



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 05:49 pm GMT

PDB ID : 8A22
EMDB ID : EMD-15100
Title : Structure of the mitochondrial ribosome from *Polytomella magna*
Authors : Tobiasson, V.; Berzina, I.; Amunts, A.
Deposited on : 2022-06-02
Resolution : 2.91 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

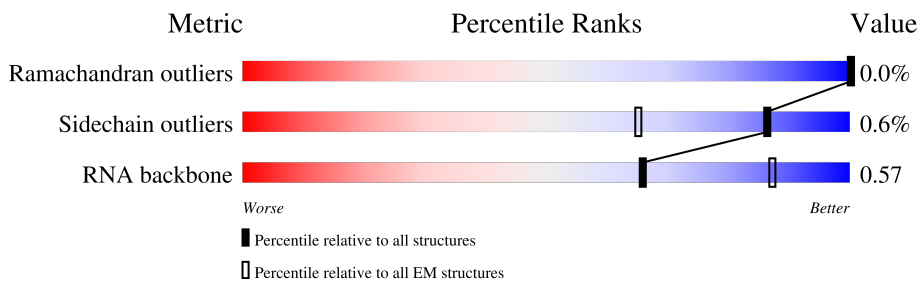
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A1	109	74% 26%
2	A2	81	78% 22%
3	A3	210	84% 14%
4	A4	73	86% 14%
5	A5	142	73% 23%
6	A6	131	67% 16% 17%
7	A7	576	78% 14% 7%
8	A8	350	83% 17%

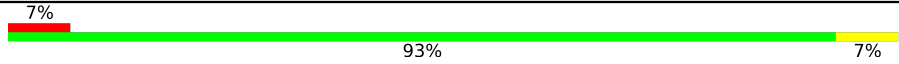
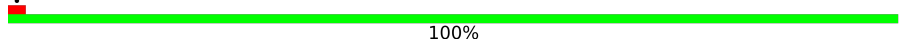
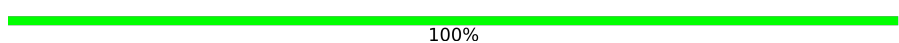
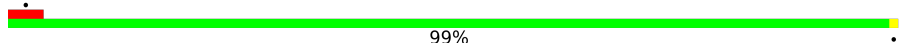
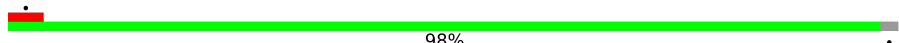
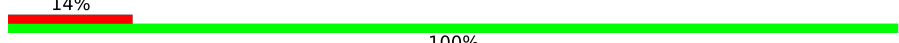
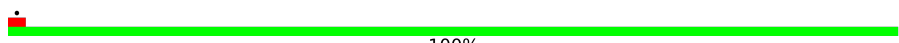

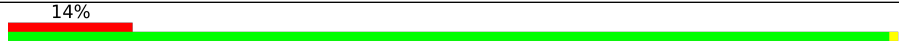

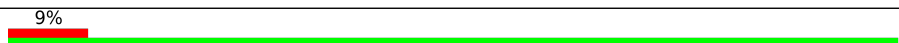

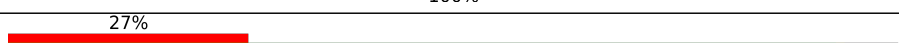
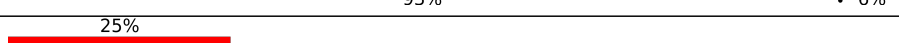
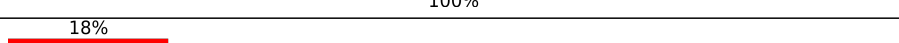
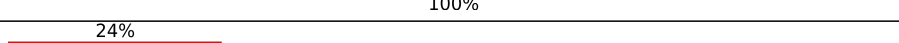
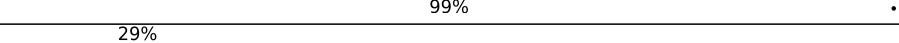
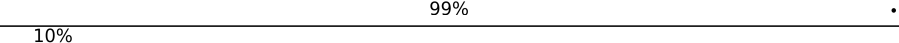
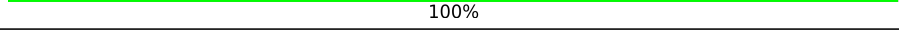
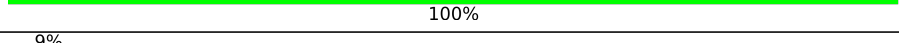
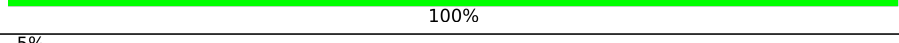
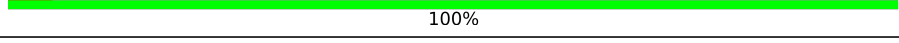
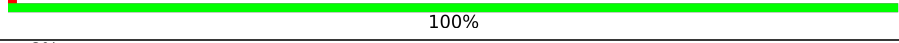
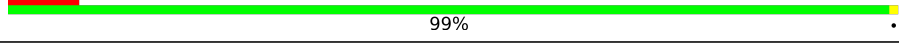
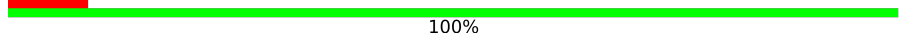
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Mol	Chain	Length	Quality of chain
9	A9	69	78% 22%
10	Aa	306	100%
11	Ab	306	100%
12	Ac	303	100%
13	Ad	193	14% 99%
14	Ae	242	8% 100%
15	Af	56	18% 98%
16	Ah	186	99%
17	Ai	121	100%
18	Aj	206	100%
19	Ak	166	99%
20	Al	173	99%
21	Am	114	100%
22	An	170	5% 100%
23	Ao	117	100%
24	Ap	200	100%
25	Aq	188	99%
26	Ar	155	99%
27	As	115	11% 100%
28	At	253	100%
29	Au	142	99%
30	Av	129	100%
31	Aw	123	98%
32	Ax	176	100%
33	Ay	72	39% 100%

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Mol	Chain	Length	Quality of chain
34	Az	59	 7% 93% 7%
35	AA	50	 100%
36	AB	50	 100%
37	AC	139	 99%
38	AD	47	 98%
39	AE	92	 14% 100%
40	AF	93	 100%
41	AG	121	 100%
42	AH	176	 14% 99%
43	AI	64	 100%
44	AJ	122	 9% 100%
45	AK	139	 100%
46	AL	420	 27% 93% 6%
46	AM	420	 25% 100%
46	AN	420	 18% 100%
47	AO	377	 24% 99%
48	Xa	199	 29% 99%
49	Xb	244	 10% 100%
50	Xc	57	 100%
51	Xd	413	 9% 100%
52	Xe	483	 5% 100%
53	Xf	201	 100%
54	Xg	410	 8% 99%
55	Xh	143	 9% 100%
56	Xi	24	 100%

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Mol	Chain	Length	Quality of chain
57	Xj	71	25% 100%
58	B1	102	25% 76% 24%
59	B2	214	17% 79% 20%
60	B3	379	85% 13%
61	B4	348	7% 80% 15% 5%
62	Ba	242	66% 98%
63	Bb	236	40% 100%
64	Bc	289	71% 99%
65	Bd	221	60% 100%
66	Be	228	33% 96%
67	Bf	119	38% 100%
68	Bg	112	40% 98%
69	Bh	374	40% 100%
70	Bi	282	67% 100%
71	Bj	401	85% 100%
72	Bk	116	16% 100%
73	Bl	123	63% 100%
74	Bm	113	73% 99%
75	Bn	118	34% 100%
76	Bo	167	13% 100%
77	Bp	123	72% 99%
78	Bq	130	18% 100%
79	Br	90	32% 99%
80	Bs	92	79% 100%
81	Bt	75	23% 100%

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Mol	Chain	Length	Quality of chain
82	Bu	167	63% 100%
83	Bv	164	53% 99%
84	Bw	349	86% 100%
85	Bx	621	95% 98%
86	By	80	62% 98%
87	Bz	119	97% 100%
88	BA	176	81% 100%
89	BB	84	64% 100%
90	BC	31	6% 100%
91	BD	270	82% 100%
92	BE	171	99% 100%
93	BF	370	80% 100%
94	Ya	180	80% 99%
95	Yb	50	96% 100%
96	Yc	159	68% 99%
97	Yd	95	94% 100%
98	Ye	106	41% 98%
99	Yf	150	71% 100%
100	Yg	67	90% 100%
101	Yh	65	82% 100%
102	Yi	132	99% 98%
103	Yj	386	96% 100%
104	Yk	92	100% 100%
105	Yl	84	63% 100%
106	Ua	32	22% 100%

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Mol	Chain	Length	Quality of chain
107	Ub	131	<p>31% 95% 5%</p>
108	Ud	43	<p>91% 100%</p>
109	Ue	47	<p>100% 100%</p>
110	Uf	81	<p>89% 90% 10%</p>
111	Ug	72	<p>81% 88% 12%</p>
112	Uh	48	<p>100% 100%</p>
113	Ui	26	<p>62% 100%</p>
114	Uj	9	<p>100% 100%</p>
115	Uk	23	<p>100% 100%</p>
116	Ul	16	<p>100% 100%</p>
117	Um	11	<p>55% 100%</p>

2 Entry composition i

There are 122 unique types of molecules in this entry. The entry contains 196554 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 RNA chain called mtLSU-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A1	109	2344	1052	444	739	109	0	0

- Molecule 2 is a RNA chain called mtLSU-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A2	81	1729	777	318	553	81	0	0

- Molecule 3 is a RNA chain called mtLSU-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A3	207	4413	1980	795	1431	207	0	0

- Molecule 4 is a RNA chain called mtLSU-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	A4	73	1572	704	302	493	73	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A4	?	-	A	deletion	GB 485474616
A4	2	A	-	insertion	GB 485474616

- Molecule 5 is a RNA chain called mtLSU-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A5	136	2897	1298	522	941	136	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	1	U	A	conflict	GB 485474616
A5	16	C	U	conflict	GB 485474616
A5	19	C	A	conflict	GB 485474616
A5	20	C	A	conflict	GB 485474616
A5	21	A	G	conflict	GB 485474616
A5	22	G	C	conflict	GB 485474616
A5	23	G	A	conflict	GB 485474616
A5	24	A	G	conflict	GB 485474616
A5	25	G	C	conflict	GB 485474616
A5	28	G	A	conflict	GB 485474616
A5	34	G	A	conflict	GB 485474616
A5	42	C	U	conflict	GB 485474616
A5	47	C	G	conflict	GB 485474616
A5	48	U	A	conflict	GB 485474616
A5	49	U	C	conflict	GB 485474616
A5	51	G	-	insertion	GB 485474616
A5	52	A	-	insertion	GB 485474616
A5	63	A	G	conflict	GB 485474616

- Molecule 6 is a RNA chain called mtLSU-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A6	109	2337	1048	433	747	109	0	0

- Molecule 7 is a RNA chain called mtLSU-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A7	534	11387	5106	2066	3681	534	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	236	A	U	conflict	GB 485474616

- Molecule 8 is a RNA chain called mtLSU-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A8	350	7452	3335	1322	2445	350	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A8	346	A	U	conflict	GB 485474616
A8	349	A	U	conflict	GB 485474616
A8	350	A	G	conflict	GB 485474616

- Molecule 9 is a RNA chain called mt-5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A9	69	1466	656	256	485	69	0	0

- Molecule 10 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Aa	306	2386	1501	470	410	5	0	0

- Molecule 11 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Ab	306	2414	1560	411	432	11	0	0

- Molecule 12 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Ac	303	2377	1499	438	435	5	0	0

- Molecule 13 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Ad	193	1537	991	256	281	9	0	0

- Molecule 14 is a protein called uL6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Ae	242	1934	1260	326	341	7	0	0

- Molecule 15 is a protein called uL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Af	56	Total	C	N	O	S	0	0
			432	274	74	83	1		

- Molecule 16 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ah	186	Total	C	N	O	S	0	0
			1517	975	274	260	8		

- Molecule 17 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ai	121	Total	C	N	O	S	0	0
			952	621	170	158	3		

- Molecule 18 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aj	206	Total	C	N	O	S	0	0
			1607	1027	290	284	6		

- Molecule 19 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ak	166	Total	C	N	O	S	0	0
			1356	870	261	216	9		

- Molecule 20 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Al	173	Total	C	N	O	S	0	0
			1412	898	272	240	2		

- Molecule 21 is a protein called uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Am	114	Total	C	N	O	S	0	0
			911	587	166	156	2		

- Molecule 22 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	An	170	1392	891	238	255	8	0	0

- Molecule 23 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Ao	117	964	607	186	168	3	0	0

- Molecule 24 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Ap	200	1566	1003	278	279	6	0	0

- Molecule 25 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Aq	188	1533	971	285	273	4	0	0

- Molecule 26 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Ar	155	1283	824	223	232	4	0	0

- Molecule 27 is a protein called bL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	As	115	920	590	157	169	4	0	0

- Molecule 28 is a protein called bL25m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	At	253	2003	1268	364	361	10	0	0

- Molecule 29 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Au	142	Total	C	N	O	S	0	0
			1149	734	212	200	3		

- Molecule 30 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Av	129	Total	C	N	O	S	0	0
			1058	670	187	198	3		

- Molecule 31 is a protein called uL29m.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Aw	123	Total	C	N	O	0	0
			1024	646	189	189		

- Molecule 32 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ax	176	Total	C	N	O	S	0	0
			1472	942	277	250	3		

- Molecule 33 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ay	72	Total	C	N	O	S	0	0
			592	387	103	100	2		

- Molecule 34 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Az	59	Total	C	N	O	S	0	0
			469	306	87	72	4		

- Molecule 35 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	50	Total	C	N	O	S	0	0
			416	276	72	66	2		

- Molecule 36 is a protein called bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	50	Total	C	N	O	S	0	0
			427	264	91	68	4		

- Molecule 37 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AC	139	Total	C	N	O	S	0	0
			1180	756	238	184	2		

- Molecule 38 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AD	46	Total	C	N	O	S	0	0
			375	236	78	57	4		

- Molecule 39 is a protein called mL40.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	AE	92	Total	C	N	O	0	0
			771	493	139	139		

- Molecule 40 is a protein called mL41.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	AF	93	Total	C	N	O	0	0
			765	495	140	130		

- Molecule 41 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AG	121	Total	C	N	O	S	0	0
			994	625	189	173	7		

- Molecule 42 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AH	176	Total	C	N	O	S	0	0
			1412	910	233	262	7		

- Molecule 43 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AI	64	Total	C	N	O	S	0	0
			505	325	92	87	1		

- Molecule 44 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AJ	122	Total	C	N	O	S	0	0
			1003	646	182	173	2		

- Molecule 45 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AK	139	Total	C	N	O	S	0	0
			1164	751	215	195	3		

- Molecule 46 is a protein called mL116.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AL	394	Total	C	N	O	S	0	0
			3093	1970	548	568	7		
46	AM	419	Total	C	N	O	S	0	0
			3282	2087	584	604	7		
46	AN	420	Total	C	N	O	S	0	0
			3286	2089	585	605	7		

- Molecule 47 is a protein called mL118.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AO	377	Total	C	N	O	S	0	0
			2881	1832	516	527	6		

- Molecule 48 is a protein called mL120.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Xa	199	Total	C	N	O	S	0	0
			1568	1000	268	296	4		

- Molecule 49 is a protein called mL121.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Xb	244	Total	C	N	O	S	0	0
			1956	1257	320	370	9		

- Molecule 50 is a protein called mL122.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	Xc	57	496	318	90	88	0	0

- Molecule 51 is a protein called mL123.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Xd	413	3236	2064	568	592	12	0	0

- Molecule 52 is a protein called mL124.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Xe	483	3675	2334	666	665	10	0	0

- Molecule 53 is a protein called mL125.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Xf	201	1615	1034	289	290	2	0	0

- Molecule 54 is a protein called mL126.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Xg	410	3081	1978	538	558	7	0	0

- Molecule 55 is a protein called mL127.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Xh	143	1147	736	208	200	3	0	0

- Molecule 56 is a protein called mL128.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Xi	24	206	131	40	34	1	0	0

- Molecule 57 is a protein called mL129.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Xj	71	Total	C	N	O	S	0	0
			582	362	104	115	1		

- Molecule 58 is a RNA chain called mtSSU-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	102	Total	C	N	O	P	0	0
			2165	969	376	718	102		

- Molecule 59 is a RNA chain called mtSSU-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	210	Total	C	N	O	P	0	0
			4484	2008	815	1451	210		

- Molecule 60 is a RNA chain called mtSSU-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	B3	373	Total	C	N	O	P	0	0
			7969	3570	1457	2569	373		

- Molecule 61 is a RNA chain called mtSSU-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	B4	332	Total	C	N	O	P	0	0
			7081	3175	1283	2291	332		

- Molecule 62 is a protein called bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Ba	242	Total	C	N	O	S	0	0
			1936	1222	344	361	9		

- Molecule 63 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bb	236	Total	C	N	O	S	0	0
			1878	1215	315	344	4		

- Molecule 64 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bc	289	Total	C	N	O	S	0	0
			2282	1451	408	416	7		

- Molecule 65 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bd	221	Total	C	N	O	S	0	0
			1793	1132	338	315	8		

- Molecule 66 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Be	228	Total	C	N	O	S	0	0
			1826	1153	336	330	7		

- Molecule 67 is a protein called uS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bf	119	Total	C	N	O	S	0	0
			969	624	170	171	4		

- Molecule 68 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bg	112	Total	C	N	O	S	0	0
			887	555	168	157	7		

- Molecule 69 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bh	374	Total	C	N	O	S	0	0
			3037	1949	549	533	6		

- Molecule 70 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bi	282	Total	C	N	O	S	0	0
			2271	1441	406	415	9		

- Molecule 71 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bj	401	Total	C	N	O	S	0	0
			3174	2020	543	597	14		

- Molecule 72 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bk	116	Total	C	N	O	S	0	0
			871	550	158	160	3		

- Molecule 73 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bl	123	Total	C	N	O	S	0	0
			962	604	190	164	4		

- Molecule 74 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bm	113	Total	C	N	O	S	0	0
			897	560	176	157	4		

- Molecule 75 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bn	118	Total	C	N	O	S	0	0
			978	613	194	167	4		

- Molecule 76 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bo	167	Total	C	N	O	S	0	0
			1212	759	234	213	6		

- Molecule 77 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bp	123	Total	C	N	O	S	0	0
			1013	655	184	172	2		

- Molecule 78 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bq	130	Total	C	N	O	S	0	0
			1053	662	200	187	4		

- Molecule 79 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Br	90	Total	C	N	O	S	0	0
			743	465	148	127	3		

- Molecule 80 is a protein called bS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bs	92	Total	C	N	O	S	0	0
			734	472	132	128	2		

- Molecule 81 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bt	75	Total	C	N	O	S	0	0
			621	396	117	107	1		

- Molecule 82 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bu	167	Total	C	N	O	S	0	0
			1366	874	240	248	4		

- Molecule 83 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bv	164	Total	C	N	O	S	0	0
			1355	846	249	256	4		

- Molecule 84 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bw	349	Total	C	N	O	S	0	0
			2749	1748	477	511	13		

- Molecule 85 is a protein called mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Bx	621	4714	2990	819	894	11	0	0

- Molecule 86 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	By	78	636	409	111	114	2	0	0

- Molecule 87 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	Bz	119	997	648	172	176	1	0	0

- Molecule 88 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	BA	176	1377	854	253	265	5	0	0

- Molecule 89 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
89	BB	84	663	411	129	118	5	0	0

- Molecule 90 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
90	BC	31	278	176	65	35	2	0	0

- Molecule 91 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
91	BD	270	2163	1364	383	406	10	0	0

- Molecule 92 is a protein called mS106.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	BE	171	Total	C	N	O	S	0	0
			1304	824	223	253	4		

- Molecule 93 is a protein called mS107.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	BF	370	Total	C	N	O	S	0	0
			2980	1897	541	533	9		

- Molecule 94 is a protein called uS4m-2 (fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
94	Ya	180	Total	C	N	O	S	0	0
			1434	904	252	272	6		

- Molecule 95 is a protein called mS108.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	Yb	50	Total	C	N	O	S	0	0
			412	260	77	74	1		

- Molecule 96 is a protein called mS109.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	Yc	159	Total	C	N	O	S	0	0
			1297	826	231	237	3		

- Molecule 97 is a protein called mS110.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	Yd	95	Total	C	N	O	S	0	0
			785	495	147	141	2		

- Molecule 98 is a protein called uS3m-2 (fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
98	Ye	106	Total	C	N	O	S	0	0
			864	559	156	147	2		

- Molecule 99 is a protein called mS111.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	Yf	150	Total	C	N	O	S	0	0
			1236	792	218	221	5		

- Molecule 100 is a protein called mS112.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	Yg	67	Total	C	N	O	S	0	0
			553	344	108	97	4		

- Molecule 101 is a protein called mS113.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	Yh	65	Total	C	N	O	S	0	0
			530	339	99	91	1		

- Molecule 102 is a protein called mS114.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	Yi	132	Total	C	N	O	S	0	0
			1075	692	197	184	2		

- Molecule 103 is a protein called mS115.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	Yj	386	Total	C	N	O	S	0	0
			2859	1796	497	559	7		

- Molecule 104 is a protein called mS116.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	Yk	92	Total	C	N	O	S	0	0
			707	460	113	133	1		

- Molecule 105 is a protein called uS7m-2 (fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
105	Yl	84	Total	C	N	O	S	0	0
			673	428	115	127	3		

- Molecule 106 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
106	Ua	32	Total	C	N	O	0	0
			166	99	35	32		

- Molecule 107 is a protein called mL105.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	Ub	131	Total	C	N	O	S	0	0
			1098	692	190	210	6		

- Molecule 108 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
108	Ud	43	Total	C	N	O	0	0
			215	129	43	43		

- Molecule 109 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
109	Ue	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 110 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
110	Uf	73	Total	C	N	O	0	0
			365	219	73	73		

- Molecule 111 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
111	Ug	63	Total	C	N	O	0	0
			315	189	63	63		

- Molecule 112 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
112	Uh	48	Total	C	N	O	0	0
			240	144	48	48		

- Molecule 113 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
113	Ui	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 114 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
114	Uj	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 115 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
115	Uk	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 116 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
116	Ul	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 117 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
117	Um	11	Total	C	N	O	0	0
			55	33	11	11		

- Molecule 118 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
118	A1	3	Total	Mg	0
			3	3	
118	A2	2	Total	Mg	0
			2	2	
118	A3	9	Total	Mg	0
			9	9	
118	A4	10	Total	Mg	0
			10	10	
118	A5	2	Total	Mg	0
			2	2	
118	A6	6	Total	Mg	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
118	A7	23	Total 23	Mg 23	0
118	A8	15	Total 15	Mg 15	0
118	Ab	1	Total 1	Mg 1	0
118	B1	3	Total 3	Mg 3	0
118	B2	8	Total 8	Mg 8	0
118	B3	14	Total 14	Mg 14	0
118	B4	14	Total 14	Mg 14	0
118	Bm	1	Total 1	Mg 1	0
118	Bw	1	Total 1	Mg 1	0

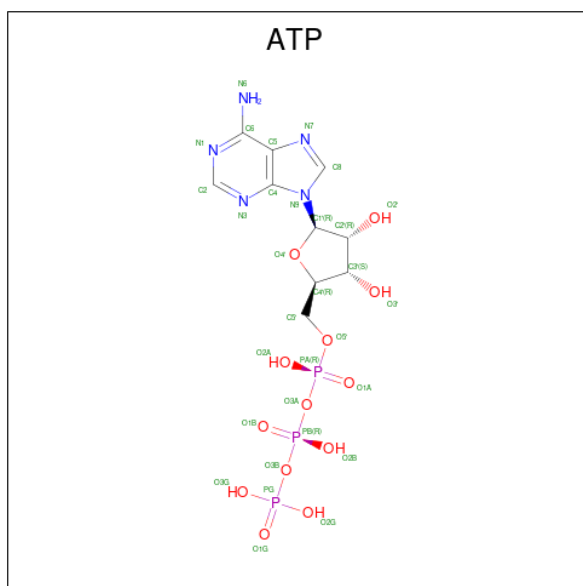
- Molecule 119 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
119	A1	1	Total 1	K 1	0
119	A3	1	Total 1	K 1	0
119	A4	2	Total 2	K 2	0
119	A7	6	Total 6	K 6	0
119	A8	5	Total 5	K 5	0
119	Ab	2	Total 2	K 2	0
119	B1	2	Total 2	K 2	0
119	B2	1	Total 1	K 1	0
119	B3	8	Total 8	K 8	0
119	B4	3	Total 3	K 3	0

- Molecule 120 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
120	AD	1	Total	Zn	0
			1	1	

- Molecule 121 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
121	Bw	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 122 is water.

