



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 09:30 am GMT

PDB ID : 6S13
EMDB ID : EMD-10079
Title : Erythromycin Resistant Staphylococcus aureus 70S ribosome (delta R88 A89 uL22).
Authors : Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on : 2019-06-18
Resolution : 3.58 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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

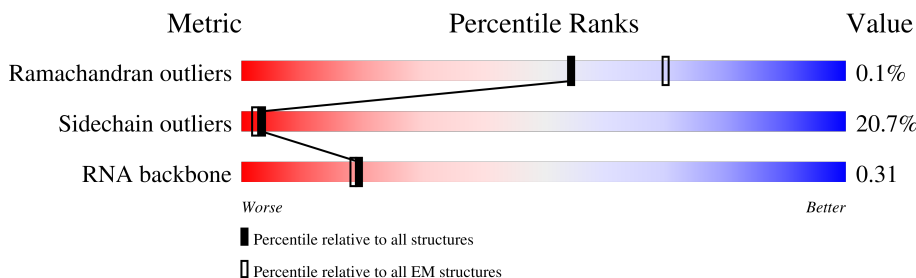
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2905	
2	B	115	
3	C	274	
4	D	215	
5	E	206	
6	F	175	
7	G	175	
8	H	145	

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Mol	Chain	Length	Quality of chain
9	I	122	62% 83% 17%
10	J	146	70% 91% 9%
11	K	137	59% 86% 14%
12	L	120	59% 88% 12%
13	M	119	63% 79% 20%
14	N	114	59% 88% 12%
15	O	116	54% 89% 11%
16	P	102	41% 78% 22%
17	Q	110	60% 73% 27%
18	R	89	72% 82% 18%
19	S	103	56% 79% 20%
20	T	94	81% 81% 19%
21	U	82	68% 78% 21%
22	V	58	78% 81% 19%
23	W	67	61% 88% 12%
24	X	58	41% 86% 14%
25	Y	59	88% 98%
26	Z	48	50% 75% 23%
27	1	47	77% 74% 26%
28	2	43	56% 91% 9%
29	3	64	66% 88% 12%
30	4	37	73% 76% 19% 5%
31	a	1539	70% 35% 54% 10%
32	b	226	93% 84% 15%
33	c	202	95% 86% 13%

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Mol	Chain	Length	Quality of chain
34	d	198	94% 81% 17% .
35	e	156	91% 87% 13%
36	f	95	95% 81% 19%
37	g	152	92% 76% 22% ..
38	h	131	88% 82% 18% .
39	i	127	87% 85% 15%
40	j	97	100% 82% 14% .
41	k	114	85% 77% 21% .
42	l	135	97% 75% 22% .
43	m	104	95% 87% 12% .
44	n	60	90% 70% 30%
45	o	88	93% 76% 22% .
46	p	89	90% 81% 19%
47	q	80	81% 78% 18% 5%
48	r	54	80% 87% 13%
49	s	80	91% 74% 24% .
50	t	81	91% 84% 16%
51	u	52	83% 75% 23% .
52	v	162	99% 78% 21% .

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 233957 atoms, of which 93218 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
1	A	2905	93564	27803	31287	11387	20182	2905	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
2	B	115	3685	1094	1240	436	801	114	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	274	4291	1301	2201	415	369	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	215	3294	1018	1667	299	305	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	206	3192	986	1620	288	296	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	175	2667	837	1342	227	255	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	175	2488	790	1225	239	231	3	0	0

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	145	2277	714	1134	208	218	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	122	1899	572	981	174	168	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	146	2211	674	1125	214	197	1	0	0

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	137	2194	689	1123	203	175	4	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	L	120	1915	576	983	182	173	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	M	119	1816	557	925	174	159	1	0	0

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
14	N	114	1826	563	937	175	151	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	O	116	1956	593	1014	189	156	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	102	1620	503	830	142	144	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Q	110	1724	523	887	158	153	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	R	89	1463	453	748	127	131	4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	103	1579	486	809	142	141	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
20	T	94	1488	463	766	130	129	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
21	U	82	1265	385	643	122	115	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
22	V	58	911	277	466	96	72	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
23	W	67	1104	333	563	102	106	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
24	X	58	940	280	491	85	84	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	Y	59	613	225	243	68	76	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	Z	48	718	222	358	77	59	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	1	47	Total	C	H	N	O	S	0	0
			784	238	394	78	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
28	2	43	Total	C	H	N	O	S	0	0
			782	225	415	89	52	1		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	3	64	Total	C	H	N	O	S	0	0
			1107	324	586	113	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
30	4	37	Total	C	H	N	O	S	0	0
			635	186	340	60	44	5		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	a	1539	Total	C	H	N	O	P	0	0
			49563	14719	16594	6017	10694	1539		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
32	b	226	Total	C	H	N	O	S	0	0
			3705	1159	1886	317	335	8		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
33	c	202	Total	C	H	N	O	S	0	0
			2965	945	1464	284	271	1		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	d	198	2946	952	1449	275	268	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	e	156	2347	723	1202	211	209	2	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
36	f	95	1553	493	775	138	145	2	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
37	g	152	2326	722	1165	218	217	4	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
38	h	131	2103	650	1077	183	189	4	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
39	i	127	1812	576	890	179	166	1	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	j	97	1527	475	775	140	136	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
41	k	114	Total	C	H	N	O	S	0	0
			1594	498	784	151	159	2		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
42	l	135	Total	C	H	N	O	S	0	0
			2128	646	1091	211	178	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
43	m	104	Total	C	H	N	O		0	0
			1401	453	674	139	135			

