wwPDB EM Validation Summary Report (i)

Sep 28, 2024 – 09:27 pm BST

PDB ID	:	4D5Y
EMDB ID	:	EMD-2810
Title	:	Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors	:	Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on	:	2014-11-07
Resolution	:	9.00 Å(reported)
Based on initial model	:	4CXD

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 (i) 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 (i)) were used in the production of this report:

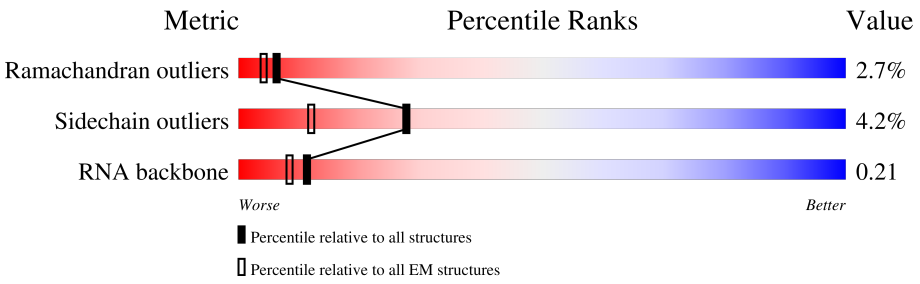
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	257	25% 93% • •
2	B	403	17% 90% 7% •
3	C	427	11% 78% 6% • 15%
4	D	297	7% 93% • •
5	E	288	13% 50% 5% 45%
6	F	248	12% 90% • 6%
7	G	266	17% 83% 5% • 12%
8	H	192	17% 95% 5%

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Mol	Chain	Length	Quality of chain
9	I	214	20% 86% 6% 8%
10	J	178	5% 85% 10%
11	L	211	16% 84% 9% 5%
12	M	215	8% 62% 35%
13	N	204	19% 98%
14	O	203	13% 94%
15	P	184	7% 78% 5% 17%
16	Q	188	14% 92% 6%
17	R	196	10% 86% 7% 7%
18	S	176	13% 91% 7%
19	T	160	18% 95%
20	U	128	13% 77% 20%
21	V	140	28% 89% 9%
22	W	157	39% 59%
23	X	156	15% 75% 24%
24	Y	145	5% 83% 6% 12%
25	Z	136	24% 93% 7%
26	a	148	14% 94% 5%
27	b	159	6% 40% 57%
28	c	115	19% 88% 10%
29	d	125	6% 83% 13%
30	e	135	14% 90% 5%
31	f	110	10% 86% 10%
32	g	117	23% 87% 10%
33	h	123	5% 94% 5%

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Mol	Chain	Length	Quality of chain
34	i	105	7% 83% 8% 8%
35	j	97	84% 12%
36	k	70	13% 97%
37	l	51	14% 94%
38	m	128	7% 38% 59%
39	n	25	12% 100%
40	o	106	24% 93% 7%
41	p	92	8% 93% 5%
42	t	137	11% 86% 7% 5%
43	u	210	48% 92% 8%
44	2	5025	30% 41% 28%
45	3	194	39% 41% 19%
46	4	119	41% 57%

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 136495 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 UL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	247	1888	1183	388	311	6	0	1

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN UL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	396	3190	2030	601	545	14	0	1

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN UL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	364	2889	1817	578	480	14	0	1

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN UL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	290	2361	1489	431	427	14	0	0

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN EL6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	158	1286	834	238	214	0	0

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN UL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	234	1949	1252	376	312	9	0	0

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN EL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	235	1881	1197	363	317	4	0	1

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN UL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	192	1535	965	286	278	6	0	0

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN UL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	196	1604	1022	308	262	12	0	0

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN UL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	170	1362	861	254	241	6	0	0

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN EL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	200	1617	1013	335	265	4	0	1

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN EL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	140	1139	730	219	183	7	0	1

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN EL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	204	1708	1077	360	266	5	0	0

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN UL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	196	1607	1034	316	252	5	0	1

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN UL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	153	1234	771	241	213	9	0	1

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN EL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	184	1493	933	311	244	5	0	0

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN UL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	183	1526	943	331	242	10	0	1

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN EL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	173	1438	916	280	232	10	0	0

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN EL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	159	1297	823	252	216	6	0	0

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN EL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	102	827	529	146	150	2	0	1

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN UL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	128	963	610	181	167	5	0	0

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	64	529	337	104	85	3	0	1

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN UL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	119	975	624	183	167	1	0	0

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN UL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	128	1065	668	217	177	3	0	1

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN EL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	136	1114	719	209	182	4	0	0

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN UL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	147	1161	736	237	185	3	0	0

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN EL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	69	560	344	123	90	3	0	1

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN EL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	104	802	508	142	145	7	0	1

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN EL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	109	904	570	174	158	2	0	0

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN EL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	128	1053	664	219	165	5	0	1

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN EL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	107	865	550	172	140	3	0	0

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN EL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	115	907	566	188	147	6	0	1

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN UL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	122	1014	641	205	167	1	0	0

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN EL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	97	783	488	168	122	5	0	1

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN EL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	85	690	423	153	109	5	0	1

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN EL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	69	568	366	103	98	1	0	0

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN EL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	50	443	281	98	63	1	0	0

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	52	428	266	90	66	6	0	0

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN EL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	25	239	145	64	27	3	0	0

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN EL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	106	870	547	176	140	7	0	0

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN EL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	91	707	445	136	119	7	0	0

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN EL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	t	130	1043	646	220	172	5	0	1

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN UL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	u	210	1621	990	278	347	6	0	0

- Molecule 44 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	2	3616	77488	34508	14153	25212	3615	0	0

- Molecule 45 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
45	3	157	3334	1489	587	1102	156	0	0

- Molecule 46 is a RNA chain called 5S Ribosomal RNA.

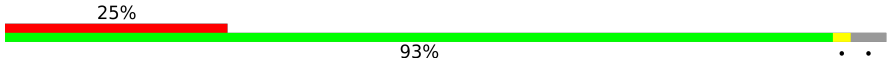
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	4	119	2538	1132	454	834	118	0	0

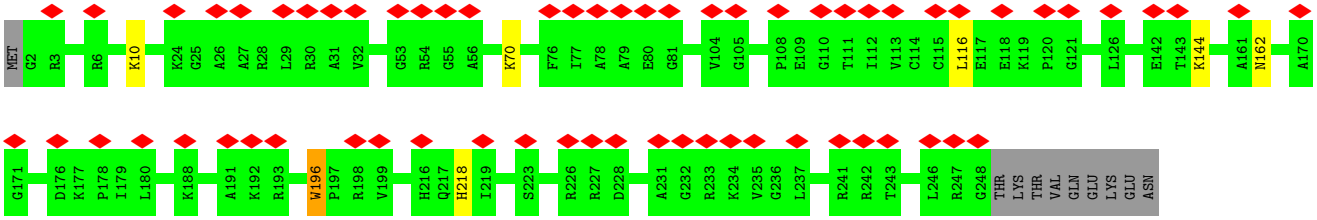
3 Residue-property plots (i)

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: 60S RIBOSOMAL PROTEIN UL2

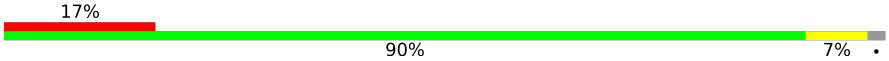
Chain A:

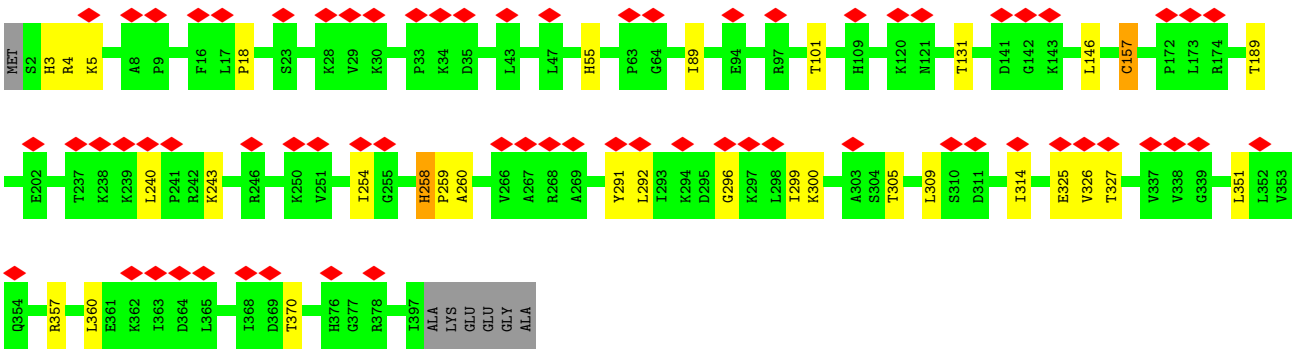




- Molecule 2: 60S RIBOSOMAL PROTEIN UL3

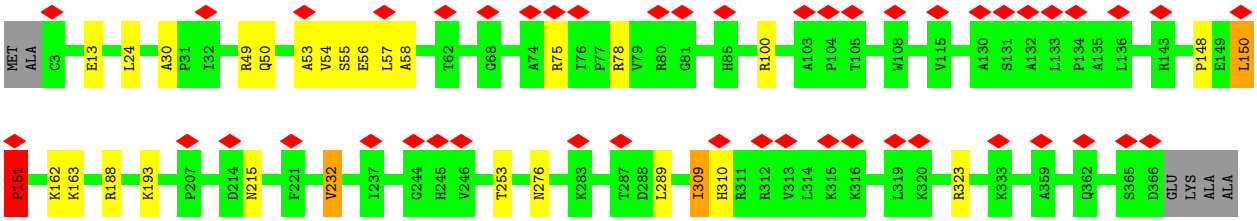
Chain B:





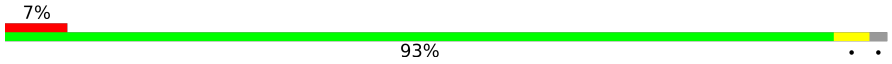
- Molecule 3: 60S RIBOSOMAL PROTEIN UL4

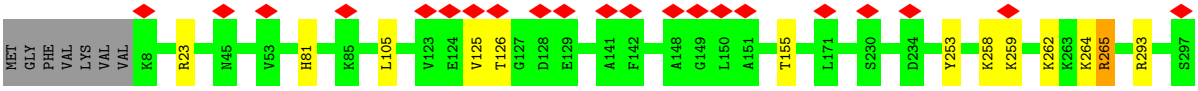
Chain C:



• Molecule 4: 60S RIBOSOMAL PROTEIN UL18

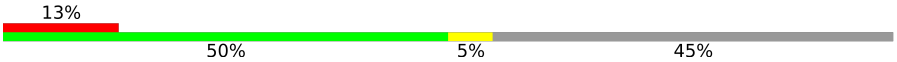
Chain D:

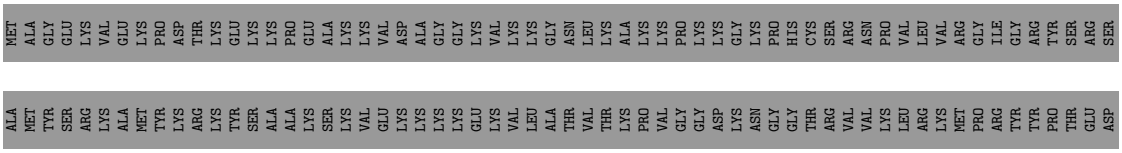


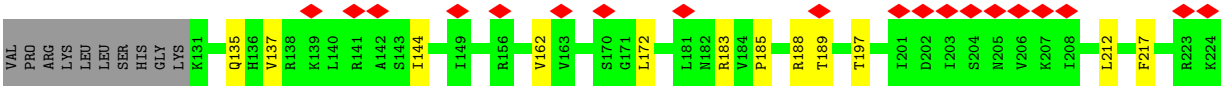


• Molecule 5: 60S RIBOSOMAL PROTEIN EL6

Chain E:

