



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 08:41 am BST

PDB ID : 8APO  
EMDB ID : EMD-15577  
Title : Structure of the mitochondrial ribosome from *Polytomella magna* with tRNAs bound to the A and P sites  
Authors : Tobiasson, V.; Berzina, I.; Amunts, A.  
Deposited on : 2022-08-10  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

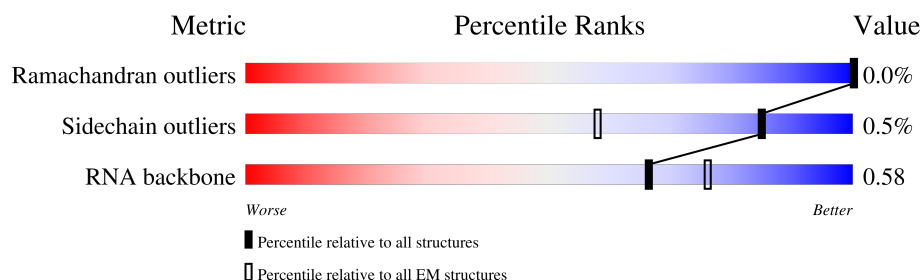
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



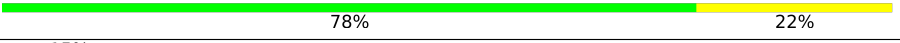
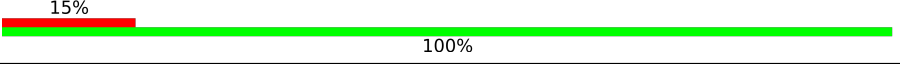
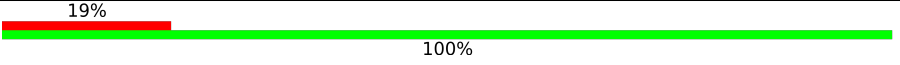
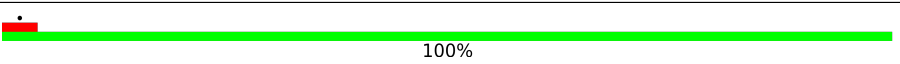
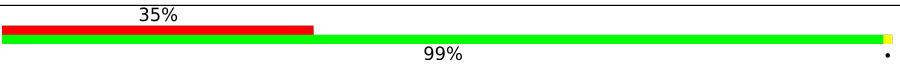
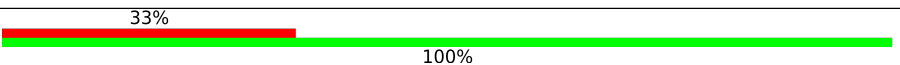
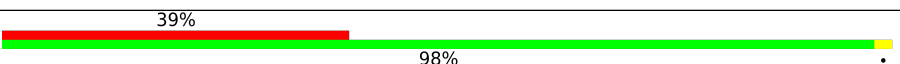
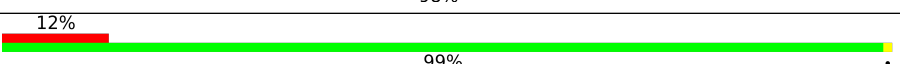
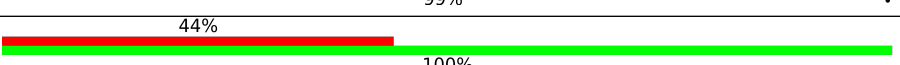
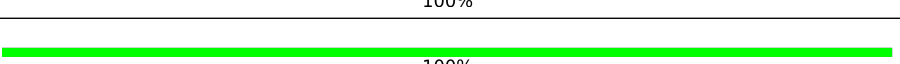
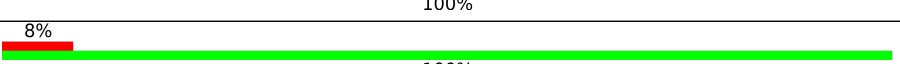
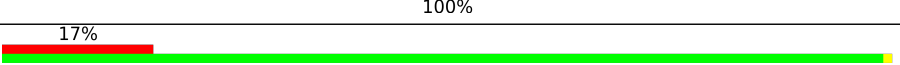
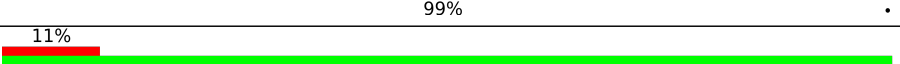
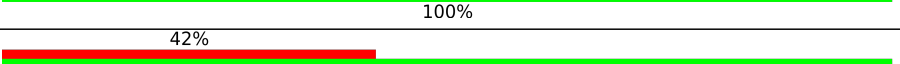
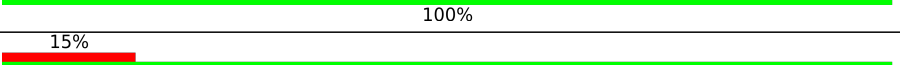
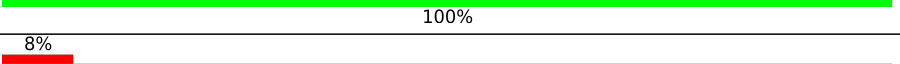
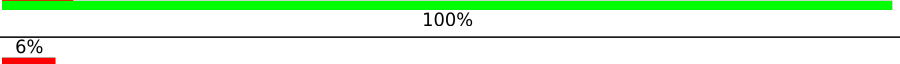
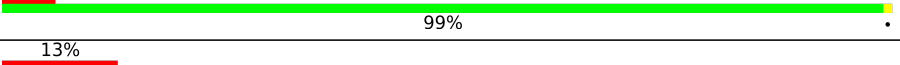
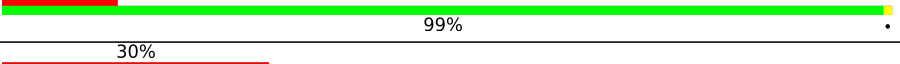
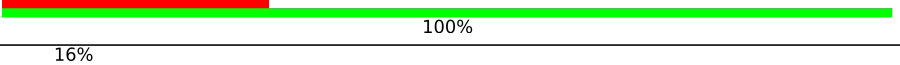
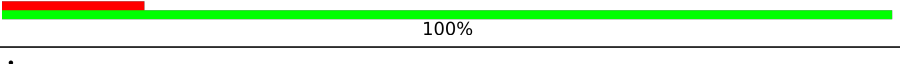
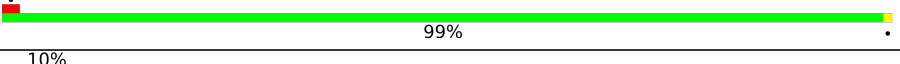
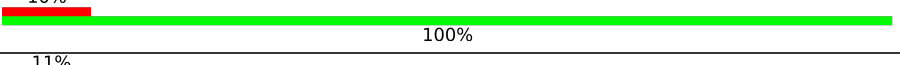
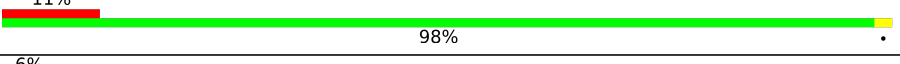
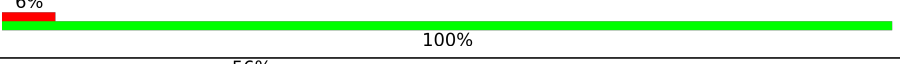
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	<div> <div>5%</div> <div>77%</div> <div>23%</div> </div>
2	A2	81	<div> <div>80%</div> <div>20%</div> </div>
3	A3	207	<div> <div>86%</div> <div>14%</div> </div>
4	A4	73	<div> <div>86%</div> <div>14%</div> </div>
5	A5	136	<div> <div>6%</div> <div>76%</div> <div>24%</div> </div>
6	A6	109	<div> <div>81%</div> <div>19%</div> </div>
7	A7	534	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
8	A8	350	<div> <div>83%</div> <div>16%</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
57	Xj	71	49% 100%
58	B1	102	72% 77% 23%
59	B2	210	61% 81% 19%
60	B3	379	25% 87% 13%
61	B4	337	36% 85% 15%
62	Ba	242	93% 99%
63	Bb	236	86% 100%
64	Bc	279	91% 100%
65	Bd	221	94% 100%
66	Be	228	78% 97%
67	Bf	119	92% 100%
68	Bg	112	82% 98%
69	Bh	374	77% 100%
70	Bi	282	91% 100%
71	Bj	401	97% 100%
72	Bk	116	70% 100%
73	Bl	123	89% 100%
74	Bm	113	98% 99%
75	Bn	118	75% 99%
76	Bo	167	56% 100%
77	Bp	123	96% 100%
78	Bq	130	68% 100%
79	Br	90	83% 100%
80	Bs	92	97% 98%
81	Bt	75	73% 100%

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Mol	Chain	Length	Quality of chain
82	Bu	167	90% 100%
83	Bv	164	80% 99% 98%
84	Bw	351	99% 99%
85	Bx	621	99% 98%
86	By	78	90% 100%
87	Bz	119	100%
88	BA	176	99% 100%
89	BB	84	93% 100%
90	BC	31	26% 100%
91	BD	270	96% 100%
92	BE	171	100%
93	BF	370	89% 100%
94	Ya	180	99% 99%
95	Yb	50	100%
96	Yc	159	94% 100%
97	Yd	95	97% 100%
98	Ye	106	83% 98%
99	Yf	150	95% 100%
100	Yg	67	100%
101	Yh	65	97% 100%
102	Yi	132	100% 98%
103	Yj	386	99% 100%
104	Yk	92	100% 99%
105	Yl	84	93% 100%
106	C1	23	91% 91% 9%

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Mol	Chain	Length	Quality of chain
107	C2	21	 90% 100%
108	C3	8	 50% 75% 25%
109	Ub	131	 48% 95% 5%
110	Ua	32	 69% 100%
111	Ud	44	 98% 98%
112	Ue	47	 100% 100%
113	Uf	73	 99% 100%
114	Ug	63	 97% 100%
115	Uh	48	 100% 100%
116	Ui	26	 96% 100%
117	Uj	9	 100% 100%
118	Uk	23	 100% 100%
119	Ul	16	 100% 100%
120	Um	11	 100% 100%

## 2 Entry composition [i](#)

There are 125 unique types of molecules in this entry. The entry contains 197823 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
1	A1	109	Total	C	N	O	P	0	0
			2344	1052	444	739	109		

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

- Molecule 10 is a protein called uL2m.

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

- Molecule 11 is a protein called uL3m.

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

- Molecule 12 is a protein called uL4m.

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

- Molecule 13 is a protein called uL5m.

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

- Molecule 14 is a protein called uL6m.

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

- 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
22	An	170	Total	C	N	O	S	0	0
			1392	891	238	255	8		

- Molecule 23 is a protein called bL20m.

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

- Molecule 24 is a protein called bL21m.

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

- Molecule 25 is a protein called uL22m.

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

- Molecule 26 is a protein called uL23m.

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

- Molecule 27 is a protein called bL24m.

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

- Molecule 28 is a protein called bL25m.

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

- 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 bL32m.

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
50	Xc	57	Total	C	N	O	0	0
			496	318	90	88		

- Molecule 51 is a protein called mL123.

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

- Molecule 52 is a protein called mL124.

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

- Molecule 53 is a protein called mL125.

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

- Molecule 54 is a protein called mL126.

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

- Molecule 55 is a protein called mL127.

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

- Molecule 56 is a protein called mL128.

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

- 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	379	Total	C	N	O	P	0	0
			8096	3627	1480	2610	379		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	B4	337	Total	C	N	O	P	0	0
			7186	3222	1300	2327	337		

- 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	279	Total	C	N	O	S	0	0
			2217	1413	398	400	6		

- 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
			2748	1748	477	510	13		

- Molecule 85 is a protein called mS31.

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

- Molecule 86 is a protein called mS33.

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

- Molecule 87 is a protein called mS34.

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

- Molecule 88 is a protein called mS35.

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

- Molecule 89 is a protein called mS37.

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

- Molecule 90 is a protein called mS38.

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

- Molecule 91 is a protein called mS45.

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

- 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.

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.

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.

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 RNA chain called P-site tRNA anticodon loop.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	C1	23	Total	C	N	O	P	0	0
			487	218	85	161	23		

- Molecule 107 is a RNA chain called A-site tRNA anticodon loop.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	C2	21	Total	C	N	O	P	0	0
			445	199	78	147	21		

- Molecule 108 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	C3	8	Total	C	N	O	P	0	0
			172	77	31	56	8		

- Molecule 109 is a protein called mL105.

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

- Molecule 110 is a protein called Unknown.

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

- Molecule 111 is a protein called Unknown.

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

- Molecule 112 is a protein called Unknown.

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

- Molecule 113 is a protein called Unknown.

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

- Molecule 114 is a protein called Unknown.

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

- Molecule 115 is a protein called Unknown.

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

- Molecule 116 is a protein called Unknown.

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

- Molecule 117 is a protein called Unknown.

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

- Molecule 118 is a protein called Unknown.

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

- Molecule 119 is a protein called Unknown.



Mol	Chain	Residues	Atoms				AltConf	Trace
119	U1	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 120 is a protein called Unknown.

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

- Molecule 121 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
121	A1	3	Total	Mg	0
			3	3	
121	A2	2	Total	Mg	0
			2	2	
121	A3	8	Total	Mg	0
			8	8	
121	A4	10	Total	Mg	0
			10	10	
121	A5	2	Total	Mg	0
			2	2	
121	A6	7	Total	Mg	0
			7	7	
121	A7	24	Total	Mg	0
			24	24	
121	A8	14	Total	Mg	0
			14	14	
121	Ab	1	Total	Mg	0
			1	1	
121	B1	4	Total	Mg	0
			4	4	
121	B2	8	Total	Mg	0
			8	8	
121	B3	12	Total	Mg	0
			12	12	
121	B4	15	Total	Mg	0
			15	15	
121	Bm	1	Total	Mg	0
			1	1	
121	Bw	1	Total	Mg	0
			1	1	

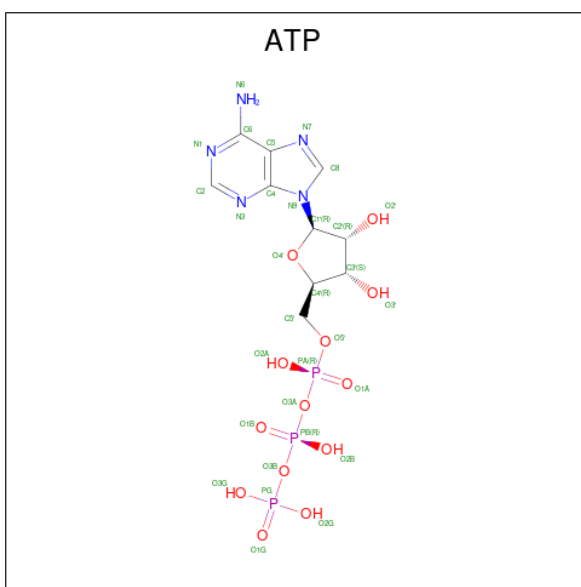
- Molecule 122 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
122	A1	1	Total 1	K 1	0
122	A3	1	Total 1	K 1	0
122	A4	2	Total 2	K 2	0
122	A7	5	Total 5	K 5	0
122	A8	4	Total 4	K 4	0
122	Aa	1	Total 1	K 1	0
122	Ab	1	Total 1	K 1	0
122	Ah	1	Total 1	K 1	0
122	AC	1	Total 1	K 1	0
122	B1	2	Total 2	K 2	0
122	B2	1	Total 1	K 1	0
122	B3	7	Total 7	K 7	0
122	B4	2	Total 2	K 2	0
122	Bl	1	Total 1	K 1	0

- Molecule 123 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 124 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 125 is water.

Mol	Chain	Residues	Atoms	AltConf
125	A1	15	Total O 15 15	0
125	A2	9	Total O 9 9	0
125	A3	34	Total O 34 34	0
125	A4	31	Total O 31 31	0
125	A5	10	Total O 10 10	0
125	A6	22	Total O 22 22	0
125	A7	109	Total O 109 109	0
125	A8	70	Total O 70 70	0
125	Aa	1	Total O 1 1	0
125	Ab	4	Total O 4 4	0
125	Ac	1	Total O 1 1	0

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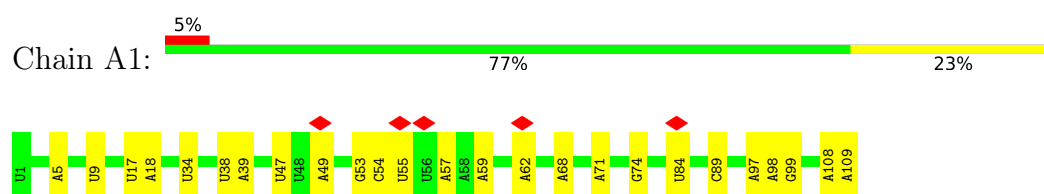
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Mol	Chain	Residues	Atoms		AltConf
125	Aj	4	Total 4	O 4	0
125	AA	1	Total 1	O 1	0
125	AC	1	Total 1	O 1	0
125	AI	4	Total 4	O 4	0
125	AK	2	Total 2	O 2	0
125	B1	10	Total 10	O 10	0
125	B2	41	Total 41	O 41	0
125	B3	55	Total 55	O 55	0
125	B4	63	Total 63	O 63	0
125	Be	3	Total 3	O 3	0
125	Bi	2	Total 2	O 2	0
125	Bl	3	Total 3	O 3	0
125	Bm	2	Total 2	O 2	0
125	Bp	2	Total 2	O 2	0
125	Ya	1	Total 1	O 1	0
125	C2	1	Total 1	O 1	0
125	C3	3	Total 3	O 3	0

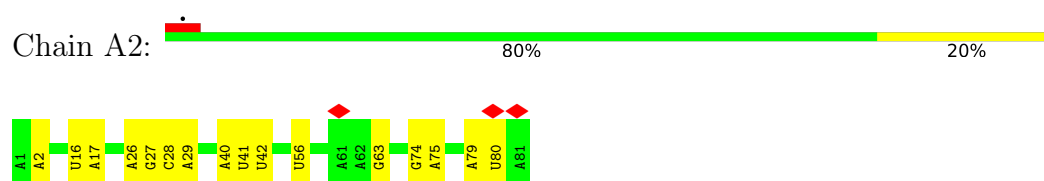
### 3 Residue-property plots [i](#)

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.

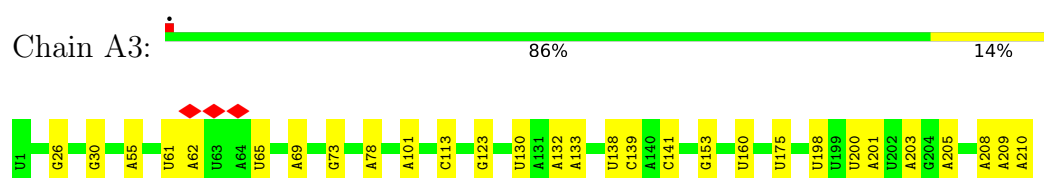
- Molecule 1: mtLSU-1



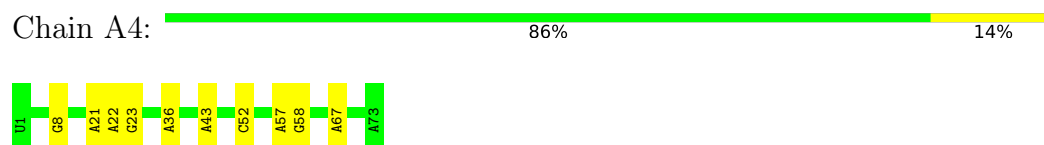
- Molecule 2: mtLSU-2



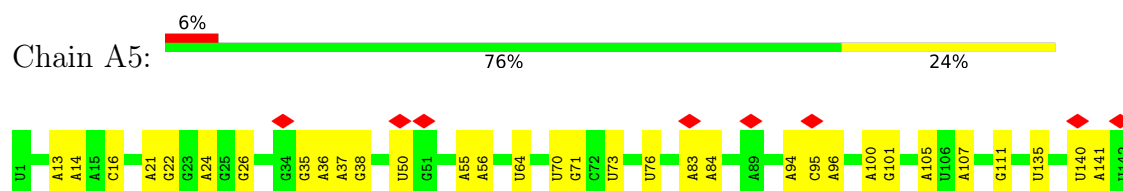
- Molecule 3: mtLSU-3



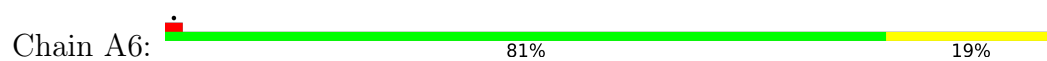
- Molecule 4: mtLSU-4



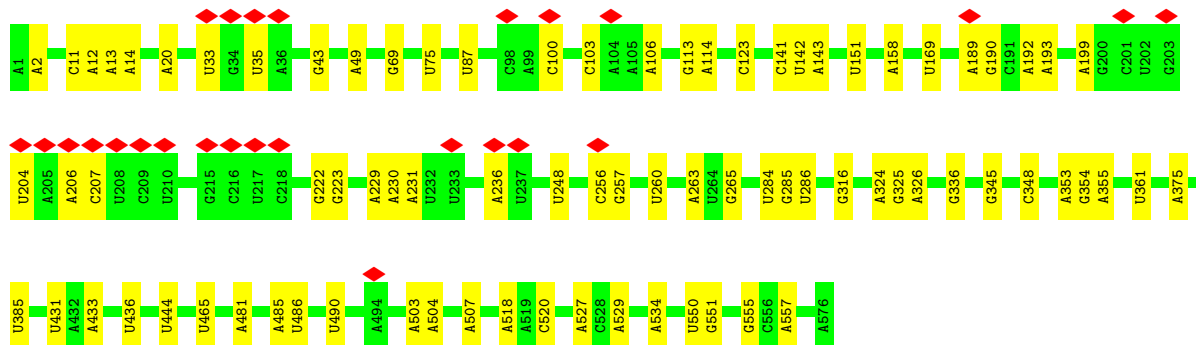
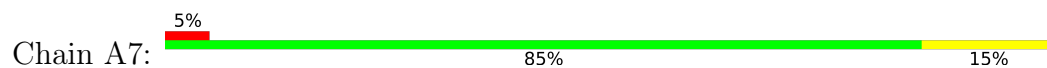
- Molecule 5: mtLSU-5



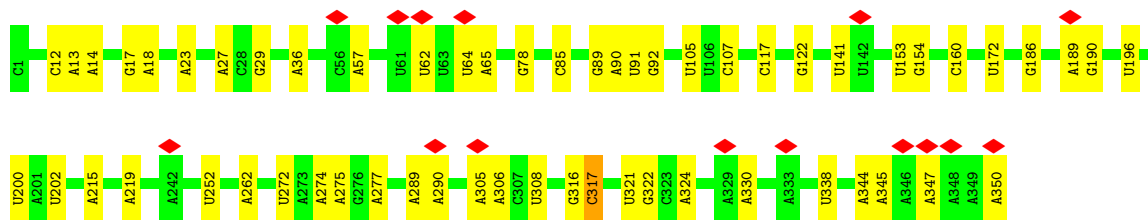
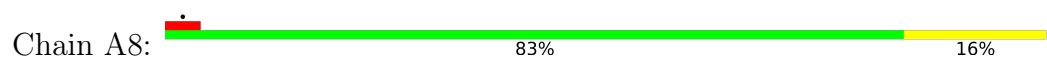
- Molecule 6: mtLSU-6



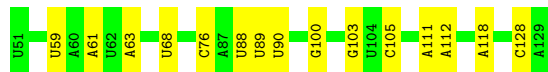
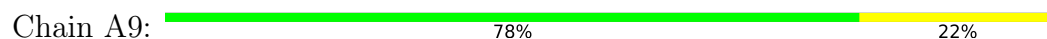
- Molecule 7: mtLSU-7



