wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 08:14 am GMT

PDB ID	:	4D67
EMDB ID	:	EMD-2813
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	:	2014-11-10
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:

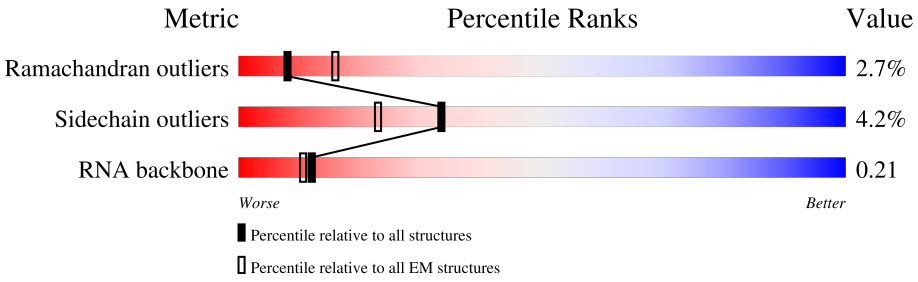
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	20% 93%
2	B	403	13% 90% 7%
3	C	427	11% 78% 6% 15%
4	D	297	15% 93%
5	E	288	15% 50% 5% 45%
6	F	248	12% 90% 6%
7	G	266	17% 83% 5% 12%
8	H	192	9% 95% 5%

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

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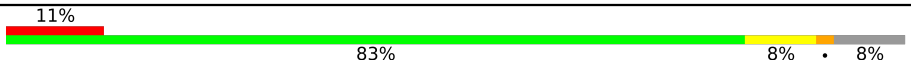
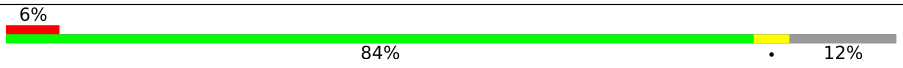
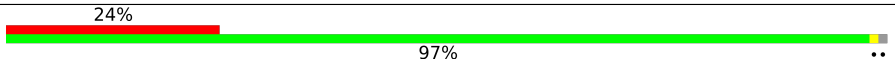
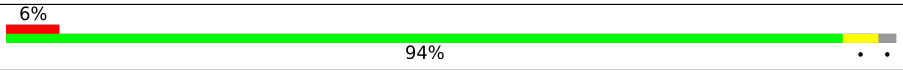
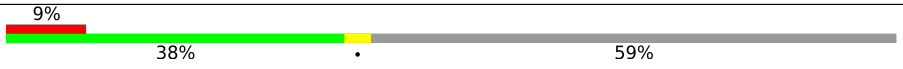
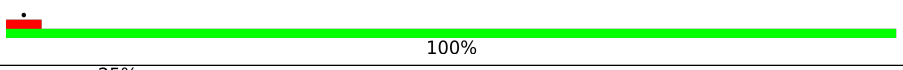
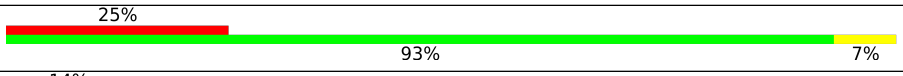
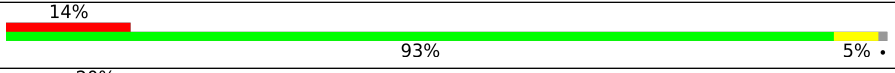
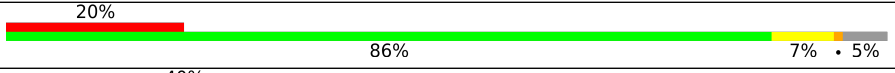
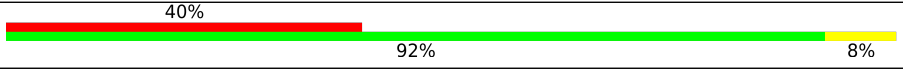
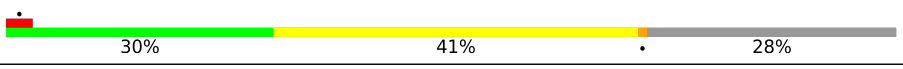
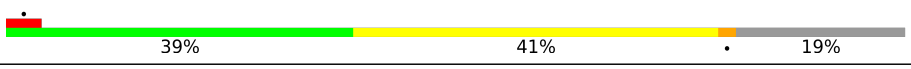
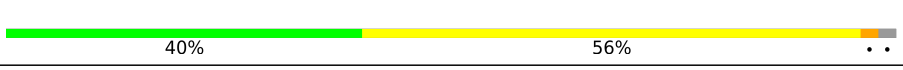
Mol	Chain	Length	Quality of chain
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	128	
39	n	25	
40	o	106	
41	p	92	
42	t	137	
43	u	210	
44	2	5025	
45	3	194	
46	4	121	

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 L8.

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 L3.

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 L4.

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 L5.

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 L6.

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 L7.

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 L7A.

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

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L9.

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

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L11.

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

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L13.

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

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L14.

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

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L15.

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

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L13A.

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

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L17.

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

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L18.

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

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN L19.

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

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L18A.

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

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN L21.

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

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN L23A.

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

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L26.

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

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L27A.

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

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L31.

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

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN L35A.

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

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L37.

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

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L38.

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

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L39.

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

- Molecule 38 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

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

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L41.

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

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L36A.

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

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L37A.

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

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L28.

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

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10A.

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

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

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

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

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

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

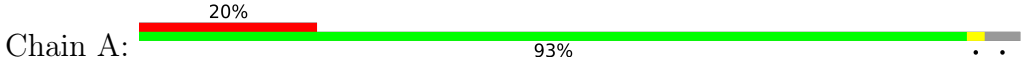
Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

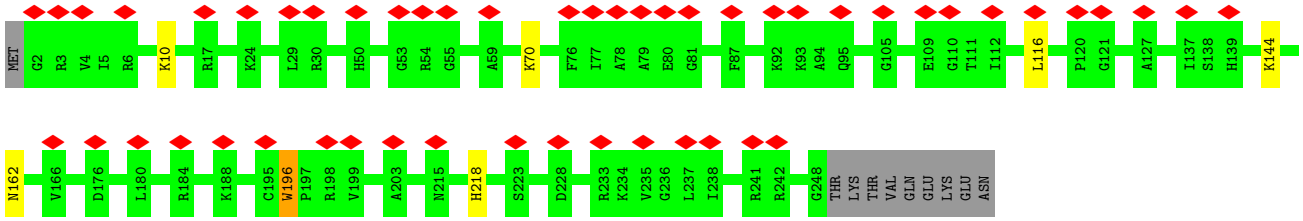
3 Residue-property plots (i)

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 L8

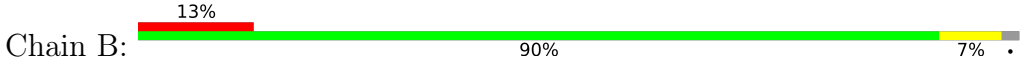
Chain A:

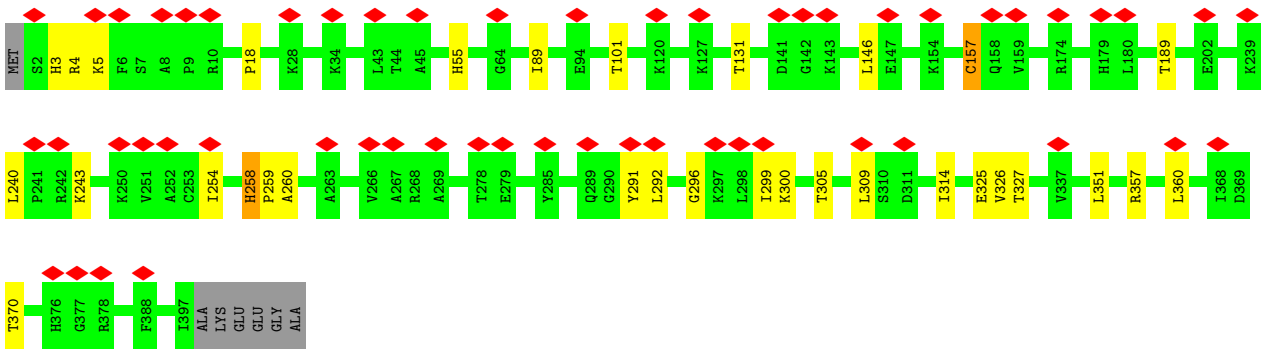




• Molecule 2: 60S RIBOSOMAL PROTEIN L3

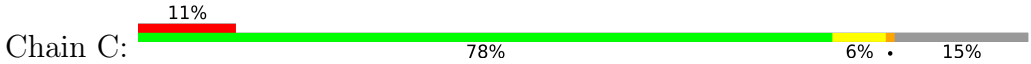
Chain B:

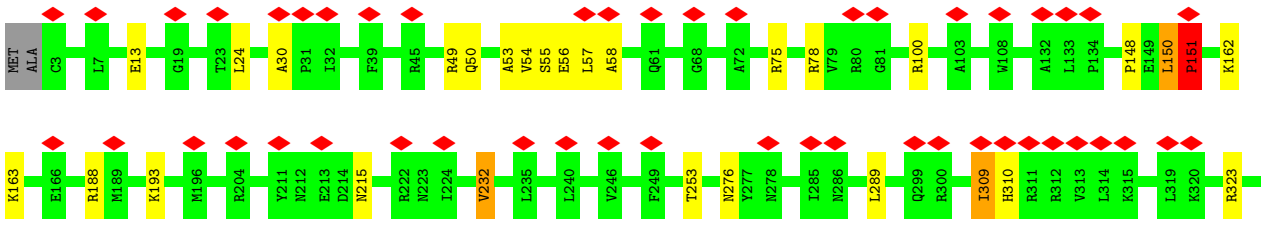


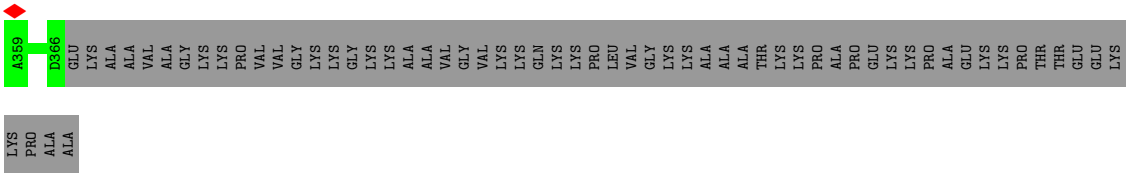


• Molecule 3: 60S RIBOSOMAL PROTEIN L4

Chain C:

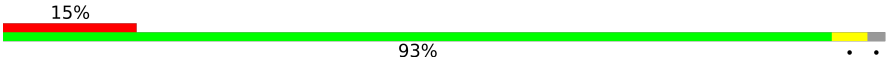


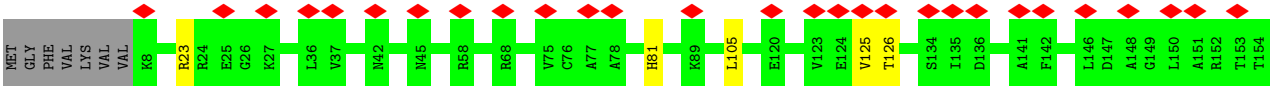


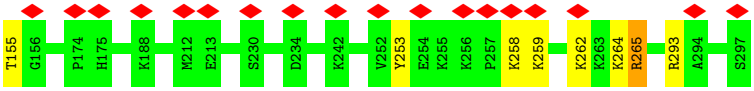


• Molecule 4: 60S RIBOSOMAL PROTEIN L5

Chain D:

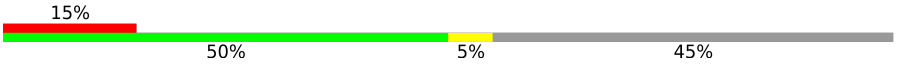


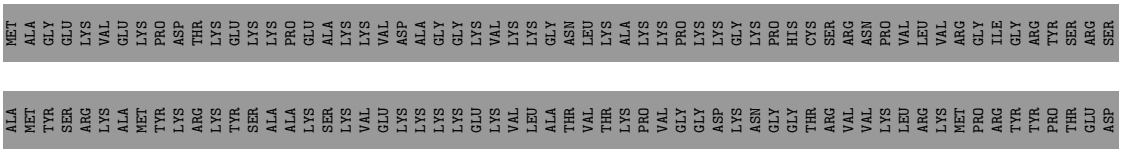


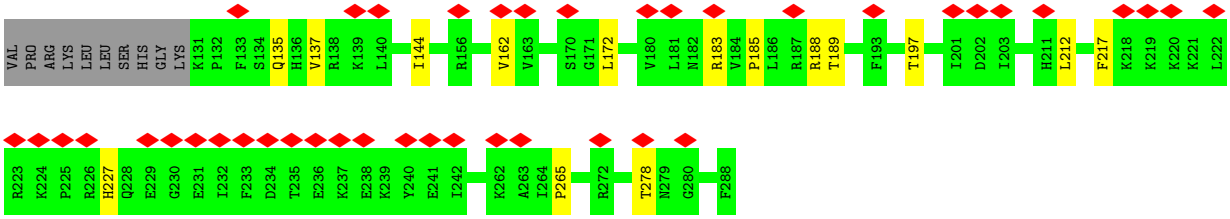


• Molecule 5: 60S RIBOSOMAL PROTEIN L6

Chain E:

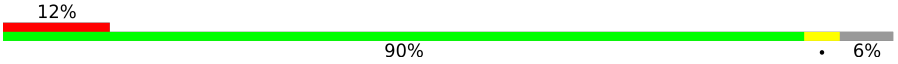


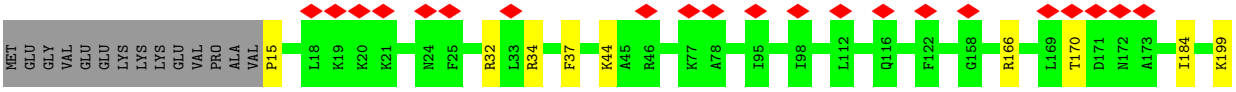


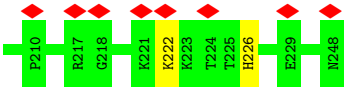


• Molecule 6: 60S RIBOSOMAL PROTEIN L7

Chain F:

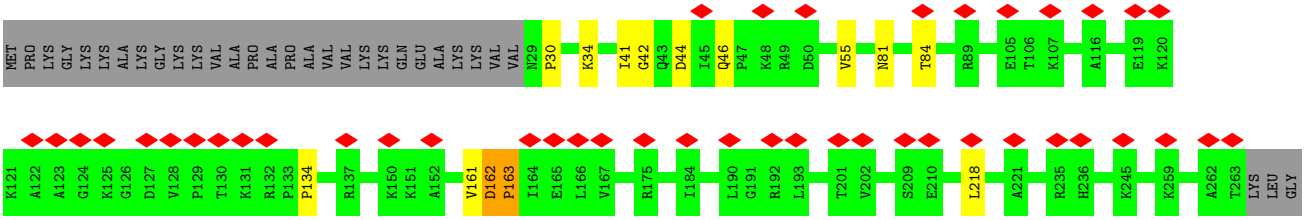




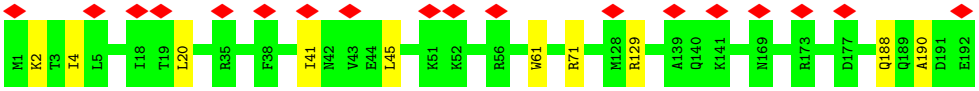


• Molecule 7: 60S RIBOSOMAL PROTEIN L7A

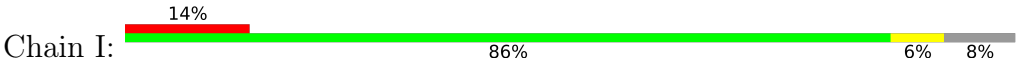
Chain G:

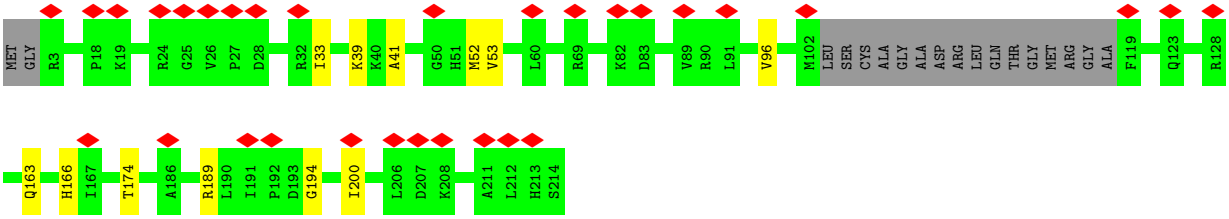


• Molecule 8: 60S RIBOSOMAL PROTEIN L9

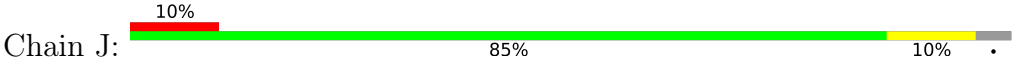


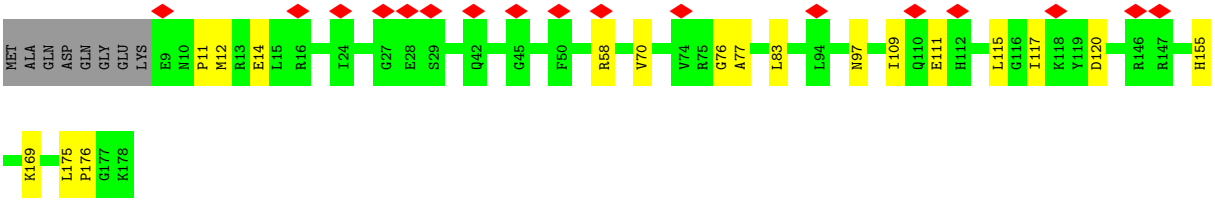
• Molecule 9: 60S RIBOSOMAL PROTEIN L10



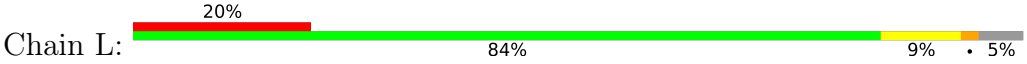


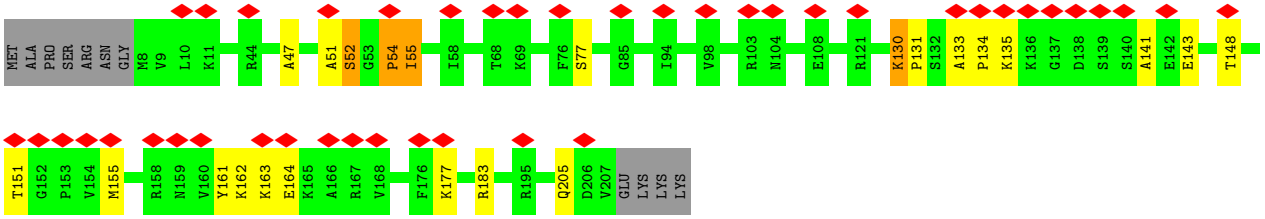
• Molecule 10: 60S RIBOSOMAL PROTEIN L11



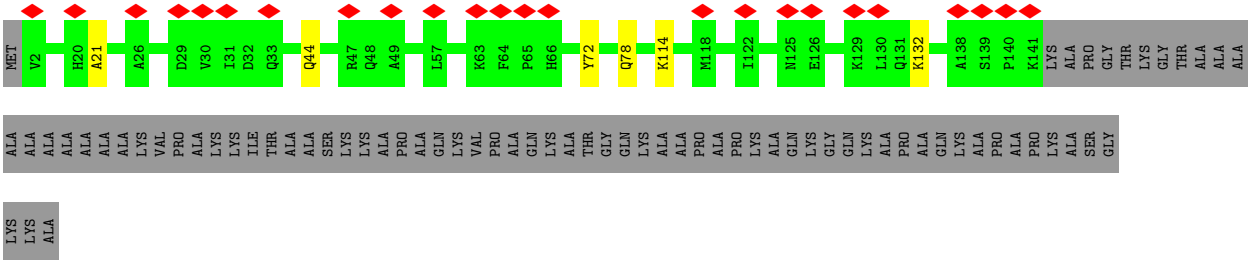


• Molecule 11: 60S RIBOSOMAL PROTEIN L13



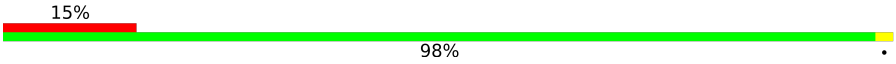


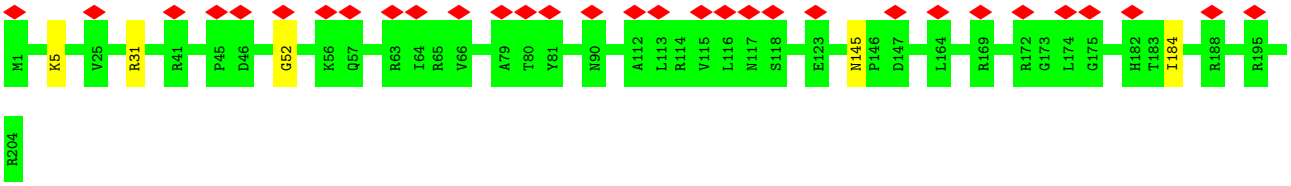
• Molecule 12: 60S RIBOSOMAL PROTEIN L14



• Molecule 13: 60S RIBOSOMAL PROTEIN L15

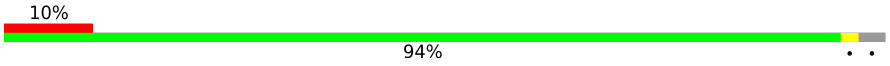
Chain N:

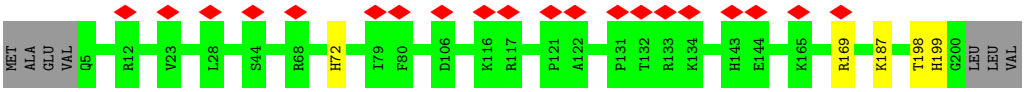




• Molecule 14: 60S RIBOSOMAL PROTEIN L13A

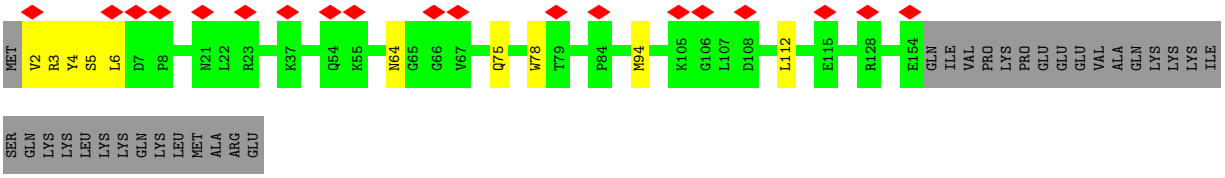
Chain O:





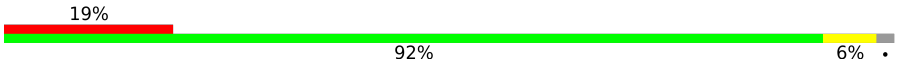
• Molecule 15: 60S RIBOSOMAL PROTEIN L17

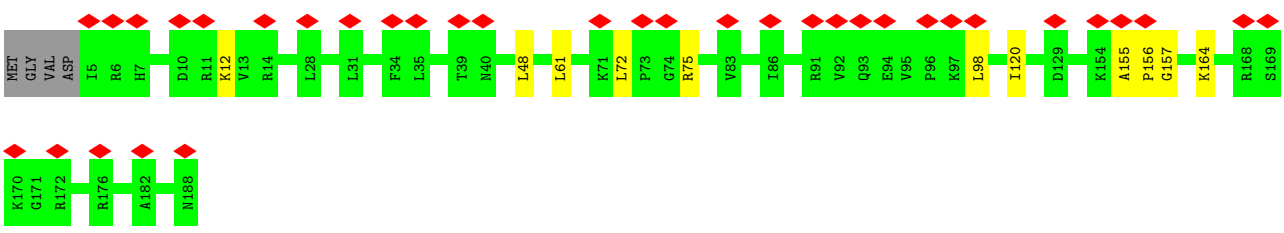
Chain P:



• Molecule 16: 60S RIBOSOMAL PROTEIN L18

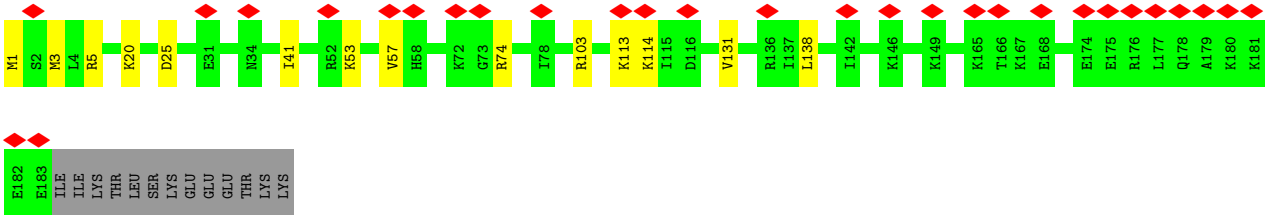
Chain Q:





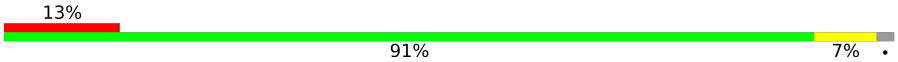
• Molecule 17: 60S RIBOSOMAL PROTEIN L19

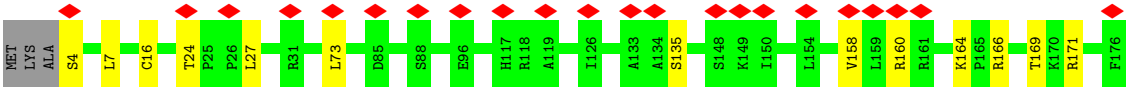
Chain R:



• Molecule 18: 60S RIBOSOMAL PROTEIN L18A

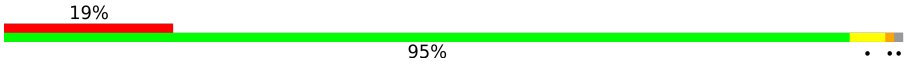
Chain S:

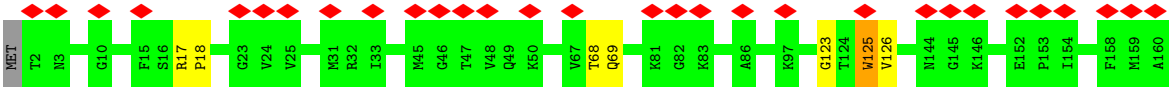




• Molecule 19: 60S RIBOSOMAL PROTEIN L21

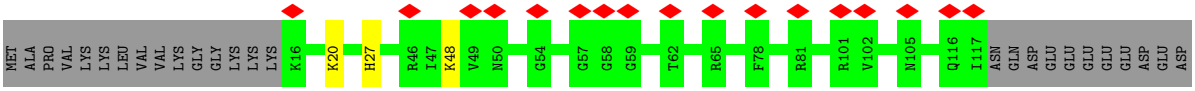
Chain T:





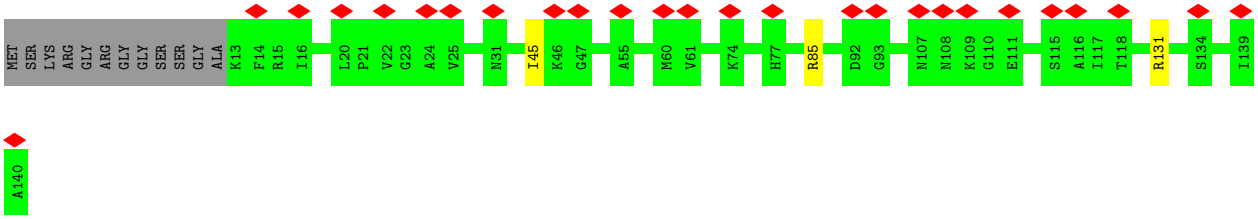
• Molecule 20: 60S RIBOSOMAL PROTEIN L22

Chain U:



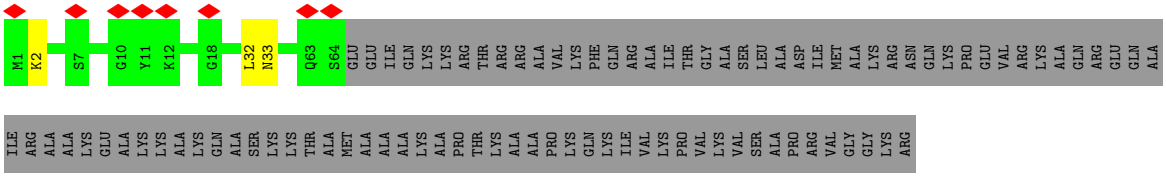
• Molecule 21: 60S RIBOSOMAL PROTEIN L23

Chain V:



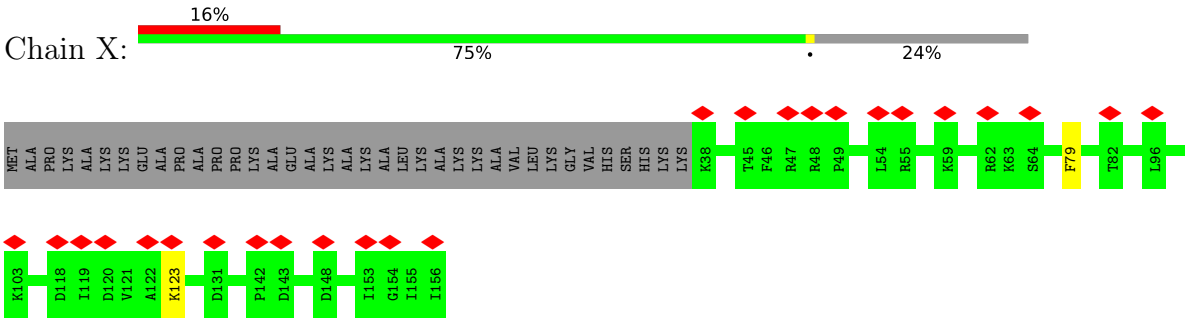
• Molecule 22: 60S RIBOSOMAL PROTEIN L24

Chain W:



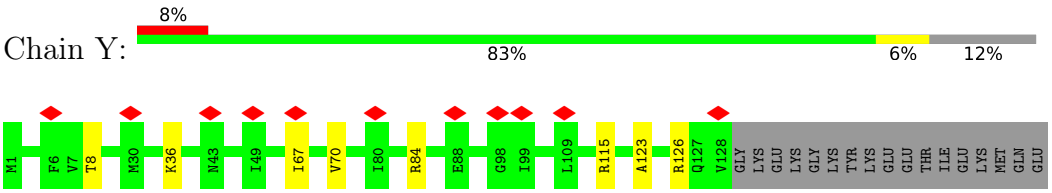
• Molecule 23: 60S RIBOSOMAL PROTEIN L23A

Chain X:



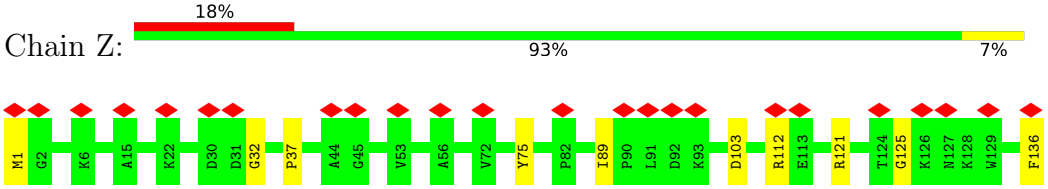
• Molecule 24: 60S RIBOSOMAL PROTEIN L26

Chain Y:



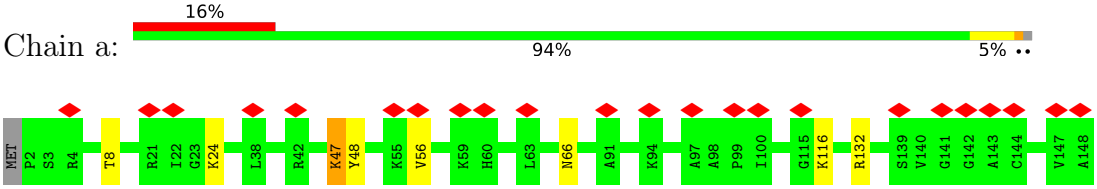
• Molecule 25: 60S RIBOSOMAL PROTEIN L27

Chain Z:



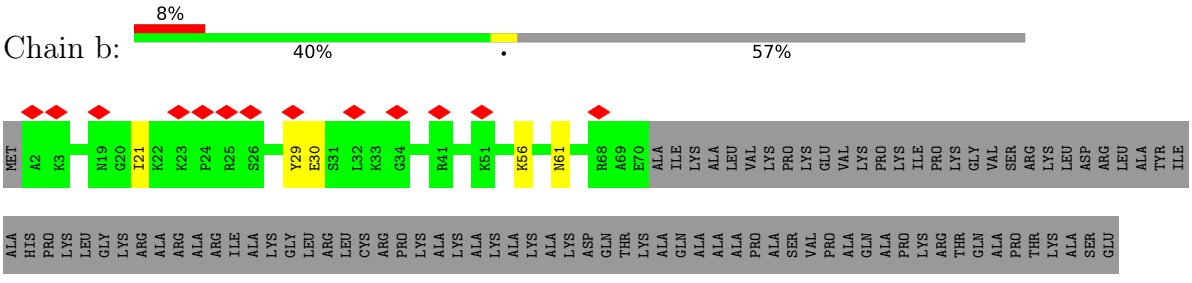
• Molecule 26: 60S RIBOSOMAL PROTEIN L27A

Chain a:



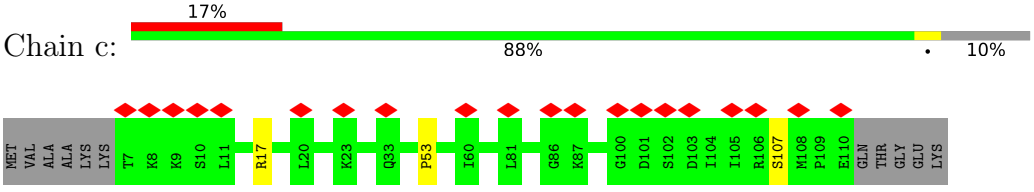
• Molecule 27: 60S RIBOSOMAL PROTEIN L29

Chain b:



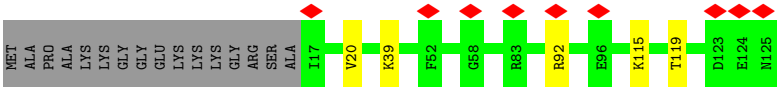
• Molecule 28: 60S RIBOSOMAL PROTEIN L30

Chain c:



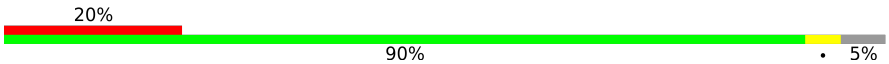
• Molecule 29: 60S RIBOSOMAL PROTEIN L31

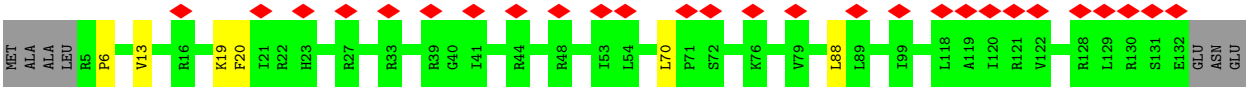
Chain d:



• Molecule 30: 60S RIBOSOMAL PROTEIN L32

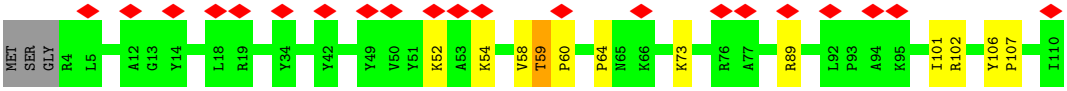
Chain e:





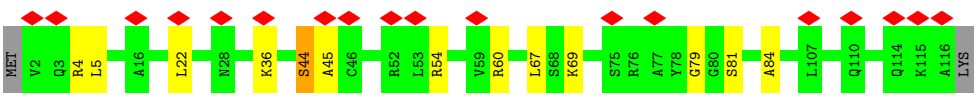
• Molecule 31: 60S RIBOSOMAL PROTEIN L35A