Mol	Chain	Residues	Atoms		AltConf
122	A1	15	Total	O	0
			15	15	
122	A2	8	Total	O	0
			8	8	
122	A3	31	Total	O	0
			31	31	
122	A4	33	Total	O	0
			33	33	
122	A5	9	Total	O	0
			9	9	
122	A6	21	Total	O	0
			21	21	

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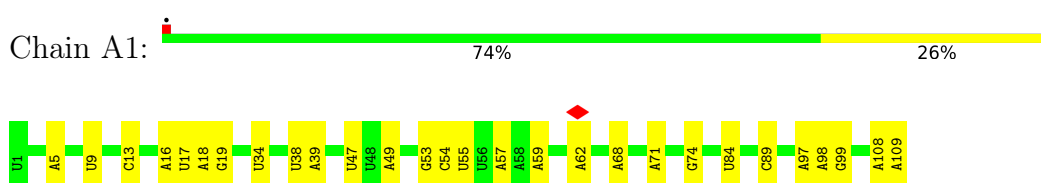
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Mol	Chain	Residues	Atoms		AltConf
122	A7	112	Total 112	O 112	0
122	A8	73	Total 73	O 73	0
122	Aa	2	Total 2	O 2	0
122	Ab	4	Total 4	O 4	0
122	Ac	1	Total 1	O 1	0
122	Aj	3	Total 3	O 3	0
122	AC	1	Total 1	O 1	0
122	AI	4	Total 4	O 4	0
122	AK	1	Total 1	O 1	0
122	B1	11	Total 11	O 11	0
122	B2	38	Total 38	O 38	0
122	B3	57	Total 57	O 57	0
122	B4	68	Total 68	O 68	0
122	Be	3	Total 3	O 3	0
122	Bi	2	Total 2	O 2	0
122	Bl	2	Total 2	O 2	0
122	Bm	1	Total 1	O 1	0
122	Bo	1	Total 1	O 1	0
122	Bp	1	Total 1	O 1	0
122	Ya	2	Total 2	O 2	0

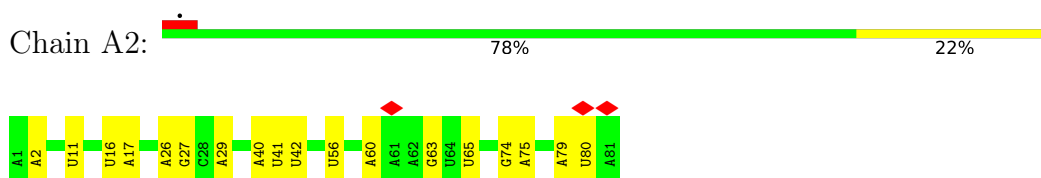
3 Residue-property plots [i](#)

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

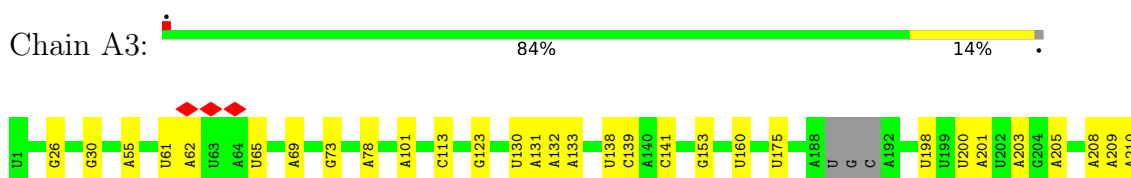
- Molecule 1: mtLSU-1



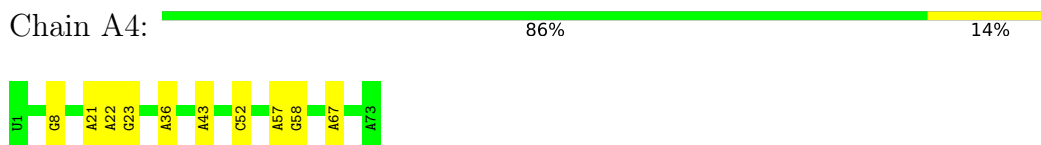
- Molecule 2: mtLSU-2



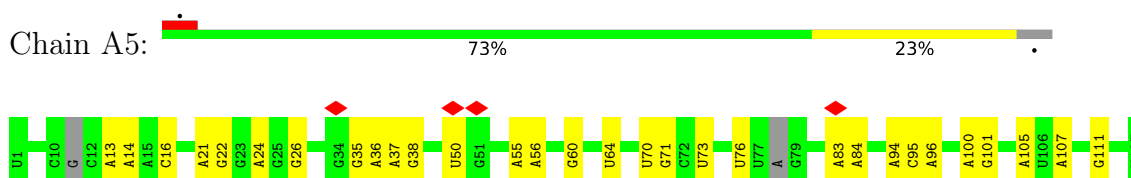
- Molecule 3: mtLSU-3

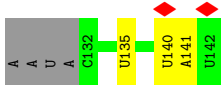


- Molecule 4: mtLSU-4



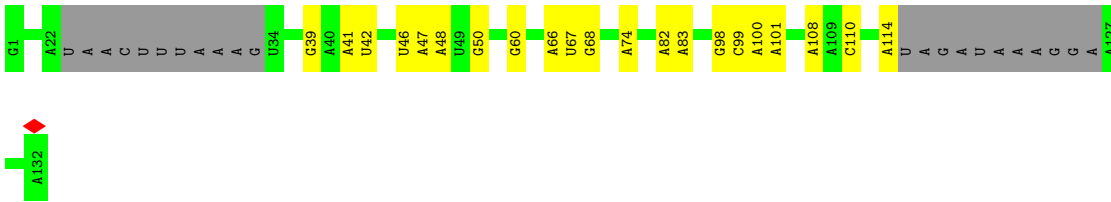
- Molecule 5: mtLSU-5





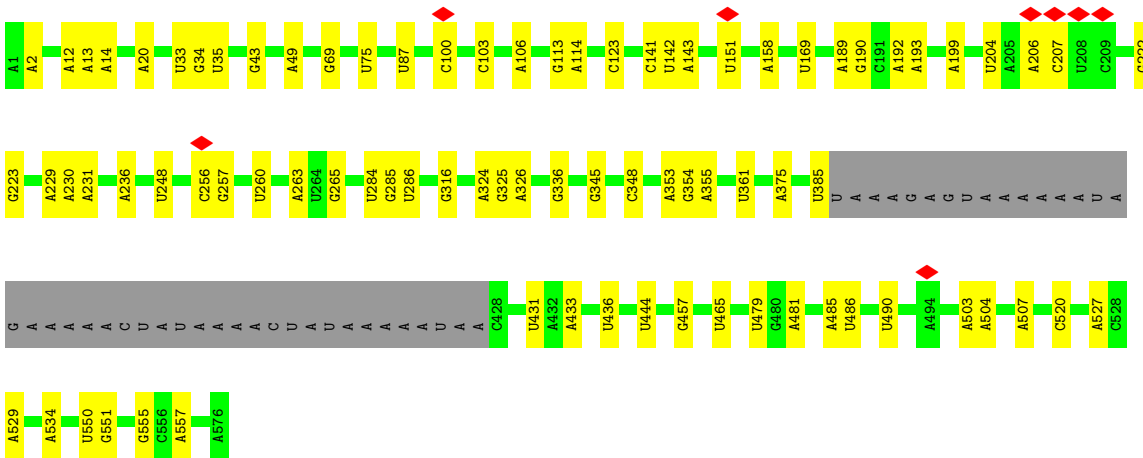
- Molecule 6: mtLSU-6

Chain A6: 67% 16% 17%



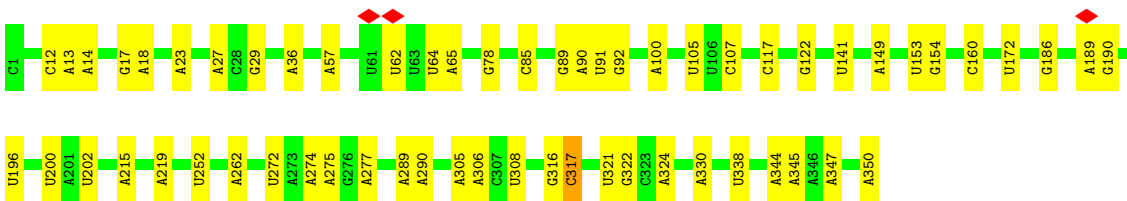
- Molecule 7: mtLSU-7

Chain A7: 78% 14% 7%



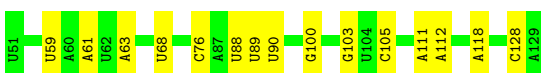
- Molecule 8: mtLSU-8

Chain A8: 83% 17%

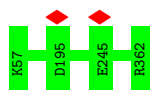


- Molecule 9: mt-5S

Chain A9: 78% 22%



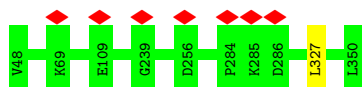
- Molecule 10: uL2m



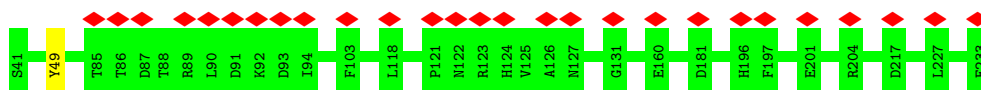
• Molecule 11: uL3m



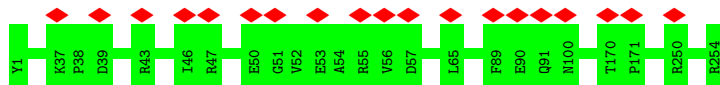
• Molecule 12: uL4m



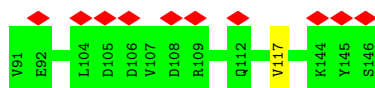
• Molecule 13: uL5m



• Molecule 14: uL6m



• Molecule 15: uL9m

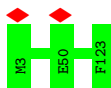


• Molecule 16: uL13m



• Molecule 17: uL14m

Chain Ai:  100%



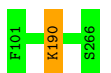
- Molecule 18: uL15m

Chain Aj:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: uL16m

Chain Ak:  99%



- Molecule 20: bL17m

Chain Al:  99%



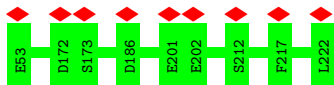
- Molecule 21: uL18m

Chain Am:  100%



- Molecule 22: bL19m

Chain An:  5%  100%

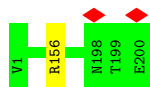


- Molecule 23: bL20m

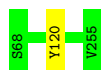
Chain Ao:  100%



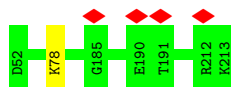
- Molecule 24: bL21m



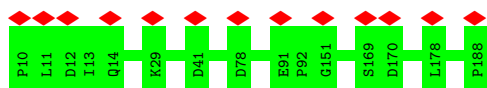
- Molecule 25: uL22m



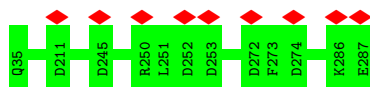
- Molecule 26: uL23m



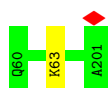
- Molecule 27: bL24m



- Molecule 28: bL25m



- Molecule 29: bL27m

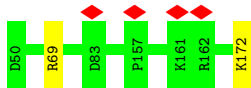


- Molecule 30: bL28m



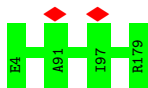
- Molecule 31: uL29m

Chain Aw:  98%

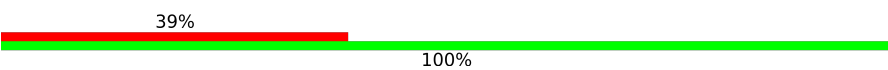


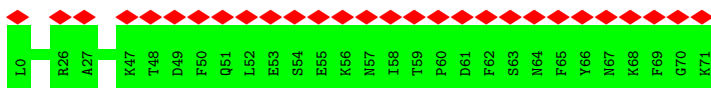
- Molecule 32: uL30m

Chain Ax:  100%



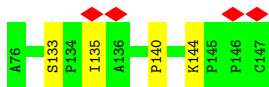
- Molecule 33: bL31m

Chain Ay:  39%
100%



- Molecule 34: bL31m

Chain Az:  7%
93% 7%



- Molecule 35: bL33m

Chain AA:  100%



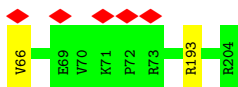
- Molecule 36: bL34m

Chain AB:  100%

There are no outlier residues recorded for this chain.

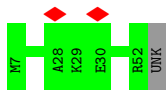
- Molecule 37: bL35m

Chain AC:  99%



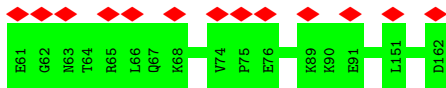
- Molecule 38: bL36m

Chain AD:  98%



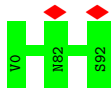
- Molecule 39: mL40

Chain AE:  14% 100%



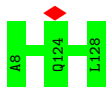
- Molecule 40: mL41

Chain AF:  100%



- Molecule 41: mL43

Chain AG:  100%



- Molecule 42: mL46

Chain AH:  14% 99%



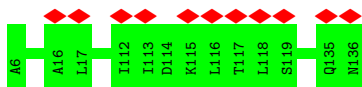
- Molecule 43: mL63

Chain AI:  100%

There are no outlier residues recorded for this chain.

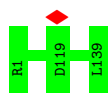
- Molecule 44: mL64

Chain AJ:  9% 100%

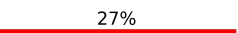




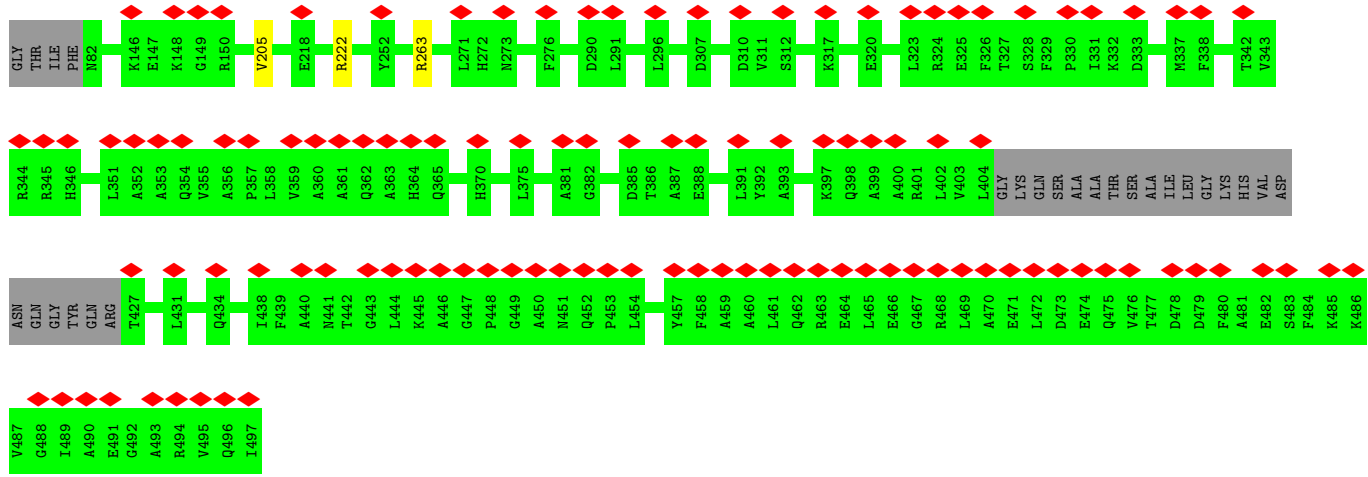
- Molecule 45: mL87

Chain AK:  100%



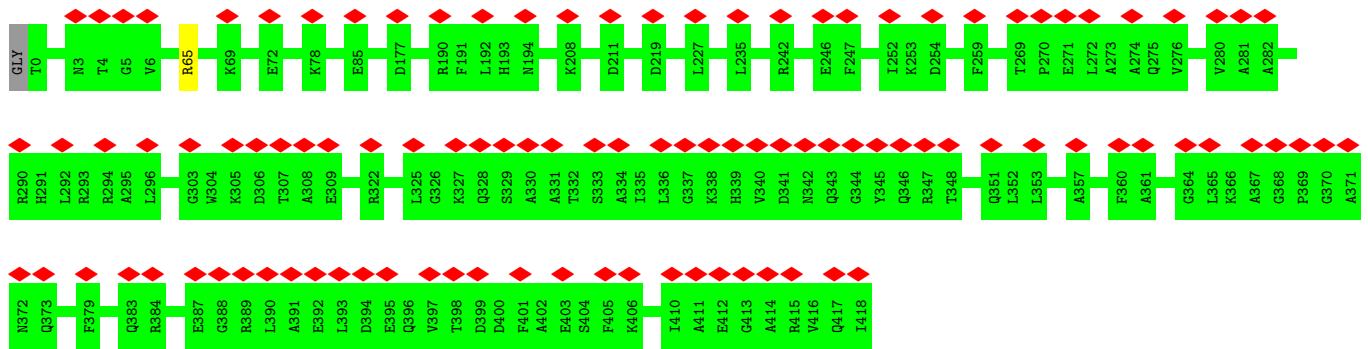
• Molecule 46: mL116

Chain AL:  27%  93%  6%



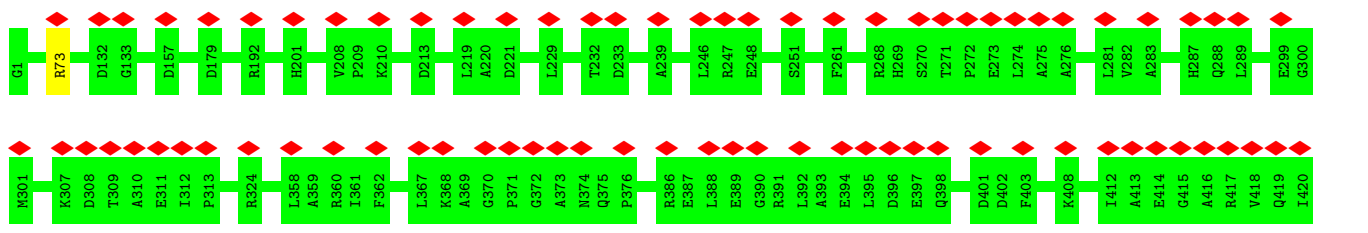
• Molecule 46: mL116

Chain AM:  25%  100%

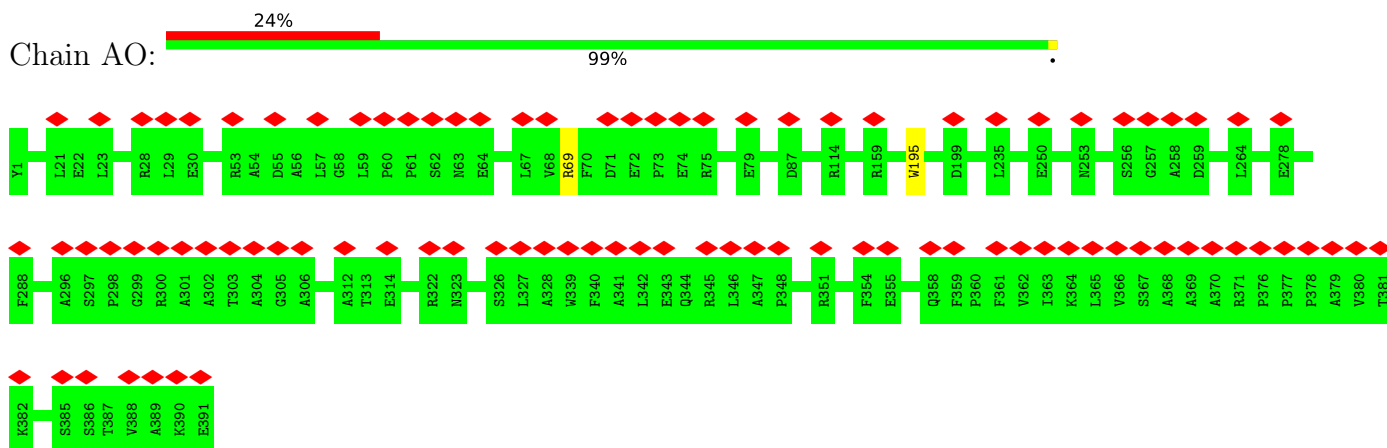


• Molecule 46: mL116

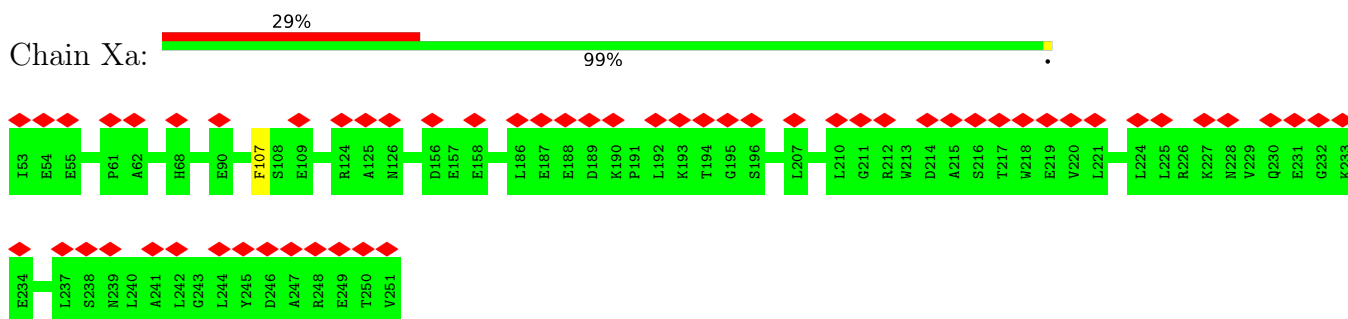
Chain AN:  18%  100%



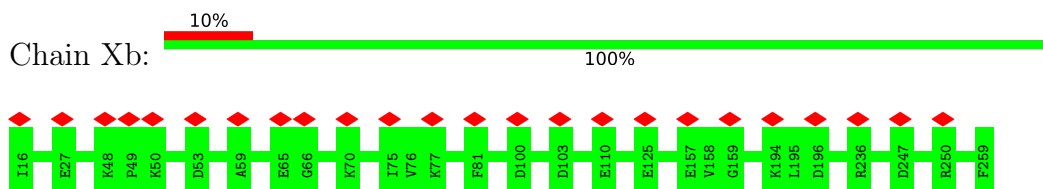
- Molecule 47: mL118



- Molecule 48: mL120



- Molecule 49: mL121

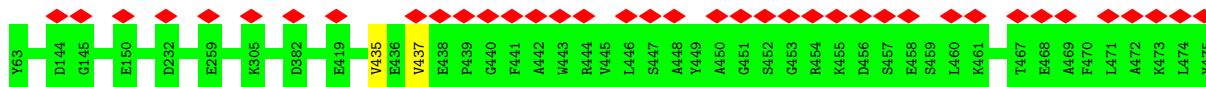


- Molecule 50: mL122



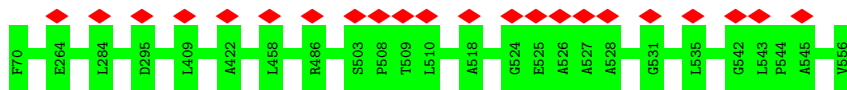
There are no outlier residues recorded for this chain.