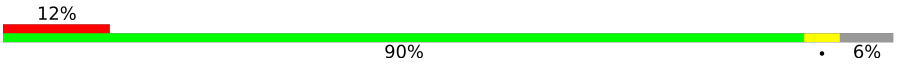


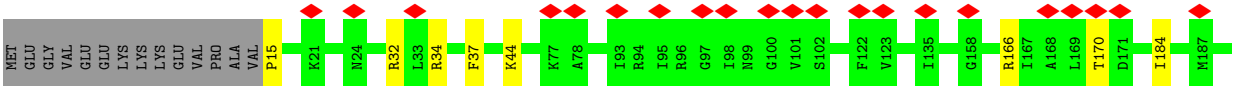




• Molecule 6: 60S RIBOSOMAL PROTEIN UL30

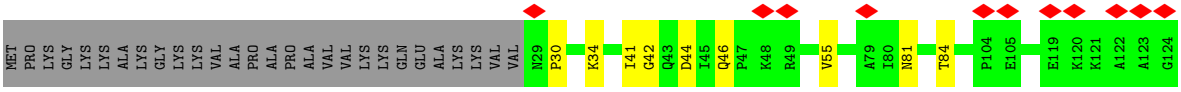
Chain F:

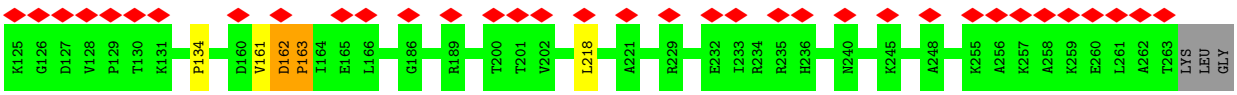




• Molecule 7: 60S RIBOSOMAL PROTEIN EL8

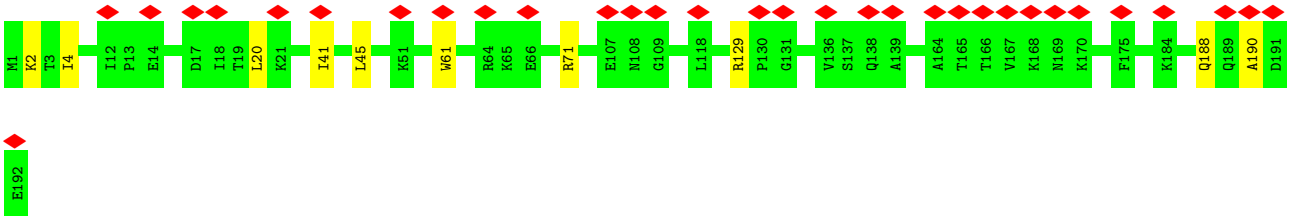
Chain G:





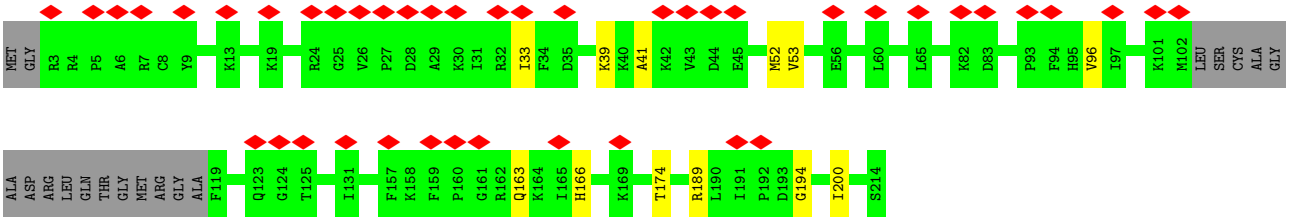
• Molecule 8: 60S RIBOSOMAL PROTEIN UL6

Chain H: 17% 95% 5%



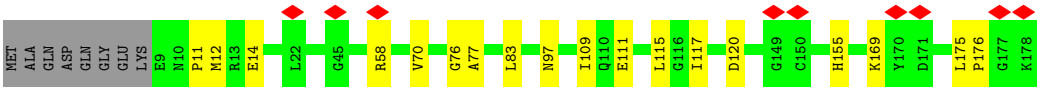
- Molecule 9: 60S RIBOSOMAL PROTEIN UL16

Chain I: 20% 86% 6% 8%



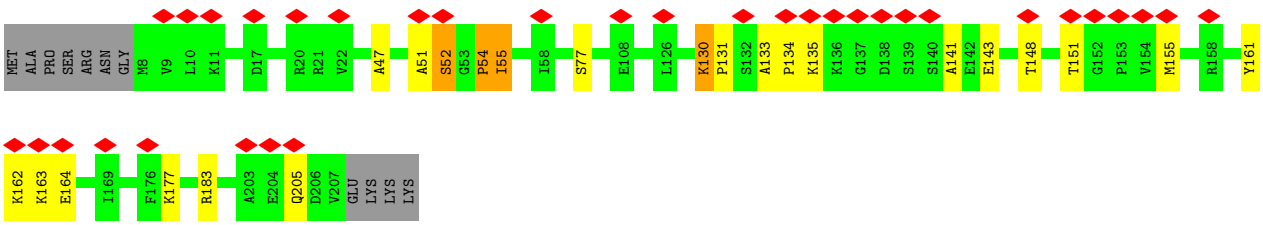
- Molecule 10: 60S RIBOSOMAL PROTEIN UL5

Chain J: 5% 85% 10%



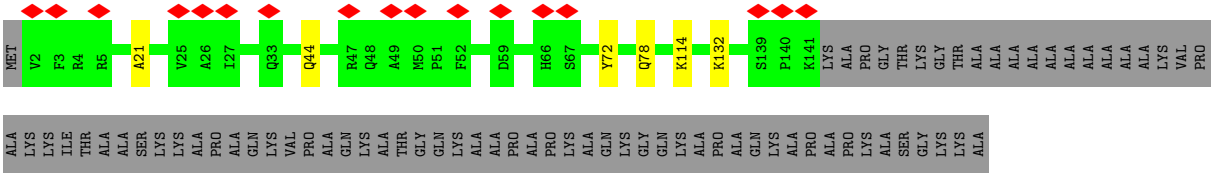
- Molecule 11: 60S RIBOSOMAL PROTEIN EL13

Chain L: 16% 84% 9% 5%



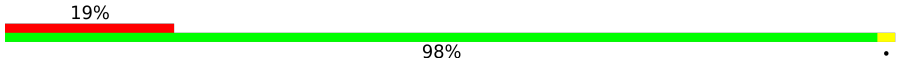
- Molecule 12: 60S RIBOSOMAL PROTEIN EL14

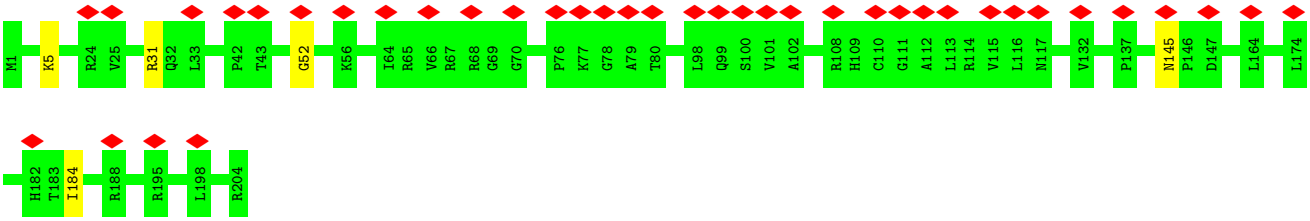
Chain M: 8% 62% 35%



- Molecule 13: 60S RIBOSOMAL PROTEIN EL15

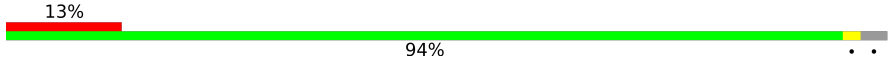
Chain N:

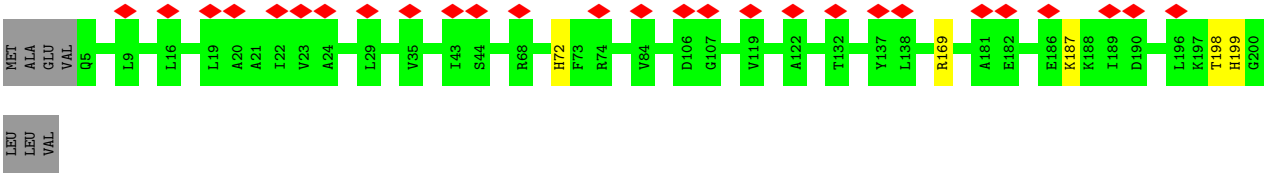




- Molecule 14: 60S RIBOSOMAL PROTEIN UL13

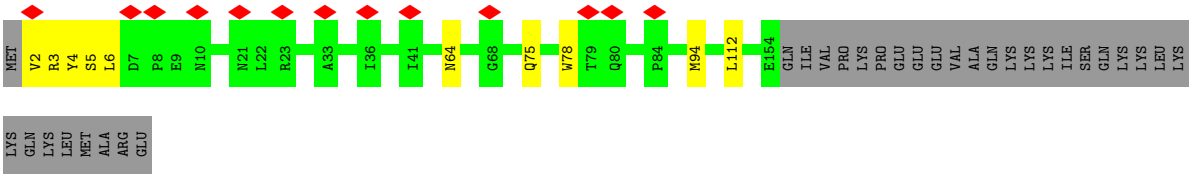
Chain O:





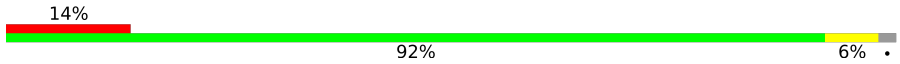
- Molecule 15: 60S RIBOSOMAL PROTEIN UL22

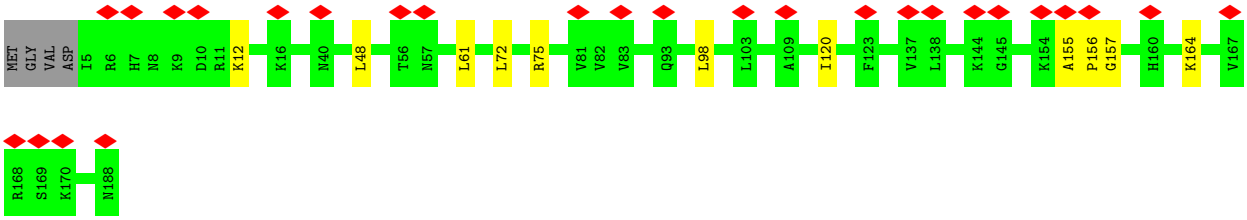
Chain P:



- Molecule 16: 60S RIBOSOMAL PROTEIN EL18

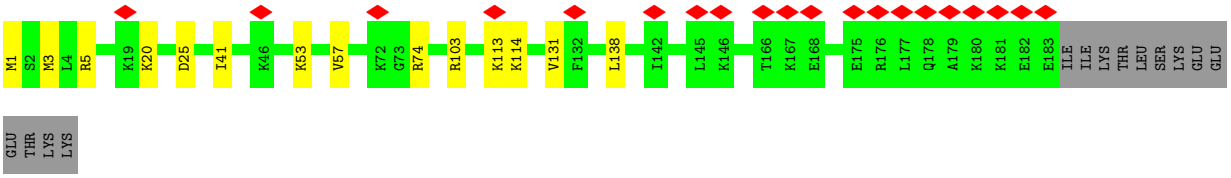
Chain Q:





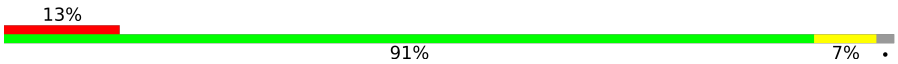
- Molecule 17: 60S RIBOSOMAL PROTEIN UL19

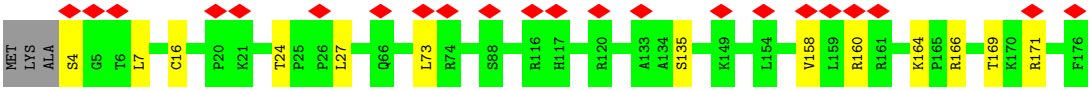
Chain R:



- Molecule 18: 60S RIBOSOMAL PROTEIN EL20

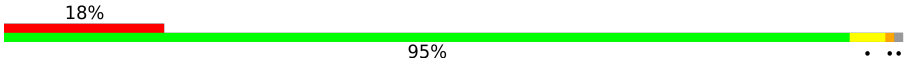
Chain S:

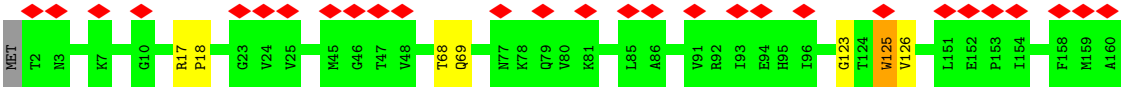




- Molecule 19: 60S RIBOSOMAL PROTEIN EL21

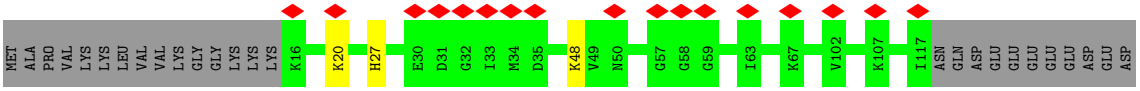
Chain T:





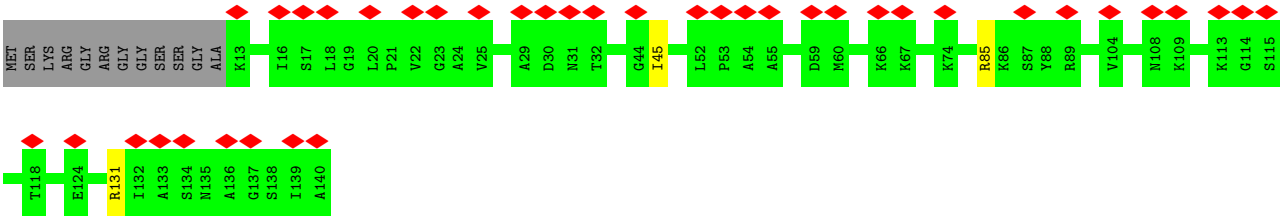
- Molecule 20: 60S RIBOSOMAL PROTEIN EL22

Chain U:



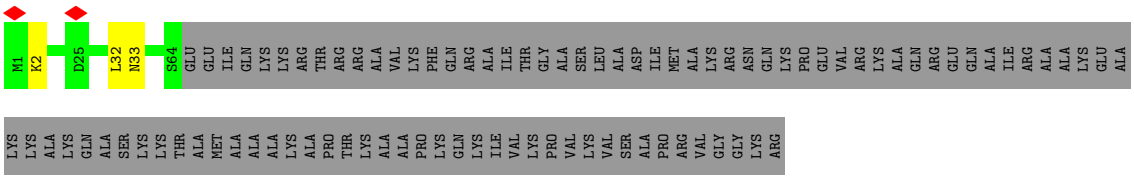
- Molecule 21: 60S RIBOSOMAL PROTEIN UL14

Chain V:



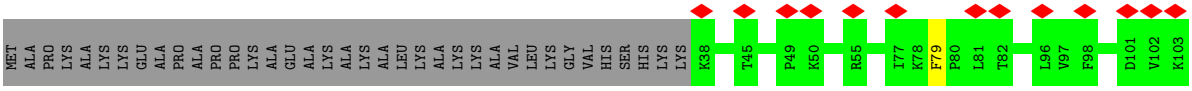
- Molecule 22: 60S RIBOSOMAL PROTEIN EL24

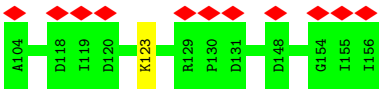
Chain W:



- Molecule 23: 60S RIBOSOMAL PROTEIN UL23

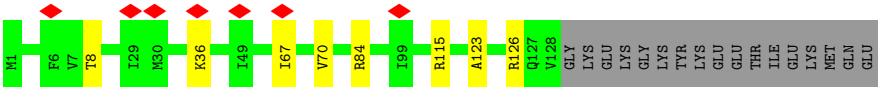
Chain X:





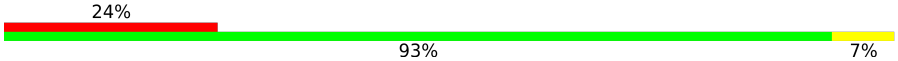
- Molecule 24: 60S RIBOSOMAL PROTEIN UL24

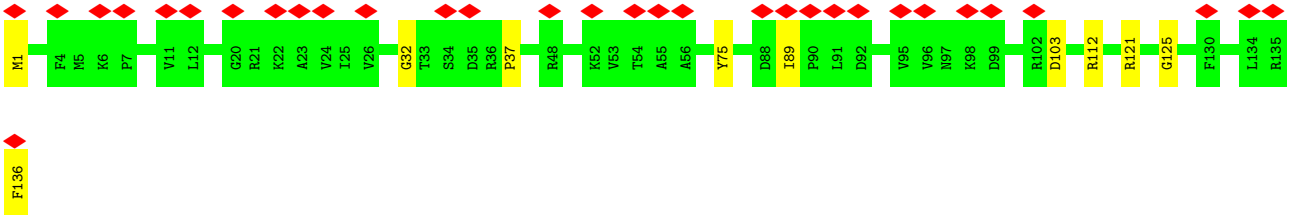
Chain Y:



- Molecule 25: 60S RIBOSOMAL PROTEIN EL27

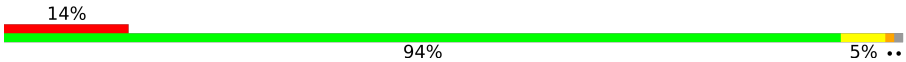
Chain Z:

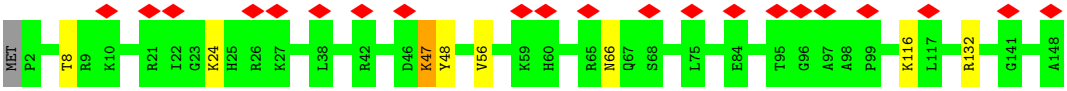




- Molecule 26: 60S RIBOSOMAL PROTEIN UL15

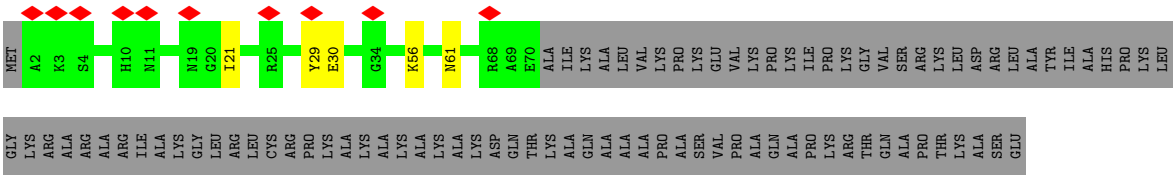
Chain a:





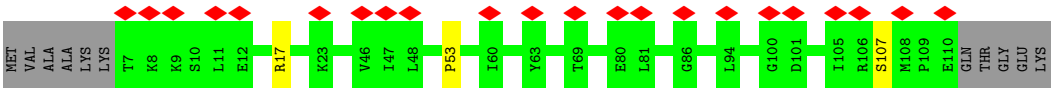
- Molecule 27: 60S RIBOSOMAL PROTEIN EL29

Chain b:



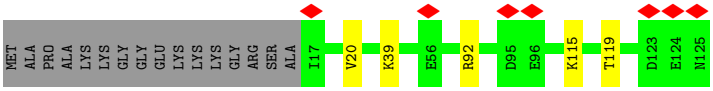
- Molecule 28: 60S RIBOSOMAL PROTEIN EL30

Chain c:



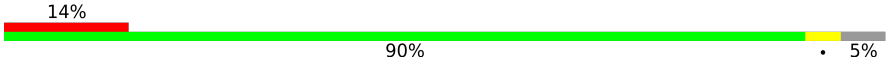
- Molecule 29: 60S RIBOSOMAL PROTEIN EL31

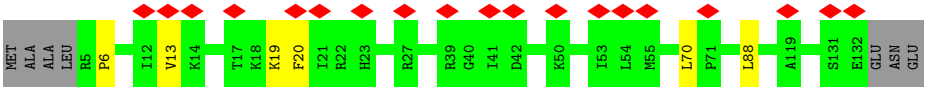
Chain d:



• Molecule 30: 60S RIBOSOMAL PROTEIN EL32

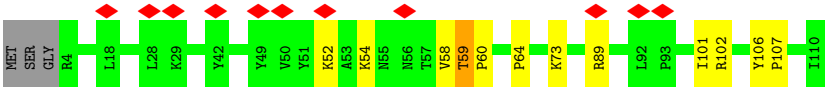
Chain e:





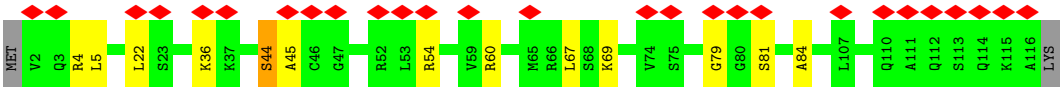
• Molecule 31: 60S RIBOSOMAL PROTEIN EL33

Chain f:



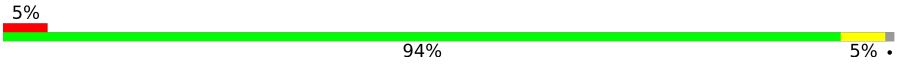
• Molecule 32: 60S RIBOSOMAL PROTEIN EL34

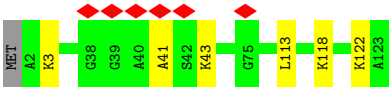
Chain g:



• Molecule 33: 60S RIBOSOMAL PROTEIN UL29

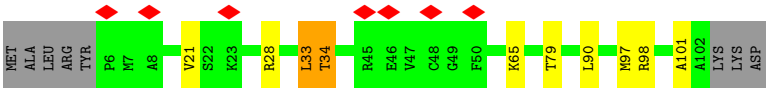
Chain h:





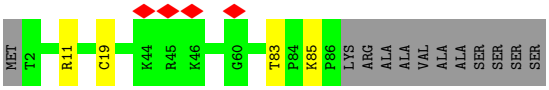
• Molecule 34: 60S RIBOSOMAL PROTEIN EL36

Chain i:



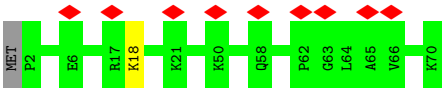
• Molecule 35: 60S RIBOSOMAL PROTEIN EL37

Chain j:



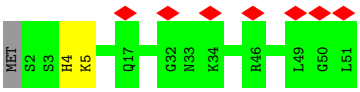
• Molecule 36: 60S RIBOSOMAL PROTEIN EL38

Chain k: 13% 97%



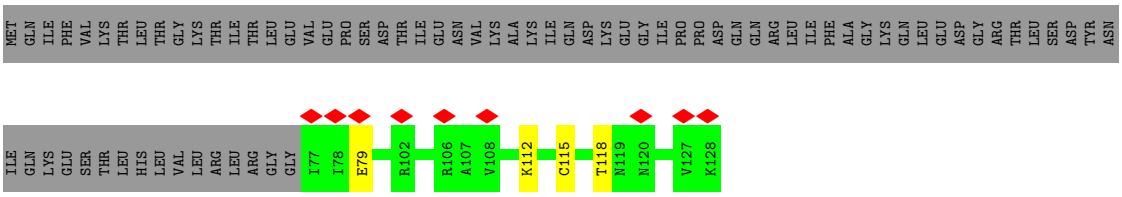
• Molecule 37: 60S RIBOSOMAL PROTEIN EL39

Chain l: 14% 94%



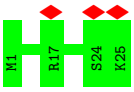
• Molecule 38: 60S RIBOSOMAL PROTEIN EL40

Chain m: 7% 38% 59%



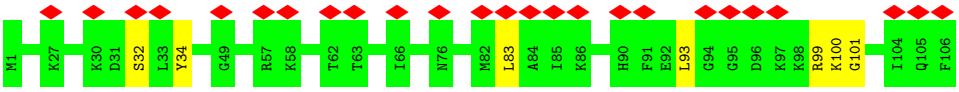
• Molecule 39: 60S RIBOSOMAL PROTEIN EL41