Chain f:



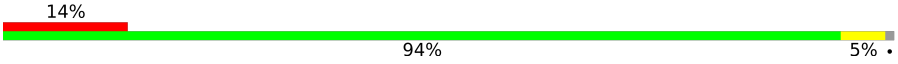
• Molecule 32: 60S RIBOSOMAL PROTEIN L34

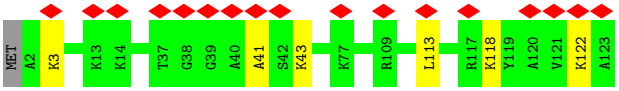
Chain g:



• Molecule 33: 60S RIBOSOMAL PROTEIN L35

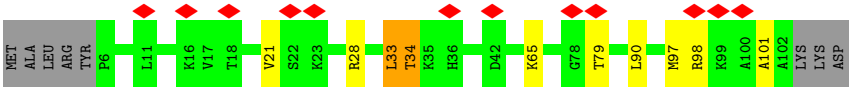
Chain h:





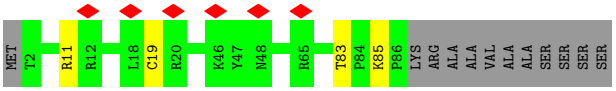
• Molecule 34: 60S RIBOSOMAL PROTEIN L36

Chain i:

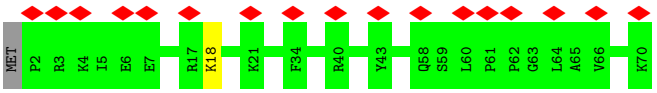


• Molecule 35: 60S RIBOSOMAL PROTEIN L37

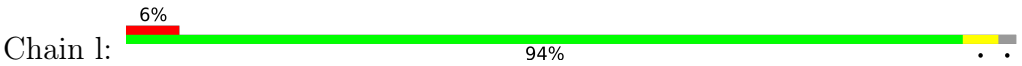
Chain j:

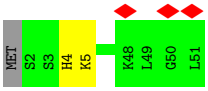


• Molecule 36: 60S RIBOSOMAL PROTEIN L38

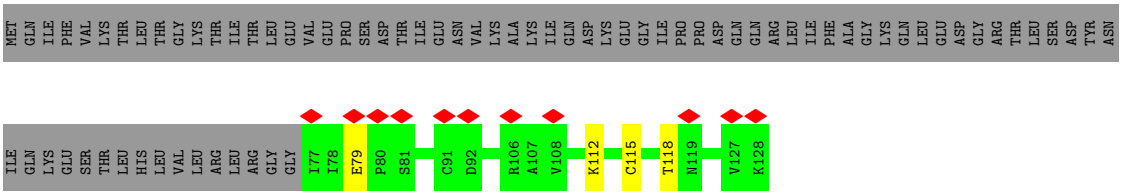


• Molecule 37: 60S RIBOSOMAL PROTEIN L39



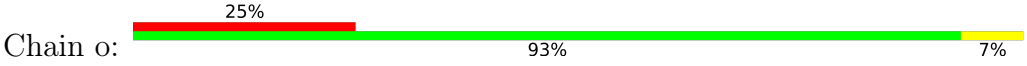


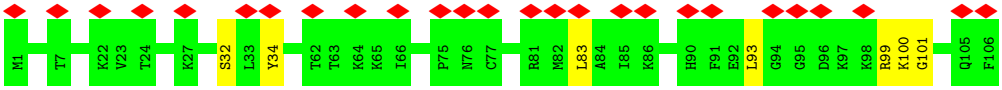
• Molecule 38: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



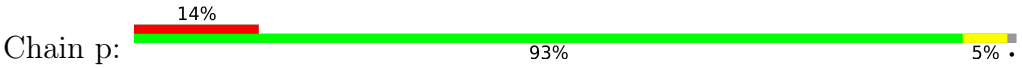
• Molecule 39: 60S RIBOSOMAL PROTEIN L41

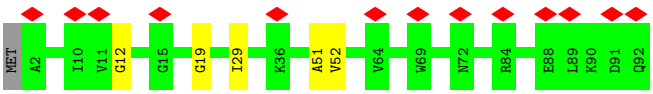
• Molecule 40: 60S RIBOSOMAL PROTEIN L36A





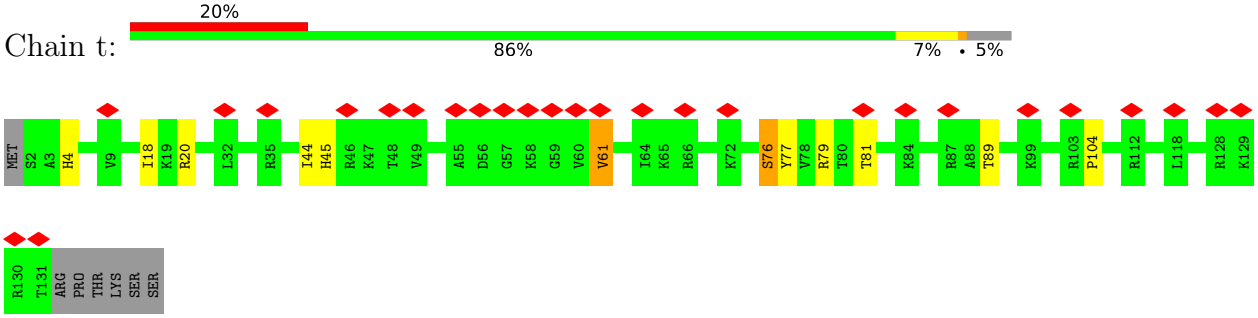
• Molecule 41: 60S RIBOSOMAL PROTEIN L37A





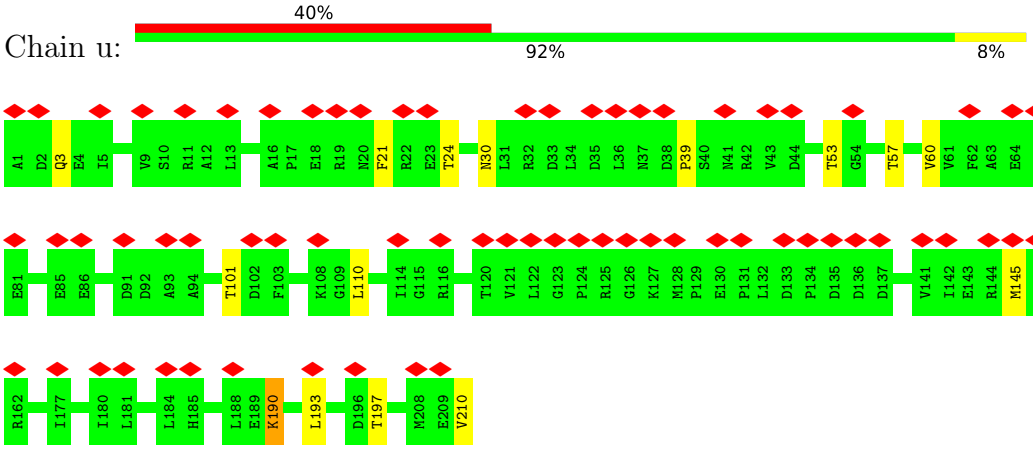
• Molecule 42: 60S RIBOSOMAL PROTEIN L28

Chain t:



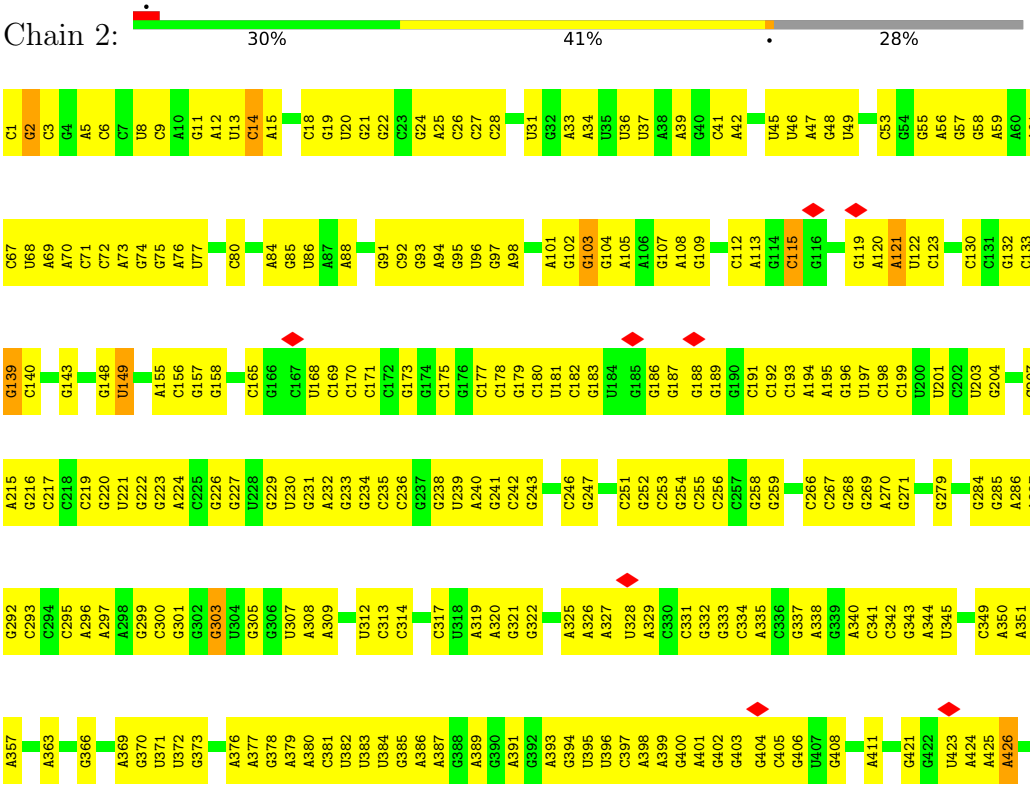
• Molecule 43: 60S RIBOSOMAL PROTEIN L10A

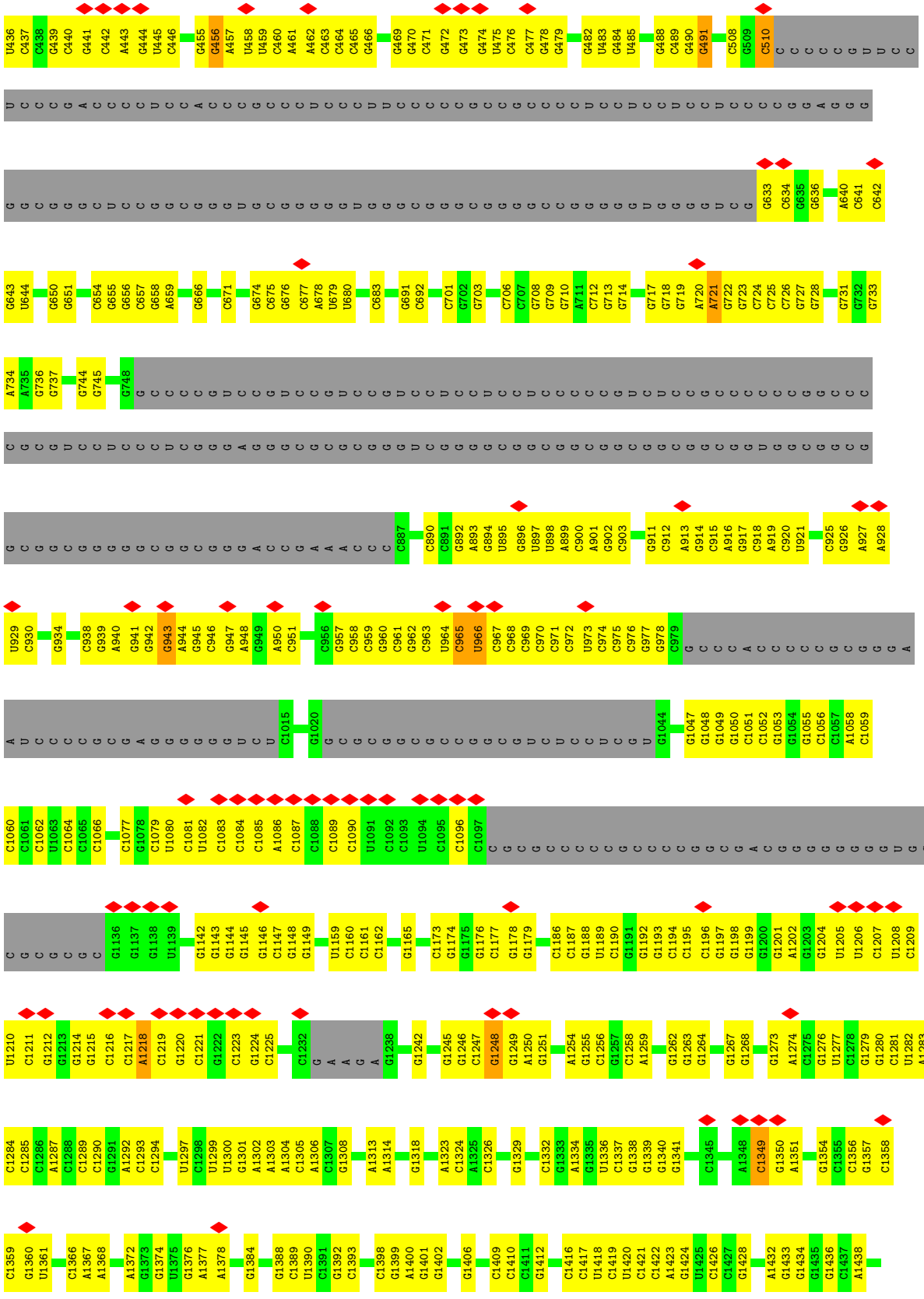
Chain u:

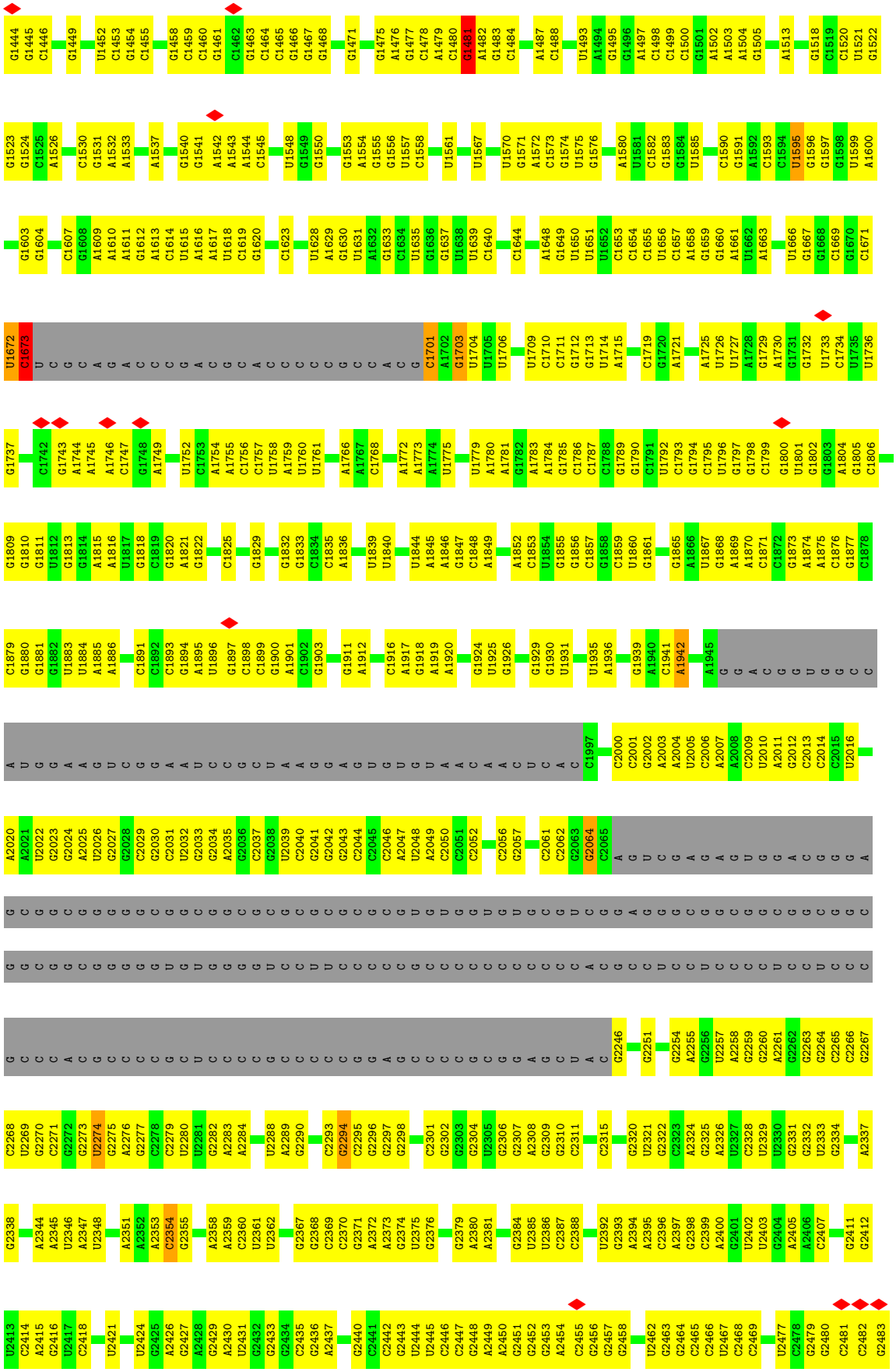


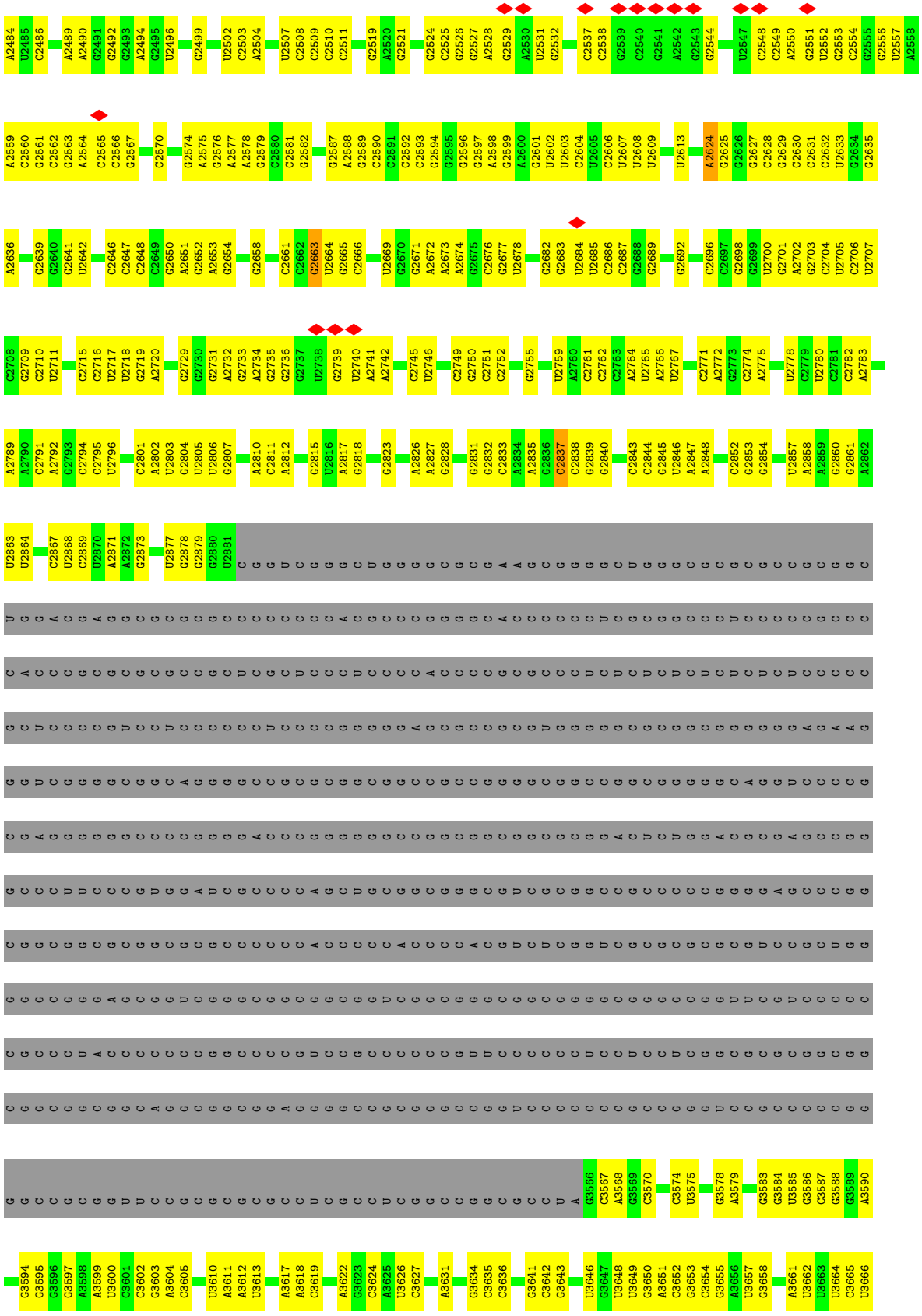
• Molecule 44: 28S RRNA

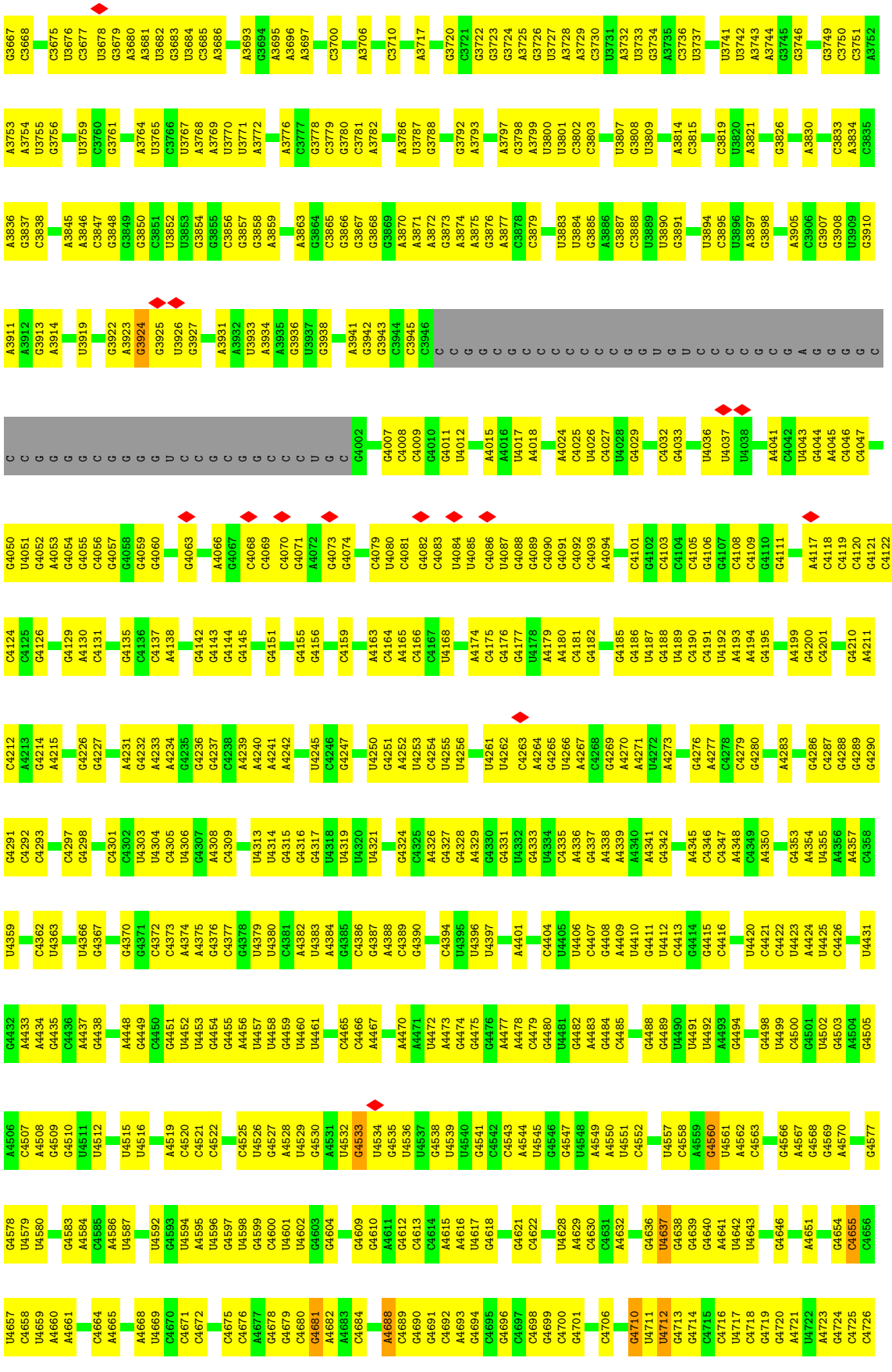
Chain 2:

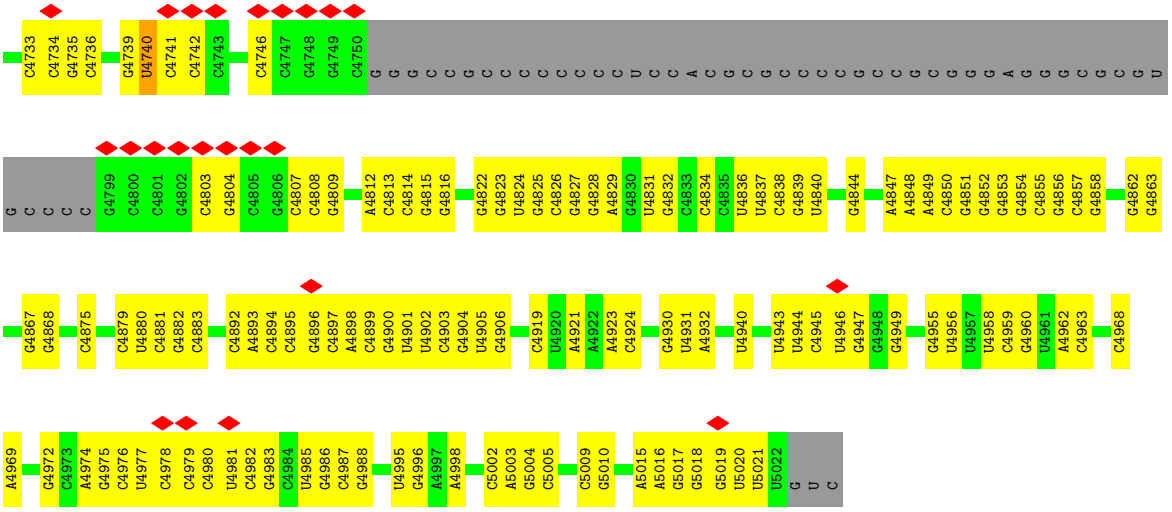






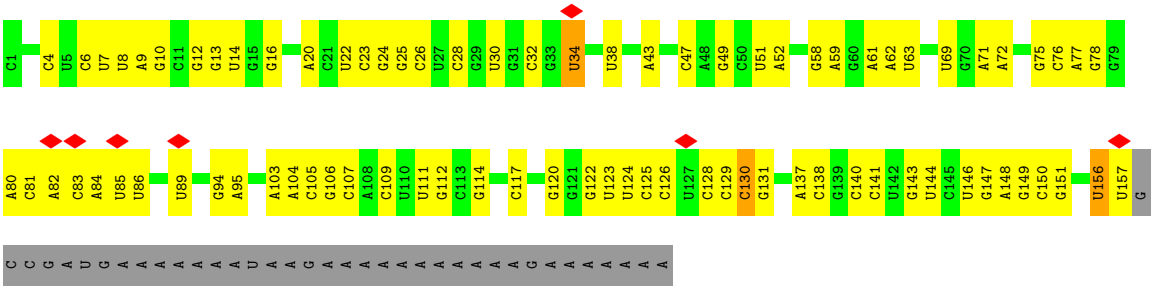






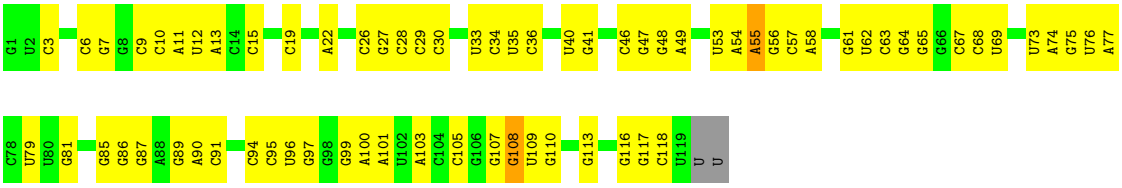
• Molecule 45: 5.8S RRNA

Chain 3:



• Molecule 46: 5S RRNA

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64902	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)	5000	Depositor
Magnification	194805	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	12.165	Depositor
Minimum map value	-4.363	Depositor
Average map value	0.164	Depositor
Map value standard deviation	0.954	Depositor
Recommended contour level	3.0	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%)	13	50
2	B	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	3	25
3	C	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	3	23
4	D	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	9	42
5	E	156/288 (54%)	141 (90%)	8 (5%)	7 (4%)	2	22
6	F	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	9	42
7	G	233/266 (88%)	217 (93%)	7 (3%)	9 (4%)	3	23
8	H	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	9	44
9	I	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	9	44
10	J	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1	14
11	L	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	2	19
12	M	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	11	46
13	N	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	10	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	10	46
15	P	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	7	38
16	Q	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	4	26
17	R	181/196 (92%)	174 (96%)	4 (2%)	3 (2%)	9	42
18	S	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	3	25
19	T	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	8	38
20	U	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
21	V	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	9	44
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%)	6	33
25	Z	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	4	28
26	a	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	3	26
27	b	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	1	17
28	c	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	7	38
29	d	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	17	57
30	e	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	6	33
31	f	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	2	21
32	g	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	3	25
33	h	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	5	32
34	i	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	1	17
35	j	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	6	33
36	k	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	10	46
37	l	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	7	36
38	m	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	7	38
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	8	38
41	p	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	3	26
42	t	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	2	19
43	u	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	11	46
All	All	6479/7422 (87%)	6102 (94%)	200 (3%)	177 (3%)	8	31

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%)	46	66
2	B	344/349 (99%)	326 (95%)	18 (5%)	23	48
3	C	302/348 (87%)	284 (94%)	18 (6%)	19	44
4	D	244/250 (98%)	237 (97%)	7 (3%)	42	64
5	E	143/252 (57%)	135 (94%)	8 (6%)	21	46
6	F	203/215 (94%)	196 (97%)	7 (3%)	37	60
7	G	199/223 (89%)	192 (96%)	7 (4%)	36	59
8	H	171/171 (100%)	164 (96%)	7 (4%)	30	55
9	I	170/181 (94%)	161 (95%)	9 (5%)	22	47
10	J	143/149 (96%)	137 (96%)	6 (4%)	30	54
11	L	167/177 (94%)	156 (93%)	11 (7%)	16	41
12	M	118/161 (73%)	114 (97%)	4 (3%)	37	60
13	N	172/172 (100%)	170 (99%)	2 (1%)	71	83
14	O	168/174 (97%)	166 (99%)	2 (1%)	71	83
15	P	133/163 (82%)	126 (95%)	7 (5%)	22	47
16	Q	162/165 (98%)	157 (97%)	5 (3%)	40	62
17	R	161/175 (92%)	150 (93%)	11 (7%)	16	41
18	S	155/157 (99%)	148 (96%)	7 (4%)	27	52
19	T	139/140 (99%)	134 (96%)	5 (4%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	91/115 (79%)	88 (97%)	3 (3%)	38	61
21	V	100/107 (94%)	99 (99%)	1 (1%)	76	86
22	W	55/126 (44%)	52 (94%)	3 (6%)	21	47
23	X	107/133 (80%)	105 (98%)	2 (2%)	57	75
24	Y	119/135 (88%)	115 (97%)	4 (3%)	37	60
25	Z	118/118 (100%)	112 (95%)	6 (5%)	24	48
26	a	120/121 (99%)	116 (97%)	4 (3%)	38	61
27	b	58/126 (46%)	57 (98%)	1 (2%)	60	78
28	c	88/97 (91%)	87 (99%)	1 (1%)	73	84
29	d	100/110 (91%)	96 (96%)	4 (4%)	31	55
30	e	115/121 (95%)	112 (97%)	3 (3%)	46	66
31	f	87/89 (98%)	79 (91%)	8 (9%)	9	29
32	g	98/100 (98%)	88 (90%)	10 (10%)	7	25
33	h	109/110 (99%)	106 (97%)	3 (3%)	43	65
34	i	82/89 (92%)	76 (93%)	6 (7%)	14	39
35	j	71/80 (89%)	69 (97%)	2 (3%)	43	65
36	k	64/65 (98%)	64 (100%)	0	100	100
37	l	47/48 (98%)	46 (98%)	1 (2%)	53	72
38	m	48/116 (41%)	45 (94%)	3 (6%)	18	43
39	n	24/24 (100%)	24 (100%)	0	100	100
40	o	94/94 (100%)	89 (95%)	5 (5%)	22	47
41	p	74/75 (99%)	72 (97%)	2 (3%)	44	65
42	t	113/121 (93%)	106 (94%)	7 (6%)	18	43
43	u	177/177 (100%)	163 (92%)	14 (8%)	12	35
All	All	5642/6318 (89%)	5403 (96%)	239 (4%)	33	54

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	118/121 (97%)	68 (57%)	9 (7%)
All	All	3879/5340 (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 monosaccharides 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.

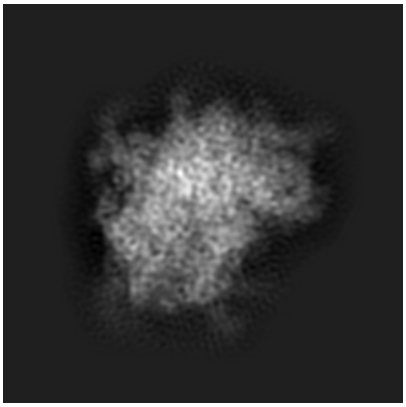
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2813. These allow visual inspection of the internal detail of the map and identification of artifacts.

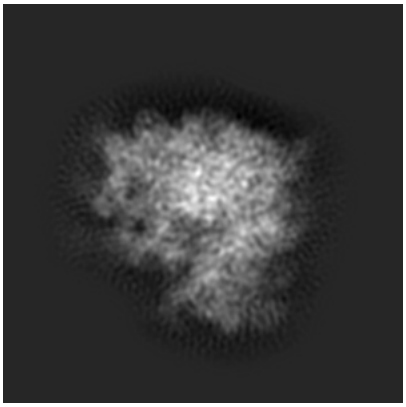
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

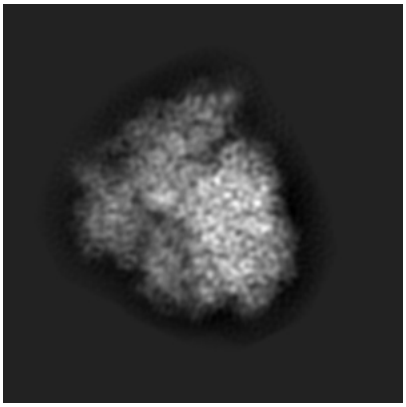
6.1.1 Primary map



X



Y

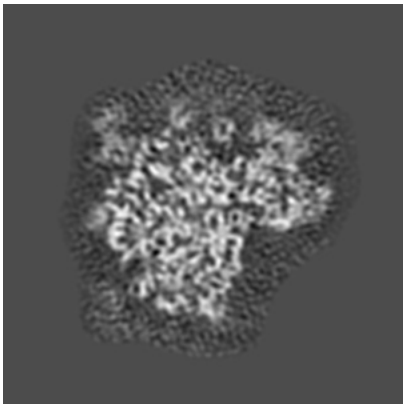


Z

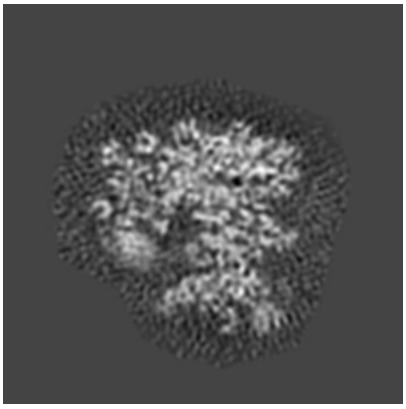
The images above show the map projected in three orthogonal directions.