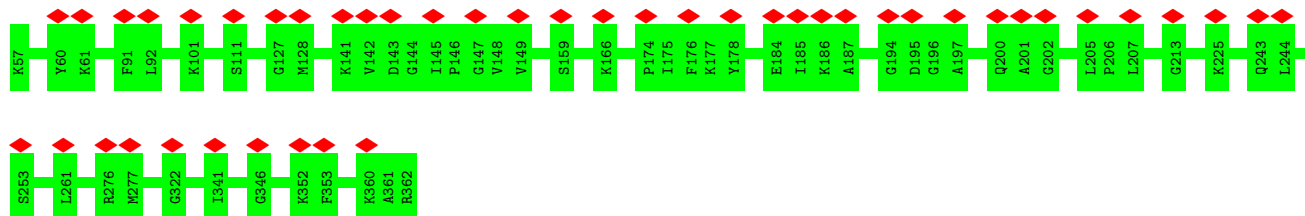
- Molecule 8: mtLSU-8



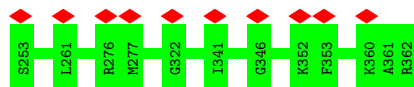
- Molecule 9: mt-5S

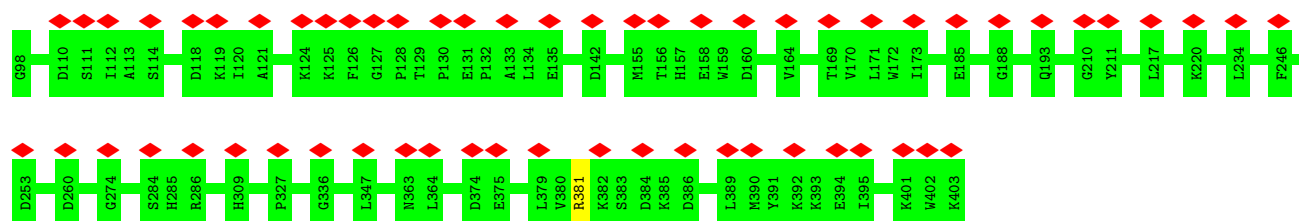


- Molecule 10: uL2m

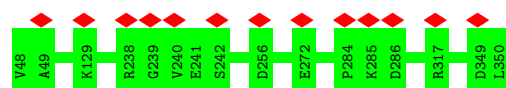


- Molecule 11: uL3m

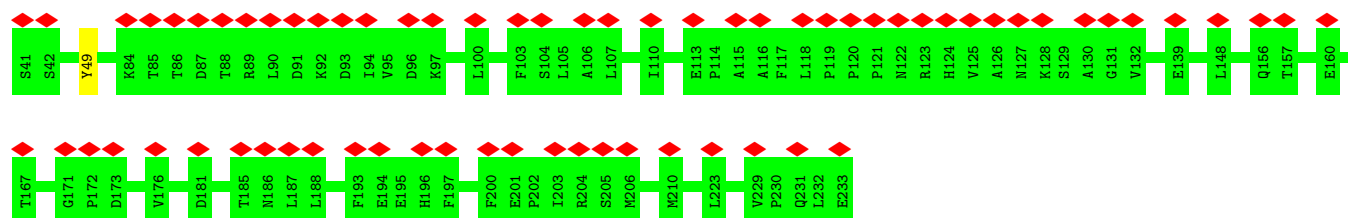




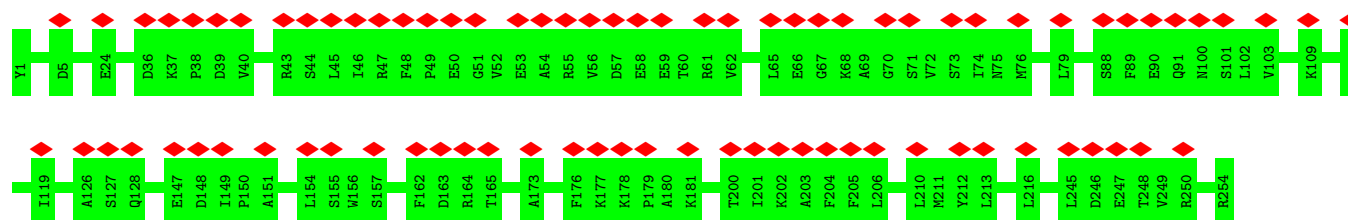
• Molecule 12: uL4m



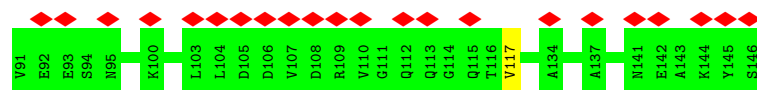
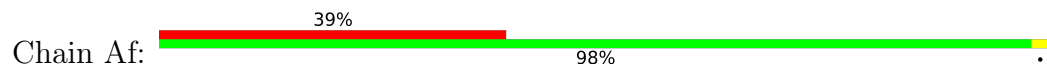
• Molecule 13: uL5m



• Molecule 14: uL6m

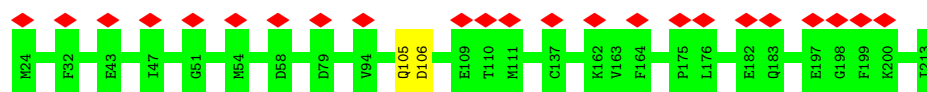


• Molecule 15: uL9m

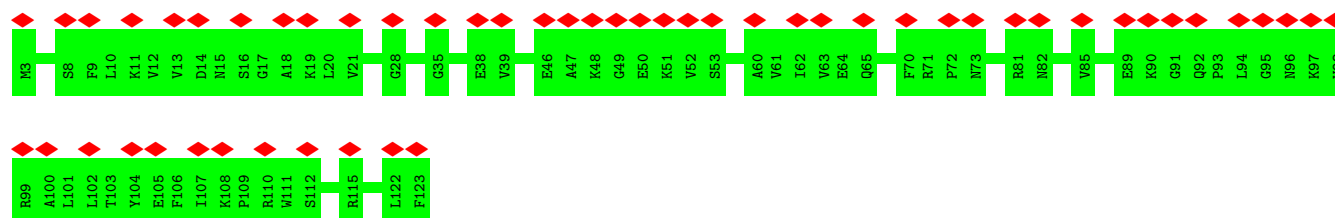


• Molecule 16: uL13m

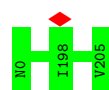




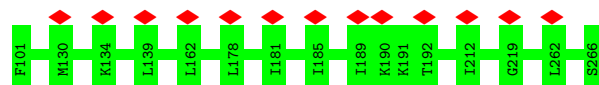
• Molecule 17: uL14m



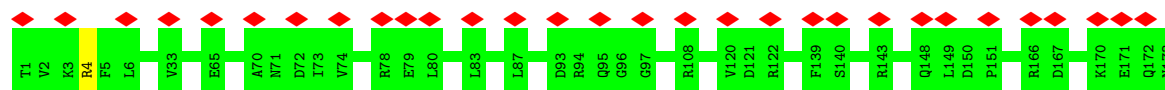
• Molecule 18: uL15m



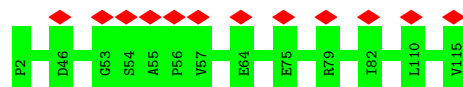
• Molecule 19: uL16m



• Molecule 20: bL17m



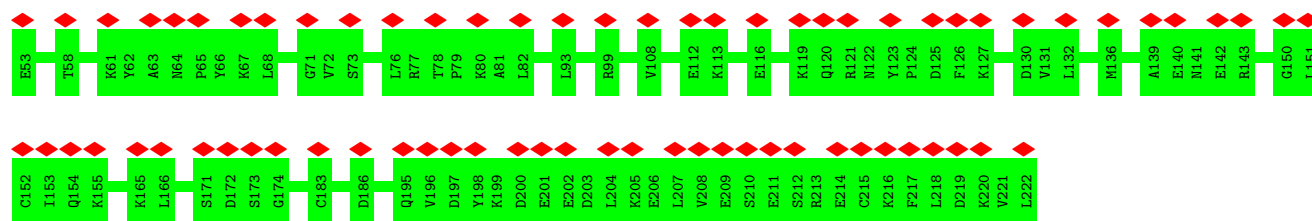
• Molecule 21: uL18m



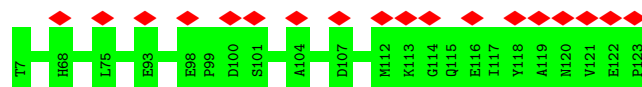
• Molecule 22: bL19m







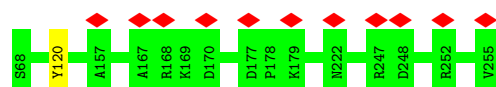
• Molecule 23: bL20m



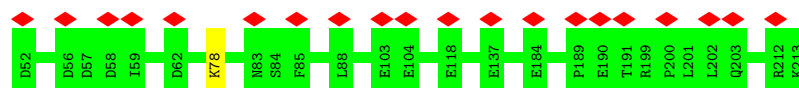
• Molecule 24: bL21m



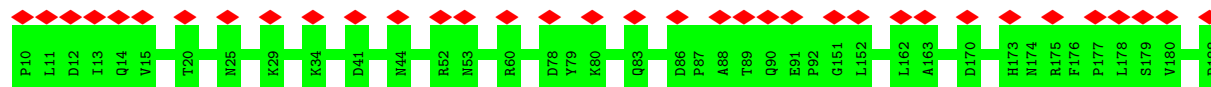
• Molecule 25: uL22m



• Molecule 26: uL23m

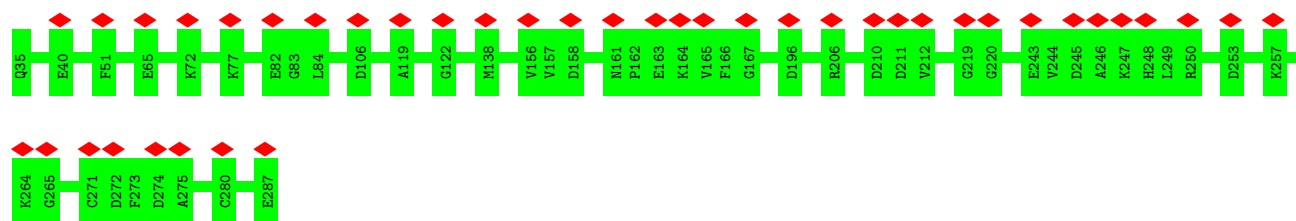


• Molecule 27: bL24m

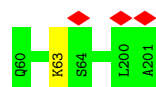


• Molecule 28: bL25m

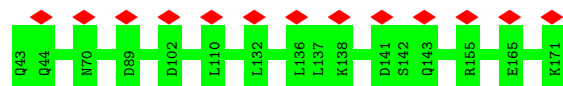




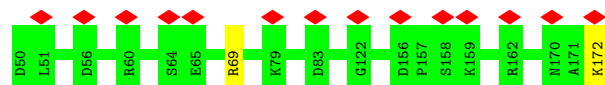
• Molecule 29: bL27m



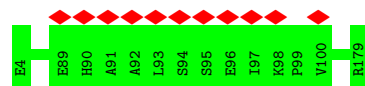
• Molecule 30: bL28m



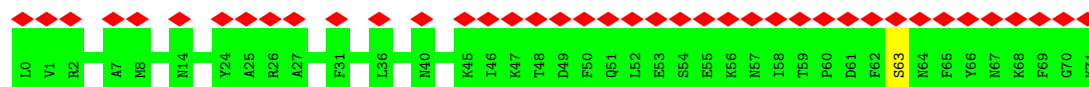
• Molecule 31: uL29m



• Molecule 32: uL30m

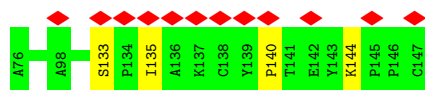


• Molecule 33: bL31m



• Molecule 34: bL32m





- Molecule 35: bL33m

Chain AA: 100%



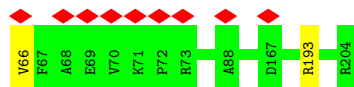
- Molecule 36: bL34m

Chain AB: 100%

There are no outlier residues recorded for this chain.

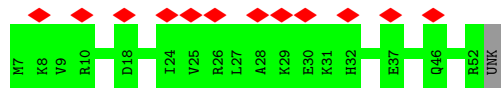
- Molecule 37: bL35m

Chain AC: 99%



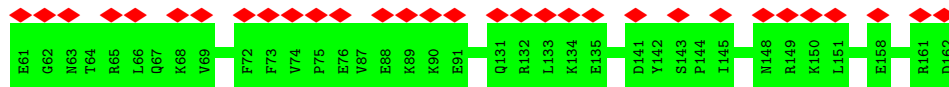
- Molecule 38: bL36m

Chain AD: 98%



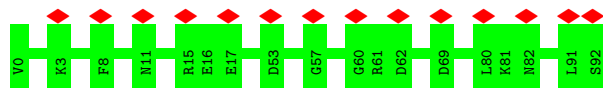
- Molecule 39: mL40

Chain AE: 100%



- Molecule 40: mL41

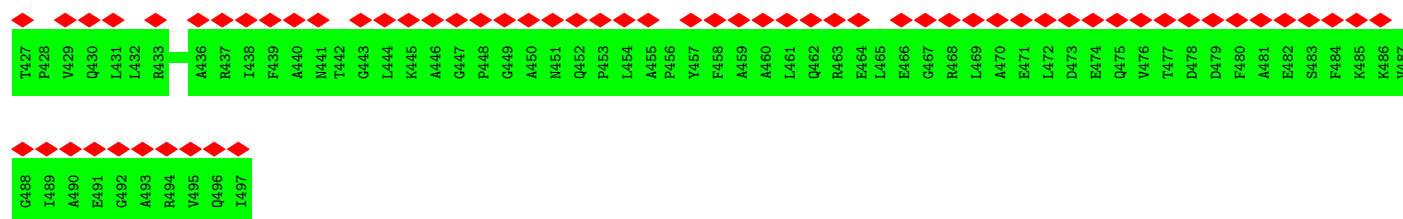
Chain AF: 100%



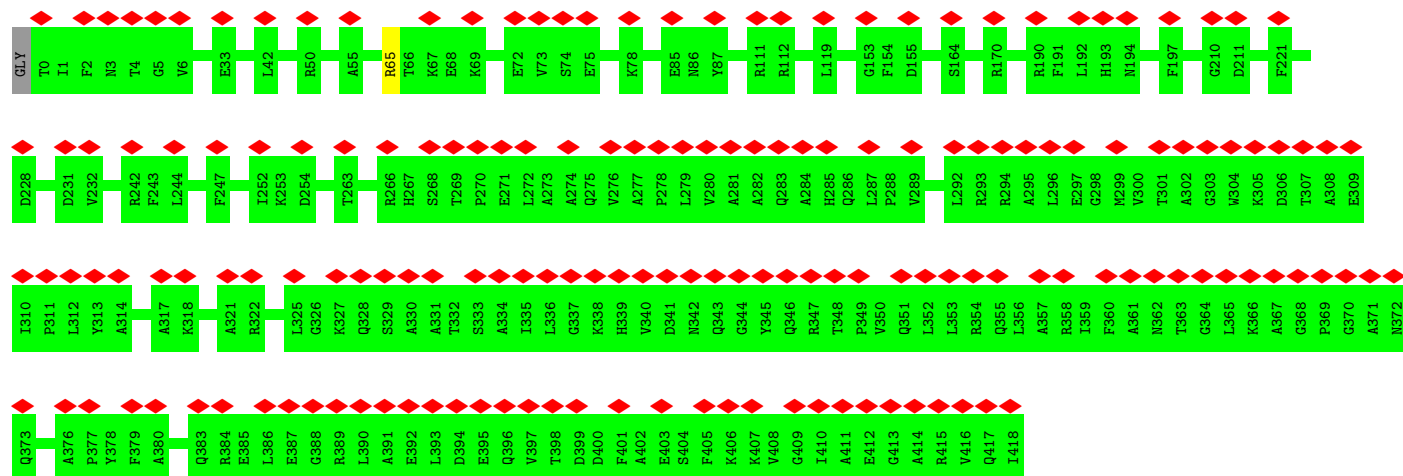
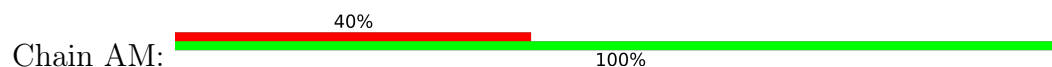
- Molecule 41: mL43

Chain AG: 100%

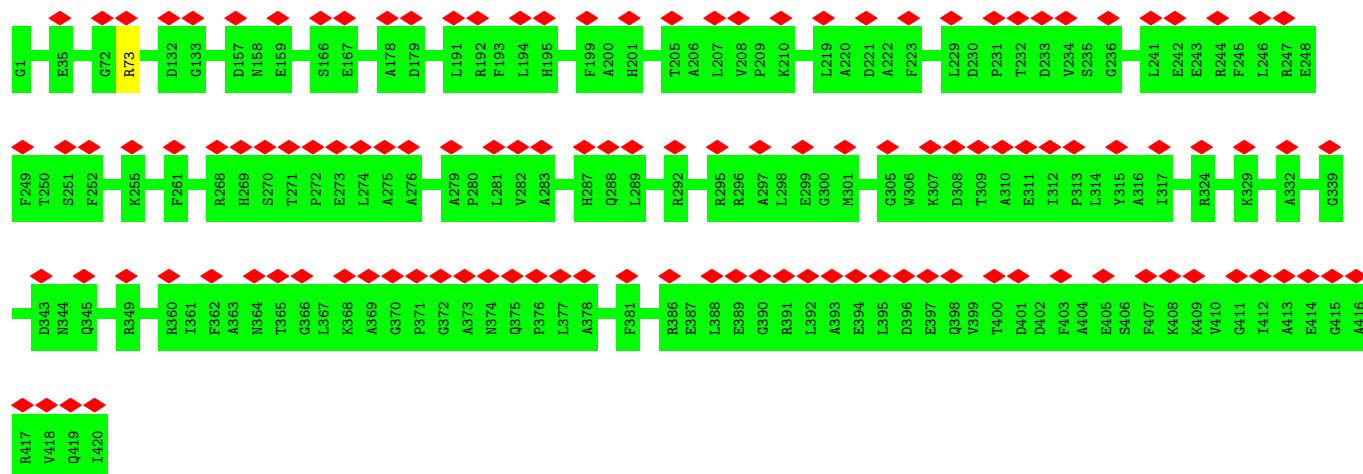




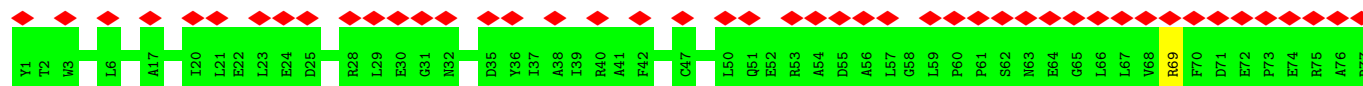
• Molecule 46: mL116

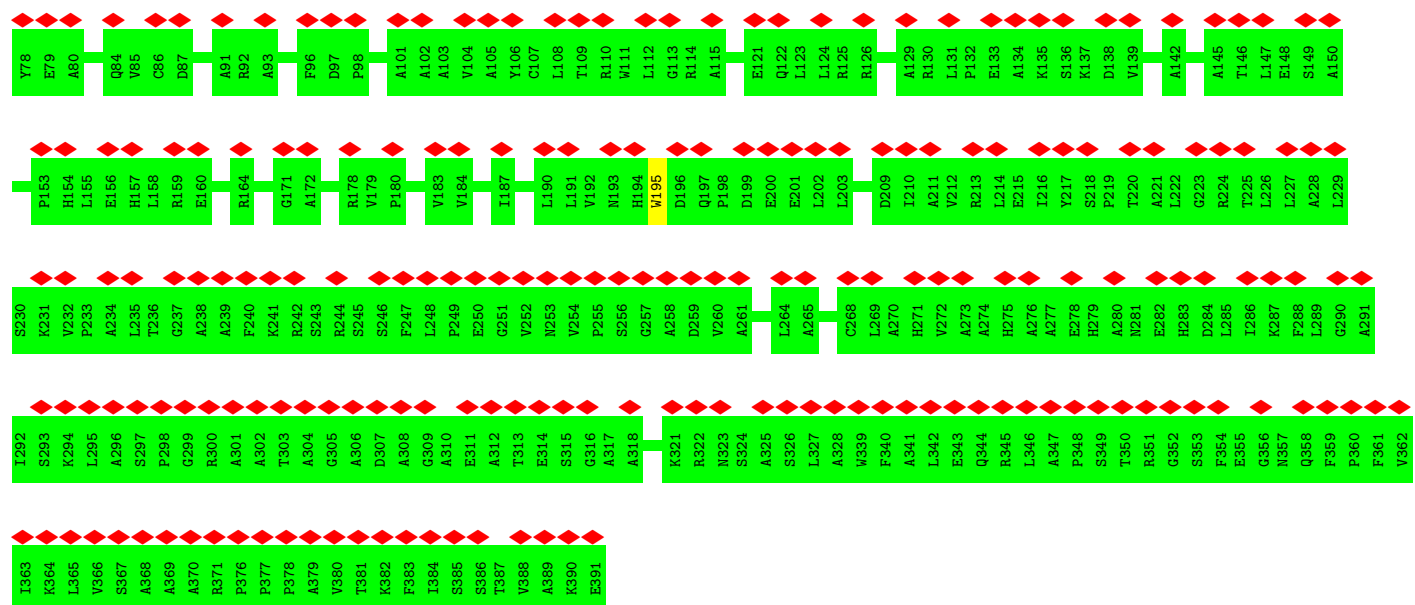


• Molecule 46: mL116



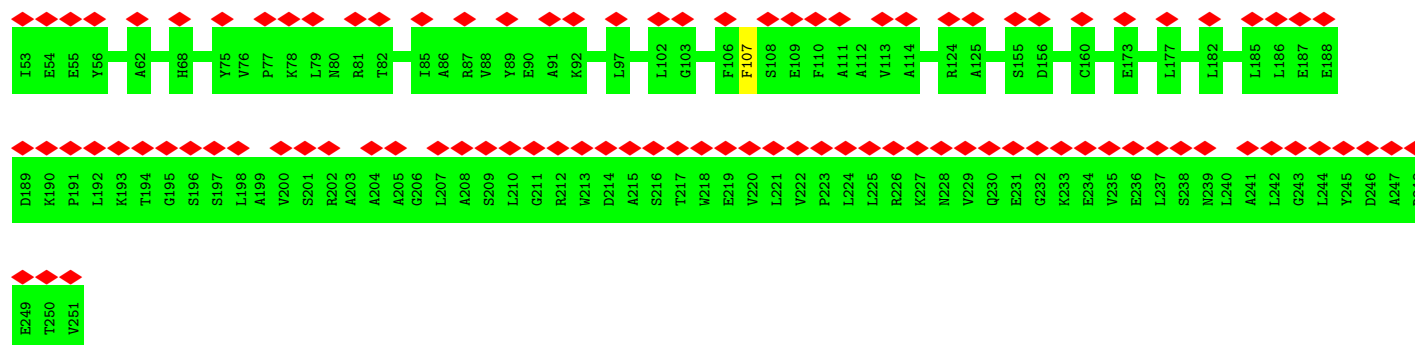
• Molecule 47: mL118





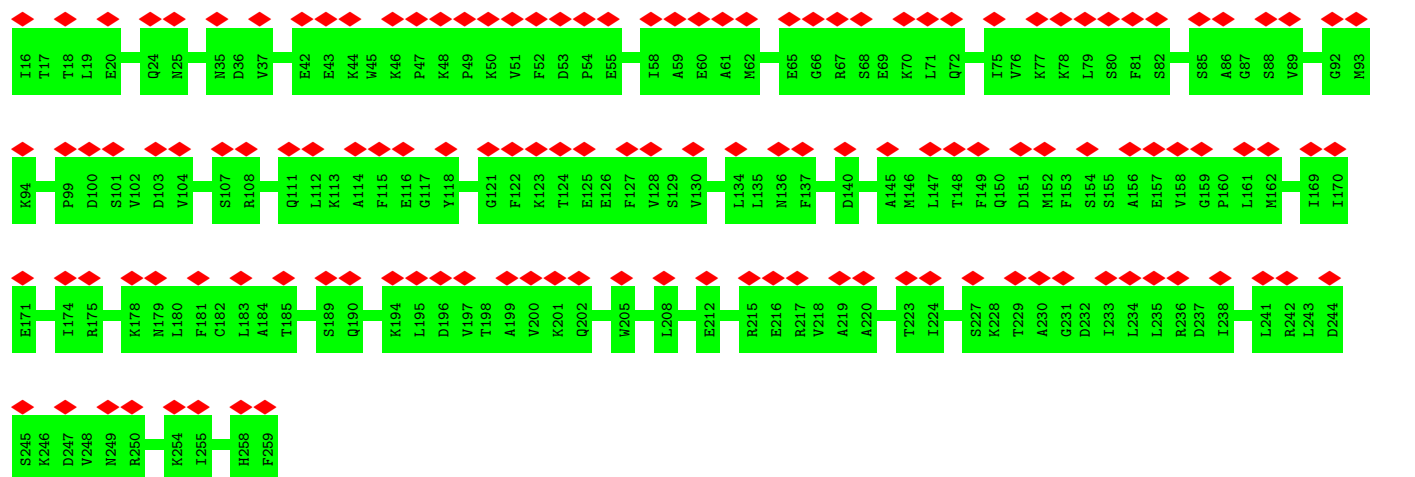
• Molecule 48: mL120

Chain Xa: 49% 99% .