Chain n: 12% 100%



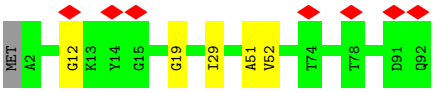
• Molecule 40: 60S RIBOSOMAL PROTEIN EL44

Chain o: 24% 93% 7%



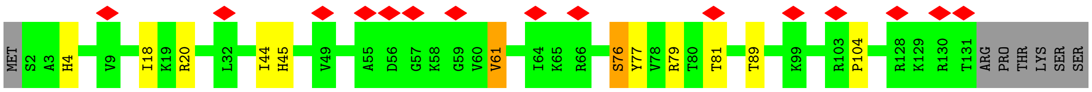
• Molecule 41: 60S RIBOSOMAL PROTEIN EL43

Chain p: 8% 93% 5%



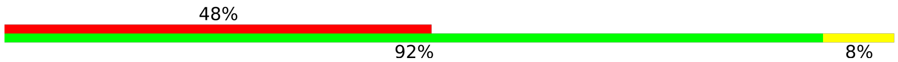
• Molecule 42: 60S RIBOSOMAL PROTEIN EL28

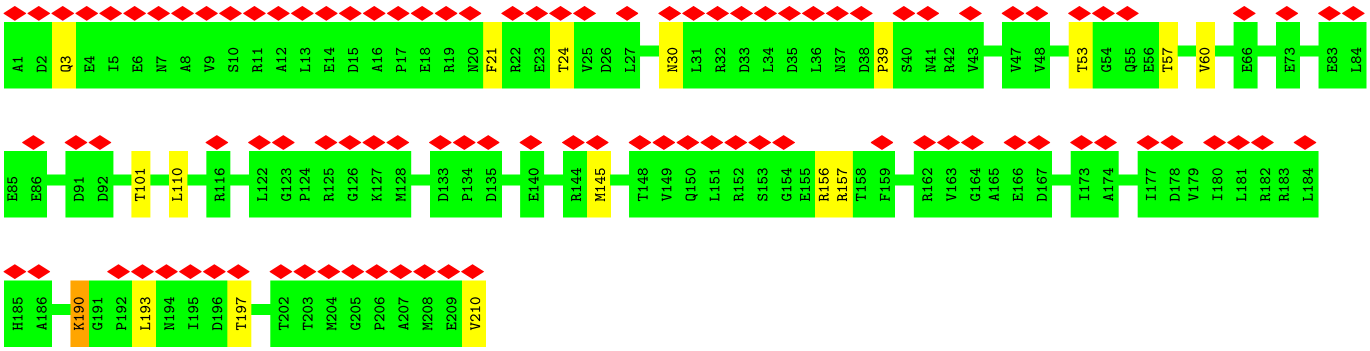
Chain t: 11% 86% 7% 5%



• Molecule 43: 60S RIBOSOMAL PROTEIN UL1

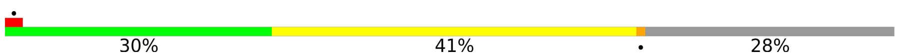
Chain u:

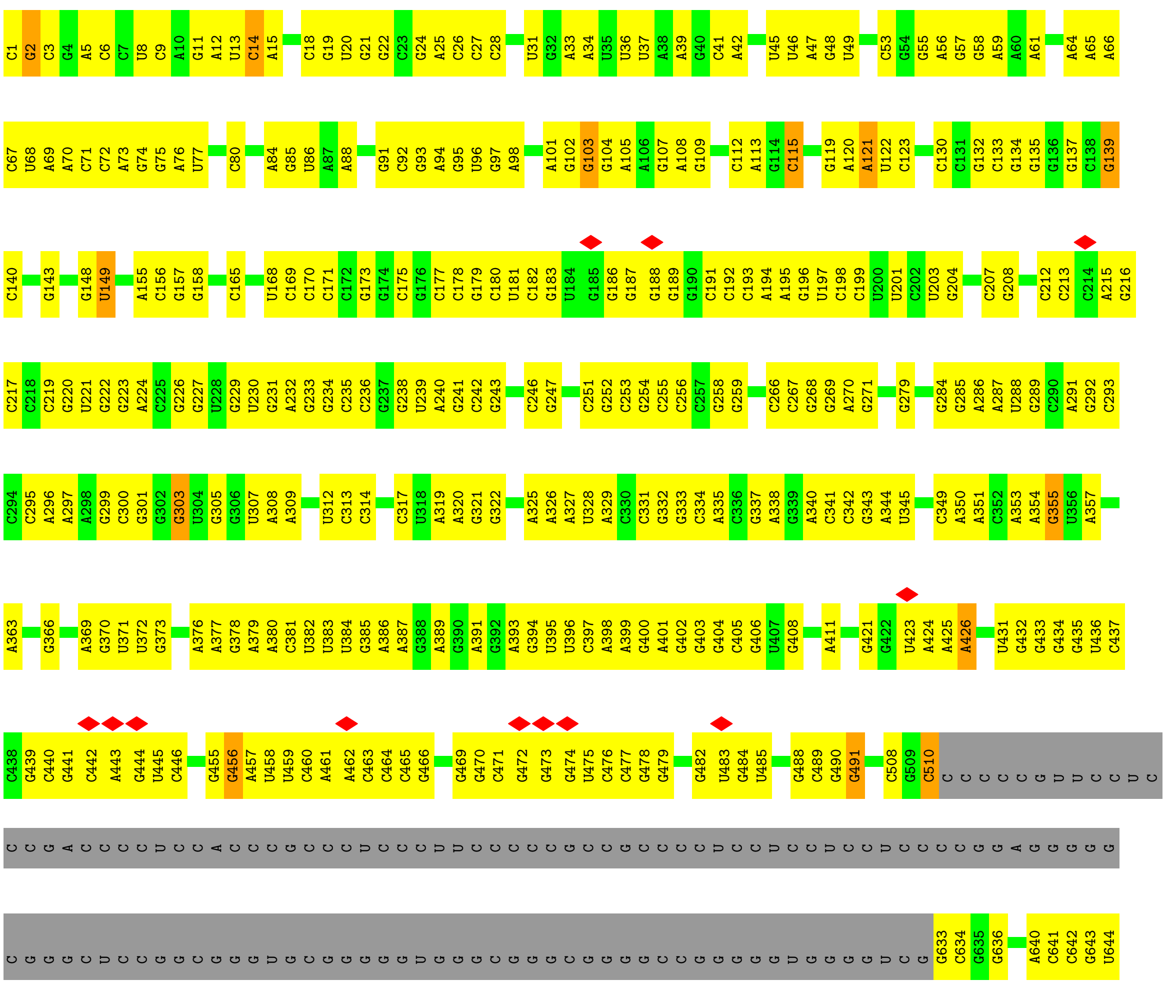


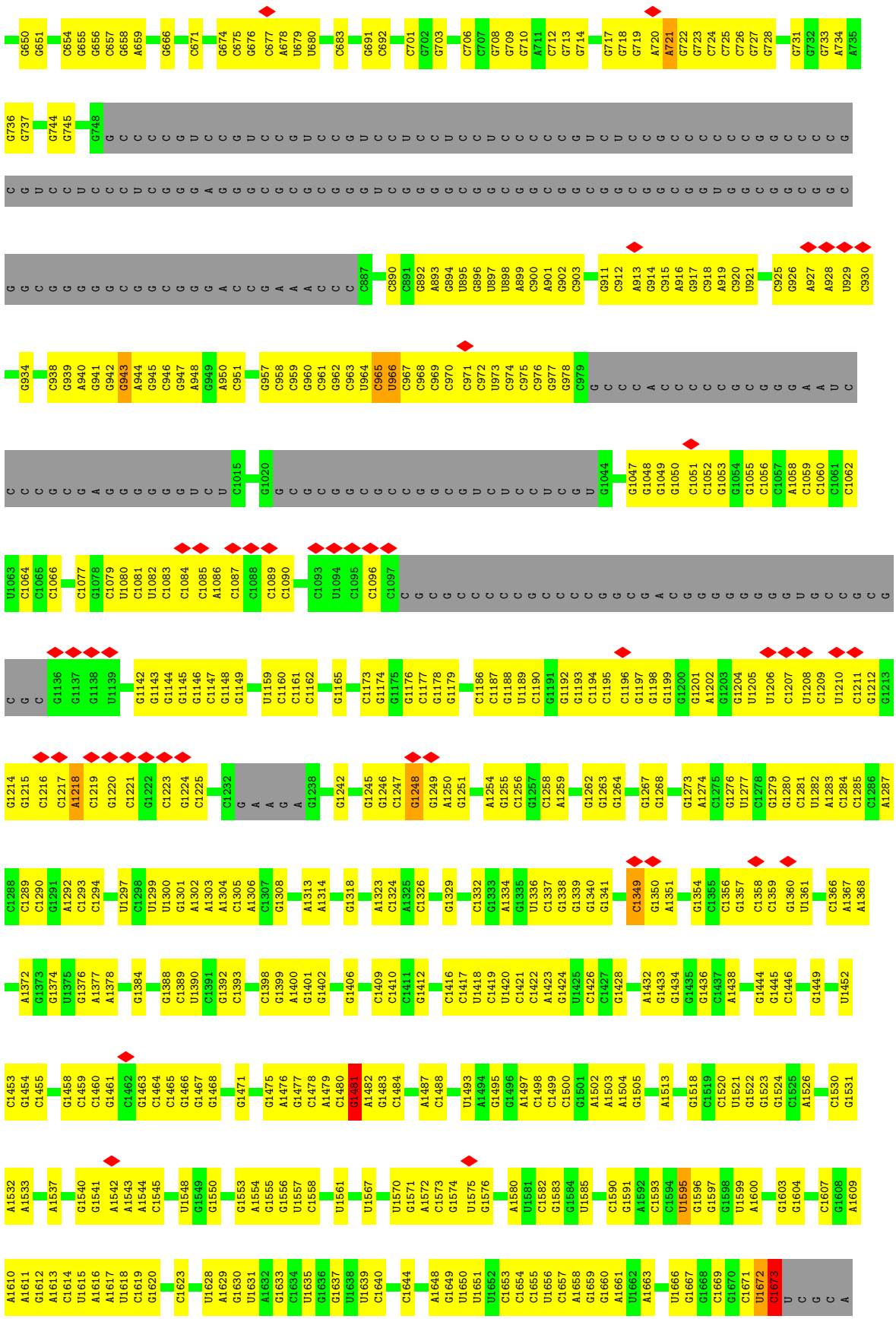


• Molecule 44: 28S Ribosomal RNA

Chain 2:






G650 G651 C654 G655 G656 C657 G658 A659 G666 C671 G674 C675 G676 C677 A678 U679 U680 C683 G691 C692 C701 G702 G703 C706 C707 G708 G709 G710 A711 C712 G713 G714 G717 G718 G719 A720 A721 G722 G723 C724 C725 C726 G727 G728 G731 G732 G733 A734 A735
G736 G737 G744 G745 G748
G934 C938 G939 A940 G941 G942 G943 A944 G945 C946 G947 A948 G949 A950 C951 G957 C958 C959 G960 C961 G962 C963 U964 C965 U966 C967 C968 C969 C970 C971 C972 U973 C974 C975 C976 G977 G978 C979
C1015 G1020 G1044 G1047 G1048 G1049 G1050 C1051 C1052 G1053 G1054 G1055 C1056 C1057 A1058 C1059 C1060 C1061 C1062
U1063 C1064 C1065 C1066 C1077 G1078 C1079 U1080 C1081 U1082 C1083 C1084 C1085 A1086 C1087 C1088 C1089 C1090 C1093 U1094 C1095 C1096 C1097
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G1214 G1215 C1216 C1217 A1218 C1219 G1220 C1221 G1222 C1223 G1224 C1225 C1232 G1238 G1242 G1245 G1246 C1247 G1248 G1249 A1250 G1251 A1254 G1255 C1256 G1257 C1258 A1259 G1262 G1263 G1264 G1267 G1268 G1273 A1274 C1275 G1276 U1277 C1278 G1279 G1280 C1281 U1282 A1283 C1284 C1285 C1286 A1287
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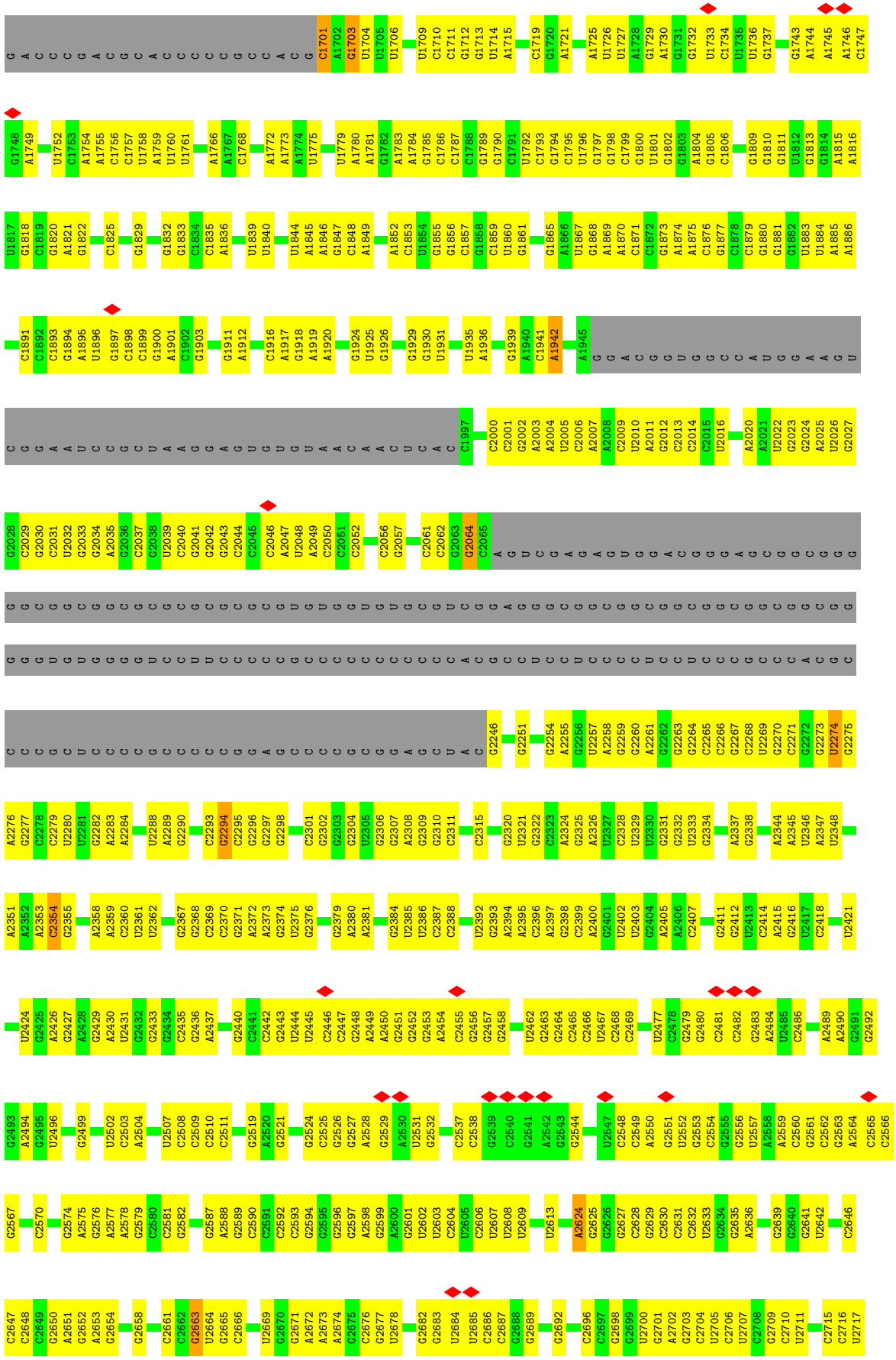

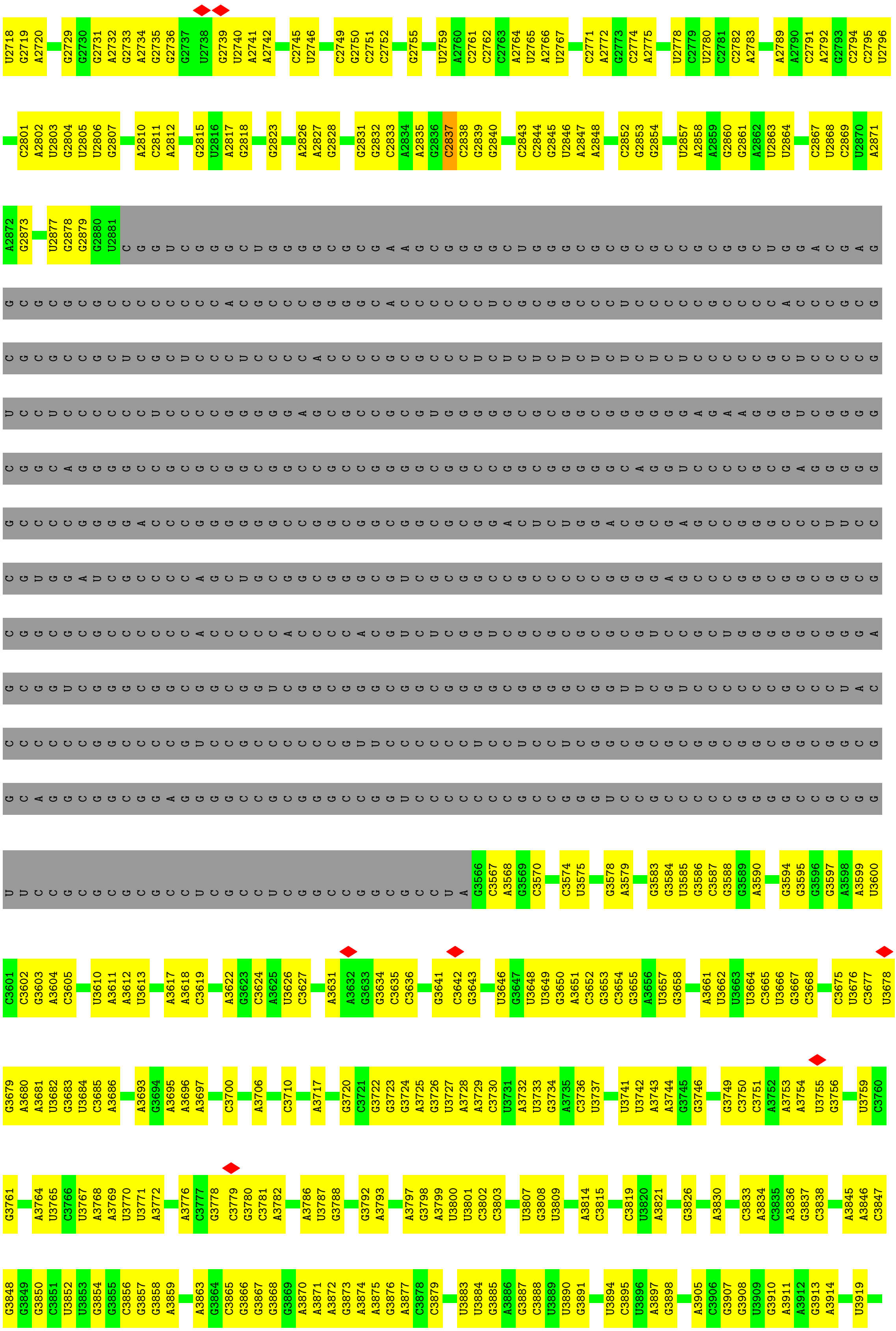
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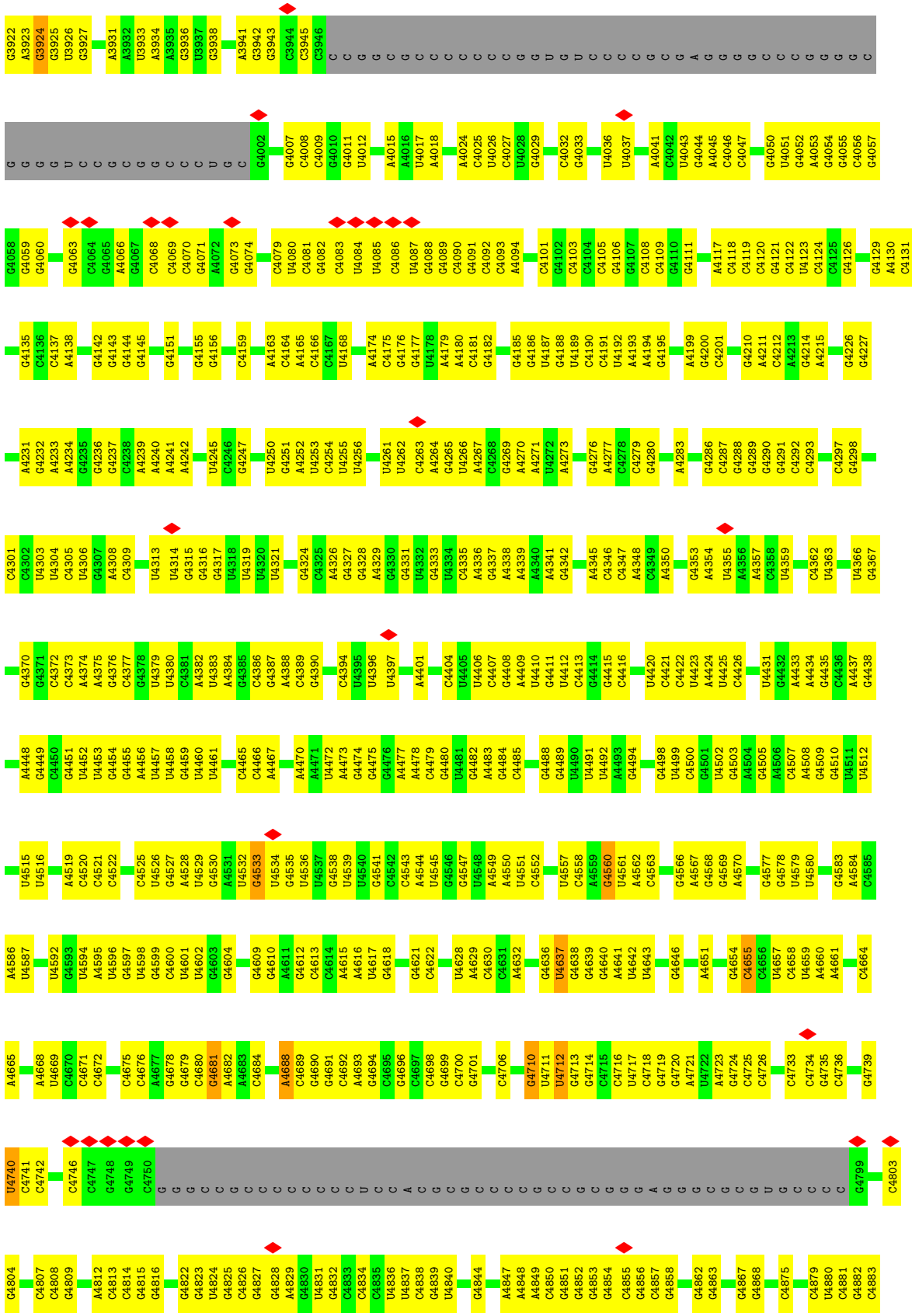
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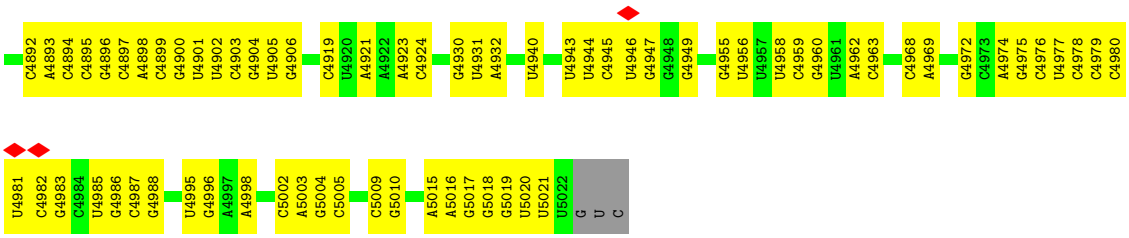
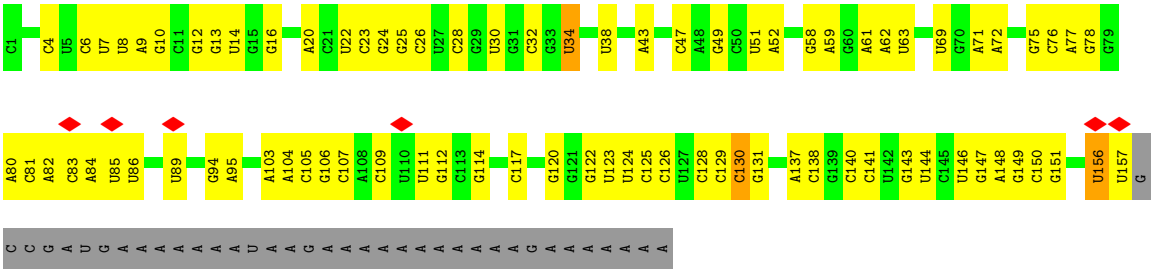


