



## wwPDB EM Validation Summary Report ⓘ

Apr 27, 2024 – 09:33 am BST

PDB ID : 8BN3  
EMDB ID : EMD-16127  
Title : Yeast 80S, ES7s delta, eIF5A, Stm1 containing  
Authors : Dimitrova-Paternoga, L.; Paternoga, H.; Wilson, D.N.  
Deposited on : 2022-11-12  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

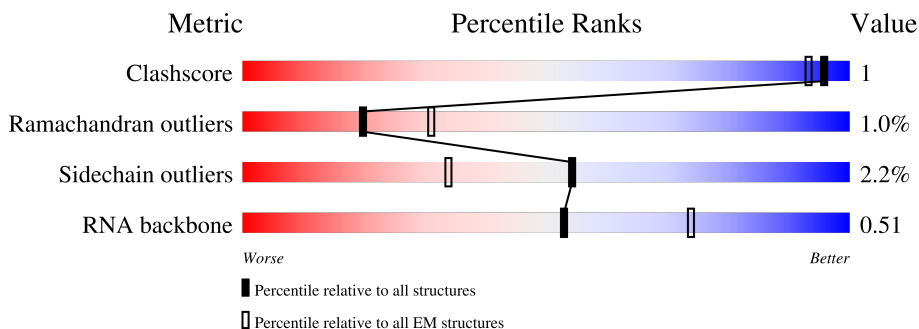
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	217	
2	S5	206	
3	C0	96	
4	C4	127	
5	C5	124	
6	C8	145	
7	D0	107	

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Mol	Chain	Length	Quality of chain
8	D5	70	99% 89% 11%
9	D8	63	86% 95%
10	P	15	100%
11	3	121	80% 19%
12	4	158	74% 22%
13	1	3162	6% 70% 25% 5%
14	2	1737	20% 64% 31%
15	S0	251	35% 77% 19%
16	S1	214	71% 92% 6%
17	S2	217	20% 93% 6%
18	S3	223	67% 92% 7%
19	S6	226	70% 94% 5%
20	S7	184	61% 96%
21	S8	188	21% 95%
22	S9	185	34% 97%
23	C1	155	12% 83% 6% 10%
24	C3	150	21% 95%
25	C6	141	76% 91% 6%
26	C7	120	62% 72% 5% 23%
27	C9	143	80% 94% 6%
28	D1	87	25% 92% 7%
29	D2	129	95% 5%
30	D3	144	5% 93% 6%
31	D4	134	60% 96%
32	D6	97	20% 88% 8%








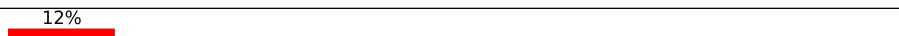
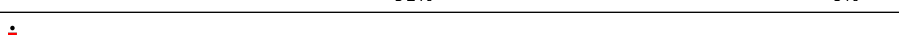
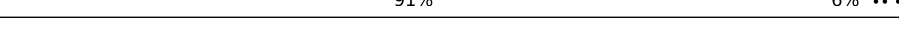
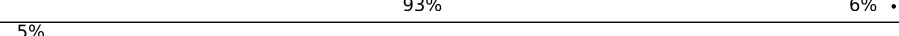

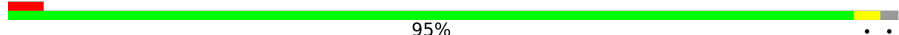
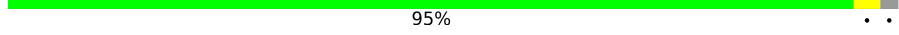








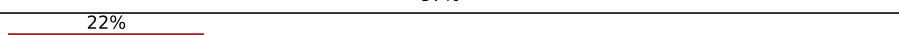
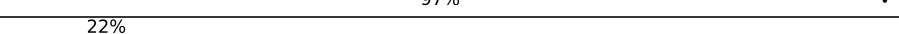
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Mol	Chain	Length	Quality of chain
33	D7	81	48% 100%
34	D9	53	17% 87% 6% 8%
35	E0	60	50% 92% 7%
36	SR	318	100% 98%
37	L2	252	93% 5%
38	L3	386	90% 9%
39	L4	361	91% 7% ...
40	L5	295	12% 92% 5% ..
41	L6	156	8% 91% 6% ..
42	L7	222	95% ..
43	L8	233	6% 88% 5% 7%
44	L9	189	5% 91% 8% .
45	M0	209	5% 91% 7% .
46	M1	168	11% 93% 5% .
47	M3	193	10% 91% 9% .
48	M4	136	90% 8% ..
49	M5	202	93% ..
50	M6	197	92% 6% ..
51	M7	183	90% .. 5%
52	M8	185	91% 6% .
53	M9	188	15% 90% 7% ..
54	N0	172	92% 7% .
55	N1	159	94% 6% .
56	N2	100	14% 97% ..
57	N3	136	91% 7% ..

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Mol	Chain	Length	Quality of chain
58	N4	98	 60% 37%
59	N5	121	 90% 7%
60	N6	126	 91% 8%
61	N7	135	 91% 7% 8%
62	N8	148	 92% 7%
63	N9	56	 93%
64	O0	97	 88% 11%
65	O1	109	 12% 91% 6%
66	O2	127	 91% 6%
67	O3	106	 93% 6%
68	O4	111	 90% 7%
69	O5	119	 92%
70	O6	99	 95%
71	O7	86	 79% 13%
72	O8	77	 17% 94% 5%
73	O9	50	 86% 12%
74	Q0	52	 92%
75	Q1	25	 8% 100%
76	Q2	105	 5% 90% 9%
77	Q3	91	 97%
78	SM	118	 64% 97%
79	eI	145	 22% 97%
80	S4	260	 22% 95% 5%
81	E1	71	 49% 46% 51%

## 2 Entry composition i

There are 87 unique types of molecules in this entry. The entry contains 201671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	216	1710	1092	298	311	9	0	0

- Molecule 2 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S5	206	1609	1007	300	299	3	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C0	96	818	530	133	153	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 4 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C4	126	933	572	185	173	3	0	0

- Molecule 5 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C5	115	912	580	170	155	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C8	145	1192	743	237	210	2	0	0

- Molecule 7 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D0	107	855	539	156	159	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	D5	70	563	360	104	99	0	0

- Molecule 9 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D8	62	490	302	98	89	1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	15	146	89	40	16	1	0	0

- Molecule 11 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	3	121	2579	1152	461	845	121	0	0

- Molecule 12 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	4	158	3353	1500	586	1109	158	0	0

- Molecule 13 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	1	3143	67219	30026	12110	21940	3143	0	0

- Molecule 14 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	2	1737	37011	16546	6549	12179	1737	0	0

- Molecule 15 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	S0	204	1598	1025	283	288	2	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S1	211	1687	1070	305	308	4	0	0

- Molecule 17 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S2	214	1615	1036	285	292	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S3	220	1709	1083	310	310	6	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein eS6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S6	226	1820	1142	350	325	3	0	0

- Molecule 20 is a protein called 40S ribosomal protein S7-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	S7	184	1481	951	265	265	0	0

- Molecule 21 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S8	188	1489	925	298	264	2	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein uS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S9	185	1494	943	289	261	1	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	C1	139	1121	721	211	186	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	C3	150	1192	759	224	207	2	0	0

- Molecule 25 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	C6	141	1105	708	203	194	0	0

- Molecule 26 is a protein called ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	C7	92	737	466	140	129	2	0	0

- Molecule 27 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	C9	143	1112	694	208	208	2	0	0

- Molecule 28 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	D1	86	673	414	121	136	2	0	0

- Molecule 29 is a protein called RPS22A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	D2	129	1021	650	188	180	3	0	0

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	D3	144	1121	708	220	191	2	0	0

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	D4	134	1073	676	208	189	0	0

- Molecule 32 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	D6	97	769	475	160	129	5	0	0

- Molecule 33 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	D7	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 34 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D9	49	Total	C	N	O	S	0	0
			404	249	86	65	4		

- Molecule 35 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E0	59	Total	C	N	O	S	0	0
			469	296	97	75	1		

- Molecule 36 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SR	318	Total	C	N	O	S	0	0
			2445	1546	419	472	8		

- Molecule 37 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L2	251	Total	C	N	O	S	0	0
			1909	1188	387	333	1		

- Molecule 38 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L3	386	Total	C	N	O	S	0	0
			3079	1954	584	533	8		

- Molecule 39 is a protein called RPL4A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L4	359	Total	C	N	O	S	0	0
			2731	1720	517	491	3		

- Molecule 40 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	L5	291	2329	1472	406	449	2	0	0

- Molecule 41 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	L6	156	1239	800	222	216	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	L7	219	1761	1138	320	302	1	0	0

- Molecule 43 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	L8	216	1706	1095	306	302	3	0	0

- Molecule 44 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	L9	189	1502	953	272	273	4	0	0

- Molecule 45 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	M0	206	1677	1066	317	289	5	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M0	?	-	LEU	deletion	UNP A0A6A5PUZ5
M0	?	-	SER	deletion	UNP A0A6A5PUZ5
M0	?	-	CYS	deletion	UNP A0A6A5PUZ5
M0	?	-	ALA	deletion	UNP A0A6A5PUZ5
M0	?	-	GLY	deletion	UNP A0A6A5PUZ5
M0	?	-	ALA	deletion	UNP A0A6A5PUZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
M0	?	-	ASP	deletion	UNP A0A6A5PUZ5
M0	?	-	ARG	deletion	UNP A0A6A5PUZ5
M0	?	-	LEU	deletion	UNP A0A6A5PUZ5

- Molecule 46 is a protein called RPL11B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	M1	168	1344	841	251	248	4	0	0

- Molecule 47 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	M3	193	1543	962	315	266	0	0

- Molecule 48 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	M4	136	1053	675	199	177	2	0	0

- Molecule 49 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	M5	202	1711	1071	359	280	1	0	0

- Molecule 50 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	M6	197	1555	1003	289	262	1	0	0

- Molecule 51 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	M7	174	1379	856	275	248	0	0

- Molecule 52 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	M8	185	1441	908	290	241	2	0	0

- Molecule 53 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	M9	184	1490	917	321	252		0	0

- Molecule 54 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	N0	172	1445	930	267	244	4	0	0

- Molecule 55 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	N1	158	1268	799	245	220	4	0	0

- Molecule 56 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	N2	98	778	505	127	146		0	0

- Molecule 57 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	N3	136	1003	628	189	179	7	0	0

- Molecule 58 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	N4	62	513	330	101	81	1	0	0

- Molecule 59 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	N5	119	954	614	167	171	2	0	0

- Molecule 60 is a protein called Large ribosomal subunit protein uL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	N6	126	993	625	192	176		0	0

- Molecule 61 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	N7	135	1092	710	202	180		0	0

- Molecule 62 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	N8	148	1173	749	231	190	3	0	0

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	N9	54	434	271	94	69		0	0

- Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	O0	97	743	479	124	139	1	0	0

- Molecule 65 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	O1	106	865	550	165	149	1	0	0

- Molecule 66 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	O2	125	Total	C	N	O	S	0	0
			1007	638	203	165	1		

- Molecule 67 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	O3	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 68 is a protein called Large ribosomal subunit protein eL34A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	O4	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 69 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	O5	118	Total	C	N	O	S	0	0
			964	612	185	166	1		

- Molecule 70 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	O6	97	Total	C	N	O	S	0	0
			750	469	149	130	2		

- Molecule 71 is a protein called Large ribosomal subunit protein eL37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	O7	84	Total	C	N	O	S	1	0
			676	411	149	111	5		

- Molecule 72 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	O8	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 73 is a protein called 60S ribosomal protein L39.



Mol	Chain	Residues	Atoms					AltConf	Trace
73	O9	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 74 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Q0	51	Total	C	N	O	S	0	0
			409	253	85	66	5		

- Molecule 75 is a protein called Large ribosomal subunit protein eL41B.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Q1	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 76 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Q2	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 77 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Q3	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 78 is a protein called STM1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	SM	118	Total	C	N	O	0	0
			893	527	180	186		

- Molecule 79 is a protein called Eukaryotic translation initiation factor 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	eI	145	Total	C	N	O	S	0	0
			1096	682	183	222	9		

- Molecule 80 is a protein called Small ribosomal subunit protein eS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	S4	260	2068	1316	389	360	3	0	0

- Molecule 81 is a protein called RPS31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	E1	35	271	165	54	48	4	0	0

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	3	3	Total 3	Mg 3	0
82	4	2	Total 2	Mg 2	0
82	1	191	Total 191	Mg 191	0
82	2	19	Total 19	Mg 19	0
82	L3	1	Total 1	Mg 1	0
82	M7	1	Total 1	Mg 1	0
82	N3	1	Total 1	Mg 1	0
82	O2	1	Total 1	Mg 1	0
82	O7	1	Total 1	Mg 1	0

- Molecule 83 is POTASSIUM ION (three-letter code: K) (formula: K).

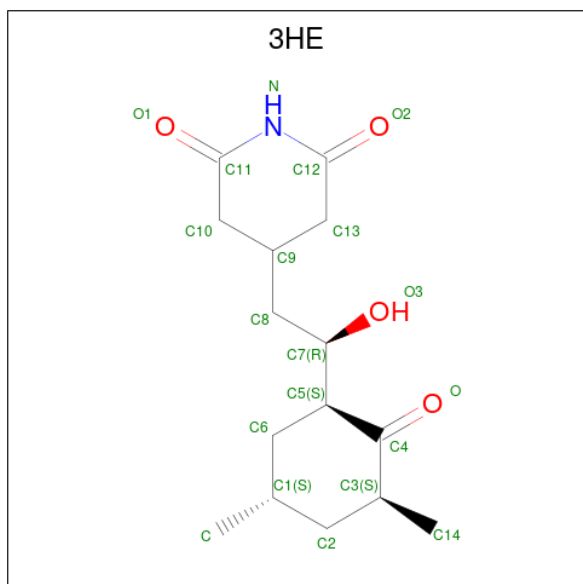
Mol	Chain	Residues	Atoms		AltConf
83	1	63	Total 63	K 63	0
83	2	1	Total 1	K 1	0
83	L2	2	Total 2	K 2	0
83	L4	1	Total 1	K 1	0

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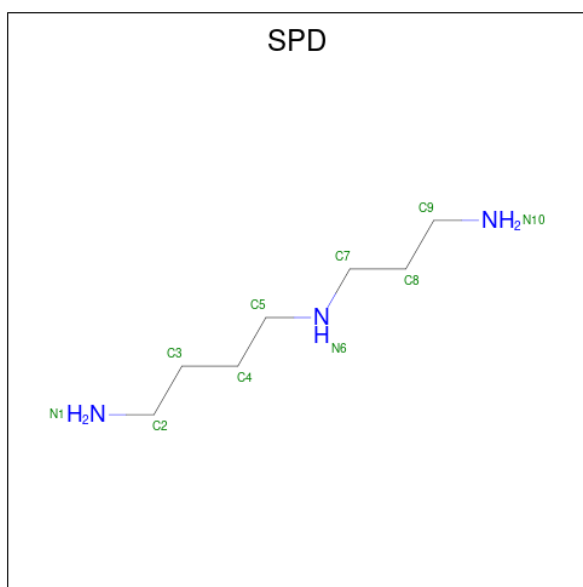
Mol	Chain	Residues	Atoms	AltConf
83	M0	1	Total K 1 1	0
83	M5	1	Total K 1 1	0
83	N9	1	Total K 1 1	0
83	O4	1	Total K 1 1	0
83	O7	1	Total K 1 1	0

- Molecule 84 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
84	1	1	Total C N O 20 15 1 4	0

- Molecule 85 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms	AltConf
85	1	1	Total C N 10 7 3	0
85	1	1	Total C N 10 7 3	0
85	1	1	Total C N 10 7 3	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
86	D6	1	Total Zn 1 1	0
86	D9	1	Total Zn 1 1	0
86	O4	1	Total Zn 1 1	0
86	O7	1	Total Zn 1 1	0
86	Q0	1	Total Zn 1 1	0
86	Q2	1	Total Zn 1 1	0
86	Q3	1	Total Zn 1 1	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	3	12	Total 12	O 12	0
87	4	40	Total 40	O 40	0
87	1	1466	Total 1466	O 1466	0
87	2	45	Total 45	O 45	0
87	C3	2	Total 2	O 2	0
87	L2	30	Total 30	O 30	0
87	L3	21	Total 21	O 21	0
87	L4	16	Total 16	O 16	0
87	L5	3	Total 3	O 3	0
87	L6	1	Total 1	O 1	0
87	L7	10	Total 10	O 10	0
87	M0	3	Total 3	O 3	0
87	M3	3	Total 3	O 3	0
87	M5	19	Total 19	O 19	0
87	M6	9	Total 9	O 9	0
87	M7	13	Total 13	O 13	0
87	M8	10	Total 10	O 10	0
87	M9	5	Total 5	O 5	0
87	N0	3	Total 3	O 3	0
87	N1	6	Total 6	O 6	0
87	N3	4	Total 4	O 4	0
87	N4	1	Total 1	O 1	0

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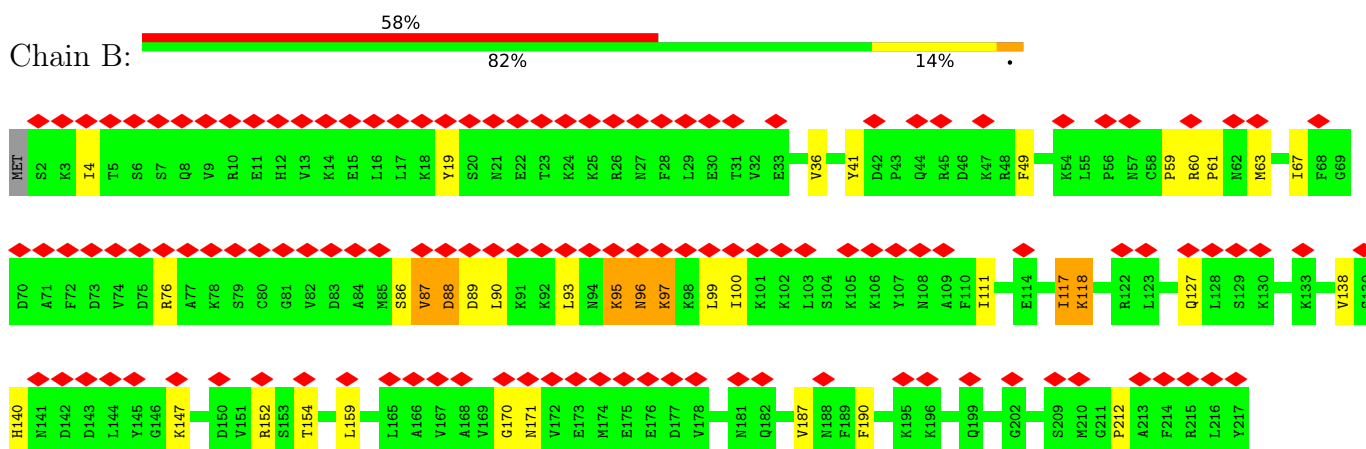
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
87	N5	4	Total 4	O 4	0
87	N8	15	Total 15	O 15	0
87	N9	5	Total 5	O 5	0
87	O1	4	Total 4	O 4	0
87	O2	20	Total 20	O 20	0
87	O3	5	Total 5	O 5	0
87	O4	6	Total 6	O 6	0
87	O6	1	Total 1	O 1	0
87	O7	11	Total 11	O 11	0
87	O8	1	Total 1	O 1	0
87	O9	1	Total 1	O 1	0
87	Q0	1	Total 1	O 1	0
87	Q2	9	Total 9	O 9	0
87	Q3	4	Total 4	O 4	0
87	eI	1	Total 1	O 1	0

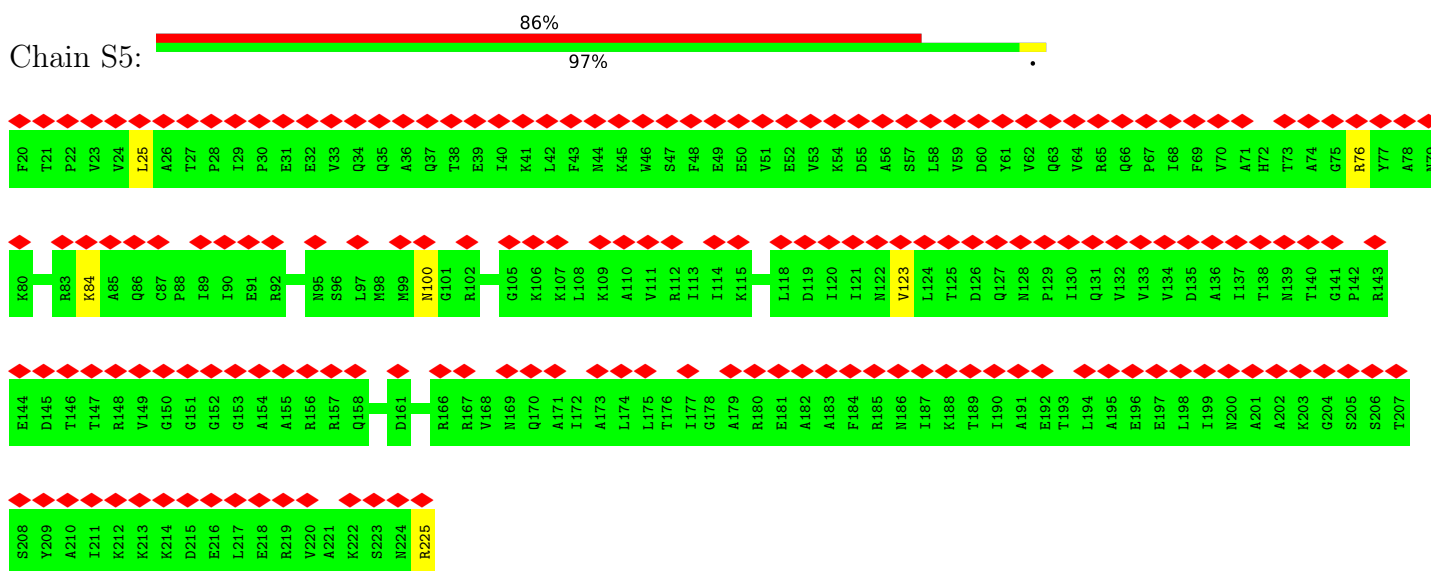
### 3 Residue-property plots

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

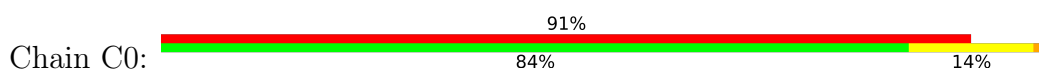
- Molecule 1: 60S ribosomal protein L1-A