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace	
44	n	60	Total	C	H	N	O	S	0	0
			979	307	492	98	77	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
45	o	88	Total	C	H	N	O	S	0	0
			1475	448	752	150	124	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
46	p	89	Total	C	H	N	O	S	0	0
			1403	436	709	128	129	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
47	q	80	Total	C	H	N	O		0	0
			1237	392	616	112	117			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
48	r	54	927	284	482	86	73	2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
49	s	80	1262	410	626	113	111	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
50	t	81	1207	358	616	117	115	1	0	0

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
51	u	52	807	249	407	79	72	0	0

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
52	v	162	2682	835	1349	242	254	2	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	PHE	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	LEU	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	MET	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

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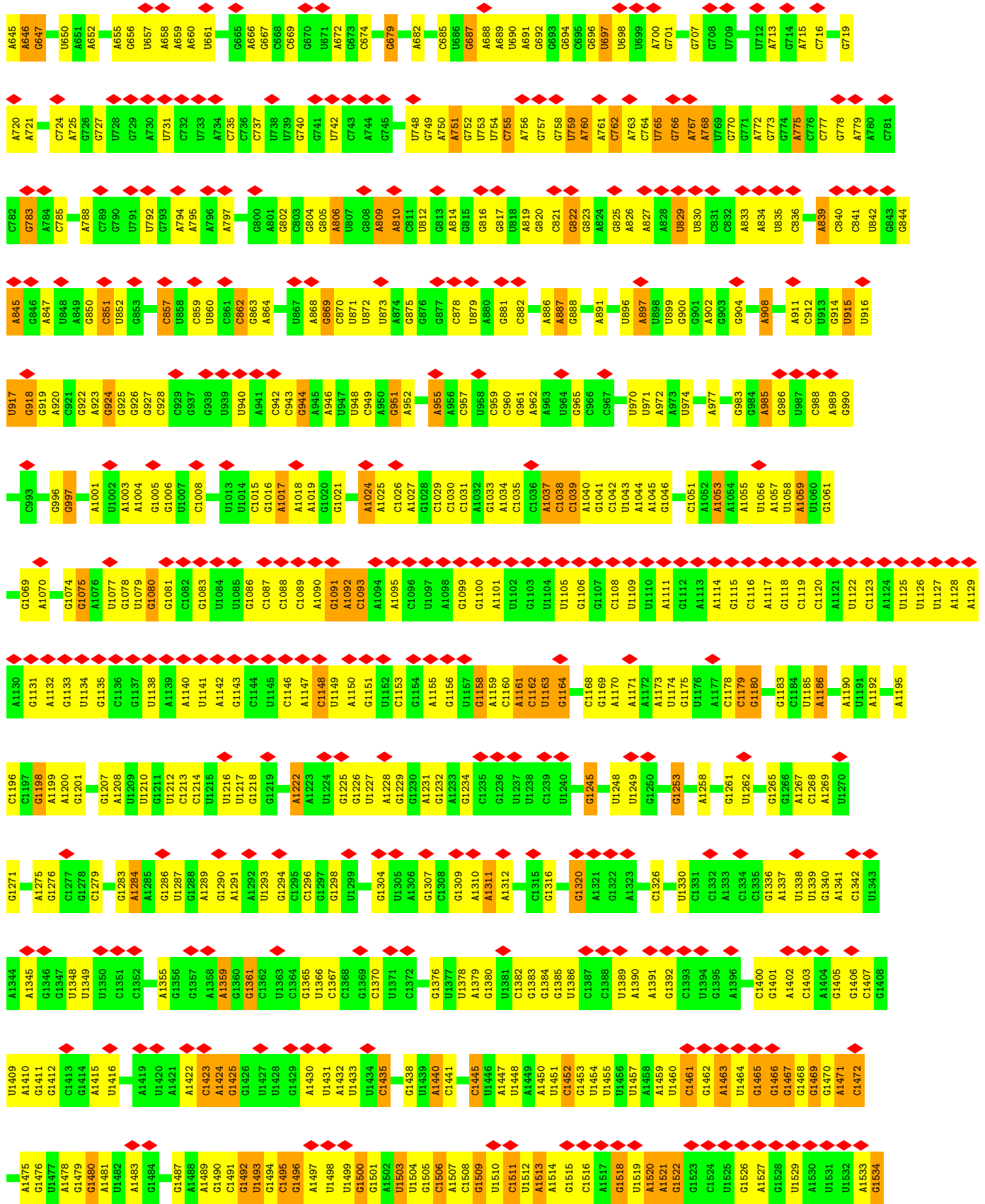
Chain	Residue	Modelled	Actual	Comment	Reference
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v	?	-	GLN	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	TYR	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