- Molecule 51: mL123



- Molecule 52: mL124

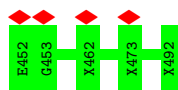




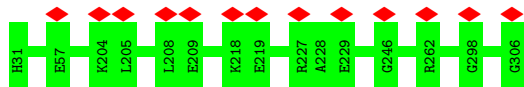
• Molecule 53: mL125



• Molecule 54: mL126



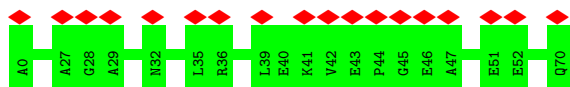
• Molecule 55: mL127



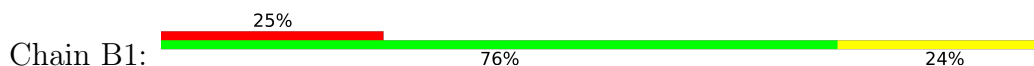
• Molecule 56: mL128

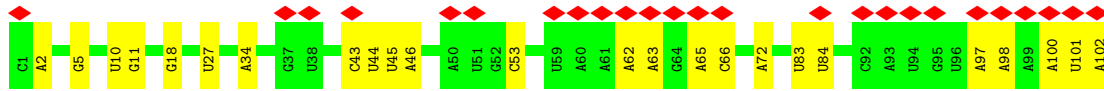


• Molecule 57: mL129

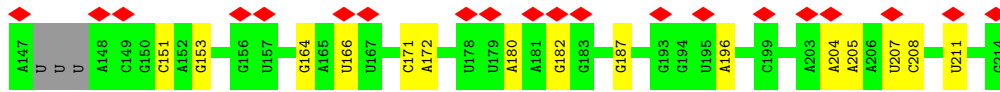
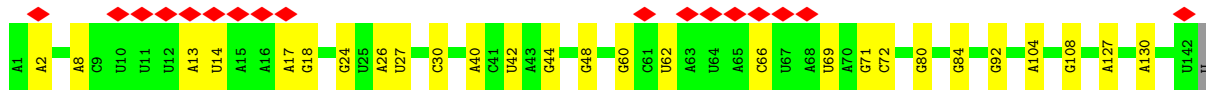
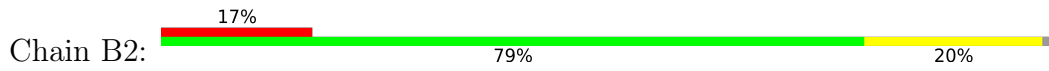


• Molecule 58: mtSSU-1

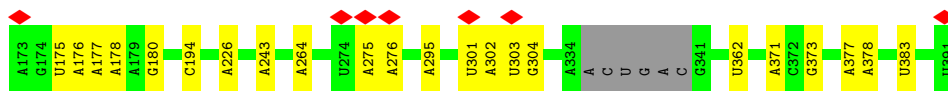
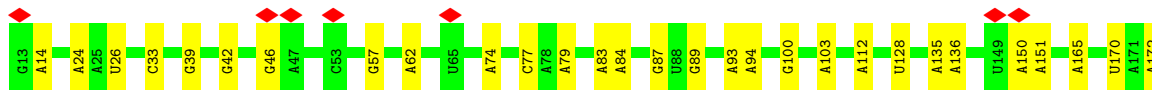
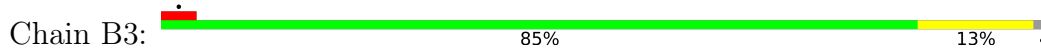




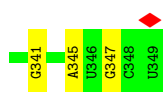
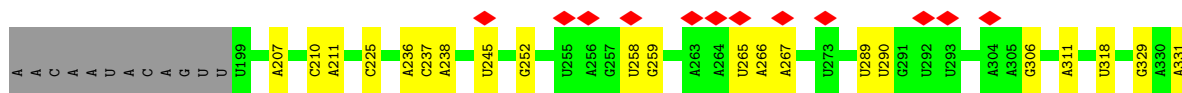
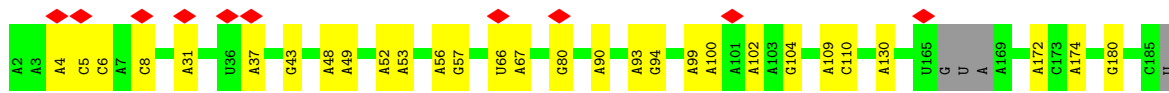
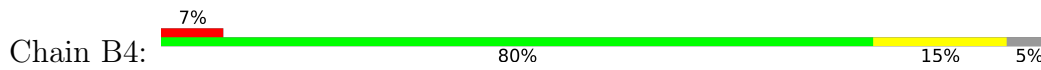
• Molecule 59: mtSSU-2



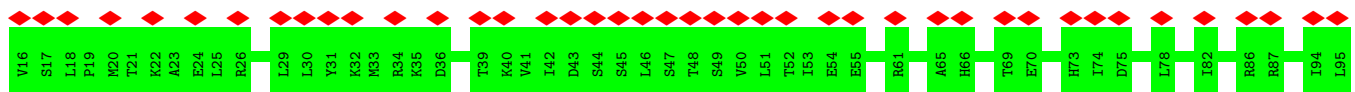
• Molecule 60: mtSSU-3

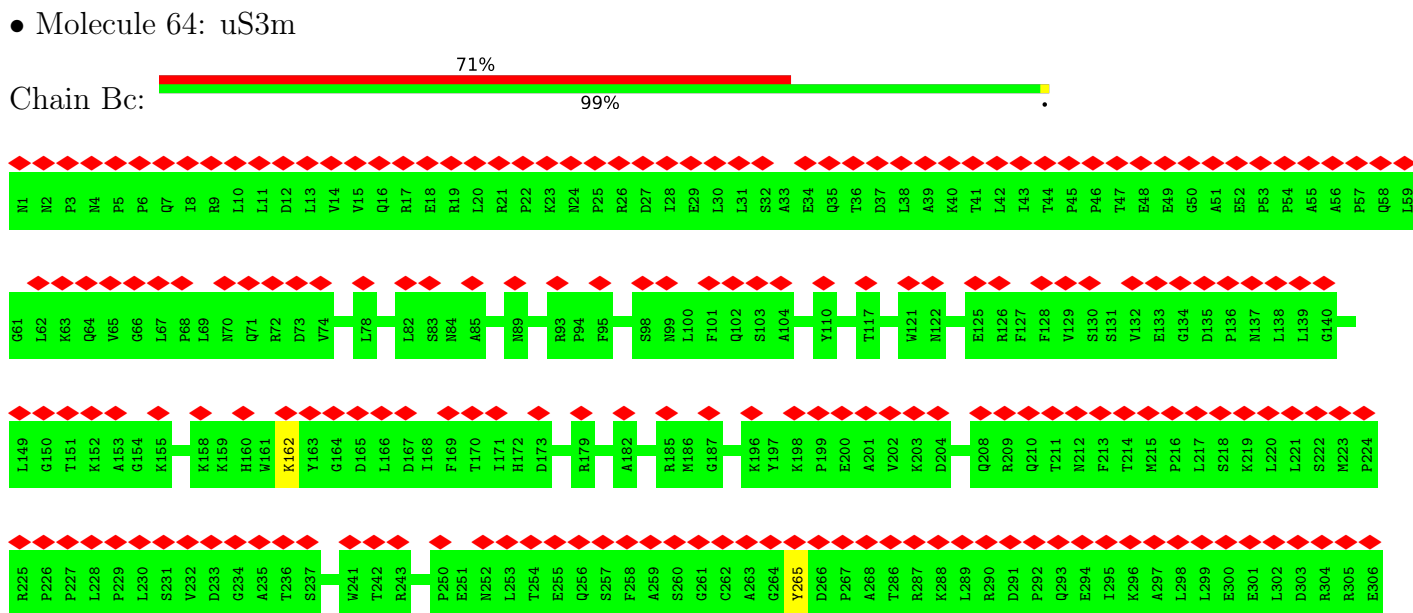
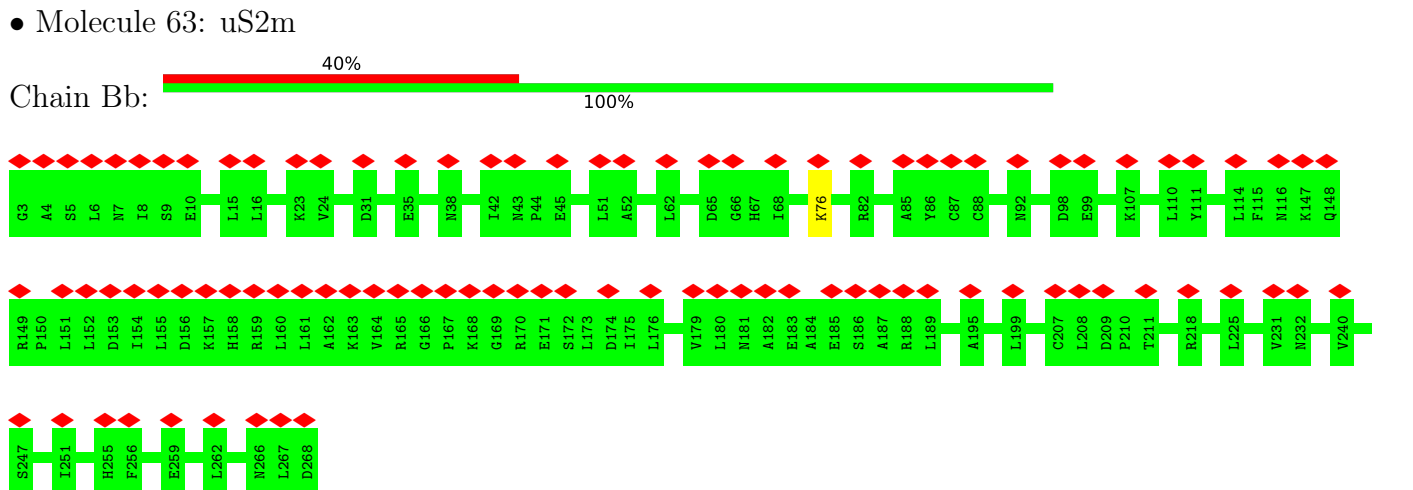


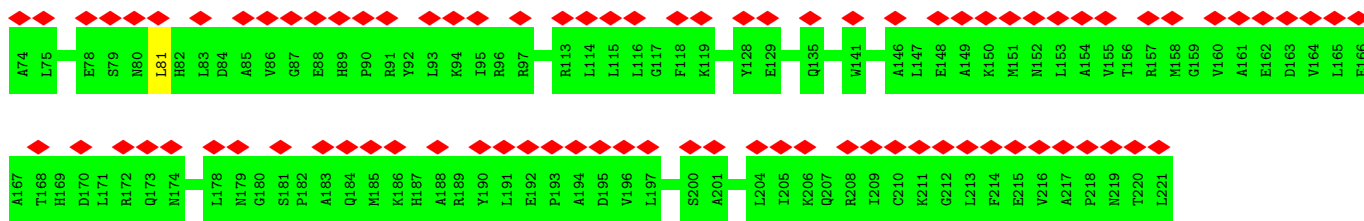
• Molecule 61: mtSSU-4



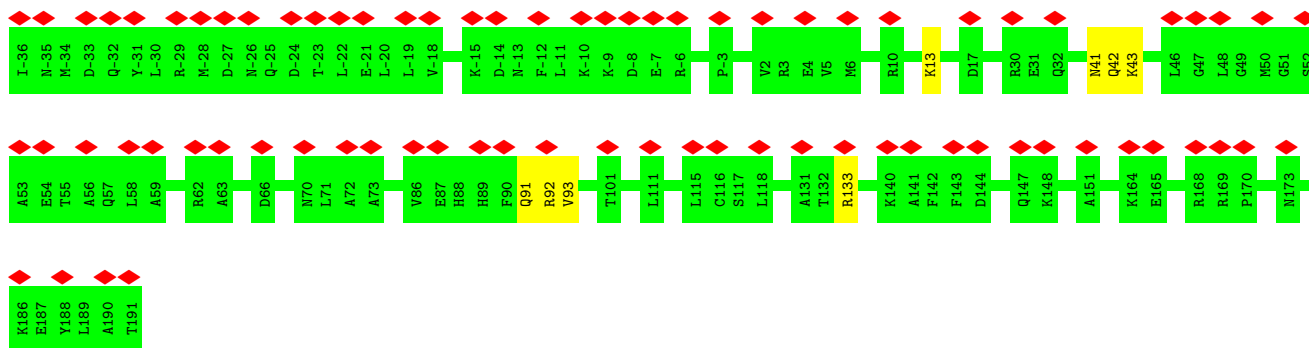
• Molecule 62: bS1m



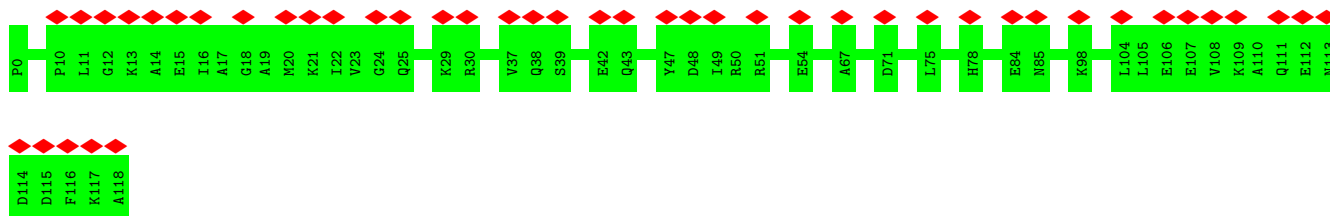
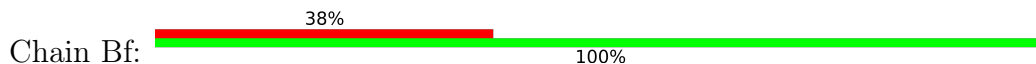




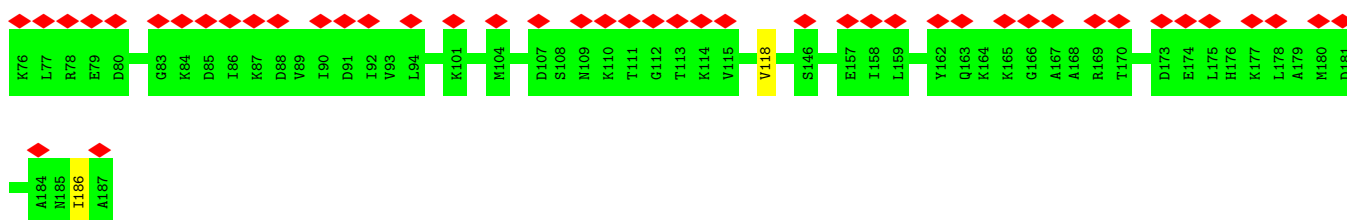
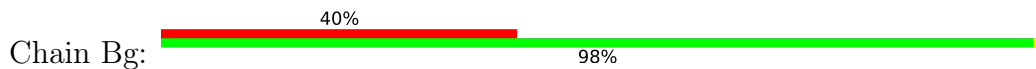
- Molecule 66: uS5m



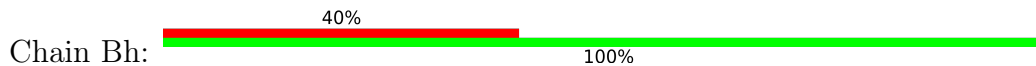
- Molecule 67: uS6m

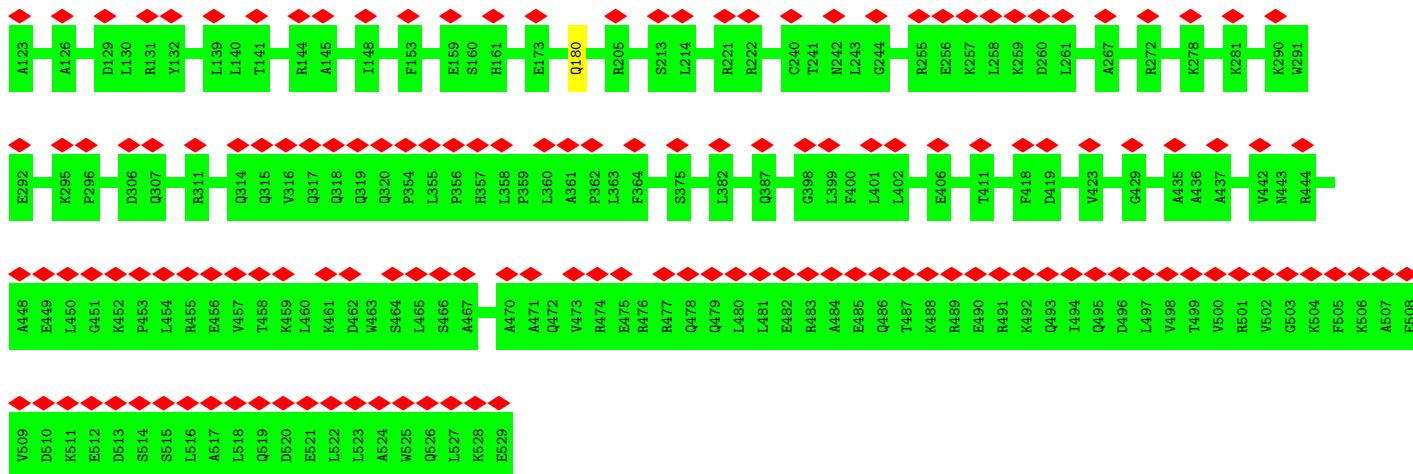


- Molecule 68: uS7m

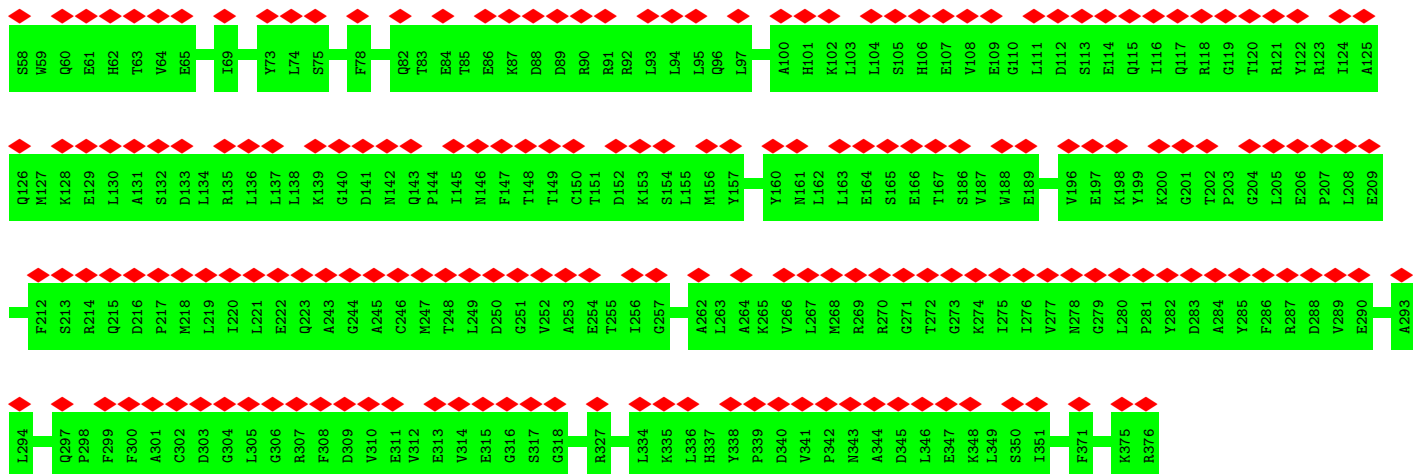


- Molecule 69: uS8m

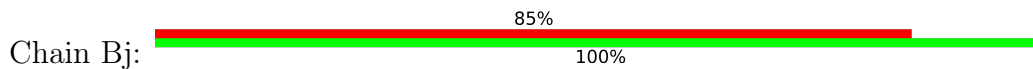


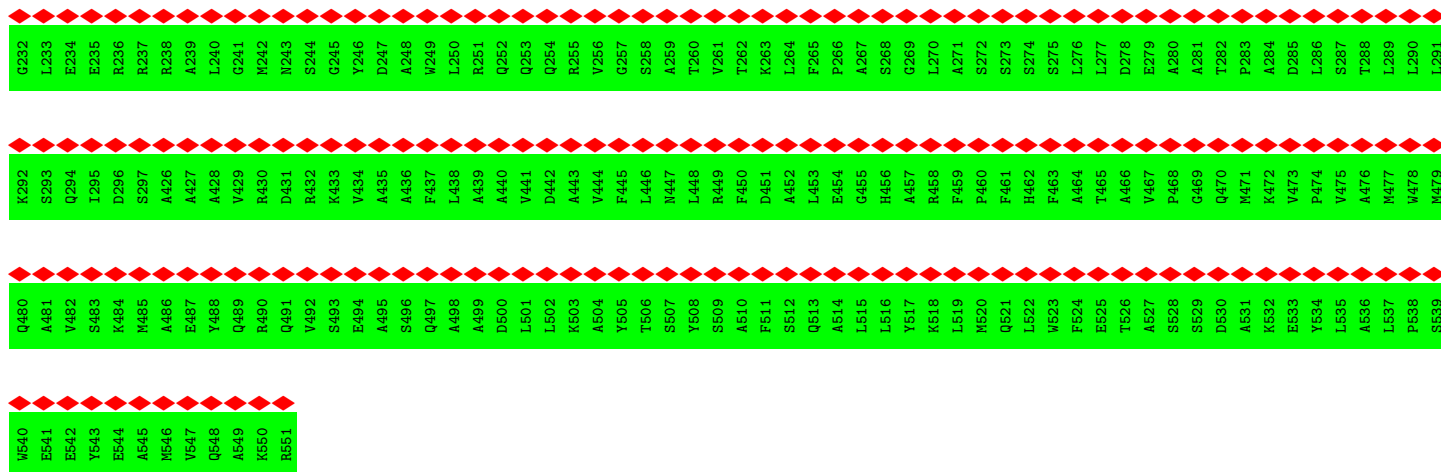


• Molecule 70: uS9m

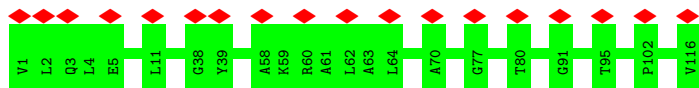


• Molecule 71: uS10m

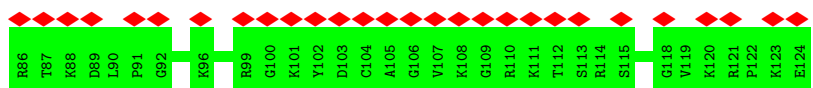
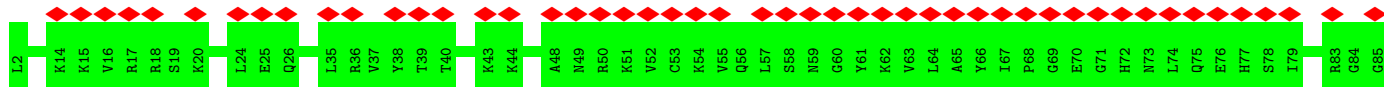