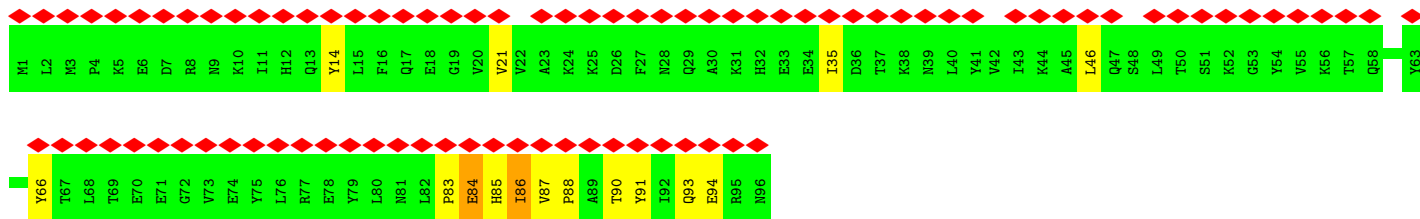


- Molecule 2: Rps5p

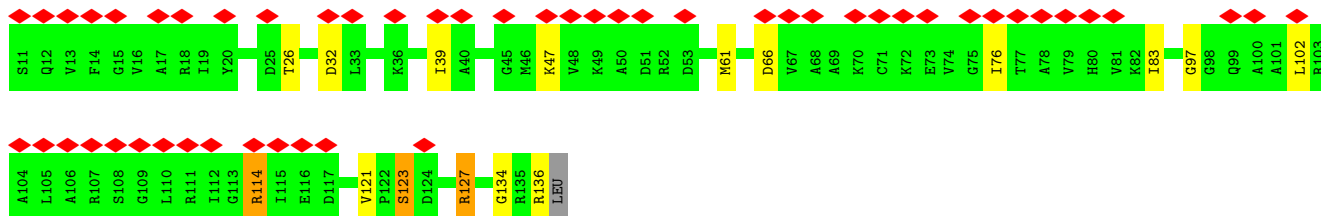
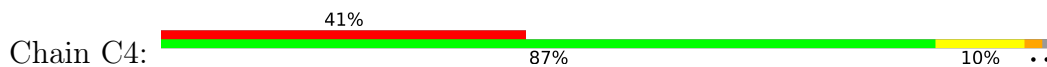


- Molecule 3: Small ribosomal subunit protein eS10A

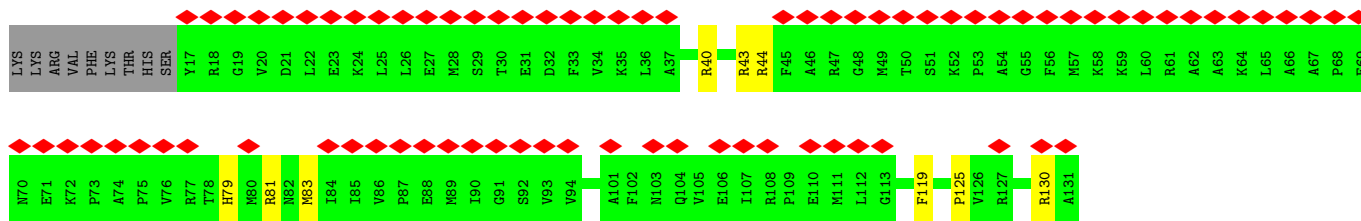
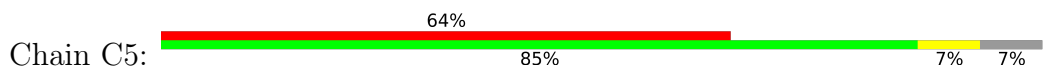




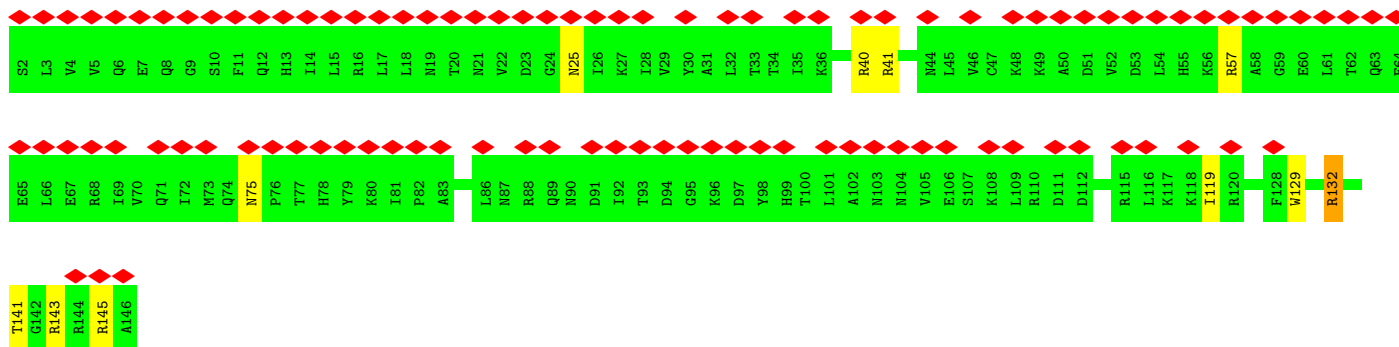
• Molecule 4: 40S ribosomal protein S14-B



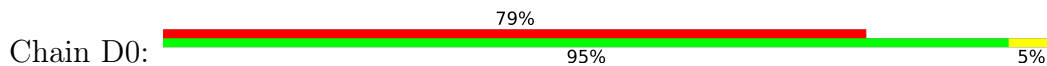
• Molecule 5: RPS15 isoform 1



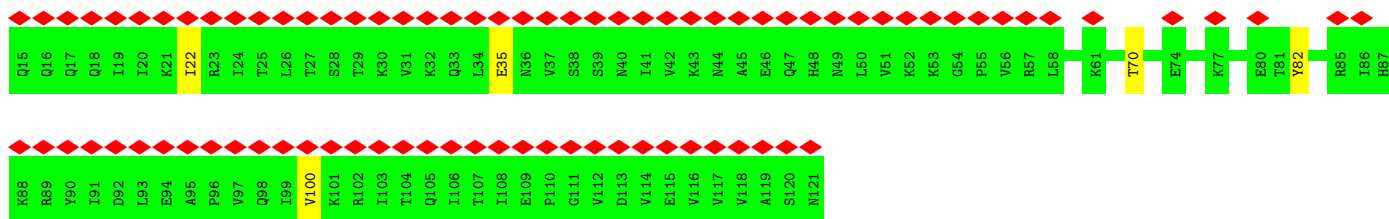
• Molecule 6: 40S ribosomal protein S18-A



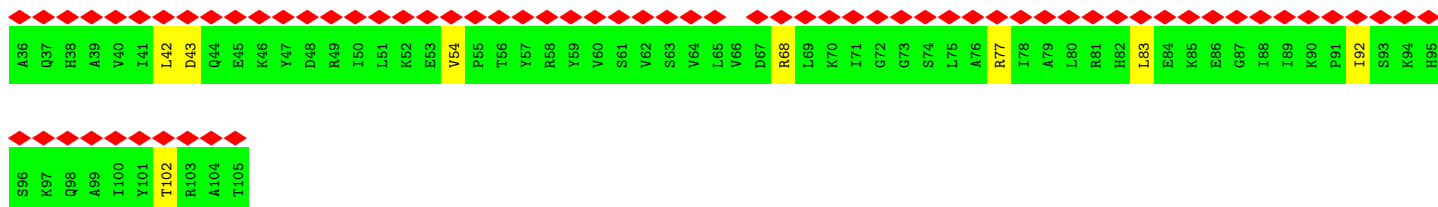
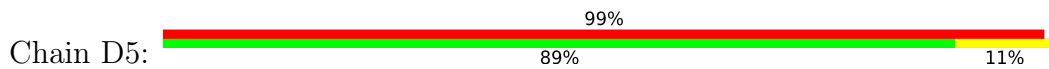
• Molecule 7: RPS20 isoform 1



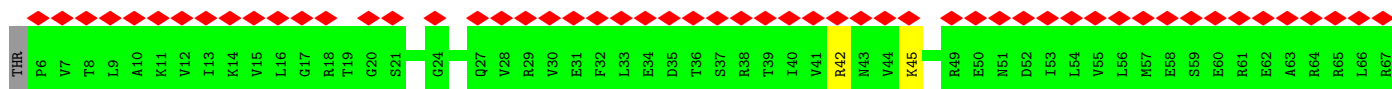
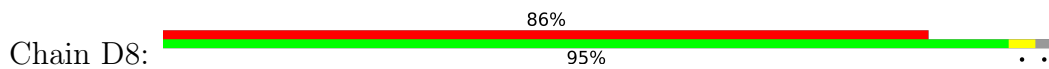




• Molecule 8: 40S ribosomal protein S25



• Molecule 9: RPS28A isoform 1

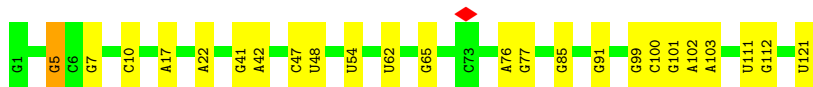
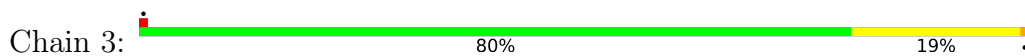


• Molecule 10: 60S ribosomal protein L41-A

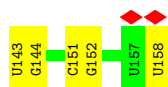
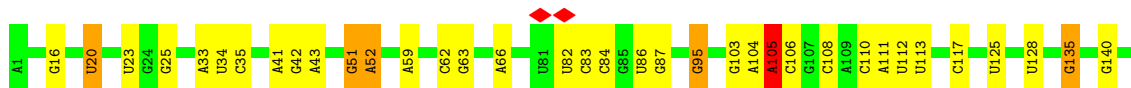


There are no outlier residues recorded for this chain.

