wwPDB EM Validation Summary Report

Jan 11, 2023 – 03:47 pm GMT

PDB ID	:	8APN
EMDB ID	:	EMD-15576
Title	:	Structure of the mitochondrial ribosome from Polytomella magna with tRNA bound to the P site
Authors	:	Tobiasson, V.; Berzina, I.; Amunts, A.
Deposited on	:	2022-08-10
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

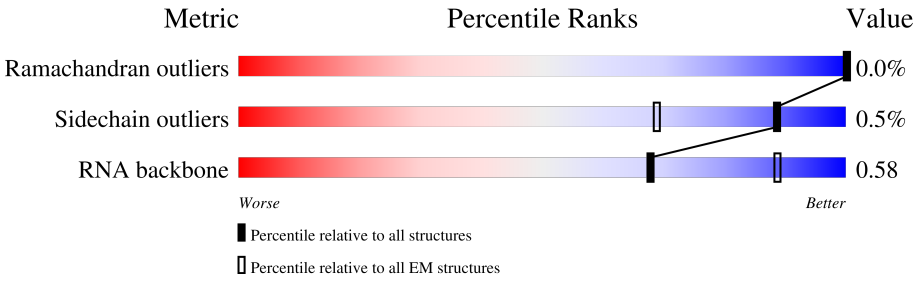
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	77% 23%
2	A2	81	5% 80% 20%
3	A3	207	86% 14%
4	A4	73	85% 15%
5	A5	136	8% 76% 24%
6	A6	109	81% 19%
7	A7	534	85% 15%
8	A8	350	83% 16%

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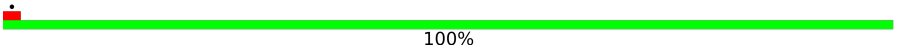
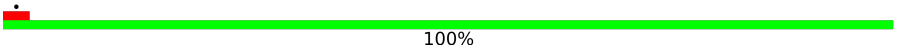
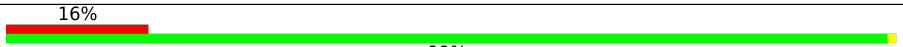
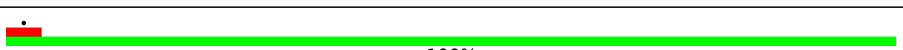
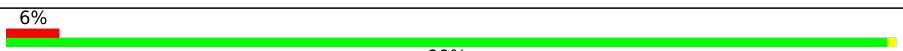
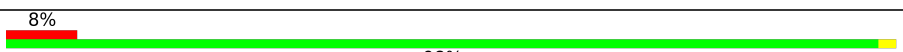
Mol	Chain	Length	Quality of chain
9	A9	69	
10	Aa	306	
11	Ab	306	
12	Ac	303	
13	Ad	193	
14	Ae	242	
15	Af	56	
16	Ah	186	
17	Ai	121	
18	Aj	206	
19	Ak	166	
20	Al	173	
21	Am	114	
22	An	170	
23	Ao	117	
24	Ap	200	
25	Aq	188	
26	Ar	155	
27	As	115	
28	At	253	
29	Au	142	
30	Av	129	
31	Aw	123	
32	Ax	176	
33	Ay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

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Mol	Chain	Length	Quality of chain
34	Az	59	8% 93% 7%
35	AA	50	100%
36	AB	50	100%
37	AC	139	5% 99%
38	AD	47	11% 98%
39	AE	92	16% 100%
40	AF	93	5% 100%
41	AG	121	100%
42	AH	176	22% 99%
43	AI	64	100%
44	AJ	122	13% 100%
45	AK	139	100%
46	AL	394	43% 99%
47	AM	419	38% 100%
48	AN	420	34% 100%
49	AO	377	34% 99%
50	Xa	199	39% 99%
51	Xb	244	18% 100%
52	Xc	57	100%
53	Xd	413	18% 100%
54	Xe	483	10% 100%
55	Xf	201	7% 100%
56	Xg	410	18% 99%
57	Xh	143	25% 100%
58	Xi	24	100%

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Mol	Chain	Length	Quality of chain
59	Xj	71	28% 100%
60	B1	102	19% 78% 22%
61	B2	210	5% 81% 19%
62	B3	379	87% 13%
63	B4	337	86% 14%
64	Ba	242	41% 98%
65	Bb	236	23% 100%
66	Bc	289	48% 99%
67	Bd	221	31% 100%
68	Be	228	8% 97%
69	Bf	119	15% 100%
70	Bg	112	16% 98%
71	Bh	374	23% 100%
72	Bi	282	32% 100%
73	Bj	401	69% 100%
74	Bk	116	100%
75	Bl	123	43% 100%
76	Bm	113	34% 99%
77	Bn	118	8% 100%
78	Bo	167	7% 100%
79	Bp	123	43% 100%
80	Bq	130	8% 100%
81	Br	90	12% 100%
82	Bs	92	50% 100%
83	Bt	75	8% 100%

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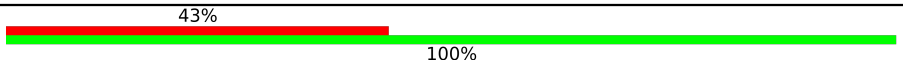
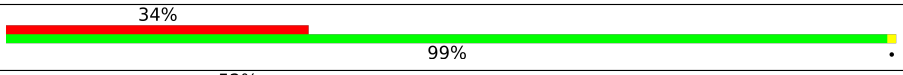
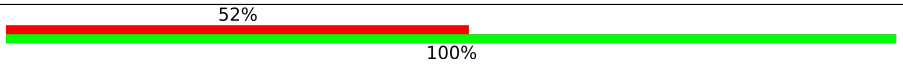
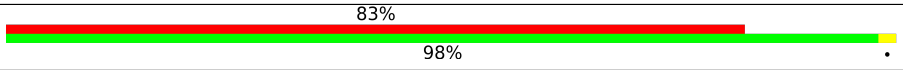
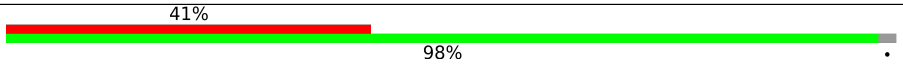
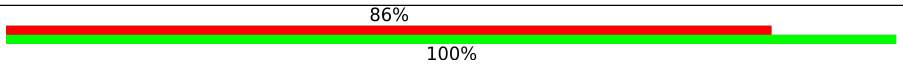
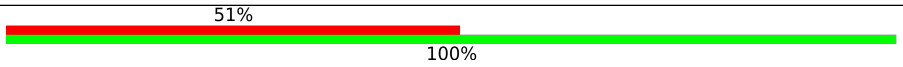
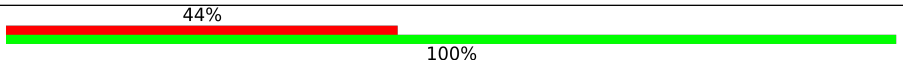
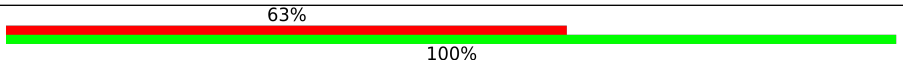
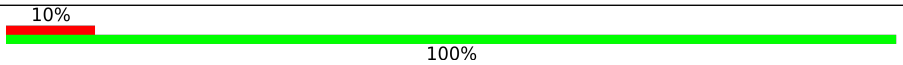
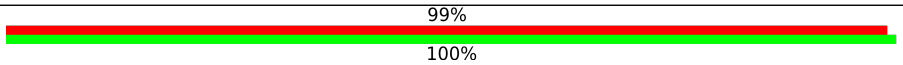
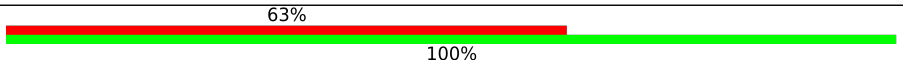
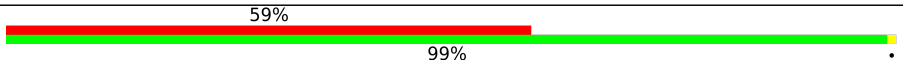
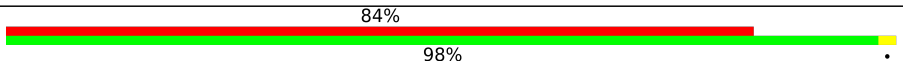
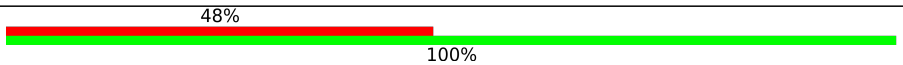
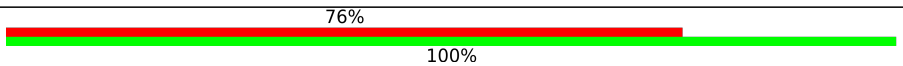
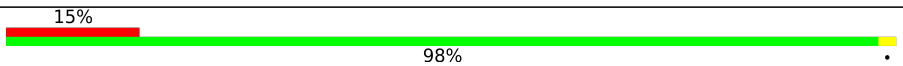
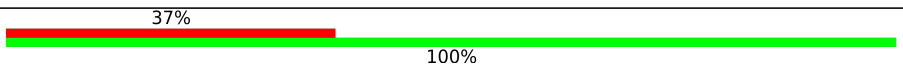
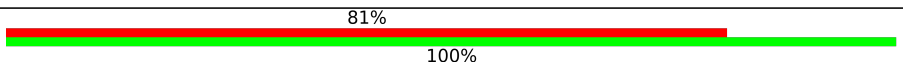
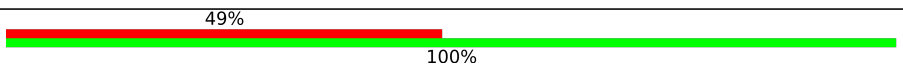
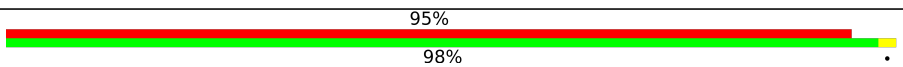
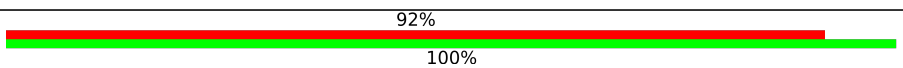
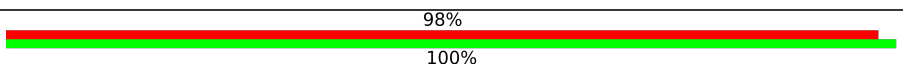
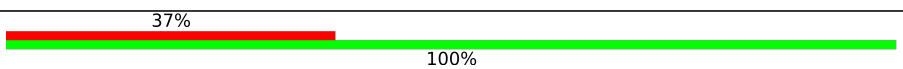
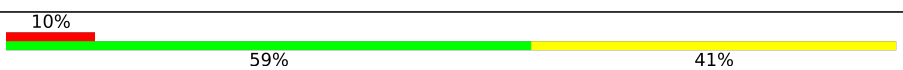
Mol	Chain	Length	Quality of chain
84	Bu	167	
85	Bv	164	
86	Bw	349	
87	Bx	621	
88	By	80	
89	Bz	119	
90	BA	176	
91	BB	84	
92	BC	270	
93	BD	31	
94	BE	171	
95	BF	370	
96	Ya	180	
97	Yb	50	
98	Yc	159	
99	Yd	95	
100	Ye	106	
101	Yf	150	
102	Yg	67	
103	Yh	65	
104	Yi	132	
105	Yj	386	
106	Yk	92	
107	Yl	84	
108	C1	73	

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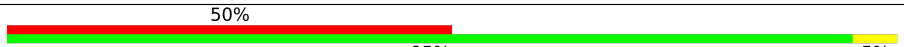
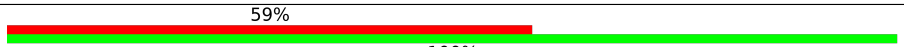
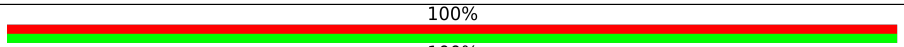
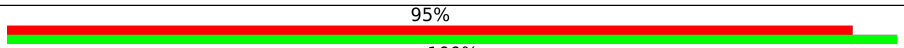
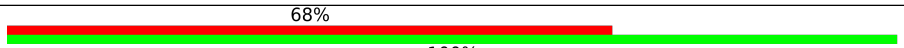
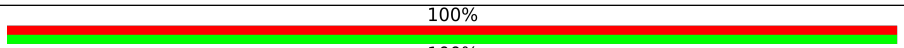
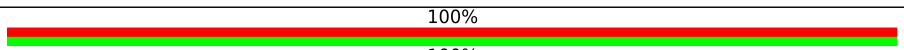
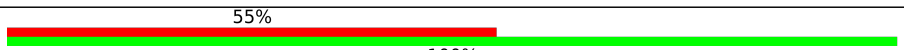
Mol	Chain	Length	Quality of chain
109	C3	4	
110	Ub	130	
111	Ua	32	
112	Ud	43	
113	Ue	47	
114	Uf	73	
115	Ug	63	
116	Uh	48	
117	Ui	26	
118	Uj	9	
119	Uk	23	
120	Ul	16	
121	Um	11	

2 Entry composition (i)

There are 126 unique types of molecules in this entry. The entry contains 198407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called mtLSU-1.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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 Hypothetical protein.

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		

- Molecule 47 is a protein called mL116.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AM	419	Total	C	N	O	S	0	0
			3282	2087	584	604	7		

- Molecule 48 is a protein called mL116.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AN	420	Total	C	N	O	S	0	0
			3286	2089	585	605	7		

- Molecule 49 is a protein called mL118.

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

- Molecule 50 is a protein called mL120.

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

- Molecule 51 is a protein called mL121.

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

- Molecule 52 is a protein called mL122.

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

- Molecule 53 is a protein called mL123.

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

- Molecule 54 is a protein called mL124.

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

- Molecule 55 is a protein called mL125.

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

- Molecule 56 is a protein called mL126.

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

- Molecule 57 is a protein called mL127.

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

- Molecule 58 is a protein called mL128.

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

- Molecule 59 is a protein called mL129.

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

- Molecule 60 is a RNA chain called mtSSU-1.

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

- Molecule 61 is a RNA chain called mtSSU-2.

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

- Molecule 62 is a RNA chain called mtSSU-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	B3	379	Total	C	N	O	P	0	0
			8096	3627	1480	2610	379		

- Molecule 63 is a RNA chain called mtSSU-4.

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

- Molecule 64 is a protein called bS1m.

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

- Molecule 65 is a protein called uS2m.

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

- Molecule 66 is a protein called uS3m.

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

- Molecule 67 is a protein called uS4m.

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

- Molecule 68 is a protein called uS5m.

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

- Molecule 69 is a protein called uS6m.

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

- Molecule 70 is a protein called uS7m.

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

- Molecule 71 is a protein called uS8m.

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

- Molecule 72 is a protein called uS9m.

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

- Molecule 73 is a protein called uS10m.

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

- Molecule 74 is a protein called uS11m.

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

- Molecule 75 is a protein called uS12m.

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

- Molecule 76 is a protein called uS13m.

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

- Molecule 77 is a protein called uS14m.

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

- Molecule 78 is a protein called uS15m.

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

- Molecule 79 is a protein called bS16m.

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

- Molecule 80 is a protein called uS17m.

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

- Molecule 81 is a protein called bS18m.

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

- Molecule 82 is a protein called bS19m.

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

- Molecule 83 is a protein called bS21m.

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

- Molecule 84 is a protein called mS23.

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

- Molecule 85 is a protein called mS26.

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

- Molecule 86 is a protein called mS29.

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

- Molecule 87 is a protein called mS31.

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

- Molecule 88 is a protein called mS33.

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

- Molecule 89 is a protein called mS34.

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

- Molecule 90 is a protein called mS35.

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

- Molecule 91 is a protein called mS37.

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

- Molecule 92 is a protein called mS45.

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

- Molecule 93 is a protein called mS38.

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

- Molecule 94 is a protein called mS106.

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

- Molecule 95 is a protein called mS107.

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

- Molecule 96 is a protein called uS4m-2.

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

- Molecule 97 is a protein called mS108.

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

- Molecule 98 is a protein called mS109.

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

- Molecule 99 is a protein called mS110.

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

- Molecule 100 is a protein called uS3m-2.

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

- Molecule 101 is a protein called mS111.

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

- Molecule 102 is a protein called mS112.

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

- Molecule 103 is a protein called mS113.

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

- Molecule 104 is a protein called mS114.

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

- Molecule 105 is a protein called mS115.

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

- Molecule 106 is a protein called mS116.

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

- Molecule 107 is a protein called uS7m-2.

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

- Molecule 108 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	C1	73	Total	C	N	O	P	0	0
			1542	693	268	509	72		

- Molecule 109 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	C3	4	Total	C	N	O	P	0	0
			87	39	17	27	4		

- Molecule 110 is a protein called mL105.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	Ub	130	Total	C	N	O	S	0	0
			1090	688	189	207	6		

- Molecule 111 is a protein called Unknown.

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

- Molecule 112 is a protein called Unknown.

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

- Molecule 113 is a protein called Unknown.

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

- Molecule 114 is a protein called Unknown.

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

- Molecule 115 is a protein called Unknown.

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

- Molecule 116 is a protein called Unknown.

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

- Molecule 117 is a protein called Unknown.

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

- Molecule 118 is a protein called Unknown.

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

- Molecule 119 is a protein called Unknown.

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

- Molecule 120 is a protein called Unknown.

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

- Molecule 121 is a protein called Unknown.

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

- Molecule 122 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
122	A1	3	Total 3	Mg 3	0
122	A2	2	Total 2	Mg 2	0
122	A3	7	Total 7	Mg 7	0
122	A4	10	Total 10	Mg 10	0
122	A5	2	Total 2	Mg 2	0
122	A6	7	Total 7	Mg 7	0
122	A7	25	Total 25	Mg 25	0
122	A8	14	Total 14	Mg 14	0
122	Ab	1	Total 1	Mg 1	0
122	B1	3	Total 3	Mg 3	0
122	B2	8	Total 8	Mg 8	0
122	B3	13	Total 13	Mg 13	0

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Mol	Chain	Residues	Atoms	AltConf
122	B4	15	Total Mg 15 15	0
122	Bm	1	Total Mg 1 1	0
122	Bw	1	Total Mg 1 1	0

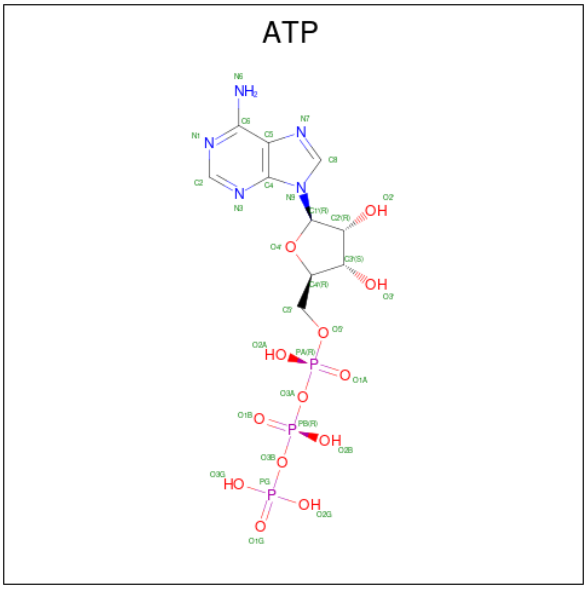
- Molecule 123 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
123	A1	1	Total K 1 1	0
123	A3	1	Total K 1 1	0
123	A4	2	Total K 2 2	0
123	A7	4	Total K 4 4	0
123	A8	5	Total K 5 5	0
123	Aa	1	Total K 1 1	0
123	Ab	1	Total K 1 1	0
123	Ah	1	Total K 1 1	0
123	AC	1	Total K 1 1	0
123	B1	2	Total K 2 2	0
123	B2	1	Total K 1 1	0
123	B3	8	Total K 8 8	0
123	B4	3	Total K 3 3	0

- Molecule 124 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 125 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 126 is water.

