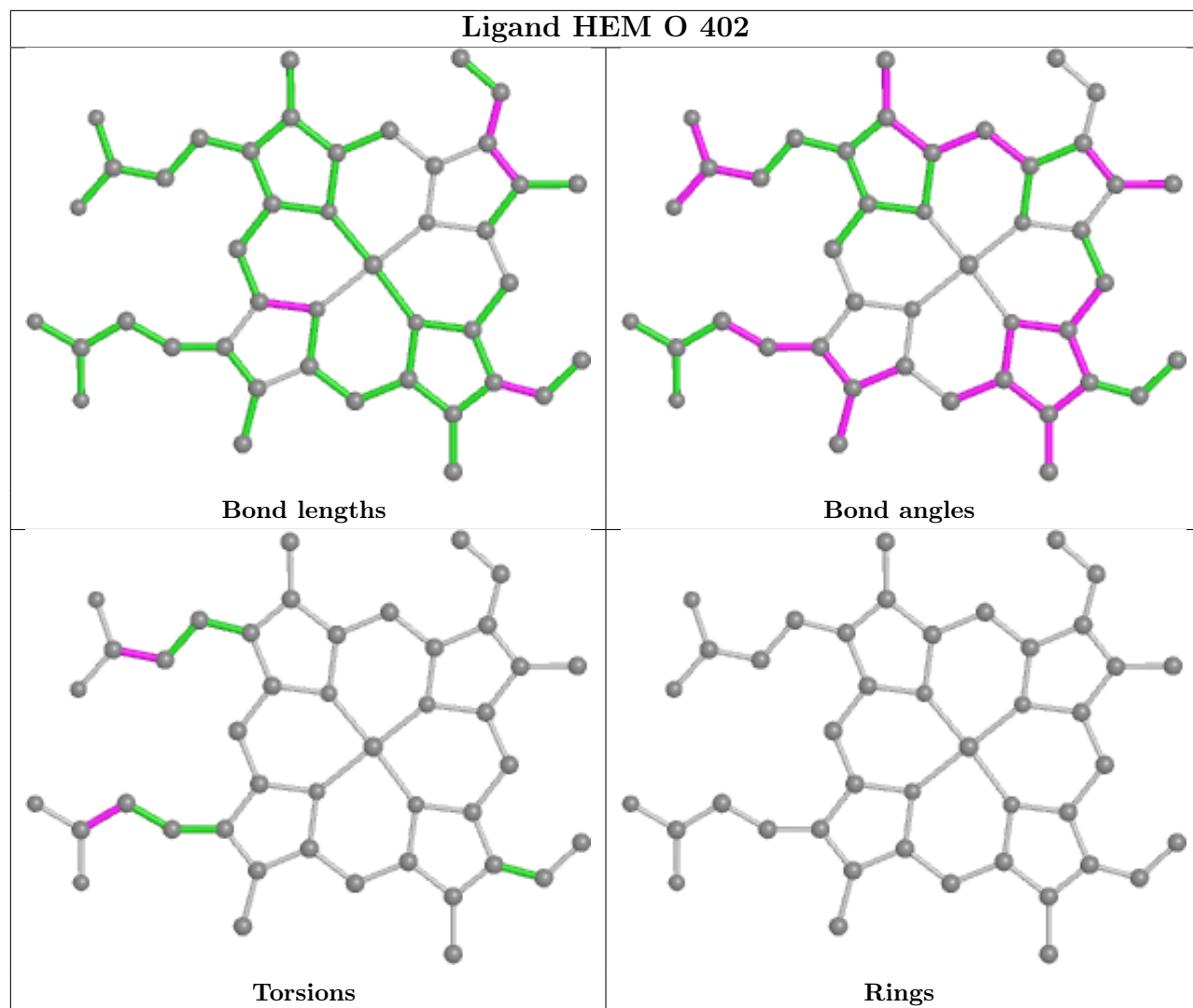
Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Y	801	SF4	4	0