6.2 Central slices

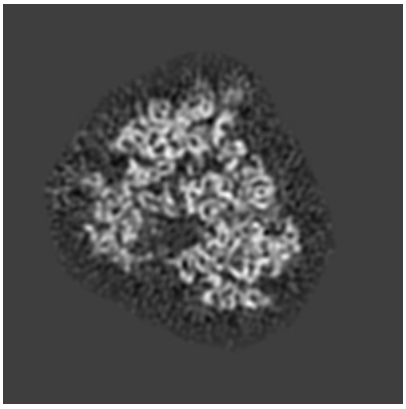
6.2.1 Primary map



X Index: 150



Y Index: 150

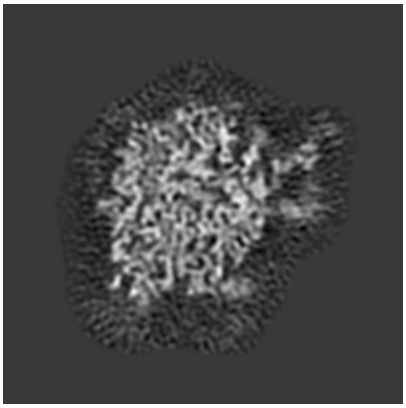


Z Index: 150

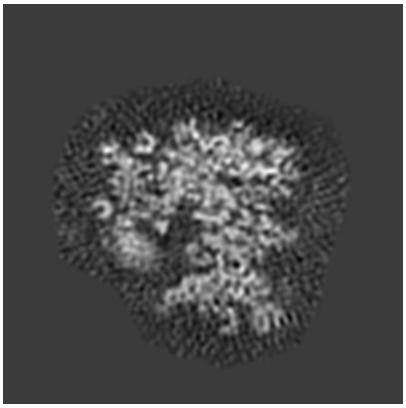
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

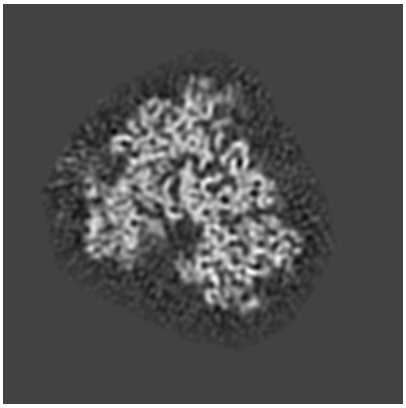
6.3.1 Primary map



X Index: 172



Y Index: 149



Z Index: 154

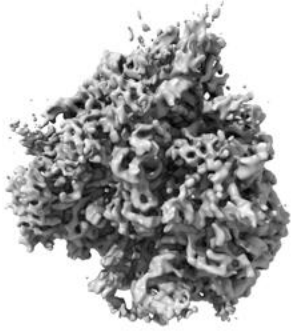
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

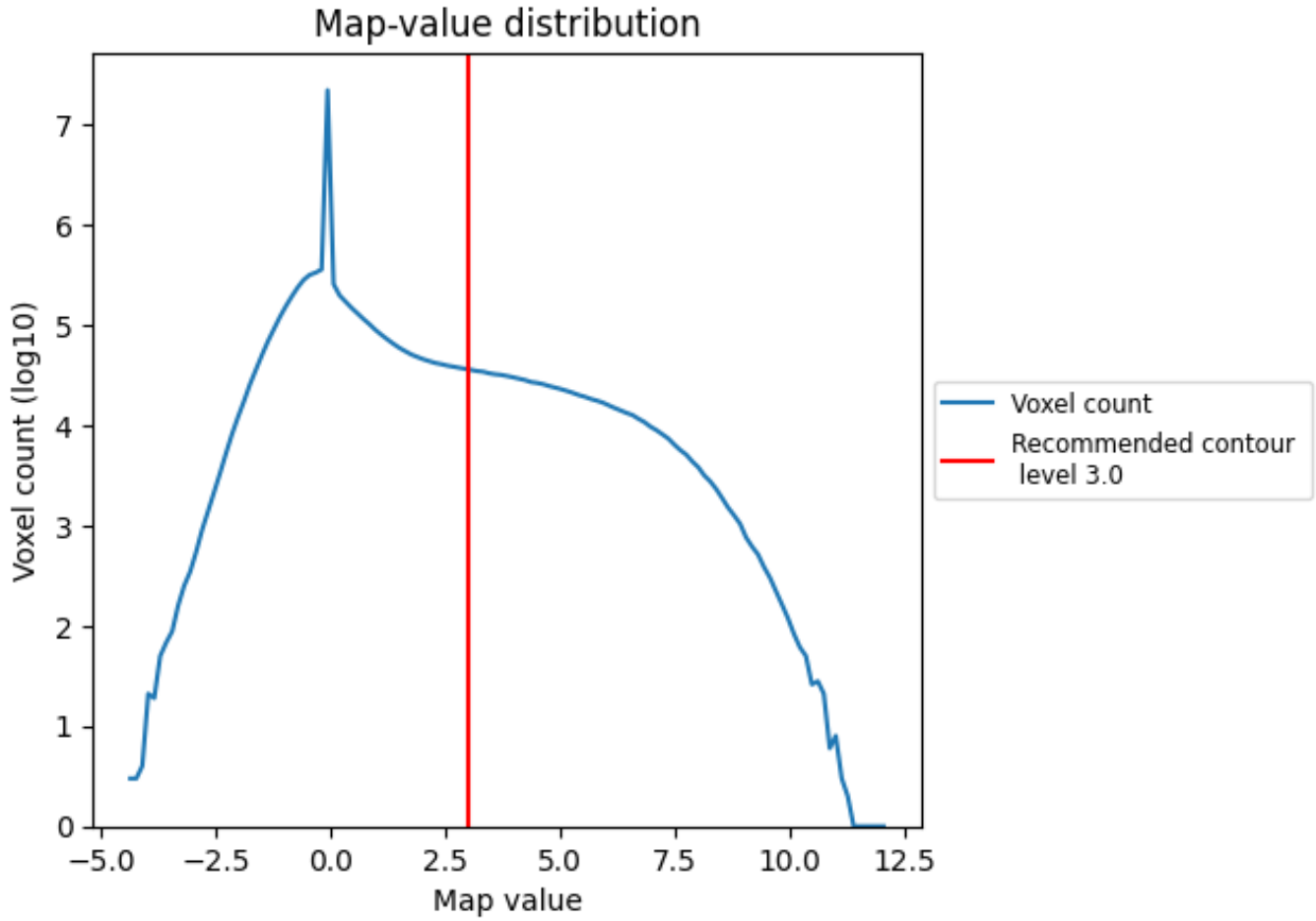
6.5 Mask visualisation (i)

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

7 Map analysis

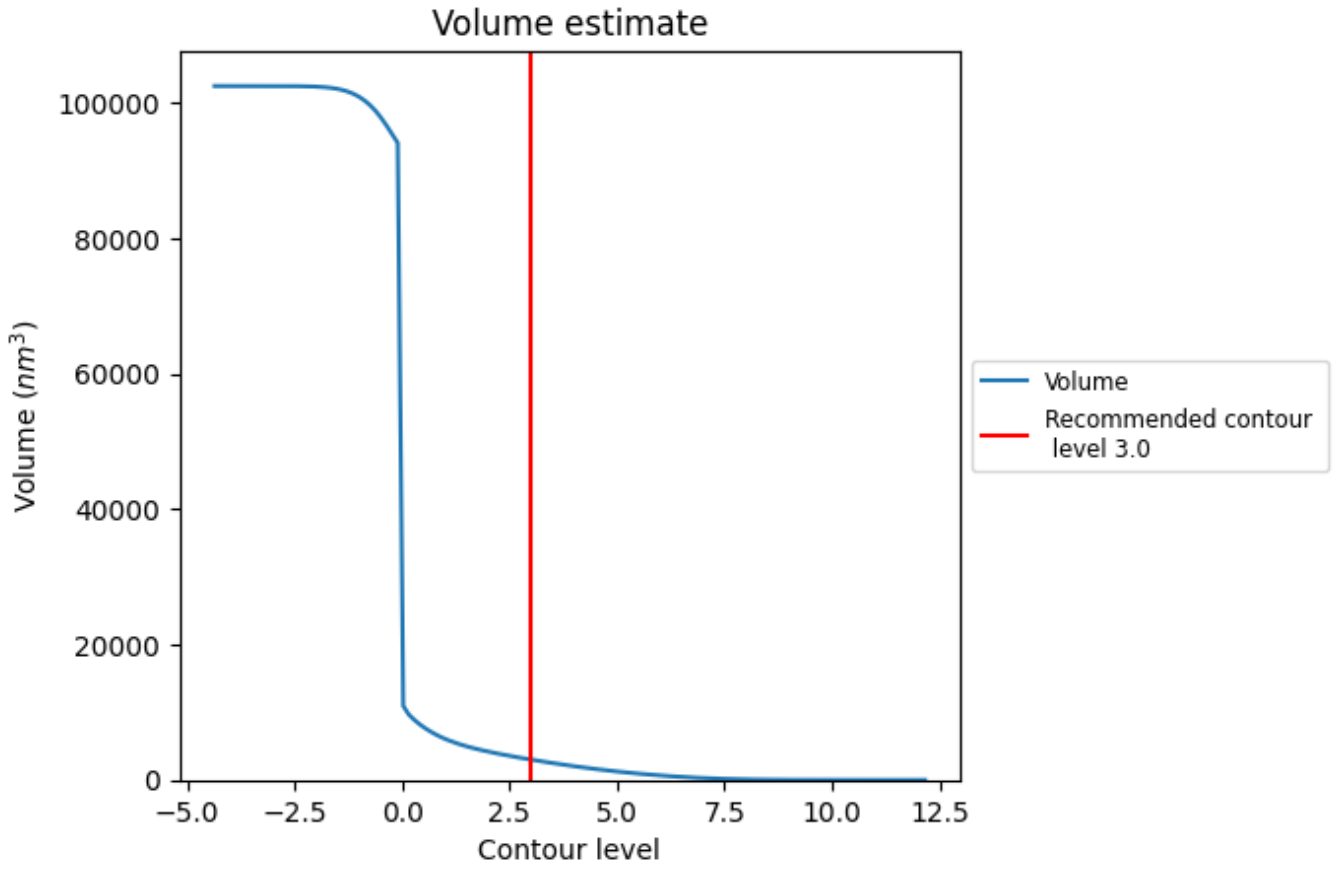
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