Mol	Chain	Residues	Atoms		AltConf
126	A1	15	Total	O	0
			15	15	
126	A2	9	Total	O	0
			9	9	
126	A3	30	Total	O	0
			30	30	
126	A4	33	Total	O	0
			33	33	
126	A5	9	Total	O	0
			9	9	
126	A6	22	Total	O	0
			22	22	
126	A7	110	Total	O	0
			110	110	
126	A8	70	Total	O	0
			70	70	
126	Aa	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
126	Ab	4	Total O 4 4	0
126	Ac	1	Total O 1 1	0
126	Aj	4	Total O 4 4	0
126	AA	1	Total O 1 1	0
126	AC	1	Total O 1 1	0
126	AI	4	Total O 4 4	0
126	AK	2	Total O 2 2	0
126	Xg	1	Total O 1 1	0
126	B1	12	Total O 12 12	0
126	B2	39	Total O 39 39	0
126	B3	57	Total O 57 57	0
126	B4	69	Total O 69 69	0
126	Be	3	Total O 3 3	0
126	Bi	2	Total O 2 2	0
126	Bl	2	Total O 2 2	0
126	Bm	1	Total O 1 1	0
126	Bp	1	Total O 1 1	0

3 Residue-property plots (i)

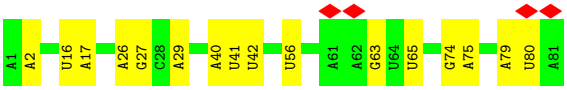
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain A1:

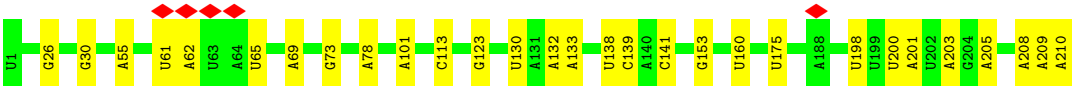
- Molecule 2: mtLSU-2

Chain A2:



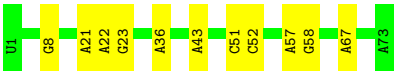
- Molecule 3: mtLSU-3

Chain A3:



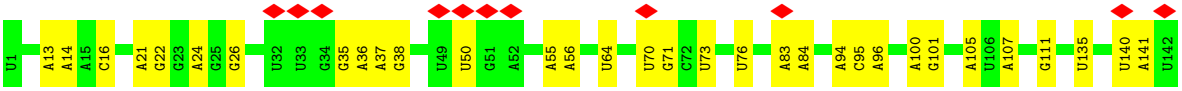
- Molecule 4: mtLSU-4

Chain A4:



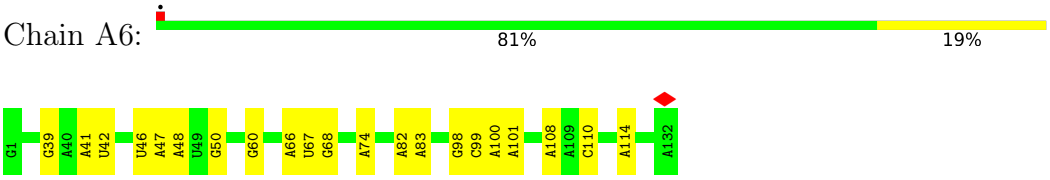
- Molecule 5: mtLSU-5

Chain A5:



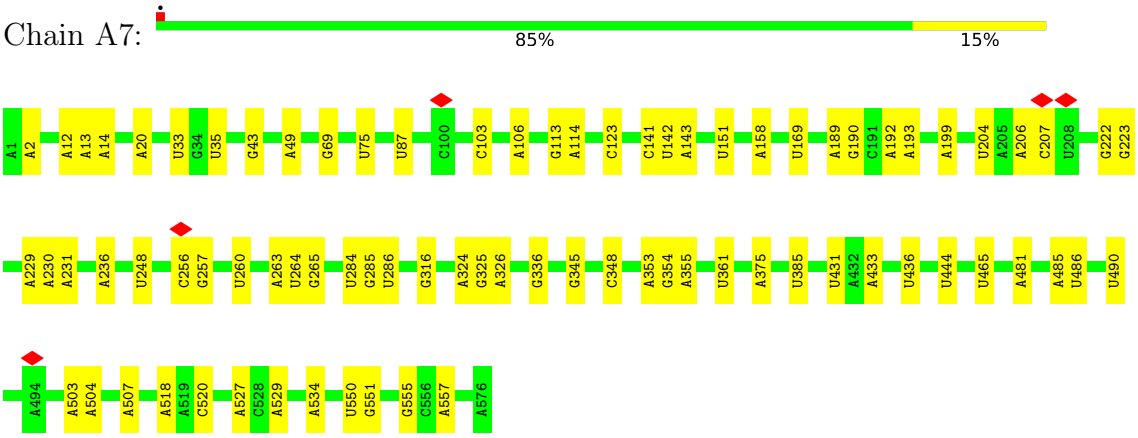
- Molecule 6: mtLSU-6

Chain A6:



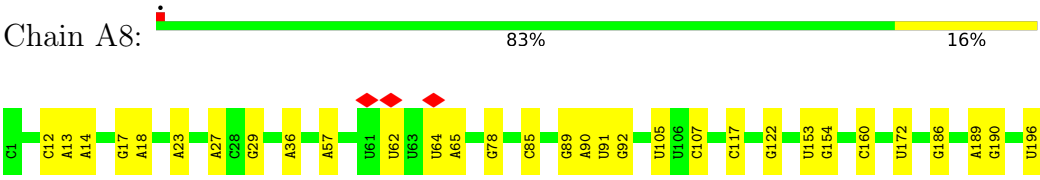
• Molecule 7: mtLSU-7

Chain A7:



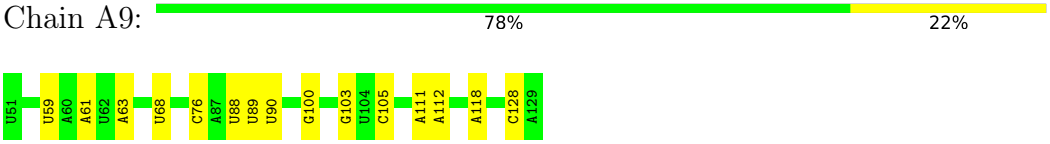
• Molecule 8: mtLSU-8

Chain A8:



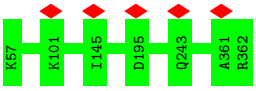
• Molecule 9: mt-5S

Chain A9:



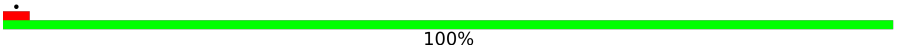
• Molecule 10: uL2m

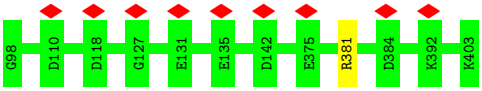
Chain Aa:



• Molecule 11: uL3m

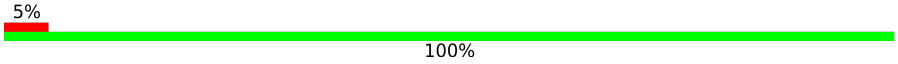
Chain Ab:

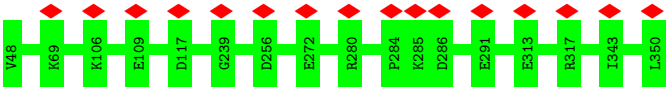




• Molecule 12: uL4m

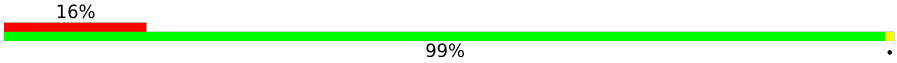
Chain Ac:

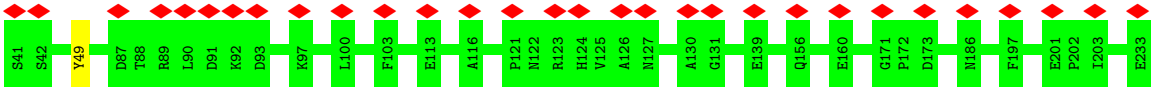




• Molecule 13: uL5m

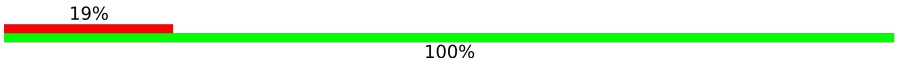
Chain Ad:

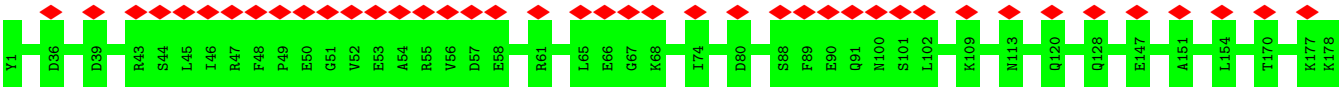


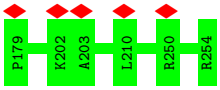


• Molecule 14: uL6m

Chain Ae:

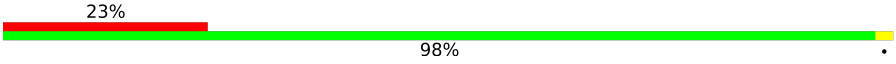


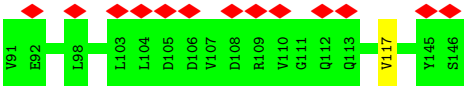




• Molecule 15: uL9m

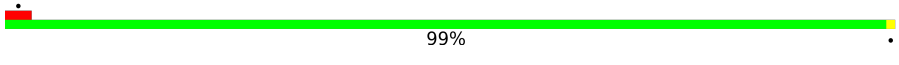
Chain Af:

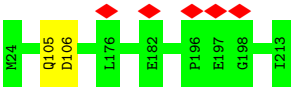




• Molecule 16: uL13m

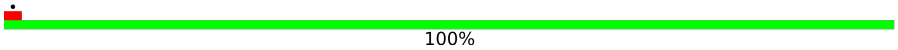
Chain Ah:

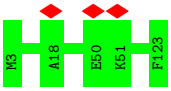




• Molecule 17: Hypothetical protein

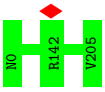
Chain Ai:





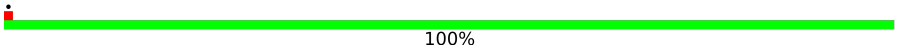
• Molecule 18: uL15m

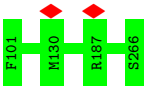
Chain Aj:



• Molecule 19: uL16m

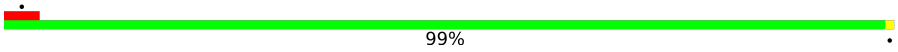
Chain Ak:

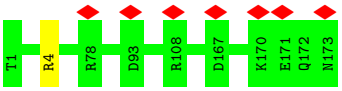




• Molecule 20: bL17m

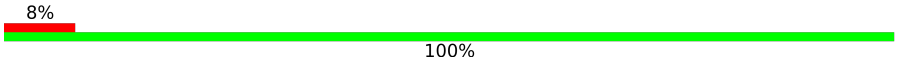
Chain Al:

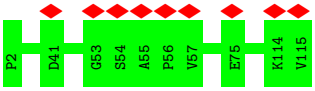




• Molecule 21: uL18m

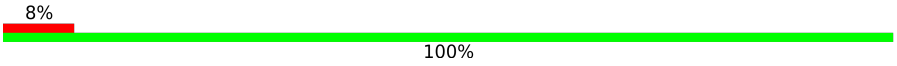
Chain Am:

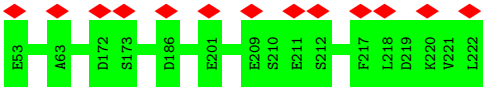




• Molecule 22: bL19m

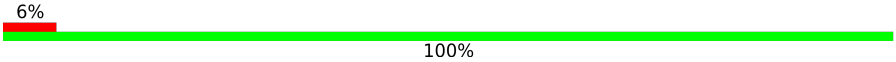
Chain An:

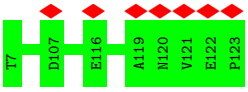




• Molecule 23: bL20m

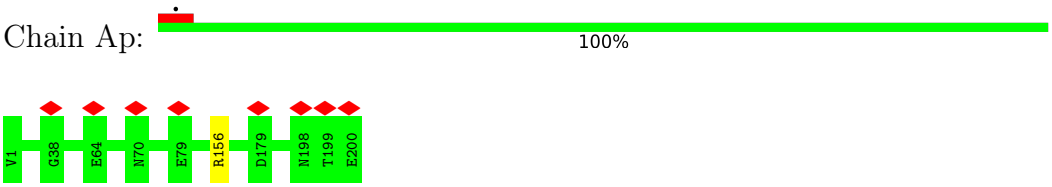
Chain Ao:





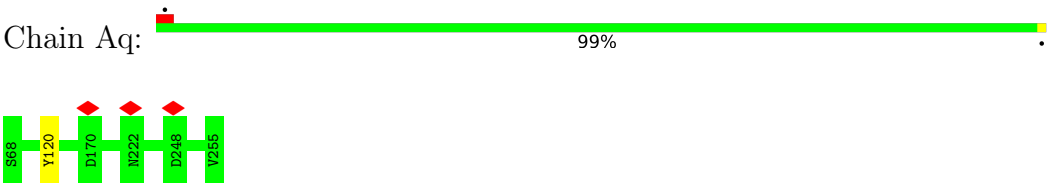
• Molecule 24: bL21m

Chain Ap:



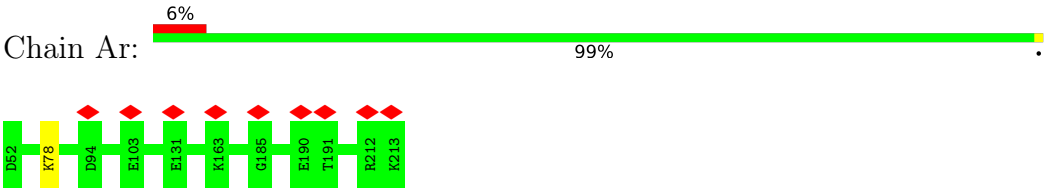
• Molecule 25: uL22m

Chain Aq:



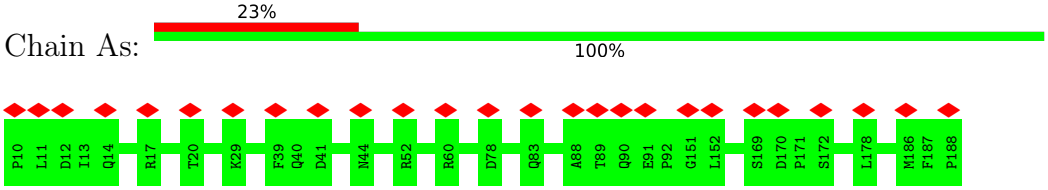
• Molecule 26: uL23m

Chain Ar:



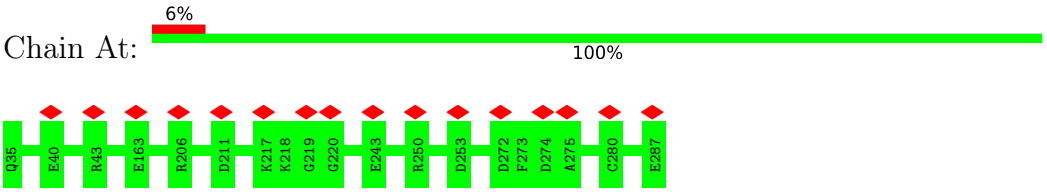
• Molecule 27: bL24m

Chain As:



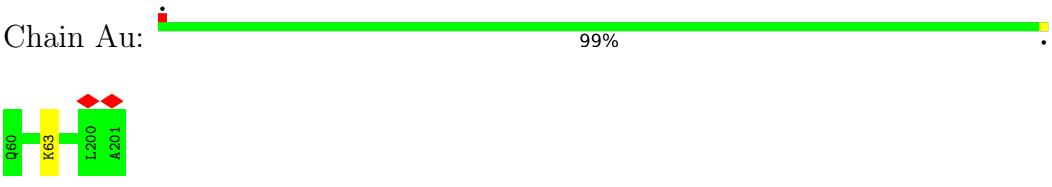
• Molecule 28: bL25m

Chain At:



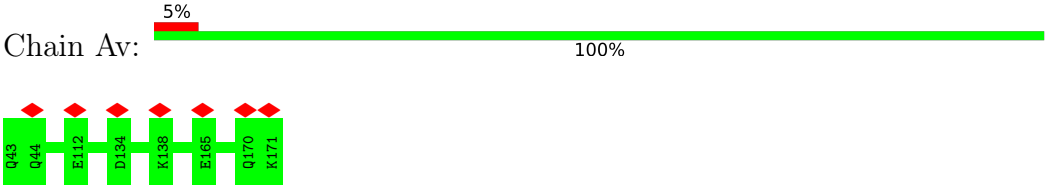
• Molecule 29: bL27m

Chain Au:



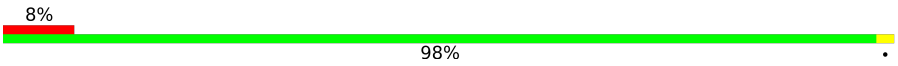
• Molecule 30: bL28m

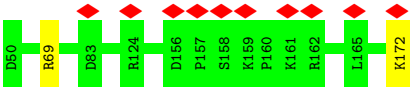
Chain Av:



• Molecule 31: uL29m

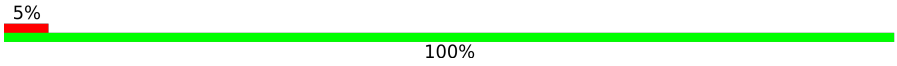
Chain Aw:

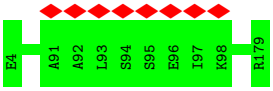




• Molecule 32: uL30m

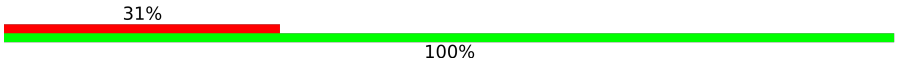
Chain Ax:

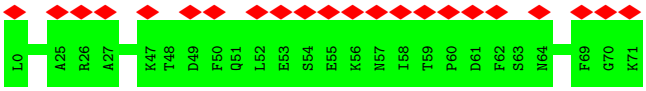




• Molecule 33: bL31m

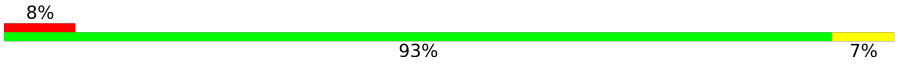
Chain Ay:

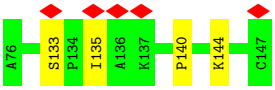




• Molecule 34: bL32m

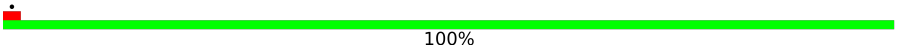
Chain Az:





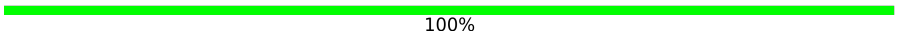
• Molecule 35: bL33m

Chain AA:



• Molecule 36: bL34m

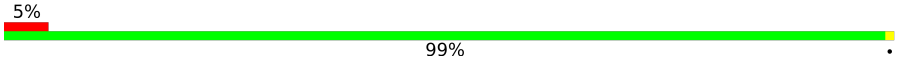
Chain AB:

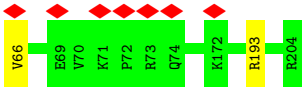


There are no outlier residues recorded for this chain.

• Molecule 37: bL35m

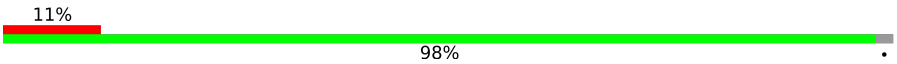
Chain AC:

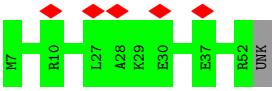




• Molecule 38: bL36m

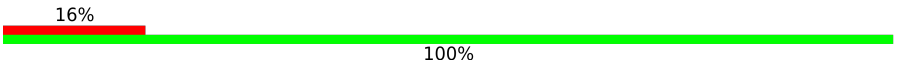
Chain AD:

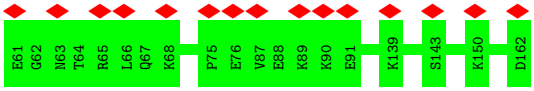




• Molecule 39: mL40

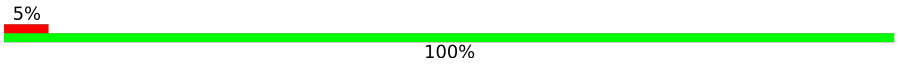
Chain AE:

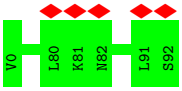




• Molecule 40: mL41

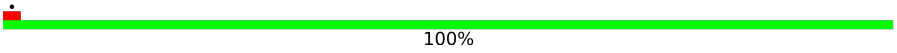
Chain AF:

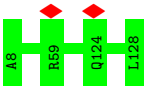




• Molecule 41: mL43

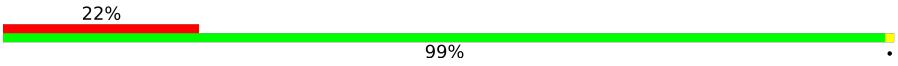
Chain AG:

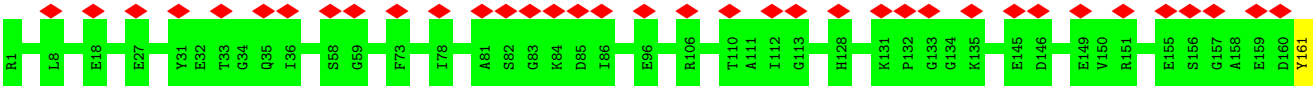


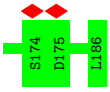


• Molecule 42: mL46

Chain AH:

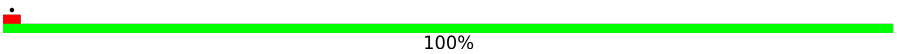


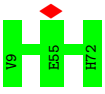




• Molecule 43: mL63

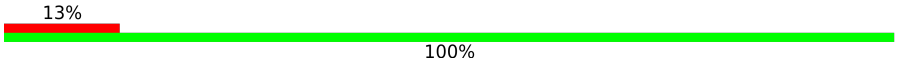
Chain AI:

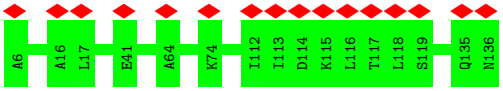




• Molecule 44: mL64

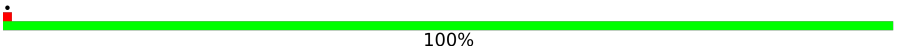
Chain AJ:

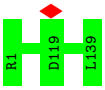




• Molecule 45: mL87

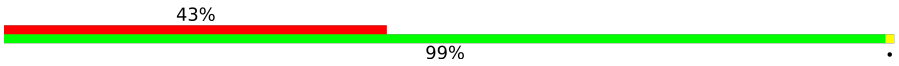
Chain AK:

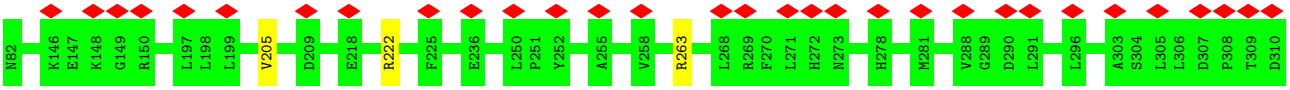


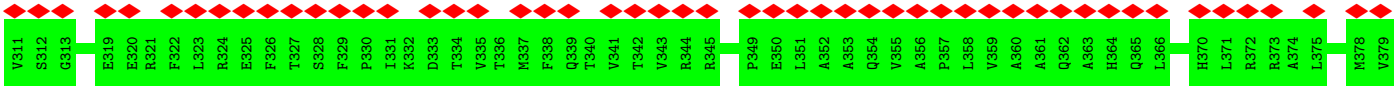


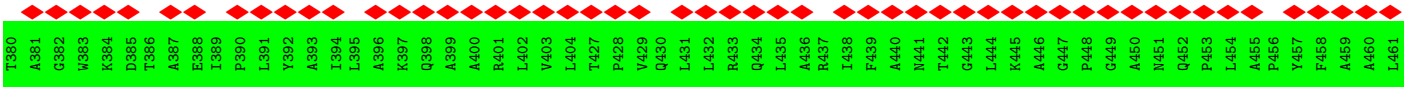
• Molecule 46: mL116

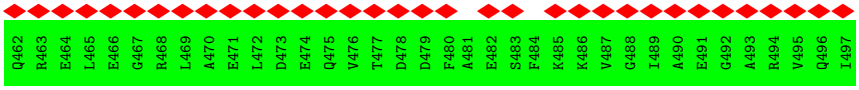
Chain AL:





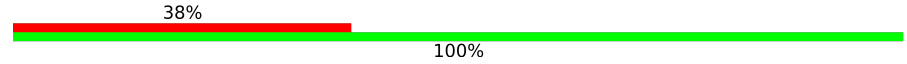


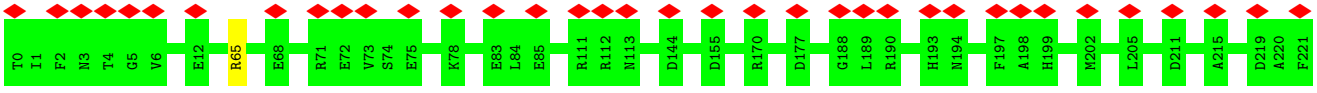


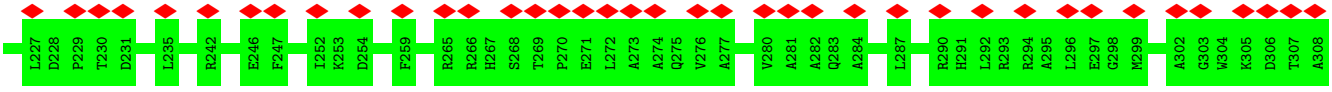


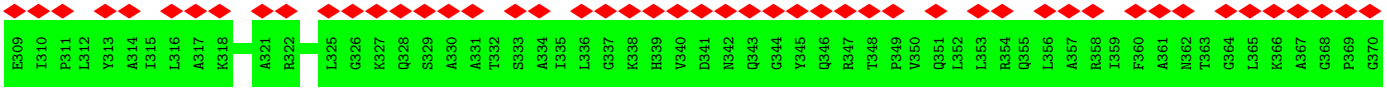
• Molecule 47: mL116

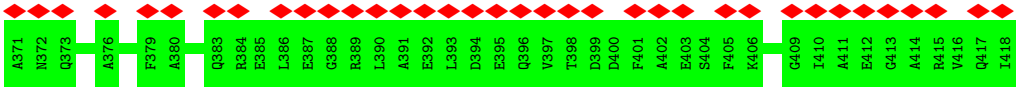
Chain AM:





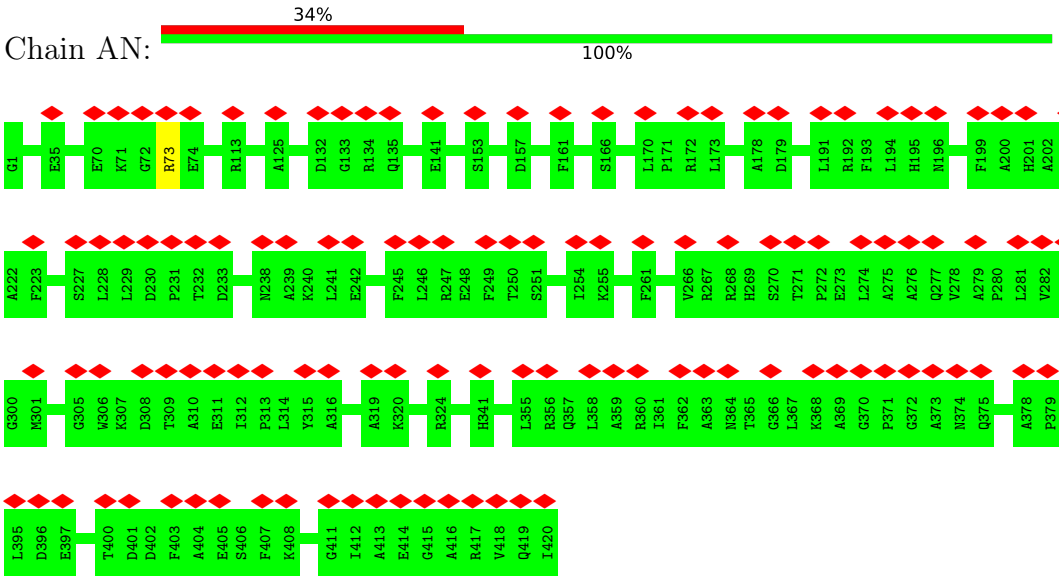






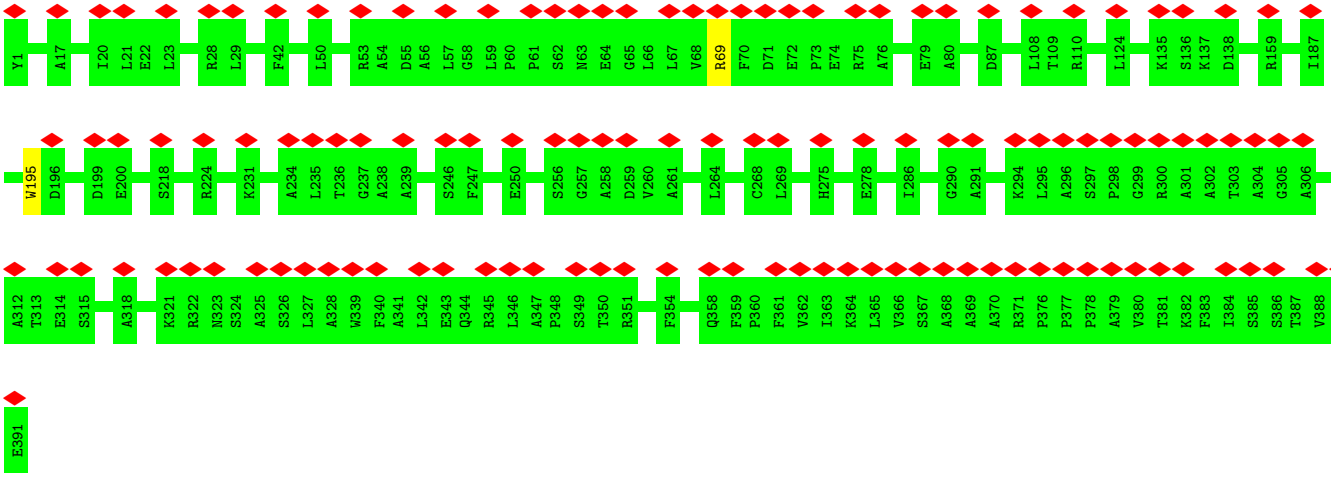
• Molecule 48: mL116

Chain AN:



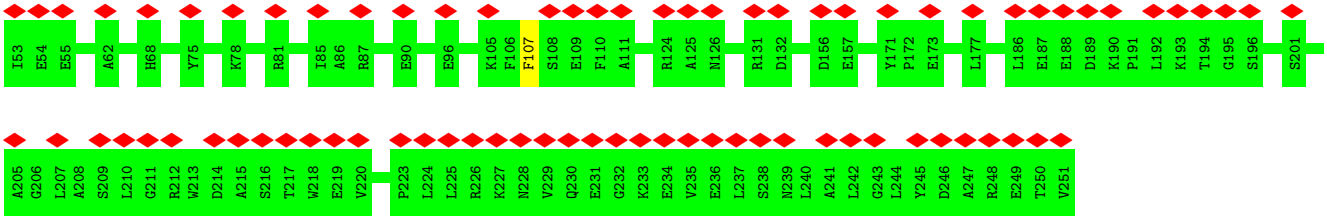
• Molecule 49: mL118

Chain AO:



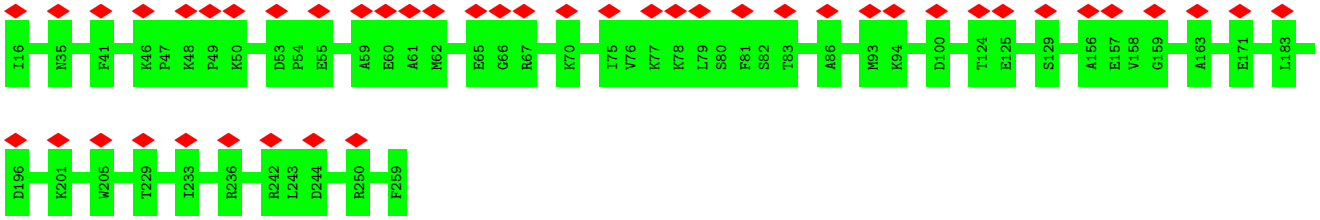
• Molecule 50: mL120

Chain Xa:



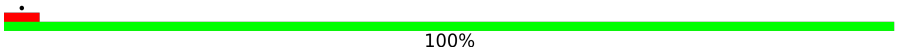
• Molecule 51: mL121

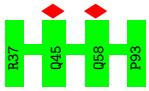
Chain Xb:



• Molecule 52: mL122

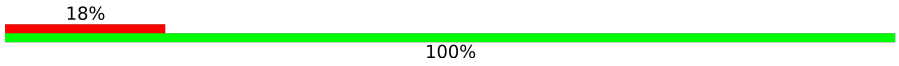
Chain Xc:

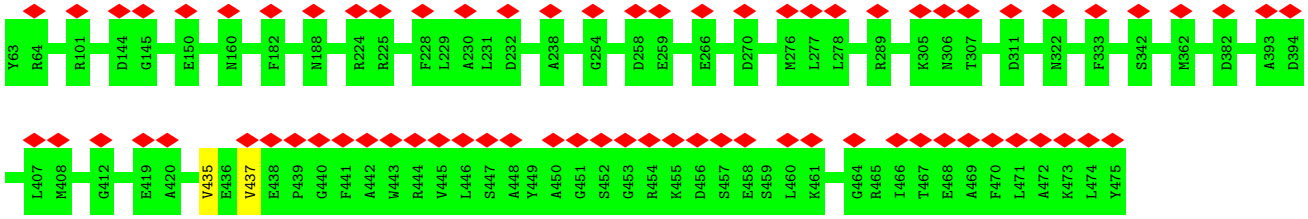




• Molecule 53: mL123

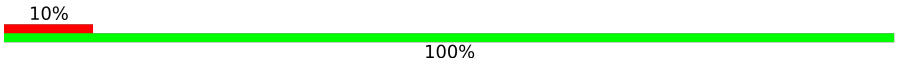
Chain Xd:

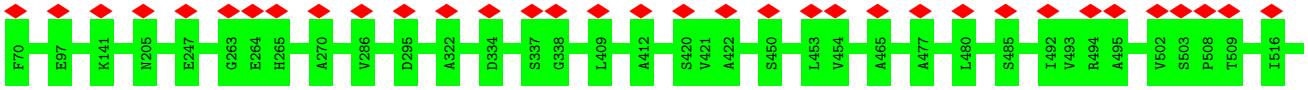


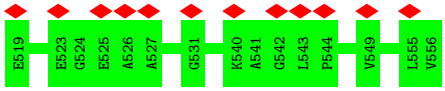


• Molecule 54: mL124

Chain Xe:

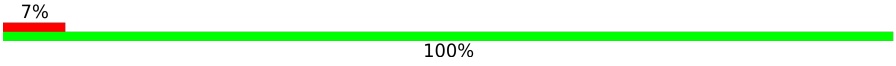


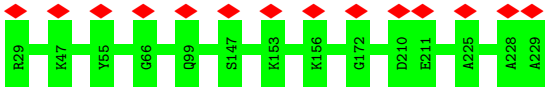




• Molecule 55: mL125

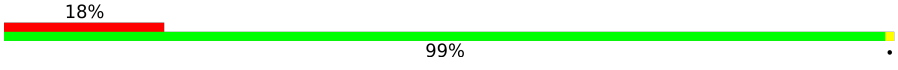
Chain Xf:

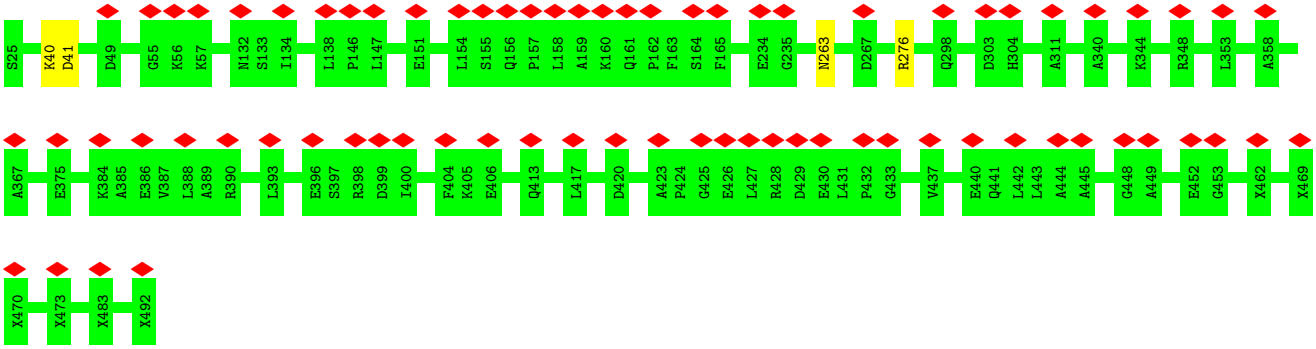




• Molecule 56: mL126

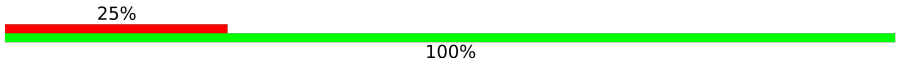
Chain Xg:

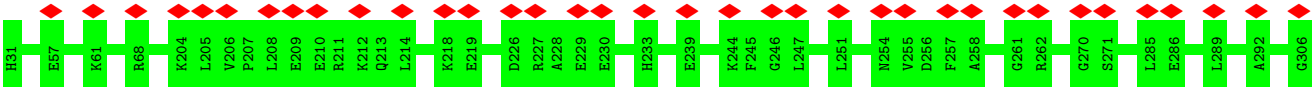




• Molecule 57: mL127

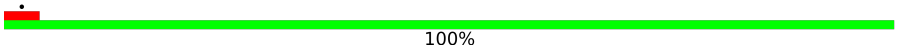
Chain Xh:





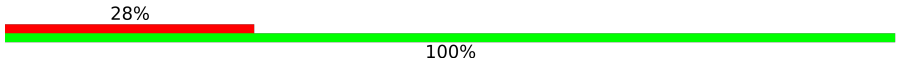
• Molecule 58: mL128

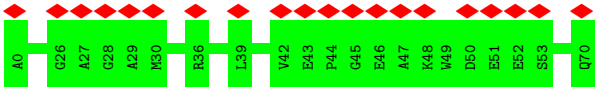
Chain Xi:



• Molecule 59: mL129

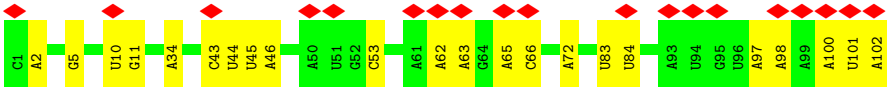
Chain Xj:





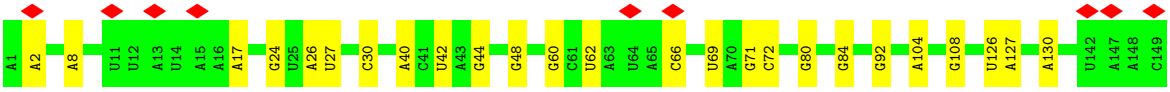
• Molecule 60: mtSSU-1

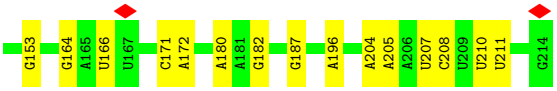
Chain B1:



• Molecule 61: mtSSU-2

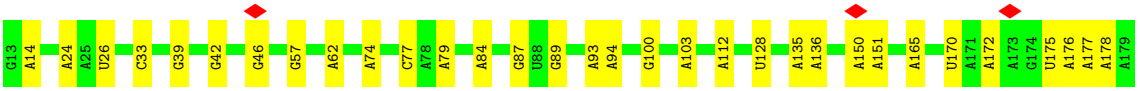
Chain B2:

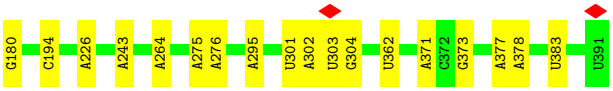




• Molecule 62: mtSSU-3

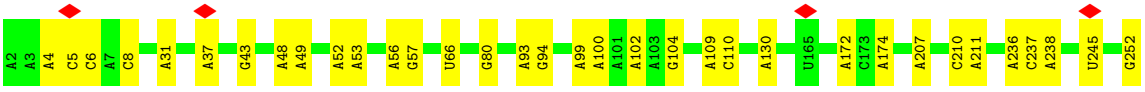
Chain B3:

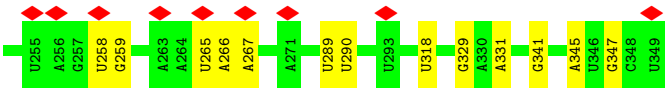




• Molecule 63: mtSSU-4

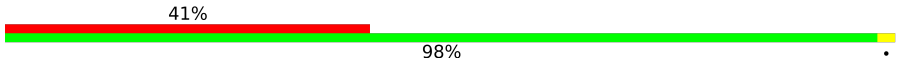
Chain B4:

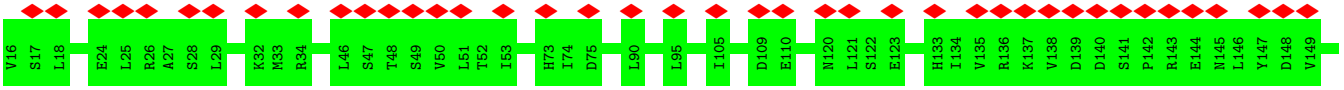


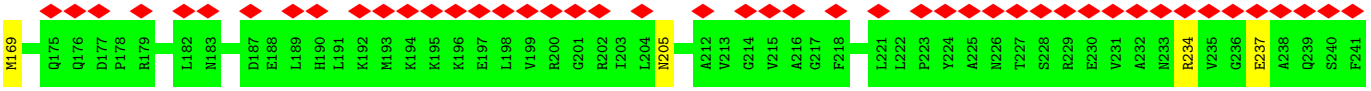


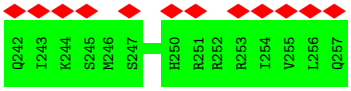
• Molecule 64: bS1m

Chain Ba:



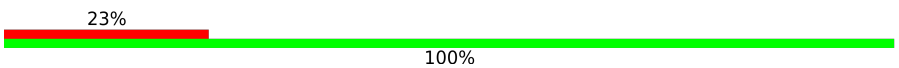


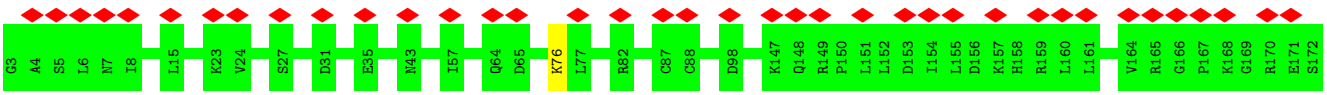


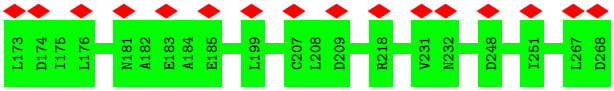


• Molecule 65: uS2m

Chain Bb:

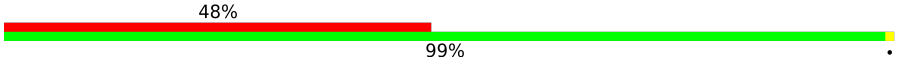


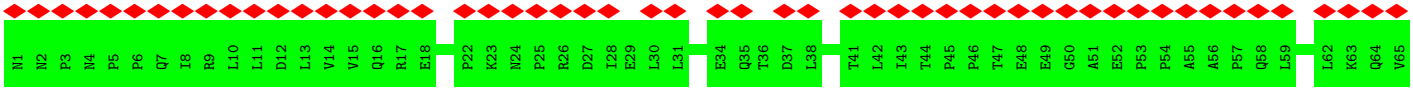


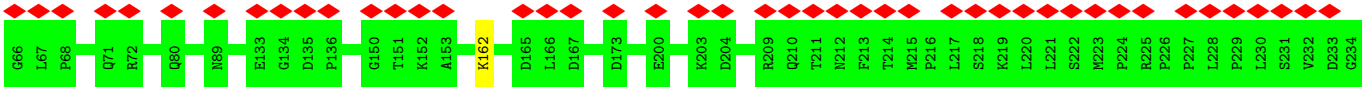


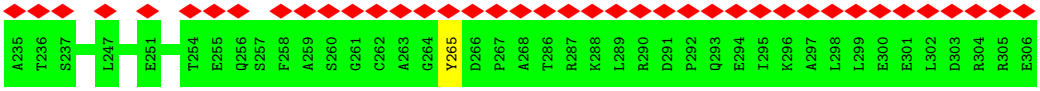
• Molecule 66: uS3m

Chain Bc:



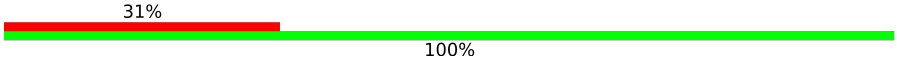


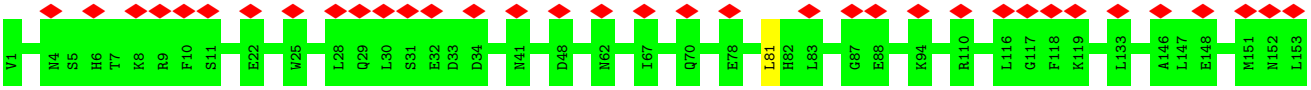


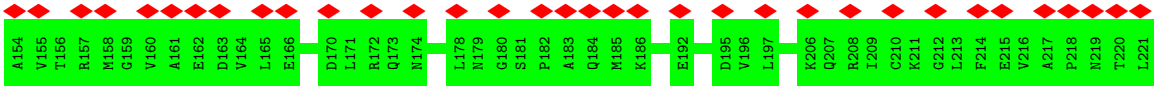


• Molecule 67: uS4m

Chain Bd:

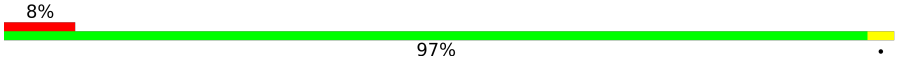


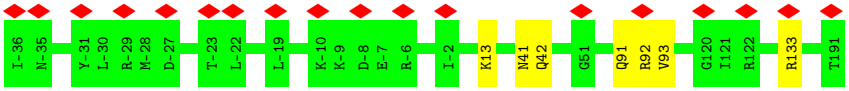




• Molecule 68: uS5m

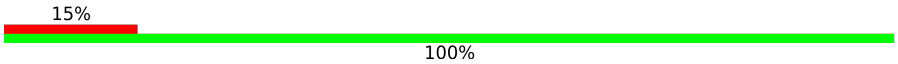
Chain Be:

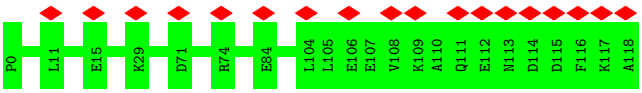




• Molecule 69: uS6m

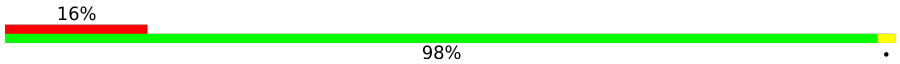
Chain Bf:

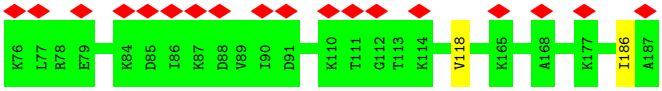




• Molecule 70: uS7m

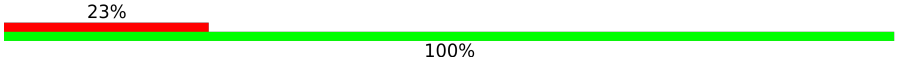
Chain Bg:

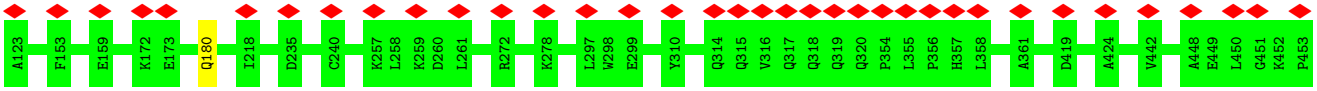


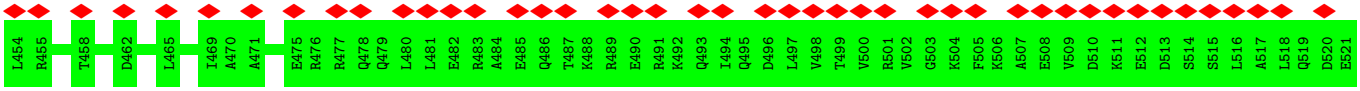


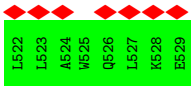
• Molecule 71: uS8m

Chain Bh:



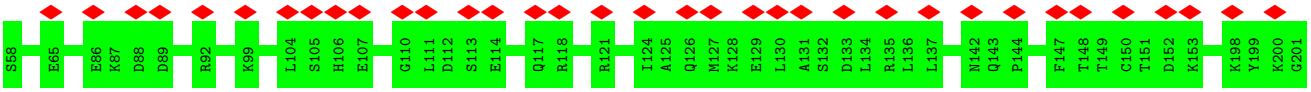


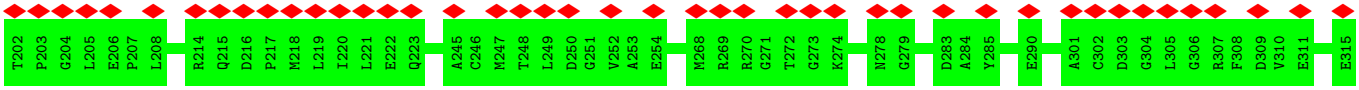


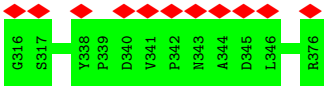


• Molecule 72: uS9m

Chain Bi:

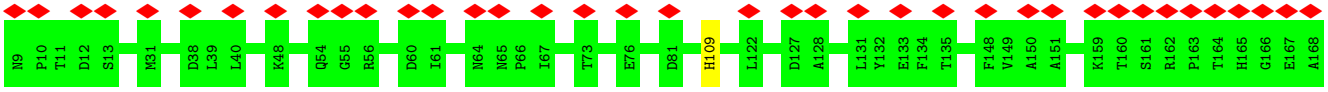


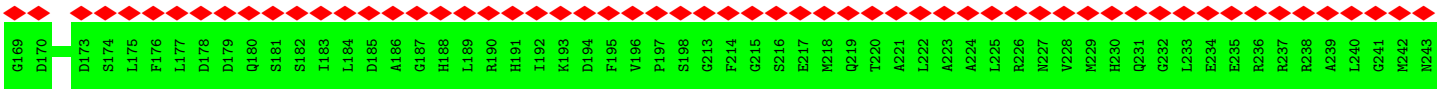


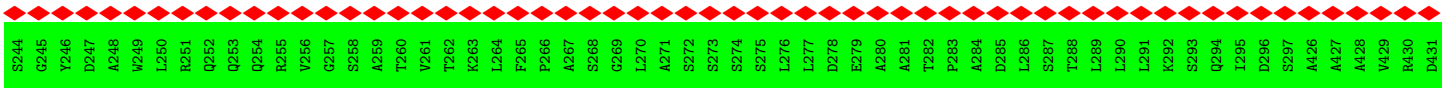


• Molecule 73: uS10m

Chain Bj:

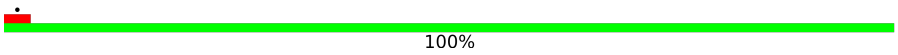


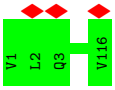




• Molecule 74: uS11m

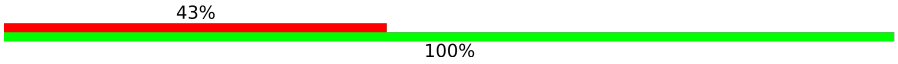
Chain Bk:

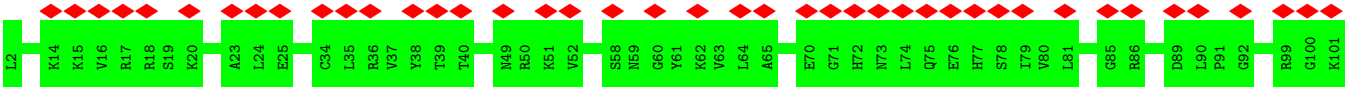


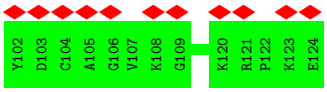


• Molecule 75: uS12m

Chain Bl:

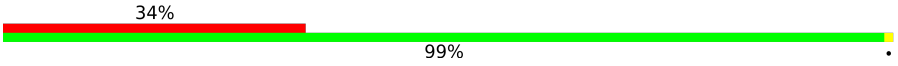


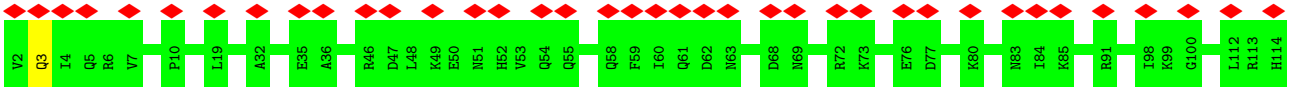




• Molecule 76: uS13m

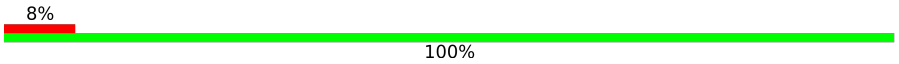
Chain Bm:

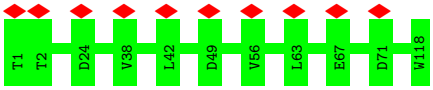




• Molecule 77: uS14m

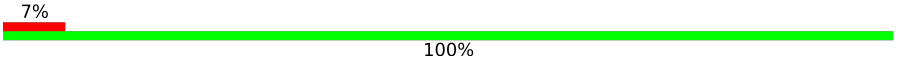
Chain Bn:

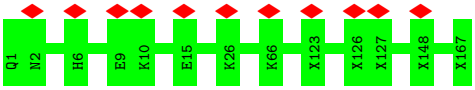




• Molecule 78: uS15m

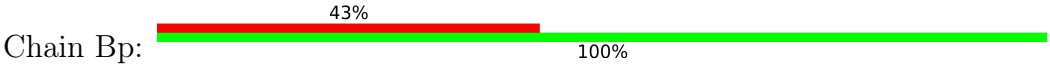
Chain Bo:

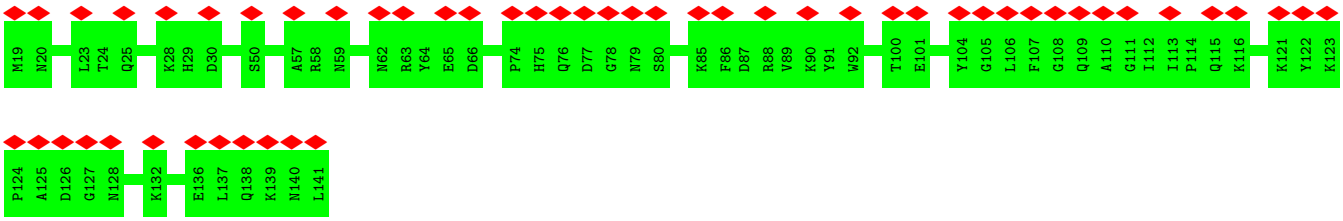




• Molecule 79: bS16m

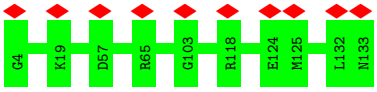
Chain Bp:





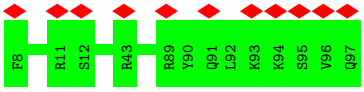
• Molecule 80: uS17m

Chain Bq:



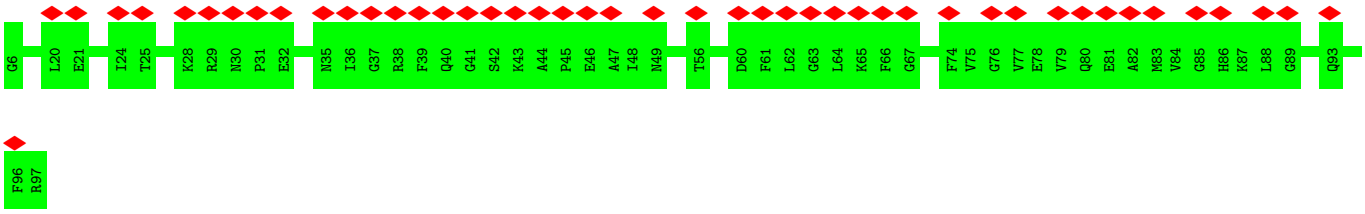
• Molecule 81: bS18m

Chain Br:



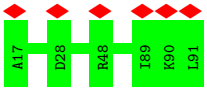
• Molecule 82: bS19m

Chain Bs:



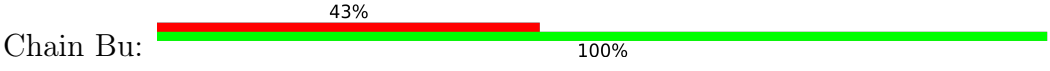
• Molecule 83: bS21m

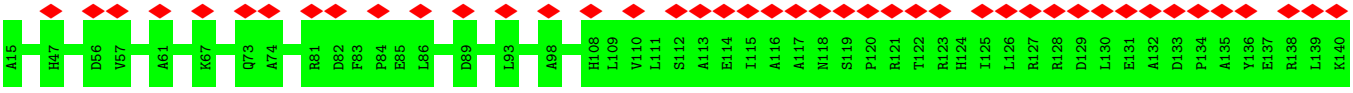
Chain Bt:

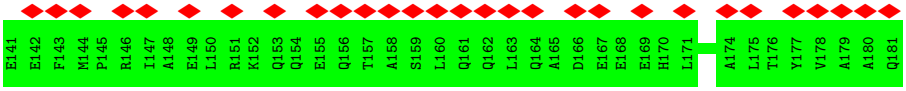


• Molecule 84: mS23

Chain Bu:

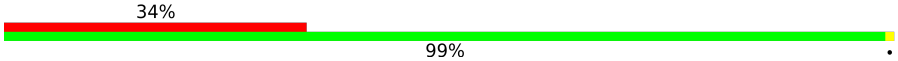


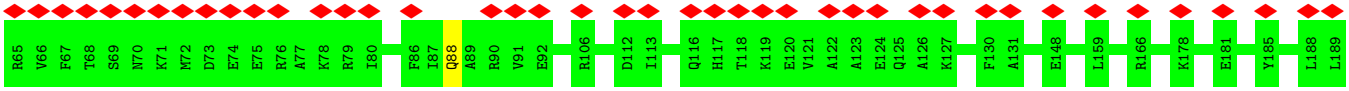


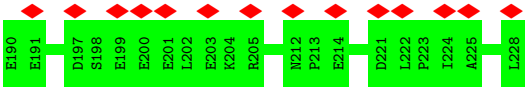


• Molecule 85: mS26

Chain Bv:

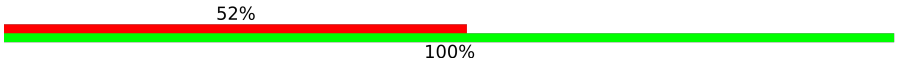


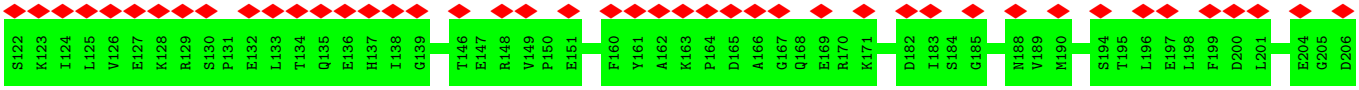


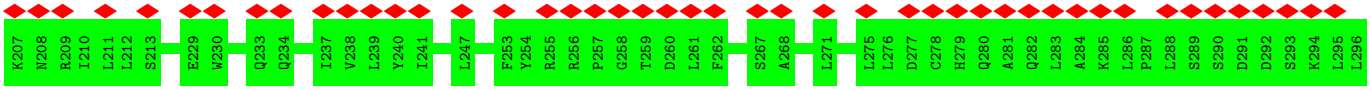


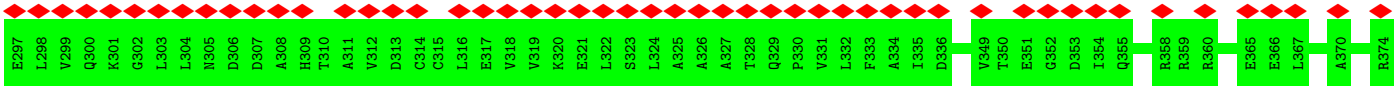
• Molecule 86: mS29

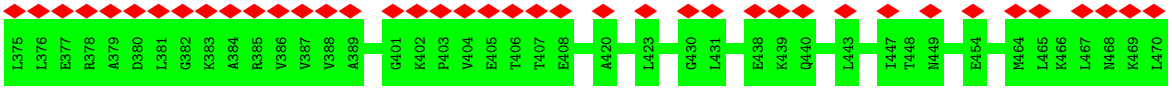
Chain Bw:





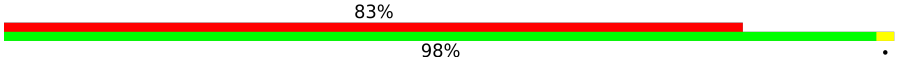


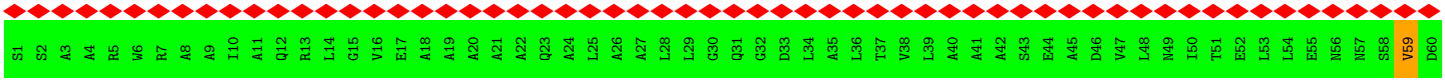


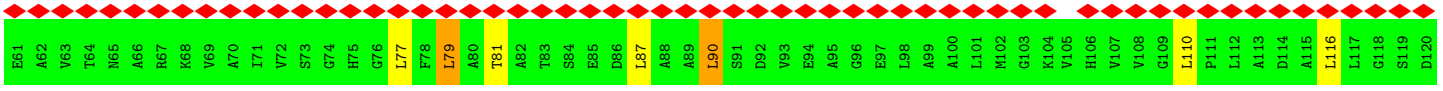


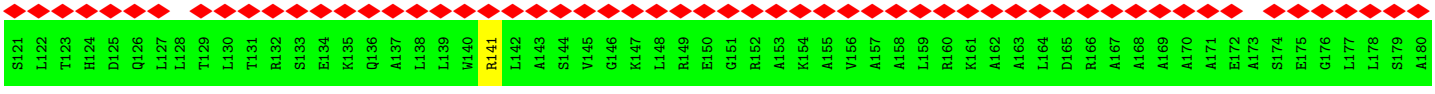
• Molecule 87: mS31

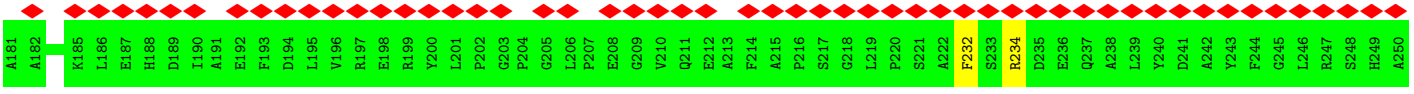
Chain Bx:

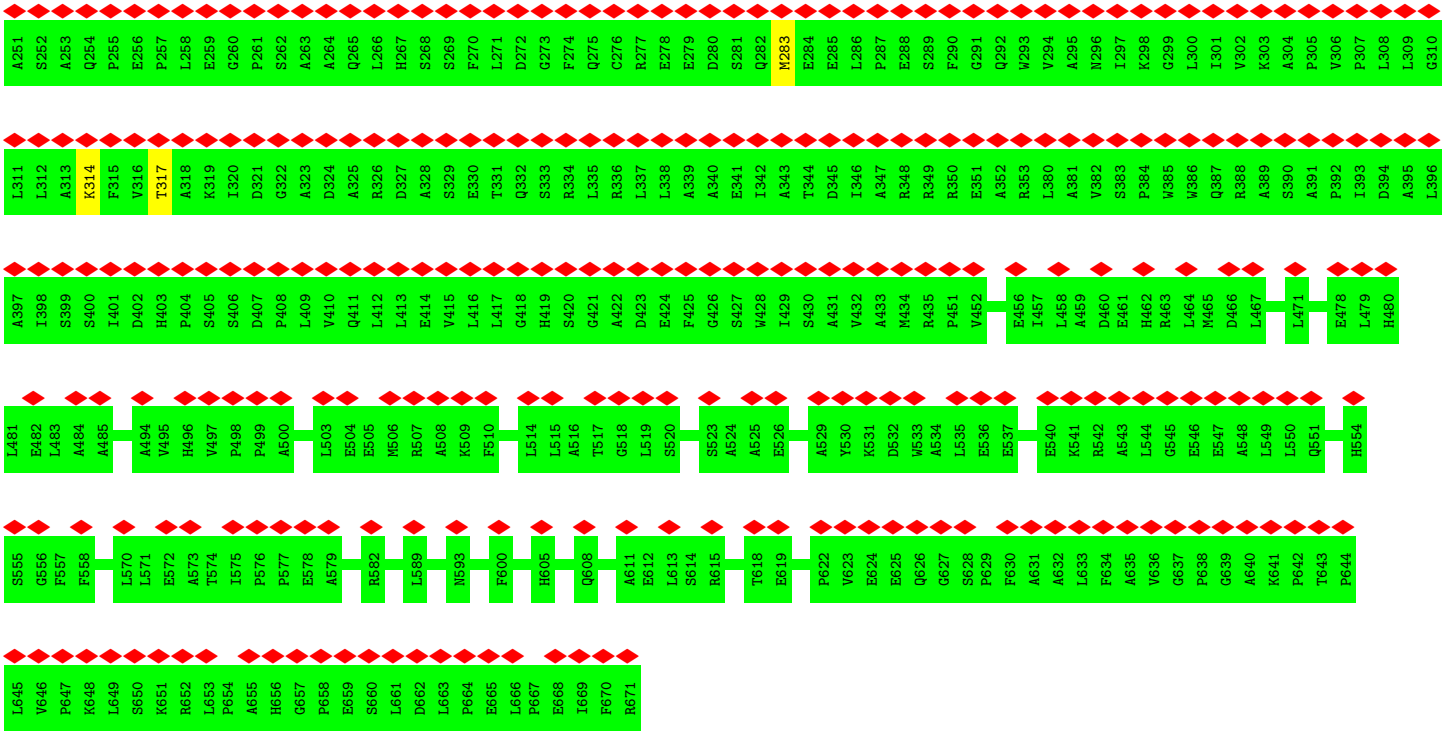




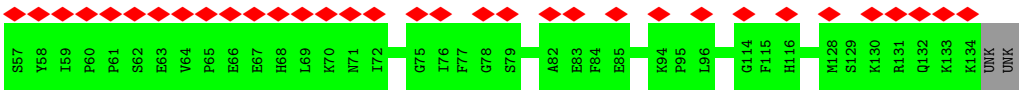




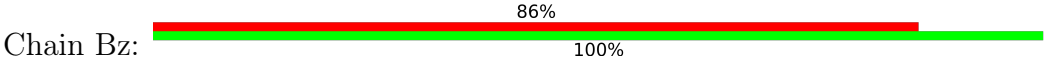


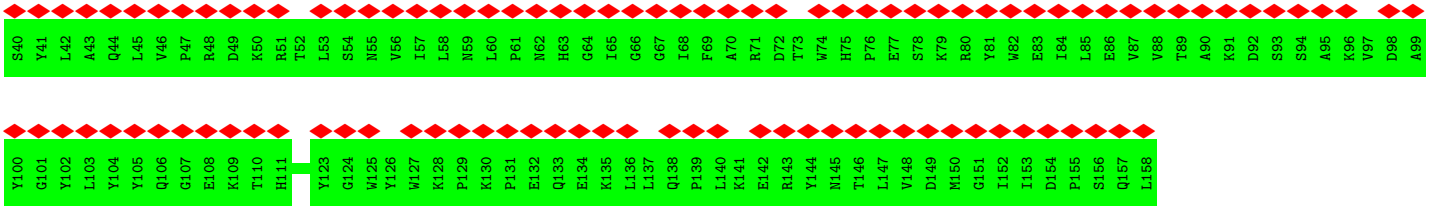


- Molecule 88: mS33

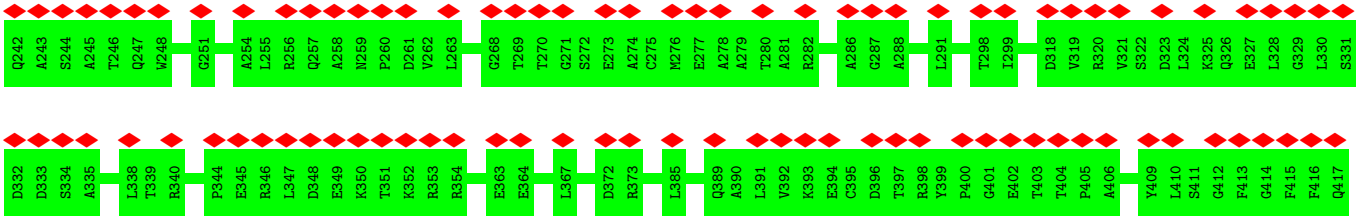


- Molecule 89: mS34



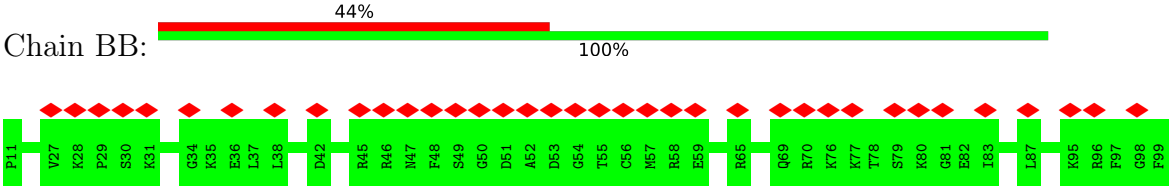


- Molecule 90: mS35



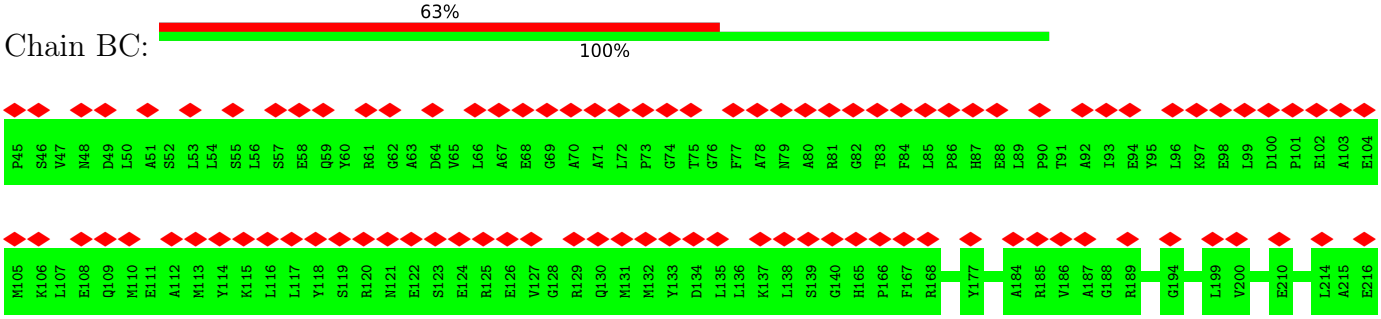
- Molecule 91: mS37

Chain BB:



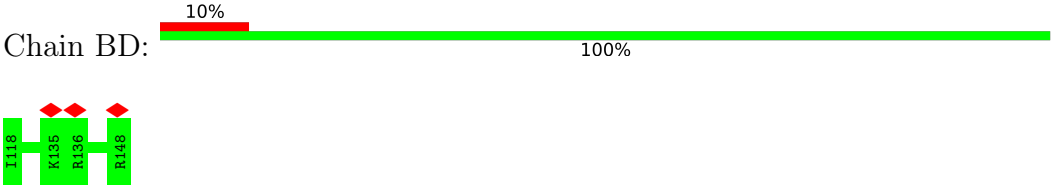
- Molecule 92: mS45

Chain BC:



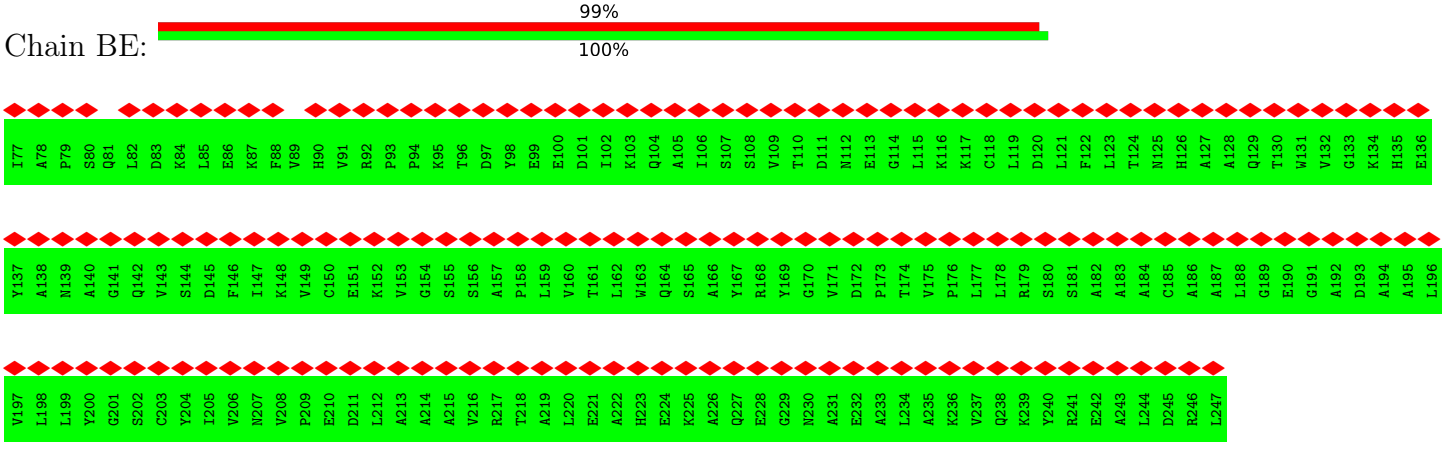
- Molecule 93: mS38

Chain BD:



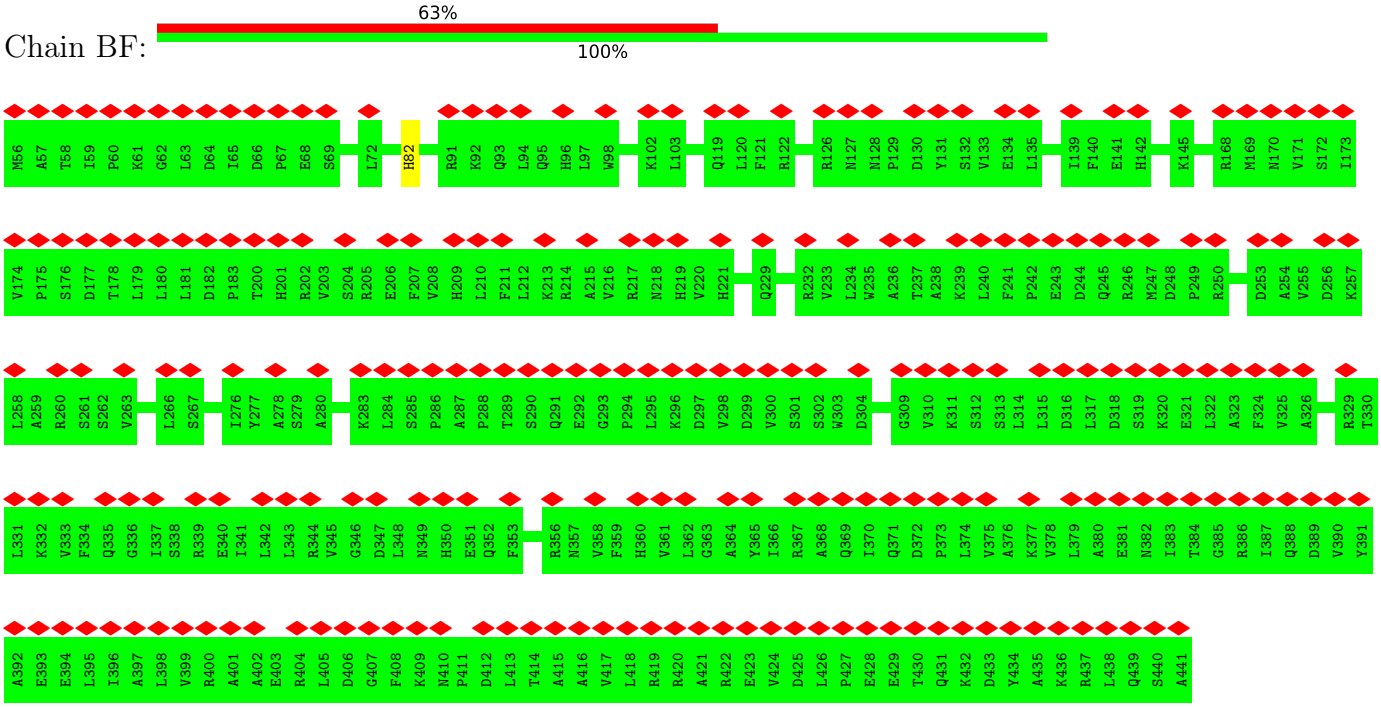
- Molecule 94: mS106

Chain BE:



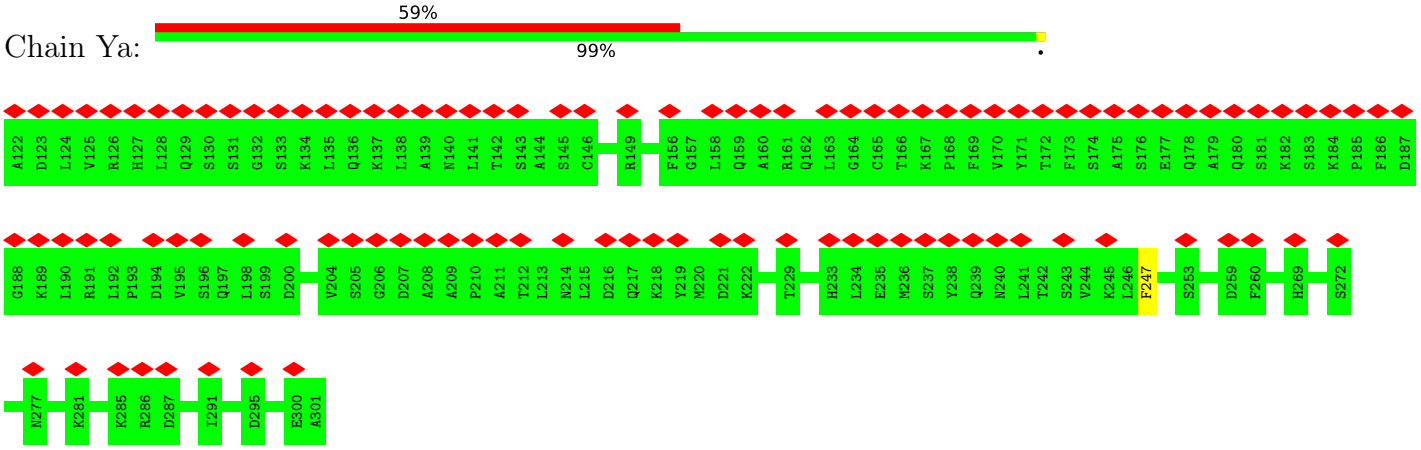
- Molecule 95: mS107

Chain BF:



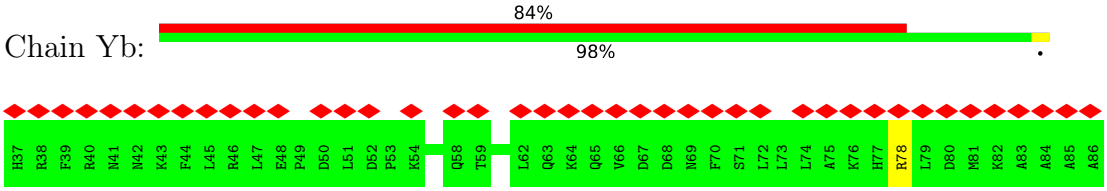
• Molecule 96: uS4m-2

Chain Ya:



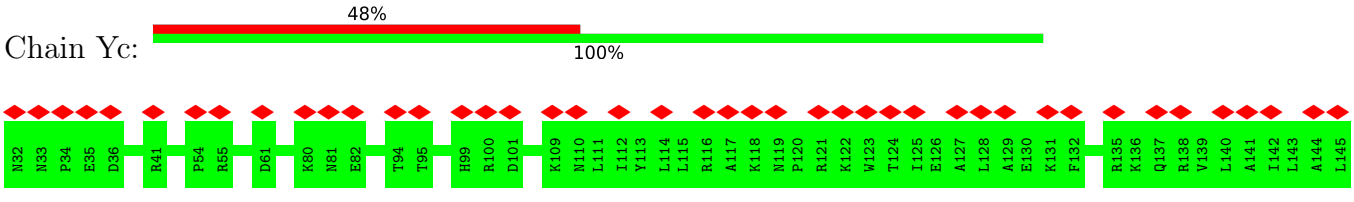
• Molecule 97: mS108

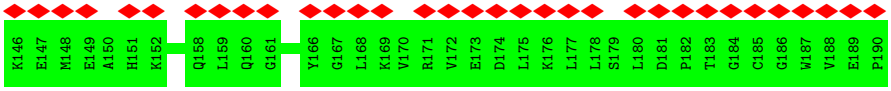
Chain Yb:



• Molecule 98: mS109

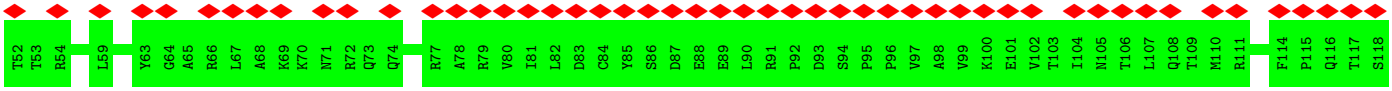
Chain Yc:

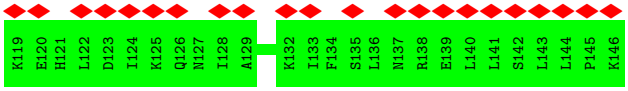




• Molecule 99: mS110

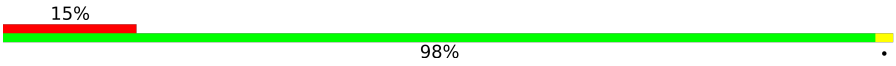
Chain Yd:

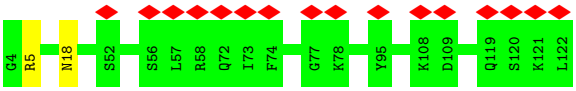




• Molecule 100: uS3m-2

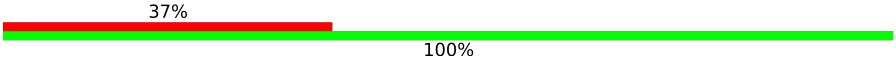
Chain Ye:

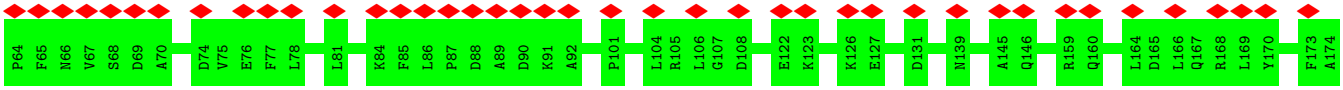


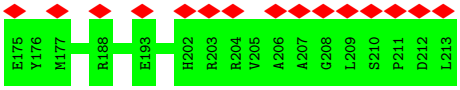


• Molecule 101: mS111

Chain Yf:

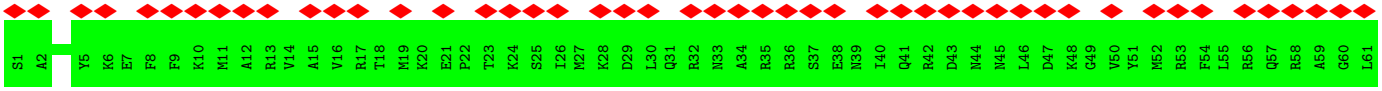


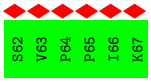




• Molecule 102: mS112

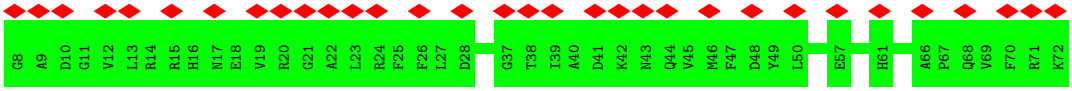
Chain Yg:





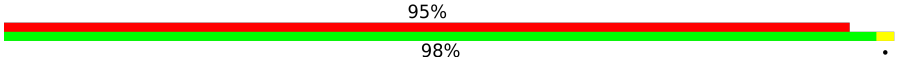
• Molecule 103: mS113

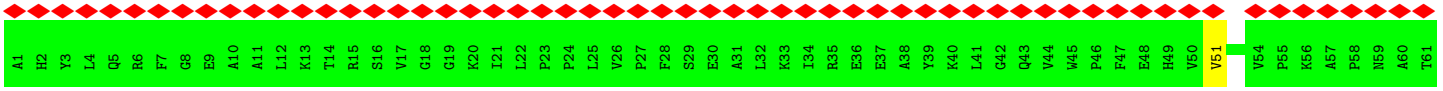
Chain Yh:

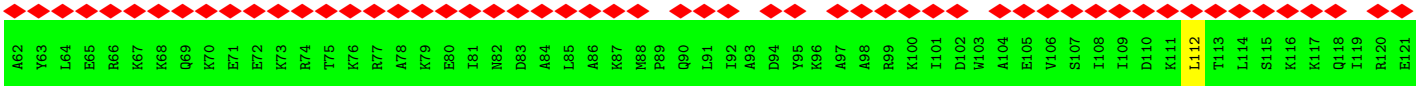


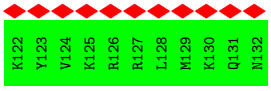
• Molecule 104: mS114

Chain Yi:



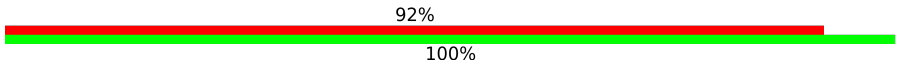


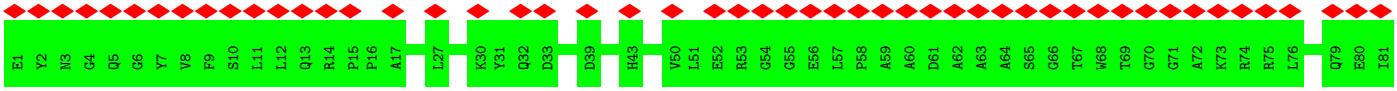


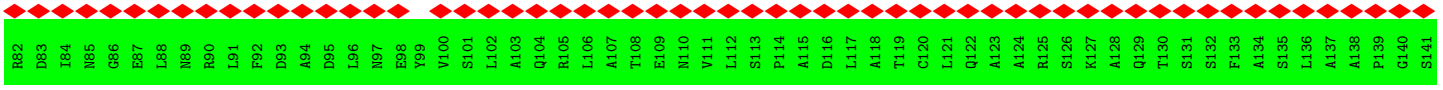


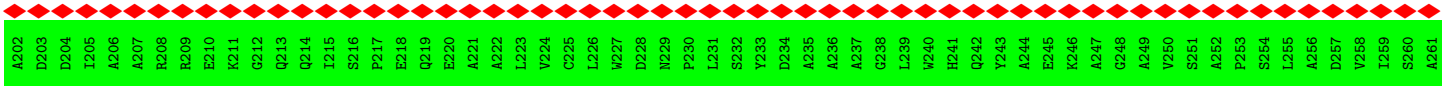
• Molecule 105: mS115

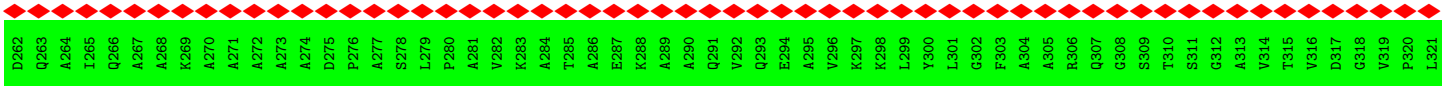
Chain Yj:

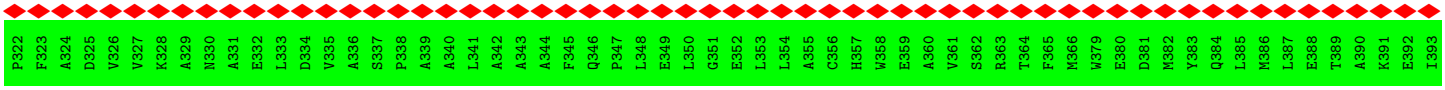


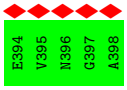






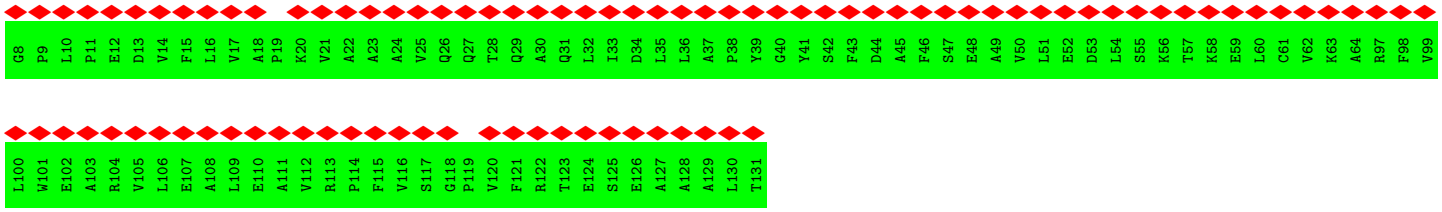






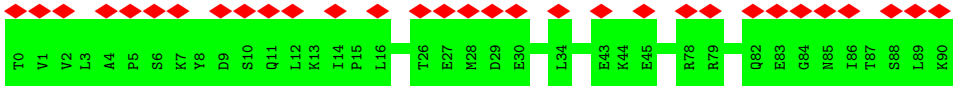
• Molecule 106: mS116

Chain Yk:



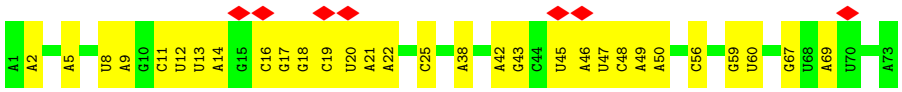
• Molecule 107: uS7m-2

Chain Yl:



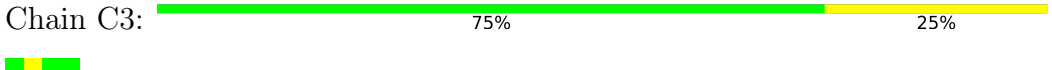
• Molecule 108: P-site tRNA

Chain C1:



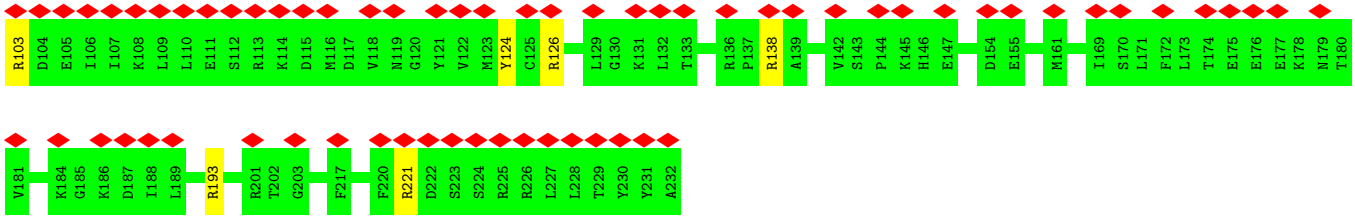
• Molecule 109: mRNA

Chain C3:



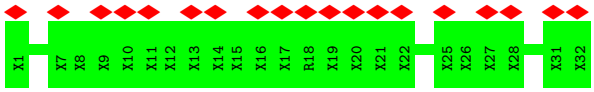
• Molecule 110: mL105

Chain Ub:



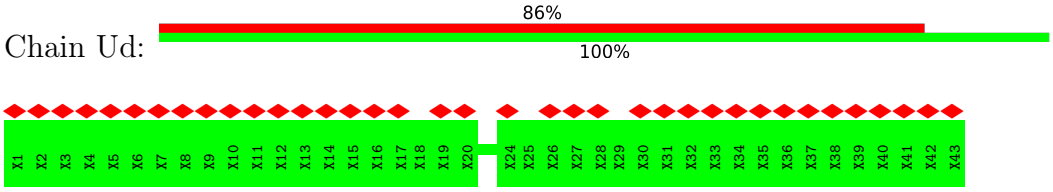
• Molecule 111: Unknown

Chain Ua:



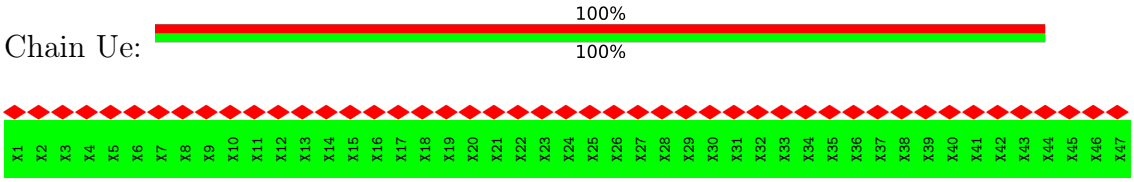
• Molecule 112: Unknown

Chain Ud:



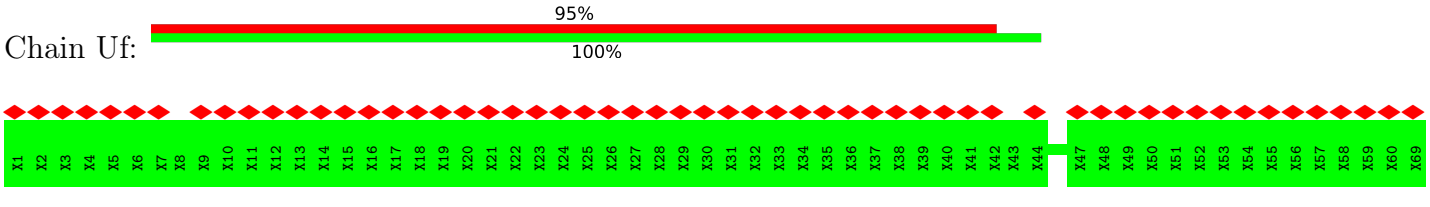
• Molecule 113: Unknown

Chain Ue:



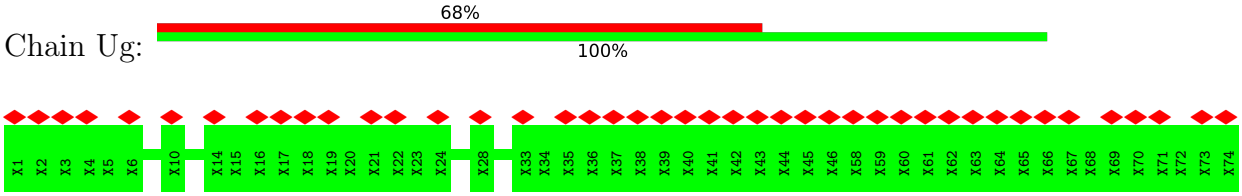
• Molecule 114: Unknown

Chain Uf:



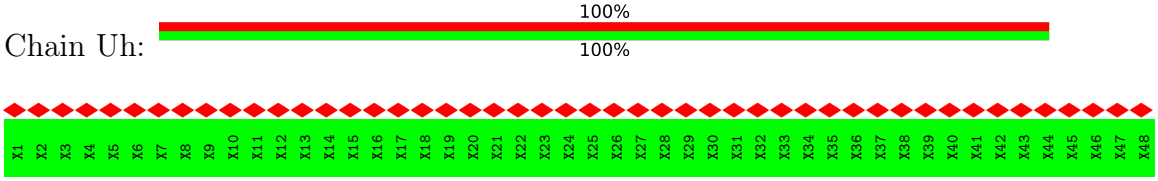
• Molecule 115: Unknown

Chain Ug:



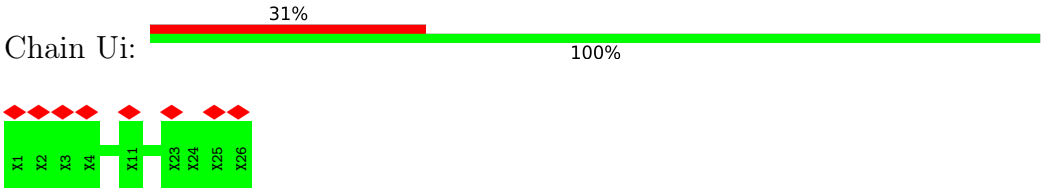
• Molecule 116: Unknown

Chain Uh:



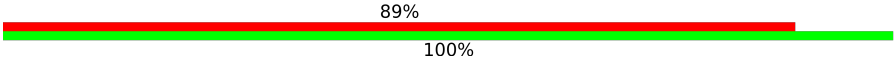
• Molecule 117: Unknown

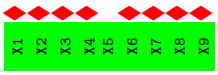
Chain Ui:



• Molecule 118: Unknown

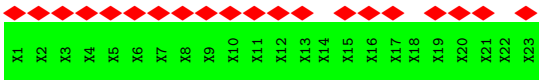
Chain Uj:





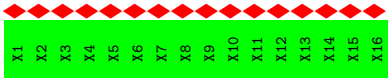
• Molecule 119: Unknown

Chain Uk:



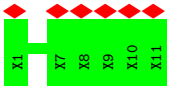
• Molecule 120: Unknown

Chain Ul:



• Molecule 121: Unknown

Chain Um:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59000	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 ($e^-/Å^2$)	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	0.048	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	592.2, 592.2, 592.2	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.846, 0.846, 0.846	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/1764	0.70	1/2749 (0.0%)
5	A5	0.16	0/3239	0.66	0/5036
6	A6	0.22	0/2619	0.67	0/4075
7	A7	0.21	0/12753	0.67	0/19862
8	A8	0.21	0/8336	0.68	1/12985 (0.0%)
9	A9	0.19	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	0.24	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	0.24	0/1643	0.43	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	0.24	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	0.23	0/2041	0.41	0/2755
29	Au	0.24	0/1182	0.41	0/1596
30	Av	0.22	0/1073	0.39	0/1443
31	Aw	0.22	0/1043	0.37	0/1401
32	Ax	0.23	0/1508	0.40	0/2028

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ay	0.24	0/610	0.38	0/827
34	Az	0.39	0/484	0.61	1/652 (0.2%)
35	AA	0.24	0/426	0.40	0/572
36	AB	0.22	0/432	0.45	0/568
37	AC	0.23	0/1217	0.40	0/1639
38	AD	0.23	0/379	0.43	0/500
39	AE	0.23	0/790	0.34	0/1066
40	AF	0.24	0/782	0.39	0/1053
41	AG	0.24	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
47	AM	0.23	0/3345	0.37	0/4532
48	AN	0.24	0/3349	0.37	0/4537
49	AO	0.23	0/2941	0.37	0/4000
50	Xa	0.23	0/1600	0.36	0/2178
51	Xb	0.23	0/1999	0.37	0/2701
52	Xc	0.23	0/509	0.40	0/684
53	Xd	0.23	0/3305	0.37	0/4478
54	Xe	0.23	0/3748	0.38	0/5096
55	Xf	0.24	0/1659	0.38	0/2253
56	Xg	0.24	0/3018	0.37	0/4098
57	Xh	0.24	0/1169	0.39	0/1578
58	Xi	0.23	0/209	0.34	0/273
59	Xj	0.25	0/596	0.39	0/802
60	B1	0.19	0/2419	0.66	0/3765
61	B2	0.19	0/5020	0.68	0/7818
62	B3	0.20	0/9069	0.67	0/14130
63	B4	0.18	0/8046	0.66	0/12527
64	Ba	0.23	0/1967	0.40	0/2662
65	Bb	0.23	0/1920	0.37	0/2615
66	Bc	0.24	0/2340	0.40	0/3182
67	Bd	0.23	0/1825	0.40	0/2459
68	Be	0.24	0/1863	0.41	0/2521
69	Bf	0.24	0/989	0.39	0/1334
70	Bg	0.22	0/898	0.36	0/1205
71	Bh	0.23	0/3109	0.38	0/4215
72	Bi	0.24	0/2317	0.39	0/3119
73	Bj	0.24	0/3243	0.37	0/4384
74	Bk	0.24	0/882	0.45	0/1193
75	Bl	0.23	0/977	0.42	0/1303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Bm	0.22	0/910	0.39	0/1223
77	Bn	0.24	0/995	0.42	0/1336
78	Bo	0.24	0/963	0.38	0/1284
79	Bp	0.23	0/1046	0.41	0/1414
80	Bq	0.23	0/1068	0.39	0/1434
81	Br	0.22	0/754	0.39	0/1009
82	Bs	0.24	0/754	0.40	0/1019
83	Bt	0.23	0/630	0.36	0/840
84	Bu	0.24	0/1395	0.36	0/1878
85	Bv	0.22	0/1372	0.35	0/1835
86	Bw	0.24	0/2804	0.39	0/3791
87	Bx	0.25	0/4813	0.43	7/6545 (0.1%)
88	By	0.25	0/655	0.38	0/883
89	Bz	0.23	0/1030	0.37	0/1400
90	BA	0.23	0/1405	0.39	0/1907
91	BB	0.23	0/673	0.36	0/896
92	BC	0.24	0/2207	0.38	0/2977
93	BD	0.21	0/280	0.36	0/365
94	BE	0.23	0/1328	0.35	0/1805
95	BF	0.23	0/3039	0.36	0/4111
96	Ya	0.23	0/1466	0.38	0/1979
97	Yb	0.34	0/419	0.50	0/562
98	Yc	0.23	0/1328	0.39	0/1799
99	Yd	0.23	0/797	0.39	0/1069
100	Ye	0.25	0/887	0.40	0/1191
101	Yf	0.23	0/1276	0.37	0/1735
102	Yg	0.24	0/560	0.37	0/744
103	Yh	0.23	0/543	0.36	0/730
104	Yi	0.24	0/1096	0.38	0/1470
105	Yj	0.23	0/2911	0.35	0/3966
106	Yk	0.26	0/721	0.37	0/982
107	Yl	0.24	0/680	0.39	0/911
108	C1	0.20	0/1723	0.75	0/2681
109	C3	0.16	0/97	0.60	0/149
110	Ub	1.00	0/1110	0.94	7/1490 (0.5%)
111	Ua	0.25	0/10	0.38	0/11
All	All	0.24	0/205350	0.51	17/291087 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
110	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
110	Ub	126	ARG	NE-CZ-NH2	-7.62	116.49	120.30
87	Bx	59	VAL	CG1-CB-CG2	7.35	122.66	110.90
110	Ub	138	ARG	NE-CZ-NH2	-6.96	116.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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%)	293 (96%)	11 (4%)	0	100	100
11	Ab	304/306 (99%)	298 (98%)	6 (2%)	0	100	100
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%)	178 (98%)	4 (2%)	0	100	100
17	Ai	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
18	Aj	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
19	Ak	164/166 (99%)	161 (98%)	3 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	An	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
23	Ao	115/117 (98%)	115 (100%)	0	0	100	100
24	Ap	198/200 (99%)	197 (100%)	1 (0%)	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%)	251 (100%)	0	0	100	100
29	Au	140/142 (99%)	140 (100%)	0	0	100	100
30	Av	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
31	Aw	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
32	Ax	174/176 (99%)	174 (100%)	0	0	100	100
33	Ay	70/72 (97%)	70 (100%)	0	0	100	100
34	Az	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
35	AA	48/50 (96%)	48 (100%)	0	0	100	100
36	AB	48/50 (96%)	48 (100%)	0	0	100	100
37	AC	137/139 (99%)	136 (99%)	1 (1%)	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%)	117 (98%)	2 (2%)	0	100	100
42	AH	172/176 (98%)	167 (97%)	4 (2%)	1 (1%)	25	59
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	390/394 (99%)	385 (99%)	5 (1%)	0	100	100
47	AM	417/419 (100%)	414 (99%)	3 (1%)	0	100	100
48	AN	418/420 (100%)	415 (99%)	3 (1%)	0	100	100
49	AO	371/377 (98%)	366 (99%)	5 (1%)	0	100	100
50	Xa	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
51	Xb	242/244 (99%)	239 (99%)	3 (1%)	0	100	100
52	Xc	55/57 (96%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	Xd	411/413 (100%)	400 (97%)	11 (3%)	0	100	100
54	Xe	479/483 (99%)	476 (99%)	3 (1%)	0	100	100
55	Xf	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
56	Xg	379/410 (92%)	377 (100%)	2 (0%)	0	100	100
57	Xh	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
58	Xi	22/24 (92%)	22 (100%)	0	0	100	100
59	Xj	69/71 (97%)	69 (100%)	0	0	100	100
64	Ba	240/242 (99%)	236 (98%)	4 (2%)	0	100	100
65	Bb	232/236 (98%)	228 (98%)	4 (2%)	0	100	100
66	Bc	285/289 (99%)	284 (100%)	1 (0%)	0	100	100
67	Bd	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
68	Be	226/228 (99%)	223 (99%)	3 (1%)	0	100	100
69	Bf	117/119 (98%)	117 (100%)	0	0	100	100
70	Bg	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
71	Bh	370/374 (99%)	367 (99%)	3 (1%)	0	100	100
72	Bi	276/282 (98%)	271 (98%)	5 (2%)	0	100	100
73	Bj	395/401 (98%)	388 (98%)	7 (2%)	0	100	100
74	Bk	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
75	Bl	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
76	Bm	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
77	Bn	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
78	Bo	113/167 (68%)	111 (98%)	2 (2%)	0	100	100
79	Bp	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
80	Bq	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
81	Br	88/90 (98%)	88 (100%)	0	0	100	100
82	Bs	90/92 (98%)	90 (100%)	0	0	100	100
83	Bt	73/75 (97%)	73 (100%)	0	0	100	100
84	Bu	165/167 (99%)	165 (100%)	0	0	100	100
85	Bv	162/164 (99%)	162 (100%)	0	0	100	100
86	Bw	347/349 (99%)	342 (99%)	5 (1%)	0	100	100
87	Bx	613/621 (99%)	604 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
88	By	76/80 (95%)	75 (99%)	1 (1%)	0	100	100
89	Bz	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
90	BA	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
91	BB	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
92	BC	266/270 (98%)	264 (99%)	2 (1%)	0	100	100
93	BD	29/31 (94%)	29 (100%)	0	0	100	100
94	BE	169/171 (99%)	169 (100%)	0	0	100	100
95	BF	366/370 (99%)	360 (98%)	6 (2%)	0	100	100
96	Ya	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
97	Yb	48/50 (96%)	48 (100%)	0	0	100	100
98	Yc	157/159 (99%)	156 (99%)	1 (1%)	0	100	100
99	Yd	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
100	Ye	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
101	Yf	148/150 (99%)	147 (99%)	1 (1%)	0	100	100
102	Yg	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
103	Yh	63/65 (97%)	63 (100%)	0	0	100	100
104	Yi	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
105	Yj	382/386 (99%)	376 (98%)	6 (2%)	0	100	100
106	Yk	88/92 (96%)	88 (100%)	0	0	100	100
107	Yl	80/84 (95%)	80 (100%)	0	0	100	100
110	Ub	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
111	Ua	1/32 (3%)	1 (100%)	0	0	100	100
All	All	16831/17200 (98%)	16637 (99%)	193 (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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	Aa	248/248 (100%)	248 (100%)	0	100 100
11	Ab	261/261 (100%)	260 (100%)	1 (0%)	91 96
12	Ac	259/259 (100%)	259 (100%)	0	100 100
13	Ad	176/176 (100%)	175 (99%)	1 (1%)	86 94
14	Ae	211/211 (100%)	211 (100%)	0	100 100
15	Af	47/47 (100%)	46 (98%)	1 (2%)	53 79
16	Ah	161/161 (100%)	159 (99%)	2 (1%)	71 88
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%)	84 93
21	Am	102/102 (100%)	102 (100%)	0	100 100
22	An	157/157 (100%)	157 (100%)	0	100 100
23	Ao	101/101 (100%)	101 (100%)	0	100 100
24	Ap	177/177 (100%)	176 (99%)	1 (1%)	86 94
25	Aq	161/161 (100%)	160 (99%)	1 (1%)	86 94
26	Ar	142/142 (100%)	141 (99%)	1 (1%)	84 93
27	As	105/105 (100%)	105 (100%)	0	100 100
28	At	223/223 (100%)	223 (100%)	0	100 100
29	Au	121/121 (100%)	120 (99%)	1 (1%)	81 92
30	Av	120/120 (100%)	120 (100%)	0	100 100
31	Aw	110/110 (100%)	108 (98%)	2 (2%)	59 82
32	Ax	161/161 (100%)	161 (100%)	0	100 100
33	Ay	66/66 (100%)	66 (100%)	0	100 100
34	Az	51/51 (100%)	48 (94%)	3 (6%)	19 50
35	AA	47/47 (100%)	47 (100%)	0	100 100
36	AB	45/45 (100%)	45 (100%)	0	100 100
37	AC	125/125 (100%)	123 (98%)	2 (2%)	62 84
38	AD	42/42 (100%)	42 (100%)	0	100 100
39	AE	84/84 (100%)	84 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	AF	82/82 (100%)	82 (100%)	0	100	100
41	AG	109/109 (100%)	109 (100%)	0	100	100
42	AH	155/155 (100%)	155 (100%)	0	100	100
43	AI	57/57 (100%)	57 (100%)	0	100	100
44	AJ	104/104 (100%)	104 (100%)	0	100	100
45	AK	117/117 (100%)	117 (100%)	0	100	100
46	AL	332/332 (100%)	329 (99%)	3 (1%)	78	91
47	AM	351/351 (100%)	350 (100%)	1 (0%)	92	96
48	AN	351/351 (100%)	350 (100%)	1 (0%)	92	96
49	AO	293/293 (100%)	291 (99%)	2 (1%)	84	93
50	Xa	173/173 (100%)	172 (99%)	1 (1%)	86	94
51	Xb	217/217 (100%)	217 (100%)	0	100	100
52	Xc	54/54 (100%)	54 (100%)	0	100	100
53	Xd	339/339 (100%)	337 (99%)	2 (1%)	86	94
54	Xe	385/385 (100%)	385 (100%)	0	100	100
55	Xf	172/172 (100%)	172 (100%)	0	100	100
56	Xg	312/312 (100%)	308 (99%)	4 (1%)	69	87
57	Xh	127/127 (100%)	127 (100%)	0	100	100
58	Xi	21/21 (100%)	21 (100%)	0	100	100
59	Xj	62/62 (100%)	62 (100%)	0	100	100
64	Ba	220/220 (100%)	216 (98%)	4 (2%)	59	82
65	Bb	214/214 (100%)	213 (100%)	1 (0%)	88	94
66	Bc	247/247 (100%)	245 (99%)	2 (1%)	81	92
67	Bd	196/196 (100%)	195 (100%)	1 (0%)	88	94
68	Be	196/196 (100%)	189 (96%)	7 (4%)	35	67
69	Bf	103/103 (100%)	103 (100%)	0	100	100
70	Bg	97/97 (100%)	95 (98%)	2 (2%)	53	79
71	Bh	327/327 (100%)	326 (100%)	1 (0%)	92	96
72	Bi	242/242 (100%)	242 (100%)	0	100	100
73	Bj	334/334 (100%)	333 (100%)	1 (0%)	92	96
74	Bk	95/95 (100%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	Bl	104/104 (100%)	104 (100%)	0	100	100
76	Bm	100/100 (100%)	99 (99%)	1 (1%)	76	90
77	Bn	106/106 (100%)	106 (100%)	0	100	100
78	Bo	104/104 (100%)	104 (100%)	0	100	100
79	Bp	107/107 (100%)	107 (100%)	0	100	100
80	Bq	113/113 (100%)	113 (100%)	0	100	100
81	Br	81/81 (100%)	81 (100%)	0	100	100
82	Bs	77/77 (100%)	77 (100%)	0	100	100
83	Bt	66/66 (100%)	66 (100%)	0	100	100
84	Bu	142/142 (100%)	142 (100%)	0	100	100
85	Bv	140/140 (100%)	139 (99%)	1 (1%)	84	93
86	Bw	298/298 (100%)	298 (100%)	0	100	100
87	Bx	481/481 (100%)	469 (98%)	12 (2%)	47	75
88	By	69/69 (100%)	69 (100%)	0	100	100
89	Bz	107/107 (100%)	107 (100%)	0	100	100
90	BA	143/143 (100%)	143 (100%)	0	100	100
91	BB	72/72 (100%)	72 (100%)	0	100	100
92	BC	225/225 (100%)	224 (100%)	1 (0%)	91	96
93	BD	30/30 (100%)	30 (100%)	0	100	100
94	BE	136/136 (100%)	136 (100%)	0	100	100
95	BF	326/326 (100%)	325 (100%)	1 (0%)	92	96
96	Ya	161/161 (100%)	160 (99%)	1 (1%)	86	94
97	Yb	44/44 (100%)	43 (98%)	1 (2%)	50	77
98	Yc	140/140 (100%)	140 (100%)	0	100	100
99	Yd	88/88 (100%)	88 (100%)	0	100	100
100	Ye	91/91 (100%)	89 (98%)	2 (2%)	52	78
101	Yf	132/132 (100%)	132 (100%)	0	100	100
102	Yg	60/60 (100%)	60 (100%)	0	100	100
103	Yh	54/54 (100%)	54 (100%)	0	100	100
104	Yi	112/112 (100%)	110 (98%)	2 (2%)	59	82
105	Yj	278/278 (100%)	278 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
106	Yk	74/74 (100%)	74 (100%)	0	100 100
107	Yl	76/76 (100%)	76 (100%)	0	100 100
110	Ub	122/122 (100%)	122 (100%)	0	100 100
111	Ua	1/1 (100%)	1 (100%)	0	100 100
All	All	14618/14618 (100%)	14546 (100%)	72 (0%)	89 94

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
87	Bx	116	LEU
104	Yi	112	LEU
87	Bx	232	PHE
95	BF	82	HIS
50	Xa	107	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
20	Al	128	GLN
87	Bx	75	HIS
100	Ye	82	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	108/109 (99%)	25 (23%)	0
108	C1	72/73 (98%)	29 (40%)	2 (2%)
109	C3	3/4 (75%)	1 (33%)	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
6	A6	106/109 (97%)	21 (19%)	0
60	B1	101/102 (99%)	22 (21%)	0
61	B2	208/210 (99%)	40 (19%)	0
62	B3	378/379 (99%)	49 (12%)	2 (0%)
63	B4	334/337 (99%)	47 (14%)	0
7	A7	532/534 (99%)	80 (15%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A8	349/350 (99%)	58 (16%)	0
9	A9	67/69 (97%)	15 (22%)	0
All	All	2747/2773 (99%)	473 (17%)	8 (0%)