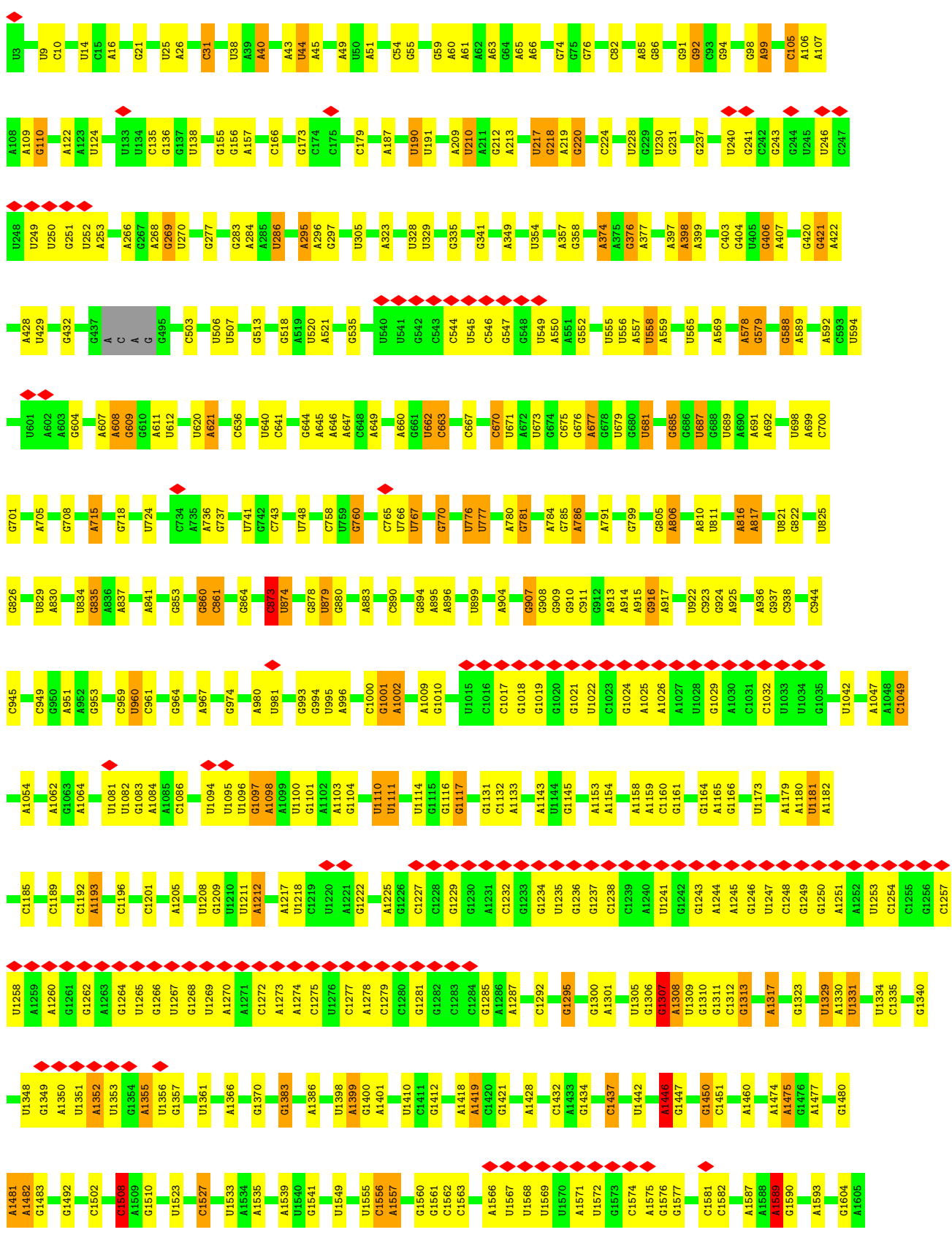
• Molecule 11: 5S ribosomal RNA

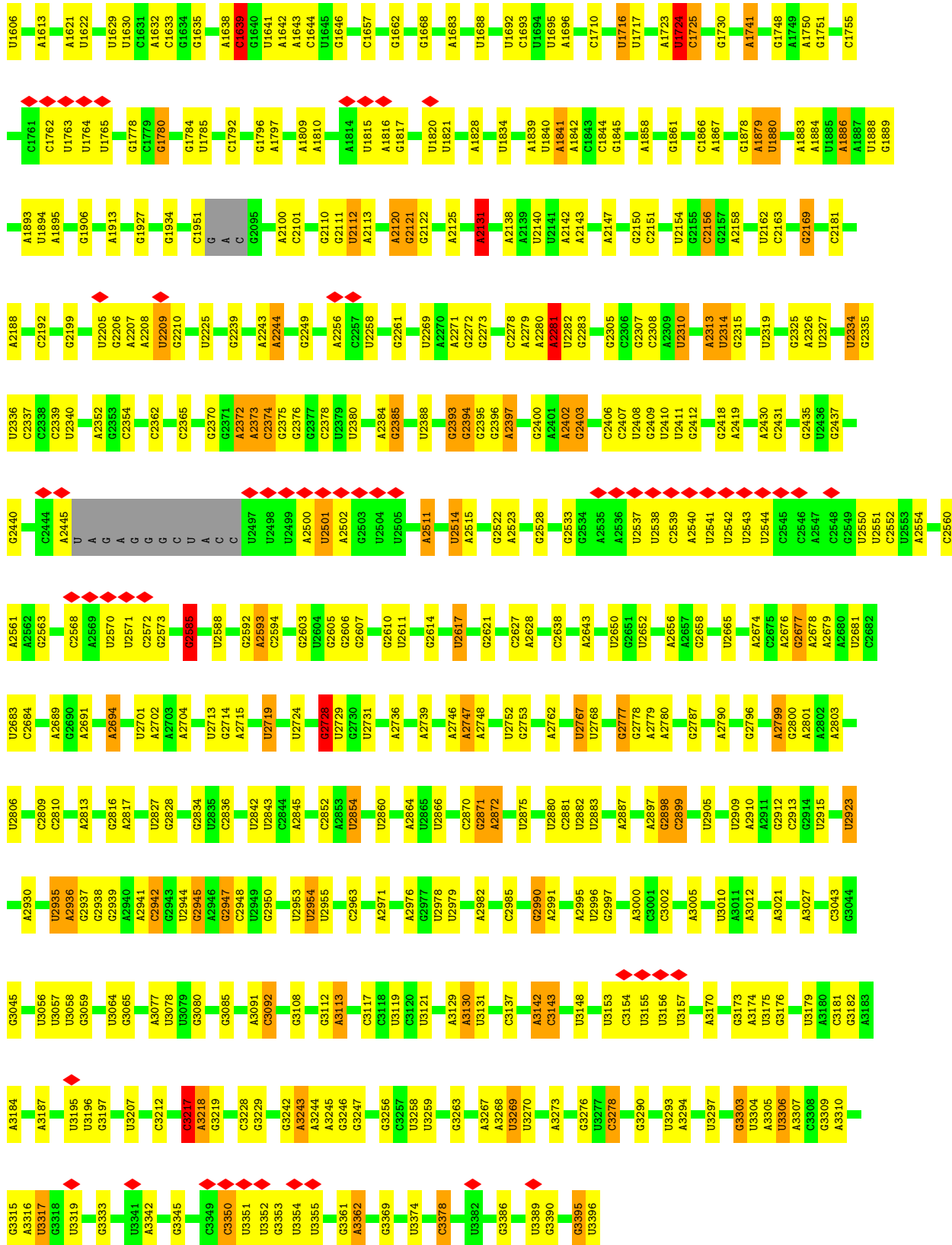


• Molecule 12: 5.8S ribosomal RNA



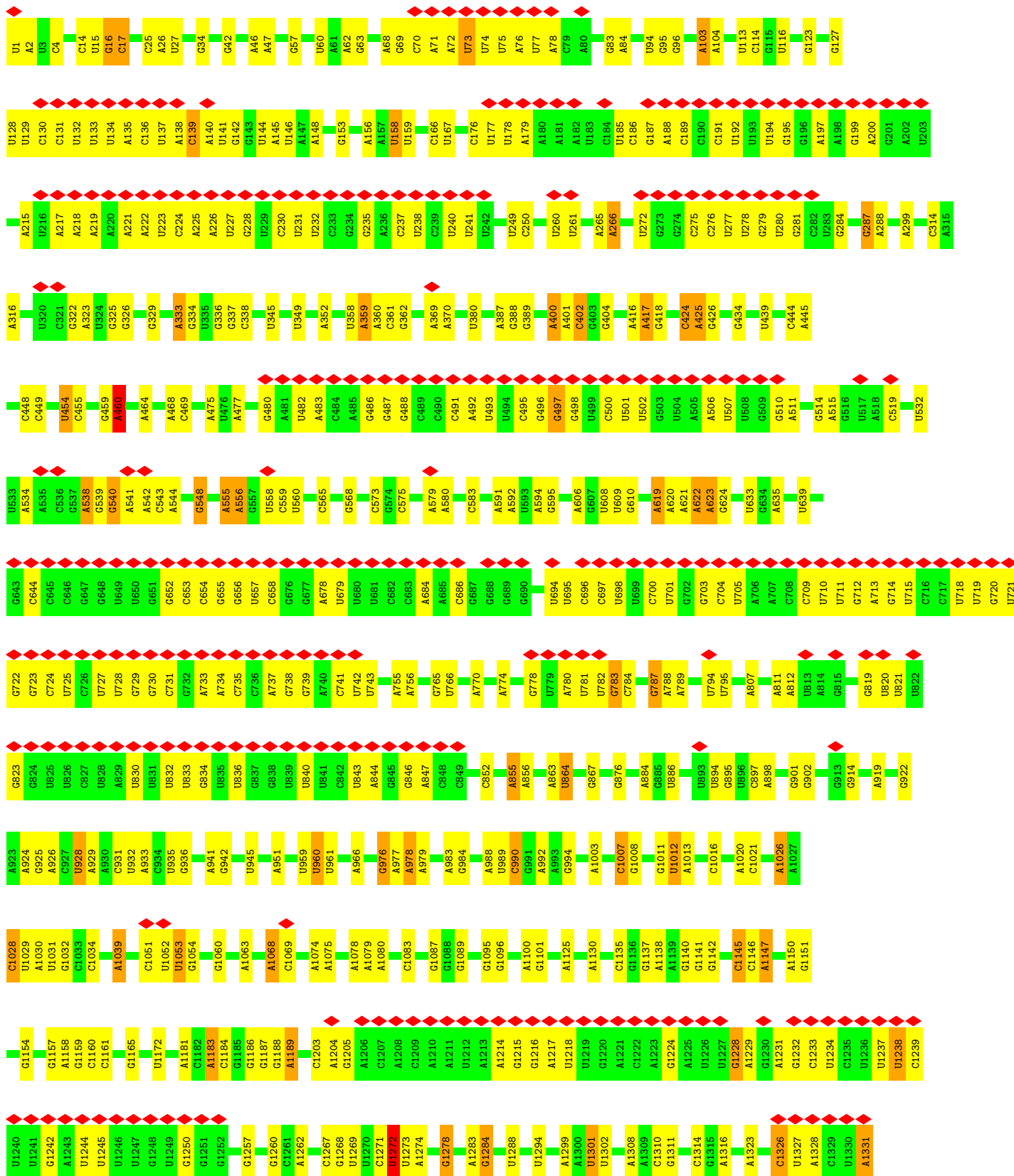
• Molecule 13: 25S ribosomal RNA

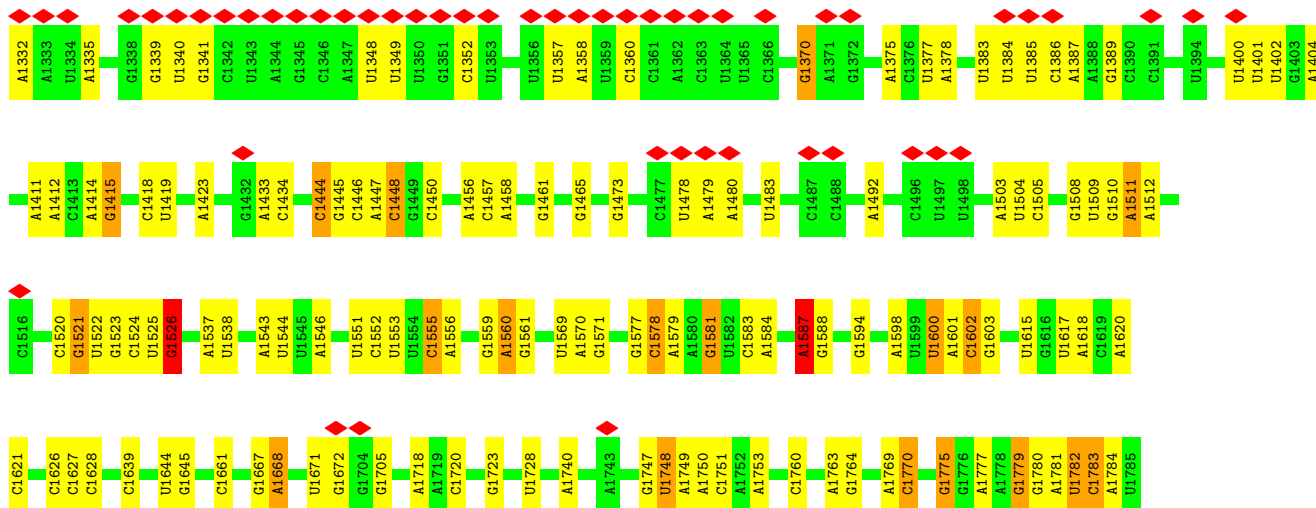




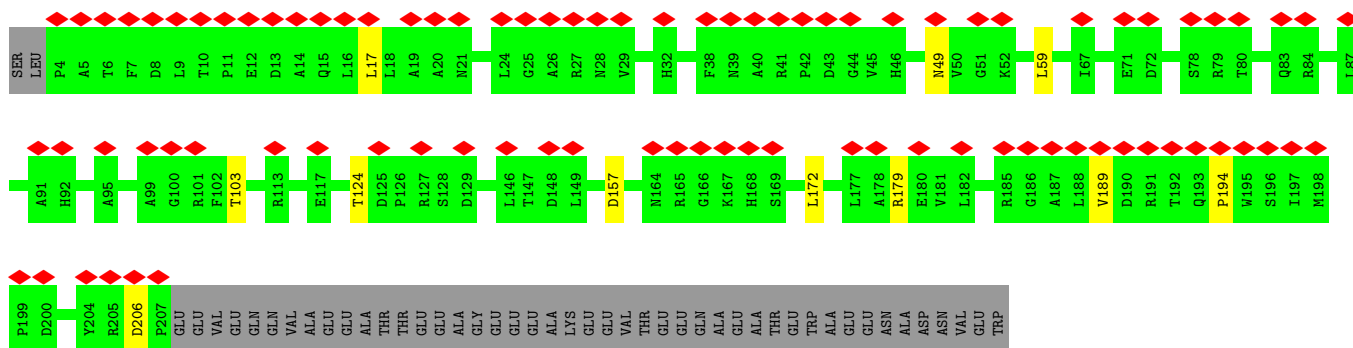
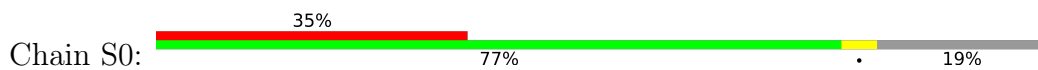
• Molecule 14: 18S ribosomal RNA



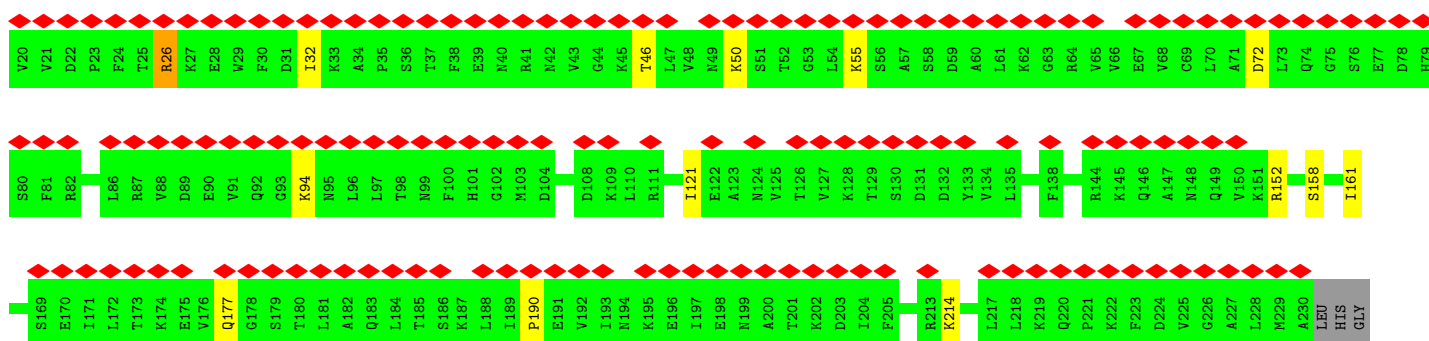
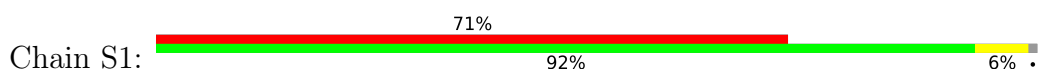




• Molecule 15: Small ribosomal subunit protein uS2A

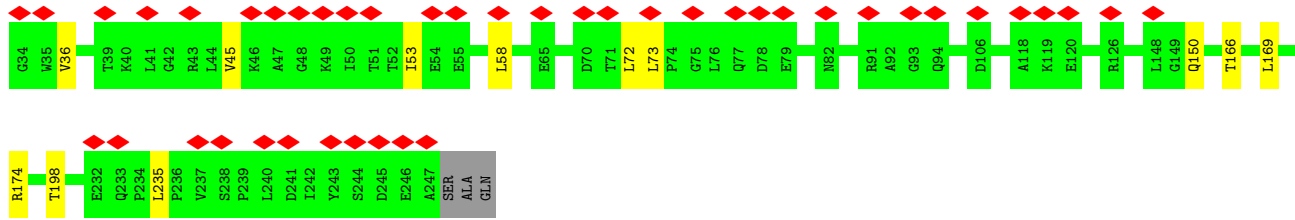


• Molecule 16: Small ribosomal subunit protein eS1

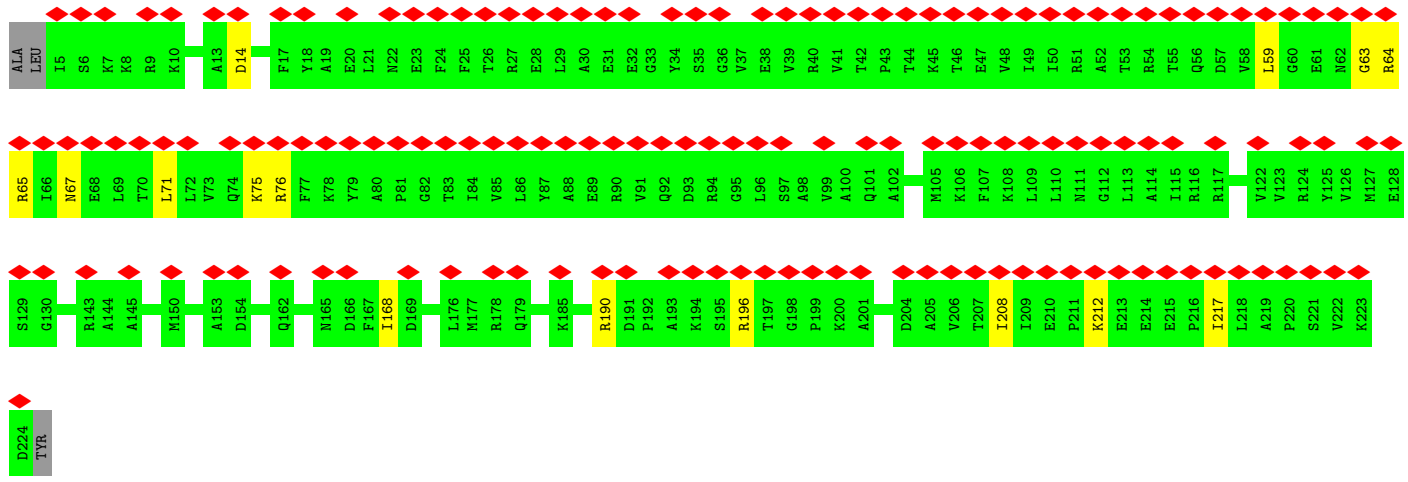
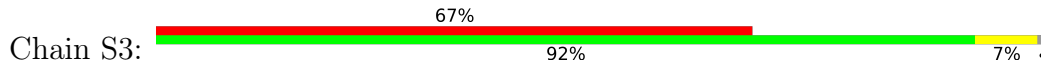


• Molecule 17: RPS2 isoform 1

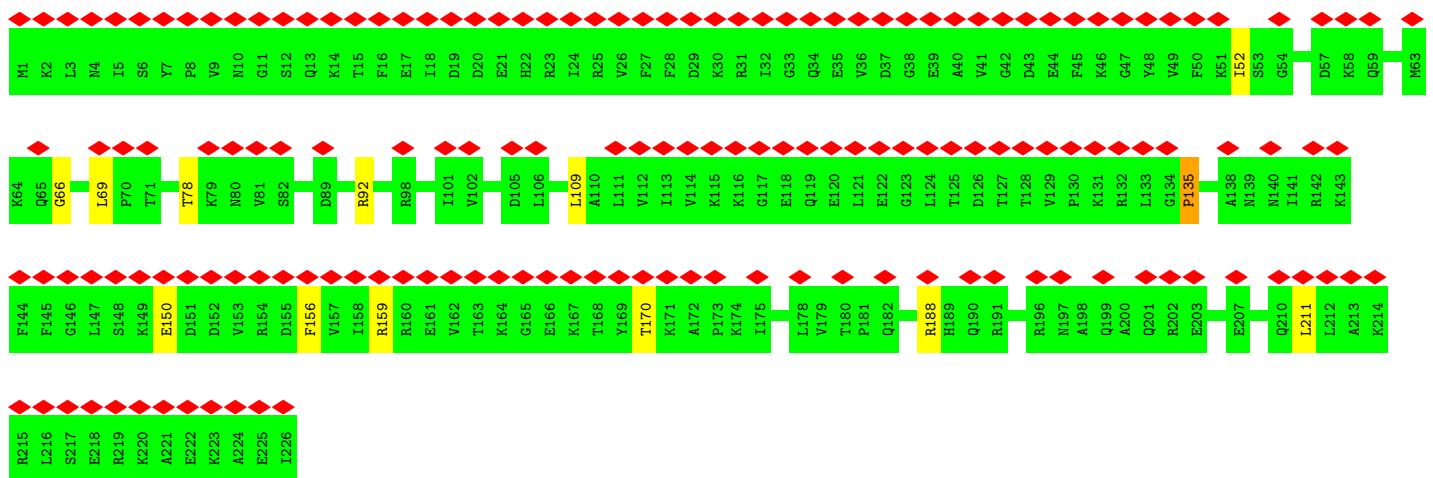




• Molecule 18: 40S ribosomal protein S3

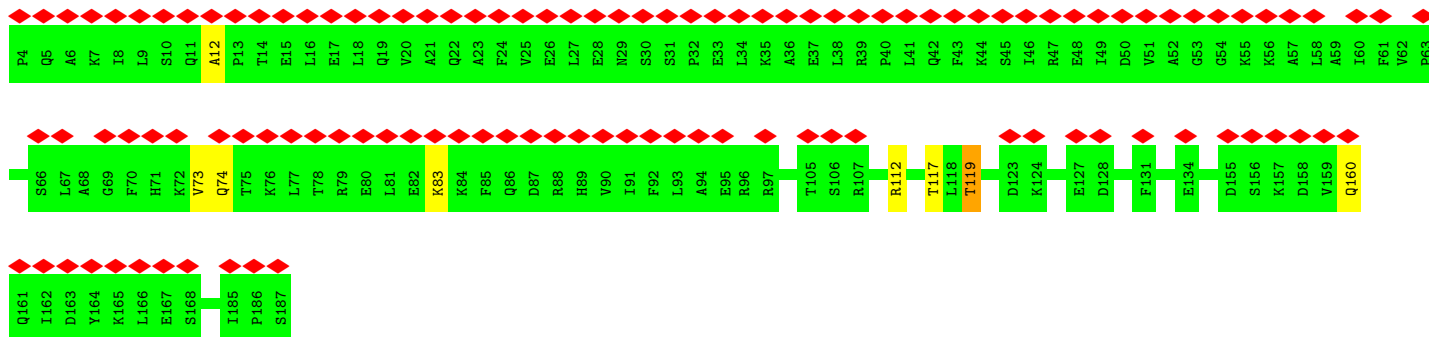


• Molecule 19: Small ribosomal subunit protein eS6A

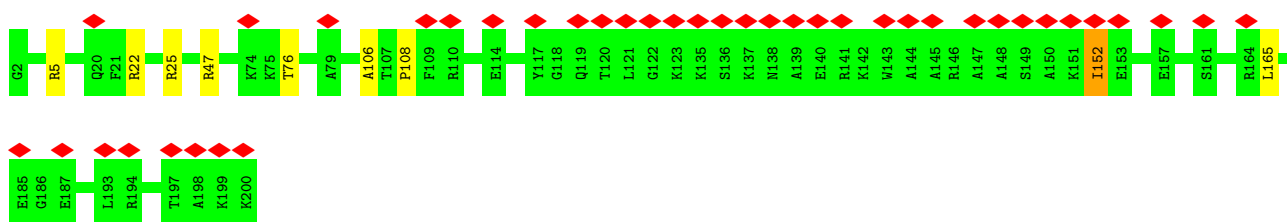


• Molecule 20: 40S ribosomal protein S7-A

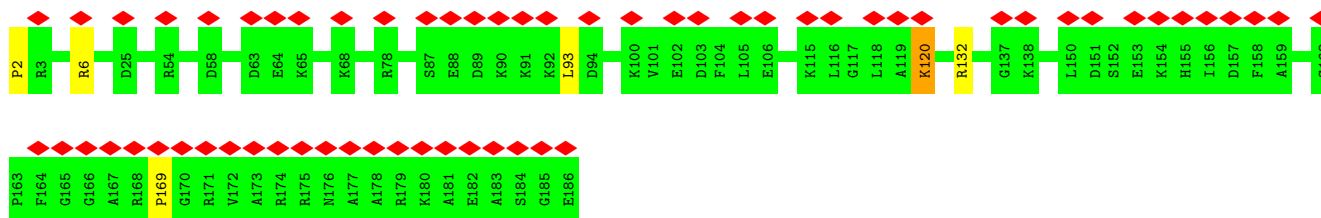




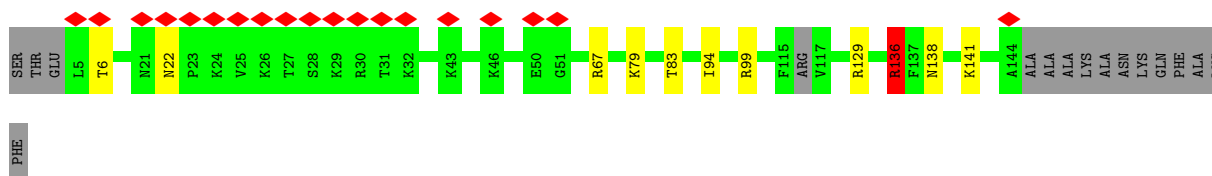
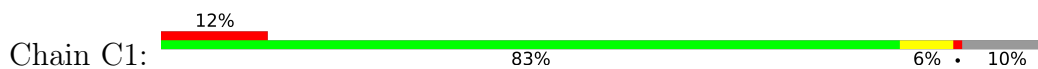
• Molecule 21: 40S ribosomal protein S8



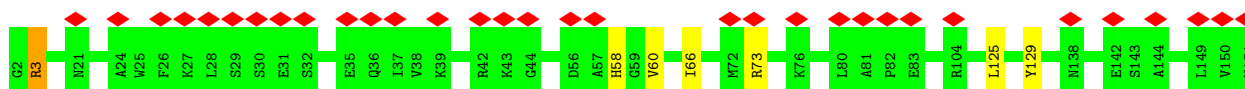
• Molecule 22: Small ribosomal subunit protein uS4A



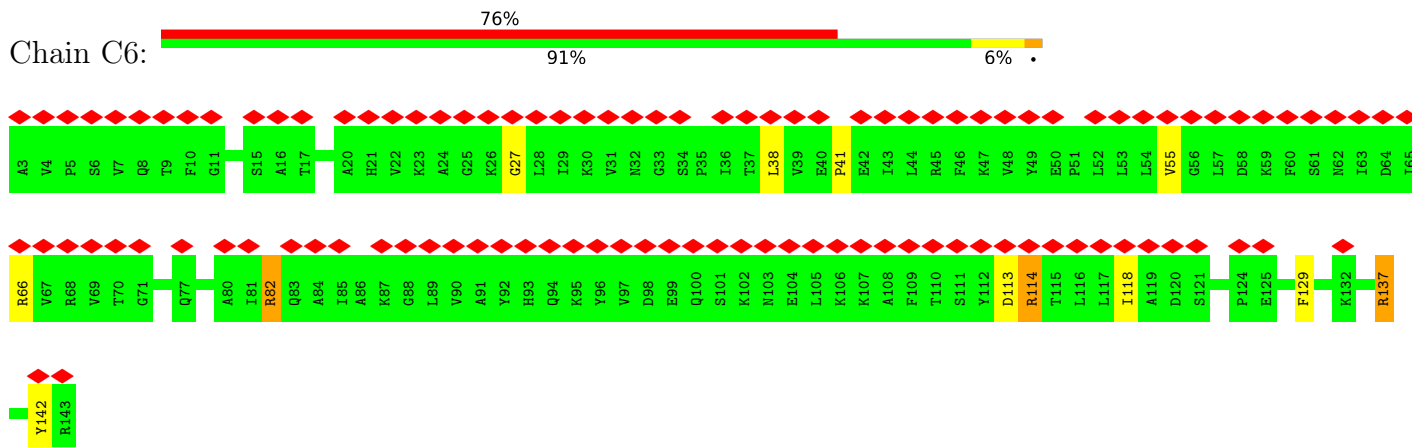
• Molecule 23: Small ribosomal subunit protein uS17A



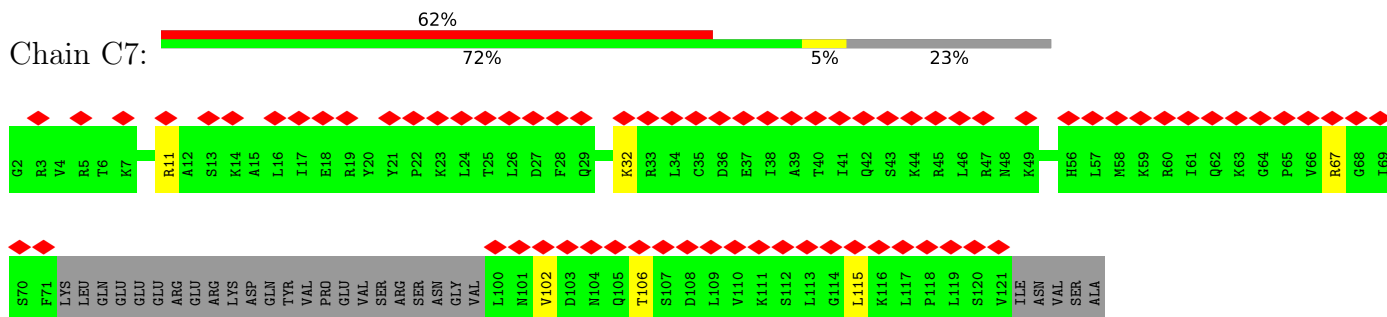
• Molecule 24: 40S ribosomal protein S13