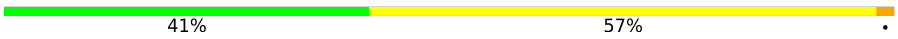
- Molecule 45: 5.8S Ribosomal RNA

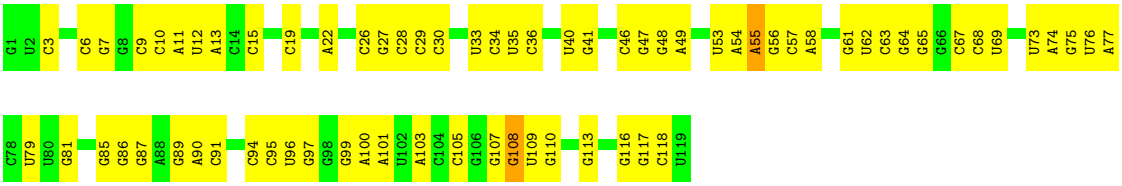
Chain 3:



- Molecule 46: 5S Ribosomal RNA

Chain 4:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109596	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	12.036	Depositor
Minimum map value	-3.841	Depositor
Average map value	0.203	Depositor
Map value standard deviation	0.880	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	467.99997, 467.99997, 467.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/1926	0.67	0/2583
2	B	0.45	0/3258	0.73	2/4361 (0.0%)
3	C	0.47	0/2943	0.73	1/3953 (0.0%)
4	D	0.49	1/2406 (0.0%)	0.70	1/3221 (0.0%)
5	E	0.52	0/1311	0.73	0/1763
6	F	0.45	0/1985	0.68	0/2644
7	G	0.46	0/1914	0.72	0/2578
8	H	0.43	0/1554	0.69	0/2089
9	I	0.42	0/1642	0.67	0/2194
10	J	0.49	0/1385	0.71	0/1852
11	L	0.53	2/1647 (0.1%)	0.73	3/2205 (0.1%)
12	M	0.49	0/1162	0.70	0/1556
13	N	0.43	0/1753	0.65	0/2348
14	O	0.44	0/1639	0.69	0/2193
15	P	0.44	0/1260	0.70	0/1691
16	Q	0.45	0/1517	0.74	0/2026
17	R	0.41	0/1542	0.64	0/2037
18	S	0.45	0/1478	0.73	0/1985
19	T	0.46	0/1325	0.72	0/1770
20	U	0.47	0/841	0.71	0/1128
21	V	0.43	0/977	0.63	0/1312
22	W	0.43	0/542	0.59	0/722
23	X	0.41	0/992	0.67	0/1334
24	Y	0.47	0/1082	0.72	1/1441 (0.1%)
25	Z	0.47	0/1137	0.79	0/1517
26	a	0.45	0/1190	0.71	0/1591
27	b	0.45	0/570	0.72	0/752
28	c	0.46	0/813	0.70	0/1091
29	d	0.45	0/919	0.67	0/1238
30	e	0.45	0/1071	0.68	0/1428
31	f	0.50	0/884	0.81	0/1185
32	g	0.48	0/917	0.74	0/1222
33	h	0.38	0/1022	0.64	0/1351
34	i	0.43	0/793	0.75	0/1048

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	j	0.49	0/704	0.76	0/931
36	k	0.43	0/574	0.73	0/761
37	l	0.40	0/453	0.61	0/599
38	m	0.42	0/434	0.70	0/575
39	n	0.40	0/240	0.50	0/305
40	o	0.46	0/884	0.74	0/1166
41	p	0.40	0/717	0.61	0/953
42	t	0.48	0/1058	0.75	0/1416
43	u	0.45	0/1638	0.69	1/2222 (0.0%)
44	2	0.41	22/86672 (0.0%)	0.81	41/135198 (0.0%)
45	3	0.36	0/3723	0.79	1/5800 (0.0%)
46	4	0.38	0/2836	0.82	3/4421 (0.1%)
All	All	0.43	25/147330 (0.0%)	0.77	54/217756 (0.0%)

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
44	2	0	34
45	3	0	2
All	All	0	36

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1701	C	C5'-C4'	18.32	1.73	1.51
44	2	1673	C	C3'-O3'	15.33	1.63	1.42
44	2	1701	C	O5'-C5'	14.40	1.67	1.44
44	2	1673	C	O3'-P	14.19	1.78	1.61
44	2	1701	C	P-O5'	13.52	1.73	1.59

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1701	C	O4'-C4'-C3'	-15.18	88.82	104.00
2	B	258	HIS	C-N-CD	-13.98	89.84	120.60
44	2	1701	C	O4'-C1'-N1	12.32	118.06	108.20
44	2	1701	C	C4'-C3'-O3'	12.21	137.41	113.00
44	2	1701	C	C2'-C3'-O3'	-10.63	86.10	109.50

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	2	1	C	Sidechain
44	2	115	C	Sidechain
44	2	121	A	Sidechain
44	2	149	U	Sidechain
44	2	2	G	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	245/257 (95%)	236 (96%)	6 (2%)	3 (1%)	11 44
2	B	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	3 20
3	C	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	2 18
4	D	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	7 37
5	E	156/288 (54%)	141 (90%)	8 (5%)	7 (4%)	2 17
6	F	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	7 37
7	G	233/266 (88%)	217 (93%)	7 (3%)	9 (4%)	2 19
8	H	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	8 38
9	I	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	8 38
10	J	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1 11
11	L	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	1 14
12	M	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	9 41
13	N	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	8 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	8	40
15	P	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	6	32
16	Q	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	3	21
17	R	181/196 (92%)	174 (96%)	4 (2%)	3 (2%)	7	37
18	S	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	3	20
19	T	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	6	32
20	U	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
21	V	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	8	38
22	W	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
23	X	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
24	Y	126/145 (87%)	119 (94%)	4 (3%)	3 (2%)	5	27
25	Z	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	3	23
26	a	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	3	21
27	b	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	1	13
28	c	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	6	32
29	d	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	14	52
30	e	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	5	27
31	f	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	2	16
32	g	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	3	20
33	h	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	4	26
34	i	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	1	13
35	j	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	5	27
36	k	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	8	40
37	l	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	30
38	m	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	6	32
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	6	32
41	p	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	3	21
42	t	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	1	15
43	u	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	9	41
All	All	6479/7422 (87%)	6102 (94%)	200 (3%)	177 (3%)	6	25

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	196	TRP
2	B	4	ARG
2	B	5	LYS
2	B	157	CYS

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	A	189/199 (95%)	184 (97%)	5 (3%)	41	59
2	B	344/349 (99%)	326 (95%)	18 (5%)	19	40
3	C	302/348 (87%)	284 (94%)	18 (6%)	16	37
4	D	244/250 (98%)	237 (97%)	7 (3%)	37	56
5	E	143/252 (57%)	135 (94%)	8 (6%)	17	38
6	F	203/215 (94%)	196 (97%)	7 (3%)	32	51
7	G	199/223 (89%)	192 (96%)	7 (4%)	31	51
8	H	171/171 (100%)	164 (96%)	7 (4%)	26	47
9	I	170/181 (94%)	161 (95%)	9 (5%)	19	40
10	J	143/149 (96%)	137 (96%)	6 (4%)	25	46
11	L	167/177 (94%)	156 (93%)	11 (7%)	14	34
12	M	118/161 (73%)	114 (97%)	4 (3%)	32	51
13	N	172/172 (100%)	170 (99%)	2 (1%)	67	78
14	O	168/174 (97%)	166 (99%)	2 (1%)	67	78
15	P	133/163 (82%)	126 (95%)	7 (5%)	19	40
16	Q	162/165 (98%)	157 (97%)	5 (3%)	35	54
17	R	161/175 (92%)	150 (93%)	11 (7%)	13	34
18	S	155/157 (99%)	148 (96%)	7 (4%)	23	45
19	T	139/140 (99%)	134 (96%)	5 (4%)	30	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	91/115 (79%)	88 (97%)	3 (3%)	33	52
21	V	100/107 (94%)	99 (99%)	1 (1%)	73	82
22	W	55/126 (44%)	52 (94%)	3 (6%)	18	39
23	X	107/133 (80%)	105 (98%)	2 (2%)	52	69
24	Y	119/135 (88%)	115 (97%)	4 (3%)	32	51
25	Z	118/118 (100%)	112 (95%)	6 (5%)	20	41
26	a	120/121 (99%)	116 (97%)	4 (3%)	33	52
27	b	58/126 (46%)	57 (98%)	1 (2%)	56	72
28	c	88/97 (91%)	87 (99%)	1 (1%)	70	80
29	d	100/110 (91%)	96 (96%)	4 (4%)	27	47
30	e	115/121 (95%)	112 (97%)	3 (3%)	41	59
31	f	87/89 (98%)	79 (91%)	8 (9%)	7	23
32	g	98/100 (98%)	88 (90%)	10 (10%)	6	20
33	h	109/110 (99%)	106 (97%)	3 (3%)	38	57
34	i	82/89 (92%)	76 (93%)	6 (7%)	11	31
35	j	71/80 (89%)	69 (97%)	2 (3%)	38	57
36	k	64/65 (98%)	64 (100%)	0	100	100
37	l	47/48 (98%)	46 (98%)	1 (2%)	48	66
38	m	48/116 (41%)	45 (94%)	3 (6%)	15	36
39	n	24/24 (100%)	24 (100%)	0	100	100
40	o	94/94 (100%)	89 (95%)	5 (5%)	19	40
41	p	74/75 (99%)	72 (97%)	2 (3%)	40	58
42	t	113/121 (93%)	106 (94%)	7 (6%)	15	36
43	u	177/177 (100%)	163 (92%)	14 (8%)	10	29
All	All	5642/6318 (89%)	5403 (96%)	239 (4%)	27	46

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	P	78	TRP
42	t	61	VAL
19	T	69	GLN
42	t	18	ILE
43	u	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
15	P	25	HIS
33	h	101	ASN
18	S	125	GLN
32	g	100	GLN
40	o	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	2	3605/5025 (71%)	2046 (56%)	325 (9%)
45	3	156/194 (80%)	81 (51%)	6 (3%)
46	4	118/119 (99%)	68 (57%)	9 (7%)
All	All	3879/5338 (72%)	2195 (56%)	340 (8%)

5 of 2195 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	2	2	G
44	2	3	C
44	2	5	A
44	2	6	C
44	2	8	U

5 of 340 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	3873	G
44	2	4659	U
44	2	4033	G
44	2	4338	A
44	2	4740	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

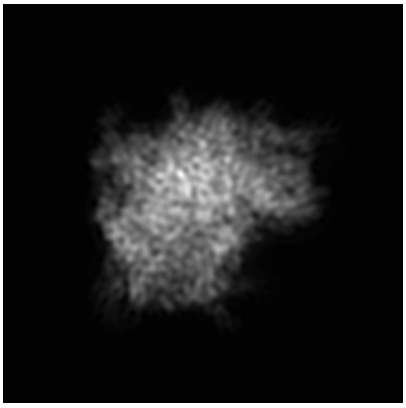
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2810. These allow visual inspection of the internal detail of the map and identification of artifacts.