5 of 473 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

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
108	C1	20	U
108	C1	16	C
62	B3	177	A
7	A7	192	A
62	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 145 ligands modelled in this entry, 144 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
125	ATP	Bw	502	122	26,33,33	0.89	1 (3%)	31,52,52	1.53	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
125	ATP	Bw	502	122	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
125	Bw	502	ATP	C5-C4	2.20	1.46	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
125	Bw	502	ATP	PA-O3A-PB	-3.80	119.80	132.83
125	Bw	502	ATP	N3-C2-N1	-3.60	123.04	128.68
125	Bw	502	ATP	PB-O3B-PG	-3.36	121.29	132.83
125	Bw	502	ATP	C3'-C2'-C1'	2.43	104.64	100.98
125	Bw	502	ATP	C4-C5-N7	-2.07	107.24	109.40

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
125	Bw	502	ATP	C5'-O5'-PA-O1A
125	Bw	502	ATP	C5'-O5'-PA-O3A
125	Bw	502	ATP	O4'-C4'-C5'-O5'
125	Bw	502	ATP	C3'-C4'-C5'-O5'
125	Bw	502	ATP	PA-O3A-PB-O1B

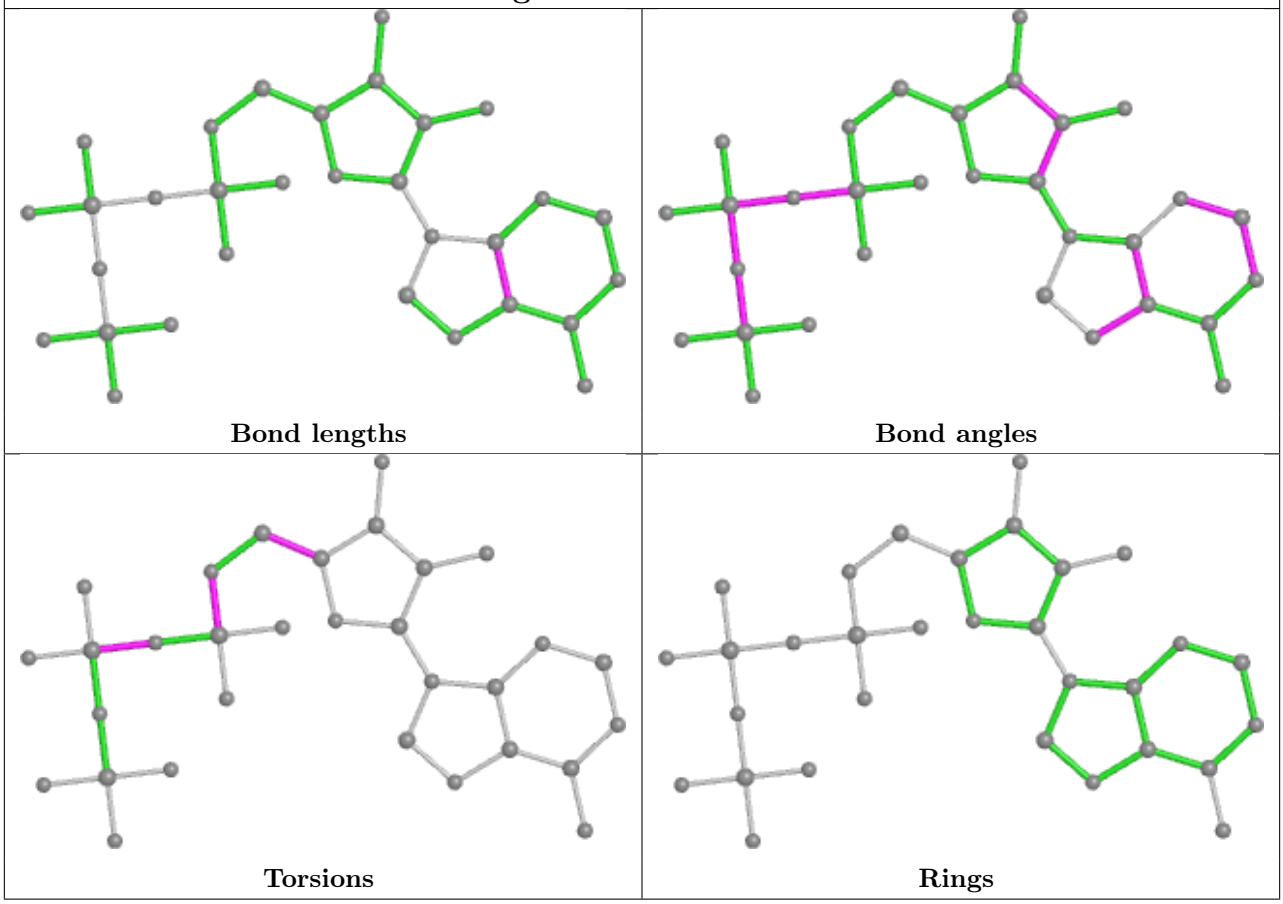
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is

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

Ligand ATP Bw 502



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
56	Xg	4

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Mol	Chain	Number of breaks
5	A5	3
87	Bx	3
27	As	2
72	Bi	2
6	A6	2
73	Bj	2
49	AO	2
63	B4	2
14	Ae	2
42	AH	1
66	Bc	1
57	Xh	1
71	Bh	1
65	Bb	1
92	BC	1
105	Yj	1
9	A9	1
107	Yl	1
26	Ar	1
39	AE	1
91	BB	1
61	B2	1
115	Ug	1
3	A3	1
114	Uf	1
34	Az	1
95	BF	1
100	Ye	1
7	A7	1
16	Ah	1
106	Yk	1
46	AL	1
44	AJ	1
54	Xe	1

The worst 5 of 49 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Xg	165:PHE	C	206:LYS	N	58.01
1	As	92:PRO	C	151:GLY	N	44.12
1	Bi	223:GLN	C	243:ALA	N	41.07
1	A6	114:A	O3’	127:A	P	35.38
1	Bj	297:SER	C	426:ALA	N	32.85

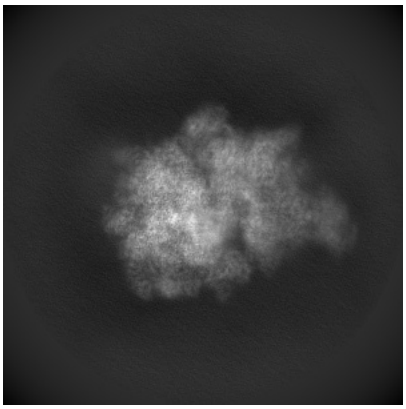
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15576. These allow visual inspection of the internal detail of the map and identification of artifacts.

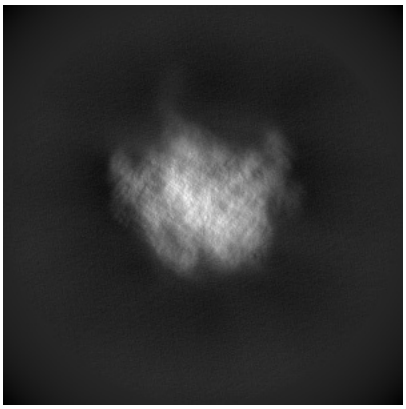
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

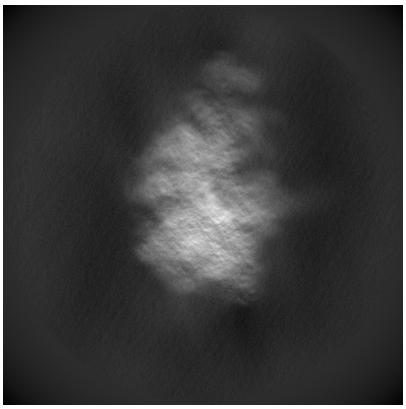
6.1.1 Primary map



X

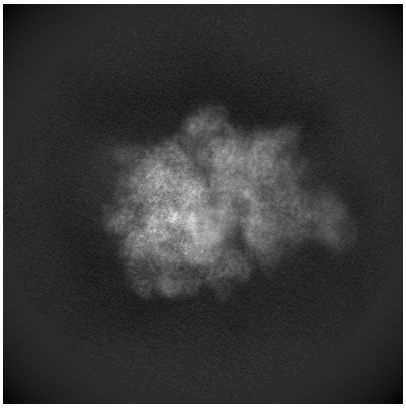


Y

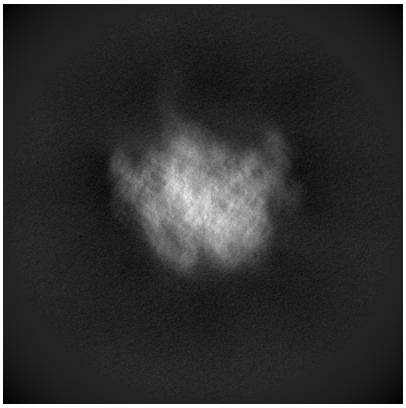


Z

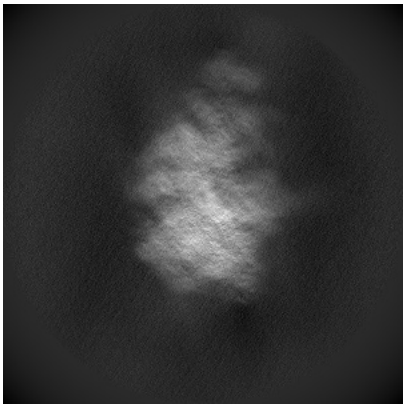
6.1.2 Raw map



X



Y

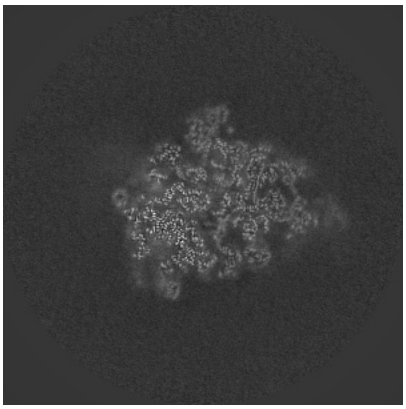


Z

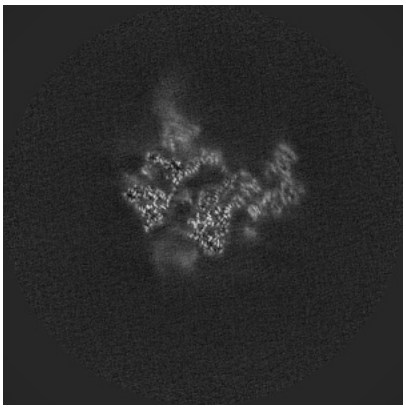
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

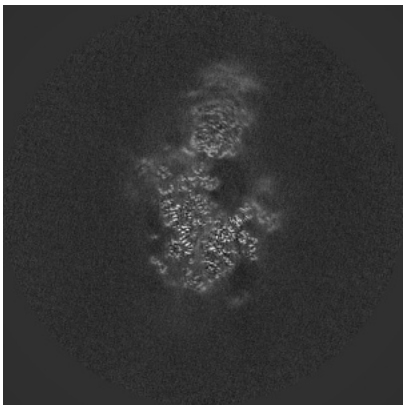
6.2.1 Primary map



X Index: 350

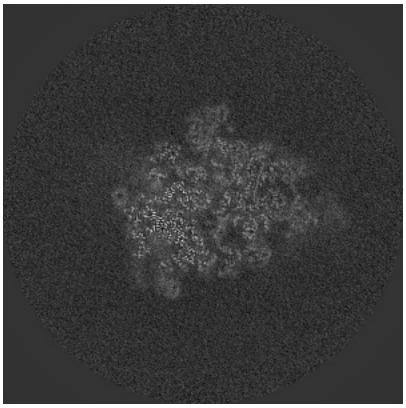


Y Index: 350

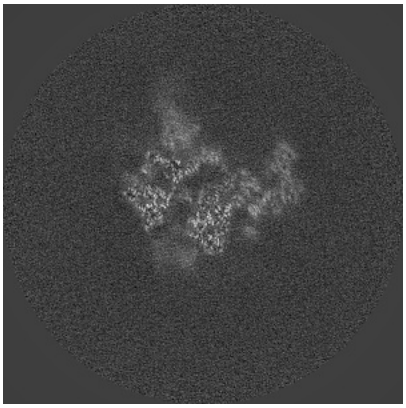


Z Index: 350

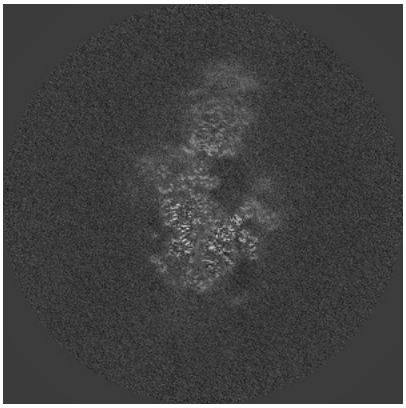
6.2.2 Raw map



X Index: 350



Y Index: 350

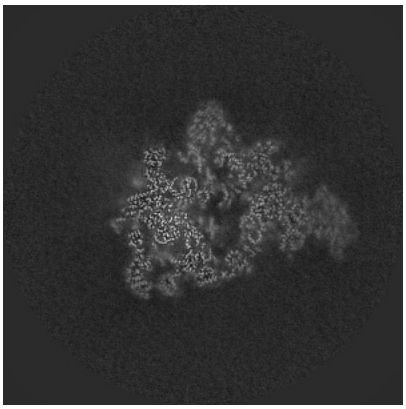


Z Index: 350

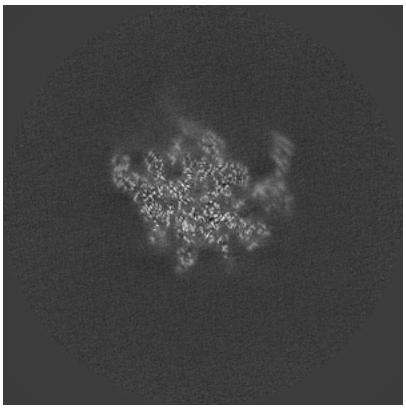
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

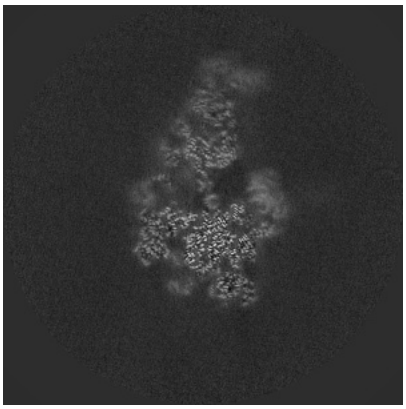
6.3.1 Primary map



X Index: 369

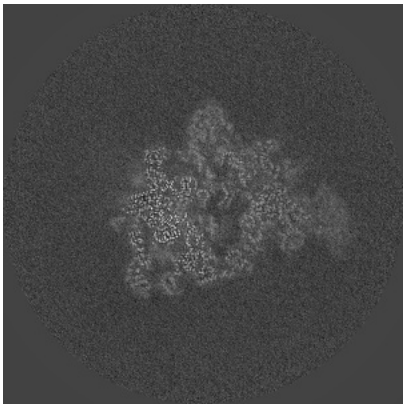


Y Index: 326

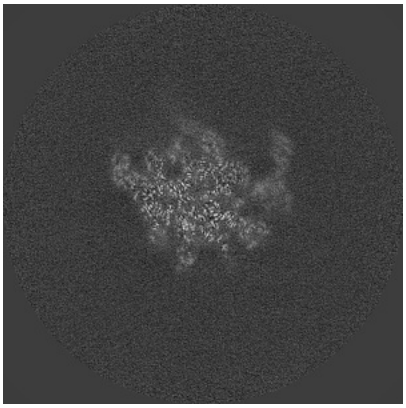


Z Index: 320

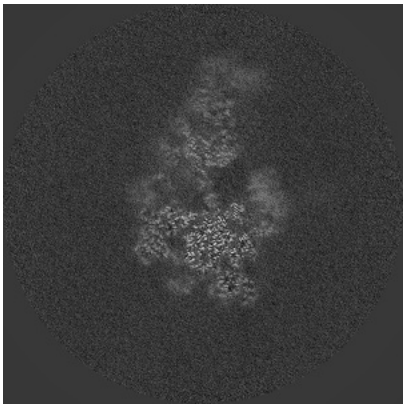
6.3.2 Raw map



X Index: 368



Y Index: 326



Z Index: 320

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

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

6.4.2 Raw map

X Y Z

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

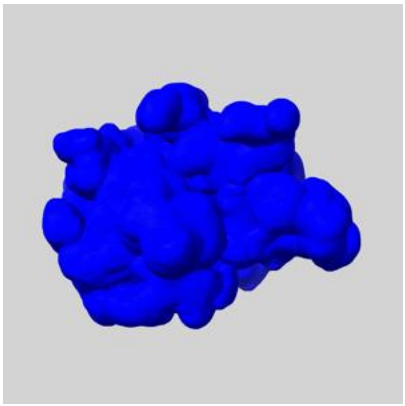
6.5 Mask visualisation

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

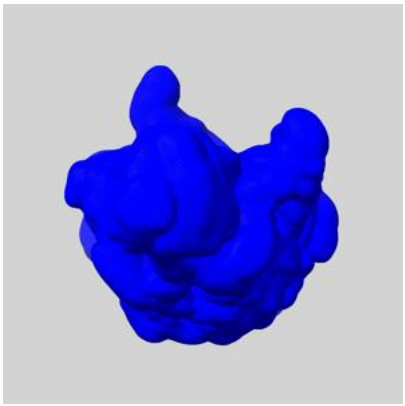
A mask typically either:

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

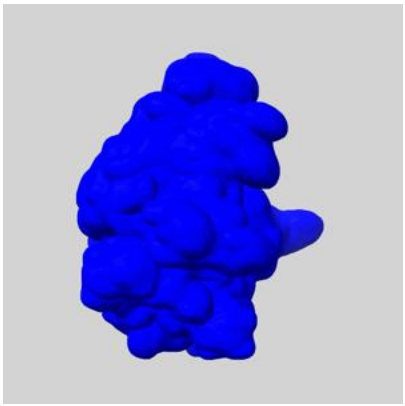
6.5.1 emd_15576_msk_1.map



X



Y

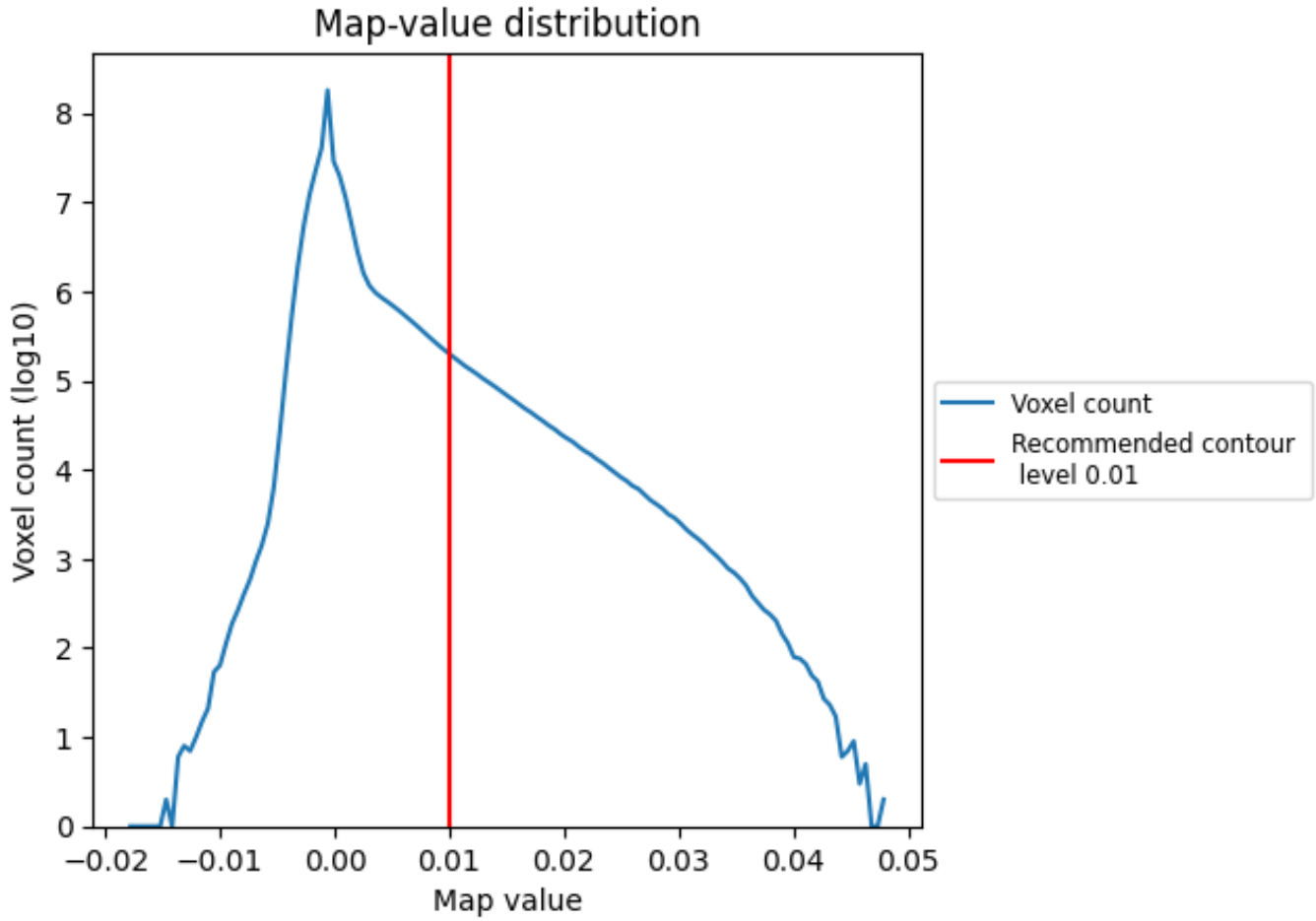


Z

7 Map analysis

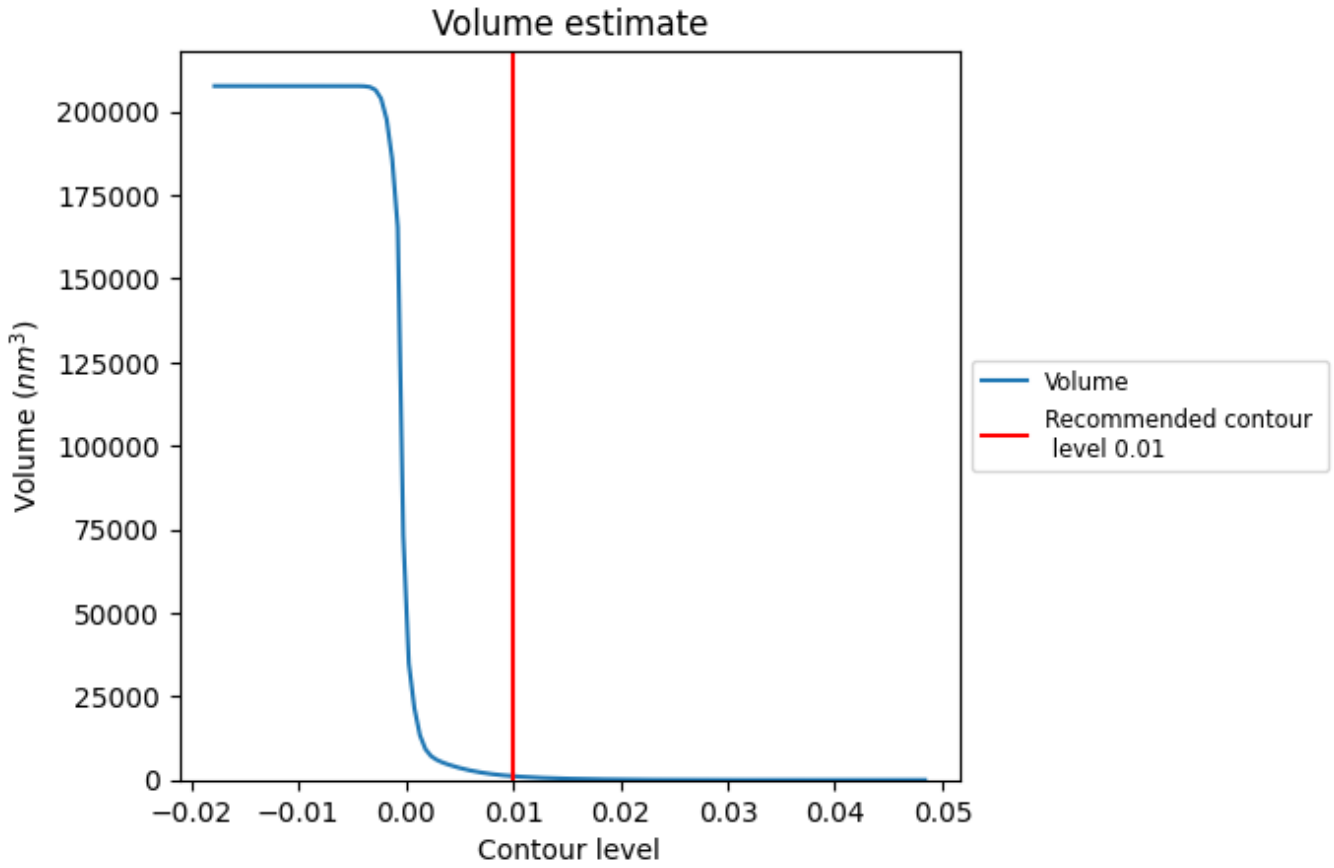
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