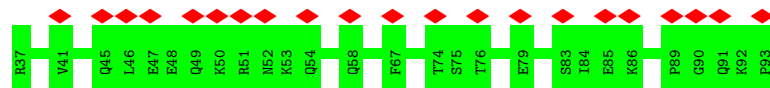
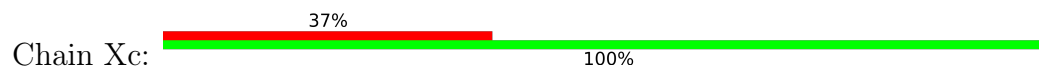


• Molecule 49: mL121

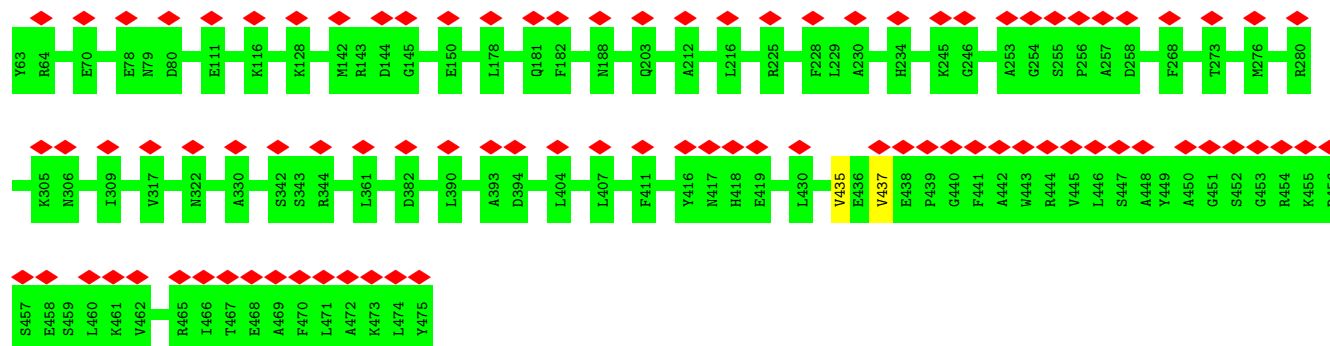
Chain Xb: 55% 100%



- Molecule 50: mL122



- Molecule 51: mL123

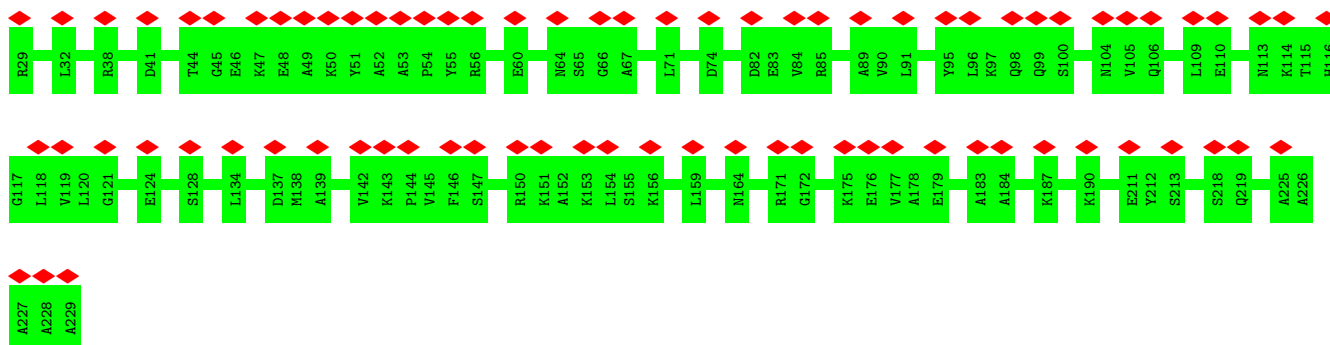


- Molecule 52: mL124

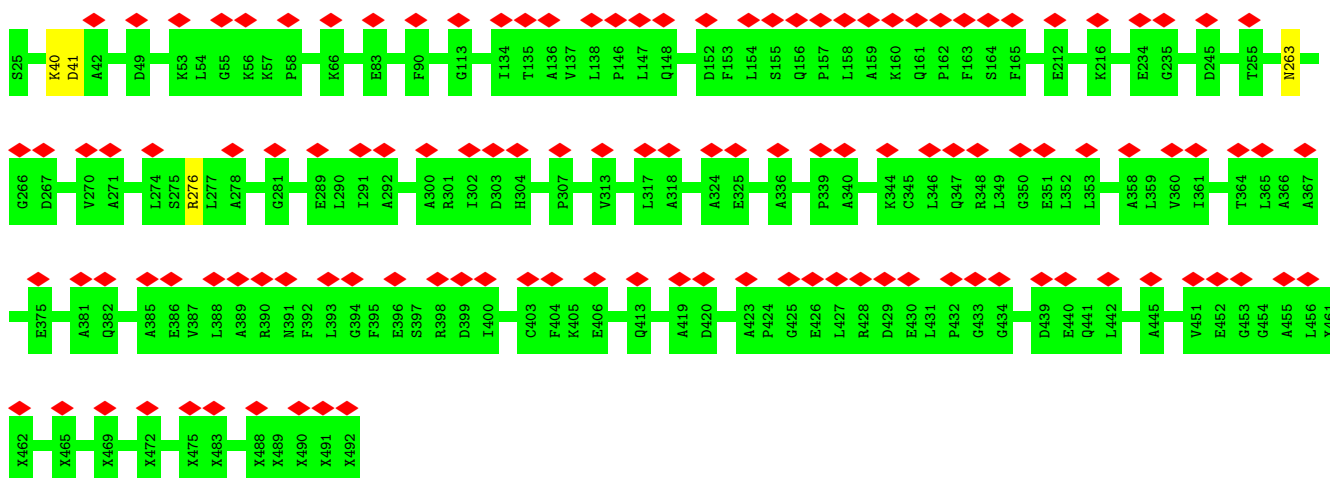


- Molecule 53: mL125

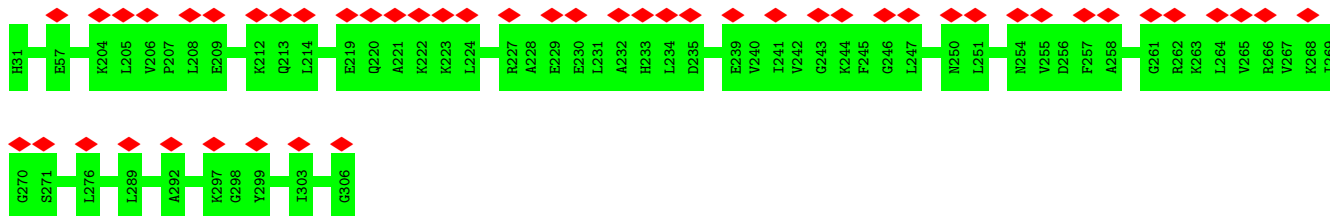




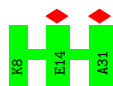
Chain Xg: 30% 99%



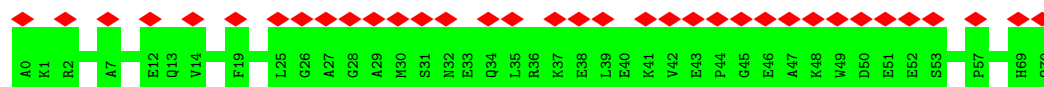
Chain Xh: 34% 100%



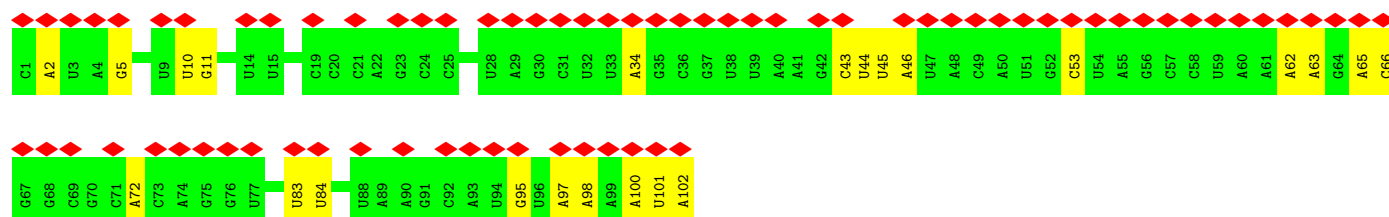
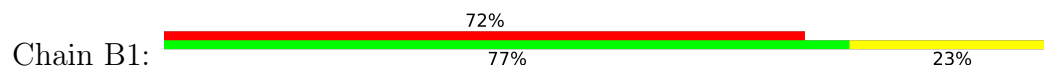
Chain Xi: 8% 100%



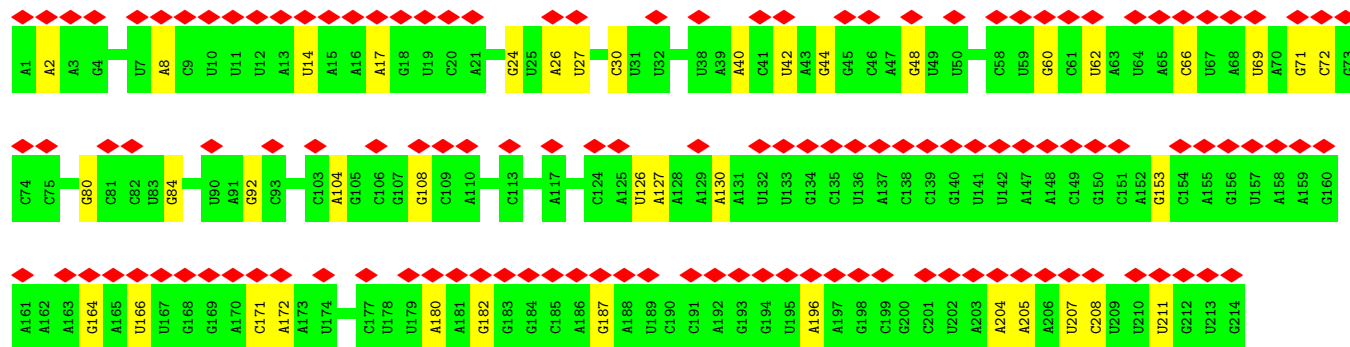
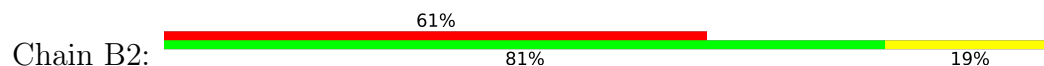




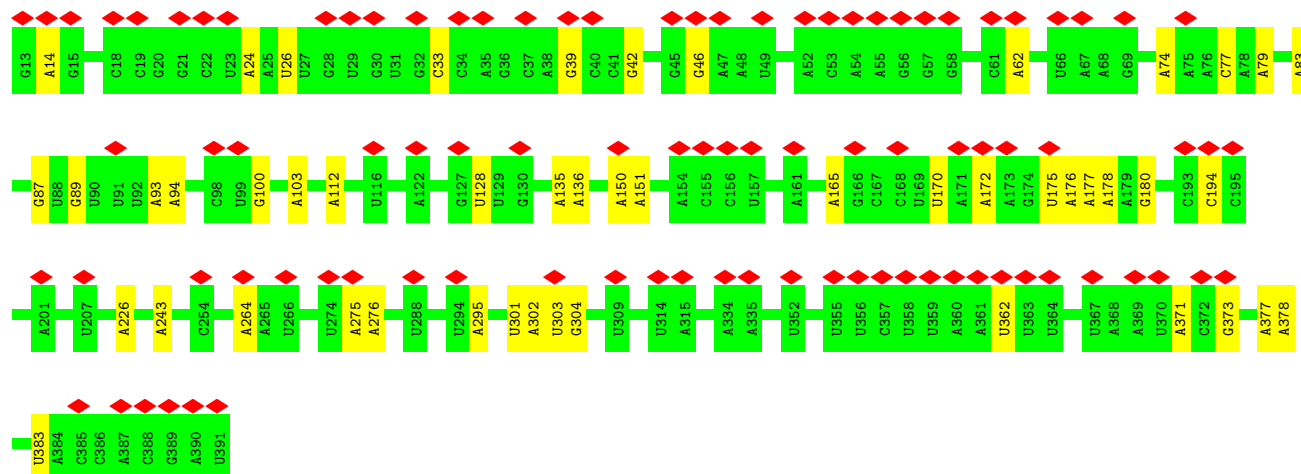
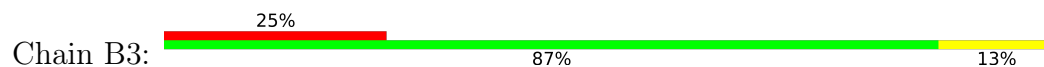
• Molecule 58: mtSSU-1



• Molecule 59: mtSSU-2

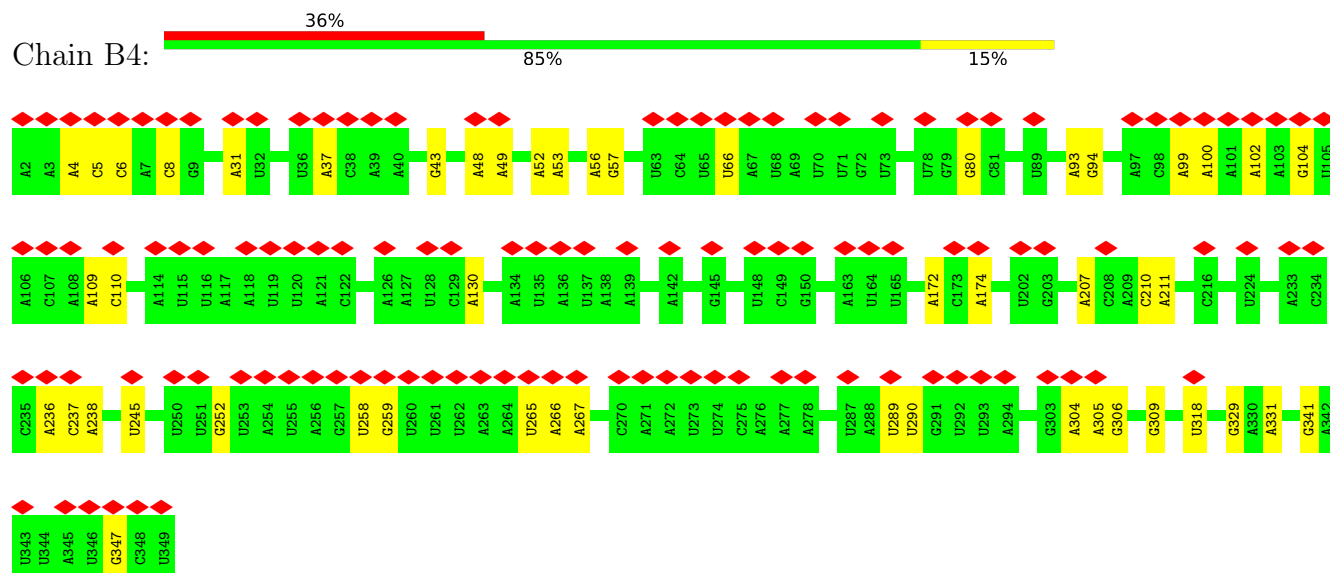


• Molecule 60: mtSSU-3



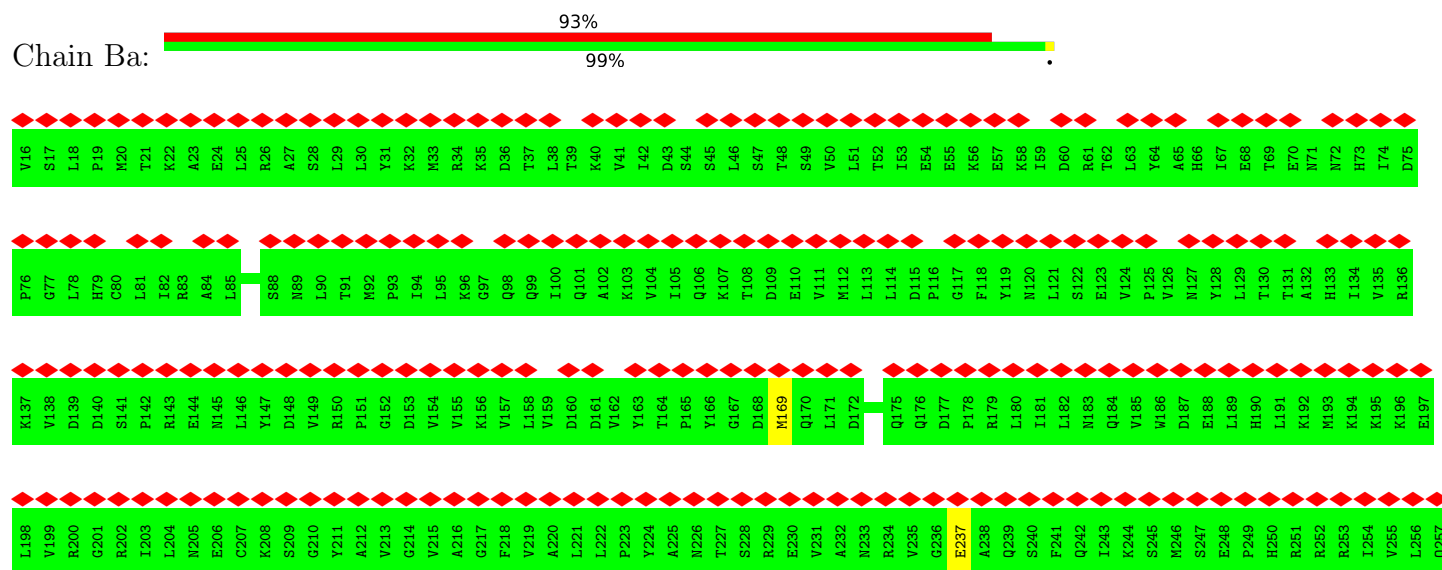
- Molecule 61: mtSSU-4

Chain B4:



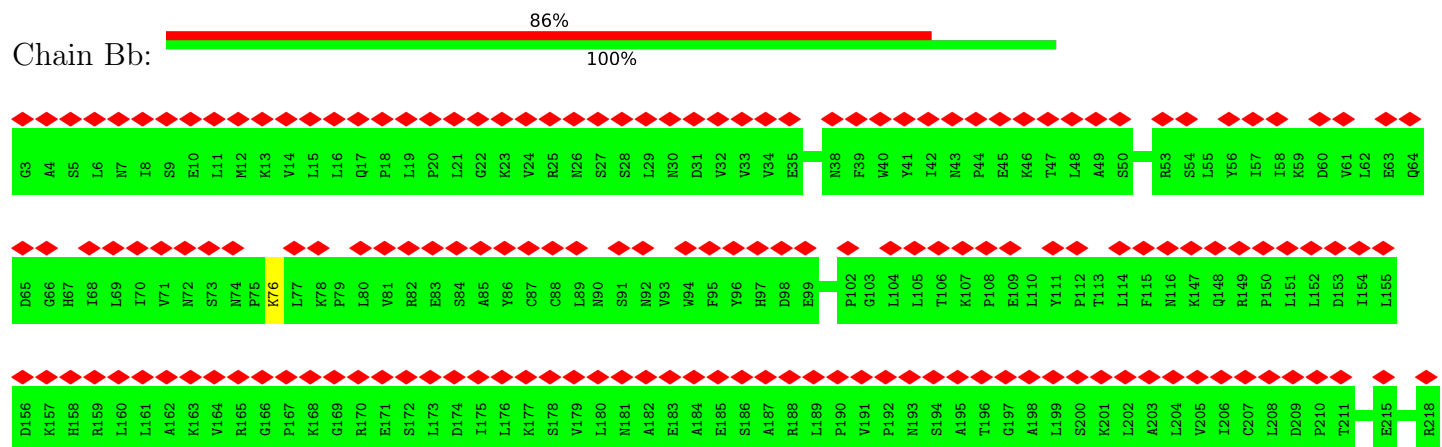
- Molecule 62: bS1m

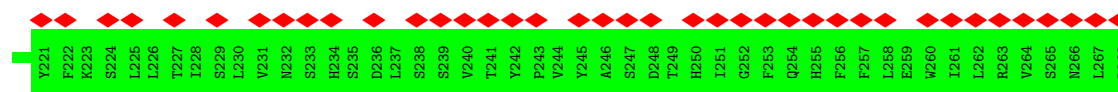
Chain Ba:



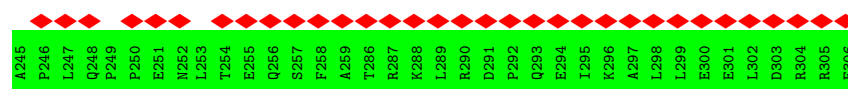
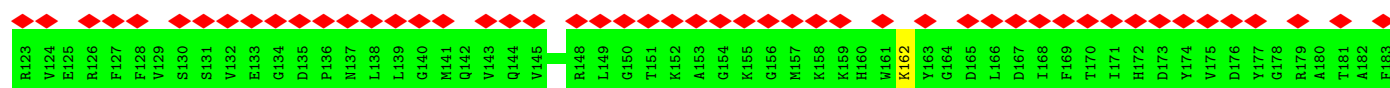
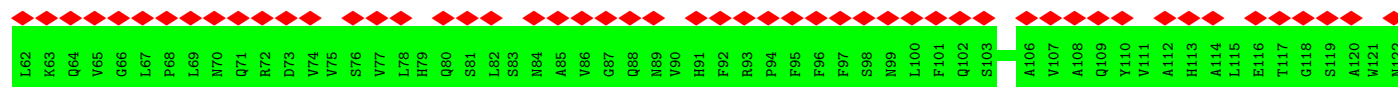
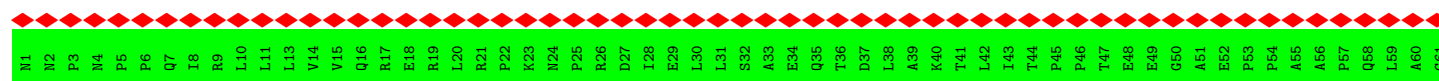
- Molecule 63: uS2m

Chain Bb:

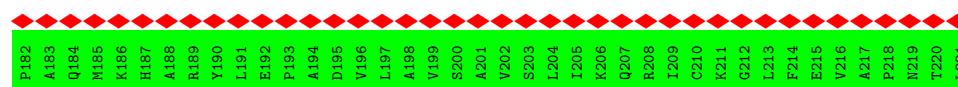
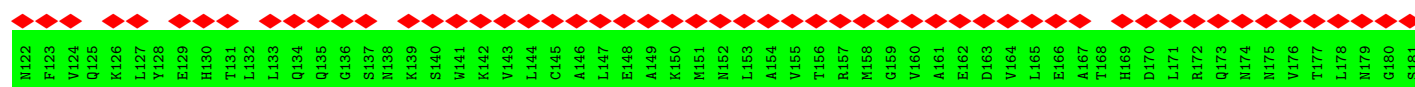
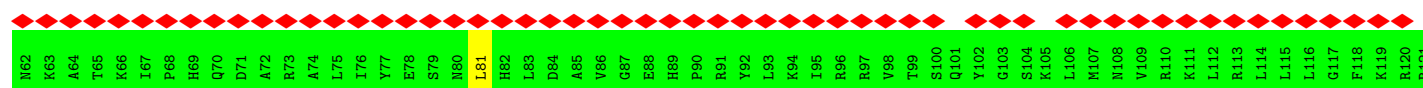
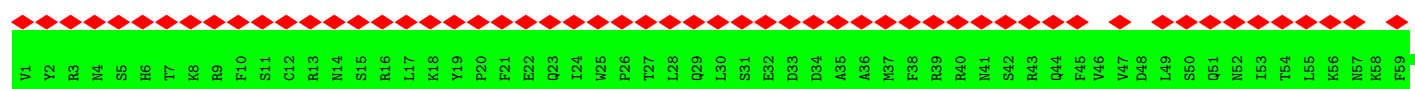




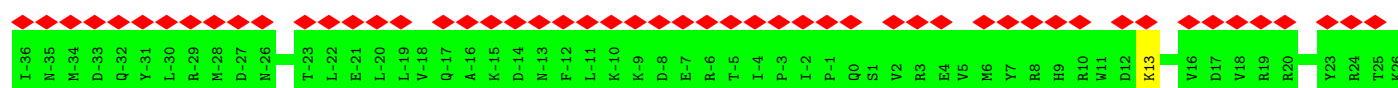
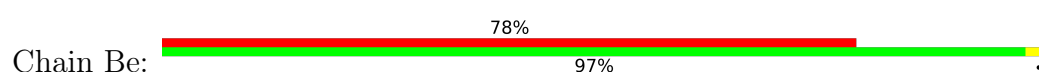
• Molecule 64: uS3m



• Molecule 65: uS4m



• Molecule 66: uS5m



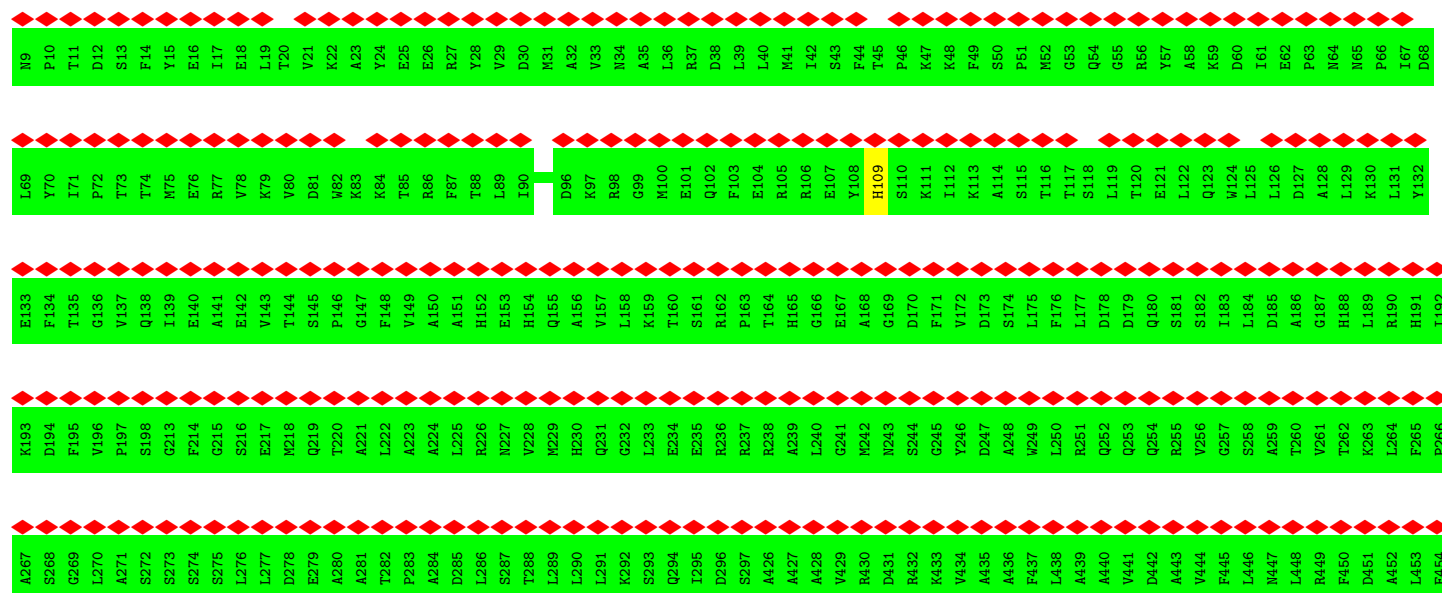




## • Molecule 70: uS9m



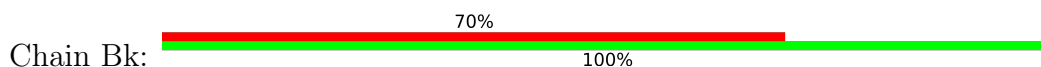
## • Molecule 71: uS10m



G455 H456 A457 R458 F459 P460 F461 H462 F463 A464 T465 A466 V467 P468 G469 Q470 M471 K472 V473 P474 V475 M477 W478 M479 Q480 A481 V482 S483 S484 K484 M485 A486 E487 Y488 Q489 R490 Q491 V492 S493 E494 A495 S496 Q497 A498 A499 D500 L501 L502 K503 Y505 T506 S507 Y508 S509 A510 F511 S512 Q513 A514