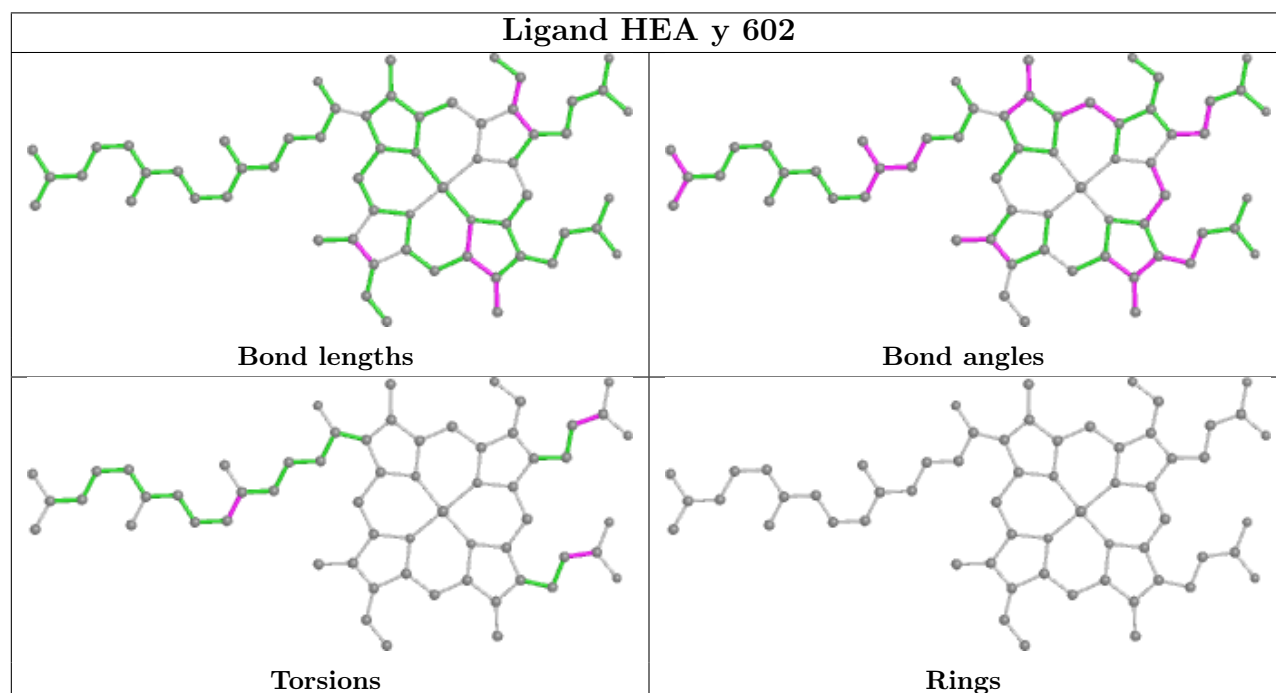
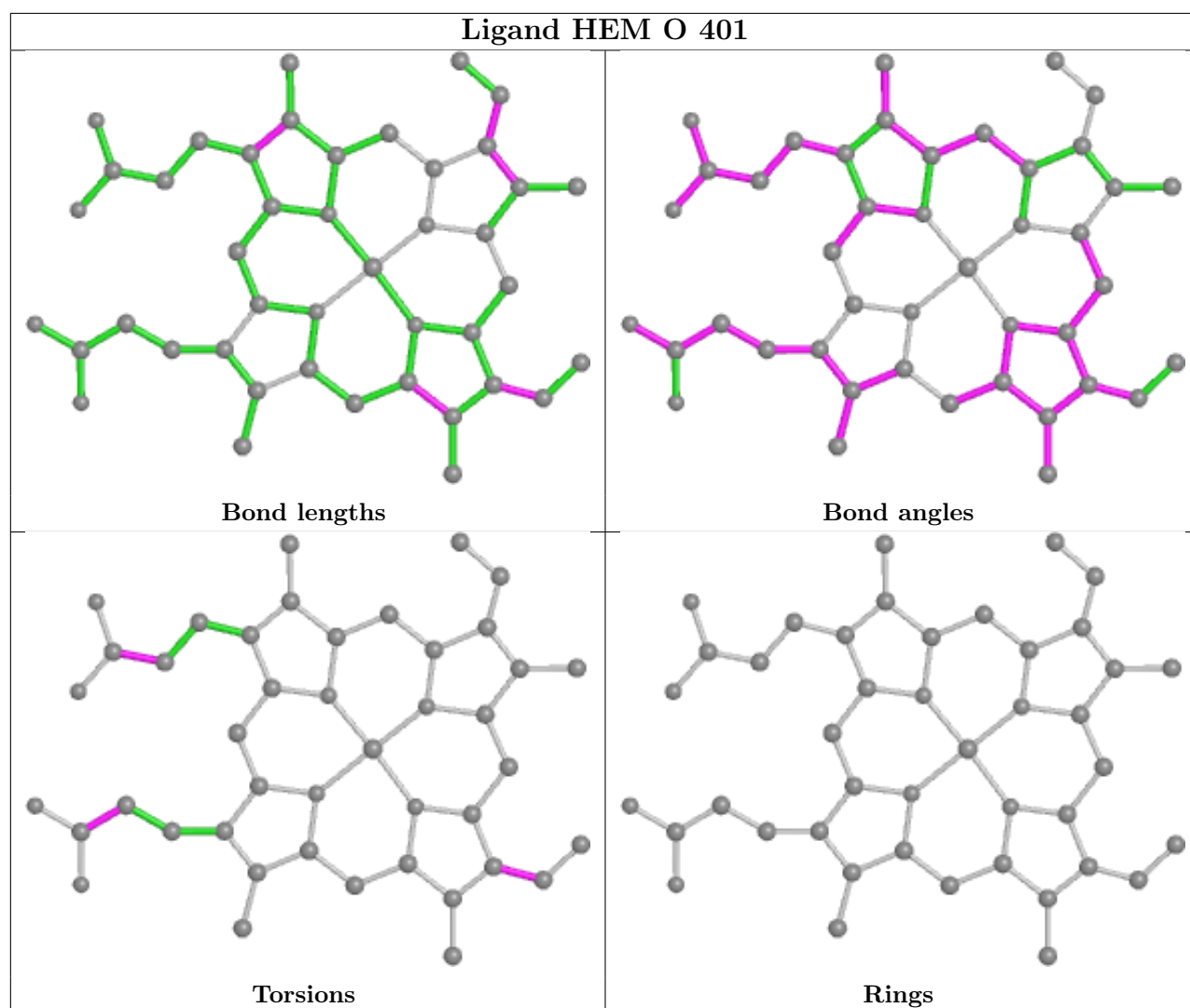
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