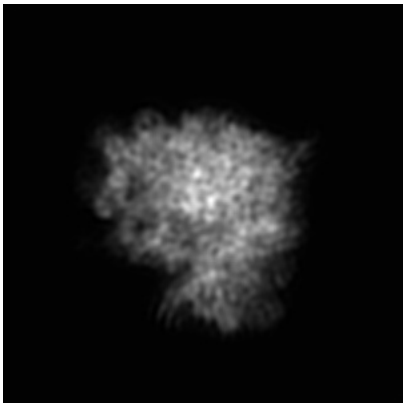
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

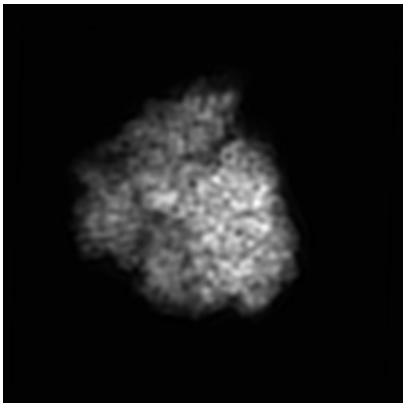
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 150

Y Index: 150

Z Index: 150

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: 173

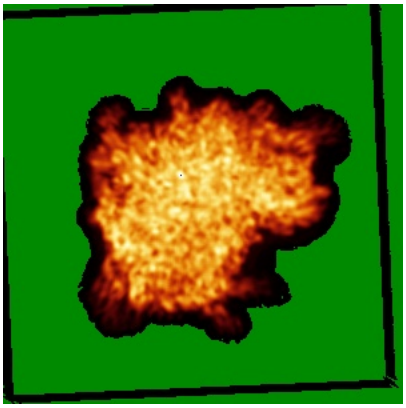
Y Index: 149

Z Index: 154

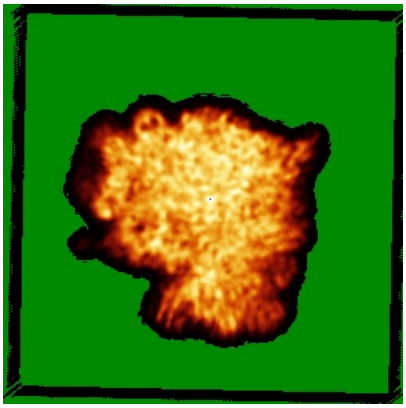
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

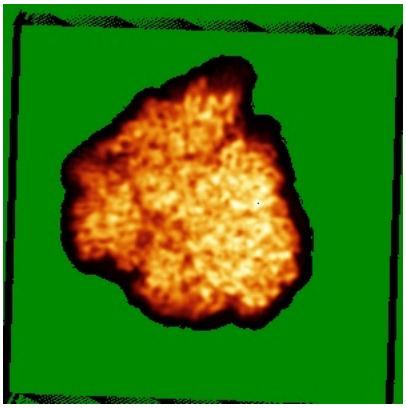
6.4.1 Primary map



X



Y

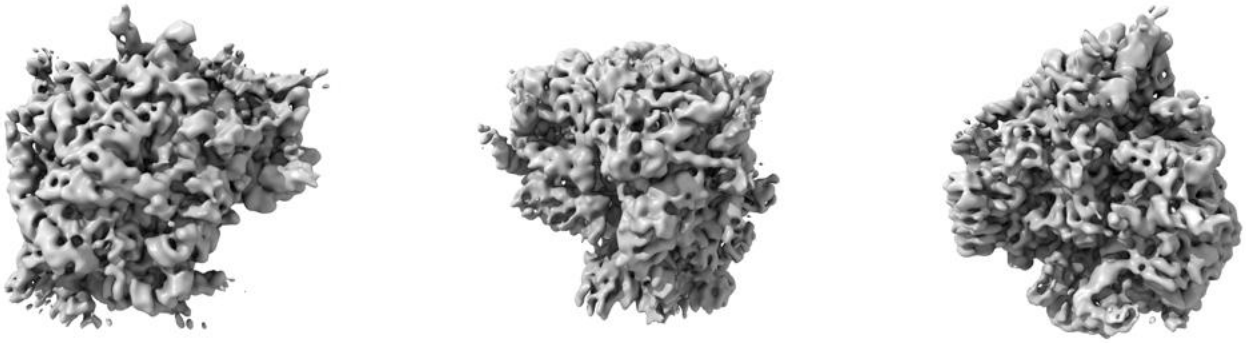


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

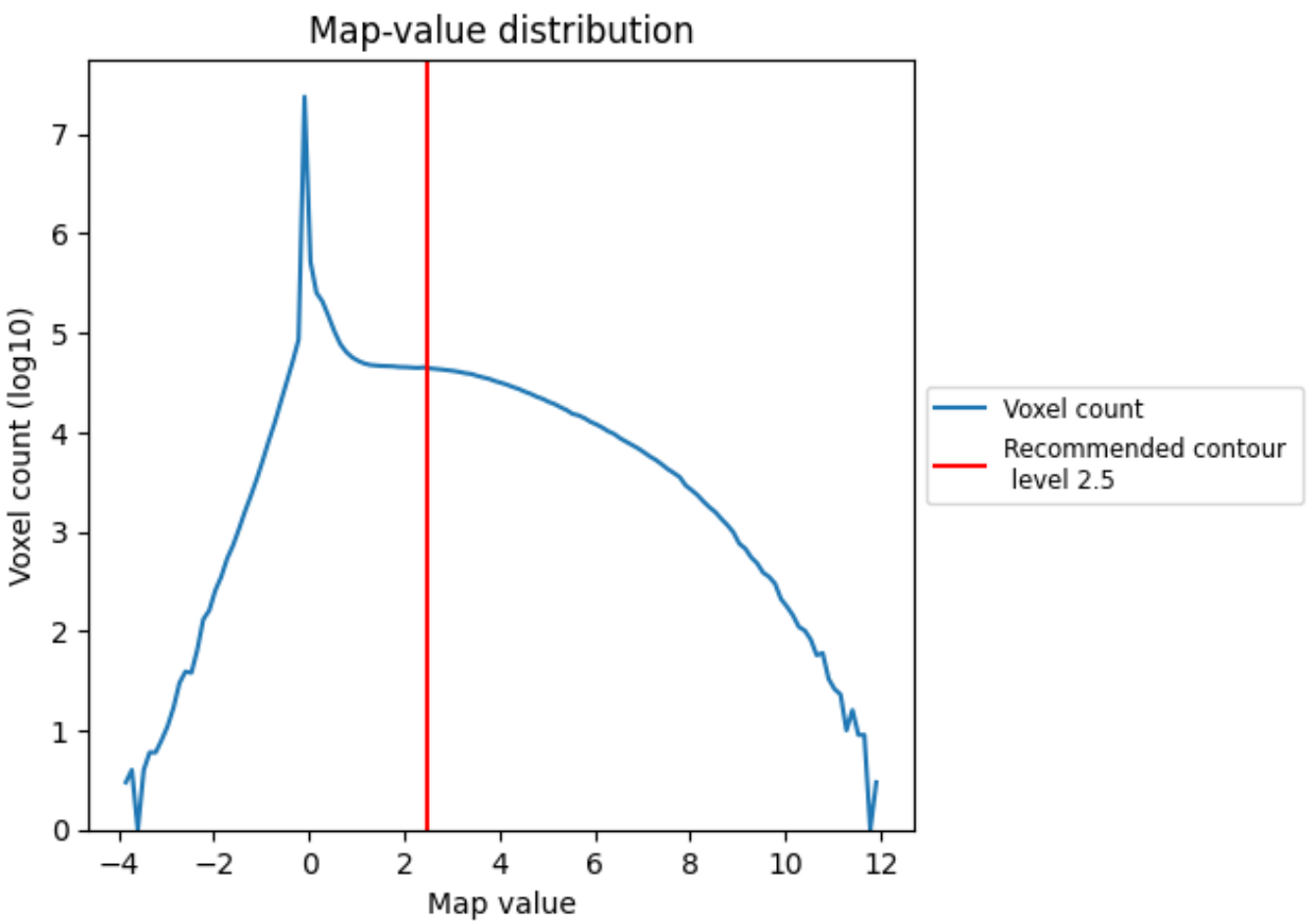
6.6 Mask visualisation (i)

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

7 Map analysis (i)

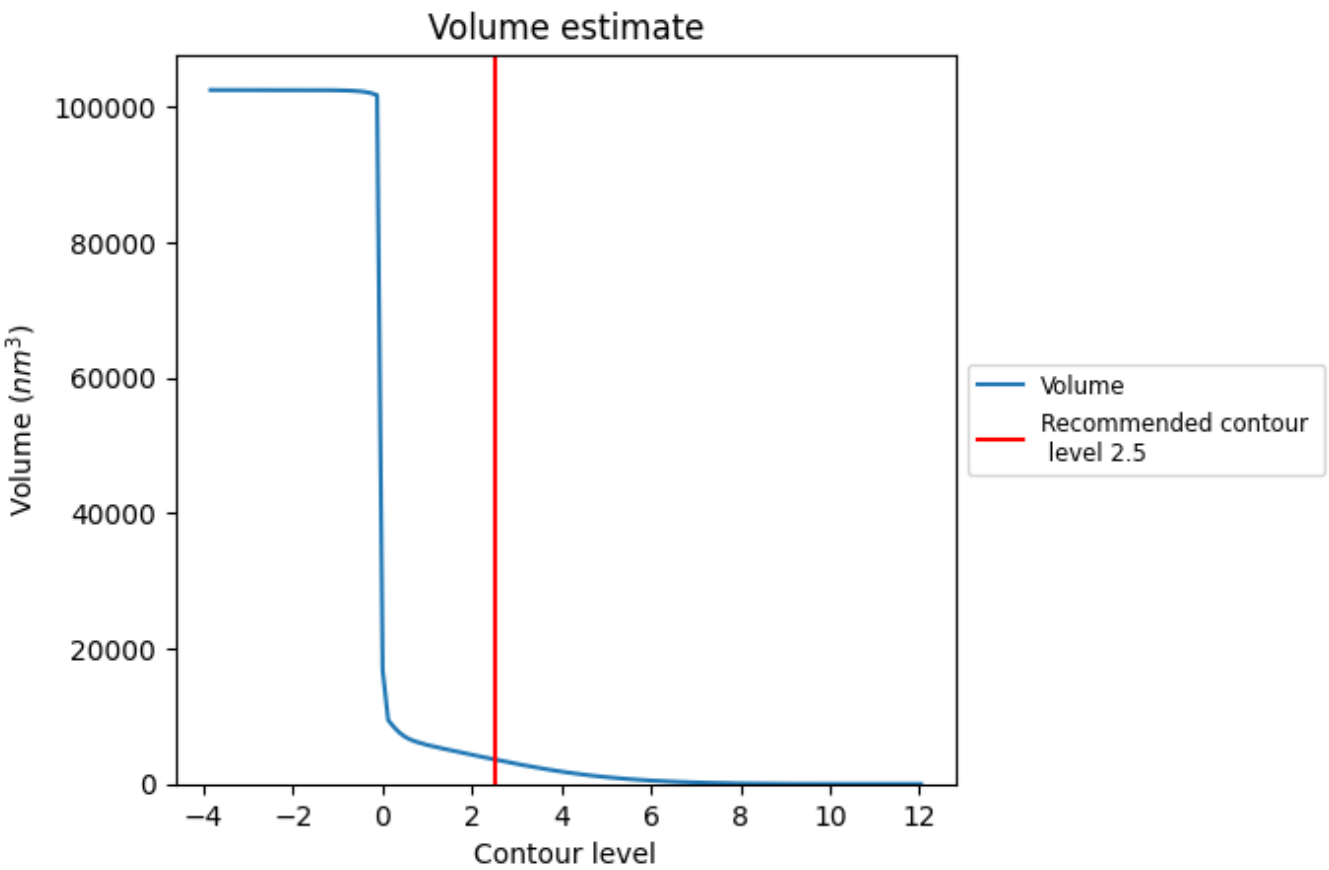
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