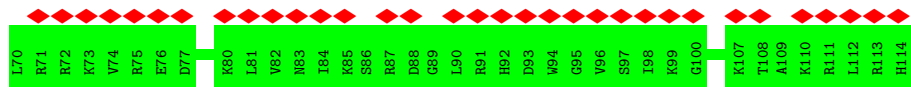
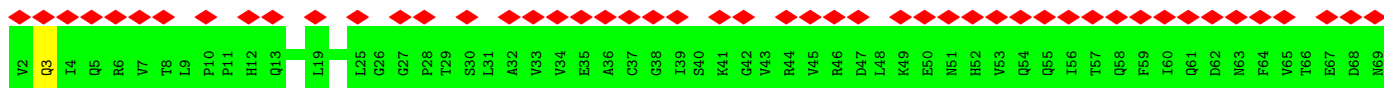
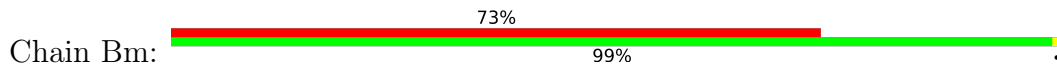
• Molecule 72: uS11m



• Molecule 73: uS12m

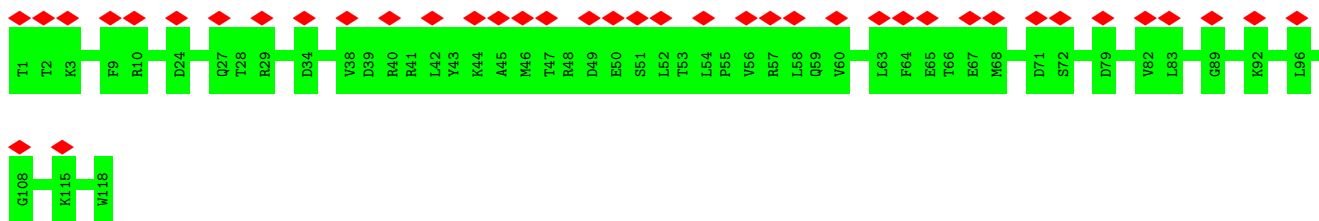


• Molecule 74: uS13m

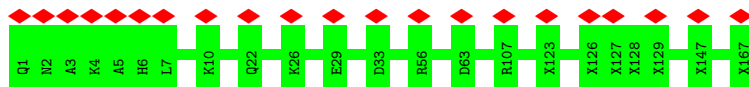


• Molecule 75: uS14m

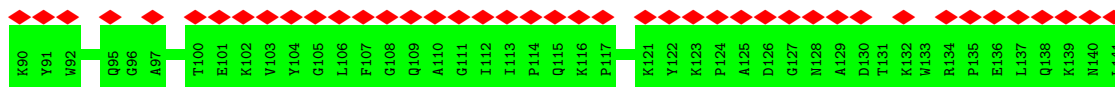
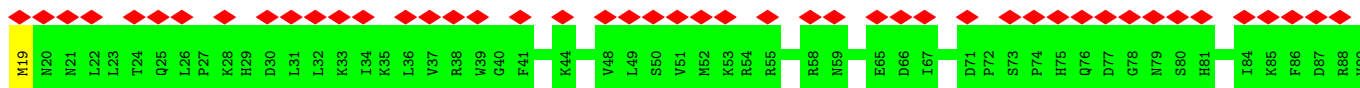
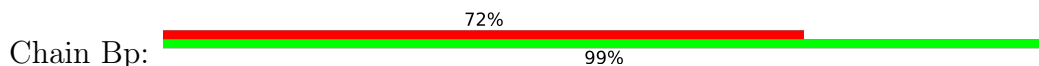




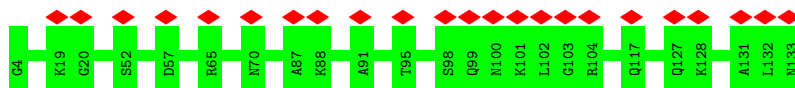
- Molecule 76: uS15m



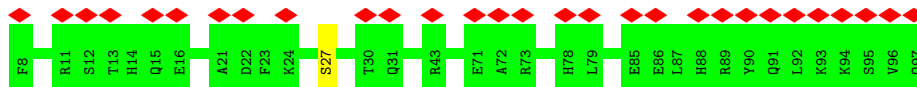
- Molecule 77: bS16m



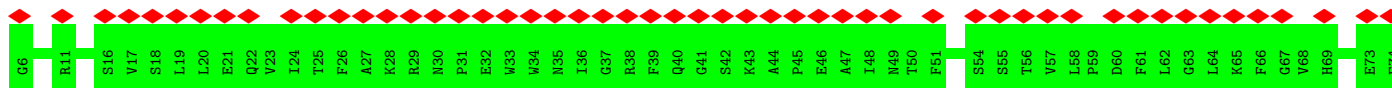
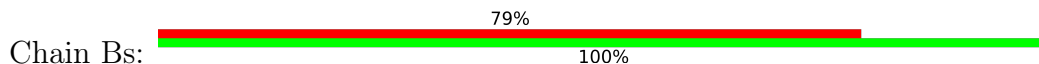
- Molecule 78: uS17m

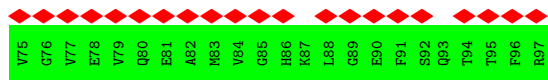


- Molecule 79: bS18m

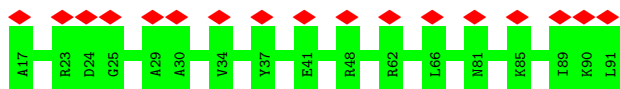


- Molecule 80: bS19m

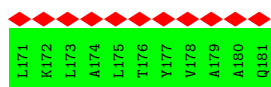
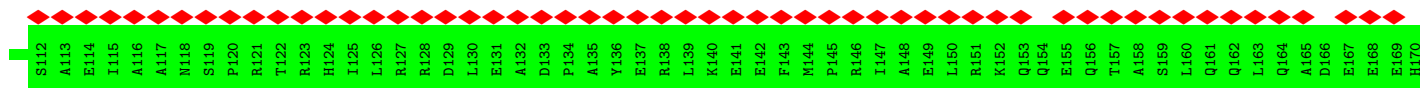
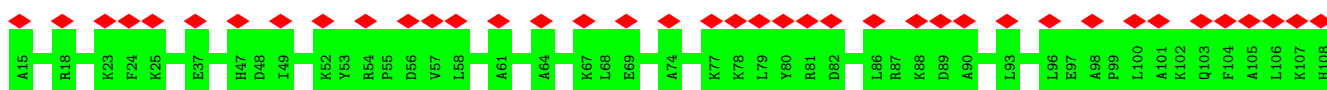




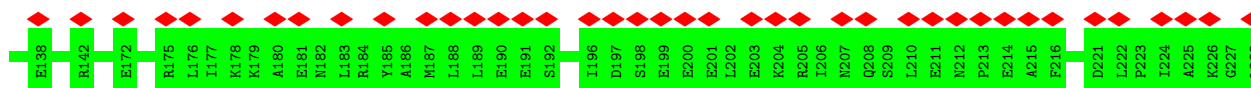
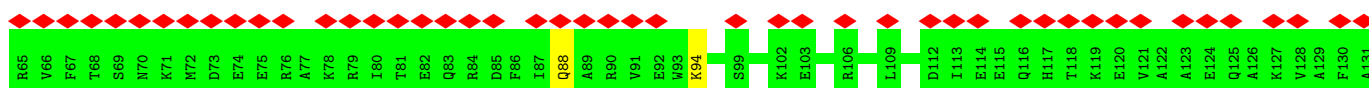
• Molecule 81: bS21m



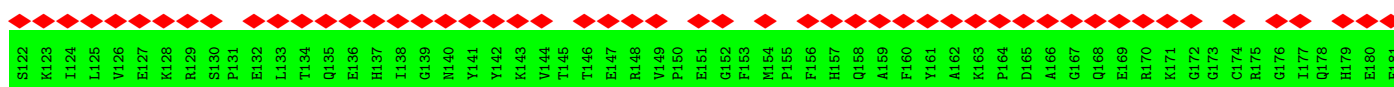
• Molecule 82: mS23

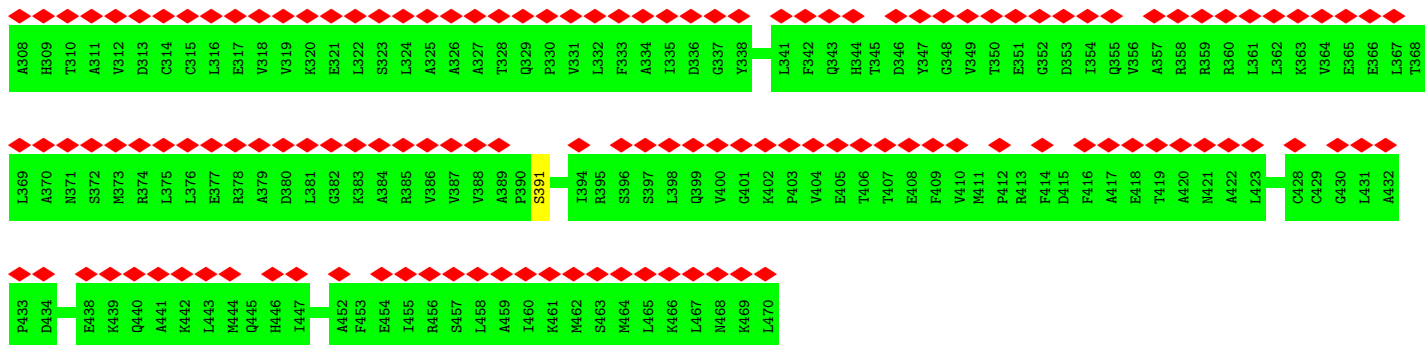


• Molecule 83: mS26

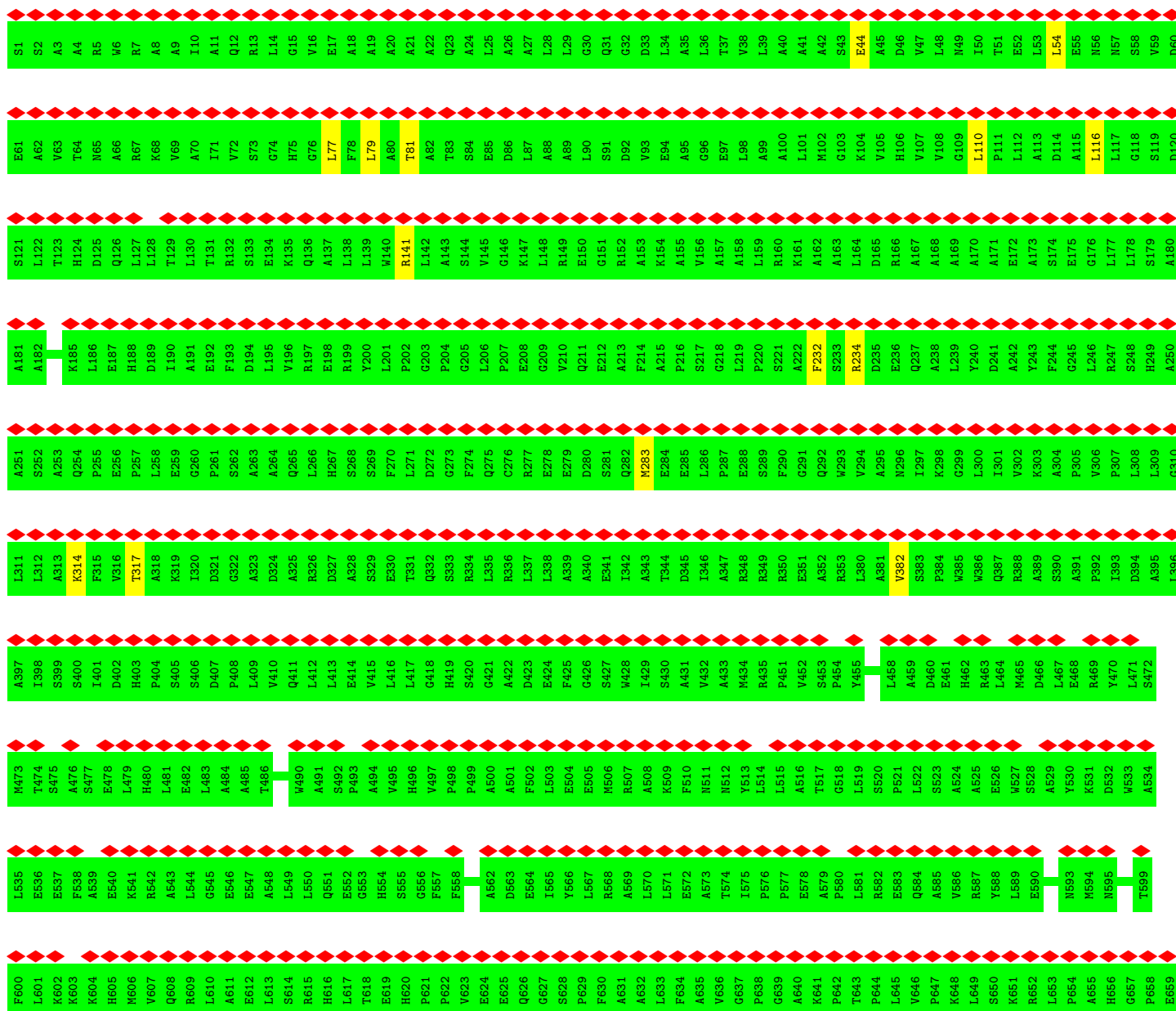


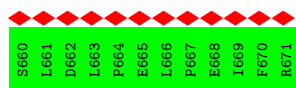
• Molecule 84: mS29



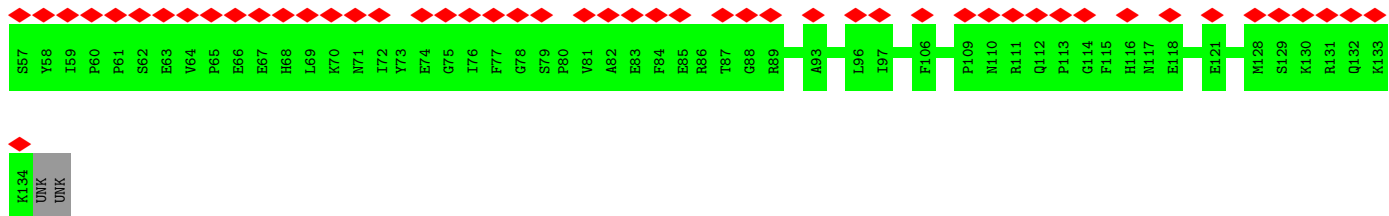


• Molecule 85: mS31

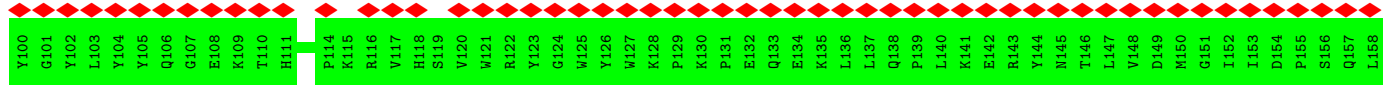
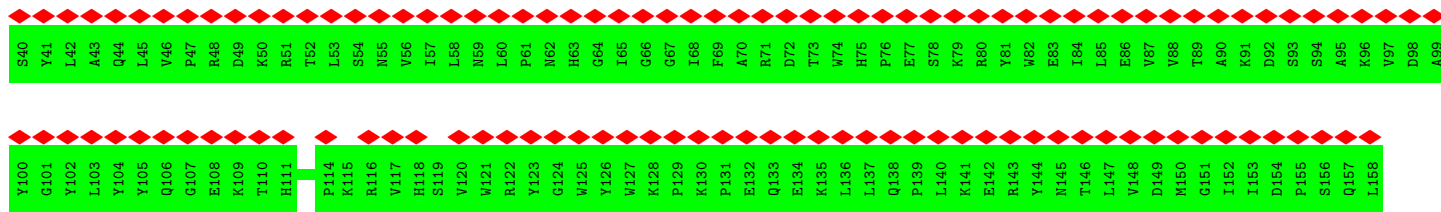




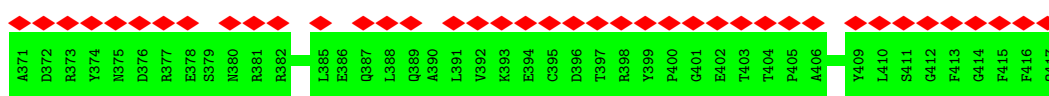
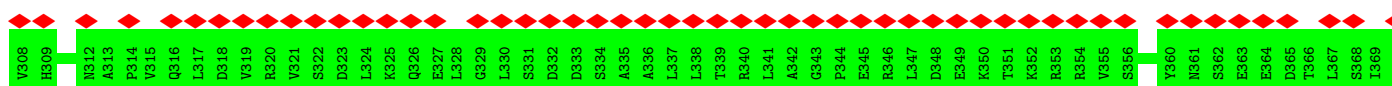
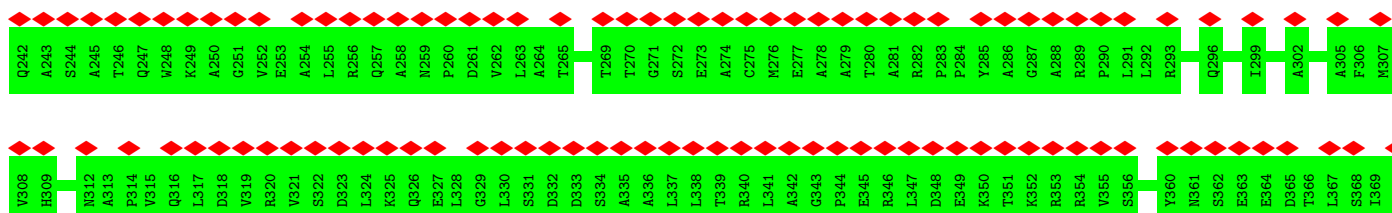
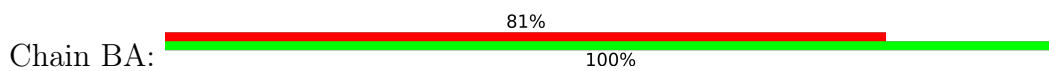
• Molecule 86: mS33



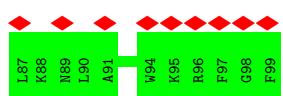
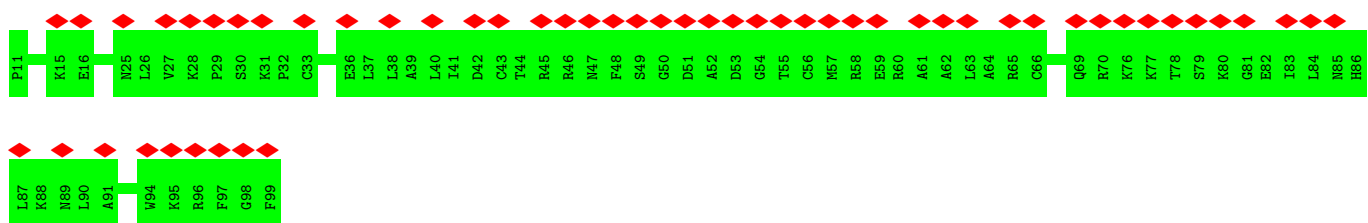
• Molecule 87: mS34