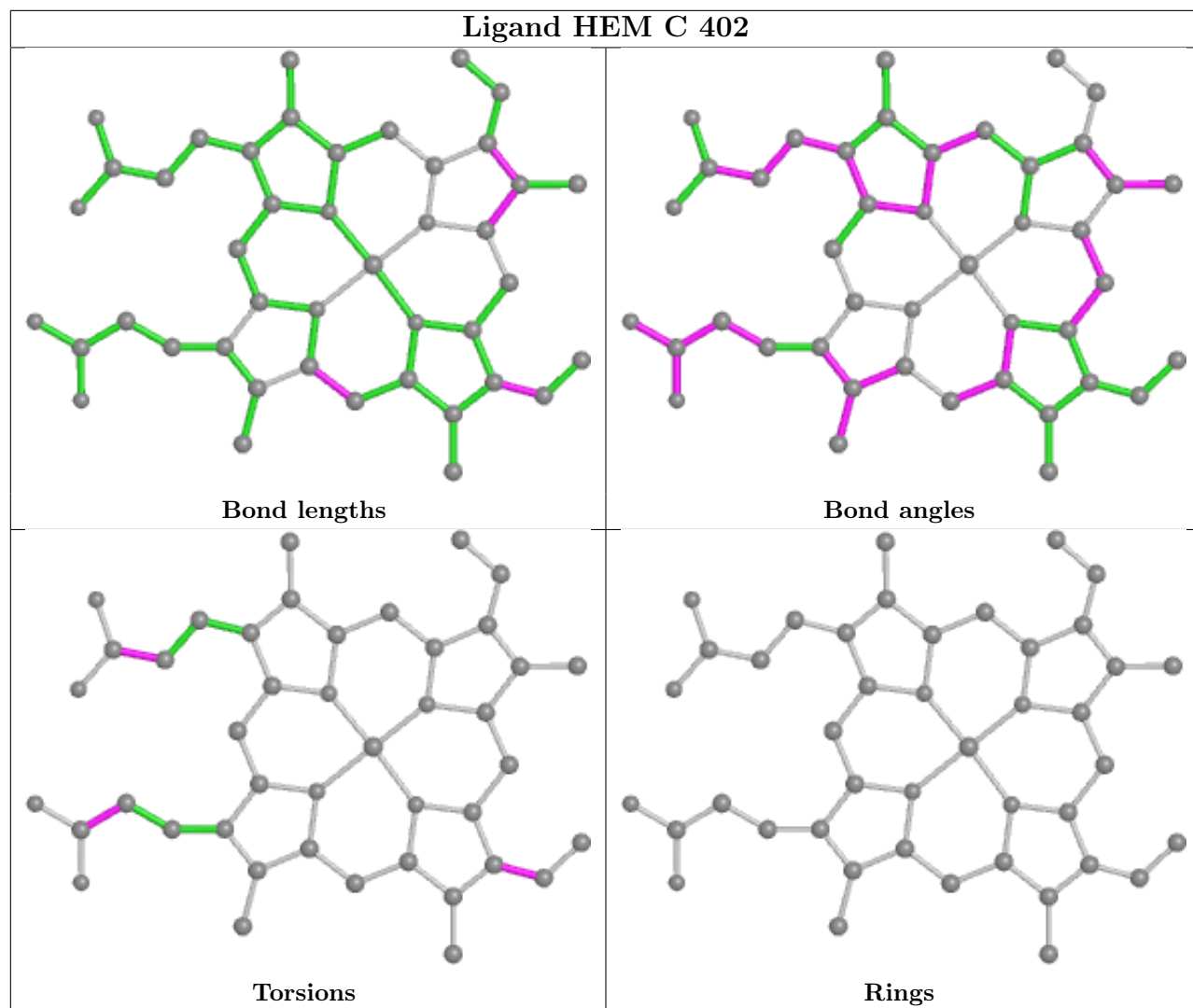


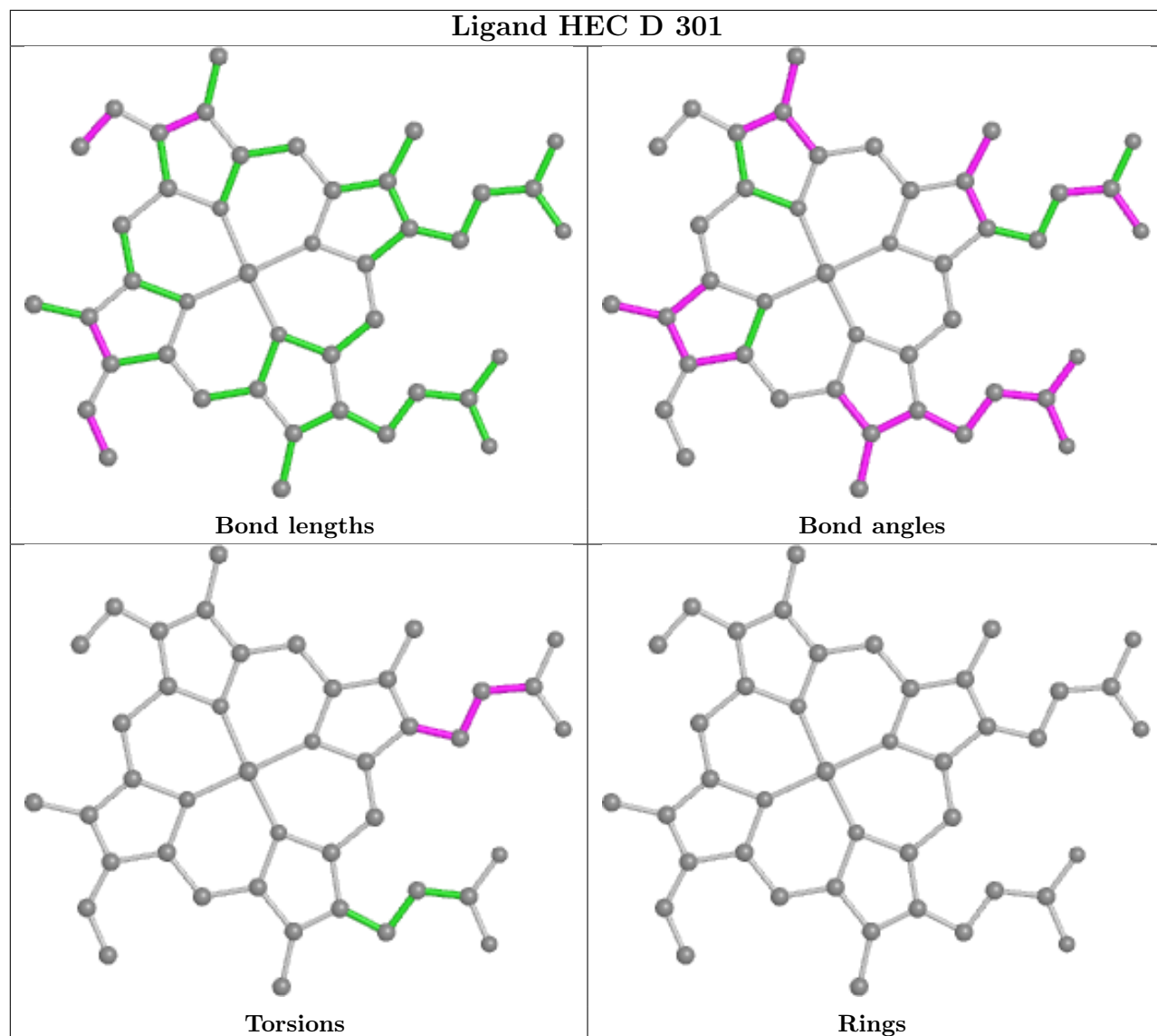


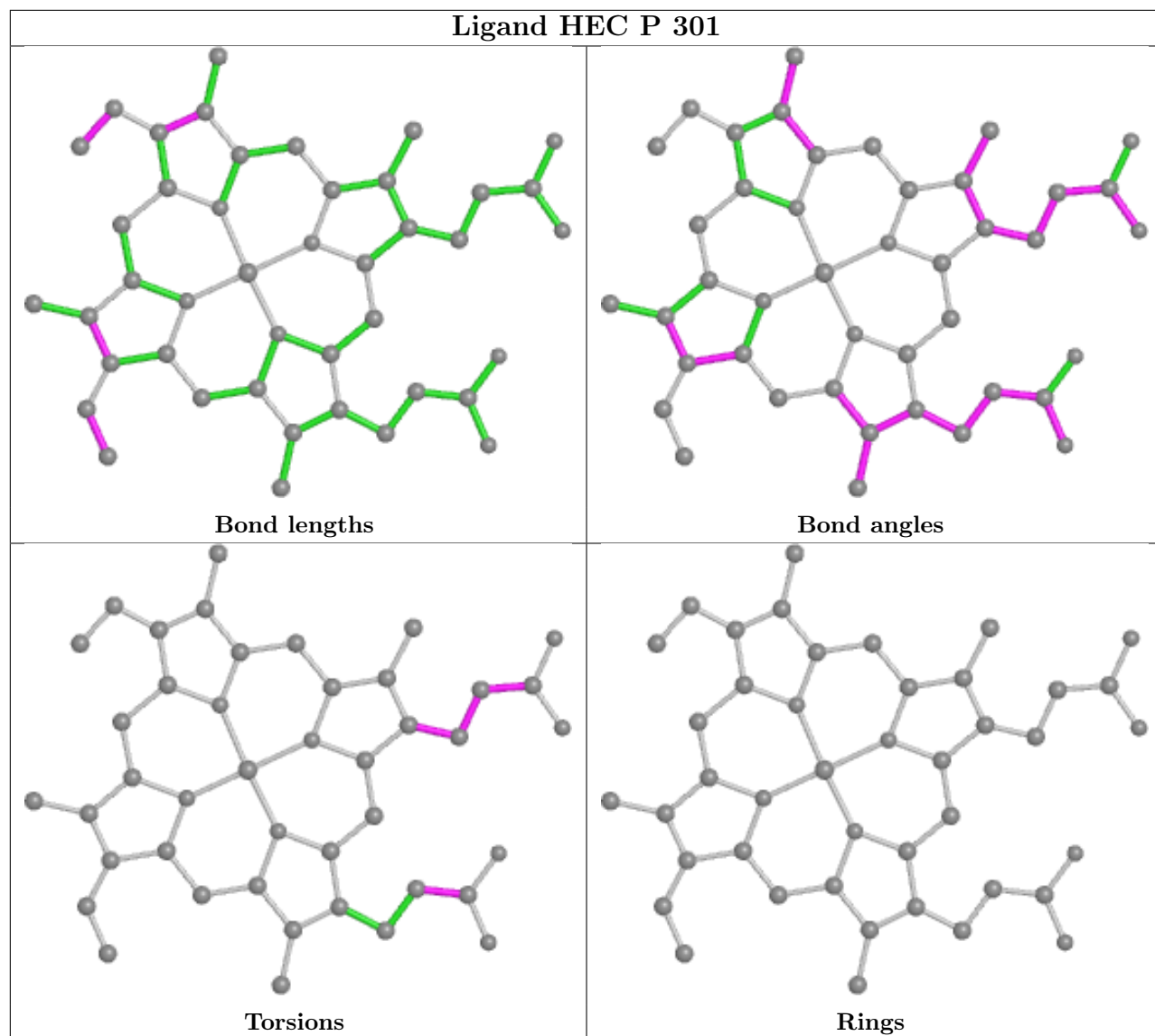


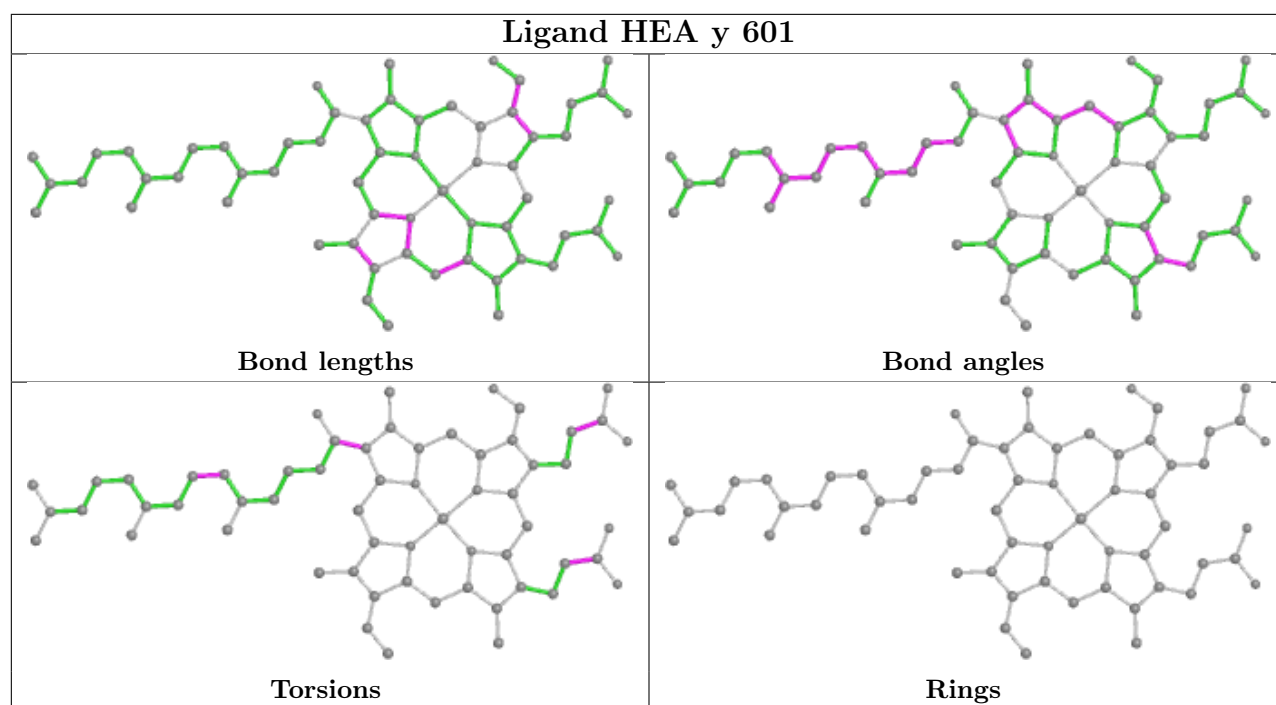












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

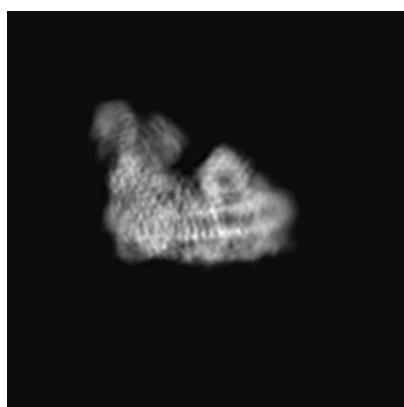
6 Map visualisation [i](#)

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.

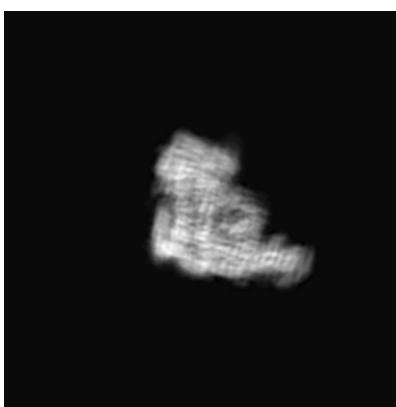
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