L515 L516 Y517 K518 L519 M520 Q521 L522 W523 F524 E525 T526 A527 S528 S529 D530 A531 K532 E533 Y534 L535 L537 P538 S539 W540 E541 E542 Y543 E544 A545 M546 V547 Q548 A549 K550 R551

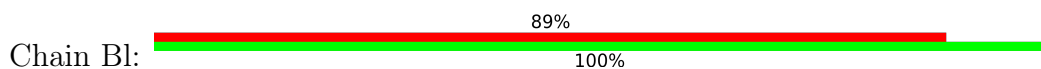
• Molecule 72: uS11m



V1 L2 Q3 L4 E5 G6 V7 W8 H9 I10 L11 M12 N13 S14 N15 M16 G91 I17 V18 L19 T20 L21 D23 K24 E25 G26 R27 V28 V31 V37 G38 R45 L46 A49 A53 A54 G55 E56 L57 A58 R60 A61 L62 Y66 S67 T68 V69 A70 I71 K72 I73 K74 G75

I76 G77 T78 W79 T80 Q81 Y82 A83 Q85 R86 L87 S88 S89 S90 G91 I92 K93 I94 L97 V98 D99 V100 T101 P102 V103 G106 R109 P110 S111 R112 K113 R114 R115 V116

• Molecule 73: uS12m



L2 T3 V4 L7 L8 R9 G10 G11 R12 T13 K14 K15 V16 R17 R18 S19 K20 S21 P22 A23 L24 E25 Y29 K30 K31 G32 I33 L35 R36 V37 Y38 T39 T40 A41 P42 K43 K44 P45 N46 S47 A48 M49 R50 K51 V52 C53 K54 V55 Q56 L57 S58 M59 Y61 K62 V63 L64

A65 Y66 I67 P68 G69 E70 G71 H72 W73 L74 T75 E76 H77 S78 I79 V80 L81 V82 R83 G84 R86 T87 K88 D89 L90 P91 G92 V93 K94 Y95 K96 V97 I98 R99 G100 K101 Y102 D103 C104 A105 G106 V107 K108 G109 R110 T111 S112 R114 S115 K116 Y117 G118 V119 K120 P122 K123 E124

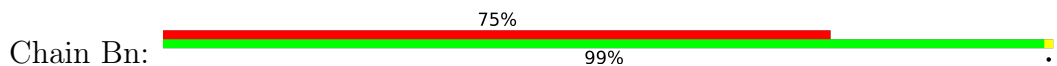
• Molecule 74: uS13m



V2 Q3 I4 Q5 R6 V7 T8 L9 P10 H12 Q13 C14 V15 Y16 M17 A18 K20 K21 V22 P23 G24 L25 G26 P28 T29 S30 L31 A32 V33 V34 E35 A36 C37 G38 I39 S40 K41 G42 V43 R44 V45 R46 D47 L48 K49 E50 N51 H52 V53 Q54 I56 T57 Q58 F59 I60 Q61

D62 M63 F64 V65 T66 E67 D68 M69 L70 R71 R72 K73 V74 R75 E76 D77 I78 V79 K80 L81 V82 M83 I84 K85 S86 R87 D88 G89 L90 R91 H92 D93 W94 G95 V96 S97 I98 K99 G100 H101 T102 S103 N105 G106 K107 T108 A109 R111 R112 R113 H114

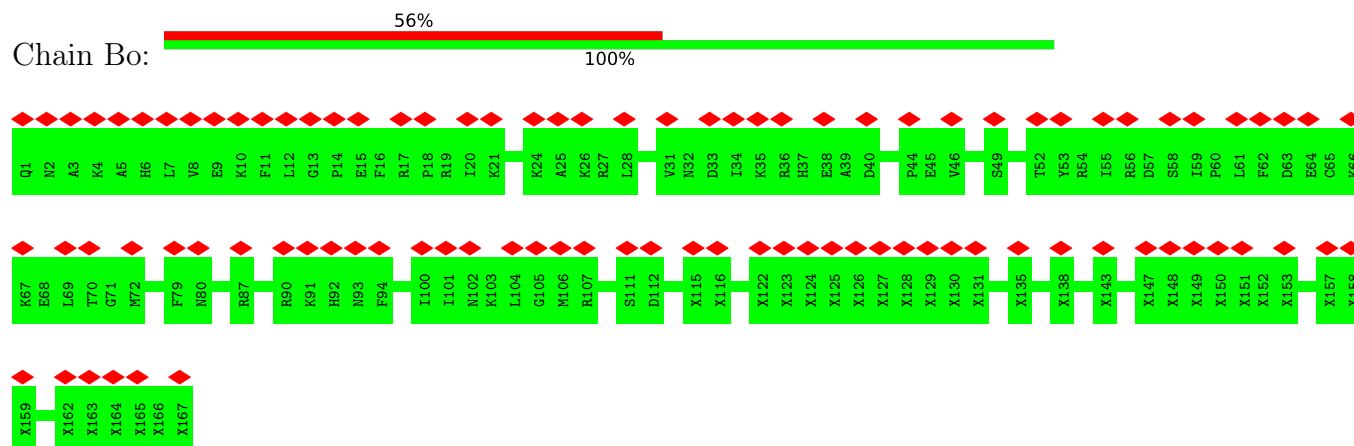
• Molecule 75: uS14m



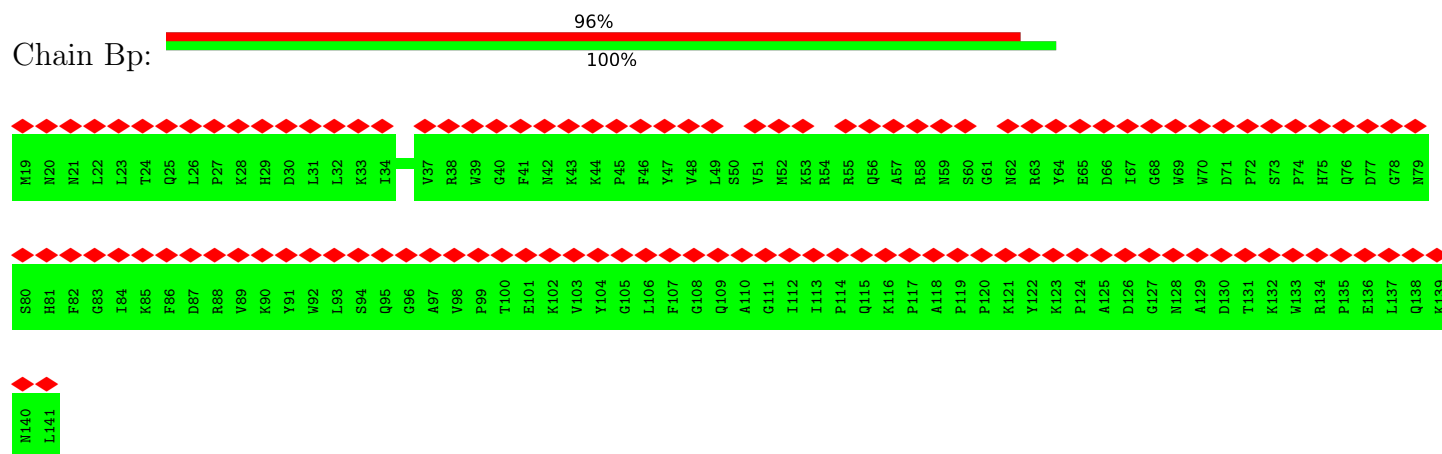
T1 T2 K3 N4 F5 R6 L7 R8 F9 R10 Q13 Y14 I17 V18 R21 R22 L23 D24 K25 D26 Q27 R28 T29 R30 V31 L32 Y33 D34 Q35 H36 E37 V38 D39 R40 R41 L42 Y43 K44 A45 M46 T47 R48 E50 S51 L52 T53 L54 P55 V56 R57 L58 Q59 V60 Q61 R62 L63

F64 E65 T66 E67 M68 P69 R70 D71 S72 A73 P74 R76 I77 V78 D79 R80 C81 V82 T83 T84 G85 R88 K92 F93 G94 G95 L96 M100 L101 R102 Q103 L104 Y107 I110 G111 A114 K115 A116 S117 W118

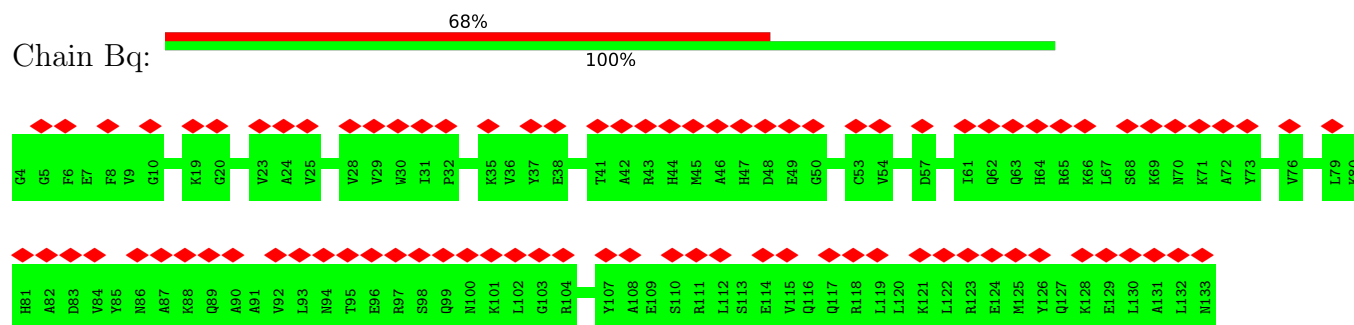
- Molecule 76: uS15m



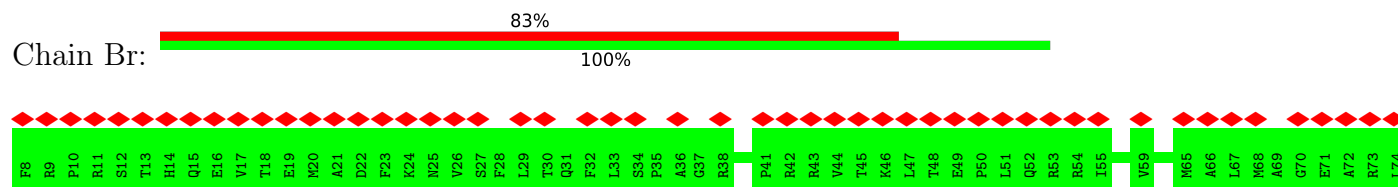
- Molecule 77: bS16m

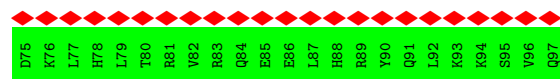


- Molecule 78: uS17m



- Molecule 79: bS18m

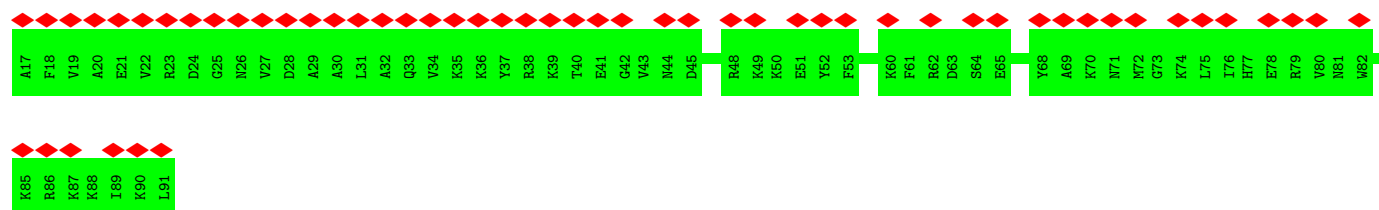
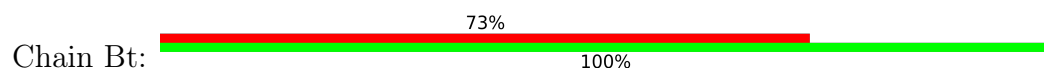




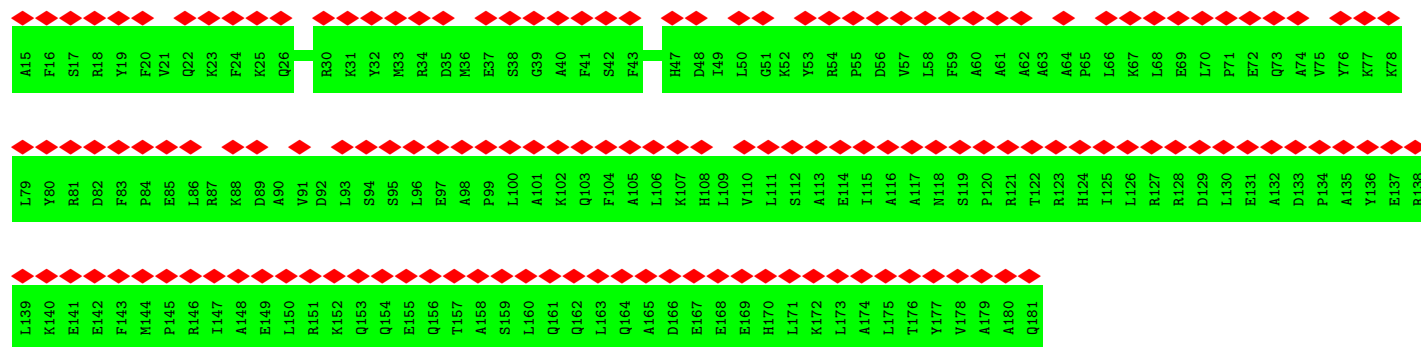
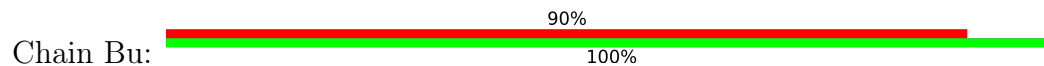
## ● Molecule 80: bS19m



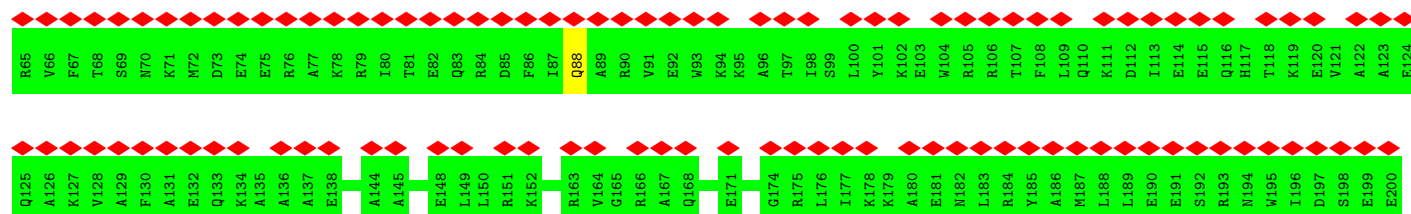
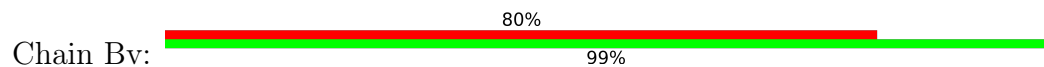
## ● Molecule 81: bS21m



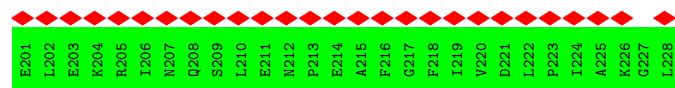
## ● Molecule 82: mS23



## ● Molecule 83: mS26

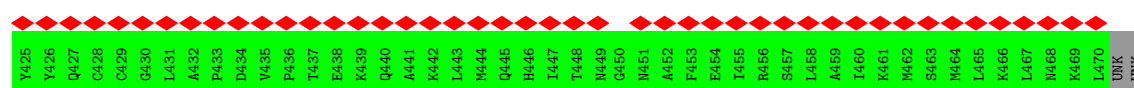
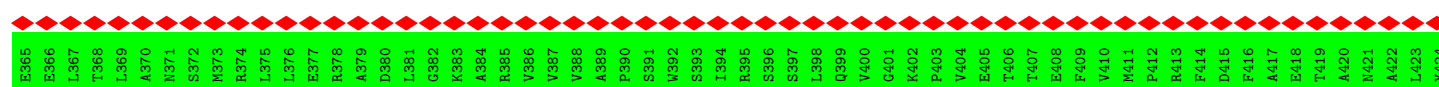
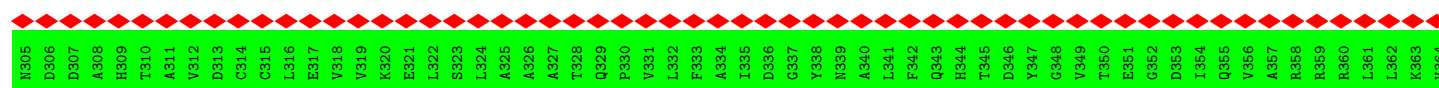
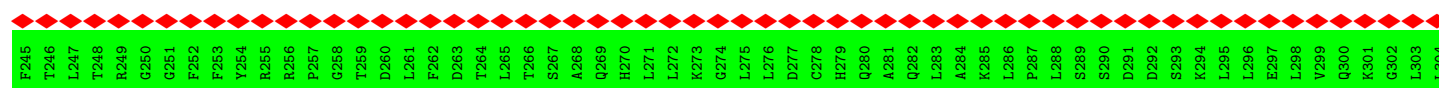
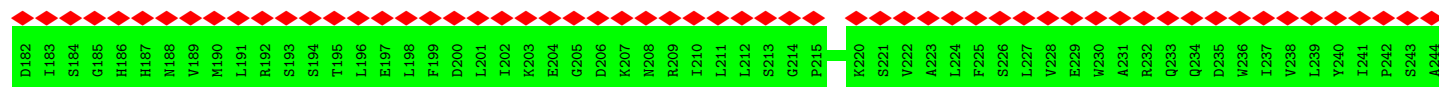
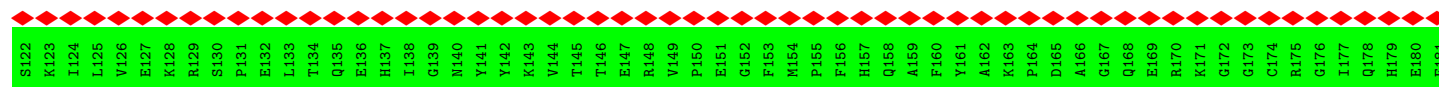






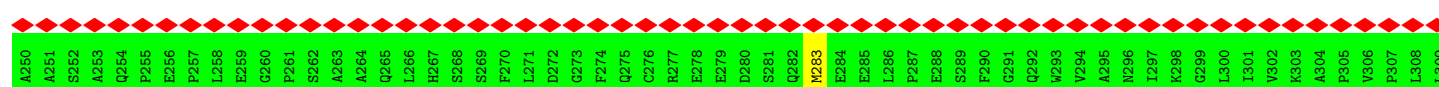
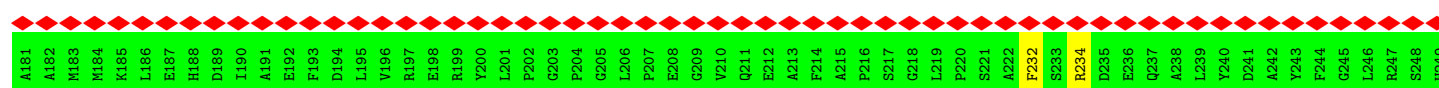
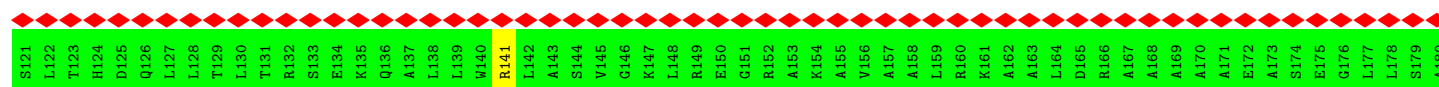
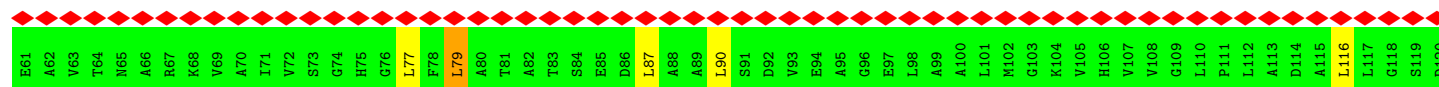
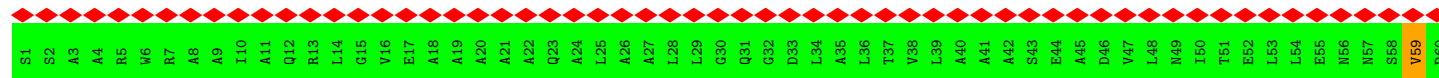
## • Molecule 84: mS29

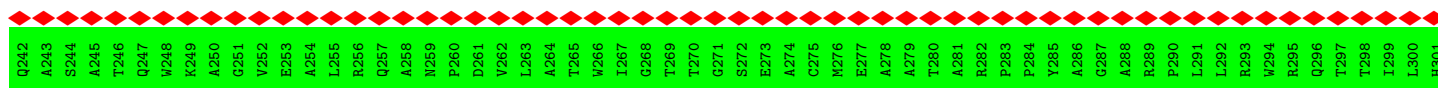
Chain Bw:



## • Molecule 85: mS31

Chain Bx:





A302 A303 A304 A305 A306 A307 A308 A309 A310 A311 A312 A313 A314 A315 A316 A317 A318 A319 A320 A321 A322 A323 A324 A325 A326 A327 A328 A329 A330 A331 A332 A333 A334 A335 A336 A337 A338 A339 A340 A341 A342 A343 A344 A345 A346 A347 A348 A349 A350 A351 A352 A353 A354 A355 A356 A357 A358 A359 A360 A361

S362 E363 E364 D365 T366 L367 S368 I369 A370 A371 D372 R373 Y374 N375 D376 R377 E378 S379 N380 R381 R382 L383 A384 L385 E386 Q387 L388 Q389 A390 A391 V392 K393 E394 C395 D396 T397 R398 Y399 P400 G401 A402 T403 T404 P405 A406 K407 Q408 Y409 L410 S411 G412 F413 G414 F415 F416 Q417

• Molecule 89: mS37



P11 W12 Q13 L14 K15 E16 P17 D18 N19 S20 R21 V22 V23 K24 N25 L26 V27 K28 P29 S30 K31 P32 C33 G34 K35 E36 L37 A39 L40 I41 D42 C43 T44 R45 R46 N47 F48 S49 G50 D51 A52 D53 G54 T55 C56 M57 R58 E59 A61 A62 L63 A64 R65 S66 S67 Q68 R70

K76 K77 T78 S79 K80 G81 E82 I83 L84 N85 H86 L87 K88 N89 L90 A91 A92 S93 W94 K95 F97 F98 F99

• Molecule 90: mS38



I118 M121 Q122 L126 K127 I128 K135 K146 V147 R148

• Molecule 91: mS45



P45 S46 V47 M48 D49 L50 A51 S52 L53 L54 E58 Q59 Y60 R61 G62 A63 D64 V65 L66 A67 E68 G69 A70 A71 L72 P73 G74 T75 G76 F77 A78 N79 A80 R81 G82 T83 F84 L85 P86 H87 E88 P90 T91 A92 I93 E94 Y95 L96 K97 E98 L99 D100 P101 A103 E104 M105 K106

L107 E108 Q109 M110 E111 A112 M113 Y114 K115 L116 L117 Y118 S119 R120 N121 E122 S123 E124 R125 E126 V127 G128 R129 Q130 M131 M132 Y133 D134 L135 L136 K137 L138 S139 G140 H145 P146 F147 R148 E149 L170 E171 E172 C173 N174 W175 D176 Y177 M178 A179 A180 F181 L182 D183 A184 R185 V186 A187 R188 R189 V190

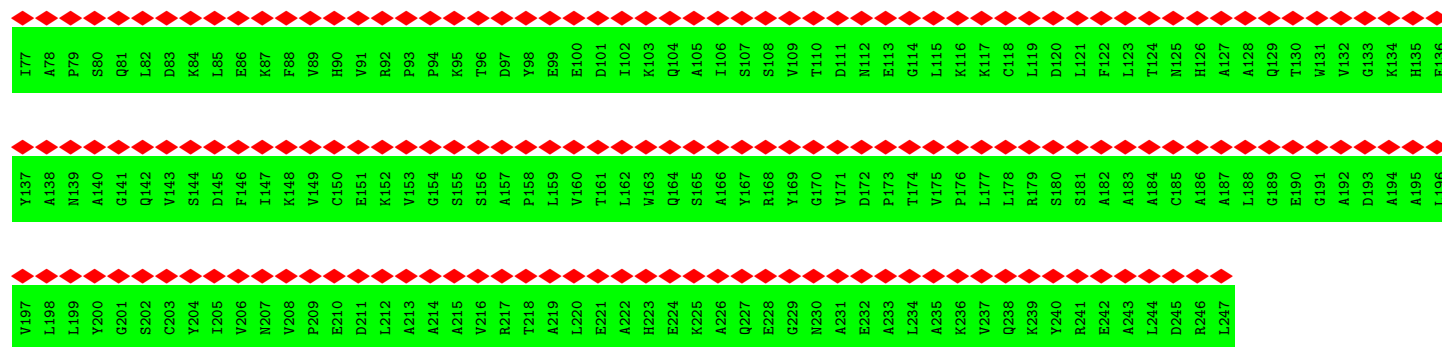
F191 H192 R193 G194 S195 G196 E197 R198 L199 V200 H201 R202 T203 A204 T205 F206 P207 A208 F209 E210 G211 Y212 P213 L214 A215 E216 V217 D218 Q219 T220 T221 E222 G223 E224 V225 K226 L228 N229 R230 E231 E232 S233 K234 R235 Q236 D237 N238 A239 M240 F241 Q242 D243 F244 R245 K246 K247 L248 F250