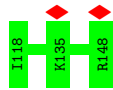
• Molecule 88: mS35



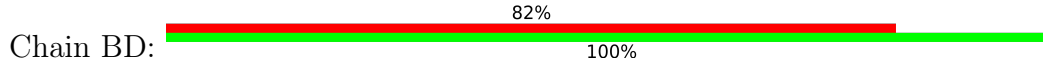
• Molecule 89: mS37



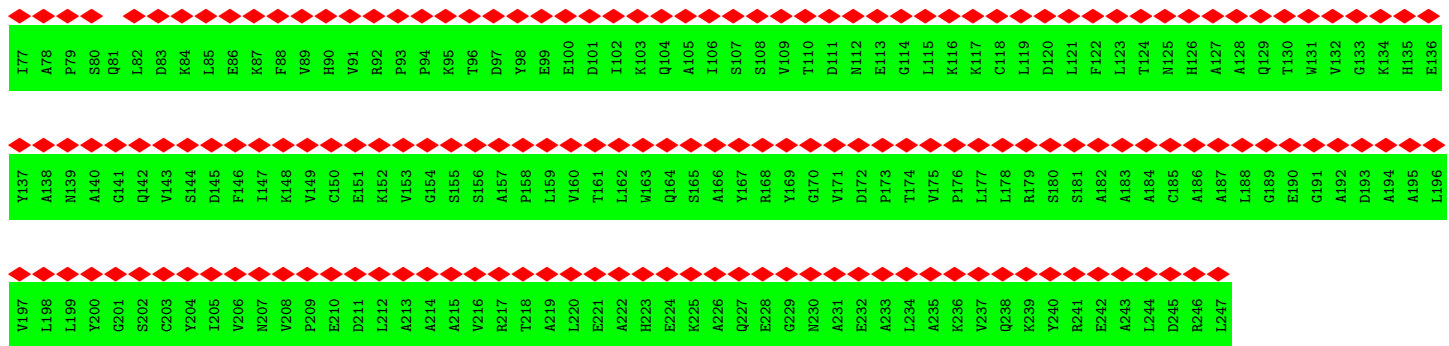
• Molecule 90: mS38



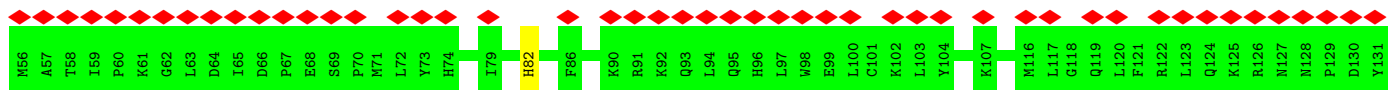
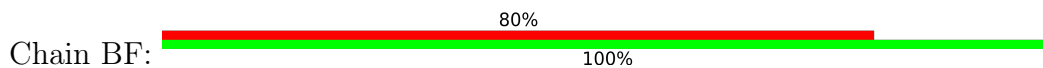
• Molecule 91: mS45



• Molecule 92: mS106

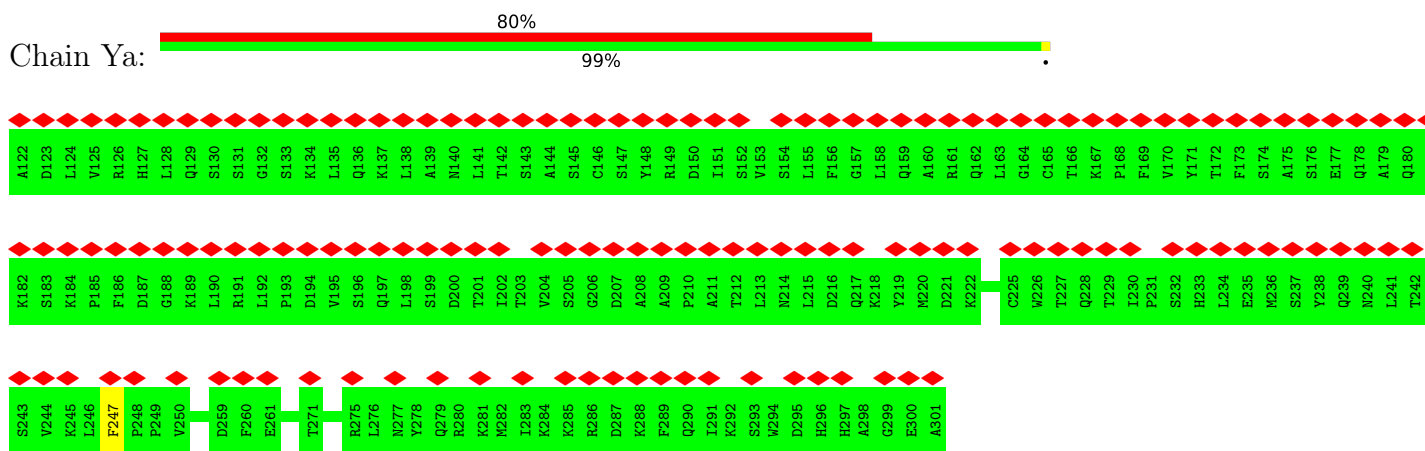


• Molecule 93: mS107

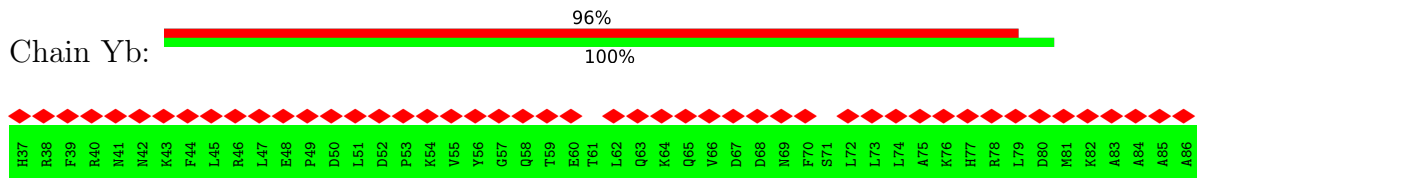




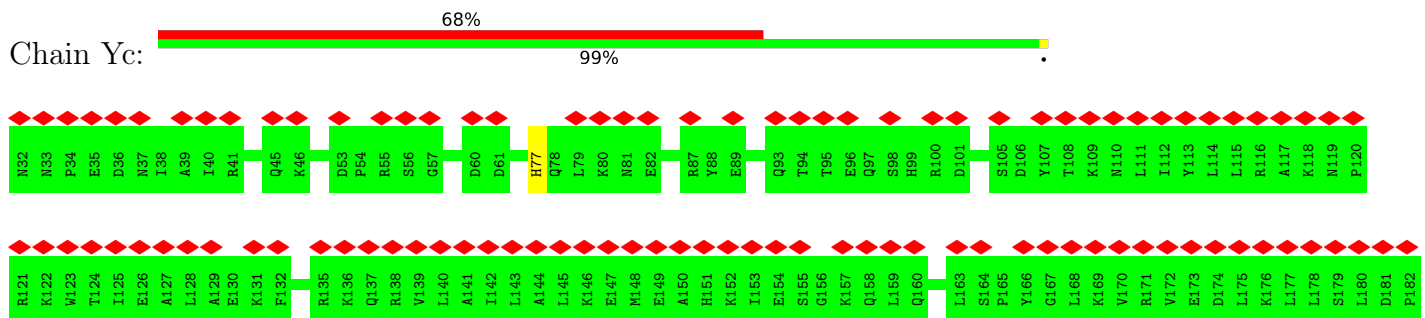
• Molecule 94: uS4m-2 (fragment)

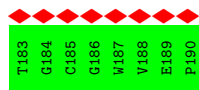


• Molecule 95: mS108

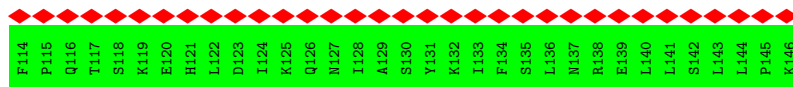
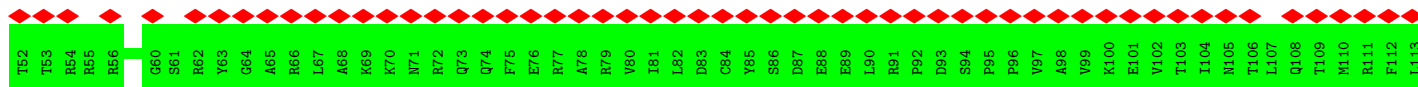


• Molecule 96: mS109

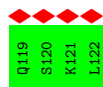
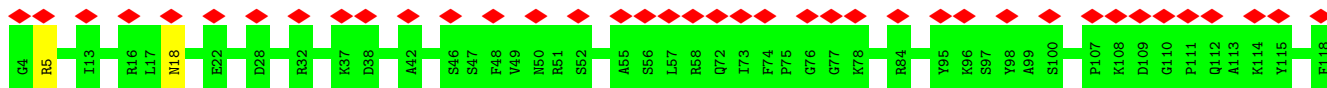
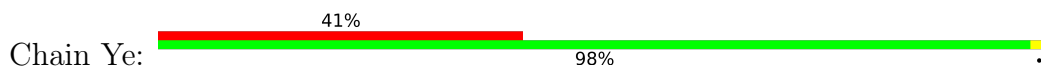




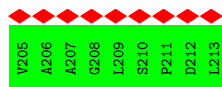
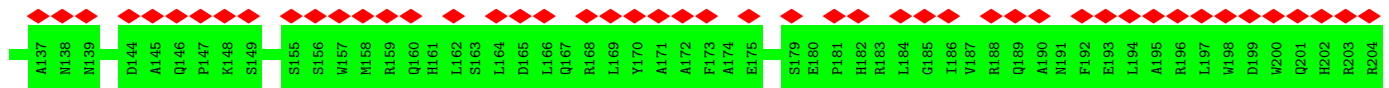
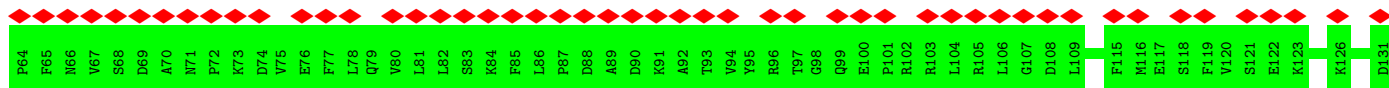
• Molecule 97: mS110



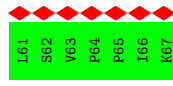
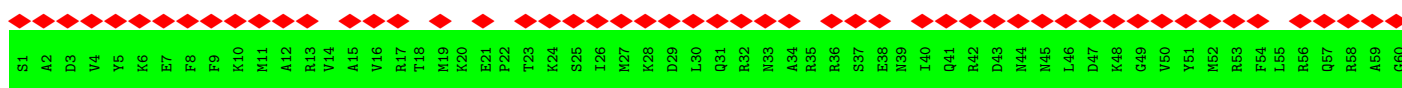
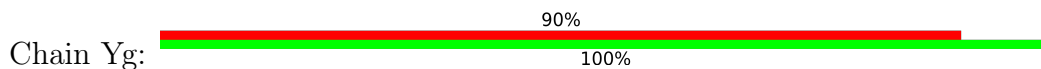
• Molecule 98: uS3m-2 (fragment)



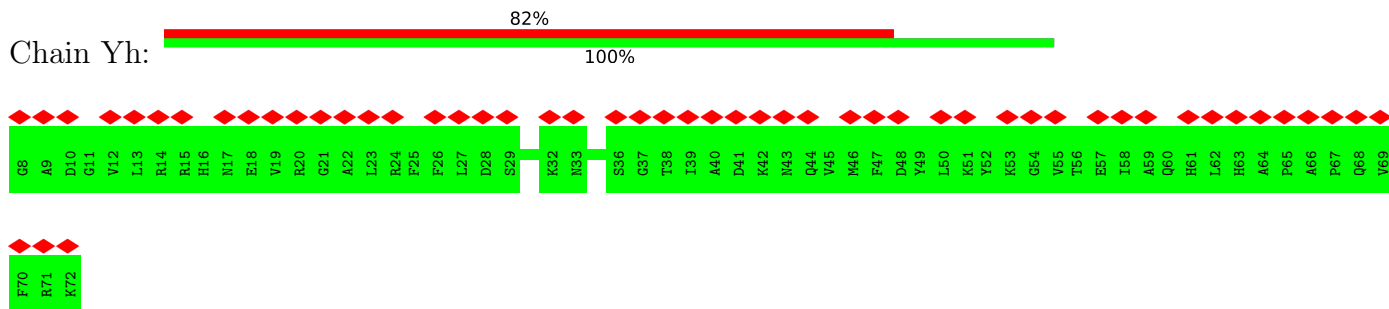
• Molecule 99: mS111



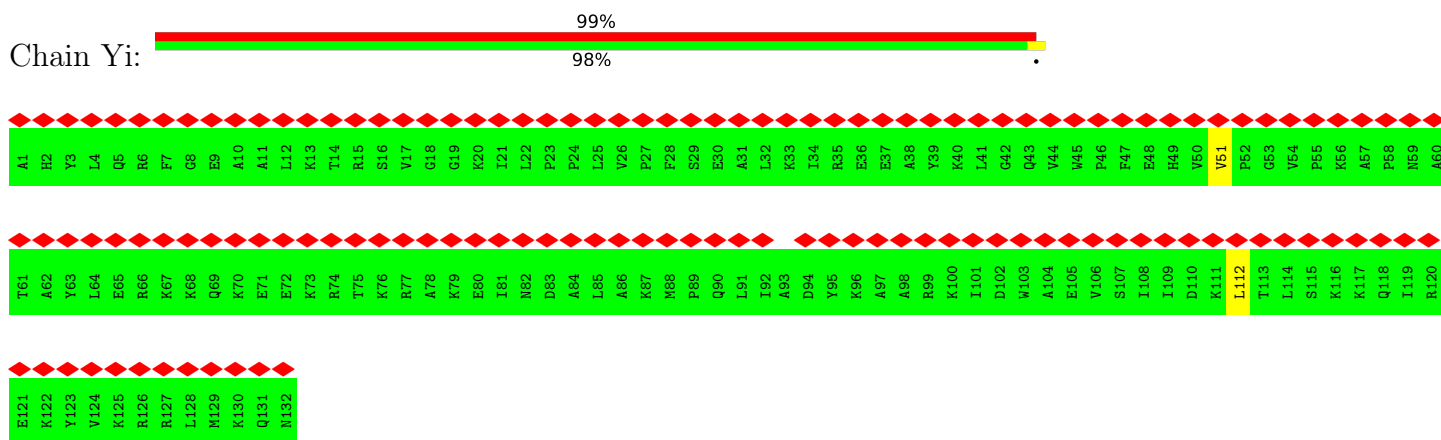
• Molecule 100: mS112



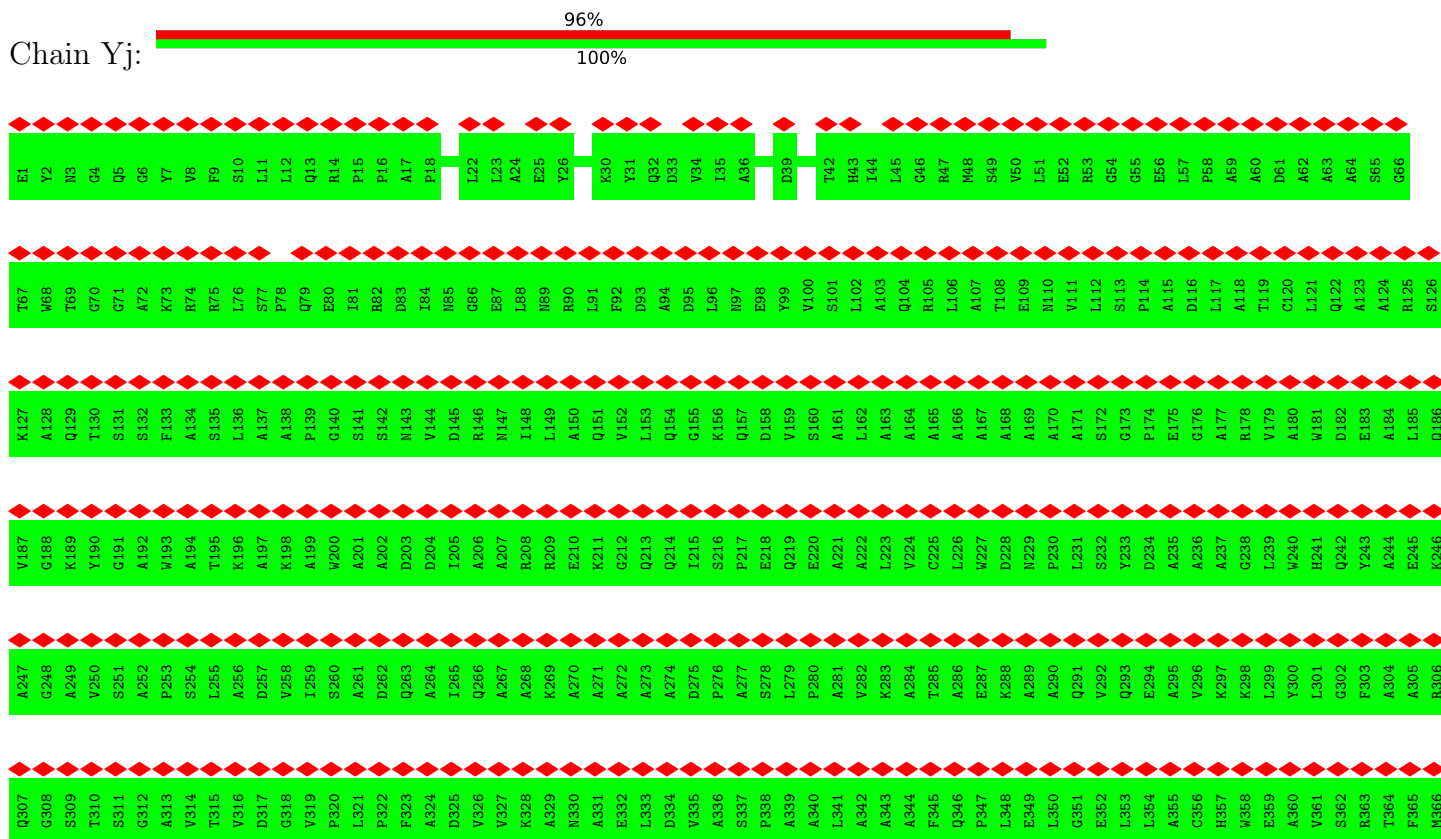
• Molecule 101: mS113

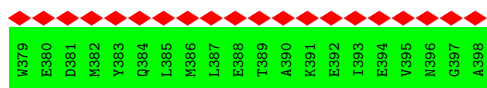


• Molecule 102: mS114

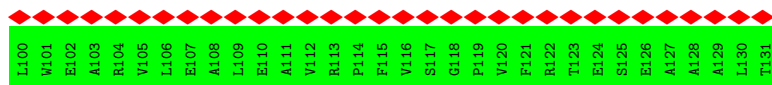
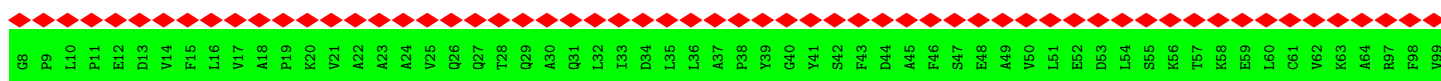


• Molecule 103: mS115

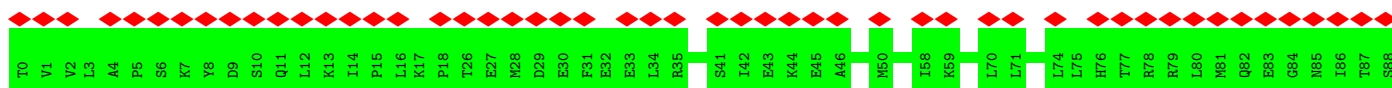




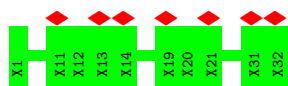
• Molecule 104: mS116



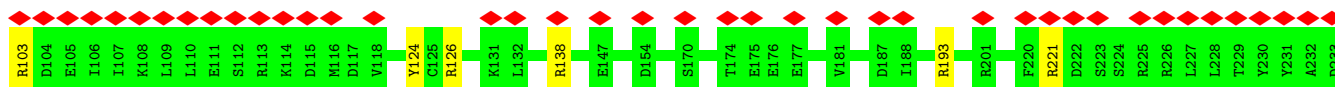
• Molecule 105: uS7m-2 (fragment)



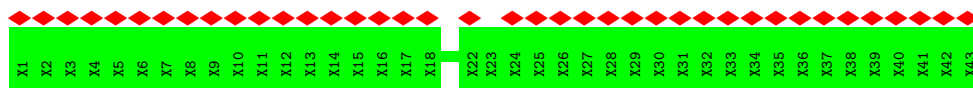
• Molecule 106: Unknown



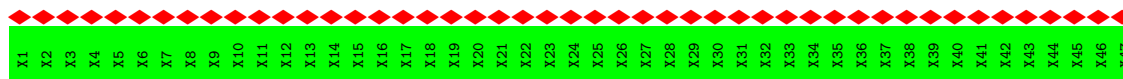
• Molecule 107: mL105



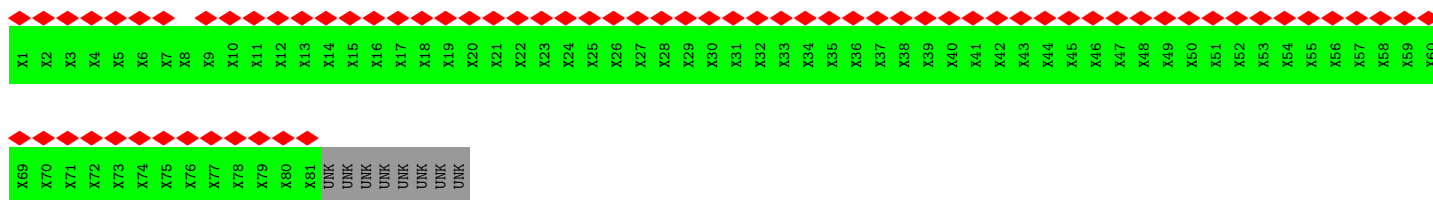
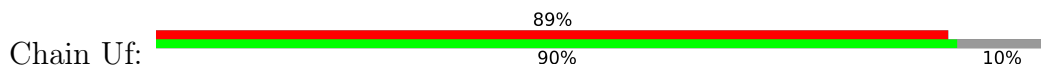
• Molecule 108: Unknown