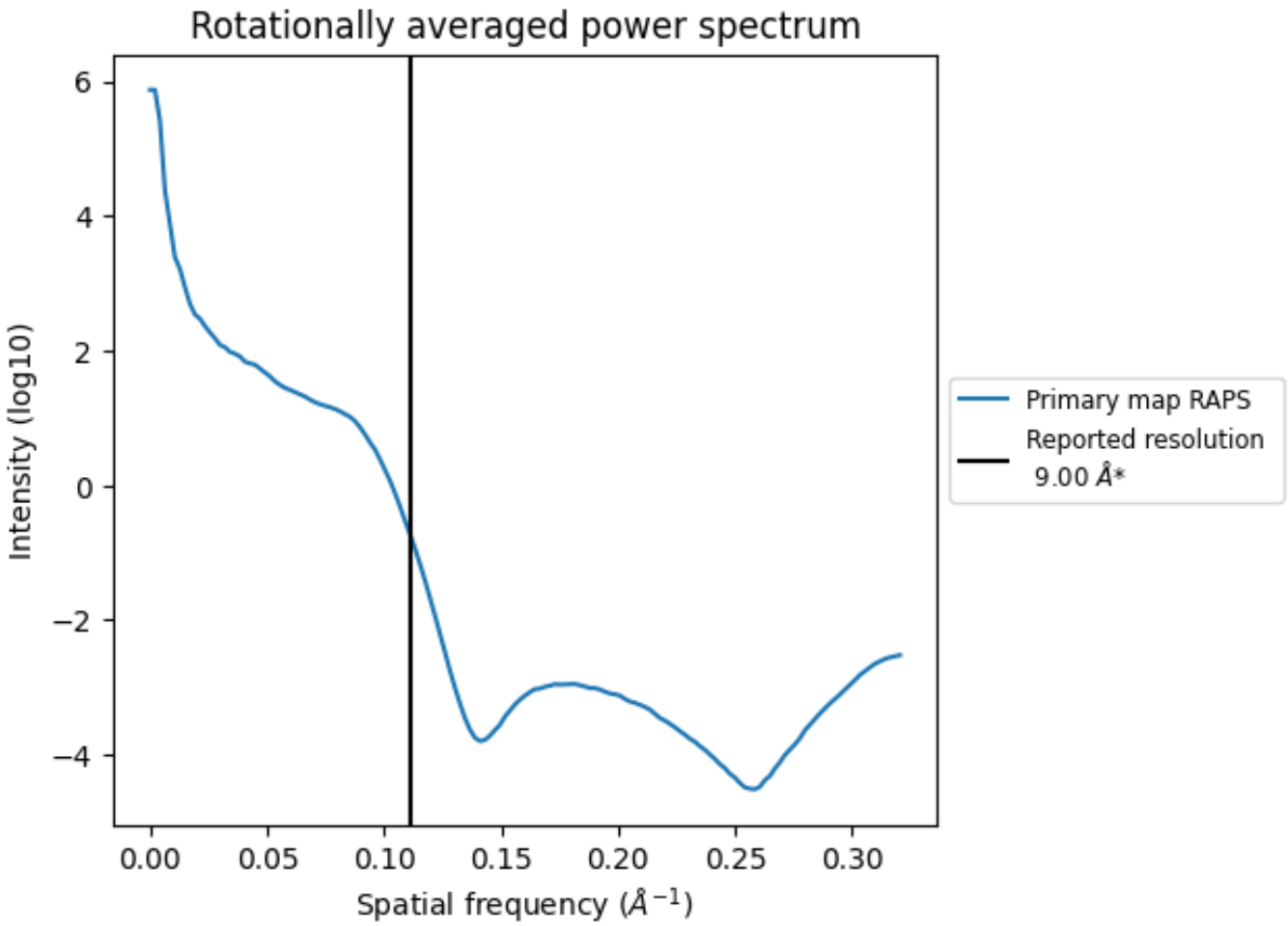
7.2 Volume estimate (i)



The volume at the recommended contour level is 3628 nm^3; this corresponds to an approximate mass of 3277 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 0.111 Å^{-1}

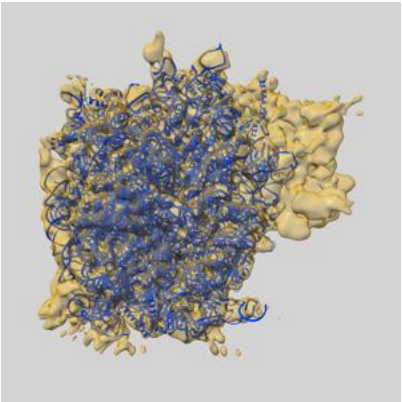
8 Fourier-Shell correlation (i)

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

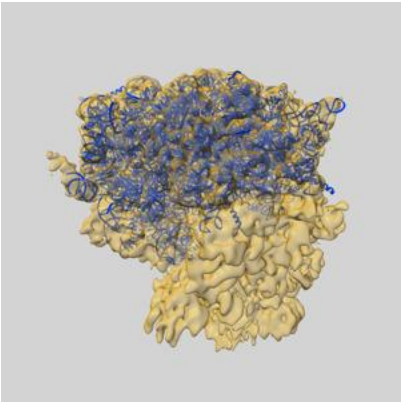
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2810 and PDB model 4D5Y. Per-residue inclusion information can be found in section 3 on page 12.

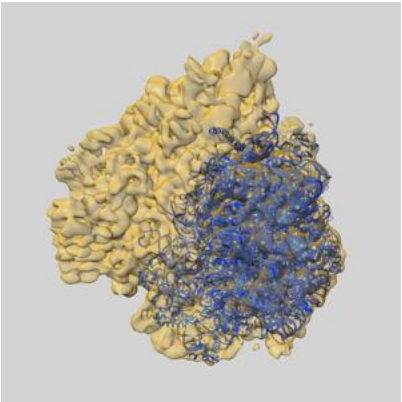
9.1 Map-model overlay (i)



X



Y



Z

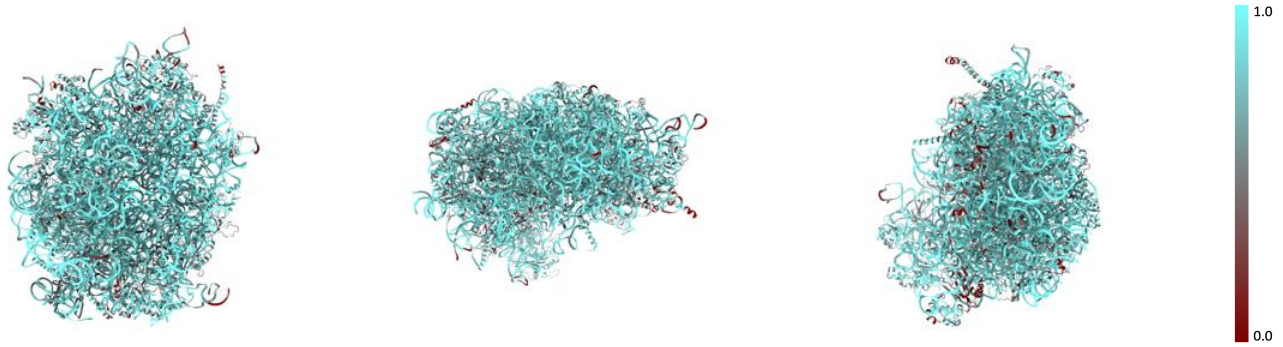
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

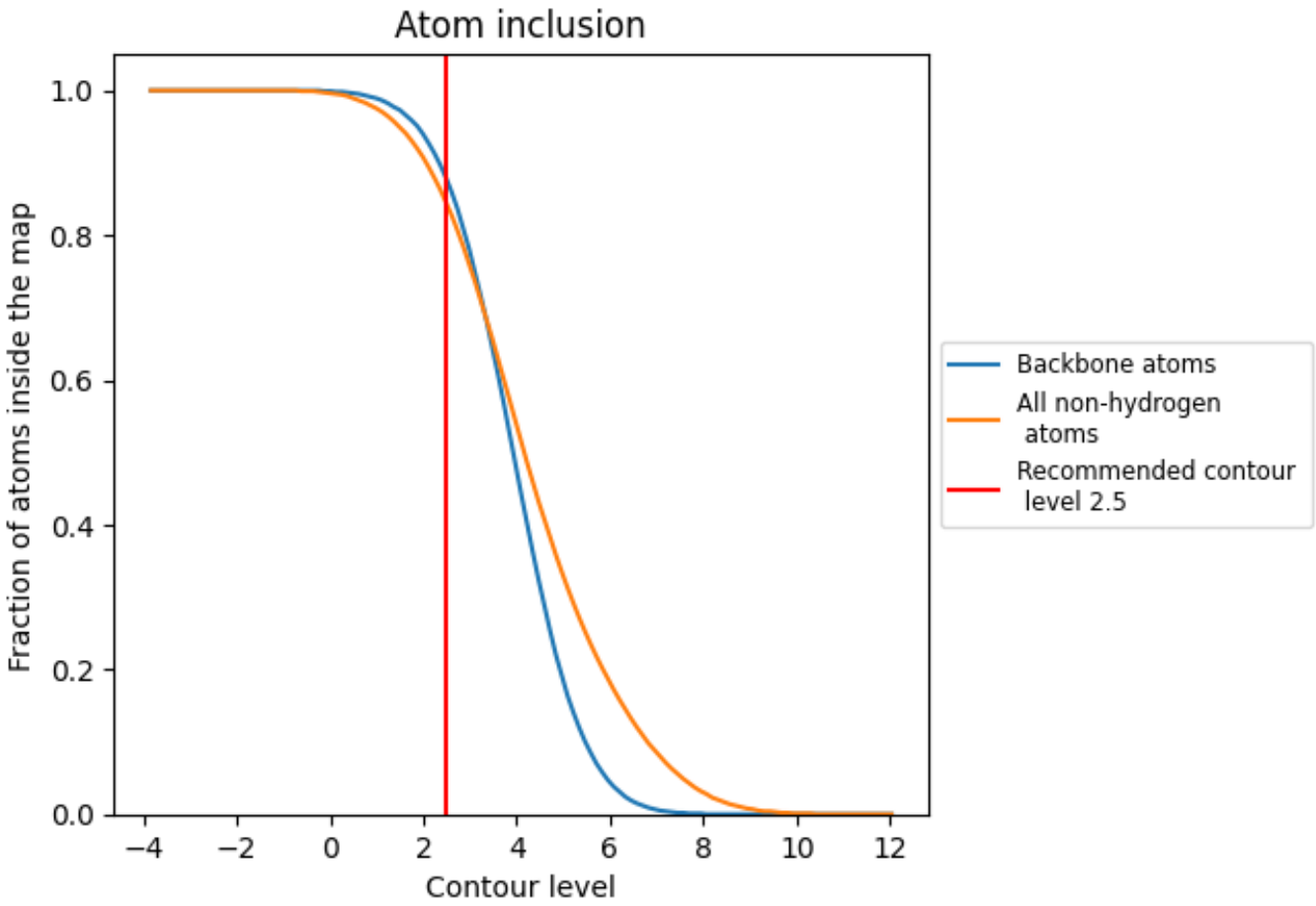
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.1160
2	0.9150	0.1330
3	0.9260	0.1360
4	0.9710	0.1440
A	0.6420	0.0660
B	0.6990	0.0730
C	0.7630	0.0770
D	0.8170	0.1040
E	0.6630	0.0560
F	0.7330	0.0970
G	0.7000	0.1150
H	0.6920	0.1120
I	0.6320	0.0940
J	0.8340	0.1070
L	0.7360	0.0930
M	0.7890	0.1210
N	0.7350	0.0510
O	0.7310	0.0970
P	0.8130	0.0830
Q	0.7230	0.0850
R	0.7470	0.1130
S	0.7390	0.0890
T	0.7090	0.0750
U	0.7330	0.1180
V	0.5930	0.0880
W	0.8240	0.1080
X	0.7020	0.0850
Y	0.8290	0.0980
Z	0.6760	0.0910
a	0.7630	0.0680
b	0.7450	0.0890
c	0.6790	0.1080
d	0.8310	0.1090
e	0.7430	0.0770
f	0.7320	0.0640

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Chain	Atom inclusion	Q-score
g	0.6340	0.0470
h	0.8150	0.1260
i	0.7550	0.1180
j	0.8480	0.0780
k	0.7180	0.1220
l	0.7770	0.0870
m	0.6790	0.0800
n	0.7200	0.0910
o	0.5900	0.0690
p	0.7380	0.1070
t	0.7950	0.0900
u	0.4640	0.0430