N251 L252 G253 M254 V255 G256 E257 Q258 L259 W260 E261 P262 V263 G264 G265 V266 L267 S268 A269 N270 L271 R272 S273 A274 L275 D276 R277 P278 L279 V280 V281 Y282 D283 L284 T285 A286 T288 G289 E290 T291 V293 P294 P295 K296 F297 V298 A299 E300 V301 D302 G303 T304 R305 R306 A307 L308 N309 E310

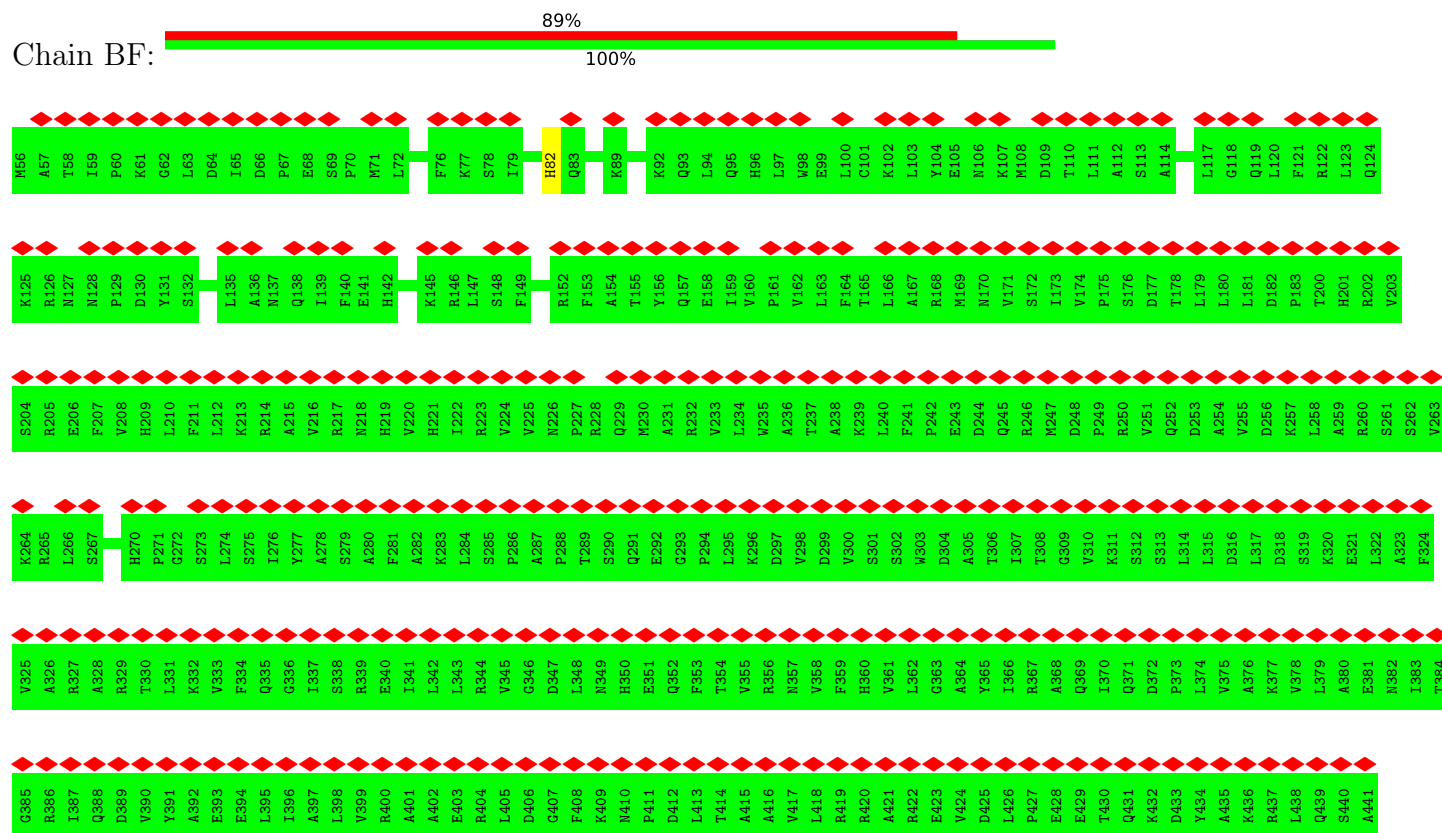
Q311 E312 R313 A314 Y315 A317 K318 R319 K320 P321 G322 P323 R324 L325 P326 Y327 Y328 K329 R330 R331 I332 A333 K335 E336 E337 L338

• Molecule 92: mS106

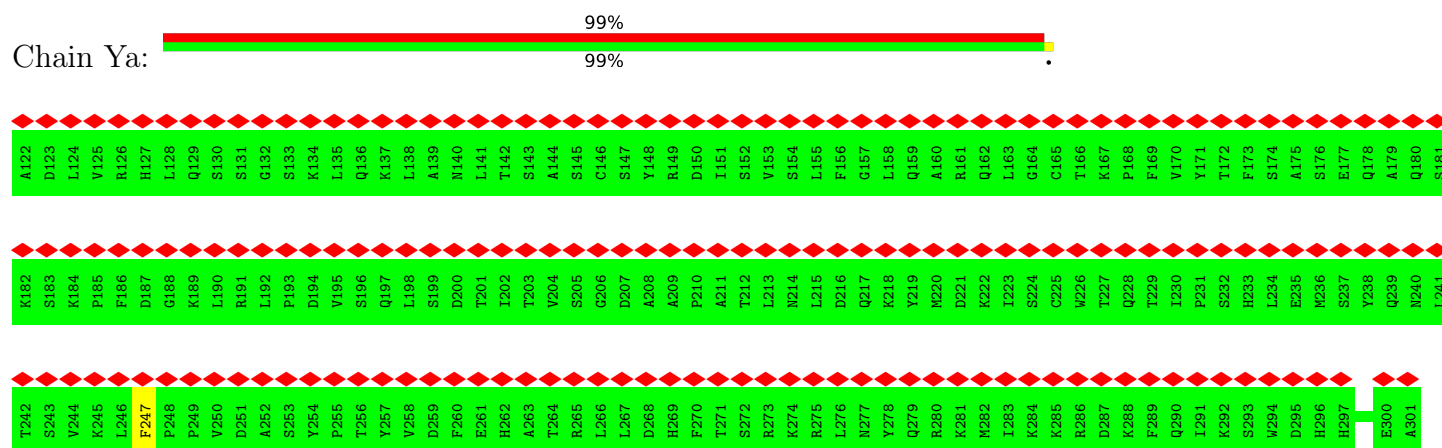




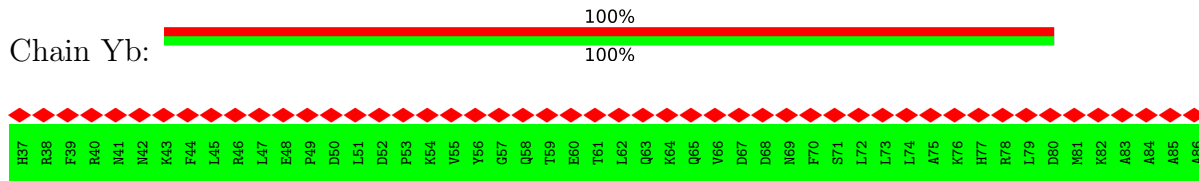
## • Molecule 93: mS107



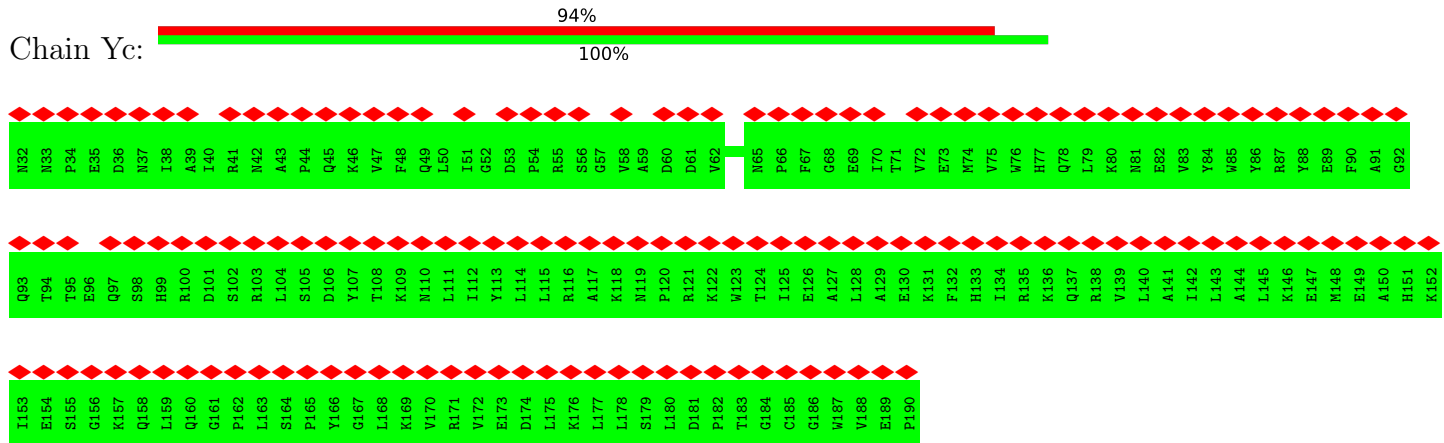
## • Molecule 94: uS4m-2



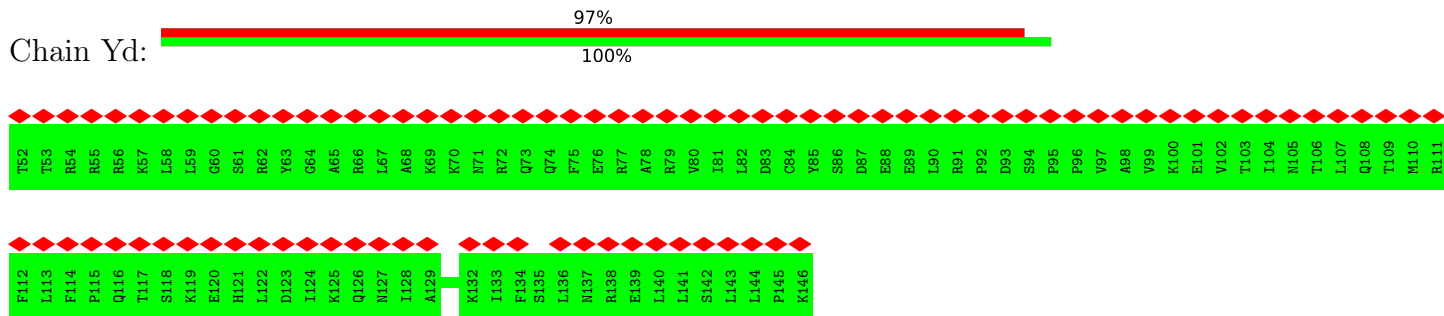
- Molecule 95: mS108



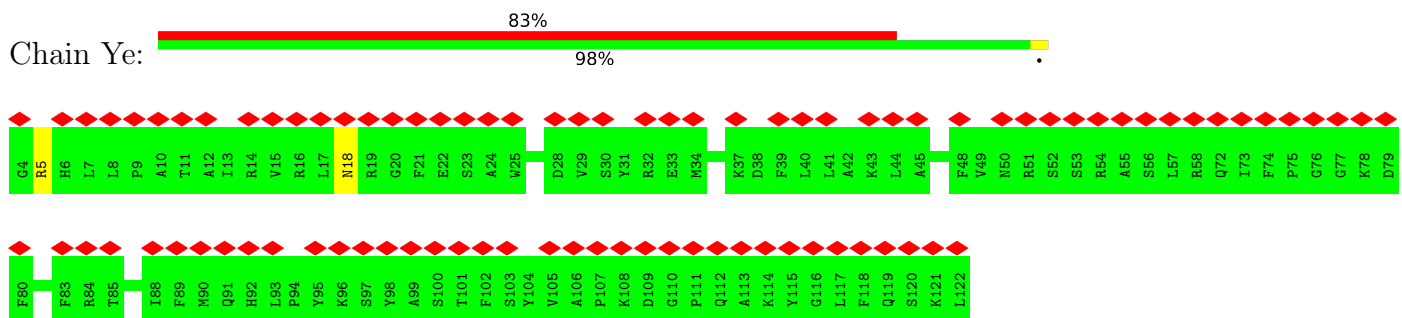
- Molecule 96: mS109



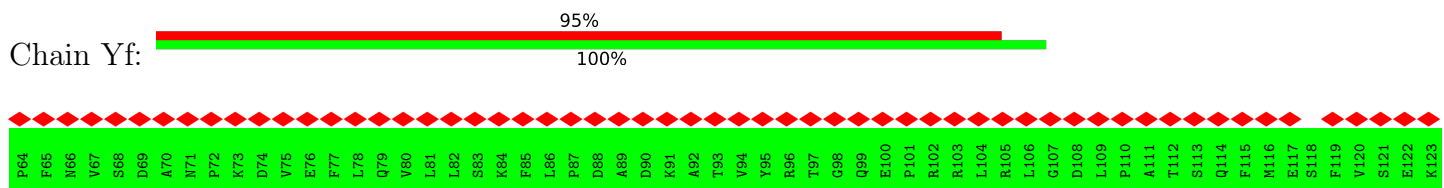
- Molecule 97: mS110



- Molecule 98: uS3m-2



- Molecule 99: mS111



L124 P125 K126 E127 P128 L129 Y130 D131 M132 P133 S134 W135 L136 A137 N138 N139 M140 P141 Y143 D144 A145 Q146 P147 K148 S149 P150 H151 Y152 H153 W154 S155 S156 W157 M158 R159 Q160 H161 S163 L164 D165 Q167 R168 L169 Y170 A171 A172 F173 A174 E175 Y176 M177 A178 S179 E180 P181 H182 R183

L184 G185 I186 V187 R188 Q189 A190 N191 F192 E193 L194 A195 R196 L197 W198 D199 W200 Q201 H202 R203 R204 V205 A206 A207 G208 L209 S210 P211 D212 L213

• Molecule 100: mS112



S1 A2 D3 V4 Y5 K6 E7 F8 F9 K10 M11 A12 R13 V14 A15 V16 R17 T18 M19 K20 E21 P22 T23 K24 S25 T26 K27 K28 D29 L30 Q31 R32 N33 A34 R35 R36 S37 E38 N39 T40 Q41 R42 D43 N44 M45 L46 D47 K48 G49 V50 Y51 M52 R53 F54 L55 R56 Q57 A59 G60

L61 S62 V63 P64 P65 T66 K67

• Molecule 101: mS113



G8 A9 D10 G11 V12 L13 R14 R15 H16 M17 E18 V19 R20 G21 A22 L23 R24 F25 F26 D28 S29 W30 K32 N33 K34 T35 S36 G37 T38 I39 A40 D41 K42 N43 Q44 V45 M46 F47 D48 Y49 L50 K51 Y52 K53 G54 T56 E57 T58 A59 Q60 H61 L62 H63 A64 P65 A66 P67

Q68 V69 F70 R71 K72

• Molecule 102: mS114



A1 H2 Y3 L4 Q5 R6 F7 G8 E9 A10 A11 L12 K13 T14 R15 S16 V17 G18 G19 K20 I21 L22 P23 P24 L25 V26 P27 F28 S29 A31 L32 K33 I34 R35 E36 E37 A38 Y39 K40 L41 L42 Q43 V44 W45 P46 F47 H49 V50 V51 P52 G53 V54 P55 K56 A57 N59 A60

T61 A62 Y63 L64 E65 R66 K67 K68 Q69 E71 E72 K73 R74 T75 K76 R77 A78 K79 E80 I81 N82 D83 A84 L85 A86 K87 M88 P89 Q90 L91 I92 D93 A94 Y95 K96 A97 A98 R99 K100 I101 T102 W103 A104 E105 V106 S107 I108 I109 D110 K111 L112 T113 L114 S115 K116 K117 Q118 I119 R120

E121 K122 Y123 V124 K125 R126 R127 L128 M129 K130 Q131 N132

• Molecule 103: mS115



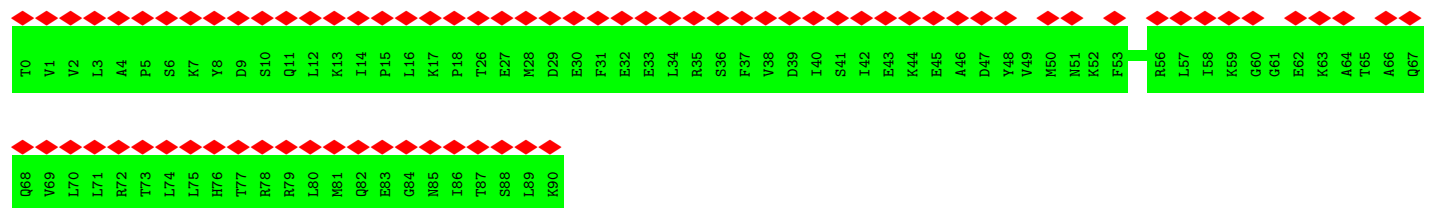
E1 Y2 N3 G4 Q5 G6 Y7 V8 S10 L11 L12 Q13 R14 P15 P16 A17 P18 T19 L20 E21 L22 L23 A24 E25 Y26 L27 T28 V29 K30 Y31 Q32 D33 V34 I35 A36 Q37 R38 D39 F40 V41 T42 H43 I44 L45 G46 R47 M48 S49 V50 L51 E52 R53 G54 G55 E56 L57 P58 A59 A60



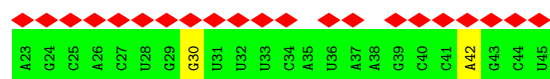
• Molecule 104: mS116



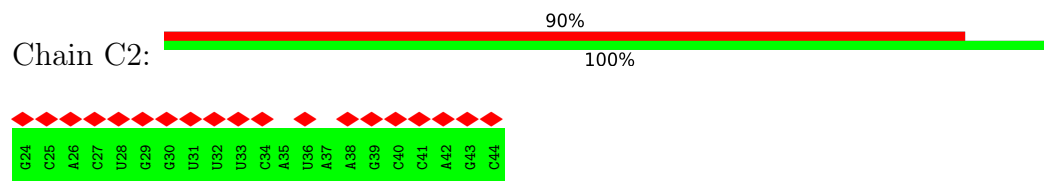
• Molecule 105: uS7m-2



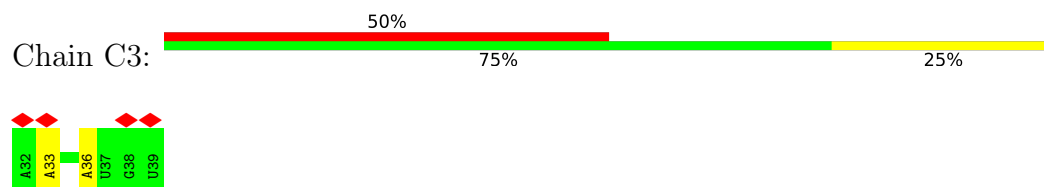
• Molecule 106: P-site tRNA anticodon loop



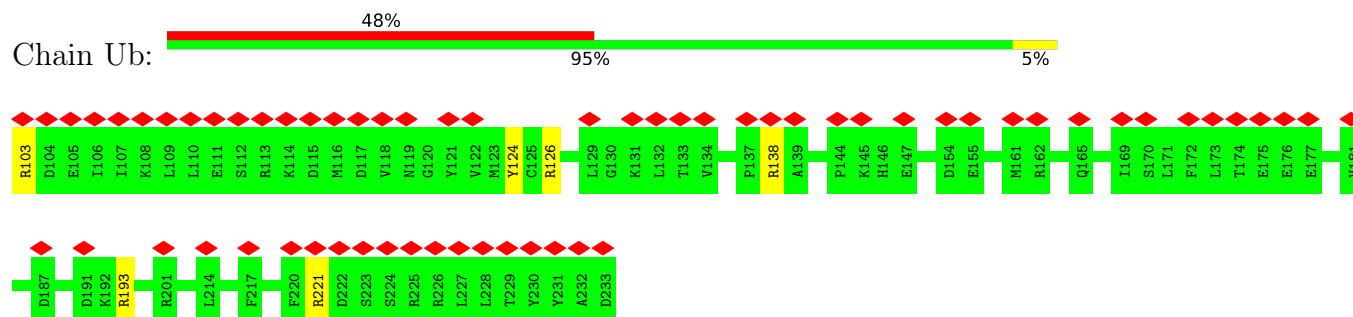
- Molecule 107: A-site tRNA anticodon loop



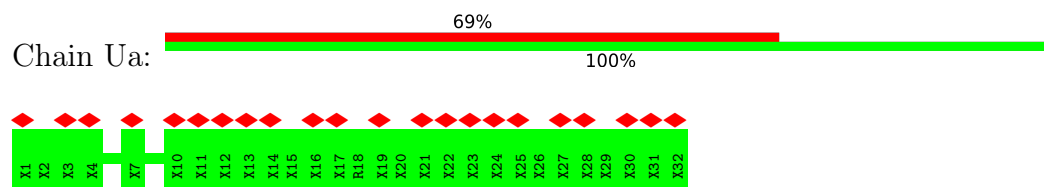
- Molecule 108: mRNA



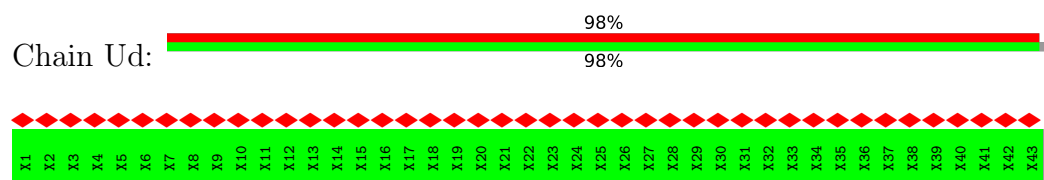
- Molecule 109: mL105



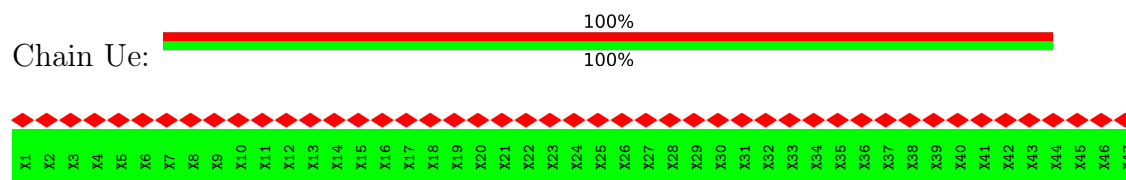
- Molecule 110: Unknown



- Molecule 111: Unknown



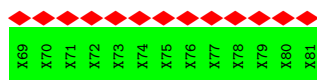
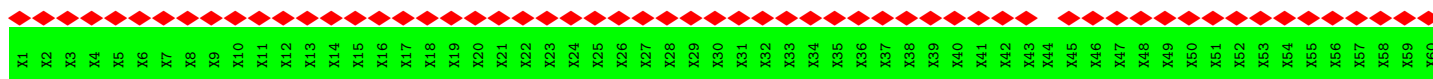
- Molecule 112: Unknown



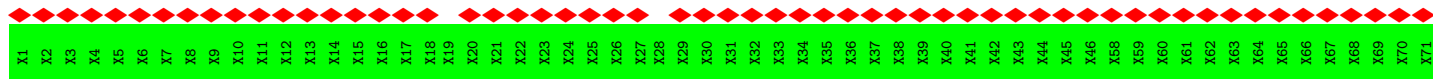
- Molecule 113: Unknown



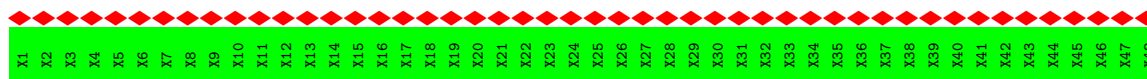




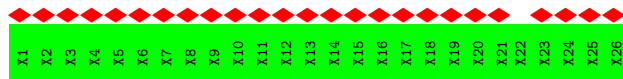
• Molecule 114: Unknown



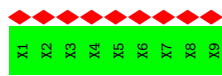
• Molecule 115: Unknown



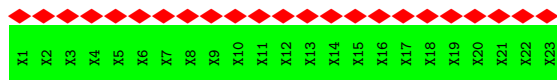
• Molecule 116: Unknown



• Molecule 117: Unknown

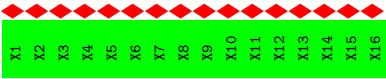


• Molecule 118: Unknown

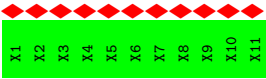


• Molecule 119: Unknown





● Molecule 120: Unknown



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76000	Depositor
Resolution determination method	OTHER	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	0.045	Depositor
Minimum map value	-0.017	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: ZN, K, ATP, MG

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	0.21	0/2632	0.67	0/4101
2	A2	0.24	0/1938	0.68	0/3016
3	A3	0.23	0/4942	0.69	0/7693
4	A4	0.28	0/1764	0.71	0/2749
5	A5	0.15	0/3239	0.66	0/5036
6	A6	0.23	0/2619	0.67	0/4075
7	A7	0.21	0/12753	0.67	0/19862
8	A8	0.20	0/8336	0.68	1/12985 (0.0%)
9	A9	0.18	0/1637	0.66	0/2545
10	Aa	0.24	0/2439	0.43	0/3287
11	Ab	0.24	0/2483	0.42	0/3369
12	Ac	0.24	0/2431	0.41	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	0.23	0/1555	0.40	0/2098
17	Ai	0.24	0/972	0.43	0/1303
18	Aj	0.25	0/1643	0.42	0/2220
19	Ak	0.23	0/1389	0.43	0/1869
20	Al	0.23	0/1438	0.39	0/1938
21	Am	0.24	0/931	0.40	0/1258
22	An	0.23	0/1420	0.40	0/1914
23	Ao	0.23	0/981	0.38	0/1314
24	Ap	0.24	0/1600	0.44	0/2176
25	Aq	0.24	0/1566	0.41	0/2106
26	Ar	0.24	0/1309	0.41	0/1759
27	As	0.24	0/938	0.39	0/1263
28	At	0.24	0/2041	0.41	0/2755
29	Au	0.24	0/1182	0.41	0/1596
30	Av	0.22	0/1073	0.38	0/1443
31	Aw	0.22	0/1043	0.37	0/1401
32	Ax	0.24	0/1508	0.40	0/2028