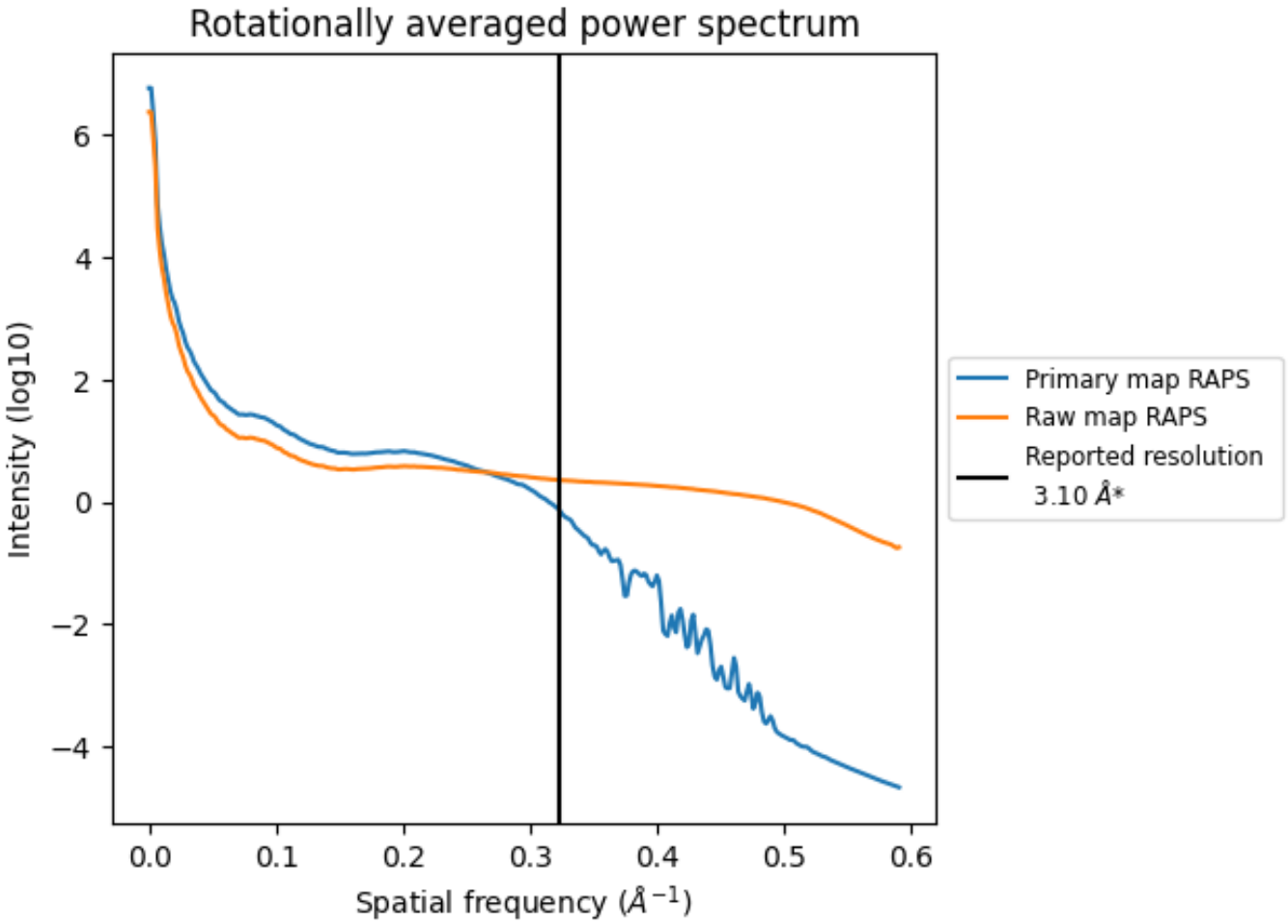
7.2 Volume estimate (i)



The volume at the recommended contour level is 1137 nm^3; this corresponds to an approximate mass of 1027 kDa.

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

7.3 Rotationally averaged power spectrum (i)

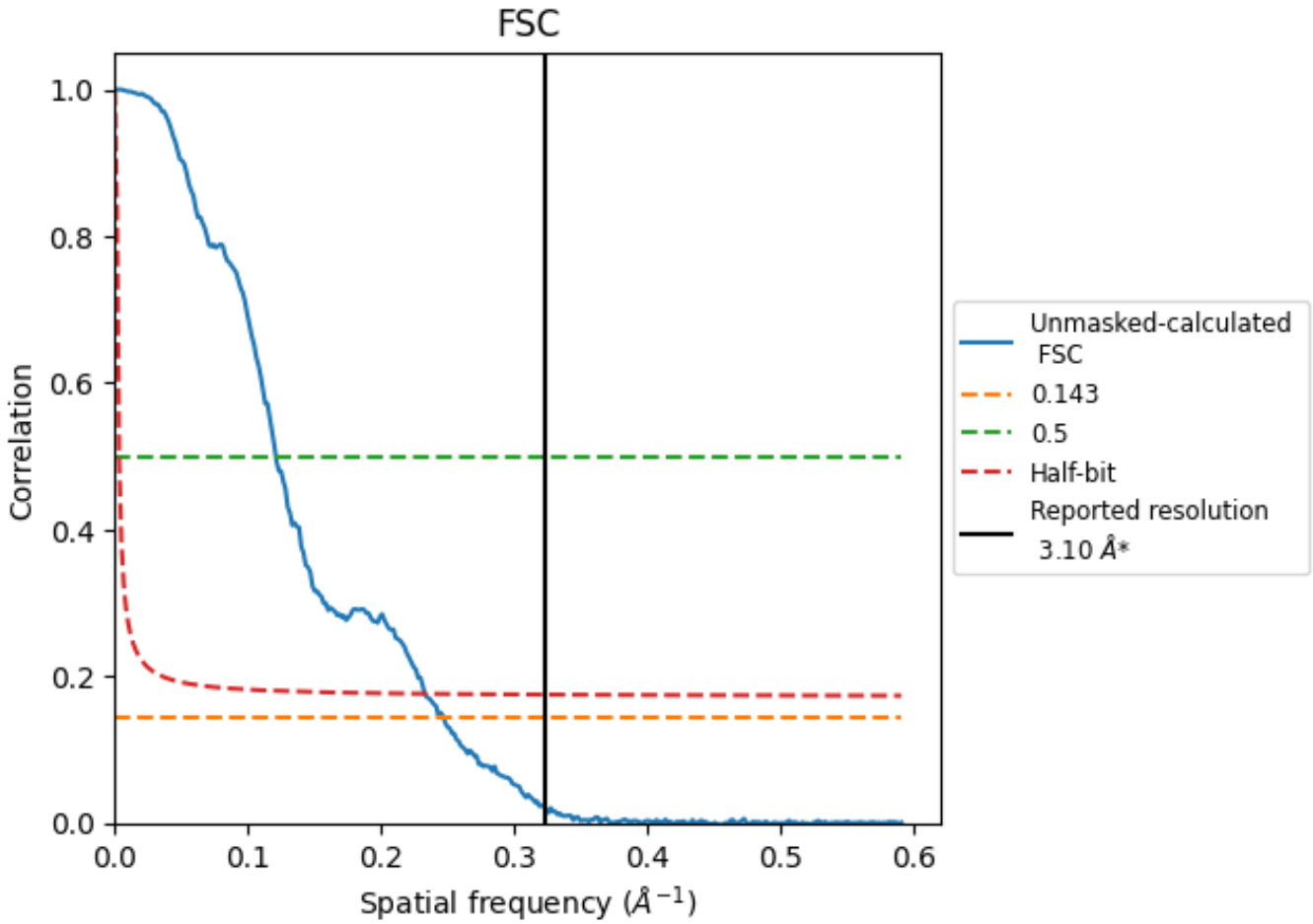


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

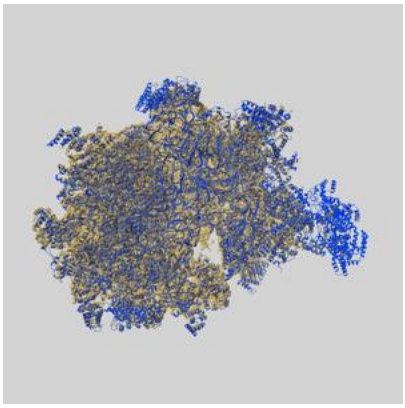
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.10
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	4.05	8.26	4.29	-

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

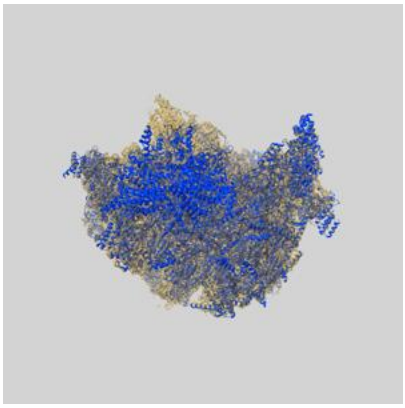
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15576 and PDB model 8APN. Per-residue inclusion information can be found in section 3 on page 29.

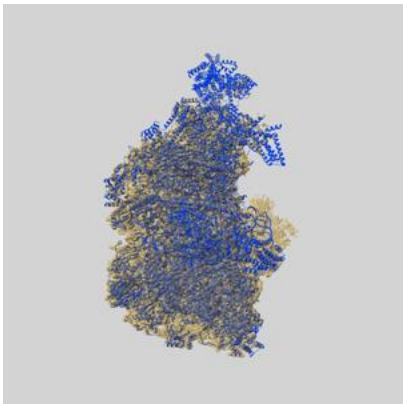
9.1 Map-model overlay



X



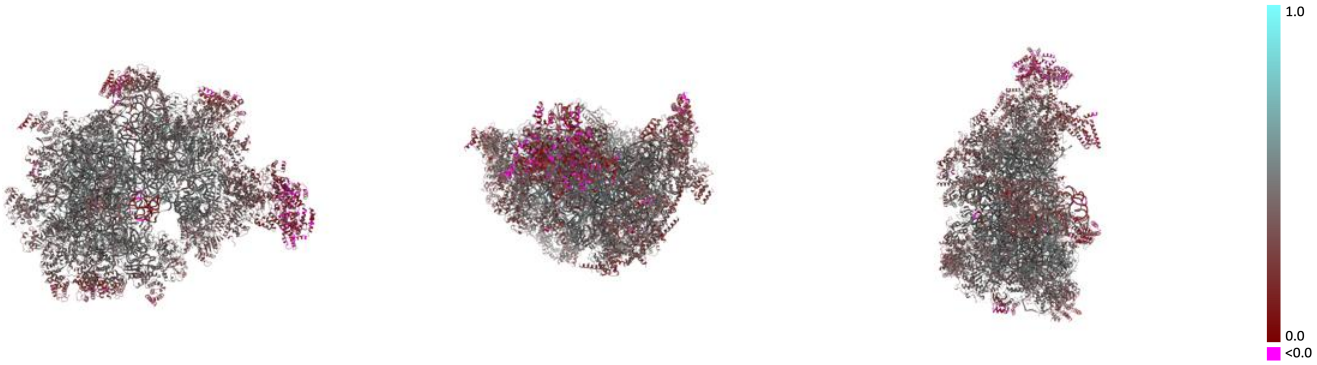
Y



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.

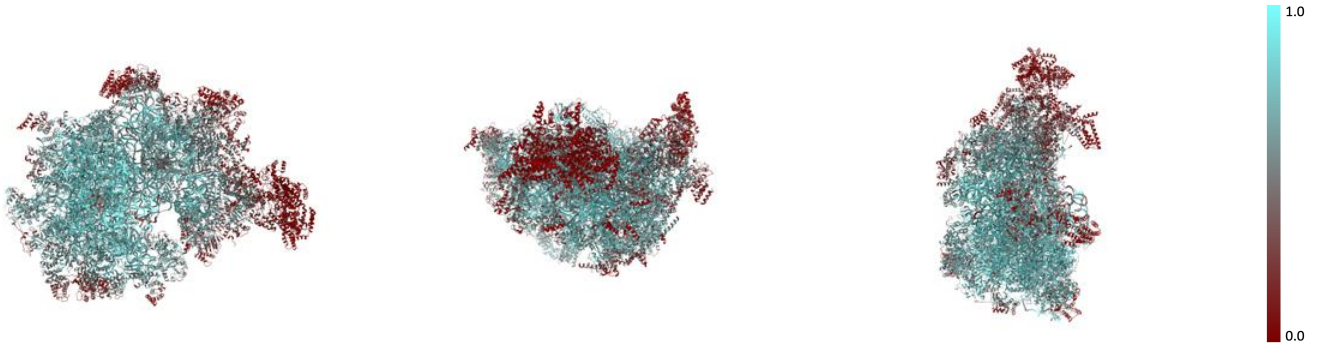
9.2 Q-score mapped to coordinate model



X Y Z

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.

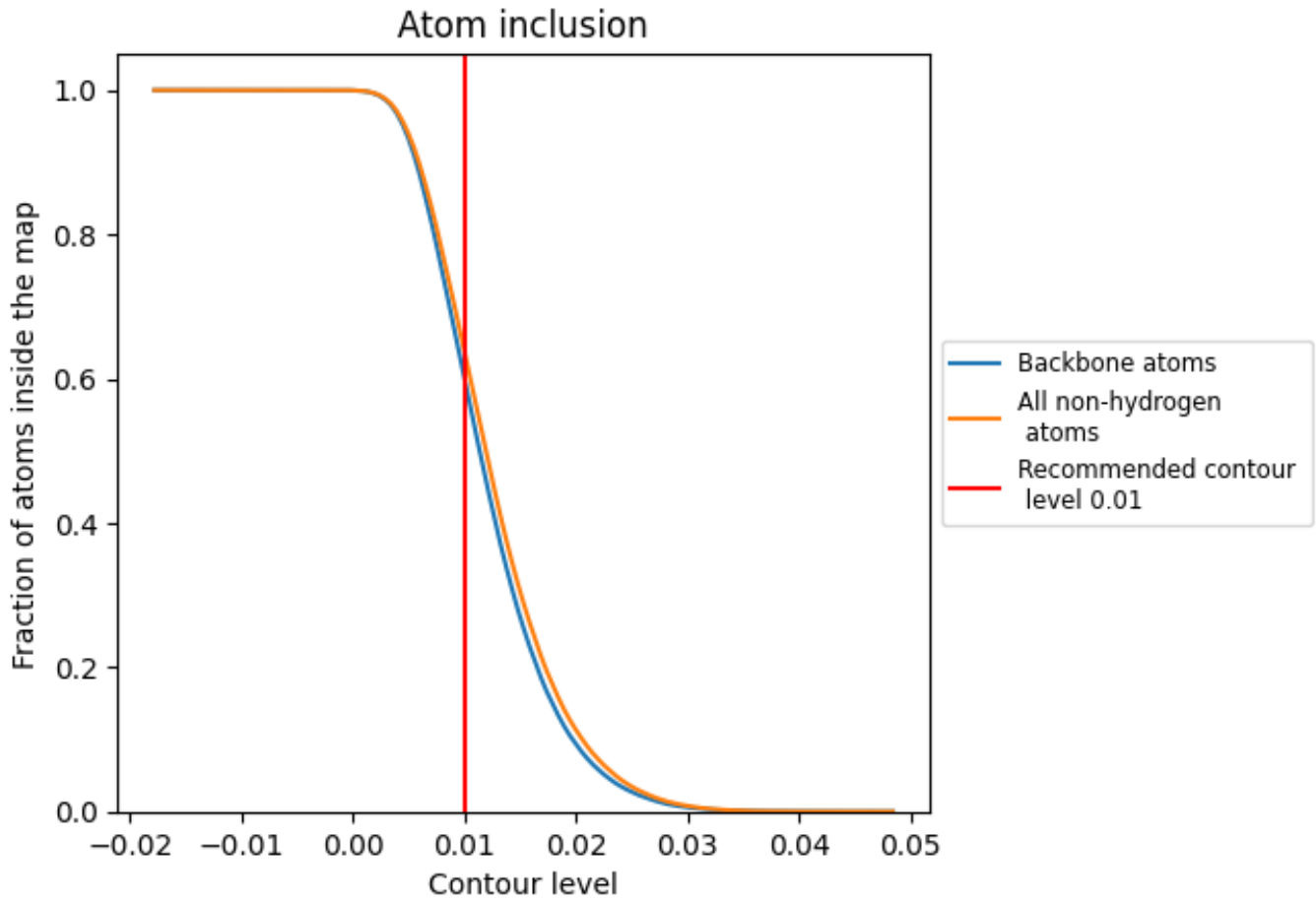
9.3 Atom inclusion mapped to coordinate model



X Y Z

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, 60% of all backbone atoms, 64% 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	0.6364	0.3990
A1	0.8641	0.4340
A2	0.8850	0.4750
A3	0.9199	0.4480
A4	0.9539	0.4800
A5	0.7903	0.2850
A6	0.9040	0.4510
A7	0.9163	0.4720
A8	0.9040	0.4660
A9	0.8868	0.4630
AA	0.8157	0.4400
AB	0.8617	0.4430
AC	0.7849	0.4460
AD	0.6923	0.4160
AE	0.5955	0.3730
AF	0.7483	0.4170
AG	0.7778	0.4420
AH	0.5494	0.3590
AI	0.7871	0.4530
AJ	0.5992	0.3790
AK	0.7998	0.4430
AL	0.4757	0.3130
AM	0.4818	0.3360
AN	0.5313	0.3460
AO	0.4929	0.3570
Aa	0.8253	0.4740
Ab	0.7780	0.4690
Ac	0.7464	0.4130
Ad	0.6053	0.4130
Ae	0.6263	0.3740
Af	0.5681	0.3680
Ah	0.7892	0.4520
Ai	0.7511	0.4810
Aj	0.8034	0.4390
Ak	0.8000	0.4770

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Chain	Atom inclusion	Q-score
Al	0.7832	0.4390
Am	0.6842	0.4160
An	0.6865	0.4520
Ao	0.7696	0.4420
Ap	0.7557	0.4460
Aq	0.8053	0.4520
Ar	0.7418	0.4260
As	0.5619	0.3300
At	0.7055	0.4470
Au	0.8079	0.4560
Av	0.7129	0.4380
Aw	0.7042	0.4150
Ax	0.7474	0.4380
Ay	0.4880	0.3800
Az	0.7379	0.4470
B1	0.7018	0.4240
B2	0.7659	0.4270
B3	0.8872	0.4720
B4	0.8455	0.4590
BA	0.3990	0.3750
BB	0.4806	0.3790
BC	0.3365	0.3570
BD	0.6768	0.4280
BE	0.0499	0.1750
BF	0.3224	0.3130
Ba	0.4308	0.3250
Bb	0.5881	0.3980
Bc	0.3996	0.3980
Bd	0.5092	0.4360
Be	0.6535	0.4510
Bf	0.6649	0.4220
Bg	0.6605	0.4540
Bh	0.6005	0.3950
Bi	0.5246	0.3970
Bj	0.2378	0.2710
Bk	0.7347	0.4670
Bl	0.4350	0.4220
Bm	0.5400	0.4120
Bn	0.6952	0.4650
Bo	0.7807	0.4240
Bp	0.4287	0.3740
Bq	0.6960	0.3960

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Chain	Atom inclusion	Q-score
Br	0.6574	0.3970
Bs	0.4092	0.3820
Bt	0.6899	0.4250
Bu	0.4512	0.3430
Bv	0.5030	0.3350
Bw	0.4004	0.3570
Bx	0.1650	0.2390
By	0.4686	0.3930
Bz	0.1713	0.2490
C1	0.6725	0.3880
C3	0.8736	0.5100
Ua	0.4268	0.4340
Ub	0.4021	0.2340
Ud	0.1907	0.2400
Ue	0.0128	0.2430
Uf	0.0795	0.1570
Ug	0.3111	0.3790
Uh	0.0000	0.1200
Ui	0.6077	0.4120
Uj	0.1556	0.3870
Uk	0.2000	0.2990
Ul	0.0500	0.2060
Um	0.5273	0.3200
Xa	0.4791	0.3520
Xb	0.5904	0.3960
Xc	0.6909	0.4040
Xd	0.6083	0.3930
Xe	0.6952	0.4140
Xf	0.7194	0.4420
Xg	0.6171	0.4010
Xh	0.5752	0.3860
Xi	0.7538	0.4040
Xj	0.5852	0.3830
Ya	0.3348	0.3640
Yb	0.2134	0.2880
Yc	0.4183	0.3790
Yd	0.2605	0.3300
Ye	0.6440	0.4740
Yf	0.4771	0.4040
Yg	0.2871	0.3360
Yh	0.4671	0.3920
Yi	0.0754	0.2610

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Chain	Atom inclusion	Q-score
Yj	0.1022	0.1840
Yk	0.0632	0.2030
Yl	0.4826	0.3880