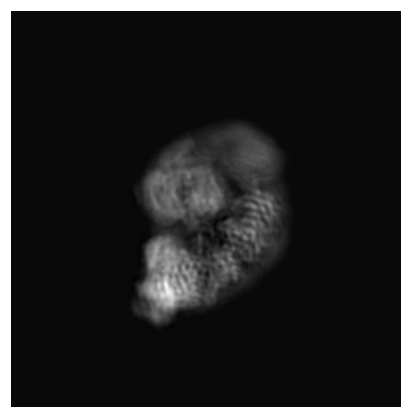
6.1.1 Primary map



X



Y

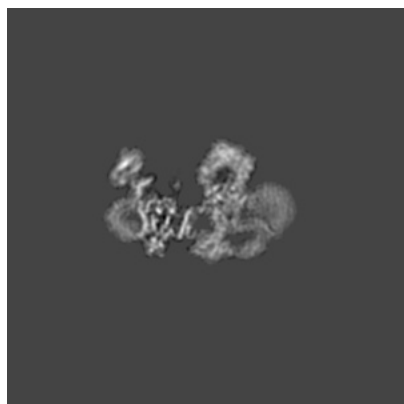


Z

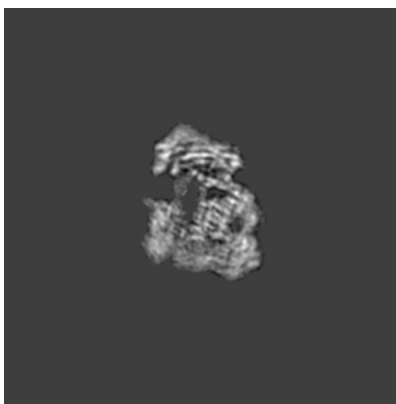
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

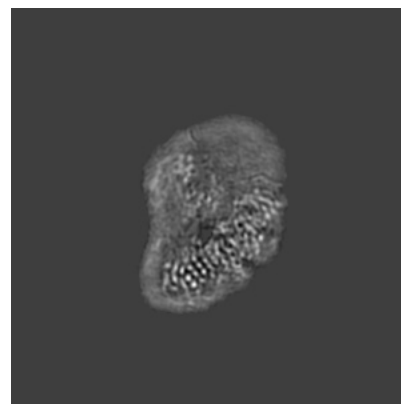
6.2.1 Primary map



X Index: 240



Y Index: 240

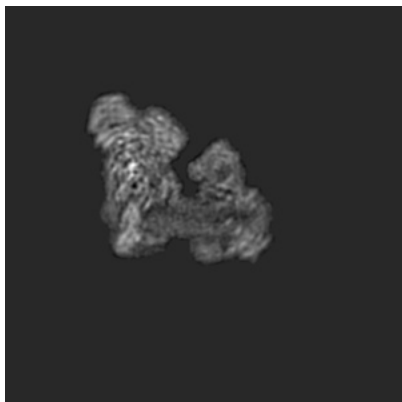


Z Index: 240

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

6.3 Largest variance slices [i](#)

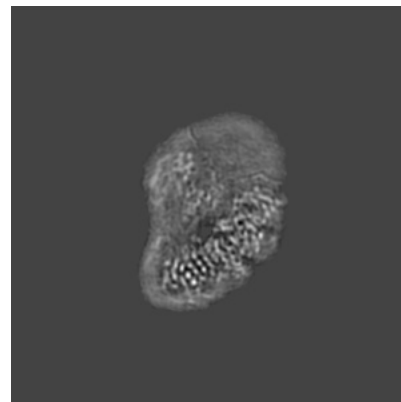
6.3.1 Primary map



X Index: 186



Y Index: 149



Z Index: 241

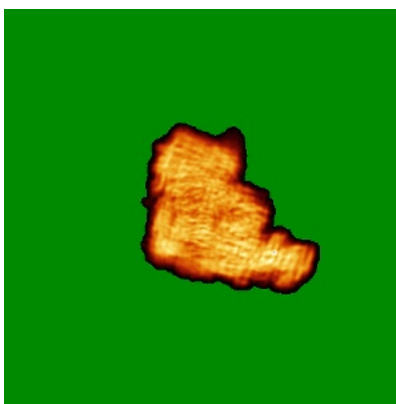
The images above show the largest variance slices of the map in three orthogonal directions.

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

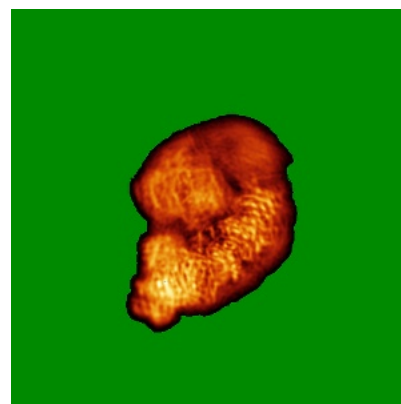
6.4.1 Primary map



X



Y

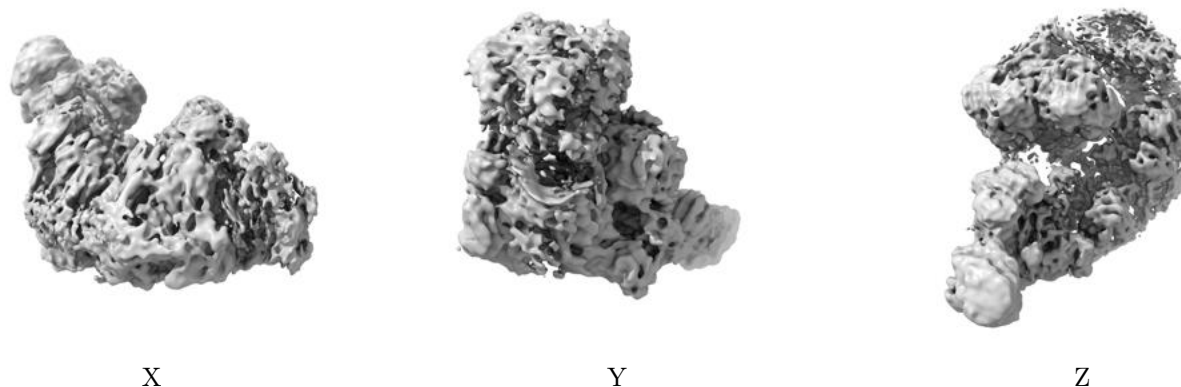


Z

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.