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Ay	0.40	0/610	0.52	0/827
34	Az	0.38	0/484	0.61	1/652 (0.2%)
35	AA	0.24	0/426	0.41	0/572
36	AB	0.22	0/432	0.44	0/568
37	AC	0.24	0/1217	0.40	0/1639
38	AD	0.22	0/379	0.43	0/500
39	AE	0.23	0/790	0.34	0/1066
40	AF	0.23	0/782	0.39	0/1053
41	AG	0.23	0/1019	0.41	0/1373
42	AH	0.24	0/1444	0.42	0/1945
43	AI	0.23	0/515	0.38	0/696
44	AJ	0.23	0/1023	0.35	0/1370
45	AK	0.24	0/1206	0.36	0/1635
46	AL	0.23	0/3152	0.37	0/4271
46	AM	0.23	0/3345	0.37	0/4532
46	AN	0.24	0/3349	0.37	0/4537
47	AO	0.23	0/2941	0.37	0/4000
48	Xa	0.23	0/1600	0.36	0/2178
49	Xb	0.23	0/1999	0.36	0/2701
50	Xc	0.23	0/509	0.39	0/684
51	Xd	0.23	0/3305	0.37	0/4478
52	Xe	0.23	0/3748	0.38	0/5096
53	Xf	0.24	0/1659	0.38	0/2253
54	Xg	0.24	0/3018	0.37	0/4098
55	Xh	0.24	0/1169	0.39	0/1578
56	Xi	0.24	0/209	0.35	0/273
57	Xj	0.25	0/596	0.39	0/802
58	B1	0.18	0/2419	0.66	0/3765
59	B2	0.19	0/5020	0.67	0/7818
60	B3	0.19	0/9069	0.67	0/14130
61	B4	0.17	0/8046	0.67	0/12527
62	Ba	0.23	0/1967	0.40	0/2662
63	Bb	0.23	0/1920	0.37	0/2615
64	Bc	0.24	0/2272	0.40	0/3087
65	Bd	0.23	0/1825	0.40	0/2459
66	Be	0.23	0/1863	0.41	0/2521
67	Bf	0.23	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	0.24	0/3243	0.37	0/4384
72	Bk	0.24	0/882	0.45	0/1193
73	Bl	0.24	0/977	0.42	0/1303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	Bm	0.23	0/910	0.40	0/1223
75	Bn	0.24	0/995	0.42	0/1336
76	Bo	0.24	0/963	0.38	0/1284
77	Bp	0.24	0/1046	0.40	0/1414
78	Bq	0.23	0/1068	0.39	0/1434
79	Br	0.22	0/754	0.38	0/1009
80	Bs	0.29	0/754	0.51	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	0.35	0/1835
84	Bw	0.24	0/2803	0.39	0/3791
85	Bx	0.25	0/4813	0.45	10/6545 (0.2%)
86	By	0.25	0/655	0.37	0/883
87	Bz	0.23	0/1030	0.37	0/1400
88	BA	0.23	0/1405	0.39	0/1907
89	BB	0.23	0/673	0.36	0/896
90	BC	0.21	0/280	0.36	0/365
91	BD	0.24	0/2207	0.38	0/2977
92	BE	0.23	0/1328	0.35	0/1805
93	BF	0.23	0/3039	0.37	0/4111
94	Ya	0.23	0/1466	0.39	0/1979
95	Yb	0.27	0/419	0.40	0/562
96	Yc	0.23	0/1328	0.39	0/1799
97	Yd	0.23	0/797	0.39	0/1069
98	Ye	0.24	0/887	0.40	0/1191
99	Yf	0.23	0/1276	0.37	0/1735
100	Yg	0.24	0/560	0.37	0/744
101	Yh	0.23	0/543	0.36	0/730
102	Yi	0.24	0/1096	0.38	0/1470
103	Yj	0.23	0/2911	0.35	0/3966
104	Yk	0.26	0/721	0.39	0/982
105	Yl	0.24	0/680	0.39	0/911
106	C1	0.15	0/543	0.67	0/843
107	C2	0.14	0/496	0.68	0/770
108	C3	0.17	0/192	0.66	0/297
109	Ub	1.00	0/1118	0.95	7/1501 (0.5%)
110	Ua	0.30	0/10	0.36	0/11
All	All	0.24	0/204700	0.51	19/290083 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
109	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
109	Ub	126	ARG	NE-CZ-NH2	-7.62	116.49	120.30
109	Ub	138	ARG	NE-CZ-NH2	-6.96	116.82	120.30
85	Bx	79	LEU	CB-CG-CD2	6.82	122.59	111.00
85	Bx	59	VAL	CG1-CB-CG2	6.75	121.71	110.90
109	Ub	193	ARG	NE-CZ-NH2	-6.52	117.04	120.30
109	Ub	103	ARG	NE-CZ-NH1	6.39	123.49	120.30
85	Bx	77	LEU	CB-CG-CD2	6.11	121.38	111.00
109	Ub	103	ARG	NE-CZ-NH2	-5.81	117.40	120.30
109	Ub	124	TYR	CB-CG-CD1	-5.70	117.58	121.00
85	Bx	87	LEU	CB-CG-CD1	5.67	120.64	111.00
85	Bx	90	LEU	CB-CG-CD2	5.59	120.50	111.00
85	Bx	79	LEU	CB-CG-CD1	5.52	120.38	111.00
8	A8	317	C	C2-N1-C1'	5.38	124.72	118.80
85	Bx	90	LEU	CB-CG-CD1	5.26	119.94	111.00
85	Bx	87	LEU	CB-CG-CD2	5.10	119.67	111.00
85	Bx	77	LEU	CB-CG-CD1	5.09	119.65	111.00
85	Bx	59	VAL	CA-CB-CG2	5.01	118.42	110.90

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%)	291 (96%)	13 (4%)	0	100	100
11	Ab	304/306 (99%)	298 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Ac	301/303 (99%)	301 (100%)	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%)	179 (98%)	3 (2%)	0	100	100
17	Ai	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
18	Aj	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
19	Ak	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
20	Al	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
21	Am	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
22	An	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
23	Ao	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
24	Ap	198/200 (99%)	196 (99%)	2 (1%)	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%)	250 (100%)	1 (0%)	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%)	121 (100%)	0	0	100	100
32	Ax	174/176 (99%)	174 (100%)	0	0	100	100
33	Ay	70/72 (97%)	68 (97%)	2 (3%)	0	100	100
34	Az	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
35	AA	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
36	AB	48/50 (96%)	48 (100%)	0	0	100	100
37	AC	137/139 (99%)	137 (100%)	0	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%)	166 (96%)	5 (3%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	385 (99%)	5 (1%)	0	100	100
46	AM	417/420 (99%)	414 (99%)	3 (1%)	0	100	100
46	AN	418/420 (100%)	416 (100%)	2 (0%)	0	100	100
47	AO	371/377 (98%)	365 (98%)	6 (2%)	0	100	100
48	Xa	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
49	Xb	242/244 (99%)	239 (99%)	3 (1%)	0	100	100
50	Xc	55/57 (96%)	55 (100%)	0	0	100	100
51	Xd	411/413 (100%)	401 (98%)	10 (2%)	0	100	100
52	Xe	479/483 (99%)	475 (99%)	4 (1%)	0	100	100
53	Xf	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
54	Xg	379/410 (92%)	377 (100%)	2 (0%)	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%)	69 (100%)	0	0	100	100
62	Ba	240/242 (99%)	236 (98%)	4 (2%)	0	100	100
63	Bb	232/236 (98%)	229 (99%)	3 (1%)	0	100	100
64	Bc	273/279 (98%)	272 (100%)	1 (0%)	0	100	100
65	Bd	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
66	Be	226/228 (99%)	224 (99%)	2 (1%)	0	100	100
67	Bf	117/119 (98%)	117 (100%)	0	0	100	100
68	Bg	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
69	Bh	370/374 (99%)	369 (100%)	1 (0%)	0	100	100
70	Bi	276/282 (98%)	271 (98%)	5 (2%)	0	100	100
71	Bj	395/401 (98%)	389 (98%)	6 (2%)	0	100	100
72	Bk	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
73	Bl	121/123 (98%)	118 (98%)	3 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	Bo	113/167 (68%)	112 (99%)	1 (1%)	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	347/351 (99%)	341 (98%)	6 (2%)	0	100	100
85	Bx	613/621 (99%)	606 (99%)	7 (1%)	0	100	100
86	By	76/78 (97%)	76 (100%)	0	0	100	100
87	Bz	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
88	BA	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
89	BB	80/84 (95%)	79 (99%)	1 (1%)	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%)	361 (99%)	5 (1%)	0	100	100
94	Ya	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
95	Yb	48/50 (96%)	48 (100%)	0	0	100	100
96	Yc	157/159 (99%)	156 (99%)	1 (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%)	126 (97%)	4 (3%)	0	100	100
103	Yj	382/386 (99%)	377 (99%)	5 (1%)	0	100	100
104	Yk	88/92 (96%)	88 (100%)	0	0	100	100
105	Yl	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
109	Ub	129/131 (98%)	128 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
110	Ua	1/32 (3%)	1 (100%)	0	0	100	100
All	All	16820/17218 (98%)	16634 (99%)	185 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	AH	161	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Aa	248/248 (100%)	248 (100%)	0	100	100
11	Ab	261/261 (100%)	260 (100%)	1 (0%)	89	94
12	Ac	259/259 (100%)	259 (100%)	0	100	100
13	Ad	176/176 (100%)	175 (99%)	1 (1%)	84	92
14	Ae	211/211 (100%)	211 (100%)	0	100	100
15	Af	47/47 (100%)	46 (98%)	1 (2%)	48	74
16	Ah	161/161 (100%)	159 (99%)	2 (1%)	67	85
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%)	146 (100%)	0	100	100
20	Al	150/150 (100%)	149 (99%)	1 (1%)	81	92
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%)	84	92
25	Aq	161/161 (100%)	160 (99%)	1 (1%)	84	92
26	Ar	142/142 (100%)	141 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	79	90
30	Av	120/120 (100%)	120 (100%)	0	100	100
31	Aw	110/110 (100%)	108 (98%)	2 (2%)	54	77
32	Ax	161/161 (100%)	161 (100%)	0	100	100
33	Ay	66/66 (100%)	65 (98%)	1 (2%)	60	81
34	Az	51/51 (100%)	48 (94%)	3 (6%)	16	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%)	58	79
38	AD	42/42 (100%)	42 (100%)	0	100	100
39	AE	84/84 (100%)	84 (100%)	0	100	100
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%)	75	89
46	AM	351/351 (100%)	350 (100%)	1 (0%)	91	96
46	AN	351/351 (100%)	350 (100%)	1 (0%)	91	96
47	AO	293/293 (100%)	291 (99%)	2 (1%)	81	92
48	Xa	173/173 (100%)	172 (99%)	1 (1%)	84	92
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%)	84	92
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%)	65	83
55	Xh	127/127 (100%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	218 (99%)	2 (1%)	75	89
63	Bb	214/214 (100%)	213 (100%)	1 (0%)	86	93
64	Bc	241/241 (100%)	240 (100%)	1 (0%)	89	94
65	Bd	196/196 (100%)	195 (100%)	1 (0%)	86	93
66	Be	196/196 (100%)	189 (96%)	7 (4%)	30	62
67	Bf	103/103 (100%)	103 (100%)	0	100	100
68	Bg	97/97 (100%)	95 (98%)	2 (2%)	48	74
69	Bh	327/327 (100%)	326 (100%)	1 (0%)	91	96
70	Bi	242/242 (100%)	242 (100%)	0	100	100
71	Bj	334/334 (100%)	333 (100%)	1 (0%)	91	96
72	Bk	95/95 (100%)	95 (100%)	0	100	100
73	Bl	104/104 (100%)	104 (100%)	0	100	100
74	Bm	100/100 (100%)	99 (99%)	1 (1%)	73	87
75	Bn	106/106 (100%)	105 (99%)	1 (1%)	75	89
76	Bo	104/104 (100%)	104 (100%)	0	100	100
77	Bp	107/107 (100%)	107 (100%)	0	100	100
78	Bq	113/113 (100%)	113 (100%)	0	100	100
79	Br	81/81 (100%)	81 (100%)	0	100	100
80	Bs	77/77 (100%)	75 (97%)	2 (3%)	41	70
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%)	139 (99%)	1 (1%)	81	92
84	Bw	298/298 (100%)	298 (100%)	0	100	100
85	Bx	481/481 (100%)	471 (98%)	10 (2%)	48	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
91	BD	225/225 (100%)	224 (100%)	1 (0%)	89	94
92	BE	136/136 (100%)	136 (100%)	0	100	100
93	BF	326/326 (100%)	325 (100%)	1 (0%)	91	96
94	Ya	161/161 (100%)	160 (99%)	1 (1%)	84	92
95	Yb	44/44 (100%)	44 (100%)	0	100	100
96	Yc	140/140 (100%)	140 (100%)	0	100	100
97	Yd	88/88 (100%)	88 (100%)	0	100	100
98	Ye	91/91 (100%)	89 (98%)	2 (2%)	47	73
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%)	54	77
103	Yj	278/278 (100%)	278 (100%)	0	100	100
104	Yk	74/74 (100%)	73 (99%)	1 (1%)	62	82
105	Yl	76/76 (100%)	76 (100%)	0	100	100
109	Ub	123/123 (100%)	123 (100%)	0	100	100
110	Ua	1/1 (100%)	1 (100%)	0	100	100
All	All	14613/14632 (100%)	14542 (100%)	71 (0%)	85	93

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Ab	381	ARG
13	Ad	49	TYR
15	Af	117	VAL
16	Ah	105	GLN
16	Ah	106	ASP
20	Al	4	ARG
24	Ap	156	ARG
25	Aq	120	TYR
26	Ar	78	LYS
29	Au	63	LYS
31	Aw	69	ARG
31	Aw	172	LYS
33	Ay	63	SER
34	Az	133	SER

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Mol	Chain	Res	Type
34	Az	135	ILE
34	Az	144	LYS
37	AC	66	VAL
37	AC	193	ARG
46	AL	205	VAL
46	AL	222	ARG
46	AL	263	ARG
46	AM	65	ARG
46	AN	73	ARG
47	AO	69	ARG
47	AO	195	TRP
48	Xa	107	PHE
51	Xd	435	VAL
51	Xd	437	VAL
54	Xg	40	LYS
54	Xg	41	ASP
54	Xg	263	ASN
54	Xg	276	ARG
62	Ba	169	MET
62	Ba	237	GLU
63	Bb	76	LYS
64	Bc	162	LYS
65	Bd	81	LEU
66	Be	13	LYS
66	Be	41	ASN
66	Be	42	GLN
66	Be	91	GLN
66	Be	92	ARG
66	Be	93	VAL
66	Be	133	ARG
68	Bg	118	VAL
68	Bg	186	ILE
69	Bh	180	GLN
71	Bj	109	HIS
74	Bm	3	GLN
75	Bn	54	LEU
80	Bs	13	PRO
80	Bs	60	ASP
83	Bv	88	GLN
85	Bx	59	VAL
85	Bx	79	LEU
85	Bx	116	LEU

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Mol	Chain	Res	Type
85	Bx	141	ARG
85	Bx	232	PHE
85	Bx	234	ARG
85	Bx	283	MET
85	Bx	314	LYS
85	Bx	317	THR
85	Bx	628	SER
91	BD	227	LYS
93	BF	82	HIS
94	Ya	247	PHE
98	Ye	5	ARG
98	Ye	18	ASN
102	Yi	51	VAL
102	Yi	112	LEU
104	Yk	104	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
10	Aa	217	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	108/109 (99%)	25 (23%)	0
106	C1	22/23 (95%)	2 (9%)	0
107	C2	20/21 (95%)	0	0
108	C3	7/8 (87%)	2 (28%)	0
2	A2	80/81 (98%)	16 (20%)	1 (1%)
3	A3	205/207 (99%)	29 (14%)	1 (0%)
4	A4	72/73 (98%)	9 (12%)	1 (1%)
5	A5	132/136 (97%)	32 (24%)	0
58	B1	101/102 (99%)	23 (22%)	0
59	B2	208/210 (99%)	40 (19%)	0
6	A6	106/109 (97%)	21 (19%)	0
60	B3	378/379 (99%)	48 (12%)	2 (0%)
61	B4	334/337 (99%)	50 (14%)	0
7	A7	532/534 (99%)	81 (15%)	1 (0%)
8	A8	349/350 (99%)	58 (16%)	0
9	A9	67/69 (97%)	15 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2721/2748 (99%)	451 (16%)	6 (0%)

All (451) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	5	A
1	A1	9	U
1	A1	17	U
1	A1	18	A
1	A1	34	U
1	A1	38	U
1	A1	39	A
1	A1	47	U
1	A1	49	A
1	A1	53	G
1	A1	54	C
1	A1	55	U
1	A1	57	A
1	A1	59	A
1	A1	62	A
1	A1	68	A
1	A1	71	A
1	A1	74	G
1	A1	84	U
1	A1	89	C
1	A1	97	A
1	A1	98	A
1	A1	99	G
1	A1	108	A
1	A1	109	A
2	A2	2	A
2	A2	16	U
2	A2	17	A
2	A2	26	A
2	A2	27	G
2	A2	28	C
2	A2	29	A
2	A2	40	A
2	A2	41	U
2	A2	42	U
2	A2	56	U
2	A2	63	G

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Mol	Chain	Res	Type
2	A2	74	G
2	A2	75	A
2	A2	79	A
2	A2	80	U
3	A3	26	G
3	A3	30	G
3	A3	55	A
3	A3	61	U
3	A3	62	A
3	A3	65	U
3	A3	69	A
3	A3	73	G
3	A3	78	A
3	A3	101	A
3	A3	113	C
3	A3	123	G
3	A3	130	U
3	A3	132	A
3	A3	133	A
3	A3	138	U
3	A3	139	C
3	A3	141	C
3	A3	153	G
3	A3	160	U
3	A3	175	U
3	A3	198	U
3	A3	200	U
3	A3	201	A
3	A3	203	A
3	A3	205	A
3	A3	208	A
3	A3	209	A
3	A3	210	A
4	A4	8	G
4	A4	21	A
4	A4	23	G
4	A4	36	A
4	A4	43	A
4	A4	52	C
4	A4	57	A
4	A4	58	G
4	A4	67	A

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Mol	Chain	Res	Type
5	A5	13	A
5	A5	14	A
5	A5	16	C
5	A5	21	A
5	A5	22	G
5	A5	24	A
5	A5	26	G
5	A5	35	G
5	A5	36	A
5	A5	37	A
5	A5	38	G
5	A5	50	U
5	A5	55	A
5	A5	56	A
5	A5	64	U
5	A5	70	U
5	A5	71	G
5	A5	73	U
5	A5	76	U
5	A5	83	A
5	A5	84	A
5	A5	94	A
5	A5	95	C
5	A5	96	A
5	A5	100	A
5	A5	101	G
5	A5	105	A
5	A5	107	A
5	A5	111	G
5	A5	135	U
5	A5	140	U
5	A5	141	A
6	A6	39	G
6	A6	41	A
6	A6	42	U
6	A6	46	U
6	A6	47	A
6	A6	48	A
6	A6	50	G
6	A6	60	G
6	A6	66	A
6	A6	67	U

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Mol	Chain	Res	Type
6	A6	68	G
6	A6	74	A
6	A6	82	A
6	A6	83	A
6	A6	98	G
6	A6	99	C
6	A6	100	A
6	A6	101	A
6	A6	108	A
6	A6	110	C
6	A6	114	A
7	A7	2	A
7	A7	11	C
7	A7	12	A
7	A7	13	A
7	A7	14	A
7	A7	20	A
7	A7	33	U
7	A7	35	U
7	A7	43	G
7	A7	49	A
7	A7	69	G
7	A7	75	U
7	A7	87	U
7	A7	100	C
7	A7	103	C
7	A7	106	A
7	A7	113	G
7	A7	114	A
7	A7	123	C
7	A7	141	C
7	A7	142	U
7	A7	143	A
7	A7	151	U
7	A7	158	A
7	A7	169	U
7	A7	189	A
7	A7	190	G
7	A7	193	A
7	A7	199	A
7	A7	204	U
7	A7	206	A

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Mol	Chain	Res	Type
7	A7	207	C
7	A7	222	G
7	A7	223	G
7	A7	229	A
7	A7	230	A
7	A7	231	A
7	A7	236	A
7	A7	248	U
7	A7	256	C
7	A7	257	G
7	A7	260	U
7	A7	263	A
7	A7	265	G
7	A7	284	U
7	A7	285	G
7	A7	286	U
7	A7	316	G
7	A7	324	A
7	A7	325	G
7	A7	326	A
7	A7	336	G
7	A7	345	G
7	A7	348	C
7	A7	353	A
7	A7	354	G
7	A7	355	A
7	A7	361	U
7	A7	375	A
7	A7	385	U
7	A7	431	U
7	A7	433	A
7	A7	436	U
7	A7	444	U
7	A7	465	U
7	A7	481	A
7	A7	485	A
7	A7	486	U
7	A7	490	U
7	A7	503	A
7	A7	504	A
7	A7	507	A
7	A7	518	A

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Mol	Chain	Res	Type
7	A7	520	C
7	A7	527	A
7	A7	529	A
7	A7	534	A
7	A7	550	U
7	A7	551	G
7	A7	555	G
7	A7	557	A
8	A8	12	C
8	A8	13	A
8	A8	14	A
8	A8	17	G
8	A8	18	A
8	A8	23	A
8	A8	27	A
8	A8	29	G
8	A8	36	A
8	A8	57	A
8	A8	62	U
8	A8	64	U
8	A8	65	A
8	A8	78	G
8	A8	85	C
8	A8	89	G
8	A8	90	A
8	A8	91	U
8	A8	92	G
8	A8	105	U
8	A8	107	C
8	A8	117	C
8	A8	122	G
8	A8	141	U
8	A8	153	U
8	A8	154	G
8	A8	160	C
8	A8	172	U
8	A8	186	G
8	A8	189	A
8	A8	190	G
8	A8	196	U
8	A8	200	U
8	A8	202	U

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Mol	Chain	Res	Type
8	A8	215	A
8	A8	219	A
8	A8	252	U
8	A8	262	A
8	A8	272	U
8	A8	274	A
8	A8	275	A
8	A8	277	A
8	A8	289	A
8	A8	290	A
8	A8	305	A
8	A8	306	A
8	A8	308	U
8	A8	316	G
8	A8	317	C
8	A8	321	U
8	A8	322	G
8	A8	324	A
8	A8	330	A
8	A8	338	U
8	A8	344	A
8	A8	345	A
8	A8	347	A
8	A8	350	A
9	A9	59	U
9	A9	61	A
9	A9	63	A
9	A9	68	U
9	A9	76	C
9	A9	88	U
9	A9	89	U
9	A9	90	U
9	A9	100	G
9	A9	103	G
9	A9	105	C
9	A9	111	A
9	A9	112	A
9	A9	118	A
9	A9	128	C
58	B1	2	A
58	B1	5	G
58	B1	10	U

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Mol	Chain	Res	Type
58	B1	11	G
58	B1	34	A
58	B1	43	C
58	B1	44	U
58	B1	45	U
58	B1	46	A
58	B1	53	C
58	B1	62	A
58	B1	63	A
58	B1	65	A
58	B1	66	C
58	B1	72	A
58	B1	83	U
58	B1	84	U
58	B1	95	G
58	B1	97	A
58	B1	98	A
58	B1	100	A
58	B1	101	U
58	B1	102	A
59	B2	2	A
59	B2	8	A
59	B2	14	U
59	B2	17	A
59	B2	24	G
59	B2	26	A
59	B2	27	U
59	B2	30	C
59	B2	40	A
59	B2	42	U
59	B2	44	G
59	B2	48	G
59	B2	60	G
59	B2	62	U
59	B2	66	C
59	B2	69	U
59	B2	71	G
59	B2	72	C
59	B2	80	G
59	B2	84	G
59	B2	92	G
59	B2	104	A

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Mol	Chain	Res	Type
59	B2	108	G
59	B2	126	U
59	B2	127	A
59	B2	130	A
59	B2	153	G
59	B2	164	G
59	B2	166	U
59	B2	171	C
59	B2	172	A
59	B2	180	A
59	B2	182	G
59	B2	187	G
59	B2	196	A
59	B2	204	A
59	B2	205	A
59	B2	207	U
59	B2	208	C
59	B2	211	U
60	B3	14	A
60	B3	24	A
60	B3	26	U
60	B3	33	C
60	B3	39	G
60	B3	42	G
60	B3	46	G
60	B3	62	A
60	B3	74	A
60	B3	77	C
60	B3	79	A
60	B3	83	A
60	B3	87	G
60	B3	89	G
60	B3	93	A
60	B3	94	A
60	B3	100	G
60	B3	103	A
60	B3	112	A
60	B3	128	U
60	B3	135	A
60	B3	136	A
60	B3	150	A
60	B3	151	A

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Mol	Chain	Res	Type
60	B3	165	A
60	B3	170	U
60	B3	172	A
60	B3	175	U
60	B3	176	A
60	B3	178	A
60	B3	180	G
60	B3	194	C
60	B3	226	A
60	B3	243	A
60	B3	264	A
60	B3	275	A
60	B3	276	A
60	B3	295	A
60	B3	301	U
60	B3	302	A
60	B3	303	U
60	B3	304	G
60	B3	362	U
60	B3	371	A
60	B3	373	G
60	B3	377	A
60	B3	378	A
60	B3	383	U
61	B4	4	A
61	B4	5	C
61	B4	6	C
61	B4	8	C
61	B4	31	A
61	B4	37	A
61	B4	43	G
61	B4	48	A
61	B4	49	A
61	B4	52	A
61	B4	53	A
61	B4	56	A
61	B4	57	G
61	B4	66	U
61	B4	80	G
61	B4	93	A
61	B4	94	G
61	B4	99	A

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Mol	Chain	Res	Type
61	B4	100	A
61	B4	102	A
61	B4	104	G
61	B4	109	A
61	B4	110	C
61	B4	130	A
61	B4	172	A
61	B4	174	A
61	B4	207	A
61	B4	210	C
61	B4	211	A
61	B4	236	A
61	B4	237	C
61	B4	238	A
61	B4	245	U
61	B4	252	G
61	B4	258	U
61	B4	259	G
61	B4	265	U
61	B4	266	A
61	B4	267	A
61	B4	289	U
61	B4	290	U
61	B4	304	A
61	B4	305	A
61	B4	306	G
61	B4	309	G
61	B4	318	U
61	B4	329	G
61	B4	331	A
61	B4	341	G
61	B4	347	G
106	C1	30	G
106	C1	42	A
108	C3	33	A
108	C3	36	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A2	79	A
3	A3	132	A

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Mol	Chain	Res	Type
4	A4	22	A
7	A7	192	A
60	B3	177	A
60	B3	275	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 143 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	$\# Z  > 2$
124	ATP	Bw	502	121	26,33,33	0.90	1 (3%)	31,52,52	1.59	5 (16%)

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
124	ATP	Bw	502	121	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
124	Bw	502	ATP	C5-C4	2.17	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
124	Bw	502	ATP	PB-O3B-PG	-3.91	119.41	132.83
124	Bw	502	ATP	PA-O3A-PB	-3.72	120.08	132.83
124	Bw	502	ATP	N3-C2-N1	-3.69	122.91	128.68
124	Bw	502	ATP	C3'-C2'-C1'	2.72	105.07	100.98
124	Bw	502	ATP	C4-C5-N7	-2.20	107.11	109.40

There are no chirality outliers.