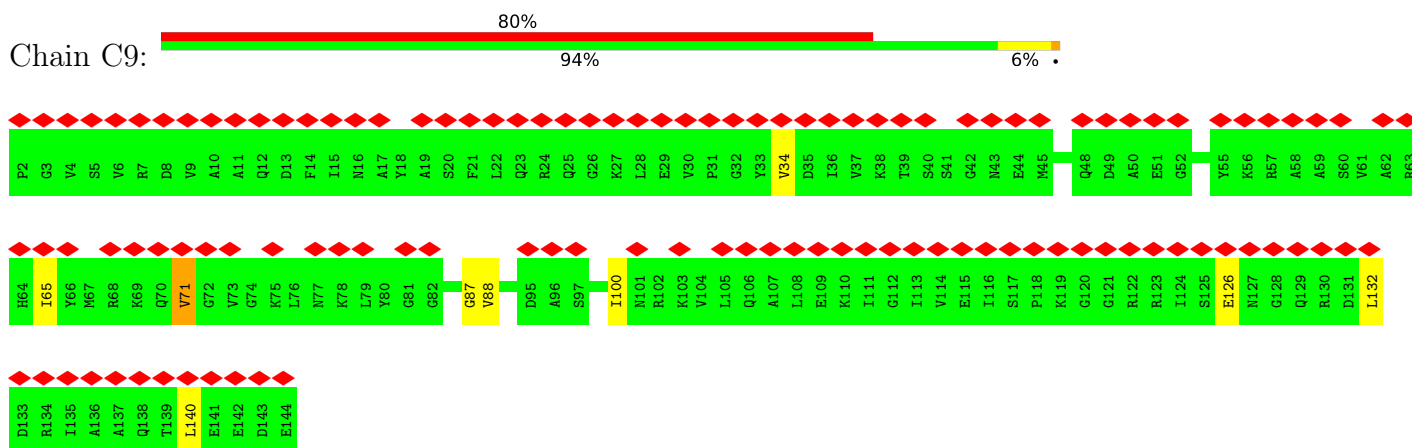
- Molecule 25: 40S ribosomal protein S16-A



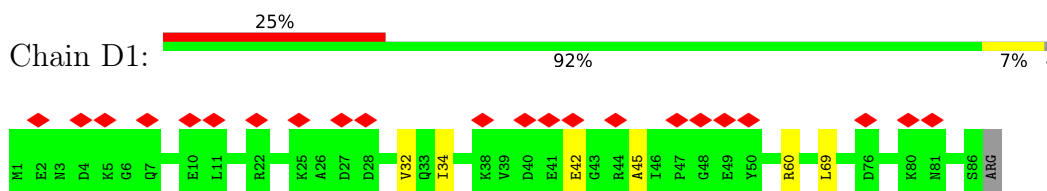
- Molecule 26: ES17



- Molecule 27: 40S ribosomal protein S19-A



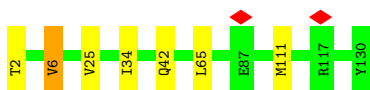
- Molecule 28: Small ribosomal subunit protein eS21A



- Molecule 29: RPS22A isoform 1

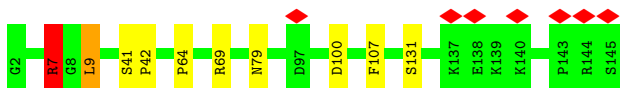


Chain D2:  95% 5%



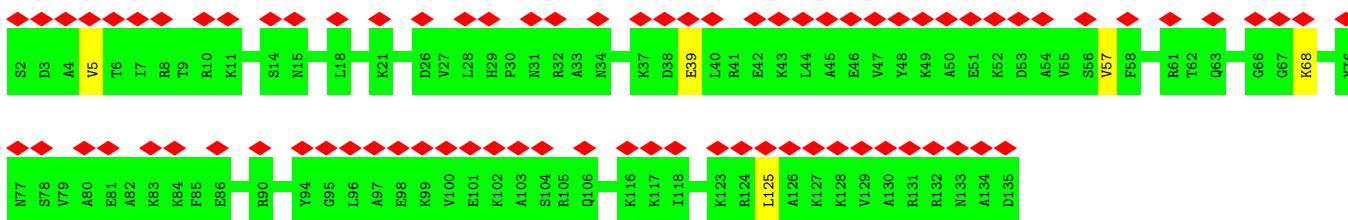
- Molecule 30: 40S ribosomal protein S23-A

Chain D3:  5% 93% 6%




- Molecule 31: 40S ribosomal protein S24-A

Chain D4:  60% 96%



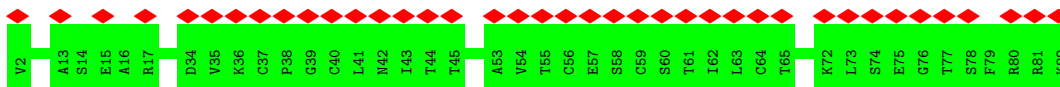
- Molecule 32: RPS26B isoform 1

Chain D6:  20% 88% 8%




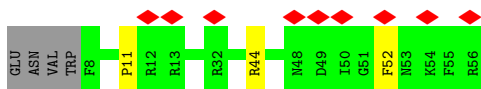
- Molecule 33: 40S ribosomal protein S27-A

Chain D7:  48% 100%



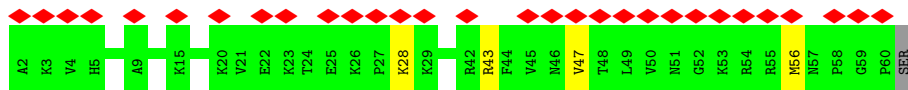
- Molecule 34: RPS29A isoform 1

Chain D9:  17% 87% 6% 8%

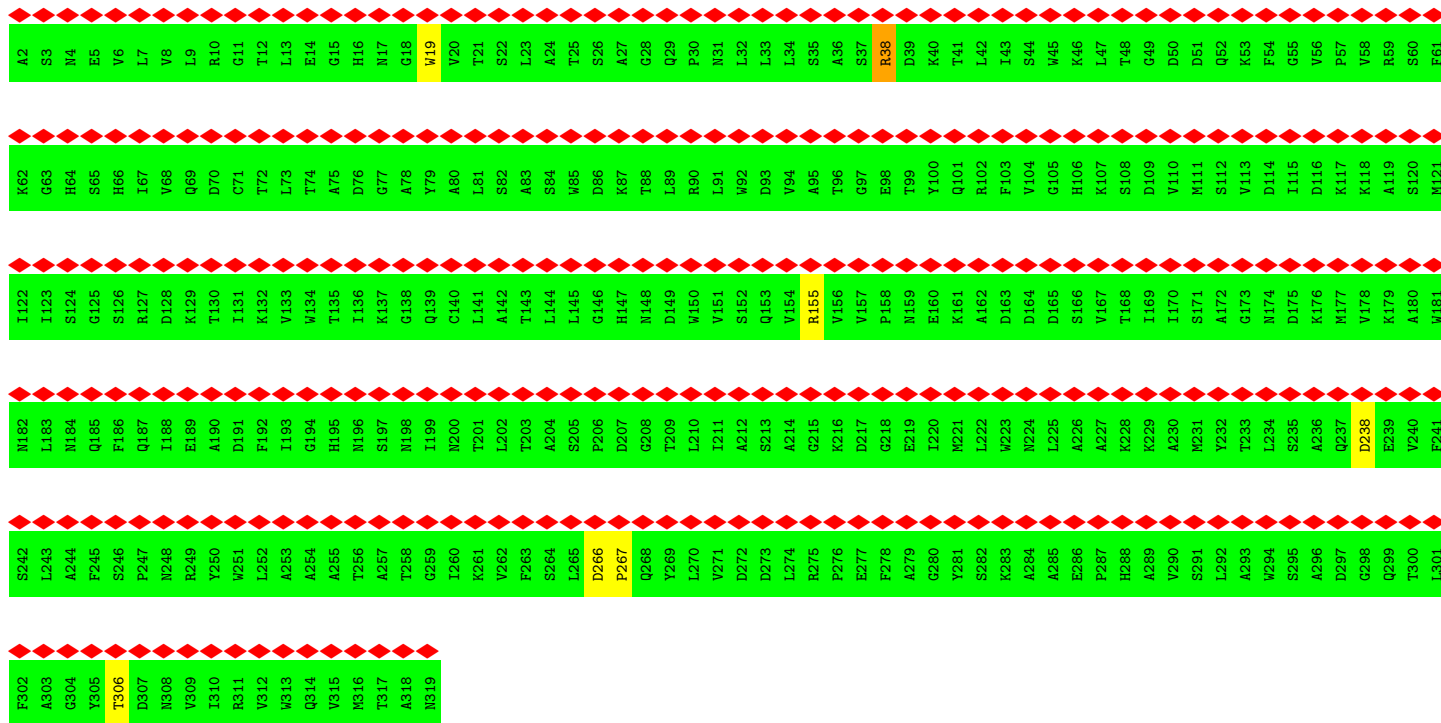


- Molecule 35: 40S ribosomal protein S30-A

Chain E0:  50% 92% 7%



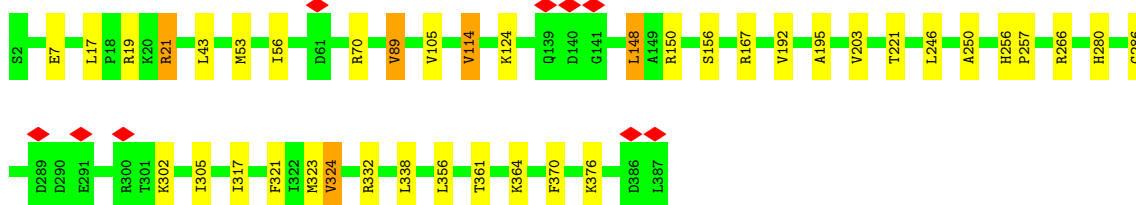
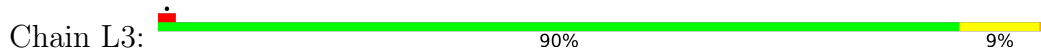
• Molecule 36: Small ribosomal subunit protein RACK1



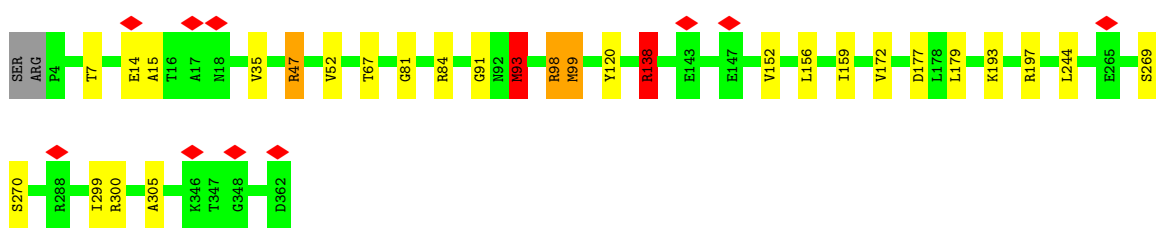
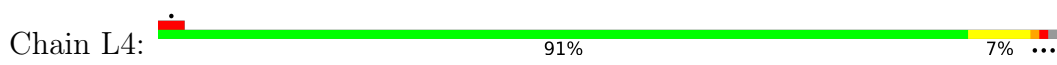
• Molecule 37: 60S ribosomal protein L2-A



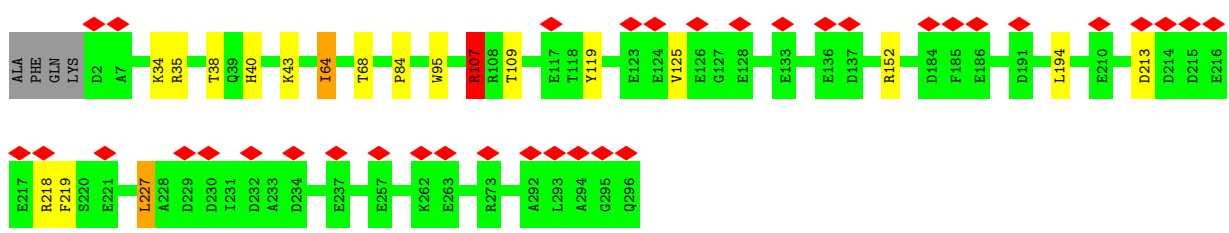
• Molecule 38: 60S ribosomal protein L3



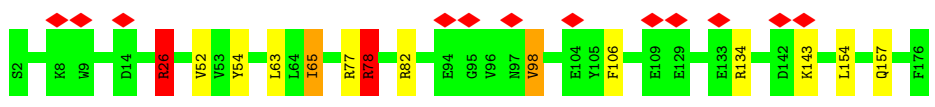
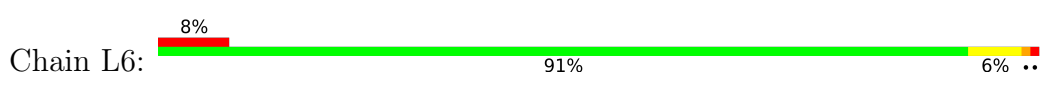
• Molecule 39: RPL4A isoform 1



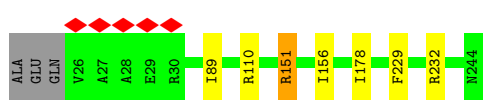
• Molecule 40: RPL5 isoform 1



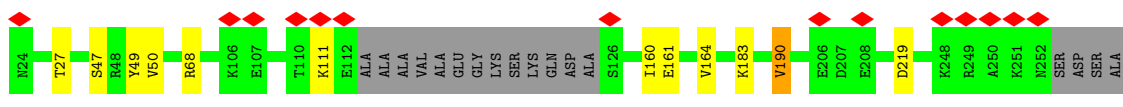
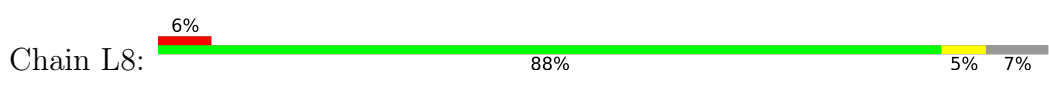
• Molecule 41: 60S ribosomal protein L6-A



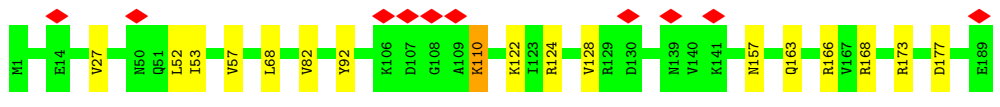
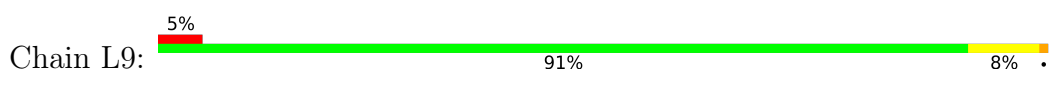
• Molecule 42: 60S ribosomal protein L7-A



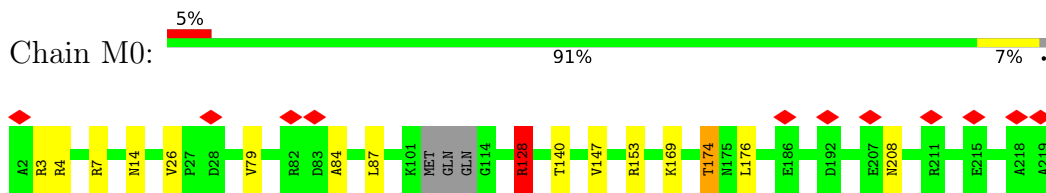
• Molecule 43: 60S ribosomal protein L8-A



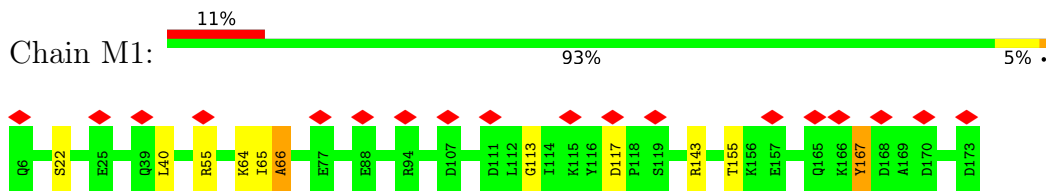
• Molecule 44: RPL9A isoform 1



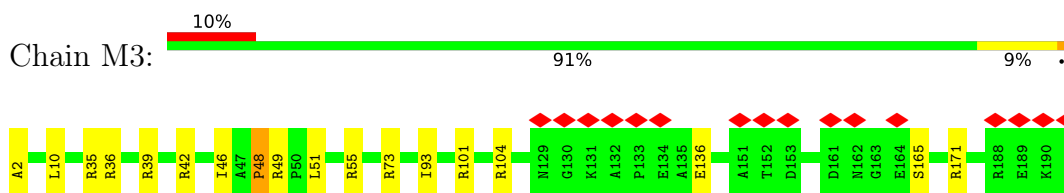
- Molecule 45: RPL10 isoform 1



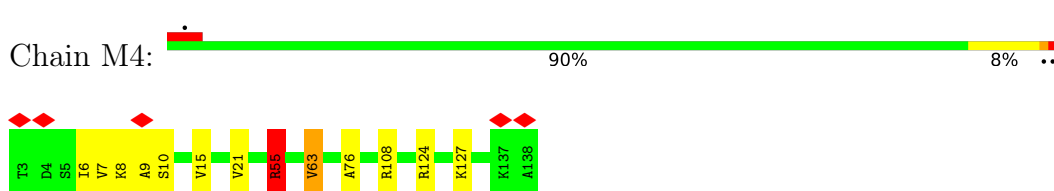
- Molecule 46: RPL11B isoform 1



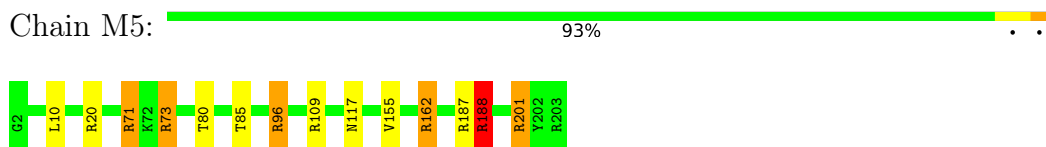
- Molecule 47: 60S ribosomal protein L13-A



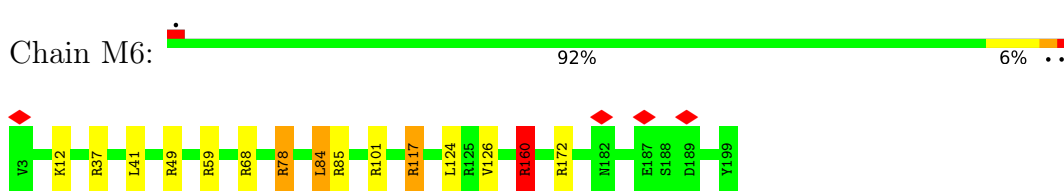
- Molecule 48: 60S ribosomal protein L14-A



- Molecule 49: Ribosomal protein L15

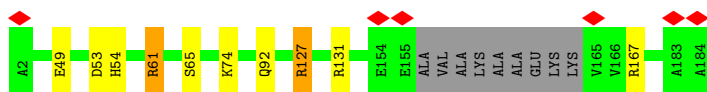


- Molecule 50: 60S ribosomal protein L16-A



- Molecule 51: 60S ribosomal protein L17-A





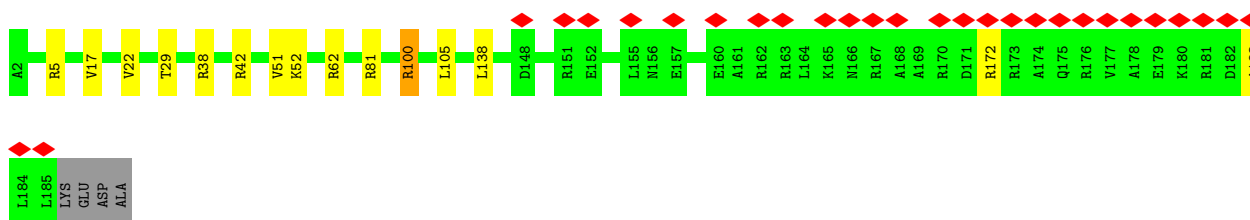
- Molecule 52: 60S ribosomal protein L18-A

Chain M8: 91% 6%



- Molecule 53: 60S ribosomal protein L19-A

Chain M9: 15% 90% 7%



- Molecule 54: 60S ribosomal protein L20-A

Chain N0: 92% 7%



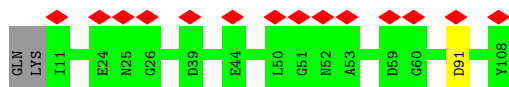
- Molecule 55: 60S ribosomal protein L21-A