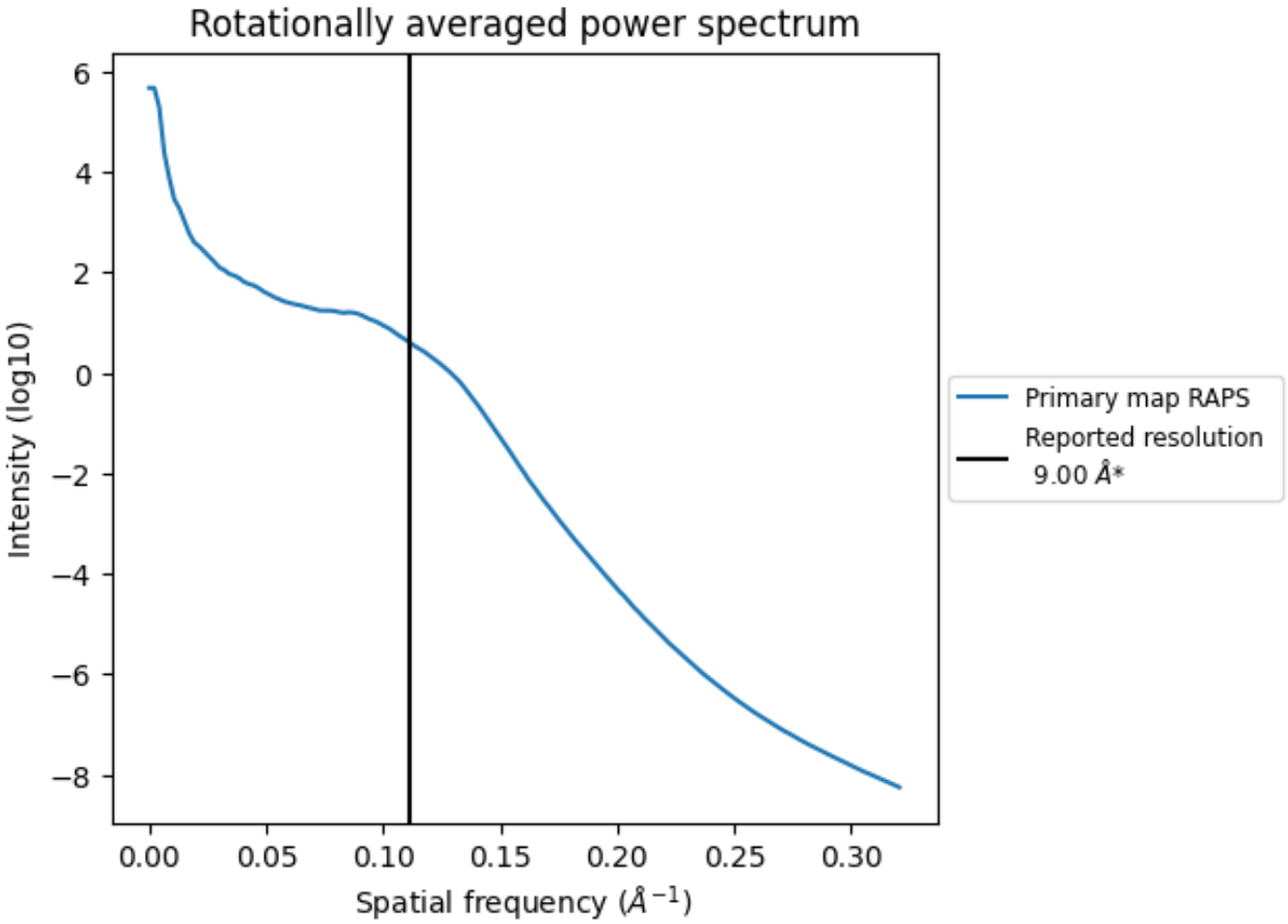
7.2 Volume estimate (i)



The volume at the recommended contour level is 3001 nm^3; this corresponds to an approximate mass of 2711 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}

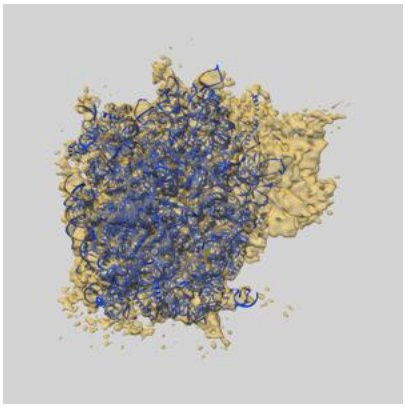
8 Fourier-Shell correlation

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

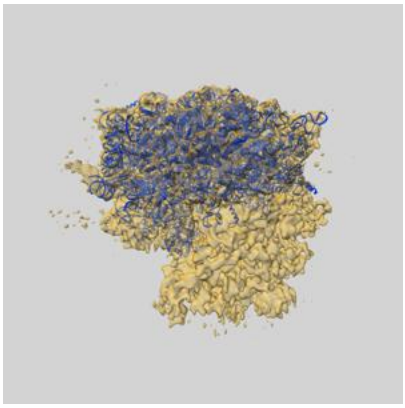
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2813 and PDB model 4D67. Per-residue inclusion information can be found in section 3 on page 12.

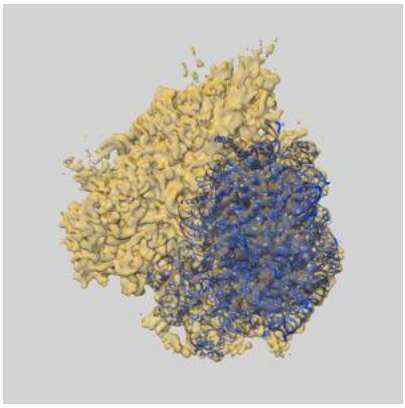
9.1 Map-model overlay



X



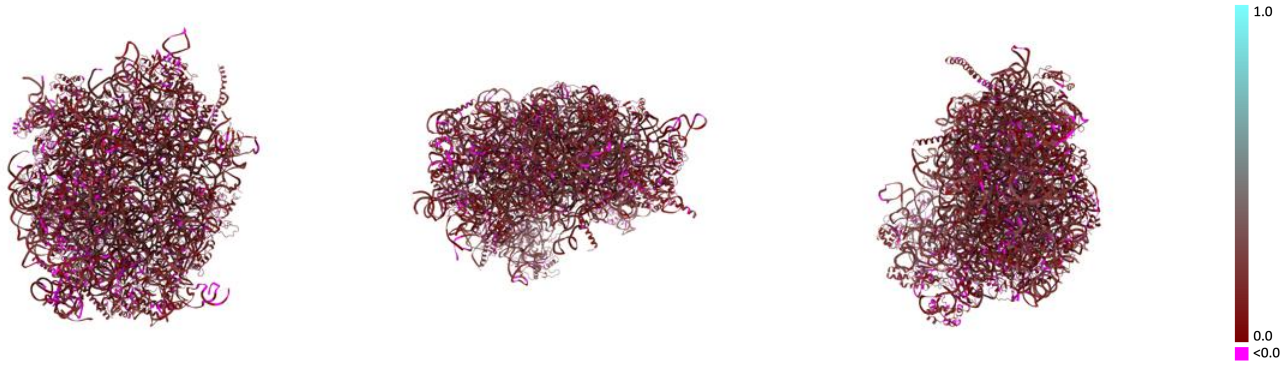
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

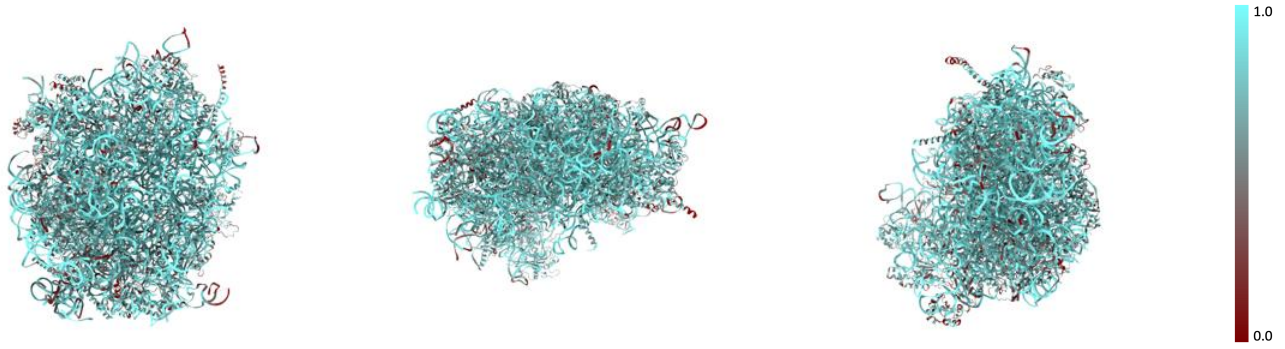
9.2 Q-score mapped to coordinate model (i)



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.

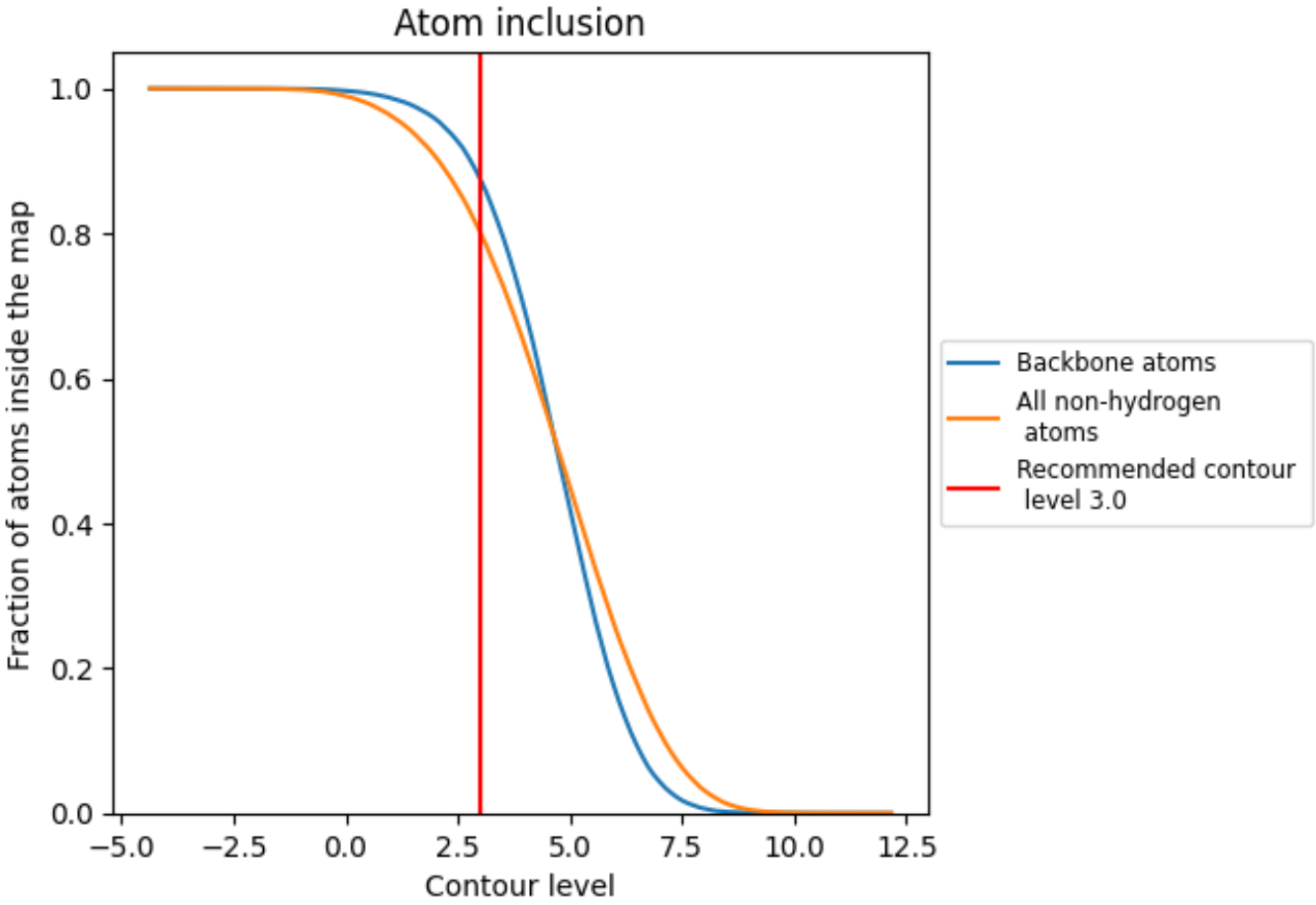
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8017	0.1420
2	0.8832	0.1660
3	0.9034	0.1700
4	0.9464	0.1820
A	0.6614	0.0870
B	0.6850	0.0980
C	0.6880	0.0900
D	0.6678	0.1060
E	0.6065	0.0930
F	0.6514	0.1020
G	0.6606	0.1250
H	0.7154	0.1300
I	0.6587	0.1180
J	0.7328	0.1140
L	0.6353	0.1020
M	0.7013	0.1110
N	0.6779	0.0780
O	0.6871	0.1080
P	0.6970	0.0890
Q	0.6583	0.0980
R	0.6724	0.1170
S	0.6818	0.1090
T	0.6656	0.1050
U	0.6230	0.1370
V	0.6312	0.1120
W	0.6863	0.1100
X	0.6350	0.1070
Y	0.7014	0.1080
Z	0.6833	0.1160
a	0.6758	0.1000
b	0.7040	0.1090
c	0.6306	0.1200
d	0.7102	0.1200
e	0.6483	0.1020
f	0.6594	0.0700

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Chain	Atom inclusion	Q-score
g	0.6828	0.0980
h	0.6622	0.1140
i	0.6596	0.1260
j	0.7534	0.0940
k	0.5881	0.1300
l	0.7630	0.1260
m	0.6981	0.1130
n	0.6468	0.1010
o	0.5865	0.0950
p	0.6623	0.1090
t	0.6670	0.0860
u	0.4884	0.0770