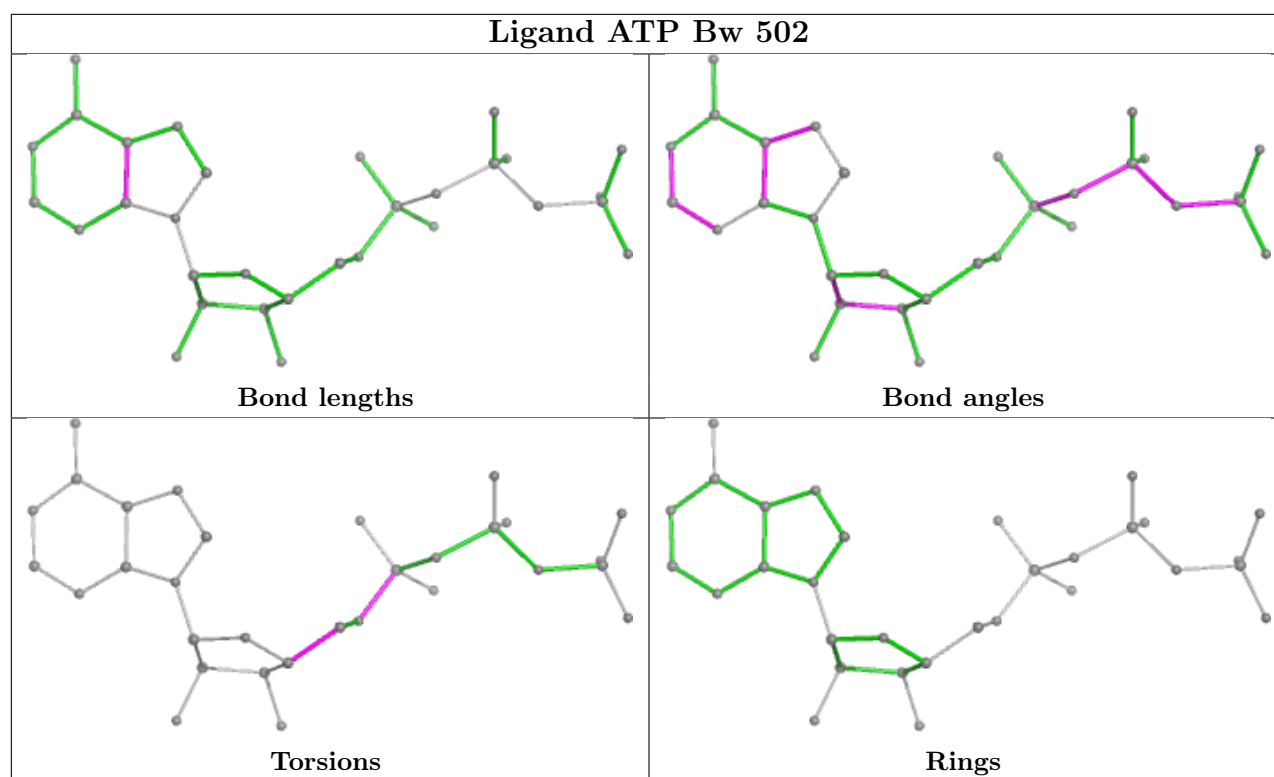
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
124	Bw	502	ATP	C5'-O5'-PA-O1A
124	Bw	502	ATP	C5'-O5'-PA-O3A
124	Bw	502	ATP	O4'-C4'-C5'-O5'
124	Bw	502	ATP	C3'-C4'-C5'-O5'
124	Bw	502	ATP	C5'-O5'-PA-O2A

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
5	A5	3
85	Bx	3
27	As	2
70	Bi	2
6	A6	2
71	Bj	2
64	Bc	2
61	B4	2
47	AO	2
14	Ae	2
42	AH	1
69	Bh	1
55	Xh	1

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Mol	Chain	Number of breaks
63	Bb	1
91	BD	1
103	Yj	1
9	A9	1
26	Ar	1
105	Yl	1
39	AE	1
89	BB	1
59	B2	1
114	Ug	1
3	A3	1
113	Uf	1
34	Az	1
93	BF	1
98	Ye	1
7	A7	1
16	Ah	1
104	Yk	1
44	AJ	1
52	Xe	1

All 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	57.97
1	As	92:PRO	C	151:GLY	N	44.14
1	Bi	223:GLN	C	243:ALA	N	41.88
1	A6	114:A	O3'	127:A	P	35.38
1	Bj	297:SER	C	426:ALA	N	32.88
1	AH	39:TYR	C	50:PRO	N	29.52
1	Bh	320:GLN	C	354:PRO	N	25.98
1	Xh	70:CYS	C	204:LYS	N	25.93
1	Bi	167:THR	C	186:SER	N	25.26
1	Bb	116:ASN	C	147:LYS	N	23.70
1	BD	140:GLY	C	165:HIS	N	22.99
1	Yj	366:MET	C	379:TRP	N	22.54
1	Bc	259:ALA	C	286:THR	N	21.15
1	A9	76:C	O3'	87:A	P	20.61
1	Ar	191:THR	C	199:ARG	N	20.57
1	Yl	18:PRO	C	26:THR	N	20.55
1	B4	185:C	O3'	194:C	P	20.47
1	AE	76:GLU	C	87:VAL	N	20.18
1	AO	328:ALA	C	339:TRP	N	19.85

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A5	127:U	O3'	132:C	P	19.41
1	Xg	475:UNK	C	483:UNK	N	18.47
1	Bj	198:SER	C	213:GLY	N	17.59
1	BB	70:ARG	C	76:LYS	N	17.51
1	B2	142:U	O3'	147:A	P	17.33
1	Ug	46:UNK	C	58:UNK	N	16.94
1	A3	188:A	O3'	192:A	P	16.68
1	Uf	60:UNK	C	69:UNK	N	16.24
1	Bx	353:ARG	C	380:LEU	N	15.92
1	Bx	222:ALA	C	232:PHE	N	15.43
1	Ae	165:THR	C	170:THR	N	15.01
1	A6	22:A	O3'	34:U	P	14.93
1	Az	119:LEU	C	133:SER	N	14.18
1	Xg	138:LEU	C	146:PRO	N	14.18
1	BF	183:PRO	C	200:THR	N	14.15
1	Ye	58:ARG	C	72:GLN	N	13.31
1	A7	385:U	O3'	428:C	P	13.20
1	AO	371:ARG	C	376:PRO	N	12.68
1	Ah	184:ARG	C	189:LYS	N	12.05
1	Xg	456:LEU	C	461:UNK	N	11.02
1	Bx	435:ARG	C	451:PRO	N	10.86
1	Yk	64:ALA	C	97:ARG	N	10.68
1	A5	77:U	O3'	79:G	P	9.36
1	AJ	17:LEU	C	27:PRO	N	7.90
1	B4	165:U	O3'	169:A	P	7.81
1	As	61:MET	C	68:PHE	N	7.23
1	Xe	503:SER	C	508:PRO	N	5.90
1	A5	10:C	O3'	12:C	P	5.77
1	Bc	11:LEU	C	13:LEU	N	3.40
1	Ae	91:GLN	C	100:ASN	N	3.07



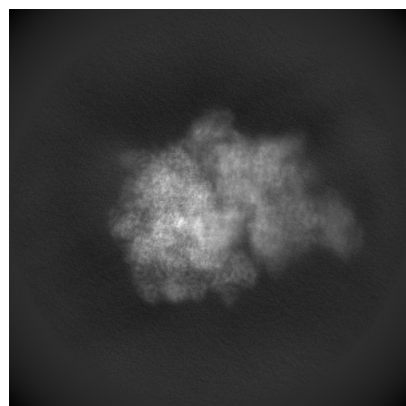
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15577. These allow visual inspection of the internal detail of the map and identification of artifacts.

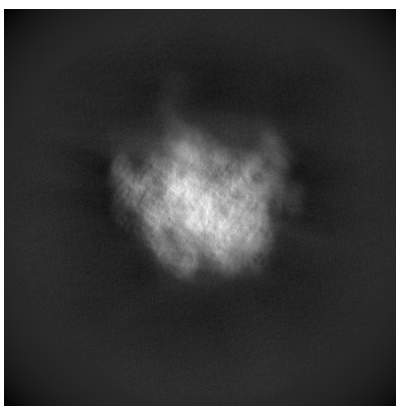
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

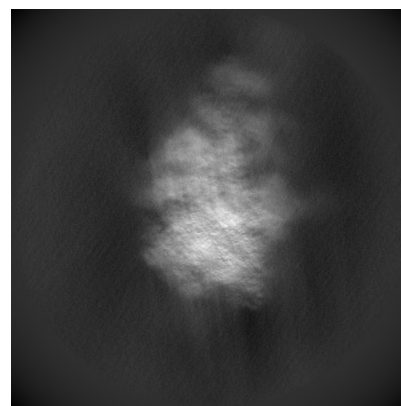
#### 6.1.1 Primary map



X

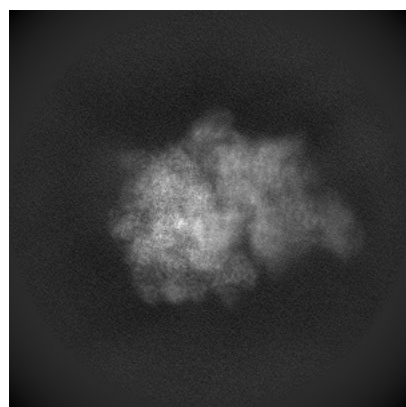


Y

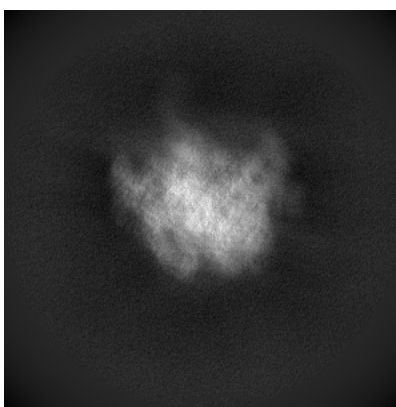


Z

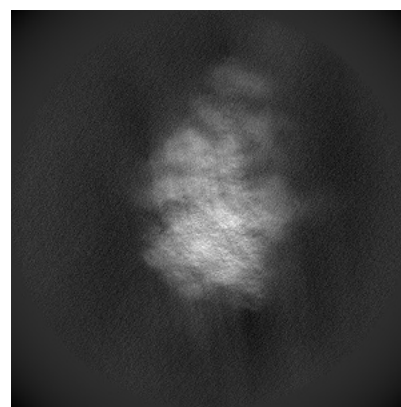
#### 6.1.2 Raw map



X



Y

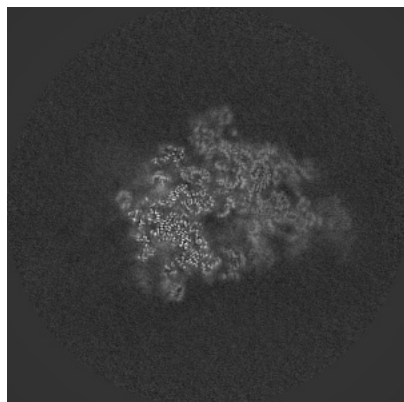


Z

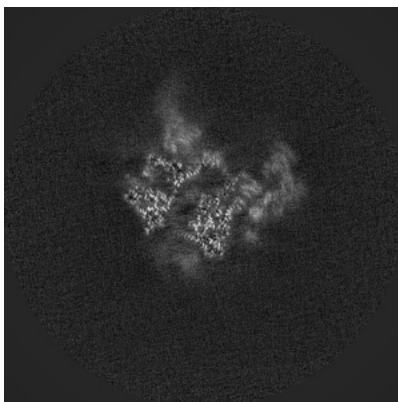
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

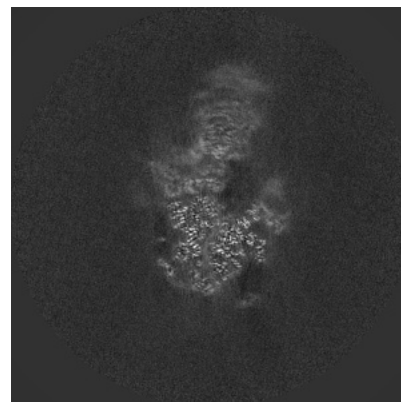
### 6.2.1 Primary map



X Index: 350

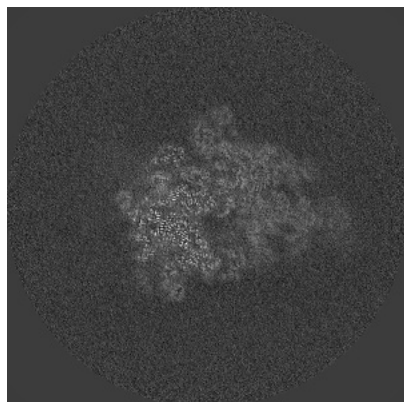


Y Index: 350

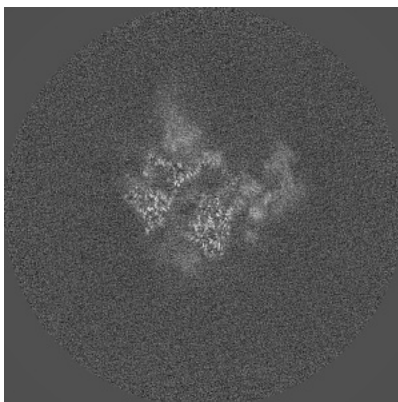


Z Index: 350

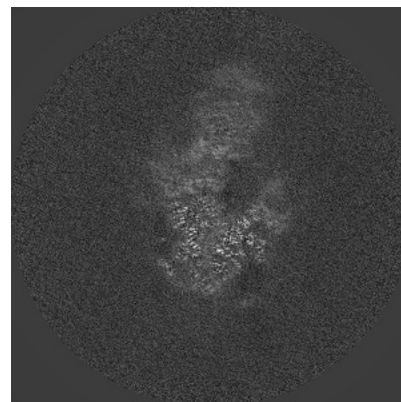
### 6.2.2 Raw map



X Index: 350



Y Index: 350

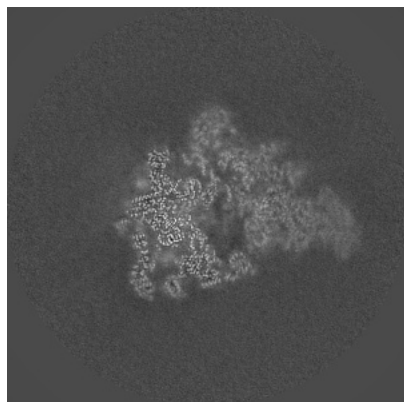


Z Index: 350

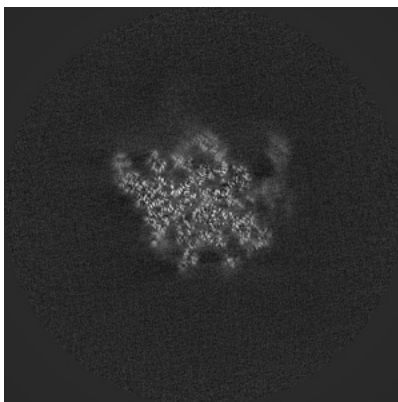
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

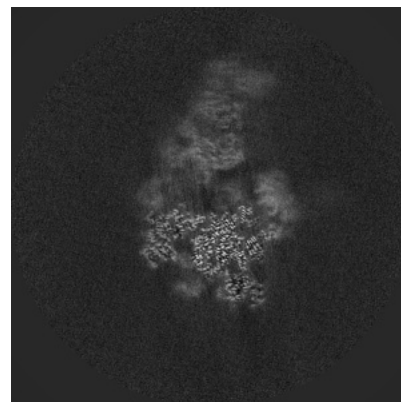
### 6.3.1 Primary map



X Index: 368

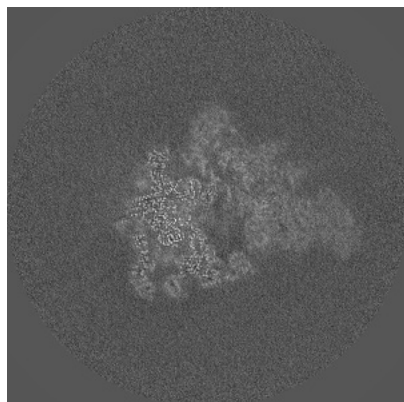


Y Index: 320

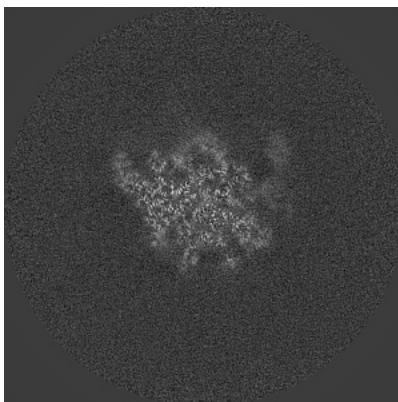


Z Index: 320

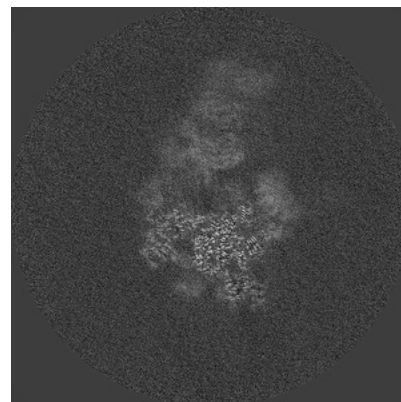
### 6.3.2 Raw map



X Index: 368



Y Index: 320



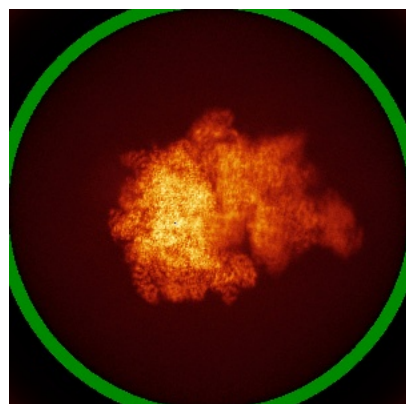
Z Index: 320

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

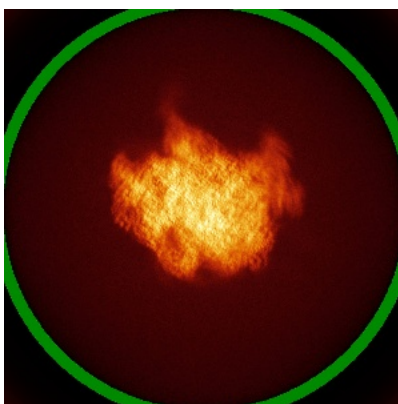


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

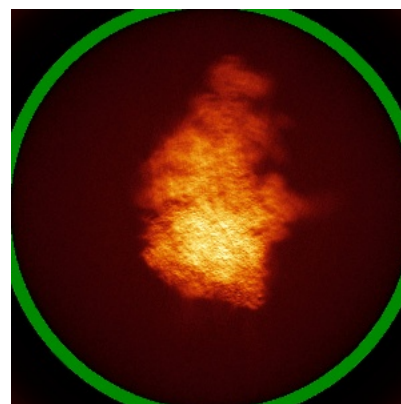
### 6.4.1 Primary map



X

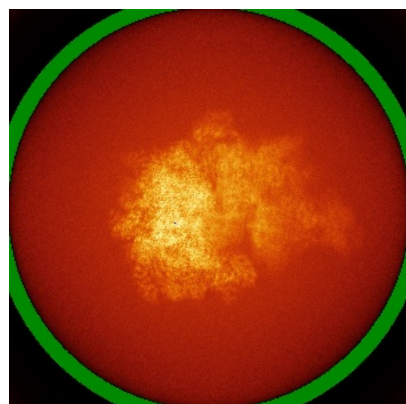


Y

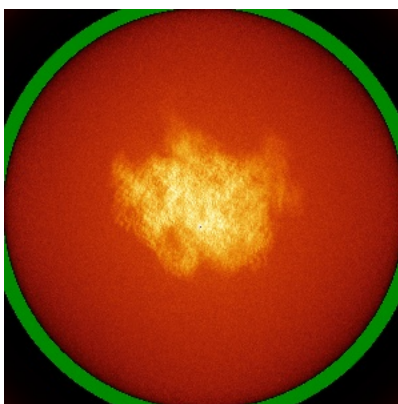


Z

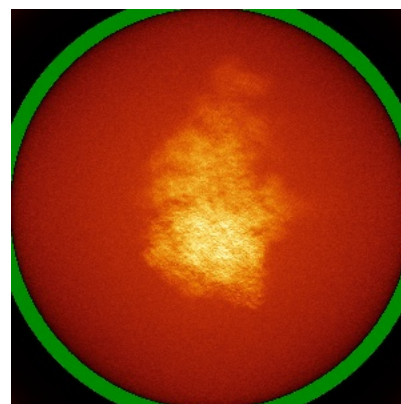
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

### 6.5.2 Raw map



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

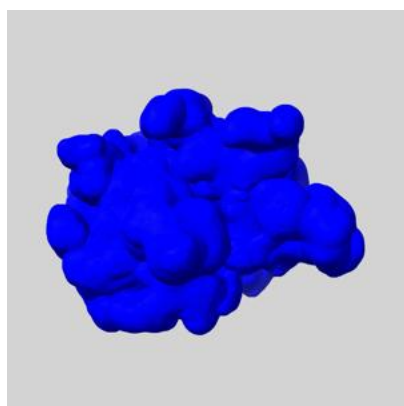
## 6.6 Mask visualisation [i](#)

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

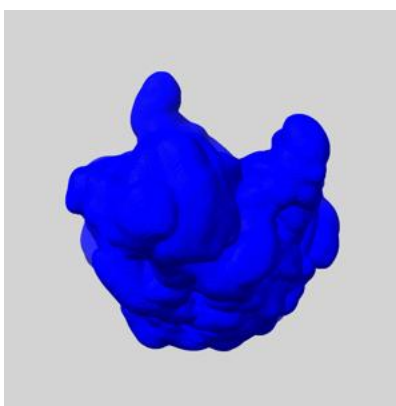
A mask typically either:

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

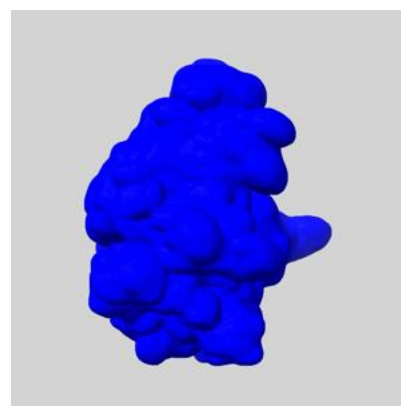
### 6.6.1 emd\_15577\_msk\_1.map [i](#)