Chain N1: 94% 6%



- Molecule 56: 60S ribosomal protein L22-A

Chain N2: 14% 97%

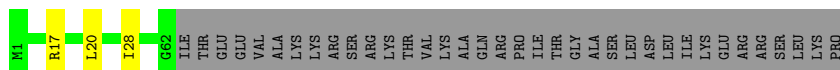


- Molecule 57: 60S ribosomal protein L23-A

Chain N3: 91% 7%



- Molecule 58: RPL24A isoform 1



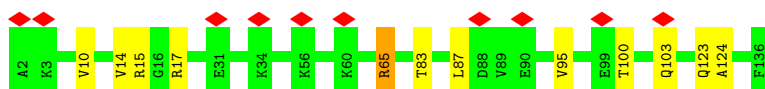
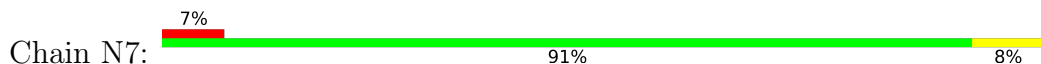
- Molecule 59: 60S ribosomal protein L25



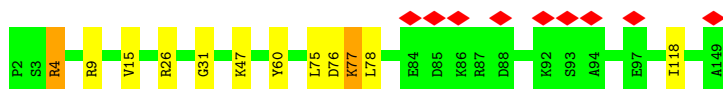
- Molecule 60: Large ribosomal subunit protein uL24A



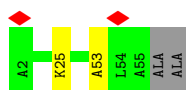
- Molecule 61: 60S ribosomal protein L27-A



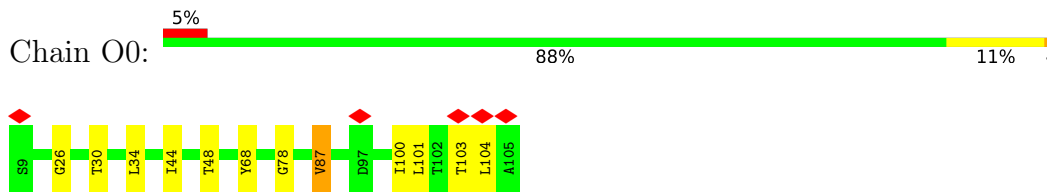
- Molecule 62: 60S ribosomal protein L28



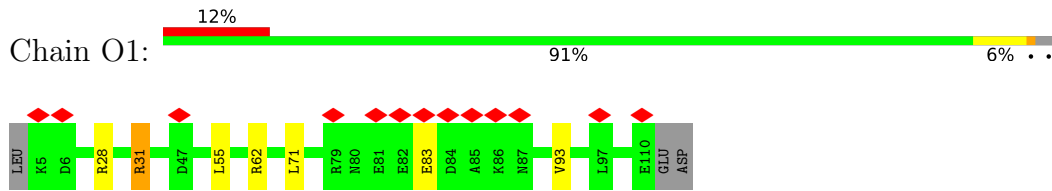
- Molecule 63: 60S ribosomal protein L29



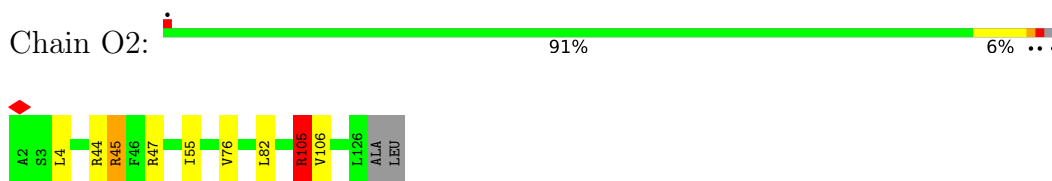
- Molecule 64: 60S ribosomal protein L30



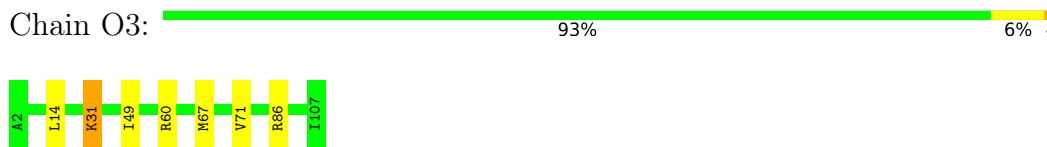
- Molecule 65: 60S ribosomal protein L31-A



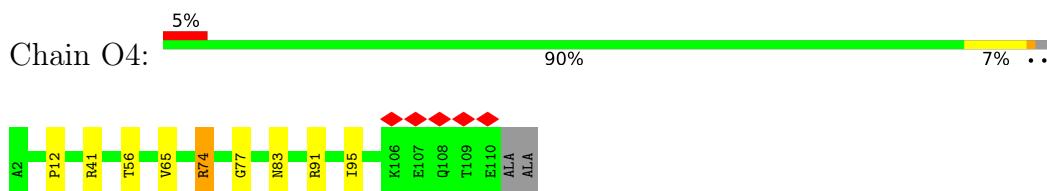
- Molecule 66: RPL32 isoform 1



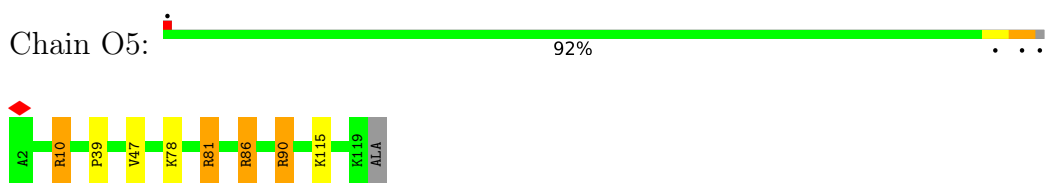
- Molecule 67: 60S ribosomal protein L33-A



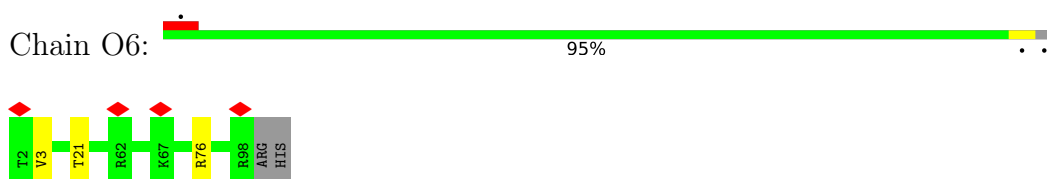
- Molecule 68: Large ribosomal subunit protein eL34A



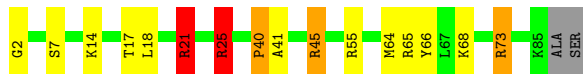
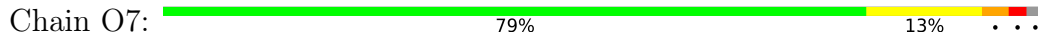
- Molecule 69: 60S ribosomal protein L35-A



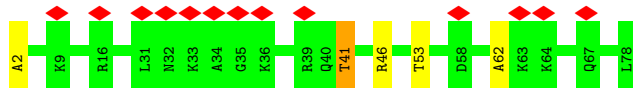
- Molecule 70: 60S ribosomal protein L36-A



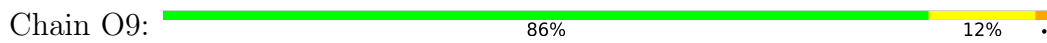
• Molecule 71: Large ribosomal subunit protein eL37A



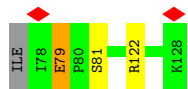
• Molecule 72: RPL38 isoform 1



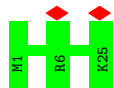
• Molecule 73: 60S ribosomal protein L39



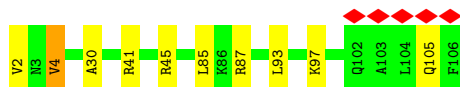
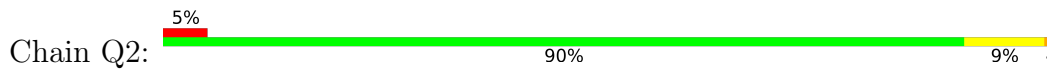
• Molecule 74: 60S ribosomal protein L40-A



• Molecule 75: Large ribosomal subunit protein eL41B



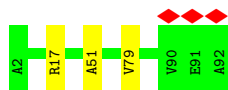
• Molecule 76: 60S ribosomal protein L42-A



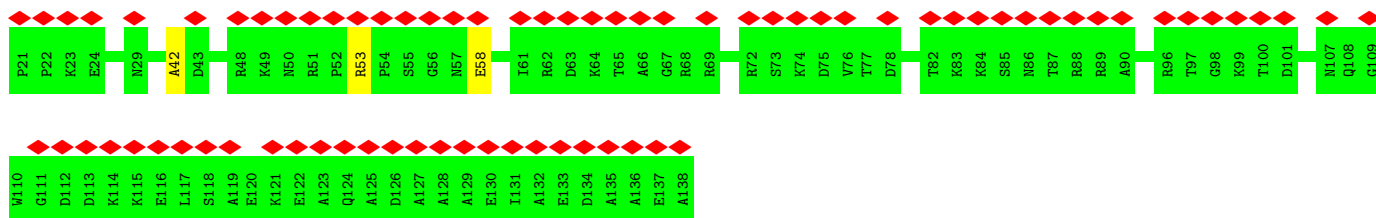
• Molecule 77: 60S ribosomal protein L43-A







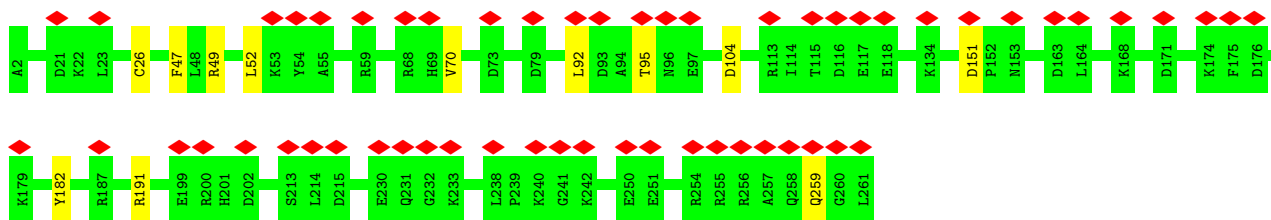
- Molecule 78: STM1 isoform 1



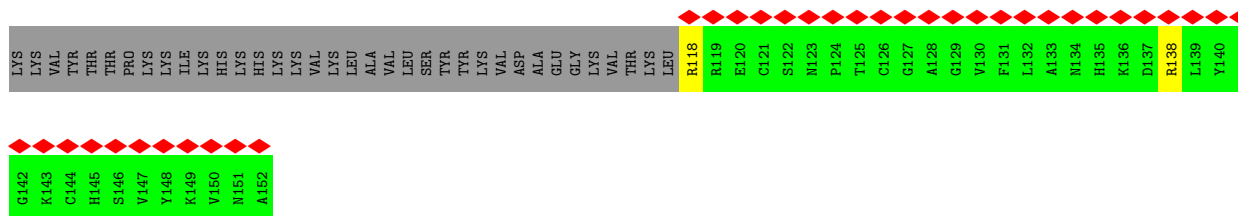
- Molecule 79: Eukaryotic translation initiation factor 5A



- Molecule 80: Small ribosomal subunit protein eS4A



- Molecule 81: RPS31 isoform 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0143	Depositor
Map size (Å)	375.84, 375.84, 375.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.783, 0.783, 0.783	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3HE, SPD, MG, 5CT, ZN, 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	B	0.35	0/1737	0.74	0/2332
2	S5	0.33	0/1629	0.68	0/2202
3	C0	0.35	0/838	0.74	0/1133
4	C4	0.38	0/944	0.77	1/1268 (0.1%)
5	C5	0.37	0/931	0.77	2/1250 (0.2%)
6	C8	0.33	0/1211	0.74	1/1628 (0.1%)
7	D0	0.31	0/865	0.69	0/1169
8	D5	0.35	0/571	0.75	0/768
9	D8	0.34	0/492	0.80	0/659
10	P	0.35	0/147	1.04	0/189
11	3	0.60	0/2883	1.28	15/4491 (0.3%)
12	4	0.64	0/3746	1.33	20/5832 (0.3%)
13	1	0.69	0/75240	1.39	602/117303 (0.5%)
14	2	0.59	0/41395	1.24	175/64501 (0.3%)
15	S0	0.35	0/1639	0.80	0/2241
16	S1	0.35	0/1712	0.83	1/2304 (0.0%)
17	S2	0.35	0/1645	0.77	0/2236
18	S3	0.35	0/1733	0.82	1/2332 (0.0%)
19	S6	0.35	0/1844	0.80	0/2464
20	S7	0.33	0/1506	0.76	1/2028 (0.0%)
21	S8	0.36	0/1514	0.84	0/2021
22	S9	0.34	0/1519	0.81	1/2035 (0.0%)
23	C1	0.37	0/1146	0.79	0/1544
24	C3	0.34	0/1215	0.75	0/1638
25	C6	0.36	0/1125	0.81	0/1510
26	C7	0.36	0/744	0.76	0/995
27	C9	0.36	0/1130	0.74	0/1517
28	D1	0.35	0/682	0.80	0/921
29	D2	0.34	0/1038	0.78	2/1395 (0.1%)
30	D3	0.37	0/1139	0.92	4/1518 (0.3%)
31	D4	0.34	0/1087	0.80	0/1449
32	D6	0.37	0/782	0.91	1/1047 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	D7	0.34	0/620	0.73	0/838
34	D9	0.38	0/412	0.86	0/544
35	E0	0.35	0/477	0.86	2/635 (0.3%)
36	SR	0.34	0/2498	0.65	0/3398
37	L2	0.49	0/1943	1.02	8/2610 (0.3%)
38	L3	0.48	0/3150	0.97	4/4235 (0.1%)
39	L4	0.45	0/2783	0.91	8/3767 (0.2%)
40	L5	0.36	0/2377	0.79	1/3206 (0.0%)
41	L6	0.37	0/1260	0.81	2/1694 (0.1%)
42	L7	0.44	0/1798	0.85	2/2420 (0.1%)
43	L8	0.36	0/1737	0.80	2/2343 (0.1%)
44	L9	0.36	0/1523	0.84	1/2051 (0.0%)
45	M0	0.41	0/1713	0.91	2/2297 (0.1%)
46	M1	0.36	0/1365	0.85	1/1831 (0.1%)
47	M3	0.44	0/1568	0.94	3/2106 (0.1%)
48	M4	0.36	0/1068	0.84	1/1438 (0.1%)
49	M5	0.52	0/1748	1.08	8/2343 (0.3%)
50	M6	0.49	0/1585	1.05	9/2128 (0.4%)
51	M7	0.51	0/1401	1.01	4/1882 (0.2%)
52	M8	0.44	0/1465	1.03	5/1965 (0.3%)
53	M9	0.45	0/1507	0.90	5/2009 (0.2%)
54	N0	0.43	0/1481	0.91	3/1990 (0.2%)
55	N1	0.47	0/1292	0.88	0/1732
56	N2	0.35	0/794	0.79	0/1076
57	N3	0.47	0/1018	0.98	4/1369 (0.3%)
58	N4	0.44	0/525	0.80	0/696
59	N5	0.40	0/969	0.89	2/1307 (0.2%)
60	N6	0.43	0/1004	0.89	2/1341 (0.1%)
61	N7	0.36	0/1118	0.85	2/1497 (0.1%)
62	N8	0.51	0/1204	0.94	4/1612 (0.2%)
63	N9	0.43	0/445	0.98	0/593
64	O0	0.37	0/751	0.77	0/1008
65	O1	0.45	0/879	0.95	2/1179 (0.2%)
66	O2	0.49	0/1028	1.02	4/1376 (0.3%)
67	O3	0.47	0/868	0.85	1/1168 (0.1%)
68	O4	0.47	0/871	0.96	3/1164 (0.3%)
69	O5	0.38	0/973	0.95	4/1294 (0.3%)
70	O6	0.38	0/756	0.91	0/1005
71	O7	0.57	0/691	1.28	8/915 (0.9%)
72	O8	0.37	0/618	0.78	0/826
73	O9	0.49	0/443	1.07	2/588 (0.3%)
74	Q0	0.39	0/415	0.90	2/551 (0.4%)
75	Q1	0.39	0/234	1.04	0/300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Q2	0.41	0/860	0.99	2/1136 (0.2%)
77	Q3	0.45	0/701	0.88	0/934
78	SM	0.35	0/903	0.75	0/1210
79	eI	0.36	0/1095	0.79	0/1473
80	S4	0.34	0/2109	0.79	0/2839
81	E1	0.39	0/276	0.74	1/368 (0.3%)
All	All	0.56	0/214148	1.18	941/314207 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	S5	0	2
4	C4	0	3
6	C8	0	2
8	D5	0	1
9	D8	0	1
13	1	0	9
15	S0	0	1
16	S1	0	1
17	S2	0	1
20	S7	0	1
21	S8	0	2
22	S9	0	1
23	C1	0	3
24	C3	0	1
25	C6	0	2
30	D3	0	2
32	D6	0	2
34	D9	0	1
36	SR	0	3
37	L2	0	5
38	L3	0	3
39	L4	0	5
40	L5	0	3
41	L6	0	5
42	L7	0	3
43	L8	0	1
44	L9	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	M0	0	2
47	M3	0	6
48	M4	0	1
49	M5	0	7
50	M6	0	6
51	M7	0	3
52	M8	0	4
53	M9	0	3
54	N0	0	5
55	N1	0	2
57	N3	0	3
58	N4	0	1
59	N5	0	2
60	N6	0	2
61	N7	0	2
62	N8	0	3
65	O1	0	2
66	O2	0	4
67	O3	0	2
69	O5	0	3
71	O7	0	4
73	O9	0	1
76	Q2	0	1
80	S4	0	2
All	All	0	141

There are no bond length outliers.

The worst 5 of 941 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	2403	G	O5'-P-OP2	-23.53	82.47	110.70
13	1	806	A	O5'-P-OP1	-19.93	86.78	110.70
13	1	1639	C	O5'-P-OP2	-19.57	87.22	110.70
13	1	2373	A	O5'-P-OP1	-17.61	89.57	110.70
13	1	1117	G	O5'-P-OP1	-17.14	90.13	110.70

There are no chirality outliers.