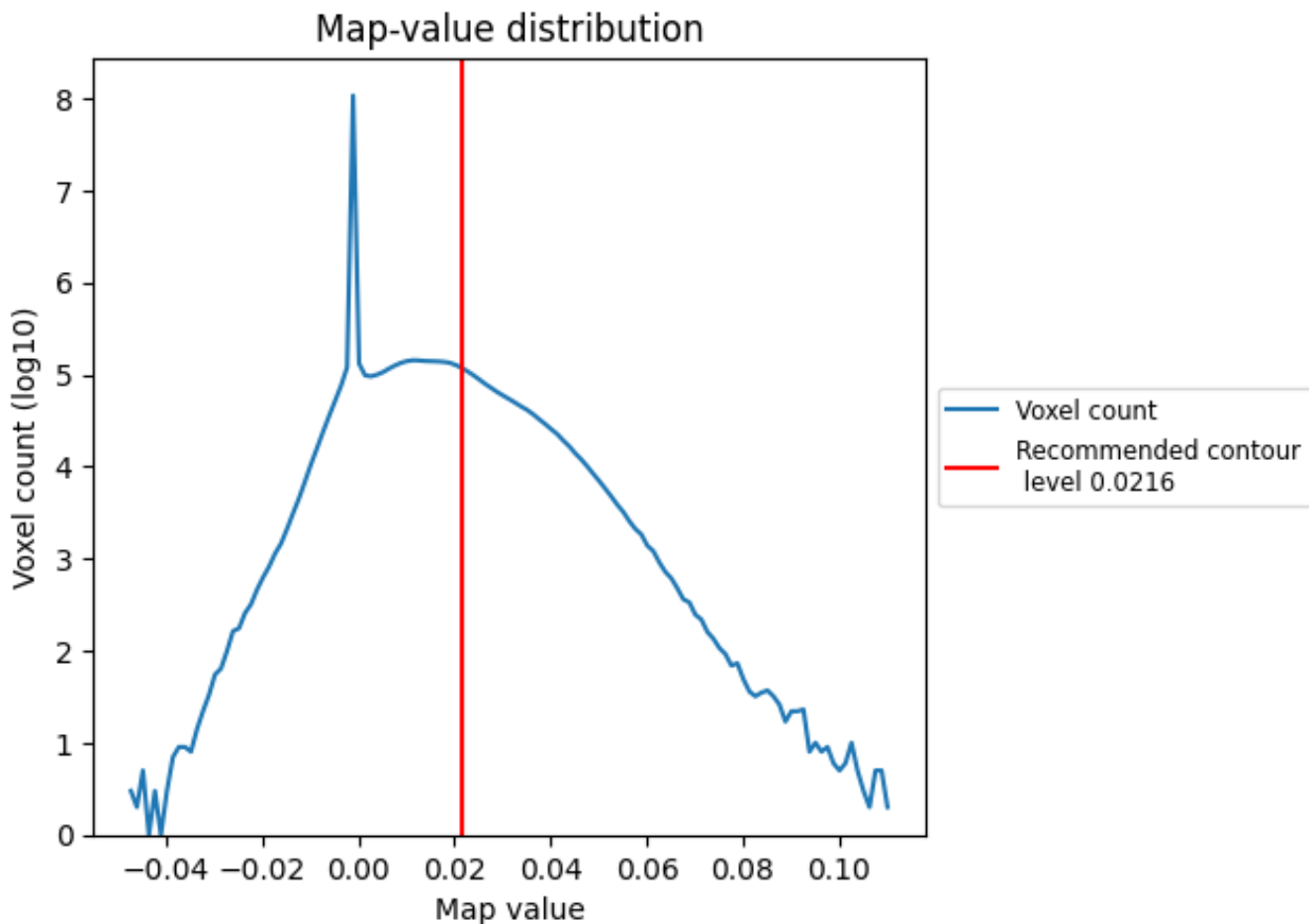
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

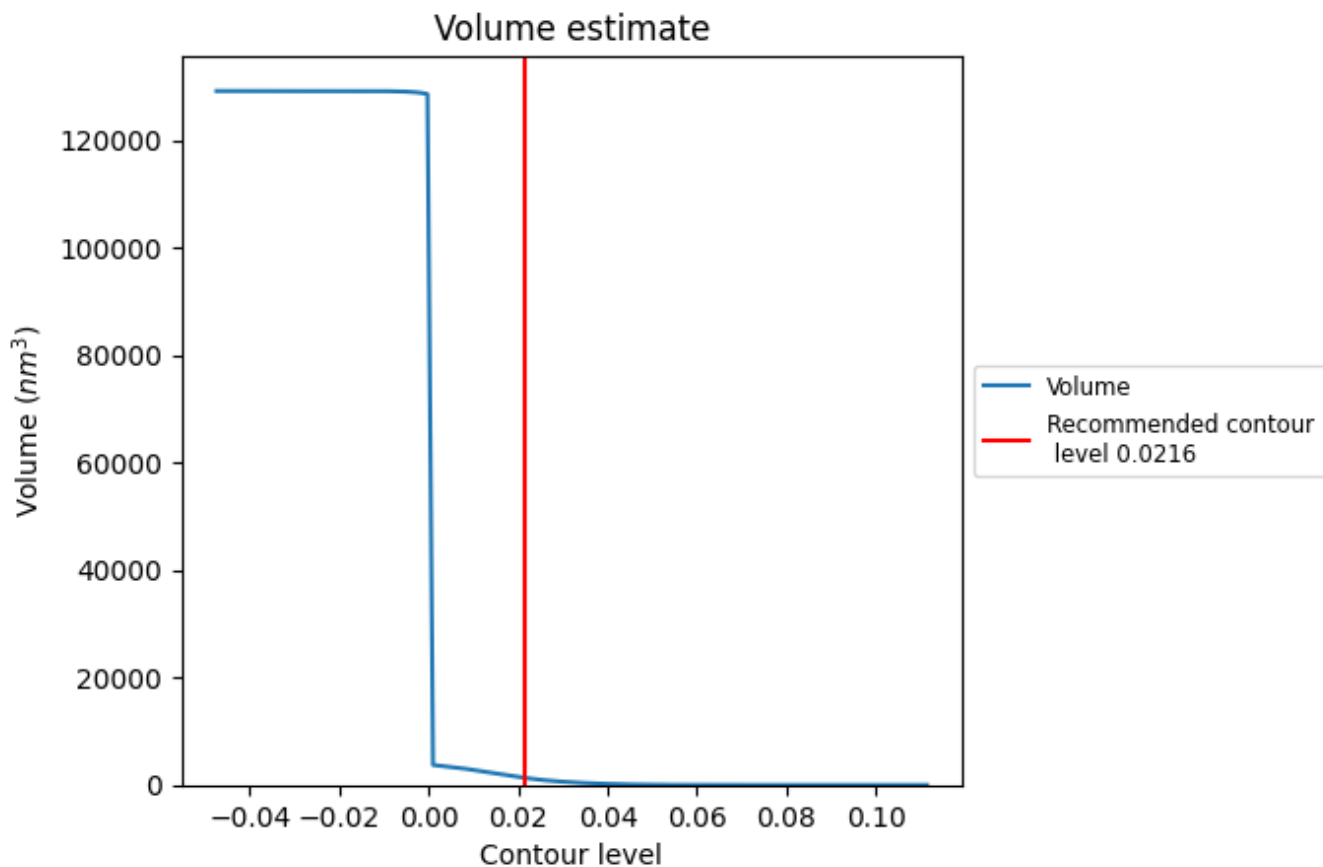
This section contains the results of statistical analysis of the map.