X



Y

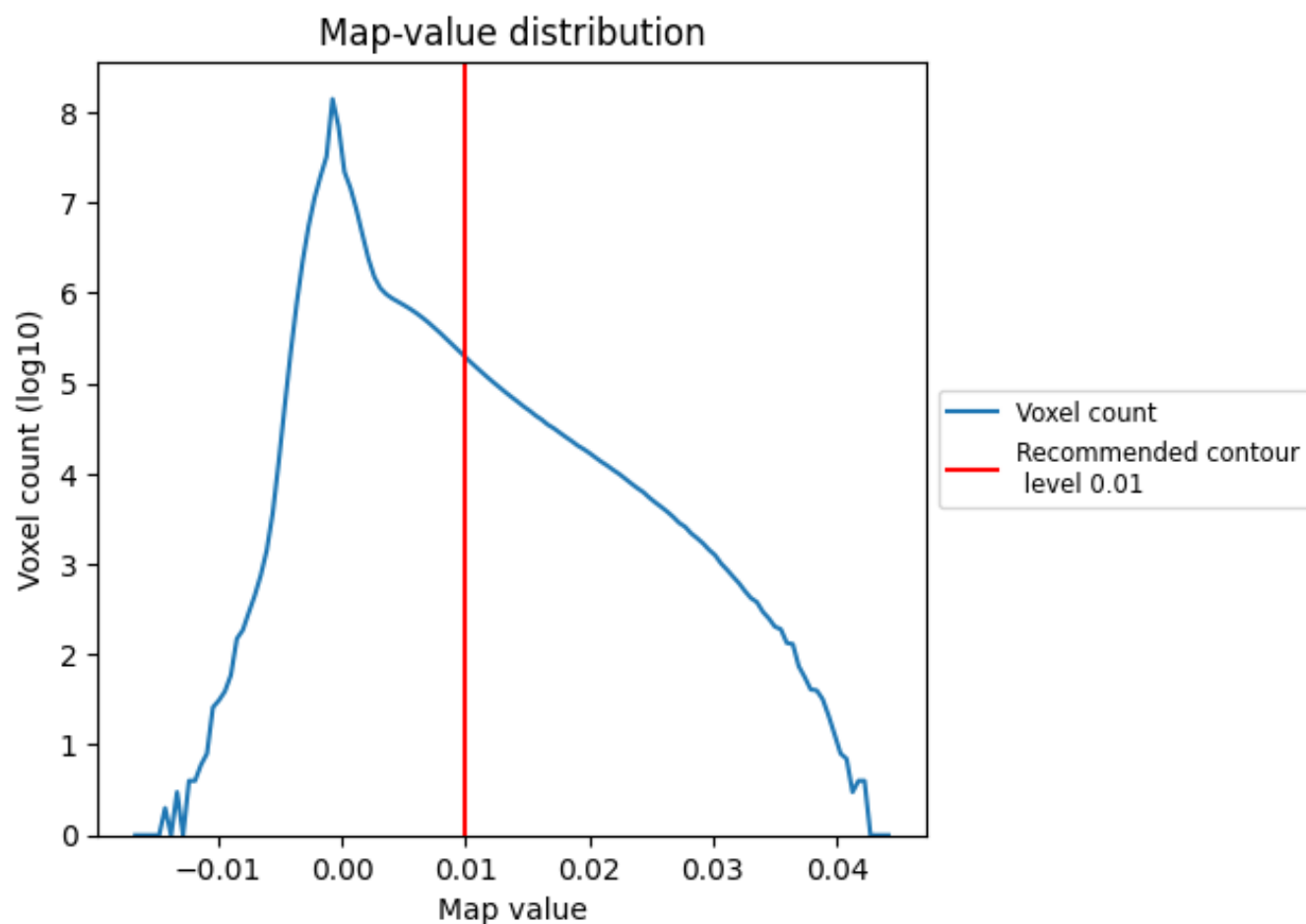


Z

## 7 Map analysis [i](#)

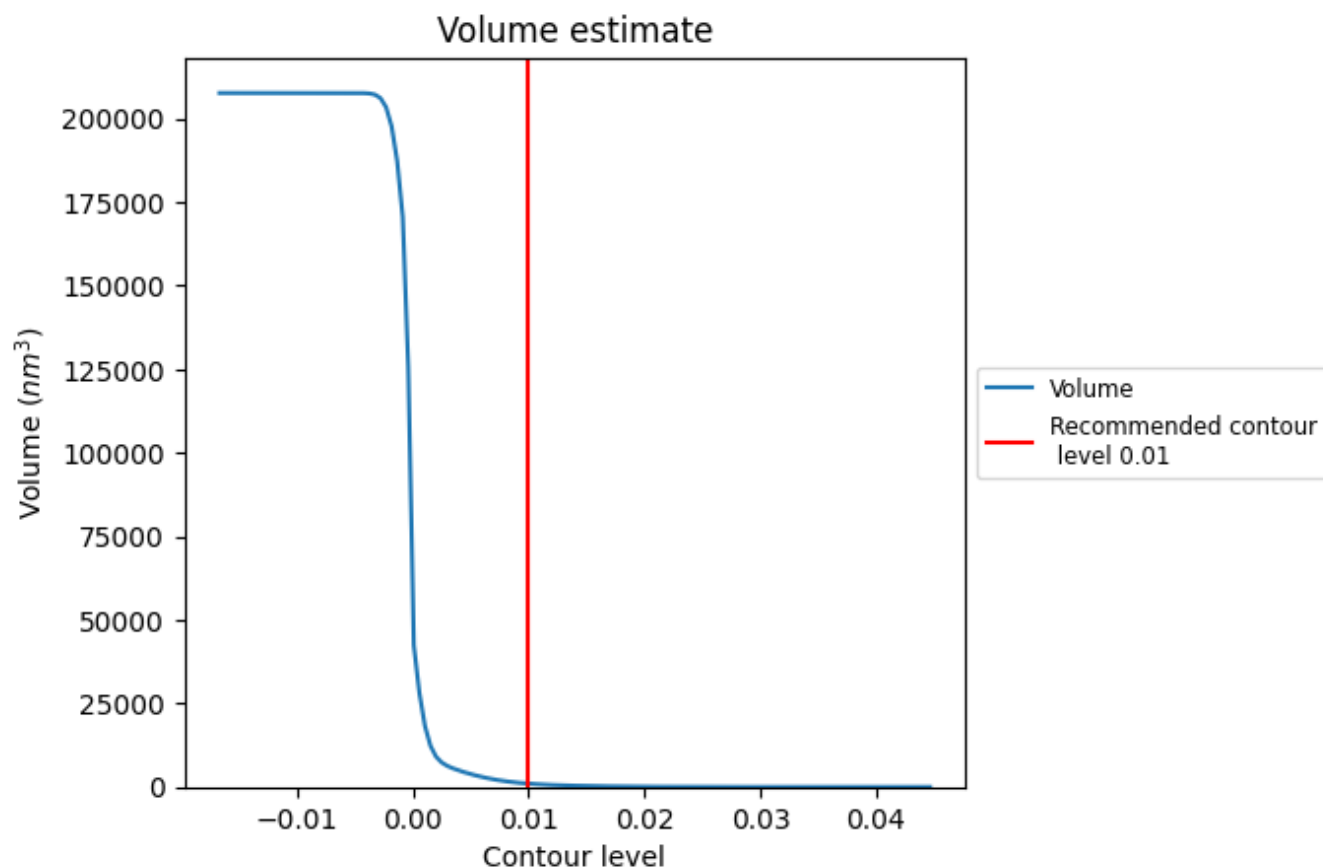
This section contains the results of statistical analysis of the map.

### 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](#)

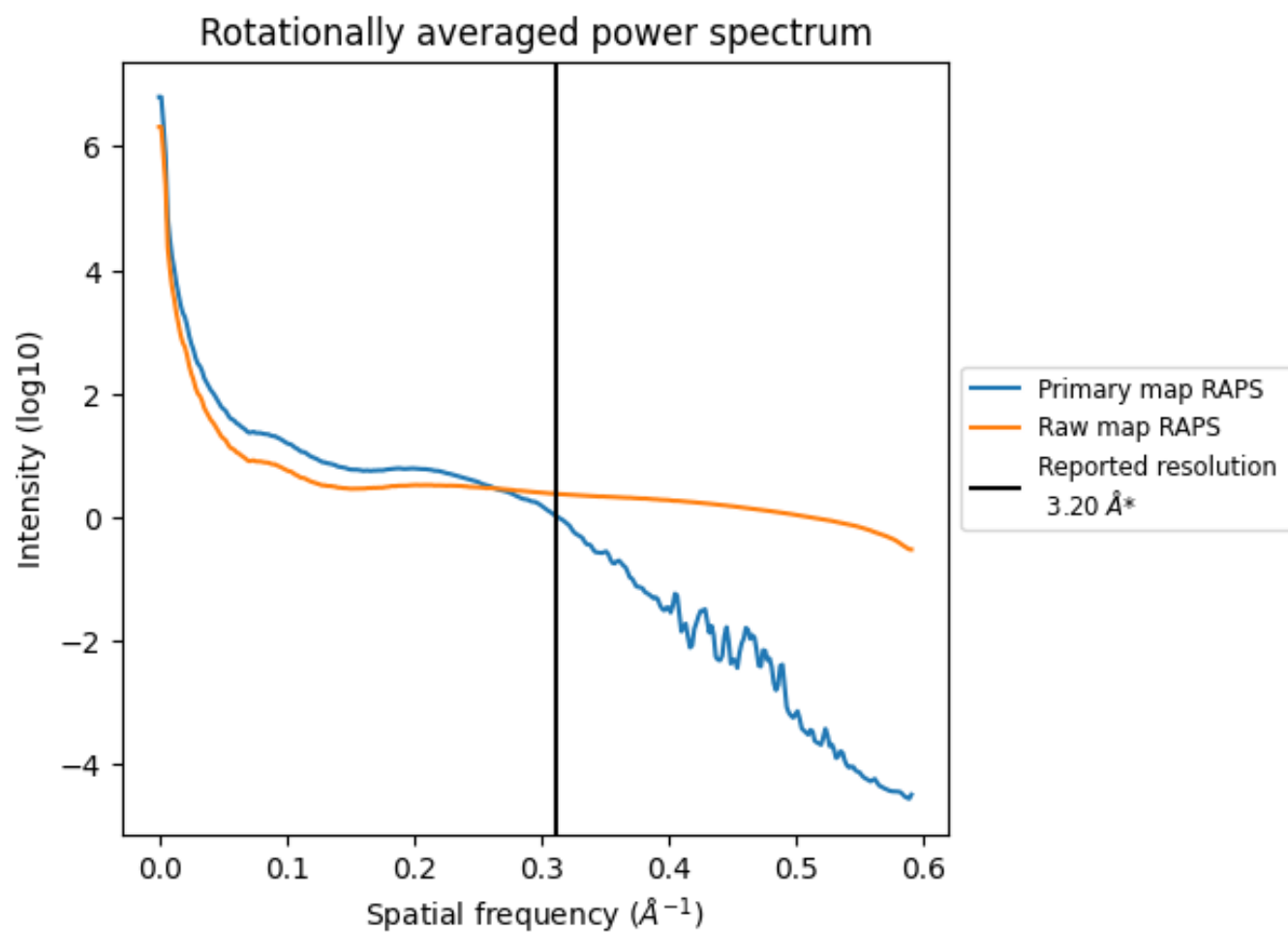


The volume at the recommended contour level is 1000  $\text{nm}^3$ ; this corresponds to an approximate mass of 903 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

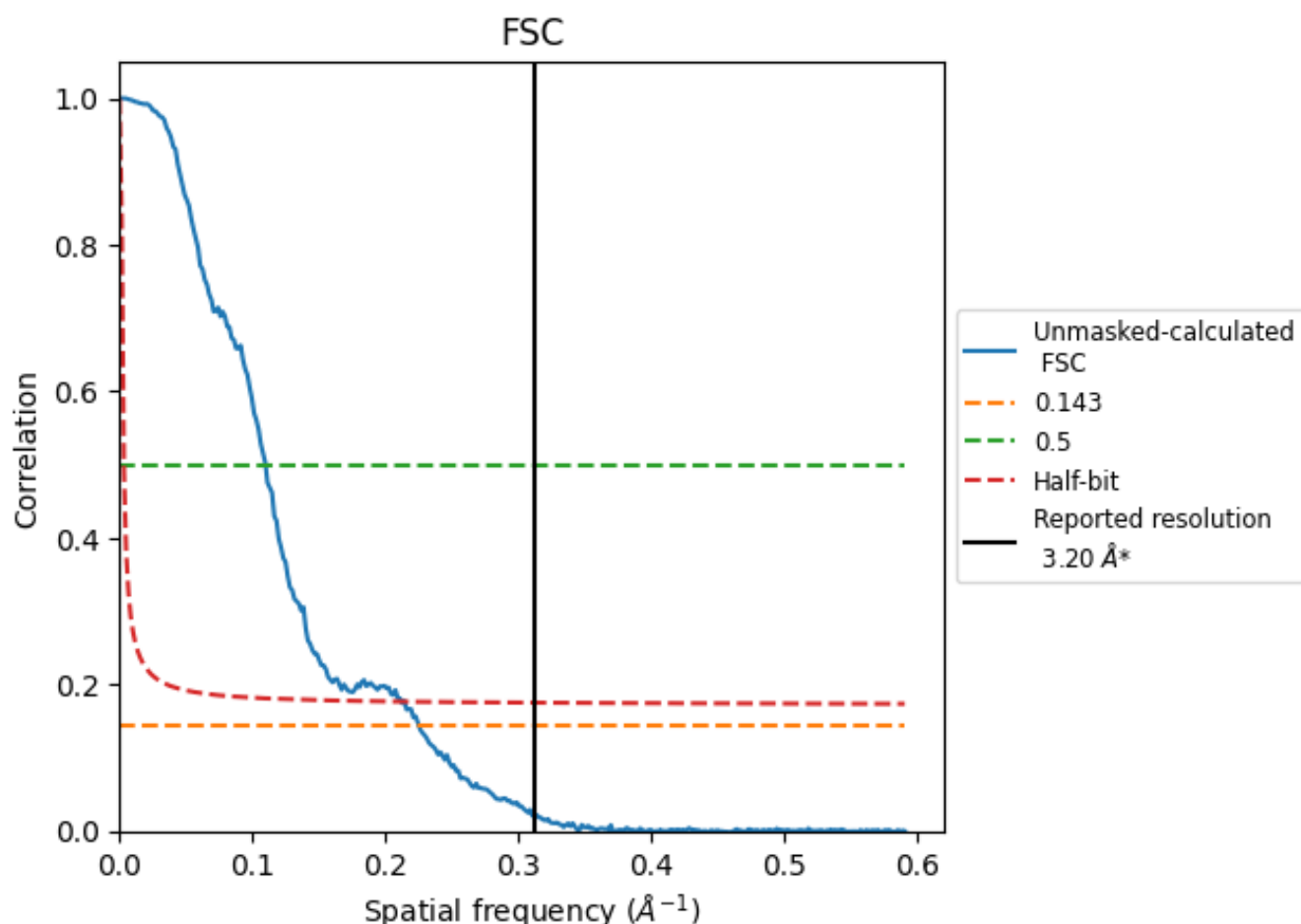


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

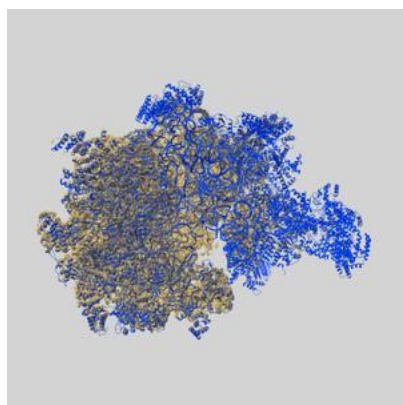
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.20
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	4.44	9.10	4.71	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

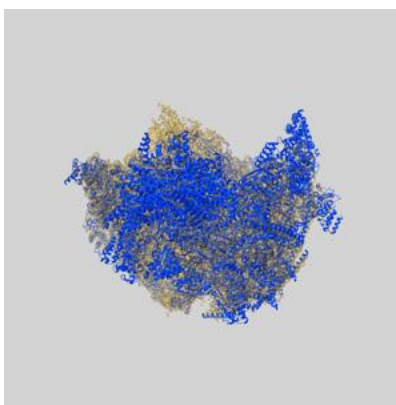
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15577 and PDB model 8APO. Per-residue inclusion information can be found in section [3](#) on page [29](#).

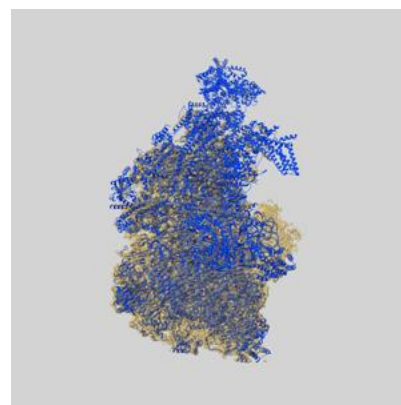
### 9.1 Map-model overlay [i](#)



X



Y



Z

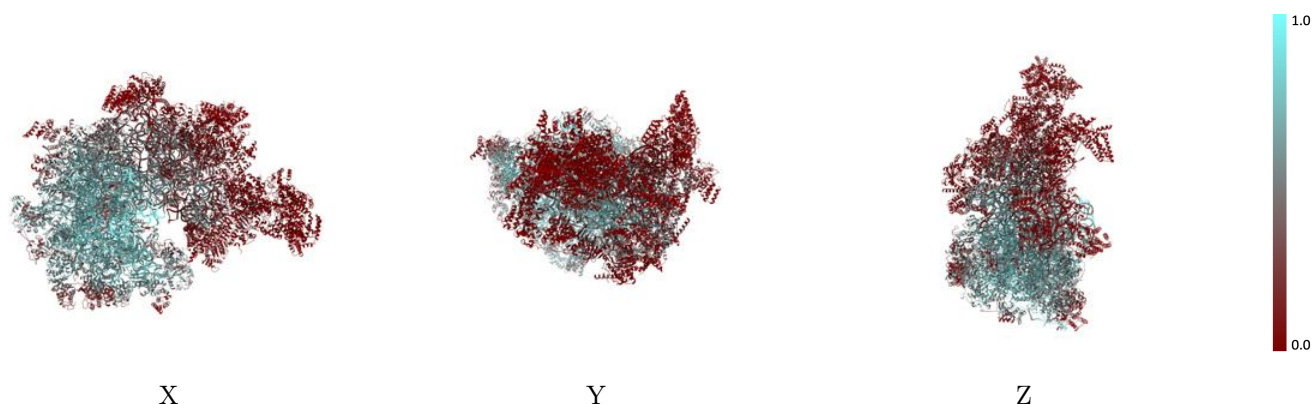
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



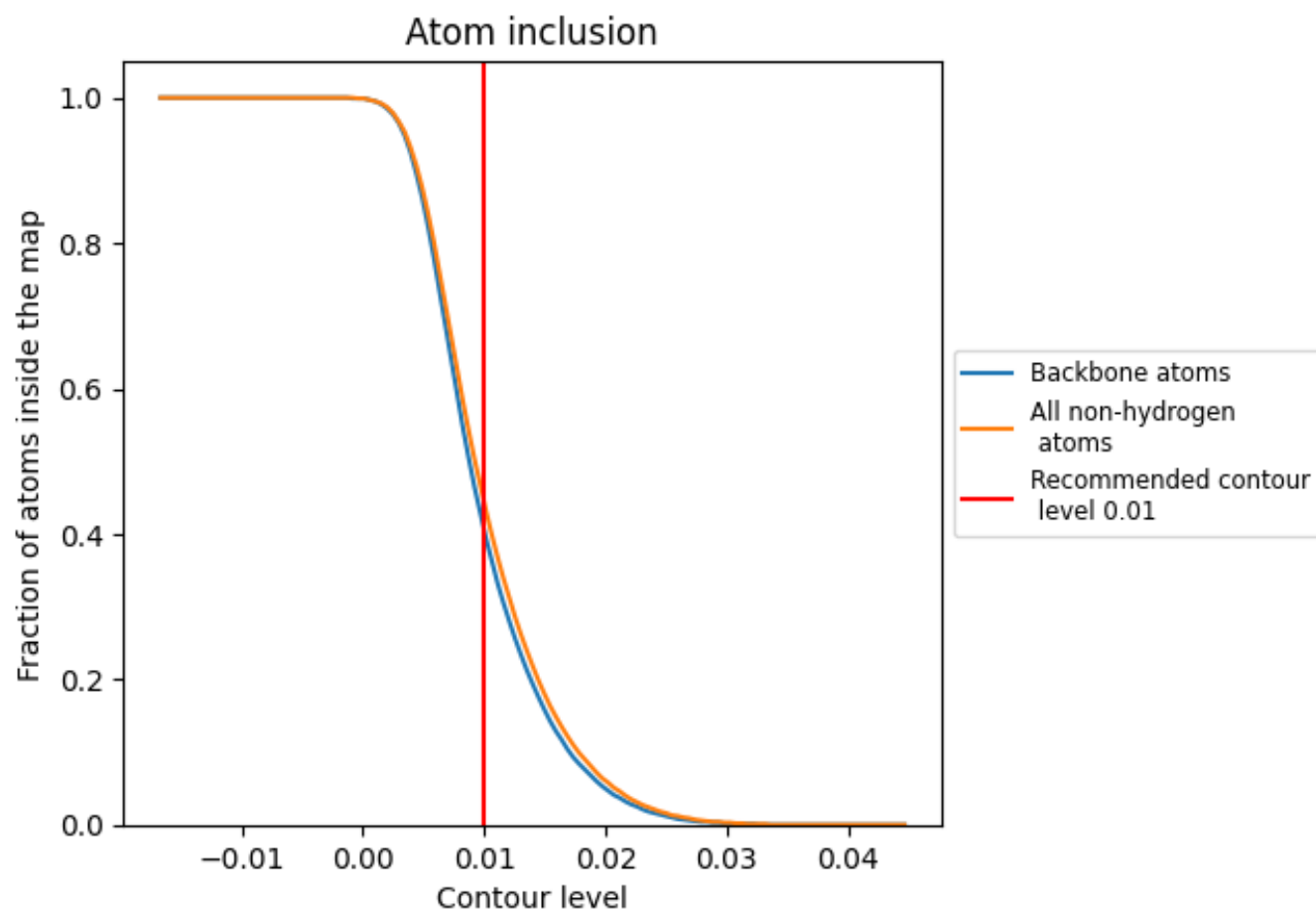
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 41% of all backbone atoms, 44% 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	 0.4440	 0.2310
A1	 0.8330	 0.4050
A2	 0.8750	 0.4510
A3	 0.8330	 0.3350
A4	 0.9150	 0.4530
A5	 0.7760	 0.2660
A6	 0.8380	 0.3660
A7	 0.7910	 0.3230
A8	 0.7600	 0.3090
A9	 0.8550	 0.4260
AA	 0.7910	 0.4330
AB	 0.8170	 0.3360
AC	 0.7780	 0.4400
AD	 0.5270	 0.2590
AE	 0.5360	 0.3400
AF	 0.6760	 0.3210
AG	 0.7640	 0.4130
AH	 0.4710	 0.3270
AI	 0.7230	 0.3900
AJ	 0.5540	 0.3730
AK	 0.6310	 0.2510
AL	 0.4590	 0.3010
AM	 0.4700	 0.3400
AN	 0.5440	 0.3800
AO	 0.3110	 0.2130
Aa	 0.6410	 0.2720
Ab	 0.5750	 0.2630
Ac	 0.7430	 0.4420
Ad	 0.4600	 0.3530
Ae	 0.5080	 0.2300
Af	 0.4510	 0.2610
Ah	 0.6550	 0.3080
Ai	 0.4370	 0.2010
Aj	 0.8370	 0.4730
Ak	 0.7110	 0.3940



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Chain	Atom inclusion	Q-score
Al	 0.6110	 0.2270
Am	 0.6840	 0.4270
An	 0.4310	 0.2080
Ao	 0.7100	 0.3550
Ap	 0.7130	 0.3960
Aq	 0.7350	 0.3570
Ar	 0.6550	 0.3030
As	 0.5190	 0.2790
At	 0.6150	 0.3570
Au	 0.8090	 0.4720
Av	 0.6350	 0.3550
Aw	 0.6410	 0.3260
Ax	 0.7130	 0.3880
Ay	 0.2970	 0.2630
Az	 0.6190	 0.3200
B1	 0.2860	 0.1020
B2	 0.3340	 0.1290
B3	 0.5610	 0.1440
B4	 0.5080	 0.1850
BA	 0.0610	 0.2070
BB	 0.1010	 0.0850
BC	 0.5170	 0.2100
BD	 0.0500	 0.0710
BE	 0.0020	 0.0580
BF	 0.1100	 0.0920
Ba	 0.0950	 0.0510
Bb	 0.1800	 0.1020
Bc	 0.1290	 0.1520
Bd	 0.1020	 0.0930
Be	 0.2220	 0.1020
Bf	 0.1290	 0.0080
Bg	 0.1920	 0.0800
Bh	 0.2240	 0.1030
Bi	 0.1080	 0.1060
Bj	 0.0420	 0.1410
Bk	 0.2640	 0.1210
Bl	 0.1090	 0.1570
Bm	 0.0360	 0.0970
Bn	 0.2200	 0.2100
Bo	 0.3990	 0.0920
Bp	 0.0760	 0.0960
Bq	 0.2760	 0.0970

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Chain	Atom inclusion	Q-score
Br	 0.1530	 0.0580
Bs	 0.0430	 0.1100
Bt	 0.2260	 0.0590
Bu	 0.1220	 0.0670
Bv	 0.1790	 0.0710
Bw	 0.0240	 0.0840
Bx	 0.0220	 0.1030
By	 0.1400	 0.2080
Bz	 0.0130	 0.0830
C1	 0.1270	 0.1480
C2	 0.1480	 0.2020
C3	 0.3900	 0.2450
Ua	 0.3480	 0.3410
Ub	 0.3960	 0.2050
Ud	 0.0000	 0.0710
Ue	 0.0000	 0.0400
Uf	 0.0140	 0.0540
Ug	 0.0410	 0.1210
Uh	 0.0000	 0.0290
Ui	 0.0540	 0.0640
Uj	 0.0000	 -0.0740
Uk	 0.0430	 0.1290
Ul	 0.0000	 -0.0270
Um	 0.0180	 0.1960
Xa	 0.4130	 0.3230
Xb	 0.3840	 0.2110
Xc	 0.5190	 0.2780
Xd	 0.5710	 0.3600
Xe	 0.4350	 0.1560
Xf	 0.4880	 0.1900
Xg	 0.5400	 0.3270
Xh	 0.5180	 0.3230
Xi	 0.6880	 0.3180
Xj	 0.3880	 0.1630
Ya	 0.0470	 0.0820
Yb	 0.0050	 0.0760
Yc	 0.0600	 0.0710
Yd	 0.0400	 0.0830
Ye	 0.1830	 0.2050
Yf	 0.1080	 0.1500
Yg	 0.0210	 0.1140
Yh	 0.1140	 0.1990

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Chain	Atom inclusion	Q-score
Yi	 0.0070	 0.0950
Yj	 0.0170	 0.0970
Yk	 0.0030	 0.0410
Yl	 0.0740	 0.0850