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	60	ARG	Sidechain
4	C4	114	ARG	Sidechain
2	S5	225	ARG	Sidechain
2	S5	76	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1710	0	1799	22	0
2	S5	1609	0	1675	2	0
3	C0	818	0	806	10	0
4	C4	933	0	968	12	0
5	C5	912	0	946	6	0
6	C8	1192	0	1222	7	0
7	D0	855	0	917	6	0
8	D5	563	0	603	4	0
9	D8	490	0	529	0	0
10	P	146	0	174	0	0
11	3	2579	0	1303	1	0
12	4	3353	0	1695	7	0
13	1	67219	0	33762	72	0
14	2	37011	0	18622	55	0
15	S0	1598	0	1608	2	0
16	S1	1687	0	1763	4	0
17	S2	1615	0	1705	3	0
18	S3	1709	0	1792	2	0
19	S6	1820	0	1918	5	0
20	S7	1481	0	1572	0	0
21	S8	1489	0	1525	3	0
22	S9	1494	0	1573	1	0
23	C1	1121	0	1188	2	0
24	C3	1192	0	1255	2	0
25	C6	1105	0	1166	2	0
26	C7	737	0	802	1	0
27	C9	1112	0	1124	1	0
28	D1	673	0	659	2	0
29	D2	1021	0	1060	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D3	1121	0	1196	3	0
31	D4	1073	0	1132	0	0
32	D6	769	0	814	6	0
33	D7	610	0	633	0	0
34	D9	404	0	397	1	0
35	E0	469	0	520	0	0
36	SR	2445	0	2401	2	0
37	L2	1909	0	1979	8	0
38	L3	3079	0	3157	15	0
39	L4	2731	0	2842	13	0
40	L5	2329	0	2279	6	0
41	L6	1239	0	1326	5	0
42	L7	1761	0	1843	1	0
43	L8	1706	0	1802	5	0
44	L9	1502	0	1572	5	0
45	M0	1677	0	1715	7	0
46	M1	1344	0	1370	2	0
47	M3	1543	0	1608	5	0
48	M4	1053	0	1149	4	0
49	M5	1711	0	1765	6	0
50	M6	1555	0	1659	2	0
51	M7	1379	0	1410	3	0
52	M8	1441	0	1543	11	0
53	M9	1490	0	1589	1	0
54	N0	1445	0	1487	3	0
55	N1	1268	0	1312	3	0
56	N2	778	0	791	0	0
57	N3	1003	0	1048	4	0
58	N4	513	0	540	1	0
59	N5	954	0	1018	3	0
60	N6	993	0	1081	1	0
61	N7	1092	0	1155	3	0
62	N8	1173	0	1215	3	0
63	N9	434	0	454	0	0
64	O0	743	0	797	4	0
65	O1	865	0	917	2	0
66	O2	1007	0	1074	2	0
67	O3	850	0	880	2	0
68	O4	861	0	918	4	0
69	O5	964	0	1073	3	0
70	O6	750	0	829	0	0
71	O7	676	0	678	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	O8	612	0	682	6	0
73	O9	436	0	475	4	0
74	Q0	409	0	444	0	0
75	Q1	233	0	284	0	0
76	Q2	847	0	914	3	0
77	Q3	694	0	734	2	0
78	SM	893	0	895	0	0
79	eI	1096	0	1094	0	0
80	S4	2068	0	2154	2	0
81	E1	271	0	263	2	0
82	1	191	0	0	0	0
82	2	19	0	0	0	0
82	3	3	0	0	0	0
82	4	2	0	0	0	0
82	L3	1	0	0	0	0
82	M7	1	0	0	0	0
82	N3	1	0	0	0	0
82	O2	1	0	0	0	0
82	O7	1	0	0	0	0
83	1	63	0	0	0	0
83	2	1	0	0	0	0
83	L2	2	0	0	0	0
83	L4	1	0	0	0	0
83	M0	1	0	0	0	0
83	M5	1	0	0	0	0
83	N9	1	0	0	0	0
83	O4	1	0	0	0	0
83	O7	1	0	0	0	0
84	1	20	0	23	0	0
85	1	30	0	57	0	0
86	D6	1	0	0	0	0
86	D9	1	0	0	0	0
86	O4	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q0	1	0	0	0	0
86	Q2	1	0	0	0	0
86	Q3	1	0	0	0	0
87	1	1466	0	0	0	0
87	2	45	0	0	0	0
87	3	12	0	0	0	0
87	4	40	0	0	1	0
87	C3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	L2	30	0	0	0	0
87	L3	21	0	0	0	0
87	L4	16	0	0	0	0
87	L5	3	0	0	0	0
87	L6	1	0	0	0	0
87	L7	10	0	0	0	0
87	M0	3	0	0	0	0
87	M3	3	0	0	0	0
87	M5	19	0	0	0	0
87	M6	9	0	0	0	0
87	M7	13	0	0	0	0
87	M8	10	0	0	0	0
87	M9	5	0	0	0	0
87	N0	3	0	0	0	0
87	N1	6	0	0	0	0
87	N3	4	0	0	0	0
87	N4	1	0	0	0	0
87	N5	4	0	0	0	0
87	N8	15	0	0	0	0
87	N9	5	0	0	0	0
87	O1	4	0	0	0	0
87	O2	20	0	0	0	0
87	O3	5	0	0	0	0
87	O4	6	0	0	0	0
87	O6	1	0	0	0	0
87	O7	11	0	0	0	0
87	O8	1	0	0	0	0
87	O9	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	9	0	0	1	0
87	Q3	4	0	0	0	0
87	eI	1	0	0	0	0
All	All	201671	0	148718	320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 320 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:O	1:B:89:ASP:N	1.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:1639:C:OP2	68:O4:74:ARG:NH2	1.99	0.94
52:M8:71:LEU:HD13	52:M8:99:THR:HG21	1.48	0.93
4:C4:39:ILE:HD13	4:C4:76:ILE:HD11	1.60	0.83
1:B:76:ARG:HH22	1:B:140:HIS:HA	1.49	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	214/217 (99%)	195 (91%)	14 (6%)	5 (2%)	6	7
2	S5	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	29	41
3	C0	94/96 (98%)	85 (90%)	5 (5%)	4 (4%)	2	2
4	C4	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
5	C5	113/124 (91%)	110 (97%)	2 (2%)	1 (1%)	17	25
6	C8	143/145 (99%)	138 (96%)	4 (3%)	1 (1%)	22	32
7	D0	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
8	D5	68/70 (97%)	65 (96%)	1 (2%)	2 (3%)	4	4
9	D8	60/63 (95%)	57 (95%)	2 (3%)	1 (2%)	9	11
10	P	13/15 (87%)	13 (100%)	0	0	100	100
15	S0	202/251 (80%)	179 (89%)	19 (9%)	4 (2%)	7	9
16	S1	209/214 (98%)	185 (88%)	20 (10%)	4 (2%)	8	10
17	S2	212/217 (98%)	196 (92%)	13 (6%)	3 (1%)	11	15
18	S3	218/223 (98%)	195 (89%)	19 (9%)	4 (2%)	8	10
19	S6	224/226 (99%)	198 (88%)	24 (11%)	2 (1%)	17	25
20	S7	182/184 (99%)	155 (85%)	23 (13%)	4 (2%)	6	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S8	184/188 (98%)	168 (91%)	14 (8%)	2 (1%)	14	20
22	S9	183/185 (99%)	164 (90%)	17 (9%)	2 (1%)	14	20
23	C1	135/155 (87%)	122 (90%)	10 (7%)	3 (2%)	6	7
24	C3	148/150 (99%)	136 (92%)	12 (8%)	0	100	100
25	C6	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3	3
26	C7	88/120 (73%)	79 (90%)	8 (9%)	1 (1%)	14	20
27	C9	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11	15
28	D1	84/87 (97%)	72 (86%)	10 (12%)	2 (2%)	6	6
29	D2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
30	D3	142/144 (99%)	132 (93%)	9 (6%)	1 (1%)	22	32
31	D4	132/134 (98%)	121 (92%)	9 (7%)	2 (2%)	10	14
32	D6	95/97 (98%)	81 (85%)	9 (10%)	5 (5%)	2	1
33	D7	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
34	D9	47/53 (89%)	41 (87%)	5 (11%)	1 (2%)	7	8
35	E0	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	3
36	SR	316/318 (99%)	304 (96%)	11 (4%)	1 (0%)	41	55
37	L2	249/252 (99%)	238 (96%)	11 (4%)	0	100	100
38	L3	384/386 (100%)	368 (96%)	15 (4%)	1 (0%)	41	55
39	L4	357/361 (99%)	335 (94%)	18 (5%)	4 (1%)	14	20
40	L5	288/295 (98%)	275 (96%)	11 (4%)	2 (1%)	22	32
41	L6	152/156 (97%)	144 (95%)	7 (5%)	1 (1%)	22	32
42	L7	217/222 (98%)	214 (99%)	2 (1%)	1 (0%)	29	41
43	L8	212/233 (91%)	203 (96%)	9 (4%)	0	100	100
44	L9	187/189 (99%)	180 (96%)	6 (3%)	1 (0%)	29	41
45	M0	202/209 (97%)	193 (96%)	9 (4%)	0	100	100
46	M1	166/168 (99%)	152 (92%)	8 (5%)	6 (4%)	3	3
47	M3	191/193 (99%)	180 (94%)	9 (5%)	2 (1%)	15	23
48	M4	134/136 (98%)	127 (95%)	3 (2%)	4 (3%)	4	3
49	M5	200/202 (99%)	195 (98%)	5 (2%)	0	100	100
50	M6	195/197 (99%)	193 (99%)	2 (1%)	0	100	100
51	M7	170/183 (93%)	163 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	M8	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	29	41
53	M9	182/188 (97%)	180 (99%)	1 (0%)	1 (0%)	29	41
54	N0	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25	36
55	N1	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	36
56	N2	96/100 (96%)	86 (90%)	9 (9%)	1 (1%)	15	23
57	N3	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
58	N4	60/98 (61%)	59 (98%)	1 (2%)	0	100	100
59	N5	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
60	N6	124/126 (98%)	117 (94%)	5 (4%)	2 (2%)	9	13
61	N7	133/135 (98%)	129 (97%)	3 (2%)	1 (1%)	19	29
62	N8	146/148 (99%)	134 (92%)	9 (6%)	3 (2%)	7	8
63	N9	52/56 (93%)	48 (92%)	2 (4%)	2 (4%)	3	2
64	O0	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	14	20
65	O1	104/109 (95%)	99 (95%)	4 (4%)	1 (1%)	15	23
66	O2	123/127 (97%)	117 (95%)	6 (5%)	0	100	100
67	O3	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
68	O4	107/111 (96%)	104 (97%)	2 (2%)	1 (1%)	17	25
69	O5	116/119 (98%)	114 (98%)	1 (1%)	1 (1%)	17	25
70	O6	95/99 (96%)	89 (94%)	4 (4%)	2 (2%)	7	8
71	O7	83/86 (96%)	77 (93%)	6 (7%)	0	100	100
72	O8	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
73	O9	48/50 (96%)	48 (100%)	0	0	100	100
74	Q0	49/52 (94%)	47 (96%)	0	2 (4%)	3	2
75	Q1	23/25 (92%)	23 (100%)	0	0	100	100
76	Q2	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
77	Q3	89/91 (98%)	83 (93%)	5 (6%)	1 (1%)	14	20
78	SM	116/118 (98%)	102 (88%)	12 (10%)	2 (2%)	9	11
79	eI	142/145 (98%)	127 (89%)	13 (9%)	2 (1%)	11	15
80	S4	258/260 (99%)	240 (93%)	16 (6%)	2 (1%)	19	29
81	E1	33/71 (46%)	33 (100%)	0	0	100	100
All	All	11102/11524 (96%)	10416 (94%)	571 (5%)	115 (1%)	20	23

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88	ASP
1	B	118	LYS
3	C0	85	HIS
16	S1	26	ARG
16	S1	50	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	197/198 (100%)	193 (98%)	4 (2%)	55	74
2	S5	173/173 (100%)	172 (99%)	1 (1%)	86	94
3	C0	89/89 (100%)	88 (99%)	1 (1%)	73	87
4	C4	95/96 (99%)	94 (99%)	1 (1%)	73	87
5	C5	95/104 (91%)	95 (100%)	0	100	100
6	C8	128/128 (100%)	127 (99%)	1 (1%)	81	91
7	D0	100/100 (100%)	100 (100%)	0	100	100
8	D5	61/61 (100%)	61 (100%)	0	100	100
9	D8	55/56 (98%)	55 (100%)	0	100	100
10	P	14/14 (100%)	14 (100%)	0	100	100
15	S0	171/209 (82%)	168 (98%)	3 (2%)	59	76
16	S1	189/191 (99%)	186 (98%)	3 (2%)	62	79
17	S2	174/176 (99%)	172 (99%)	2 (1%)	73	87
18	S3	180/182 (99%)	172 (96%)	8 (4%)	28	45
19	S6	193/193 (100%)	188 (97%)	5 (3%)	46	66
20	S7	165/165 (100%)	162 (98%)	3 (2%)	59	76
21	S8	150/150 (100%)	148 (99%)	2 (1%)	69	84
22	S9	158/158 (100%)	156 (99%)	2 (1%)	69	84
23	C1	125/136 (92%)	120 (96%)	5 (4%)	31	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	C3	127/127 (100%)	124 (98%)	3 (2%)	49	68
25	C6	117/117 (100%)	113 (97%)	4 (3%)	37	56
26	C7	83/109 (76%)	80 (96%)	3 (4%)	35	54
27	C9	115/115 (100%)	109 (95%)	6 (5%)	23	38
28	D1	73/74 (99%)	72 (99%)	1 (1%)	67	82
29	D2	110/110 (100%)	109 (99%)	1 (1%)	78	90
30	D3	119/119 (100%)	114 (96%)	5 (4%)	30	47
31	D4	112/112 (100%)	109 (97%)	3 (3%)	44	65
32	D6	83/83 (100%)	82 (99%)	1 (1%)	71	85
33	D7	70/70 (100%)	70 (100%)	0	100	100
34	D9	43/47 (92%)	43 (100%)	0	100	100
35	E0	50/51 (98%)	49 (98%)	1 (2%)	55	74
36	SR	261/261 (100%)	260 (100%)	1 (0%)	91	96
37	L2	193/194 (100%)	190 (98%)	3 (2%)	62	79
38	L3	322/322 (100%)	307 (95%)	15 (5%)	26	42
39	L4	286/288 (99%)	280 (98%)	6 (2%)	53	72
40	L5	239/243 (98%)	232 (97%)	7 (3%)	42	62
41	L6	134/134 (100%)	131 (98%)	3 (2%)	52	71
42	L7	184/186 (99%)	182 (99%)	2 (1%)	73	87
43	L8	181/191 (95%)	177 (98%)	4 (2%)	52	71
44	L9	169/169 (100%)	165 (98%)	4 (2%)	49	68
45	M0	176/179 (98%)	171 (97%)	5 (3%)	43	63
46	M1	146/146 (100%)	143 (98%)	3 (2%)	53	72
47	M3	154/154 (100%)	151 (98%)	3 (2%)	57	75
48	M4	107/107 (100%)	103 (96%)	4 (4%)	34	53
49	M5	174/174 (100%)	170 (98%)	4 (2%)	50	70
50	M6	160/160 (100%)	155 (97%)	5 (3%)	40	60
51	M7	140/145 (97%)	137 (98%)	3 (2%)	53	72
52	M8	150/150 (100%)	147 (98%)	3 (2%)	55	74
53	M9	150/153 (98%)	144 (96%)	6 (4%)	31	49
54	N0	156/156 (100%)	152 (97%)	4 (3%)	46	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	N1	135/136 (99%)	132 (98%)	3 (2%)	52	71
56	N2	85/87 (98%)	85 (100%)	0	100	100
57	N3	104/104 (100%)	101 (97%)	3 (3%)	42	62
58	N4	54/86 (63%)	54 (100%)	0	100	100
59	N5	104/105 (99%)	99 (95%)	5 (5%)	25	41
60	N6	109/109 (100%)	105 (96%)	4 (4%)	34	53
61	N7	115/115 (100%)	111 (96%)	4 (4%)	36	55
62	N8	118/118 (100%)	116 (98%)	2 (2%)	60	78
63	N9	44/44 (100%)	44 (100%)	0	100	100
64	O0	81/81 (100%)	77 (95%)	4 (5%)	25	40
65	O1	93/96 (97%)	92 (99%)	1 (1%)	73	87
66	O2	108/109 (99%)	105 (97%)	3 (3%)	43	63
67	O3	90/90 (100%)	89 (99%)	1 (1%)	73	87
68	O4	94/94 (100%)	93 (99%)	1 (1%)	73	87
69	O5	104/104 (100%)	102 (98%)	2 (2%)	57	75
70	O6	79/81 (98%)	78 (99%)	1 (1%)	69	84
71	O7	70/70 (100%)	66 (94%)	4 (6%)	20	33
72	O8	68/68 (100%)	67 (98%)	1 (2%)	65	80
73	O9	45/45 (100%)	44 (98%)	1 (2%)	52	71
74	Q0	46/47 (98%)	46 (100%)	0	100	100
75	Q1	23/23 (100%)	23 (100%)	0	100	100
76	Q2	90/90 (100%)	85 (94%)	5 (6%)	21	34
77	Q3	71/71 (100%)	71 (100%)	0	100	100
78	SM	95/95 (100%)	94 (99%)	1 (1%)	73	87
79	eI	120/120 (100%)	118 (98%)	2 (2%)	60	78
80	S4	221/221 (100%)	217 (98%)	4 (2%)	59	76
81	E1	29/62 (47%)	29 (100%)	0	100	100
All	All	9491/9696 (98%)	9285 (98%)	206 (2%)	54	71

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	M0	87	LEU

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Mol	Chain	Res	Type
52	M8	86	THR
78	SM	58	GLU
46	M1	22	SER
49	M5	80	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
41	L6	157	GLN
80	S4	130	GLN
47	M3	19	GLN
78	SM	86	ASN
61	N7	57	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	3	120/121 (99%)	10 (8%)	2 (1%)
12	4	157/158 (99%)	21 (13%)	2 (1%)
13	1	3139/3162 (99%)	495 (15%)	93 (2%)
14	2	1735/1737 (99%)	467 (26%)	90 (5%)
All	All	5151/5178 (99%)	993 (19%)	187 (3%)

5 of 993 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	3	22	A
11	3	41	G
11	3	42	A
11	3	54	U
11	3	65	G

5 of 187 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	2	260	U
14	2	794	U
14	2	280	U
14	2	501	U
14	2	959	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
79	5CT	eI	51	79	13,14,15	0.45	0	9,15,17	1.09	1 (11%)

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
79	5CT	eI	51	79	-	6/13/14/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	eI	51	5CT	C4-C3-C2	2.76	119.29	113.47

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
79	eI	51	5CT	C1-C2-C3-C4
79	eI	51	5CT	O1-C2-C3-C4
79	eI	51	5CT	C2-C1-NZ-CE
79	eI	51	5CT	C2-C3-C4-N1
79	eI	51	5CT	NZ-C1-C2-O1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 299 are monoatomic - leaving 4 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
85	SPD	1	3467	-	9,9,9	0.24	0	8,8,8	0.32	0
85	SPD	1	3466	-	9,9,9	0.48	0	8,8,8	0.88	0
85	SPD	1	3465	-	9,9,9	0.26	0	8,8,8	0.34	0
84	3HE	1	3464	-	21,21,21	0.72	0	19,30,30	0.82	0

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
85	SPD	1	3467	-	-	1/7/7/7	-
85	SPD	1	3466	-	-	3/7/7/7	-
85	SPD	1	3465	-	-	0/7/7/7	-
84	3HE	1	3464	-	-	0/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	1	3466	SPD	N6-C7-C8-C9
85	1	3466	SPD	C3-C4-C5-N6
85	1	3466	SPD	C8-C7-N6-C5

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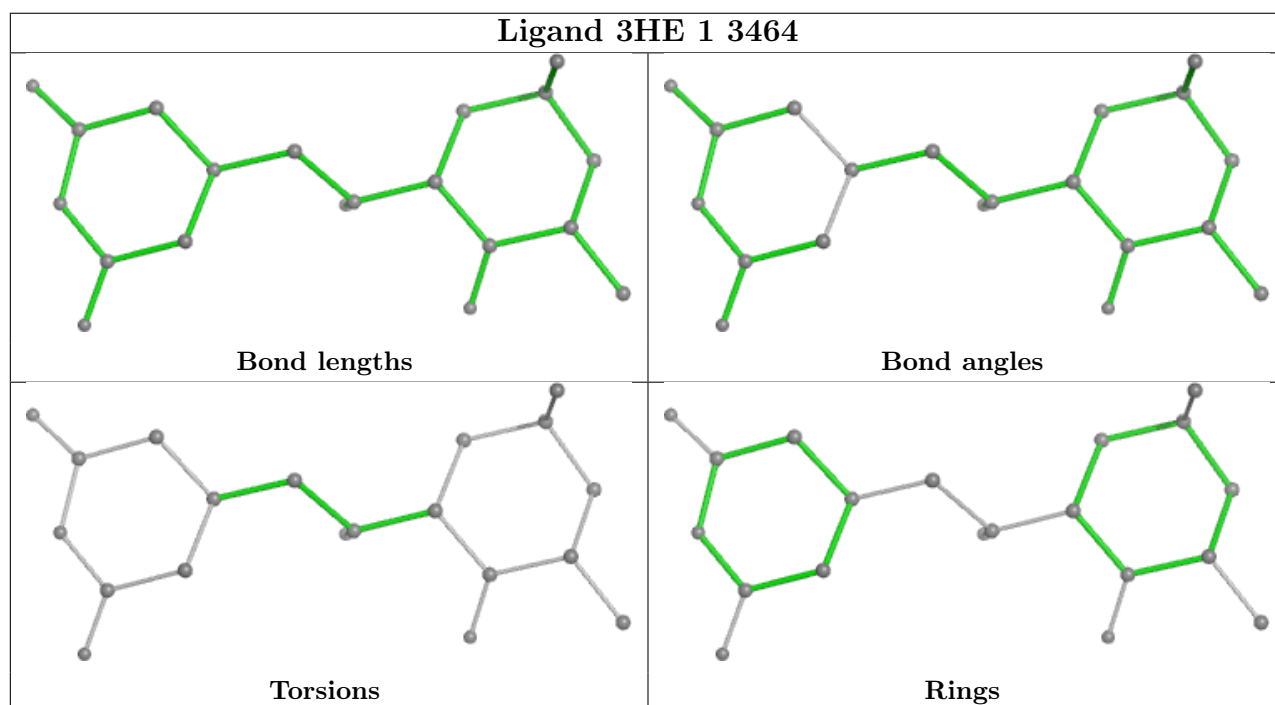
Continued from previous page...

Mol	Chain	Res	Type	Atoms
85	1	3467	SPD	C7-C8-C9-N10

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	2	2
21	S8	1
41	L6	1
40	L5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S8	123:LYS	C	135:LYS	N	22.02
1	L6	109:GLU	C	129:GLU	N	15.02
1	L5	2:ASP	C	7:ALA	N	7.28
1	2	658:C	O3'	676:G	P	4.28
1	2	1672:G	O3'	1704:G	P	3.36

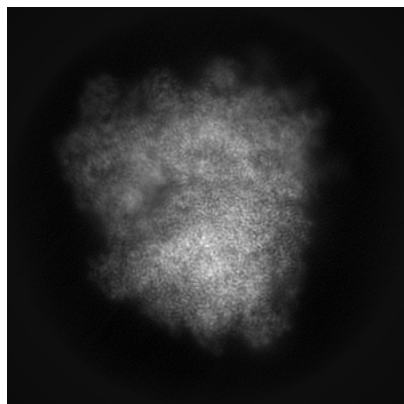
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16127. These allow visual inspection of the internal detail of the map and identification of artifacts.