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.

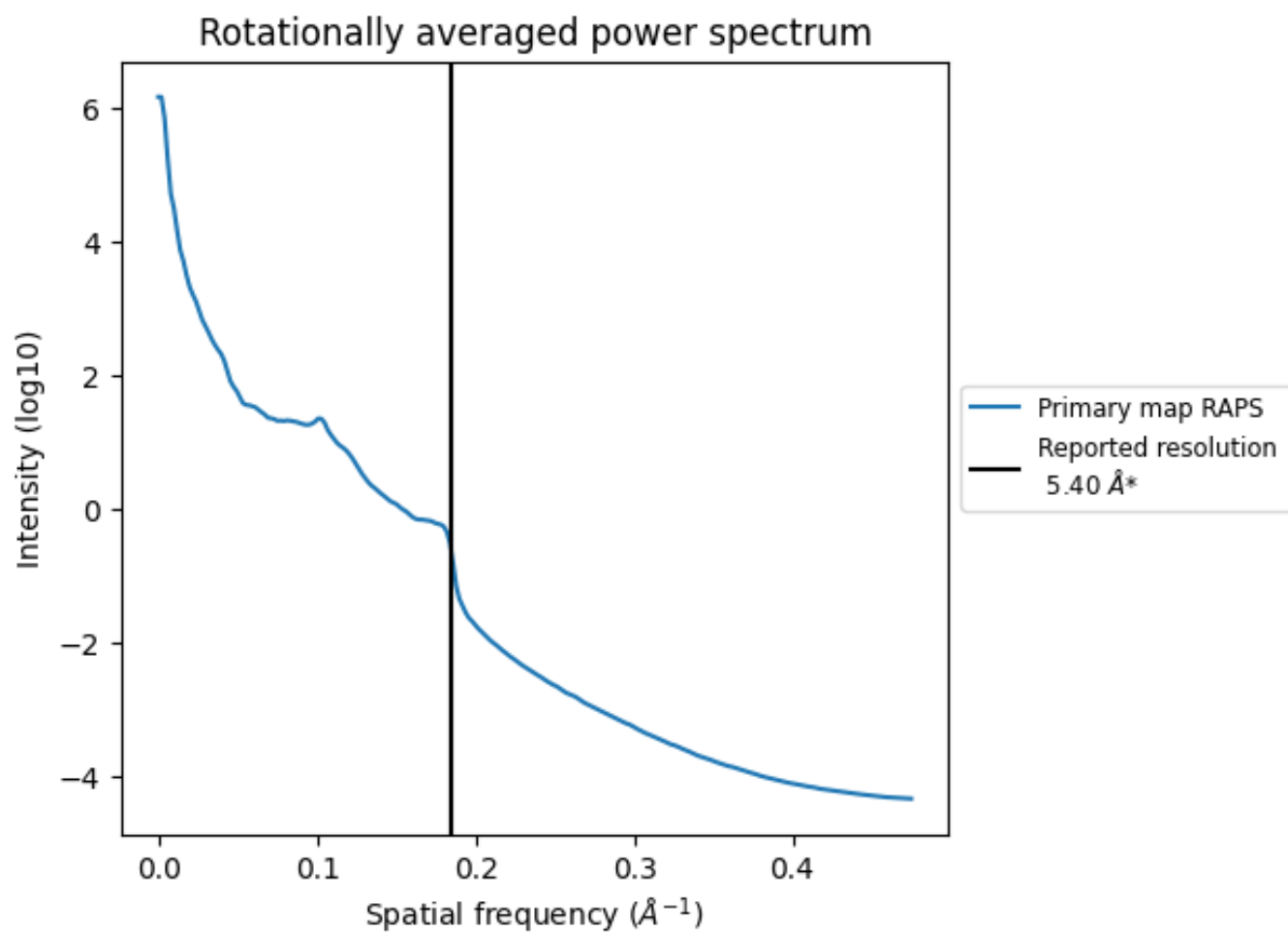
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1312 nm³; 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.185\AA^{-1}

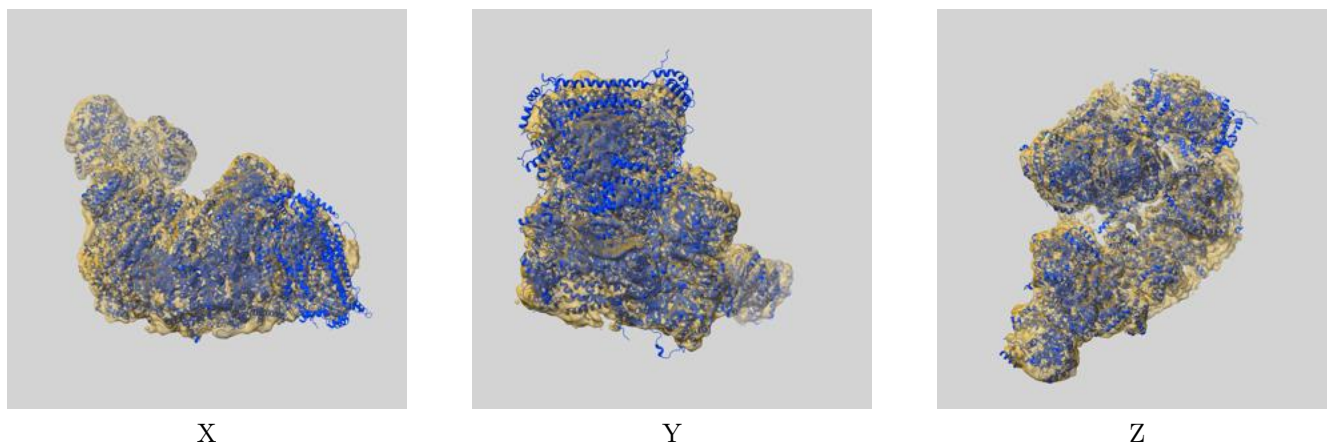
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