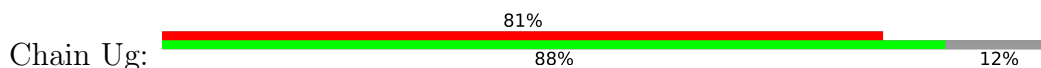
• Molecule 109: Unknown



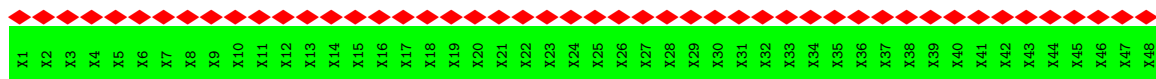
● Molecule 110: Unknown



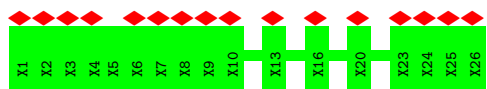
● Molecule 111: Unknown



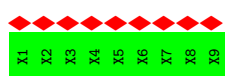
● Molecule 112: Unknown



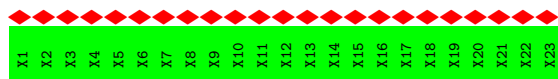
● Molecule 113: Unknown



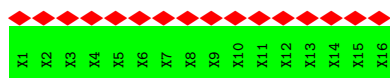
● Molecule 114: Unknown



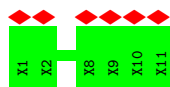
● Molecule 115: Unknown



• Molecule 116: Unknown



• Molecule 117: Unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184300	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	592.2, 592.2, 592.2	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.846, 0.846, 0.846	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, ATP, ZN

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	A1	0.28	0/2632	0.68	0/4101
2	A2	0.30	0/1938	0.70	0/3016
3	A3	0.26	0/4942	0.70	0/7693
4	A4	0.31	0/1764	0.72	0/2749
5	A5	0.17	0/3239	0.66	0/5036
6	A6	0.26	0/2619	0.70	0/4075
7	A7	0.25	0/12753	0.69	3/19862 (0.0%)
8	A8	0.24	0/8336	0.69	1/12985 (0.0%)
9	A9	0.21	0/1637	0.66	0/2545
10	Aa	0.24	0/2439	0.44	0/3287
11	Ab	0.25	0/2483	0.43	0/3369
12	Ac	0.26	0/2431	0.44	0/3290
13	Ad	0.24	0/1574	0.40	0/2136
14	Ae	0.25	0/1982	0.40	0/2683
15	Af	0.23	0/437	0.42	0/589
16	Ah	0.24	0/1555	0.41	0/2098
17	Ai	0.24	0/972	0.43	0/1303
18	Aj	0.25	0/1643	0.43	0/2220
19	Ak	0.23	0/1389	0.44	0/1869
20	Al	0.23	0/1438	0.41	0/1938
21	Am	0.24	0/931	0.40	0/1258
22	An	0.24	0/1420	0.41	0/1914
23	Ao	0.23	0/981	0.39	0/1314
24	Ap	0.24	0/1600	0.45	0/2176
25	Aq	0.25	0/1566	0.42	0/2106
26	Ar	0.28	0/1309	0.45	0/1759
27	As	0.24	0/938	0.39	0/1263
28	At	0.24	0/2041	0.42	0/2755
29	Au	0.24	0/1182	0.42	0/1596
30	Av	0.22	0/1073	0.39	0/1443
31	Aw	0.22	0/1043	0.37	0/1401
32	Ax	0.24	0/1508	0.41	0/2028

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ay	0.25	0/610	0.38	0/827
34	Az	0.41	0/484	0.69	1/652 (0.2%)
35	AA	0.24	0/426	0.41	0/572
36	AB	0.23	0/432	0.47	0/568
37	AC	0.24	0/1217	0.42	0/1639
38	AD	0.23	0/379	0.44	0/500
39	AE	0.23	0/790	0.34	0/1066
40	AF	0.27	0/782	0.45	0/1053
41	AG	0.24	0/1019	0.41	0/1373
42	AH	0.25	0/1444	0.43	0/1945
43	AI	0.23	0/515	0.39	0/696
44	AJ	0.23	0/1023	0.35	0/1370
45	AK	0.24	0/1206	0.37	0/1635
46	AL	0.24	0/3152	0.38	0/4271
46	AM	0.24	0/3345	0.37	0/4532
46	AN	0.24	0/3349	0.37	0/4537
47	AO	0.24	0/2941	0.38	0/4000
48	Xa	0.23	0/1600	0.37	0/2178
49	Xb	0.24	0/1999	0.37	0/2701
50	Xc	0.24	0/509	0.41	0/684
51	Xd	0.24	0/3305	0.38	0/4478
52	Xe	0.23	0/3748	0.38	0/5096
53	Xf	0.24	0/1659	0.39	0/2253
54	Xg	0.25	0/3018	0.39	0/4098
55	Xh	0.23	0/1169	0.38	0/1578
56	Xi	0.24	0/209	0.35	0/273
57	Xj	0.25	0/596	0.40	0/802
58	B1	0.23	0/2419	0.67	0/3765
59	B2	0.23	0/5020	0.68	0/7818
60	B3	0.23	0/8926	0.68	0/13905
61	B4	0.20	0/7929	0.67	0/12345
62	Ba	0.23	0/1967	0.41	0/2662
63	Bb	0.23	0/1920	0.38	0/2615
64	Bc	0.24	0/2340	0.40	0/3182
65	Bd	0.23	0/1825	0.41	0/2459
66	Be	0.24	0/1863	0.42	0/2521
67	Bf	0.24	0/989	0.39	0/1334
68	Bg	0.22	0/898	0.36	0/1205
69	Bh	0.23	0/3109	0.38	0/4215
70	Bi	0.24	0/2317	0.39	0/3119
71	Bj	0.25	0/3243	0.38	0/4384
72	Bk	0.25	0/882	0.46	0/1193
73	Bl	0.24	0/977	0.43	0/1303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Bm	0.22	0/910	0.39	0/1223
75	Bn	0.24	0/995	0.43	0/1336
76	Bo	0.24	0/963	0.39	0/1284
77	Bp	0.24	0/1046	0.41	0/1414
78	Bq	0.24	0/1068	0.40	0/1434
79	Br	0.22	0/754	0.39	0/1009
80	Bs	0.25	0/754	0.41	0/1019
81	Bt	0.23	0/630	0.36	0/840
82	Bu	0.24	0/1395	0.36	0/1878
83	Bv	0.23	0/1372	0.36	0/1835
84	Bw	0.28	0/2804	0.43	0/3791
85	Bx	0.44	0/4813	0.47	0/6545
86	By	0.26	0/655	0.38	0/883
87	Bz	0.23	0/1030	0.38	0/1400
88	BA	0.23	0/1405	0.40	0/1907
89	BB	0.23	0/673	0.36	0/896
90	BC	0.21	0/280	0.39	0/365
91	BD	0.24	0/2207	0.39	0/2977
92	BE	0.23	0/1328	0.35	0/1805
93	BF	0.23	0/3039	0.37	0/4111
94	Ya	0.26	0/1466	0.41	0/1979
95	Yb	0.23	0/419	0.35	0/562
96	Yc	0.23	0/1328	0.39	0/1799
97	Yd	0.23	0/797	0.39	0/1069
98	Ye	0.25	0/887	0.40	0/1191
99	Yf	0.24	0/1276	0.38	0/1735
100	Yg	0.25	0/560	0.36	0/744
101	Yh	0.24	0/543	0.37	0/730
102	Yi	0.24	0/1096	0.40	0/1470
103	Yj	0.23	0/2911	0.36	0/3966
104	Yk	0.24	0/721	0.35	0/982
105	Yl	0.24	0/680	0.39	0/911
106	Ua	0.54	0/10	0.78	0/11
107	Ub	1.00	0/1118	0.95	7/1501 (0.5%)
All	All	0.26	0/203278	0.52	12/287861 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
107	Ub	221	ARG	NE-CZ-NH2	-9.79	115.40	120.30
34	Az	140	PRO	CA-N-CD	-9.16	98.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
107	Ub	126	ARG	NE-CZ-NH2	-7.62	116.49	120.30
107	Ub	138	ARG	NE-CZ-NH2	-6.96	116.82	120.30
7	A7	457	G	N3-C2-N2	6.86	124.70	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Aa	304/306 (99%)	295 (97%)	9 (3%)	0	100	100
11	Ab	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
12	Ac	301/303 (99%)	300 (100%)	1 (0%)	0	100	100
13	Ad	191/193 (99%)	187 (98%)	4 (2%)	0	100	100
14	Ae	236/242 (98%)	235 (100%)	1 (0%)	0	100	100
15	Af	54/56 (96%)	54 (100%)	0	0	100	100
16	Ah	182/186 (98%)	178 (98%)	4 (2%)	0	100	100
17	Ai	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
18	Aj	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
19	Ak	164/166 (99%)	160 (98%)	3 (2%)	1 (1%)	25	57
20	Al	171/173 (99%)	168 (98%)	3 (2%)	0	100	100
21	Am	112/114 (98%)	112 (100%)	0	0	100	100
22	An	168/170 (99%)	165 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Ao	115/117 (98%)	115 (100%)	0	0	100	100
24	Ap	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
25	Aq	186/188 (99%)	186 (100%)	0	0	100	100
26	Ar	151/155 (97%)	151 (100%)	0	0	100	100
27	As	109/115 (95%)	109 (100%)	0	0	100	100
28	At	251/253 (99%)	248 (99%)	3 (1%)	0	100	100
29	Au	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
30	Av	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
31	Aw	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
32	Ax	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
33	Ay	70/72 (97%)	70 (100%)	0	0	100	100
34	Az	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
35	AA	48/50 (96%)	48 (100%)	0	0	100	100
36	AB	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
37	AC	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
38	AD	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
39	AE	88/92 (96%)	88 (100%)	0	0	100	100
40	AF	91/93 (98%)	91 (100%)	0	0	100	100
41	AG	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
42	AH	172/176 (98%)	167 (97%)	4 (2%)	1 (1%)	25	57
43	AI	62/64 (97%)	62 (100%)	0	0	100	100
44	AJ	118/122 (97%)	118 (100%)	0	0	100	100
45	AK	137/139 (99%)	137 (100%)	0	0	100	100
46	AL	390/420 (93%)	387 (99%)	3 (1%)	0	100	100
46	AM	417/420 (99%)	416 (100%)	1 (0%)	0	100	100
46	AN	418/420 (100%)	414 (99%)	4 (1%)	0	100	100
47	AO	371/377 (98%)	362 (98%)	9 (2%)	0	100	100
48	Xa	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
49	Xb	242/244 (99%)	240 (99%)	2 (1%)	0	100	100
50	Xc	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
51	Xd	411/413 (100%)	399 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Xe	479/483 (99%)	474 (99%)	5 (1%)	0	100	100
53	Xf	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
54	Xg	379/410 (92%)	375 (99%)	4 (1%)	0	100	100
55	Xh	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
56	Xi	22/24 (92%)	22 (100%)	0	0	100	100
57	Xj	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
62	Ba	240/242 (99%)	234 (98%)	6 (2%)	0	100	100
63	Bb	232/236 (98%)	226 (97%)	6 (3%)	0	100	100
64	Bc	285/289 (99%)	283 (99%)	2 (1%)	0	100	100
65	Bd	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
66	Be	226/228 (99%)	222 (98%)	4 (2%)	0	100	100
67	Bf	117/119 (98%)	117 (100%)	0	0	100	100
68	Bg	110/112 (98%)	110 (100%)	0	0	100	100
69	Bh	370/374 (99%)	366 (99%)	4 (1%)	0	100	100
70	Bi	276/282 (98%)	270 (98%)	6 (2%)	0	100	100
71	Bj	395/401 (98%)	387 (98%)	8 (2%)	0	100	100
72	Bk	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
73	Bl	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
74	Bm	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
75	Bn	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
76	Bo	113/167 (68%)	110 (97%)	3 (3%)	0	100	100
77	Bp	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
78	Bq	128/130 (98%)	128 (100%)	0	0	100	100
79	Br	88/90 (98%)	88 (100%)	0	0	100	100
80	Bs	90/92 (98%)	90 (100%)	0	0	100	100
81	Bt	73/75 (97%)	73 (100%)	0	0	100	100
82	Bu	165/167 (99%)	165 (100%)	0	0	100	100
83	Bv	162/164 (99%)	162 (100%)	0	0	100	100
84	Bw	347/349 (99%)	343 (99%)	4 (1%)	0	100	100
85	Bx	613/621 (99%)	594 (97%)	19 (3%)	0	100	100
86	By	76/80 (95%)	76 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	Bz	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
88	BA	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
89	BB	80/84 (95%)	80 (100%)	0	0	100	100
90	BC	29/31 (94%)	29 (100%)	0	0	100	100
91	BD	266/270 (98%)	264 (99%)	2 (1%)	0	100	100
92	BE	169/171 (99%)	169 (100%)	0	0	100	100
93	BF	366/370 (99%)	360 (98%)	6 (2%)	0	100	100
94	Ya	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
95	Yb	48/50 (96%)	48 (100%)	0	0	100	100
96	Yc	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
97	Yd	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
98	Ye	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
99	Yf	148/150 (99%)	147 (99%)	1 (1%)	0	100	100
100	Yg	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
101	Yh	63/65 (97%)	63 (100%)	0	0	100	100
102	Yi	130/132 (98%)	127 (98%)	3 (2%)	0	100	100
103	Yj	382/386 (99%)	376 (98%)	6 (2%)	0	100	100
104	Yk	88/92 (96%)	88 (100%)	0	0	100	100
105	Yl	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
106	Ua	1/32 (3%)	1 (100%)	0	0	100	100
107	Ub	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
All	All	16832/17228 (98%)	16598 (99%)	232 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	AH	161	TYR
19	Ak	190	LYS

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	
10	Aa	248/248 (100%)	248 (100%)	0	100	100
11	Ab	261/261 (100%)	260 (100%)	1 (0%)	91	97
12	Ac	259/259 (100%)	258 (100%)	1 (0%)	91	97
13	Ad	176/176 (100%)	175 (99%)	1 (1%)	86	95
14	Ae	211/211 (100%)	211 (100%)	0	100	100
15	Af	47/47 (100%)	46 (98%)	1 (2%)	53	80
16	Ah	161/161 (100%)	159 (99%)	2 (1%)	71	90
17	Ai	103/103 (100%)	103 (100%)	0	100	100
18	Aj	172/172 (100%)	172 (100%)	0	100	100
19	Ak	146/146 (100%)	145 (99%)	1 (1%)	84	95
20	Al	150/150 (100%)	149 (99%)	1 (1%)	84	95
21	Am	102/102 (100%)	102 (100%)	0	100	100
22	An	157/157 (100%)	157 (100%)	0	100	100
23	Ao	101/101 (100%)	101 (100%)	0	100	100
24	Ap	177/177 (100%)	176 (99%)	1 (1%)	86	95
25	Aq	161/161 (100%)	160 (99%)	1 (1%)	86	95
26	Ar	142/142 (100%)	141 (99%)	1 (1%)	84	95
27	As	105/105 (100%)	105 (100%)	0	100	100
28	At	223/223 (100%)	223 (100%)	0	100	100
29	Au	121/121 (100%)	120 (99%)	1 (1%)	81	93
30	Av	120/120 (100%)	120 (100%)	0	100	100
31	Aw	110/110 (100%)	108 (98%)	2 (2%)	59	83
32	Ax	161/161 (100%)	161 (100%)	0	100	100
33	Ay	66/66 (100%)	66 (100%)	0	100	100
34	Az	51/51 (100%)	48 (94%)	3 (6%)	19	48
35	AA	47/47 (100%)	47 (100%)	0	100	100
36	AB	45/45 (100%)	45 (100%)	0	100	100
37	AC	125/125 (100%)	123 (98%)	2 (2%)	62	85
38	AD	42/42 (100%)	42 (100%)	0	100	100
39	AE	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	AF	82/82 (100%)	82 (100%)	0	100	100
41	AG	109/109 (100%)	109 (100%)	0	100	100
42	AH	155/155 (100%)	155 (100%)	0	100	100
43	AI	57/57 (100%)	57 (100%)	0	100	100
44	AJ	104/104 (100%)	104 (100%)	0	100	100
45	AK	117/117 (100%)	117 (100%)	0	100	100
46	AL	332/351 (95%)	329 (99%)	3 (1%)	78	92
46	AM	351/351 (100%)	350 (100%)	1 (0%)	92	98
46	AN	351/351 (100%)	350 (100%)	1 (0%)	92	98
47	AO	293/293 (100%)	291 (99%)	2 (1%)	84	95
48	Xa	173/173 (100%)	172 (99%)	1 (1%)	86	95
49	Xb	217/217 (100%)	217 (100%)	0	100	100
50	Xc	54/54 (100%)	54 (100%)	0	100	100
51	Xd	339/339 (100%)	337 (99%)	2 (1%)	86	95
52	Xe	385/385 (100%)	385 (100%)	0	100	100
53	Xf	172/172 (100%)	172 (100%)	0	100	100
54	Xg	312/312 (100%)	308 (99%)	4 (1%)	69	89
55	Xh	127/127 (100%)	127 (100%)	0	100	100
56	Xi	21/21 (100%)	21 (100%)	0	100	100
57	Xj	62/62 (100%)	62 (100%)	0	100	100
62	Ba	220/220 (100%)	215 (98%)	5 (2%)	50	79
63	Bb	214/214 (100%)	213 (100%)	1 (0%)	88	96
64	Bc	247/247 (100%)	245 (99%)	2 (1%)	81	93
65	Bd	196/196 (100%)	195 (100%)	1 (0%)	88	96
66	Be	196/196 (100%)	188 (96%)	8 (4%)	30	63
67	Bf	103/103 (100%)	103 (100%)	0	100	100
68	Bg	97/97 (100%)	95 (98%)	2 (2%)	53	80
69	Bh	327/327 (100%)	326 (100%)	1 (0%)	92	98
70	Bi	242/242 (100%)	242 (100%)	0	100	100
71	Bj	334/334 (100%)	333 (100%)	1 (0%)	92	98
72	Bk	95/95 (100%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	Bl	104/104 (100%)	104 (100%)	0	100	100
74	Bm	100/100 (100%)	99 (99%)	1 (1%)	76	91
75	Bn	106/106 (100%)	106 (100%)	0	100	100
76	Bo	104/104 (100%)	104 (100%)	0	100	100
77	Bp	107/107 (100%)	106 (99%)	1 (1%)	78	92
78	Bq	113/113 (100%)	113 (100%)	0	100	100
79	Br	81/81 (100%)	80 (99%)	1 (1%)	71	90
80	Bs	77/77 (100%)	77 (100%)	0	100	100
81	Bt	66/66 (100%)	66 (100%)	0	100	100
82	Bu	142/142 (100%)	142 (100%)	0	100	100
83	Bv	140/140 (100%)	138 (99%)	2 (1%)	67	88
84	Bw	298/298 (100%)	297 (100%)	1 (0%)	92	98
85	Bx	481/481 (100%)	467 (97%)	14 (3%)	42	74
86	By	69/69 (100%)	69 (100%)	0	100	100
87	Bz	107/107 (100%)	107 (100%)	0	100	100
88	BA	143/143 (100%)	143 (100%)	0	100	100
89	BB	72/72 (100%)	72 (100%)	0	100	100
90	BC	30/30 (100%)	30 (100%)	0	100	100
91	BD	225/225 (100%)	224 (100%)	1 (0%)	91	97
92	BE	136/136 (100%)	136 (100%)	0	100	100
93	BF	326/326 (100%)	325 (100%)	1 (0%)	92	98
94	Ya	161/161 (100%)	160 (99%)	1 (1%)	86	95
95	Yb	44/44 (100%)	44 (100%)	0	100	100
96	Yc	140/140 (100%)	139 (99%)	1 (1%)	84	95
97	Yd	88/88 (100%)	88 (100%)	0	100	100
98	Ye	91/91 (100%)	89 (98%)	2 (2%)	52	80
99	Yf	132/132 (100%)	132 (100%)	0	100	100
100	Yg	60/60 (100%)	60 (100%)	0	100	100
101	Yh	54/54 (100%)	54 (100%)	0	100	100
102	Yi	112/112 (100%)	110 (98%)	2 (2%)	59	83
103	Yj	278/278 (100%)	278 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
104	Yk	74/74 (100%)	74 (100%)	0	100	100
105	Yl	76/76 (100%)	76 (100%)	0	100	100
106	Ua	1/1 (100%)	1 (100%)	0	100	100
107	Ub	123/123 (100%)	123 (100%)	0	100	100
All	All	14619/14638 (100%)	14537 (99%)	82 (1%)	86	95

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
83	Bv	88	GLN
85	Bx	314	LYS
84	Bw	391	SER
85	Bx	110	LEU
93	BF	82	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
62	Ba	205	ASN
85	Bx	75	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	108/109 (99%)	28 (25%)	0
2	A2	80/81 (98%)	18 (22%)	1 (1%)
3	A3	205/210 (97%)	30 (14%)	1 (0%)
4	A4	72/73 (98%)	9 (12%)	1 (1%)
5	A5	132/142 (92%)	33 (25%)	0
58	B1	101/102 (99%)	24 (23%)	0
59	B2	208/214 (97%)	42 (20%)	0
6	A6	106/131 (80%)	21 (19%)	0
60	B3	371/379 (97%)	50 (13%)	2 (0%)
61	B4	329/348 (94%)	53 (16%)	0
7	A7	532/576 (92%)	80 (15%)	1 (0%)
8	A8	349/350 (99%)	60 (17%)	0
9	A9	67/69 (97%)	15 (22%)	0
All	All	2660/2784 (95%)	463 (17%)	6 (0%)

5 of 463 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	5	A
1	A1	9	U
1	A1	13	C
1	A1	16	A
1	A1	17	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A7	192	A
60	B3	177	A
60	B3	275	A
3	A3	132	A
2	A2	79	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 145 ligands modelled in this entry, 144 are monoatomic - leaving 1 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
121	ATP	Bw	502	118	26,33,33	0.76	0	31,52,52	0.74	1 (3%)

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
121	ATP	Bw	502	118	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
121	Bw	502	ATP	C5-C6-N6	2.22	123.73	120.35

There are no chirality outliers.