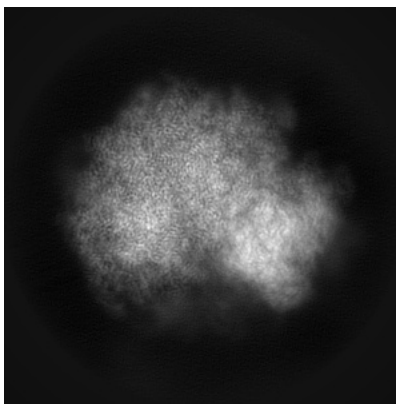
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

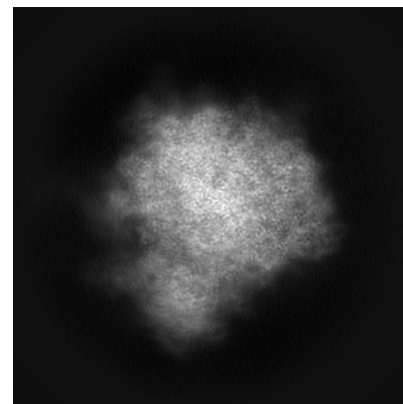
#### 6.1.1 Primary map



X

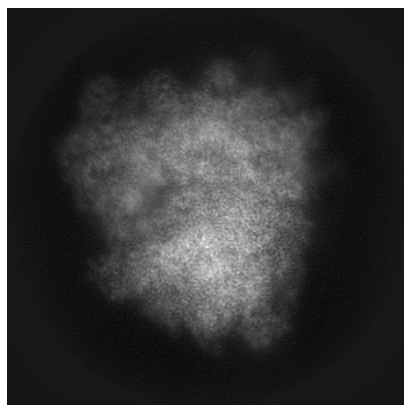


Y

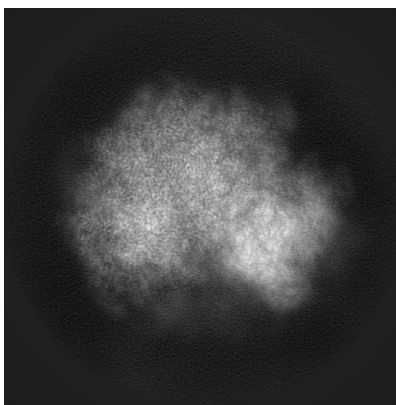


Z

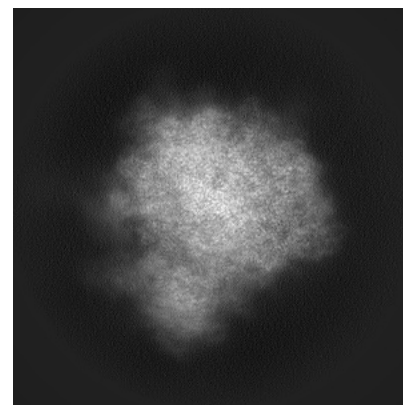
#### 6.1.2 Raw map



X



Y

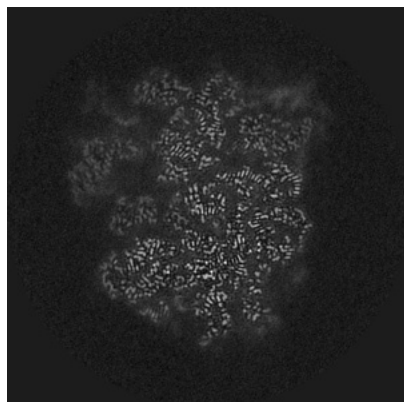


Z

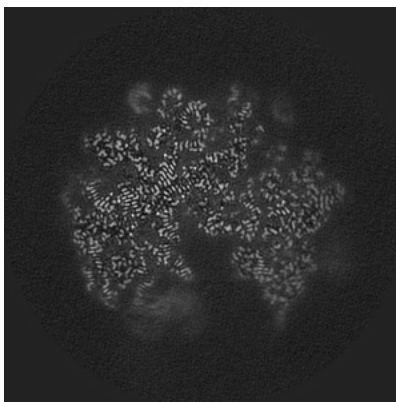
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

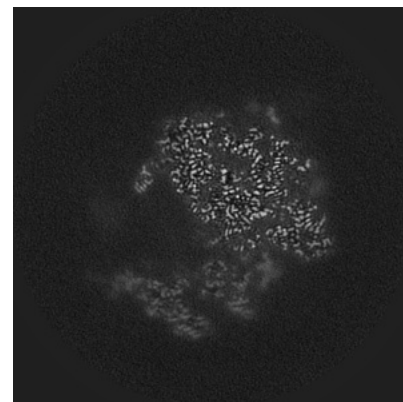
### 6.2.1 Primary map



X Index: 240

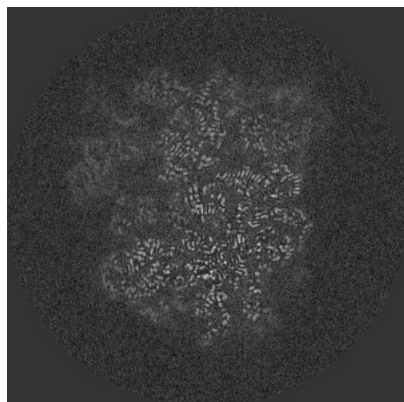


Y Index: 240

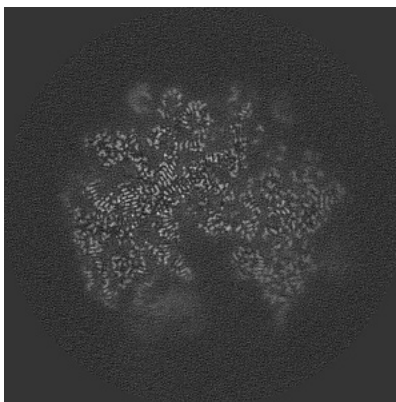


Z Index: 240

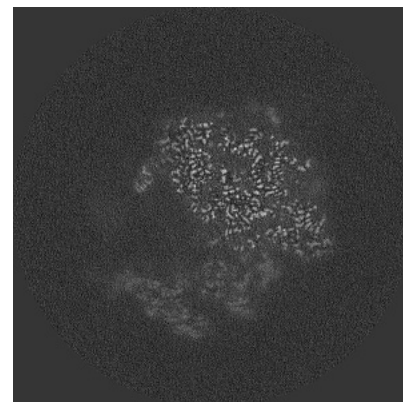
### 6.2.2 Raw map



X Index: 240



Y Index: 240

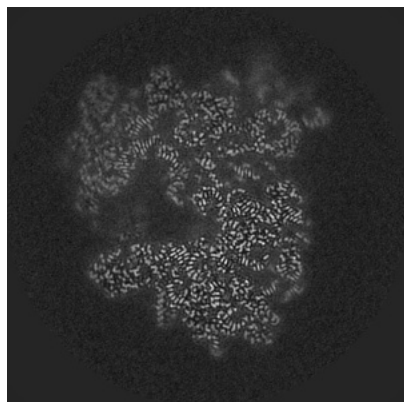


Z Index: 240

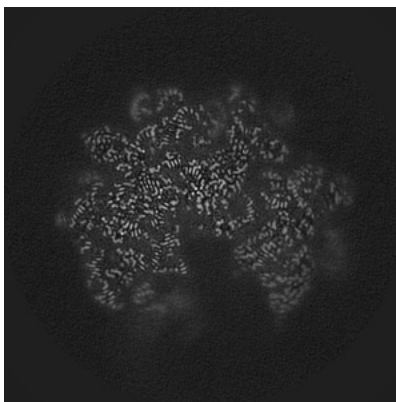
The images above show central slices of the map in three orthogonal directions.

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

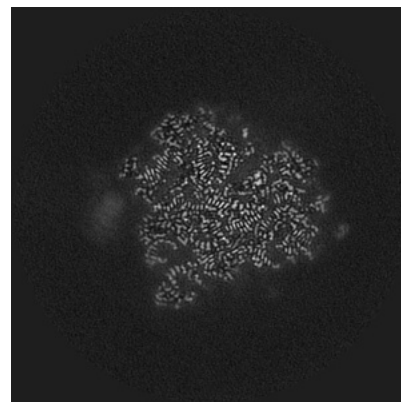
### 6.3.1 Primary map



X Index: 222

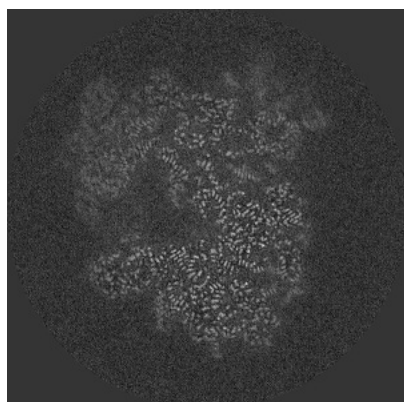


Y Index: 247

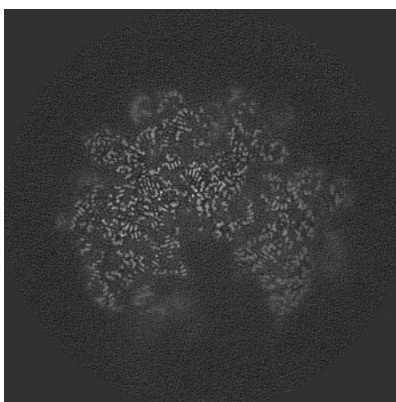


Z Index: 193

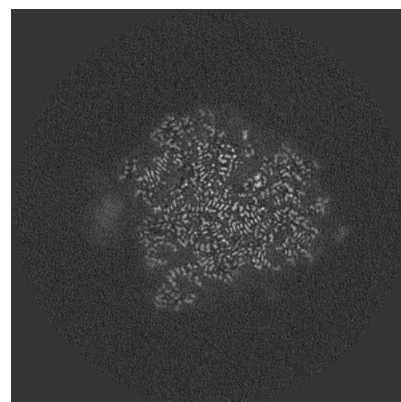
### 6.3.2 Raw map



X Index: 221



Y Index: 247



Z Index: 193

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

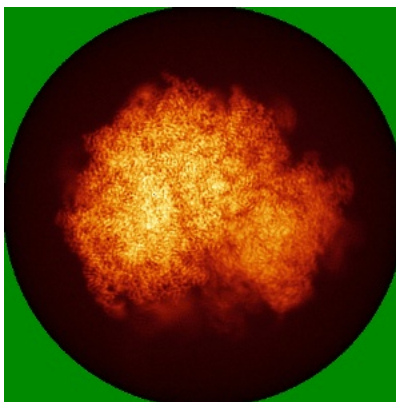


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

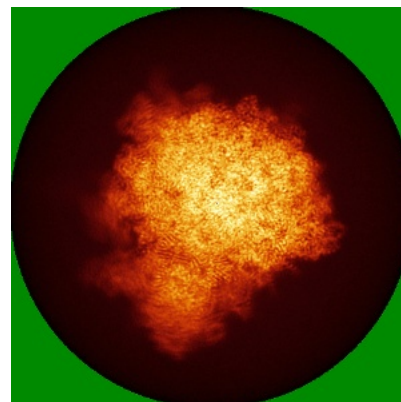
### 6.4.1 Primary map



X

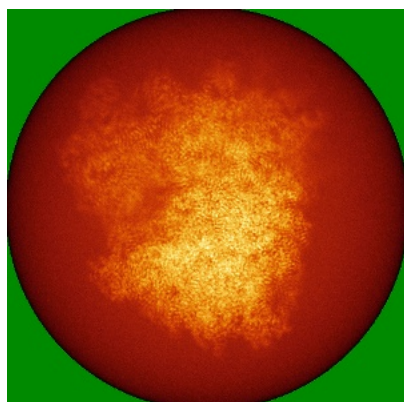


Y

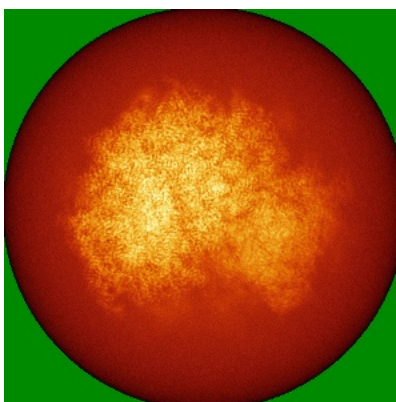


Z

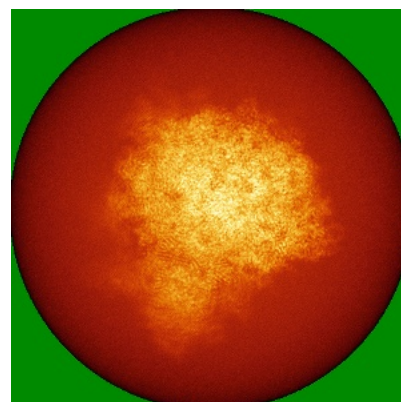
### 6.4.2 Raw map



X



Y

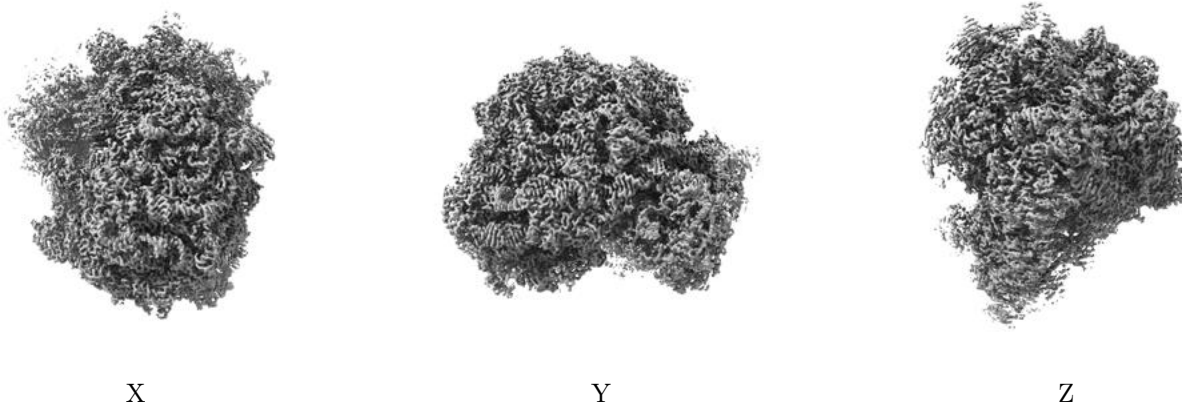


Z

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

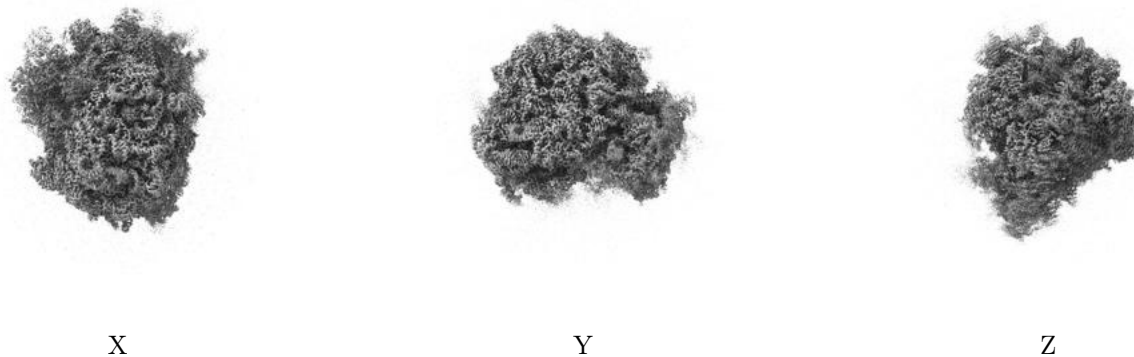
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0143. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

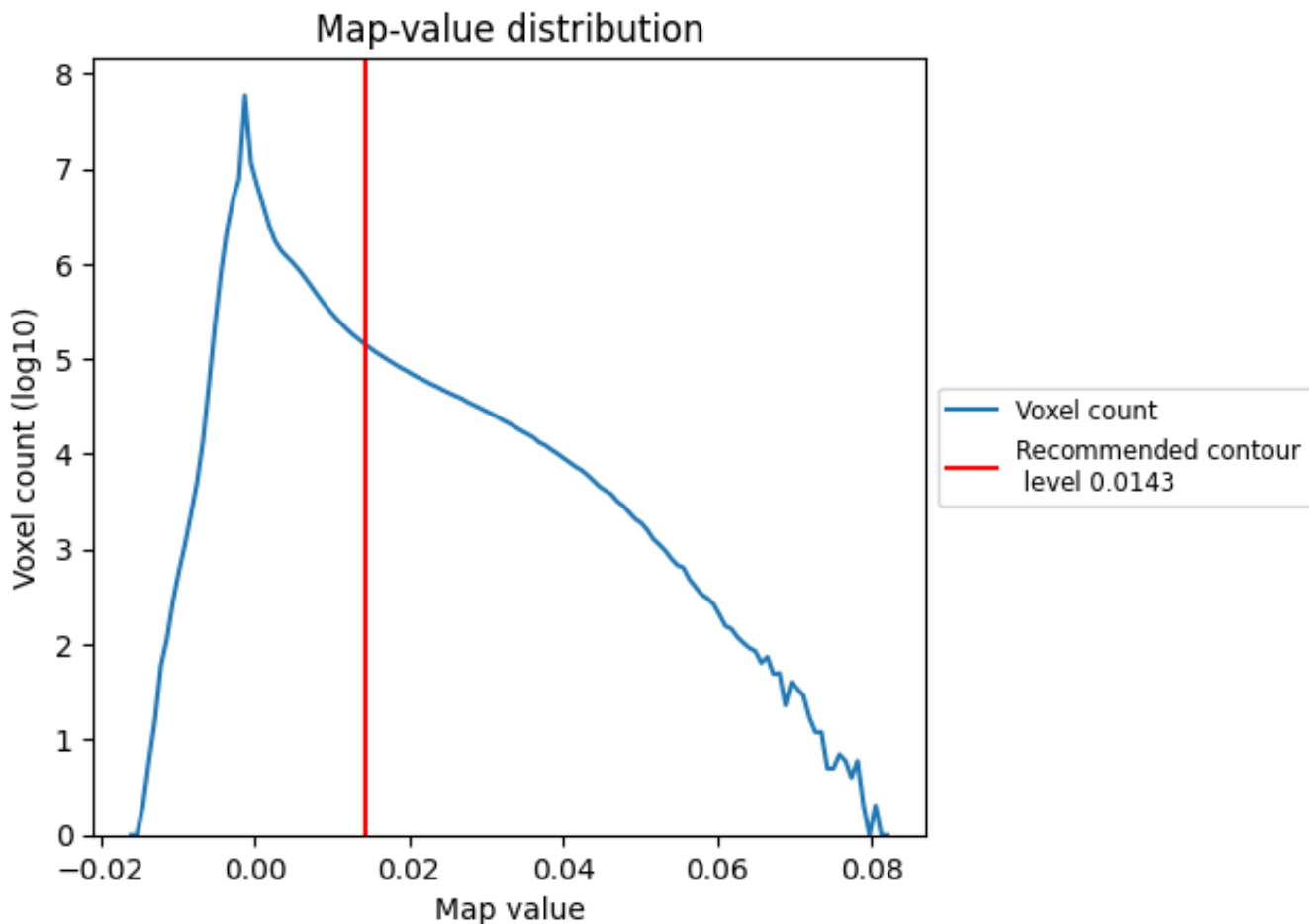
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

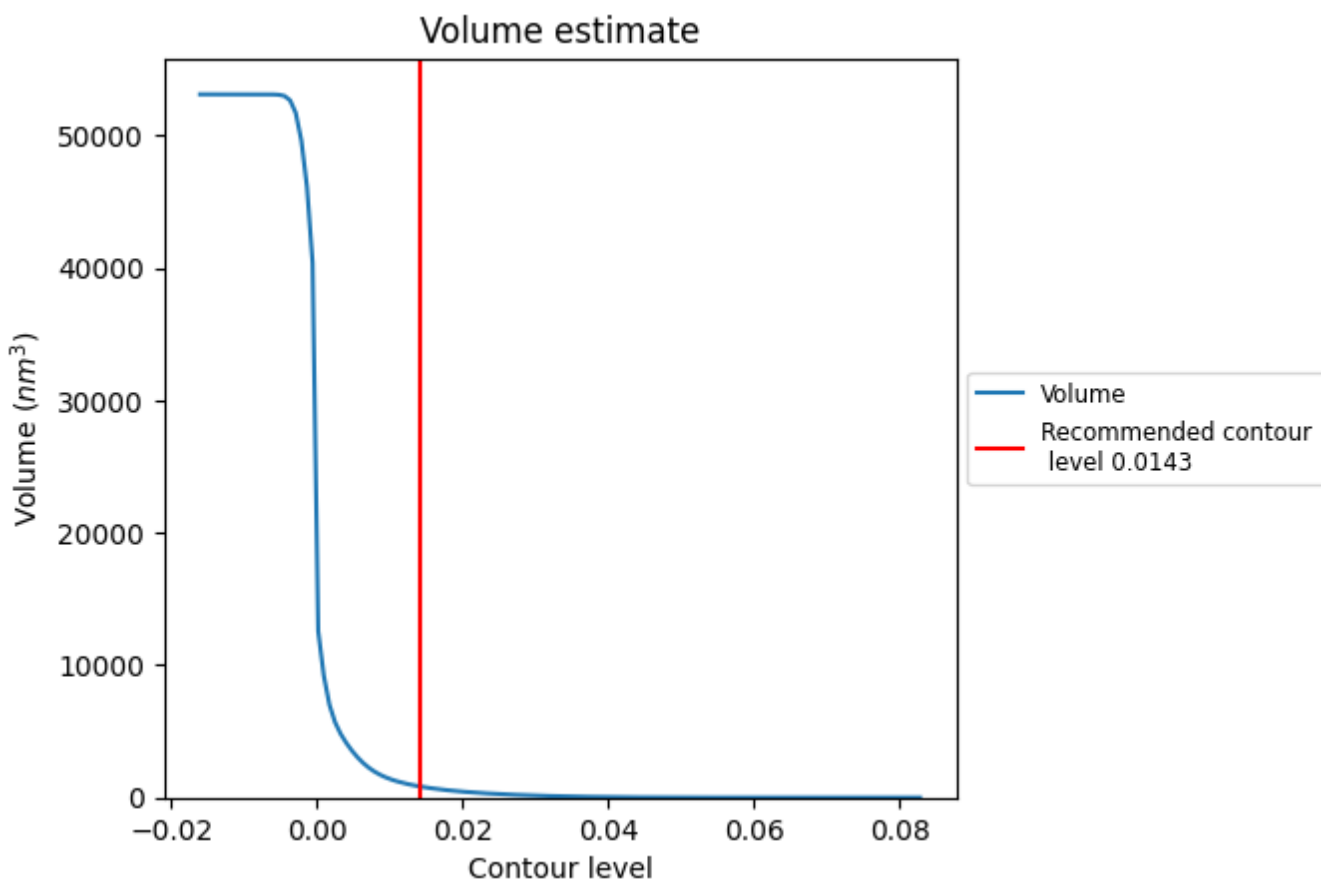
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