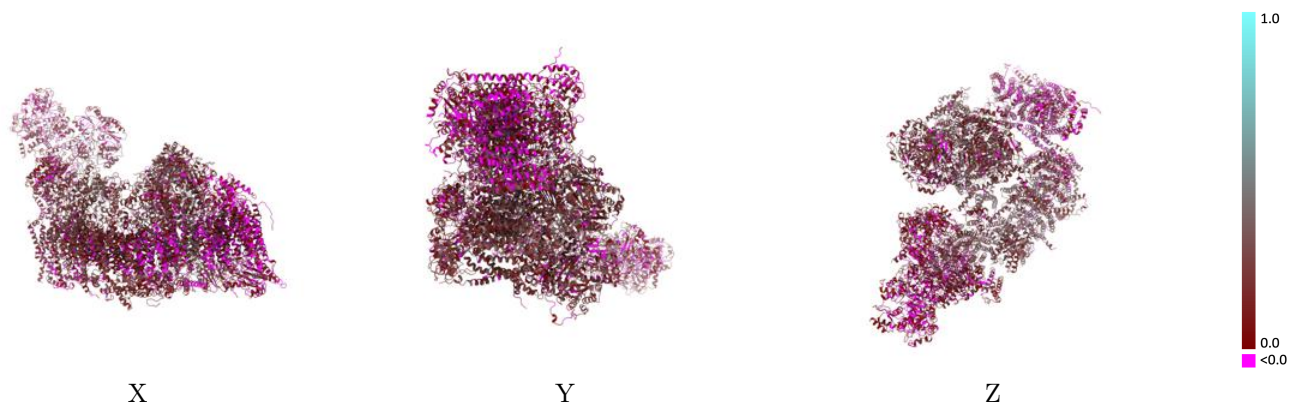
This section contains information regarding the fit between EMDB map EMD-9534 and PDB model 5GPN. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



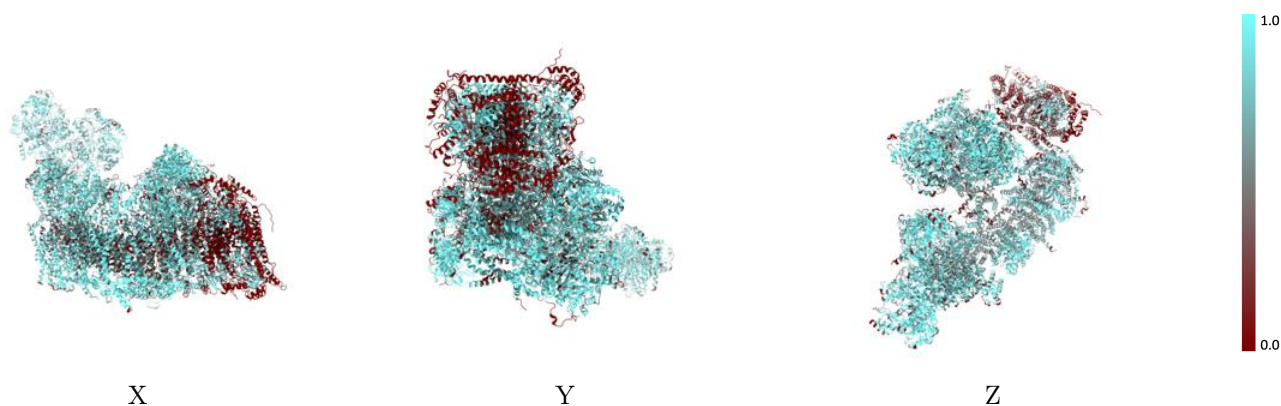
The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



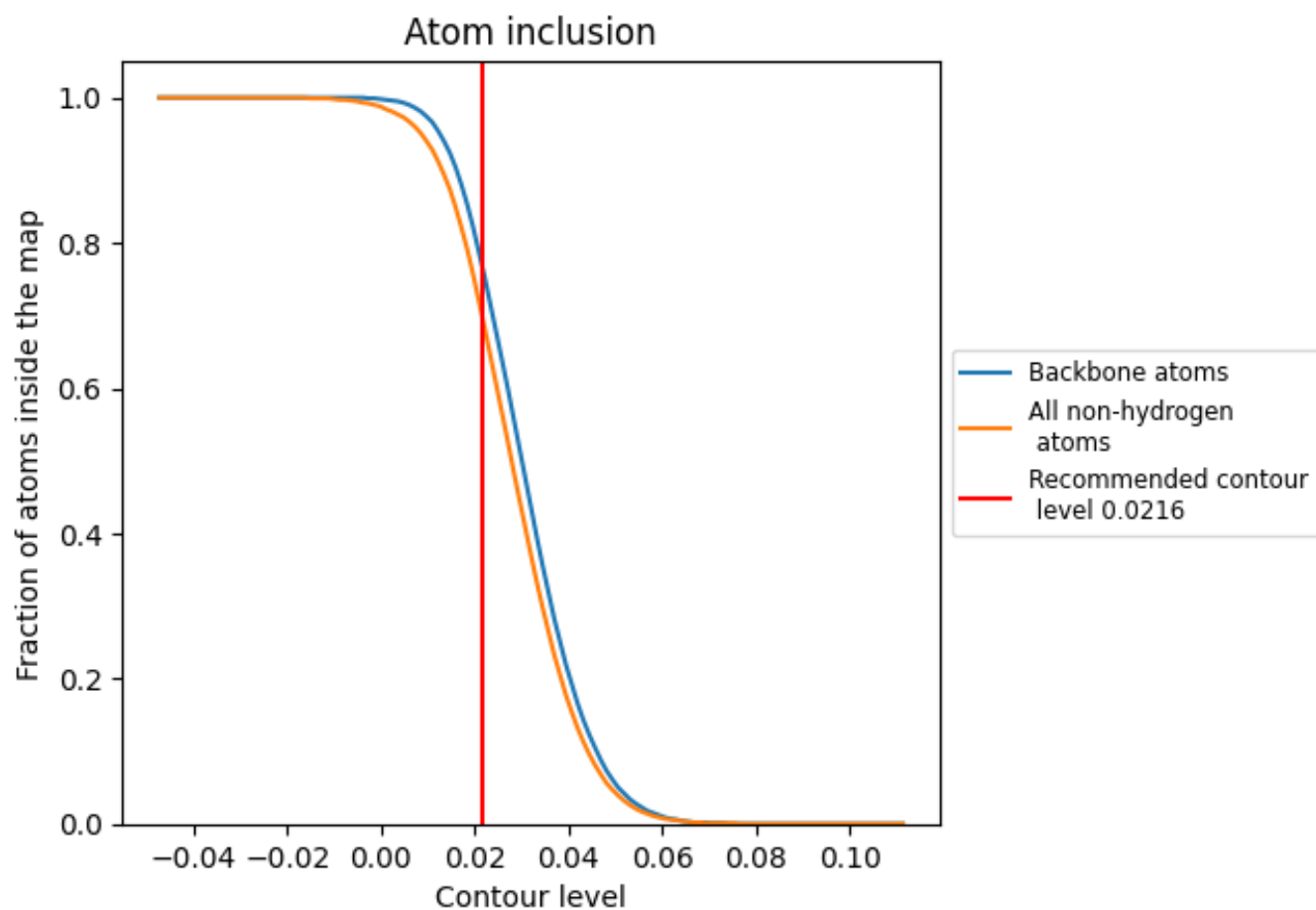
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































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



















Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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