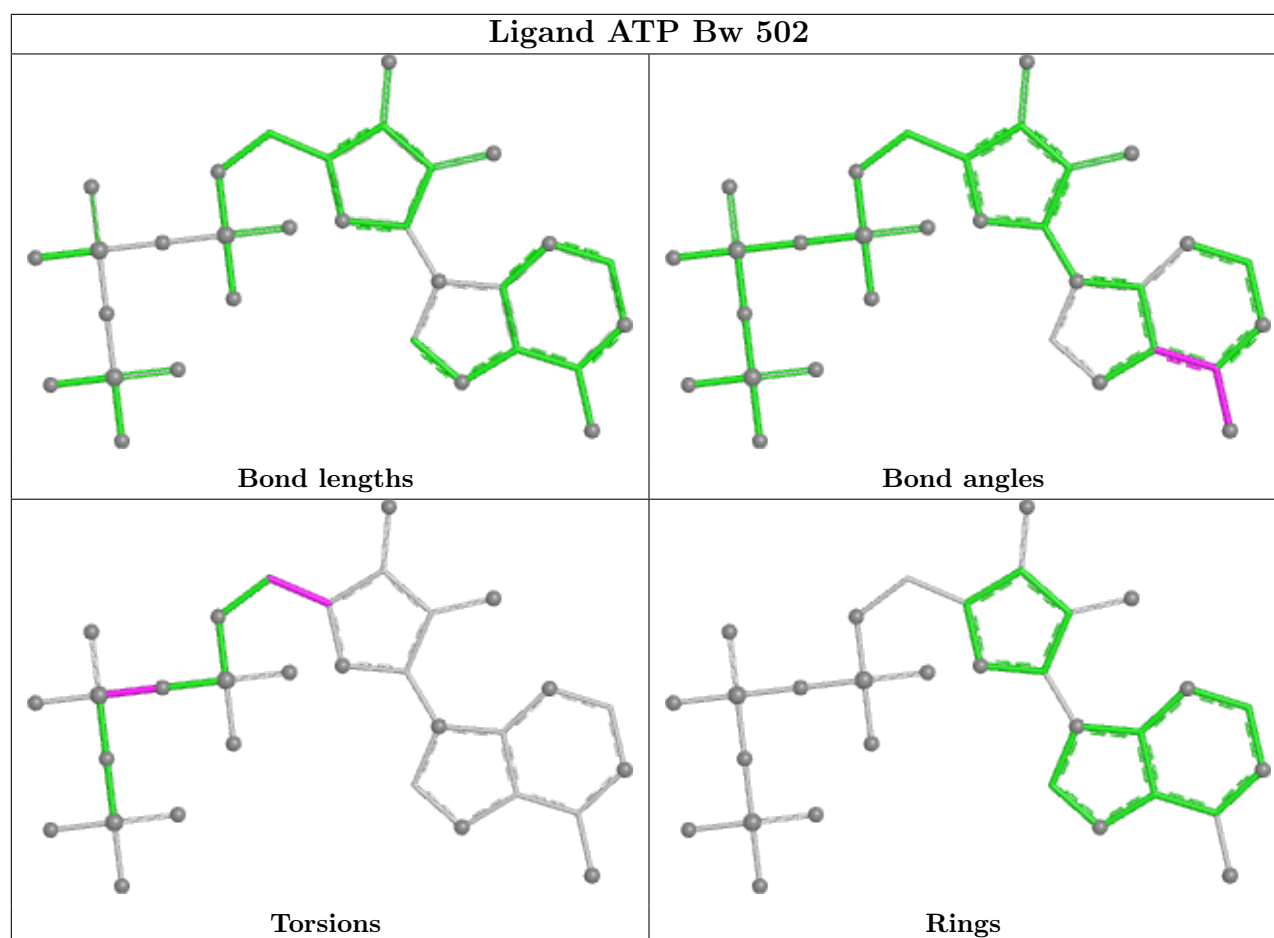
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
121	Bw	502	ATP	O4'-C4'-C5'-O5'
121	Bw	502	ATP	PA-O3A-PB-O1B
121	Bw	502	ATP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	Xg	4
85	Bx	3
27	As	2
70	Bi	2
71	Bj	2
47	AO	2
14	Ae	2
42	AH	1
64	Bc	1
69	Bh	1

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Mol	Chain	Number of breaks
55	Xh	1
63	Bb	1
91	BD	1
103	Yj	1
9	A9	1
105	Yl	1
26	Ar	1
39	AE	1
89	BB	1
111	Ug	1
110	Uf	1
34	Az	1
93	BF	1
98	Ye	1
16	Ah	1
104	Yk	1
44	AJ	1
52	Xe	1

The worst 5 of 38 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Xg	165:PHE	C	206:LYS	N	58.00
1	As	92:PRO	C	151:GLY	N	43.90
1	Bi	223:GLN	C	243:ALA	N	41.05
1	Bj	297:SER	C	426:ALA	N	32.84
1	AH	39:TYR	C	50:PRO	N	29.49

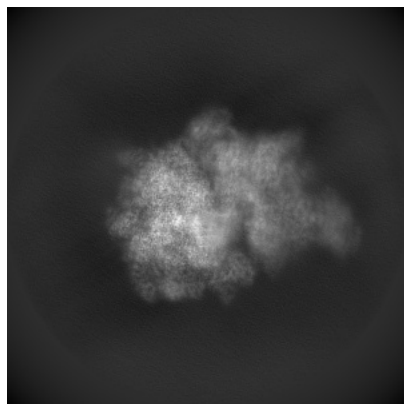
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15100. These allow visual inspection of the internal detail of the map and identification of artifacts.

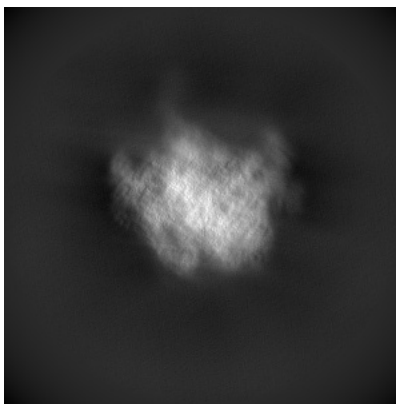
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

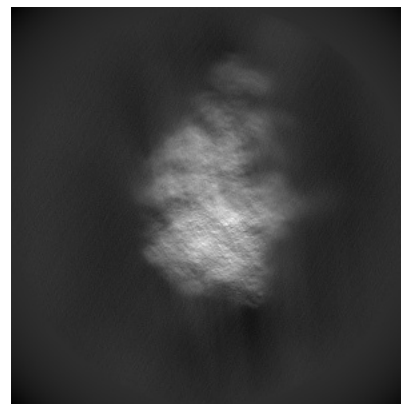
6.1.1 Primary map



X

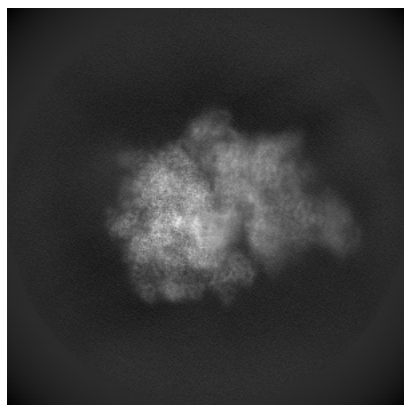


Y

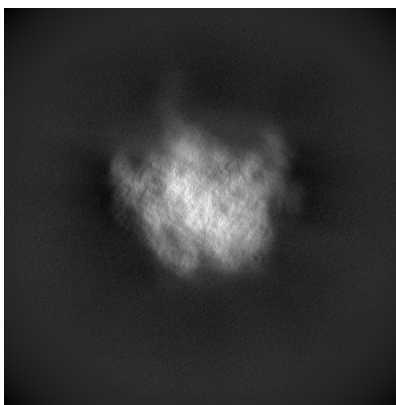


Z

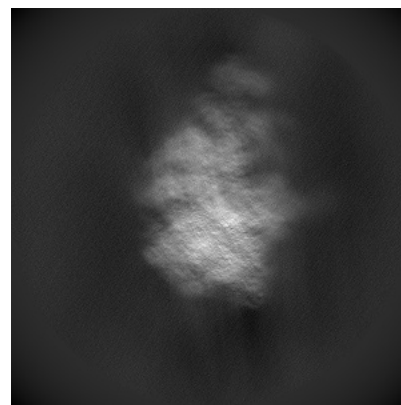
6.1.2 Raw map



X



Y

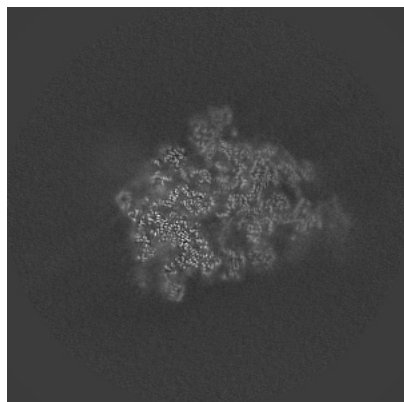


Z

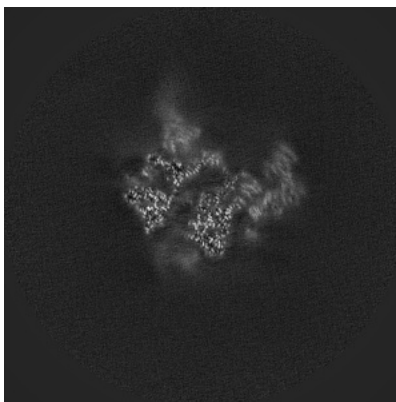
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

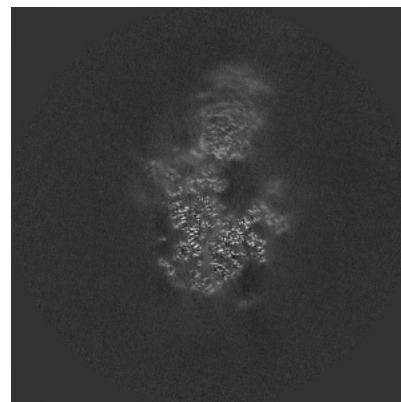
6.2.1 Primary map



X Index: 350

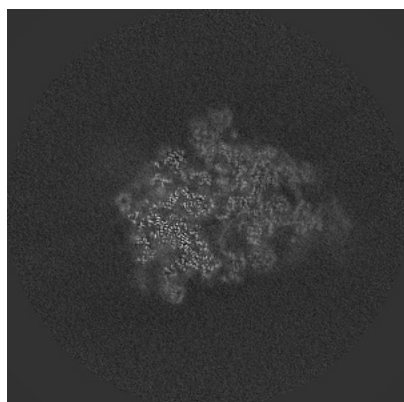


Y Index: 350

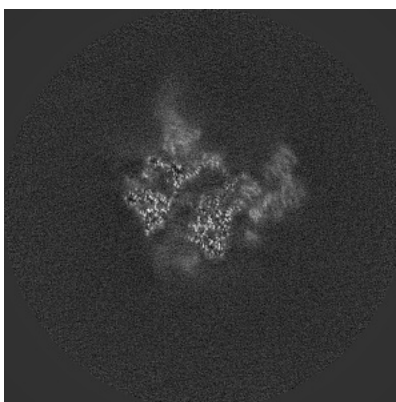


Z Index: 350

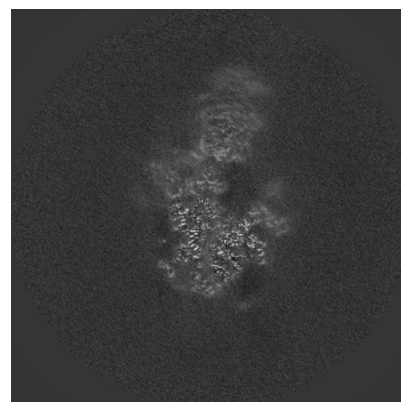
6.2.2 Raw map



X Index: 350



Y Index: 350

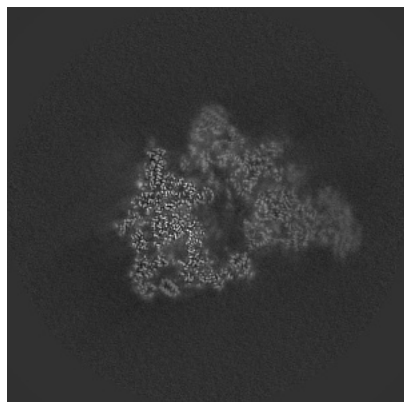


Z Index: 350

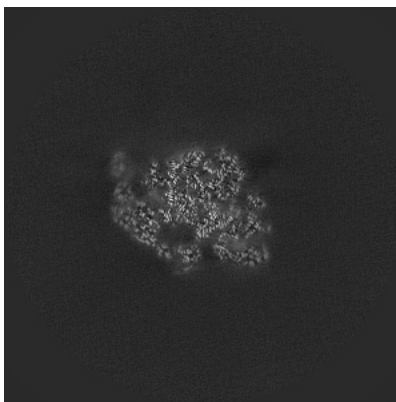
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

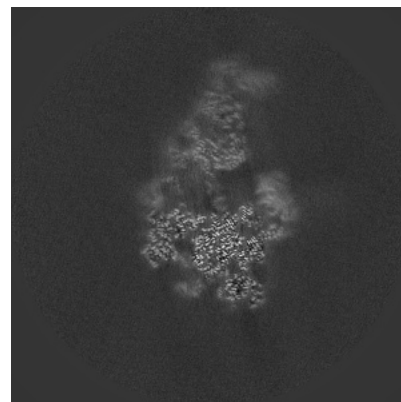
6.3.1 Primary map



X Index: 376

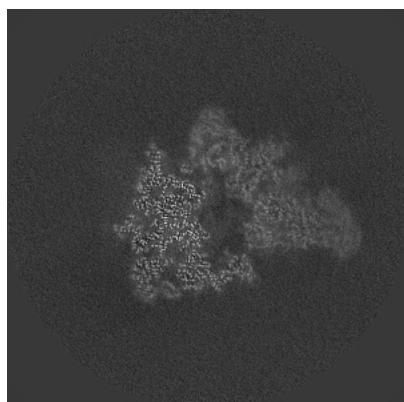


Y Index: 284

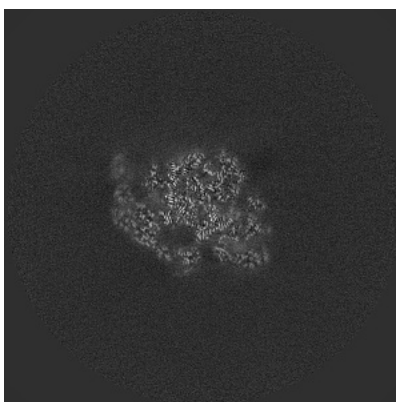


Z Index: 320

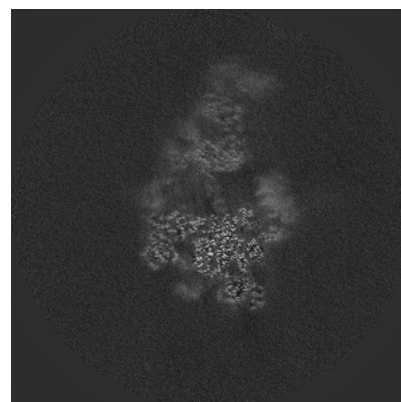
6.3.2 Raw map



X Index: 380



Y Index: 284

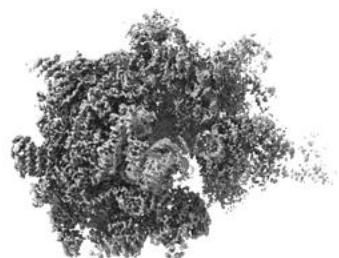


Z Index: 319

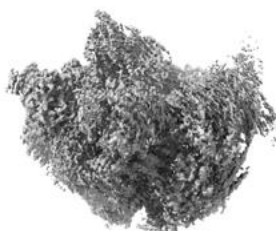
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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

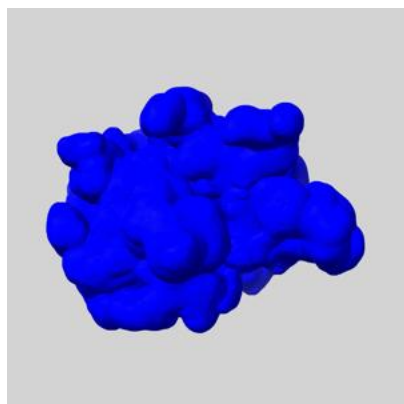
6.5 Mask visualisation [i](#)

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

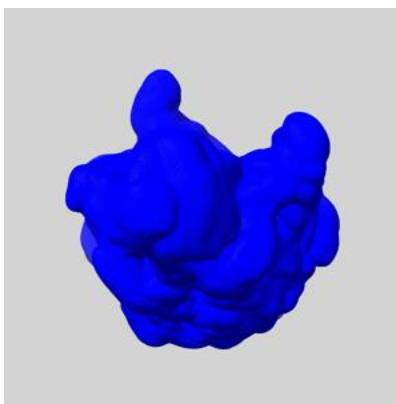
A mask typically either:

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

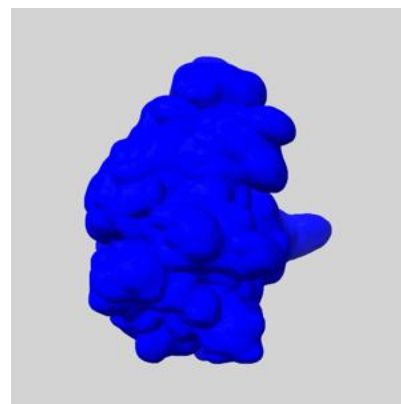
6.5.1 emd_15100_msk_1.map [i](#)



X



Y

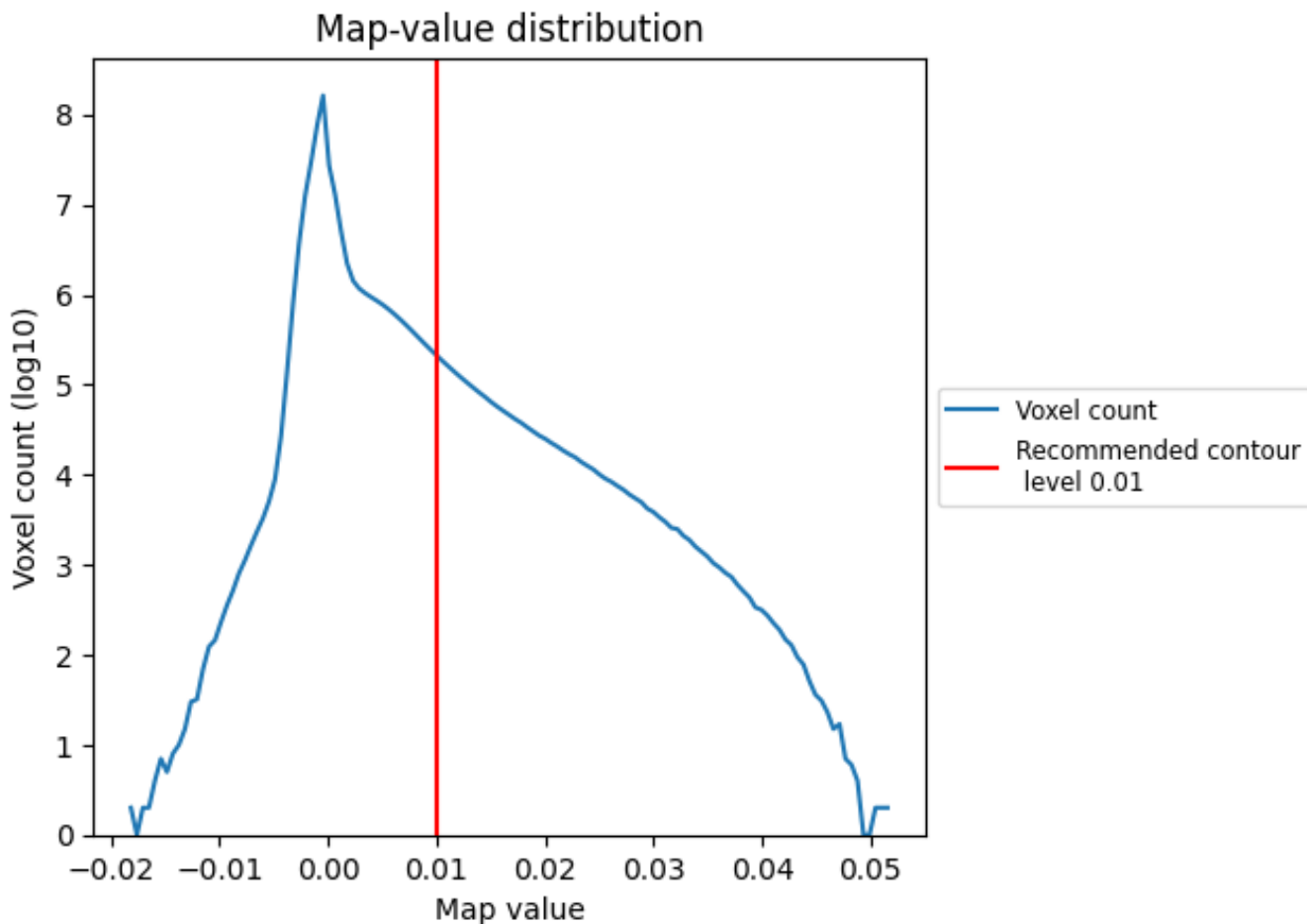


Z

7 Map analysis [i](#)

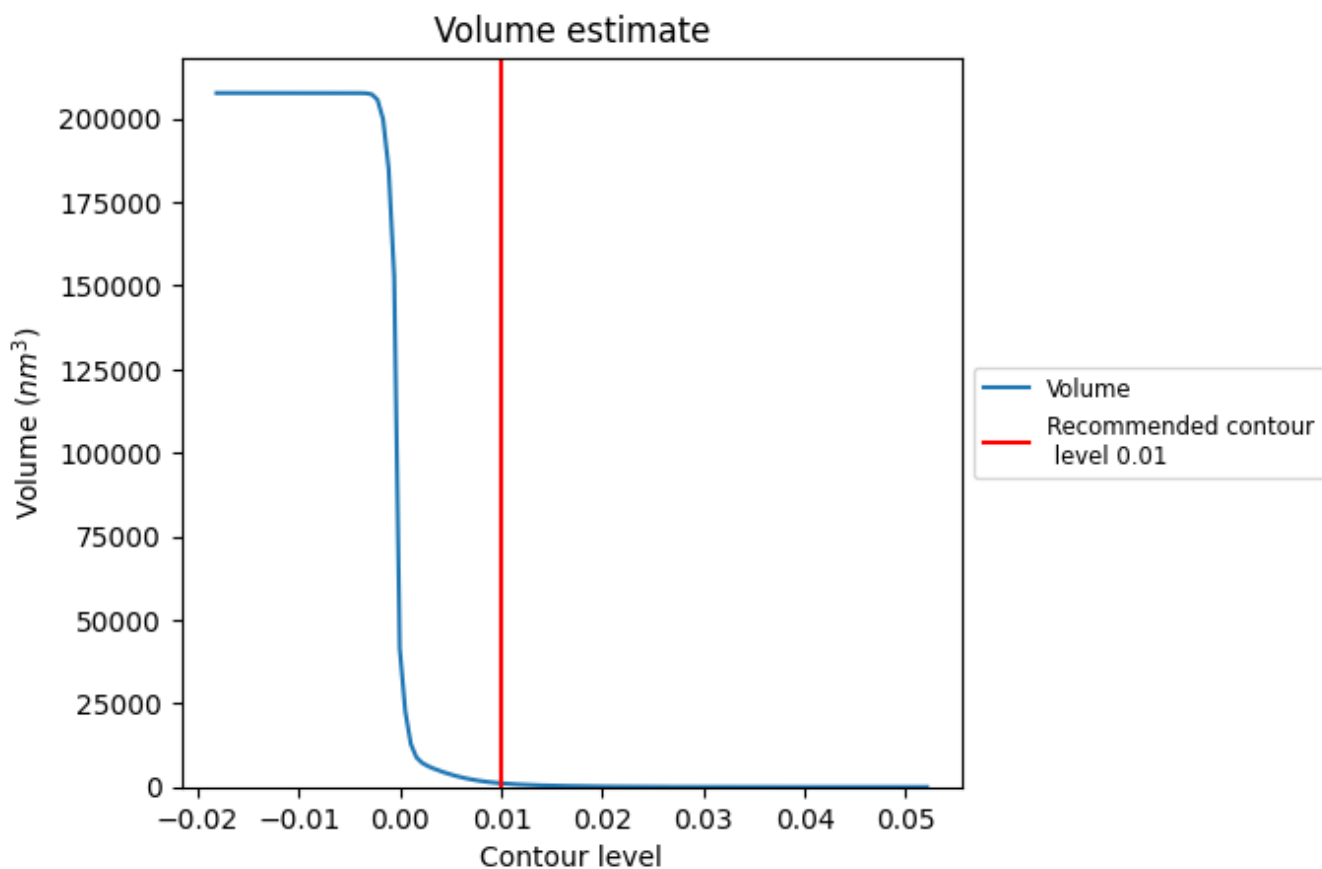
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