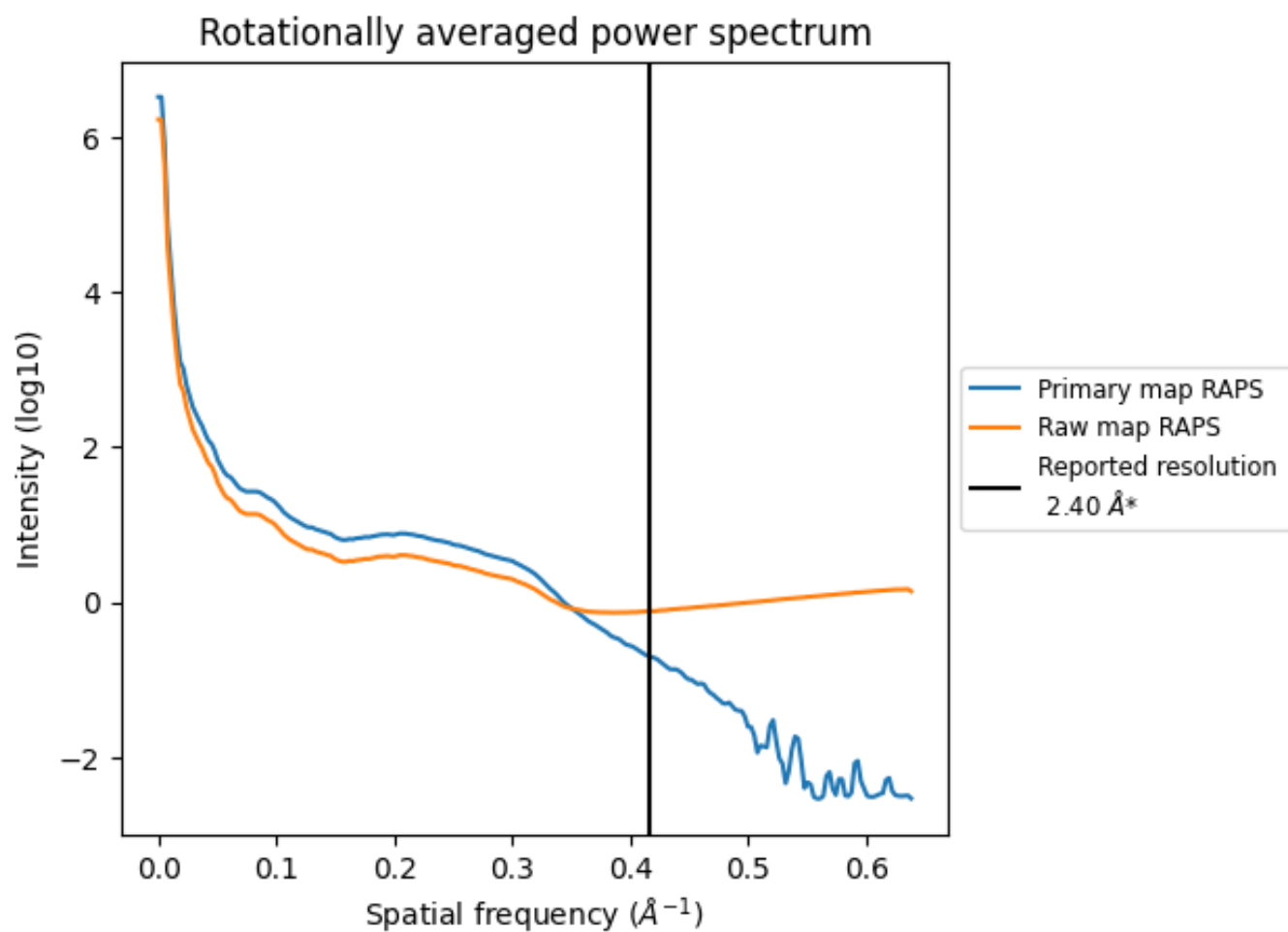
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 825  $\text{nm}^3$ ; this corresponds to an approximate mass of 745 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

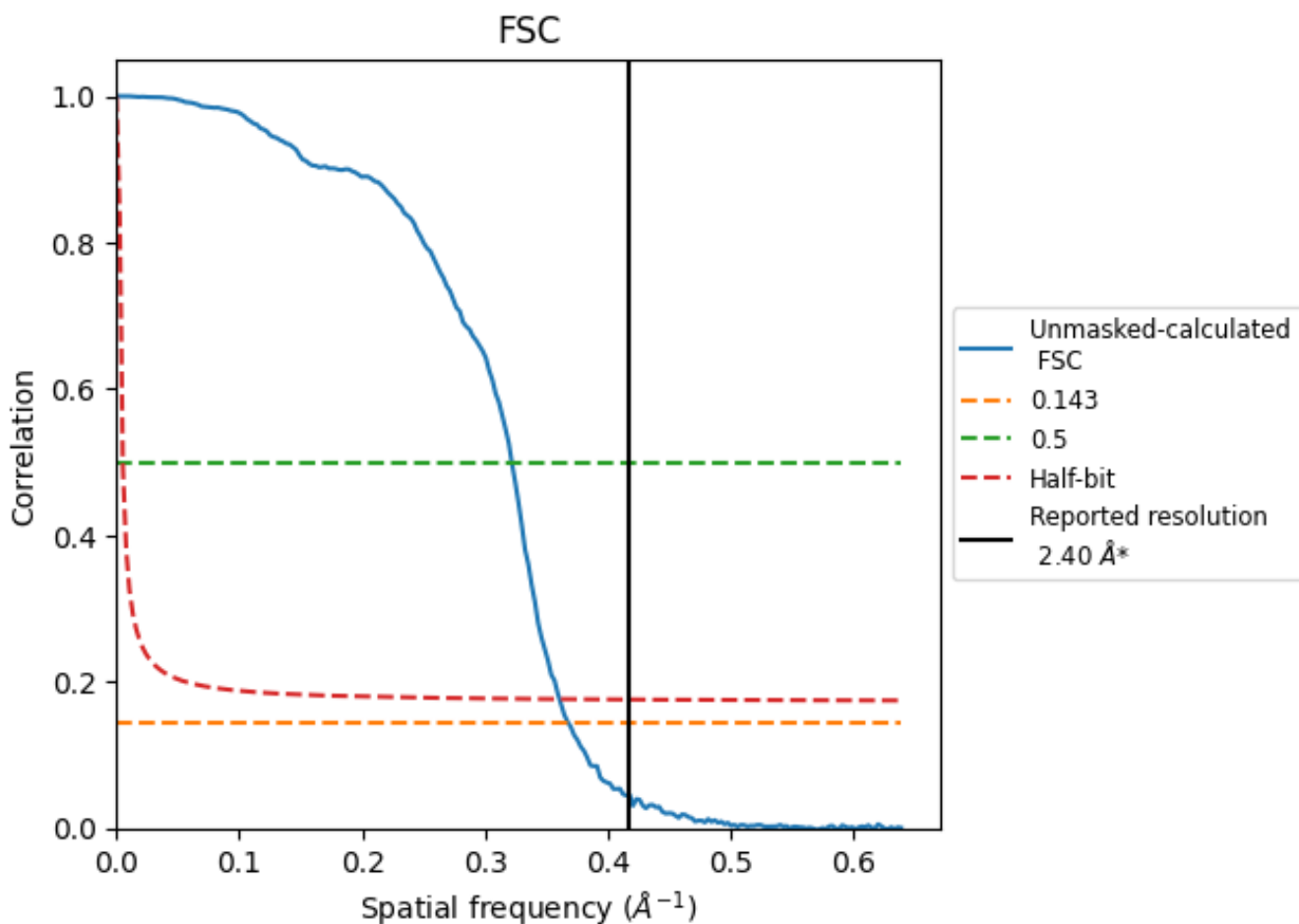


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

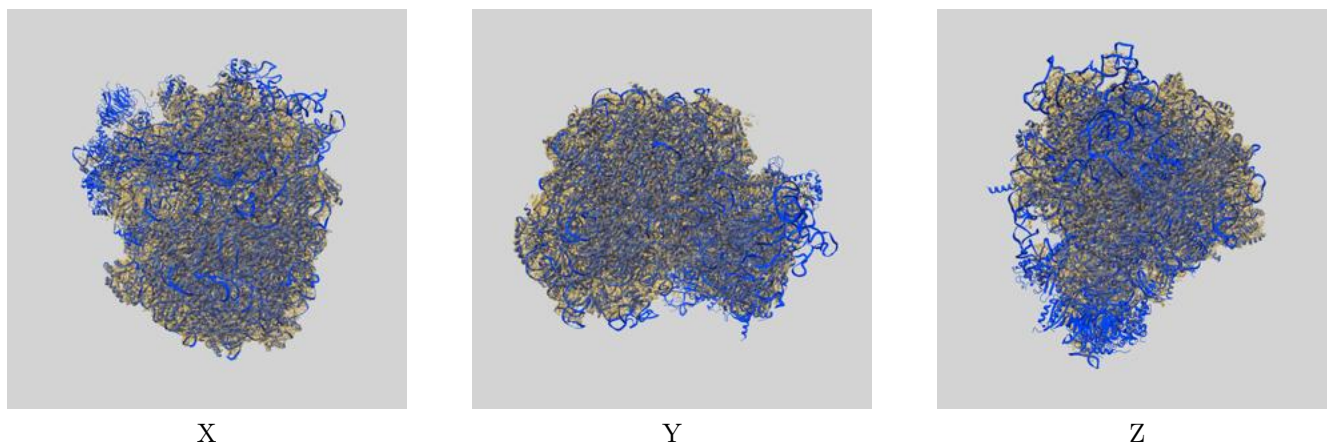
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.72	3.11	2.77

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.4 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-16127 and PDB model 8BN3. Per-residue inclusion information can be found in section 3 on page 23.

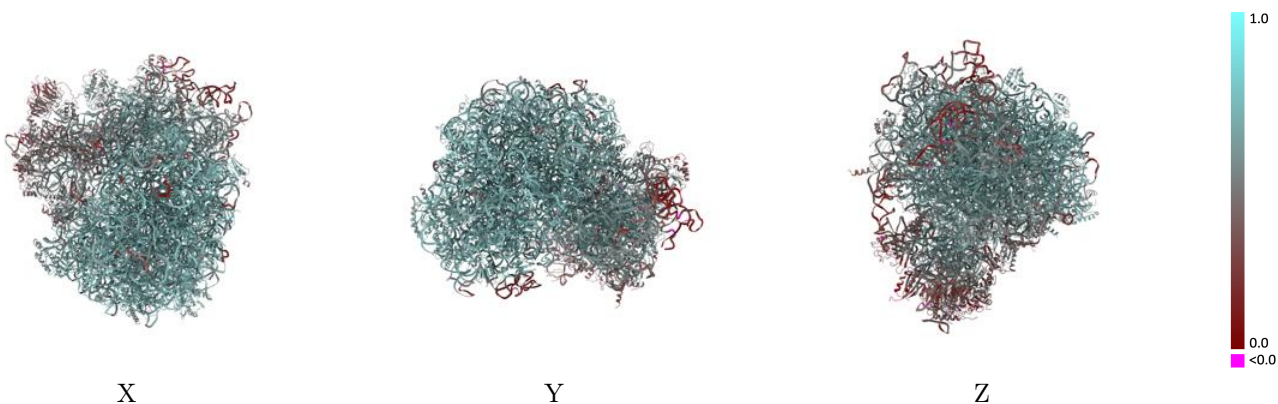
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

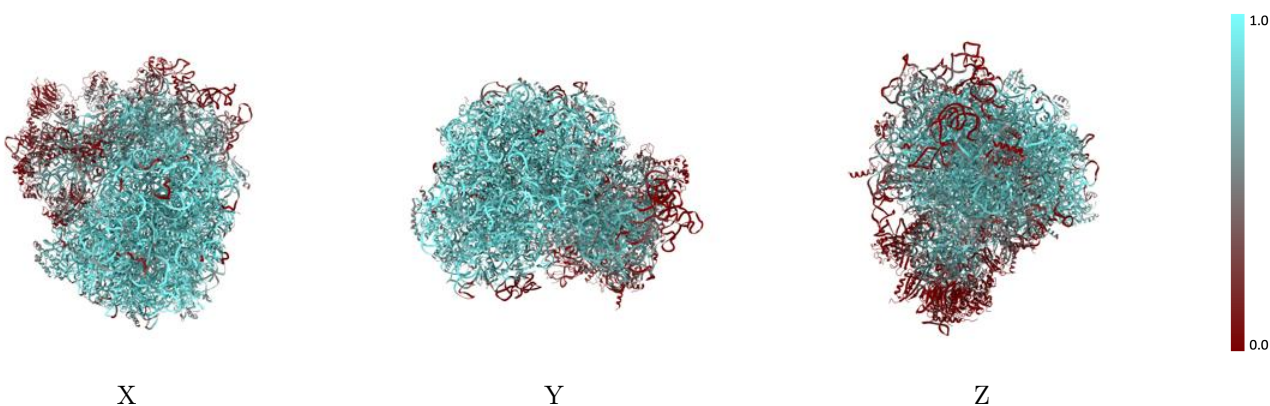


## 9.2 Q-score mapped to coordinate model [i](#)



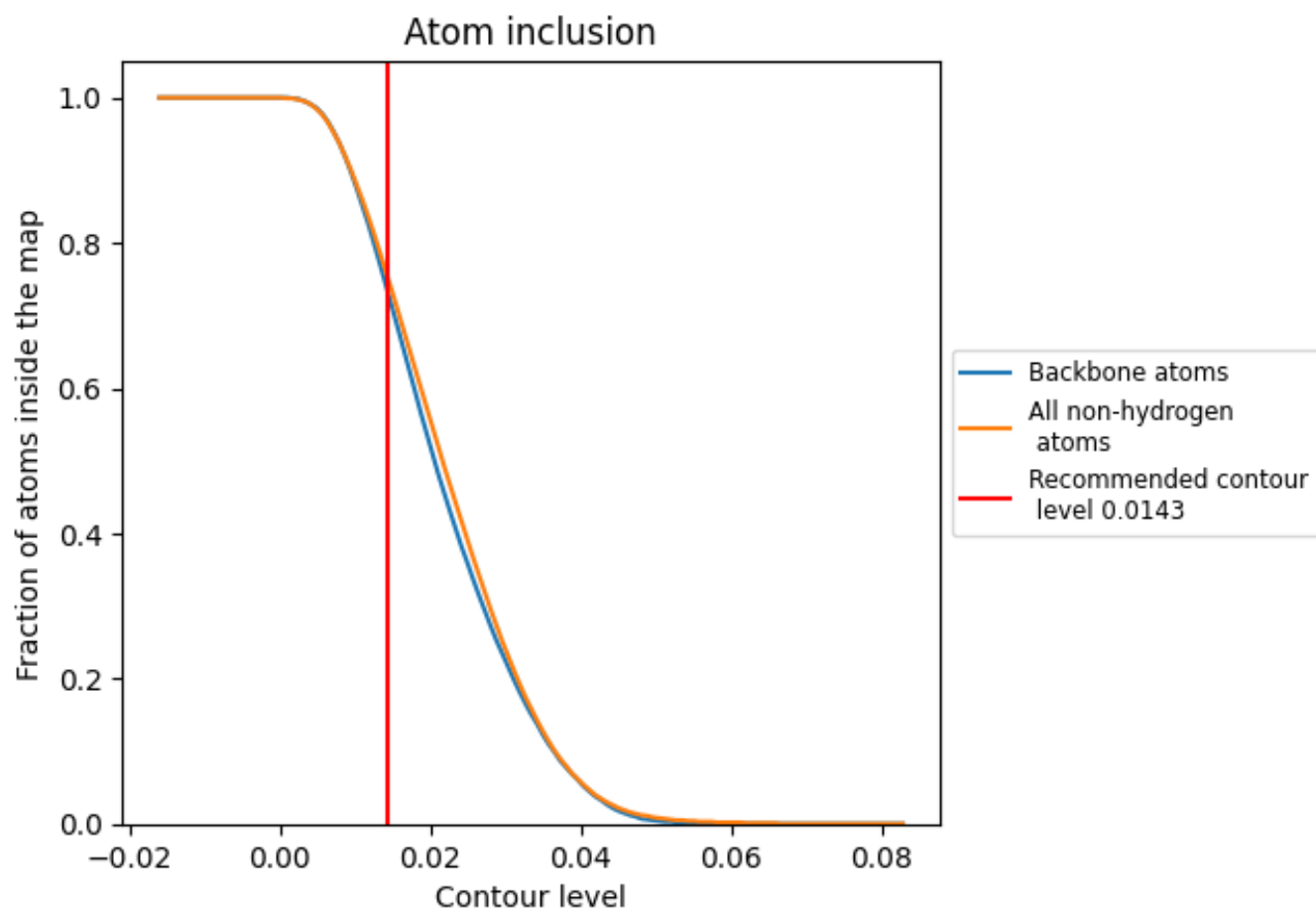
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0143).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 75% 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 (0.0143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.5970
1	 0.9120	 0.6480
2	 0.7180	 0.5400
3	 0.9590	 0.6580
4	 0.9540	 0.6630
B	 0.3520	 0.5050
C0	 0.1250	 0.3300
C1	 0.7230	 0.6110
C3	 0.6180	 0.5680
C4	 0.4530	 0.4760
C5	 0.3120	 0.4430
C6	 0.2180	 0.4240
C7	 0.2290	 0.4630
C8	 0.3150	 0.4440
C9	 0.2290	 0.4460
D0	 0.1860	 0.3210
D1	 0.5430	 0.5690
D2	 0.7950	 0.6270
D3	 0.7600	 0.6160
D4	 0.3480	 0.4840
D5	 0.0440	 0.3270
D6	 0.6580	 0.5600
D7	 0.4230	 0.5350
D8	 0.1340	 0.3520
D9	 0.6100	 0.5490
E0	 0.3860	 0.4790
E1	 0.0000	 0.1990
L2	 0.9260	 0.6860
L3	 0.8880	 0.6770
L4	 0.8610	 0.6660
L5	 0.7360	 0.6130
L6	 0.7470	 0.6230
L7	 0.9010	 0.6750
L8	 0.7650	 0.6300
L9	 0.7840	 0.6440













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Chain	Atom inclusion	Q-score
M0	0.8280	0.6490
M1	0.6910	0.6020
M3	0.8140	0.6470
M4	0.8210	0.6470
M5	0.9700	0.6950
M6	0.9070	0.6780
M7	0.8960	0.6770
M8	0.9060	0.6740
M9	0.7880	0.6200
N0	0.8860	0.6690
N1	0.8640	0.6620
N2	0.6530	0.5870
N3	0.8630	0.6600
N4	0.8890	0.6600
N5	0.8460	0.6510
N6	0.8050	0.6480
N7	0.7580	0.6310
N8	0.8890	0.6790
N9	0.8570	0.6520
O0	0.7820	0.6240
O1	0.8160	0.6530
O2	0.9000	0.6790
O3	0.9390	0.6920
O4	0.8790	0.6700
O5	0.8110	0.6440
O6	0.7950	0.6350
O7	0.9640	0.6970
O8	0.6230	0.5970
O9	0.9420	0.6740
P	0.7790	0.6370
Q0	0.8540	0.6560
Q1	0.7030	0.6310
Q2	0.8470	0.6630
Q3	0.8810	0.6720
S0	0.4310	0.5260
S1	0.2870	0.4610
S2	0.6110	0.5750
S3	0.2640	0.4220
S4	0.5900	0.5700
S5	0.1720	0.3780
S6	0.2900	0.4500
S7	0.3050	0.4690

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Chain	Atom inclusion	Q-score
S8	 0.6280	 0.5720
S9	 0.5100	 0.5230
SM	 0.3070	 0.4810
SR	 0.0130	 0.3020
eI	 0.6020	 0.5930