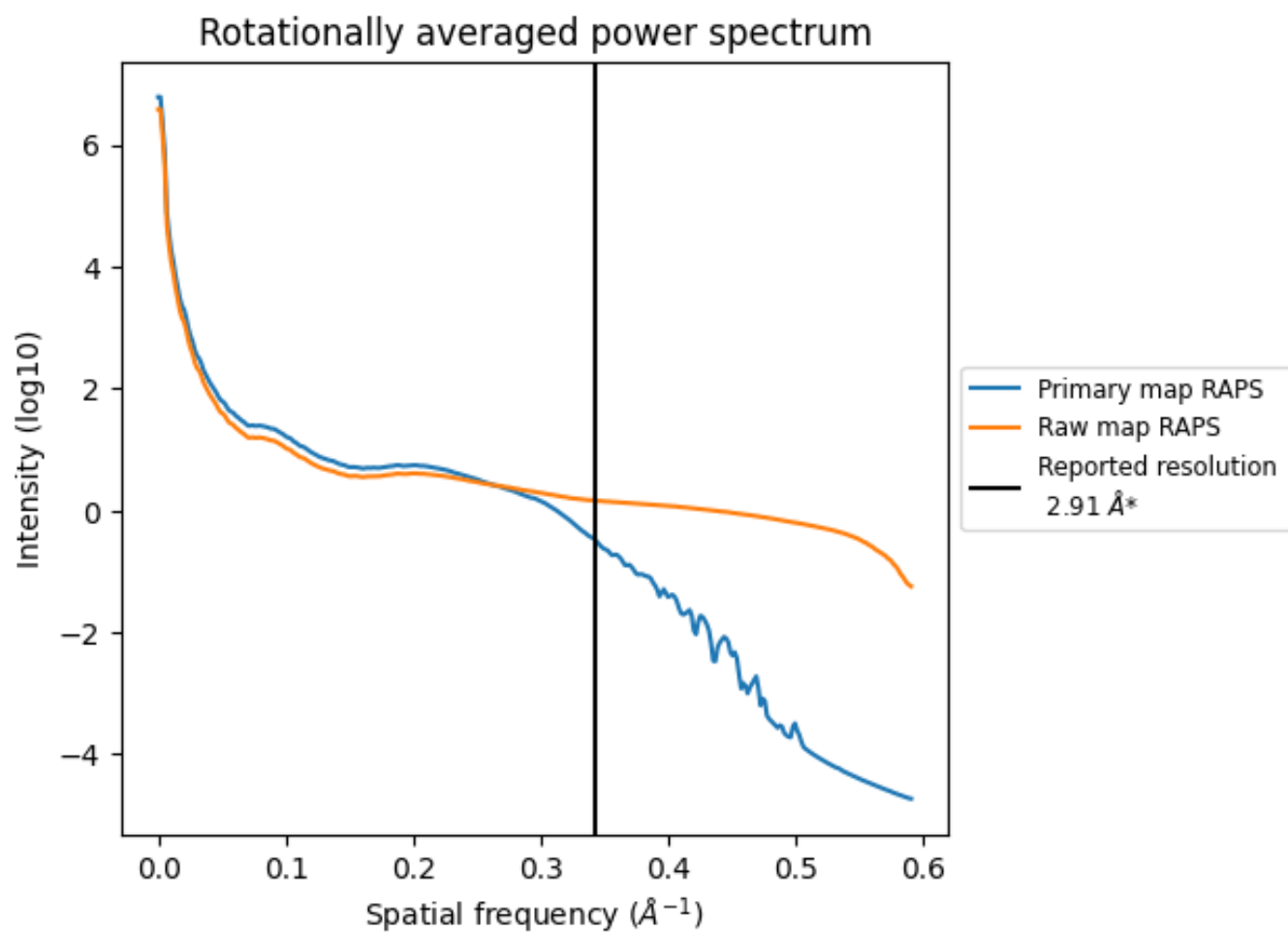
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1106 nm^3 ; this corresponds to an approximate mass of 999 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](#)

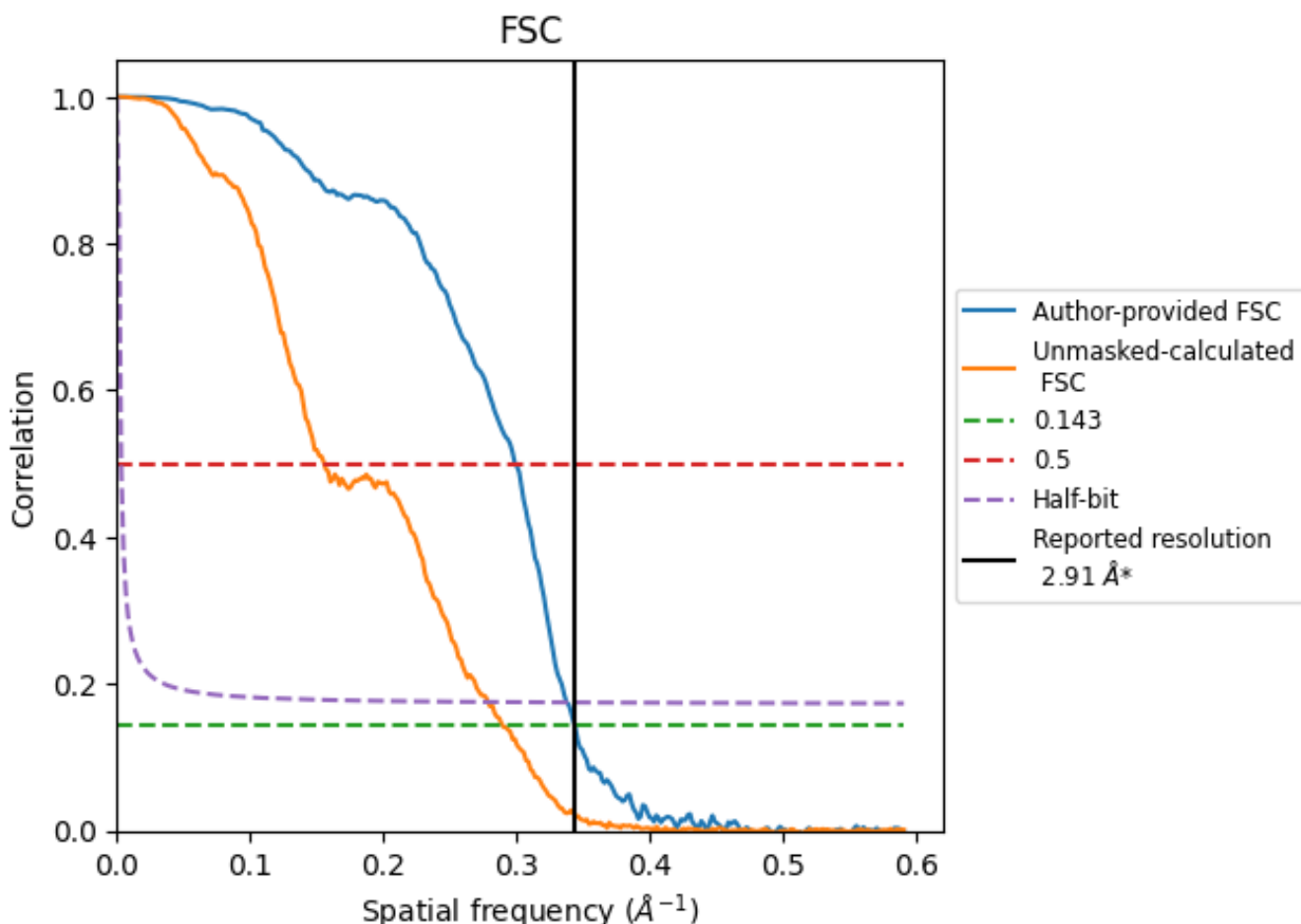


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

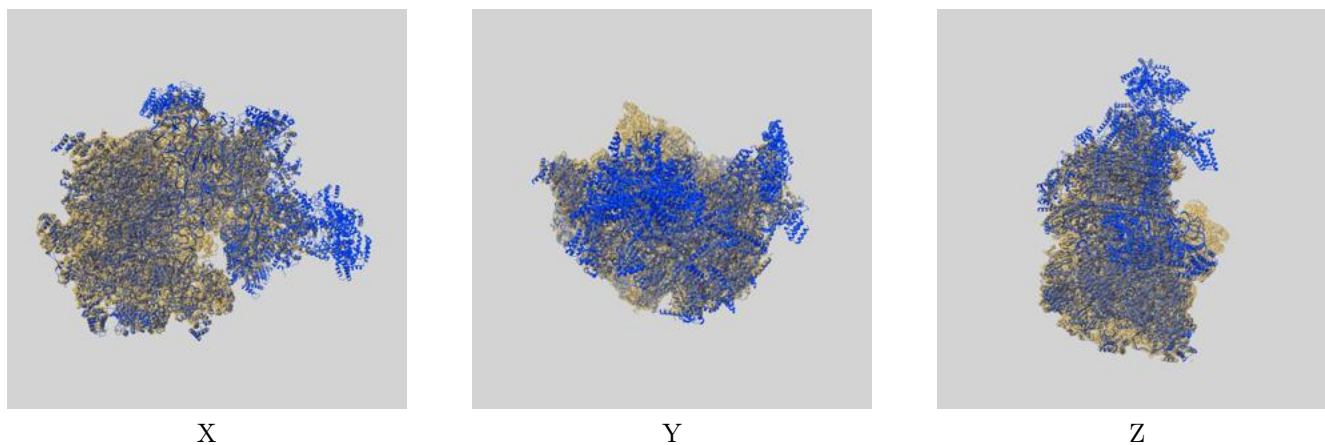
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.34	2.96
Unmasked-calculated*	3.45	6.42	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

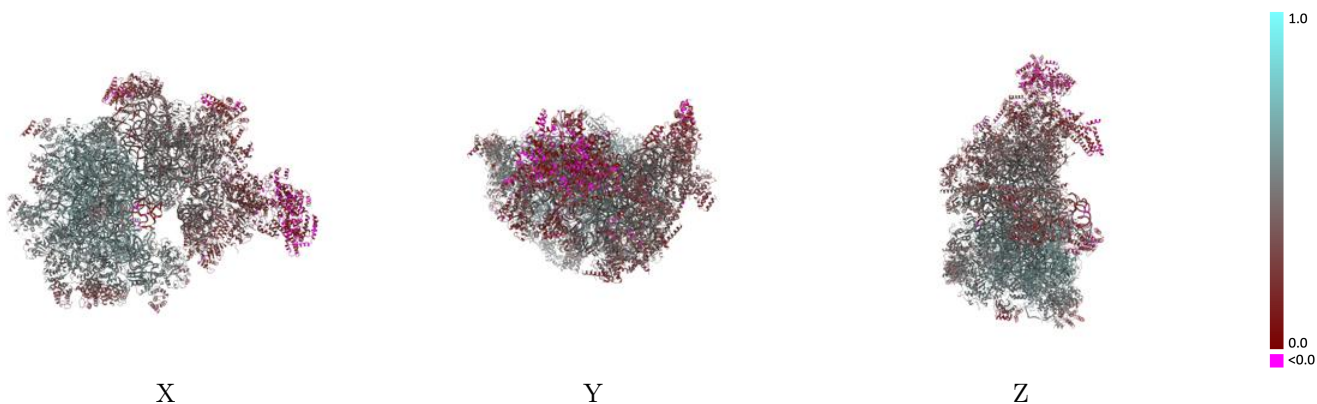
This section contains information regarding the fit between EMDB map EMD-15100 and PDB model 8A22. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



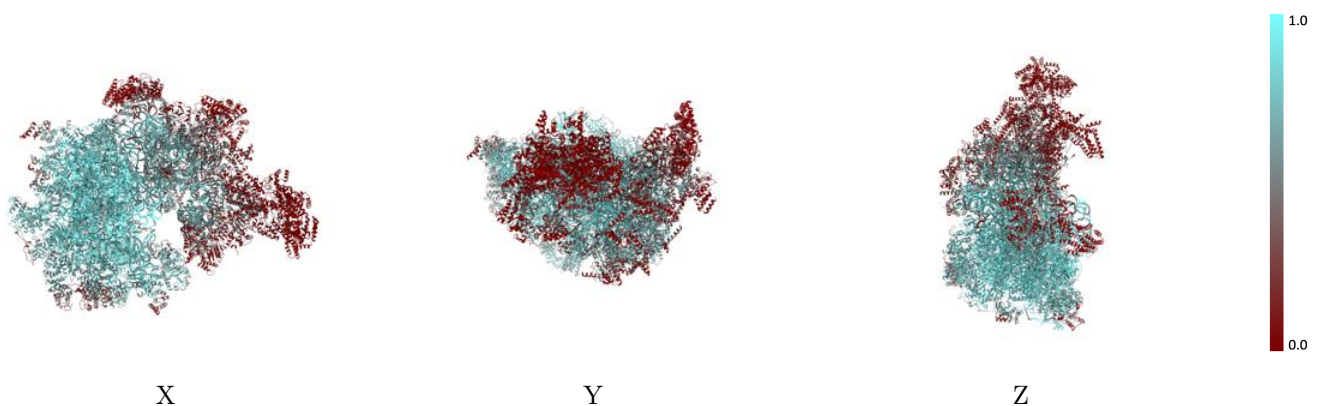
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



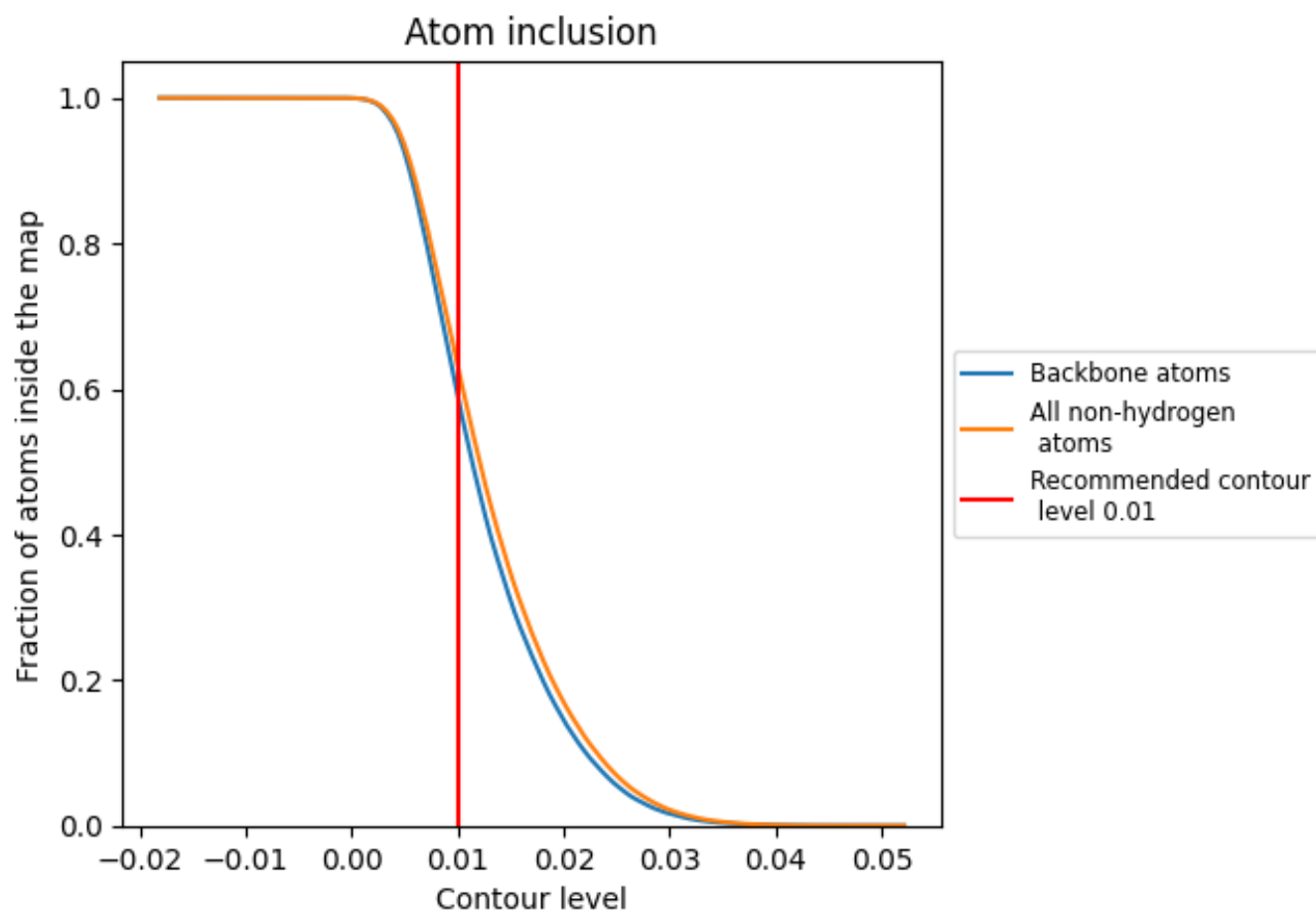
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 63% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6306	 0.4380
A1	 0.9289	 0.5420
A2	 0.9469	 0.5800
A3	 0.9575	 0.5800
A4	 0.9943	 0.6010
A5	 0.8744	 0.3630
A6	 0.9659	 0.5610
A7	 0.9479	 0.5690
A8	 0.9532	 0.5740
A9	 0.9386	 0.5570
AA	 0.9066	 0.5610
AB	 0.9333	 0.5740
AC	 0.8726	 0.5650
AD	 0.7253	 0.5230
AE	 0.6658	 0.4530
AF	 0.8474	 0.5220
AG	 0.8910	 0.5450
AH	 0.6402	 0.4350
AI	 0.9076	 0.5670
AJ	 0.6779	 0.4730
AK	 0.8902	 0.5440
AL	 0.5765	 0.3940
AM	 0.5805	 0.4230
AN	 0.6398	 0.4400
AO	 0.5868	 0.4430
Aa	 0.8772	 0.5370
Ab	 0.8941	 0.5750
Ac	 0.8314	 0.5290
Ad	 0.6475	 0.4950
Ae	 0.7458	 0.4510
Af	 0.6103	 0.4350
Ah	 0.8972	 0.5550
Ai	 0.8237	 0.5730
Aj	 0.9138	 0.5610
Ak	 0.8943	 0.5750























































































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Chain	Atom inclusion	Q-score
Al	 0.8964	 0.5580
Am	 0.7872	 0.5260
An	 0.7822	 0.5450
Ao	 0.8864	 0.5660
Ap	 0.8716	 0.5580
Aq	 0.9080	 0.5660
Ar	 0.8311	 0.5170
As	 0.6571	 0.4150
At	 0.7970	 0.5240
Au	 0.9017	 0.5740
Av	 0.8035	 0.5090
Aw	 0.8159	 0.5010
Ax	 0.8688	 0.5490
Ay	 0.4639	 0.4220
Az	 0.8458	 0.5520
B1	 0.6286	 0.4160
B2	 0.6677	 0.4220
B3	 0.8346	 0.4570
B4	 0.7780	 0.4360
BA	 0.2081	 0.3120
BB	 0.3426	 0.3240
BC	 0.7376	 0.4620
BD	 0.1918	 0.3260
BE	 0.0109	 0.1590
BF	 0.1889	 0.2860
Ba	 0.3018	 0.3130
Bb	 0.4531	 0.3700
Bc	 0.2439	 0.3180
Bd	 0.3477	 0.3990
Be	 0.5239	 0.4070
Bf	 0.5042	 0.4090
Bg	 0.4925	 0.3760
Bh	 0.4756	 0.3810
Bi	 0.3068	 0.3140
Bj	 0.1422	 0.2240
Bk	 0.6444	 0.4270
Bl	 0.3201	 0.4050
Bm	 0.2500	 0.3270
Bn	 0.5198	 0.3870
Bo	 0.7307	 0.4470
Bp	 0.2720	 0.3740
Bq	 0.6217	 0.4020



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Chain	Atom inclusion	Q-score
Br	 0.5390	 0.3980
Bs	 0.1899	 0.3050
Bt	 0.5738	 0.4110
Bu	 0.3258	 0.3250
Bv	 0.3915	 0.3330
Bw	 0.1575	 0.2390
Bx	 0.0765	 0.1850
By	 0.2963	 0.3520
Bz	 0.0619	 0.2220
Ua	 0.6707	 0.5150
Ub	 0.5296	 0.3080
Ud	 0.1116	 0.2100
Ue	 0.0000	 0.2090
Uf	 0.0247	 0.1420
Ug	 0.1016	 0.2830
Uh	 0.0000	 0.0560
Ui	 0.4000	 0.3880
Uj	 0.0000	 0.3640
Uk	 0.0261	 0.2440
Ul	 0.0125	 0.2120
Um	 0.3818	 0.2990
Xa	 0.5620	 0.4230
Xb	 0.6861	 0.4520
Xc	 0.7427	 0.4860
Xd	 0.7216	 0.4720
Xe	 0.7720	 0.4830
Xf	 0.8222	 0.5340
Xg	 0.7358	 0.4970
Xh	 0.7008	 0.4820
Xi	 0.8342	 0.5390
Xj	 0.6538	 0.4500
Ya	 0.2118	 0.3340
Yb	 0.0844	 0.2380
Yc	 0.2526	 0.3680
Yd	 0.1066	 0.3250
Ye	 0.4743	 0.3950
Yf	 0.2934	 0.3250
Yg	 0.1426	 0.2500
Yh	 0.2287	 0.2740
Yi	 0.0229	 0.1890
Yj	 0.0438	 0.1500
Yk	 0.0043	 0.1500

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Chain	Atom inclusion	Q-score
Y1	 0.2995	 0.3200