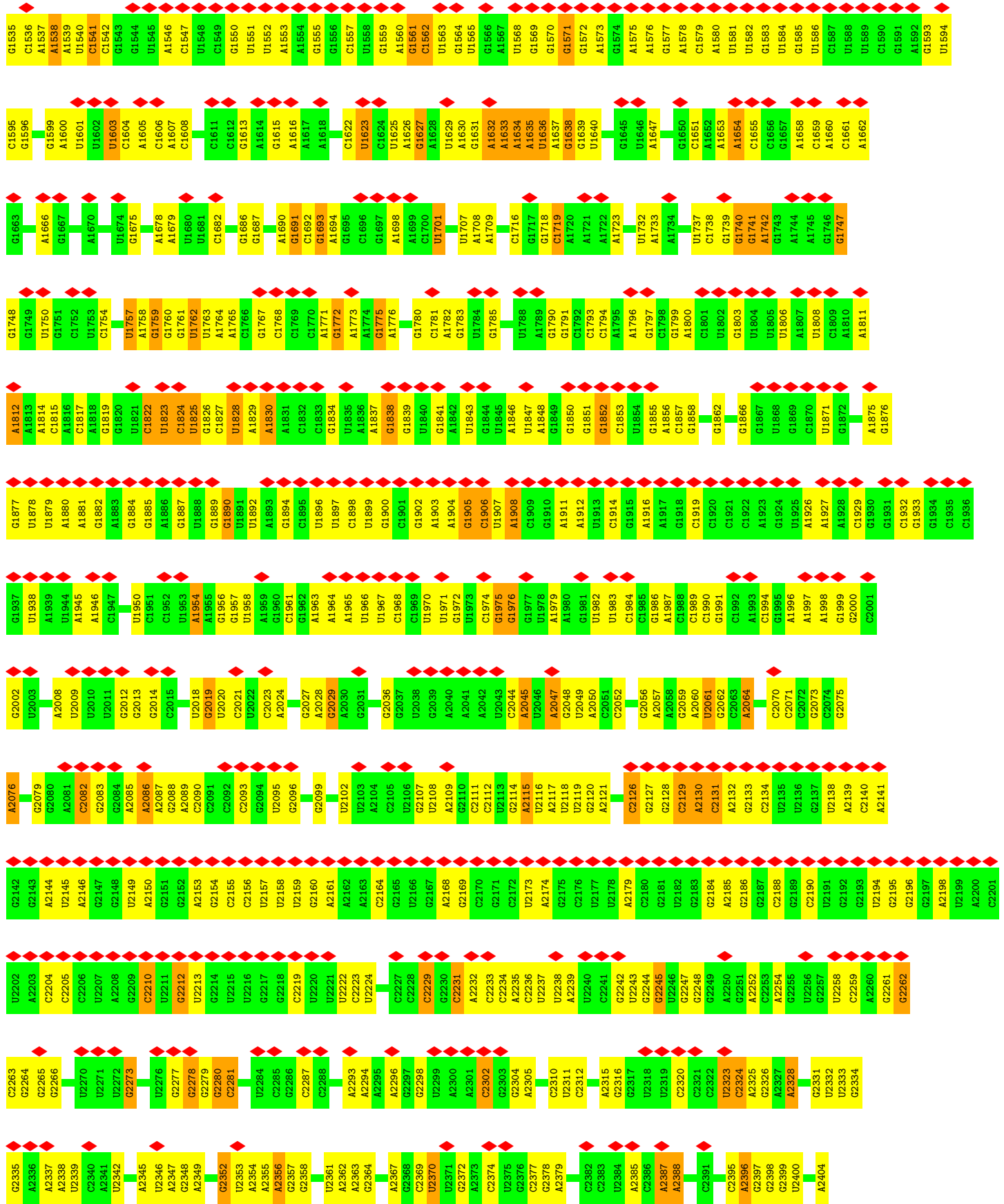
3 Residue-property plots

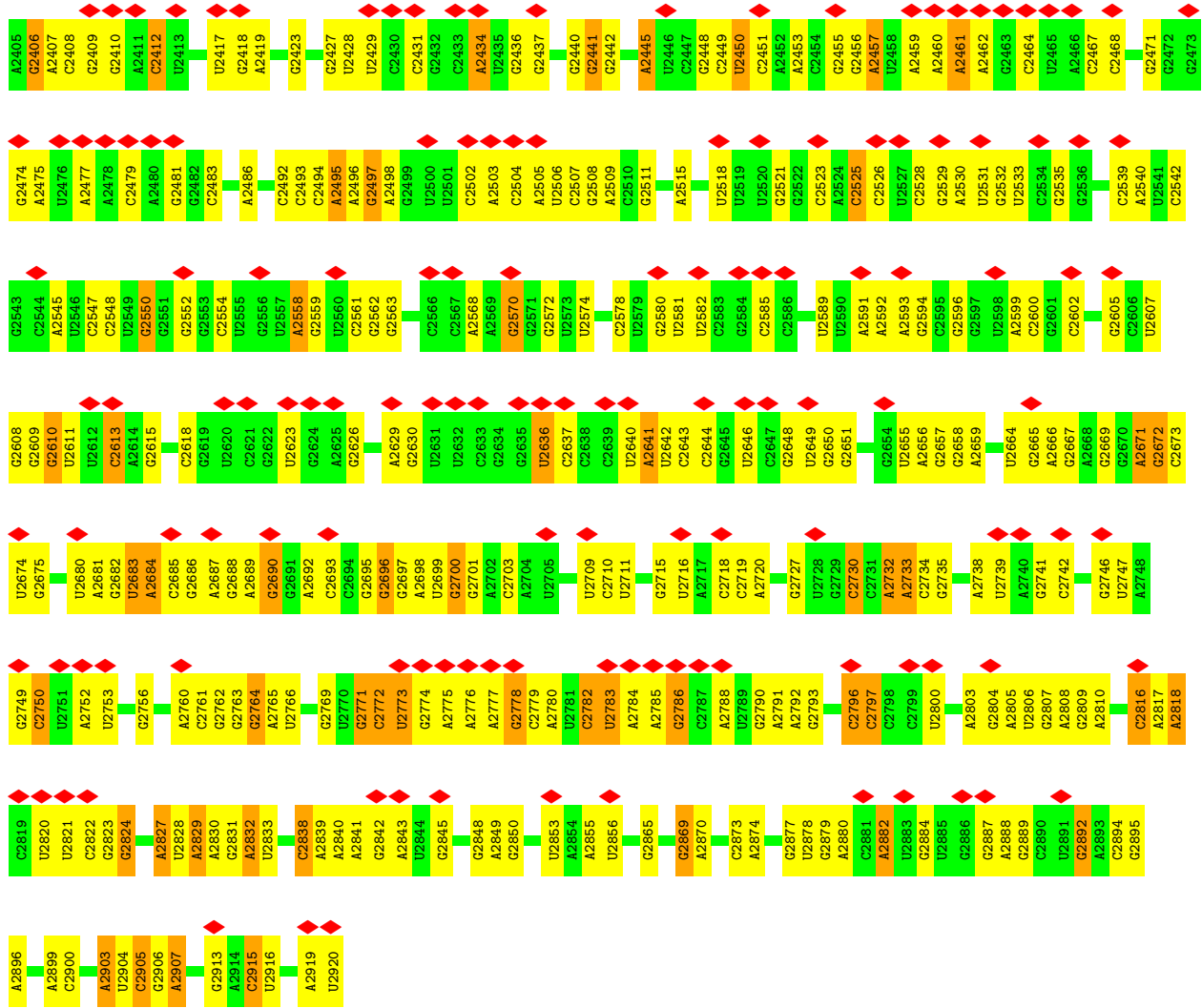
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S ribosomal RNA

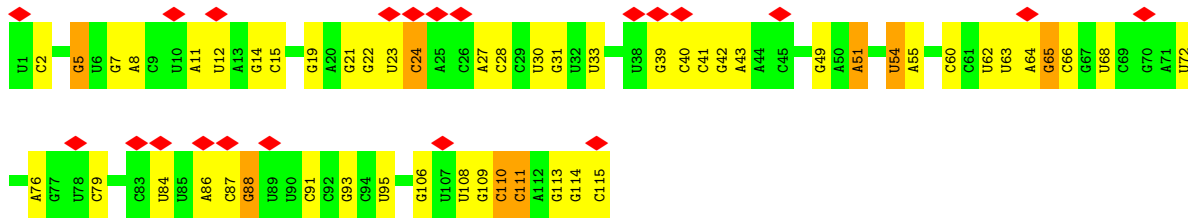




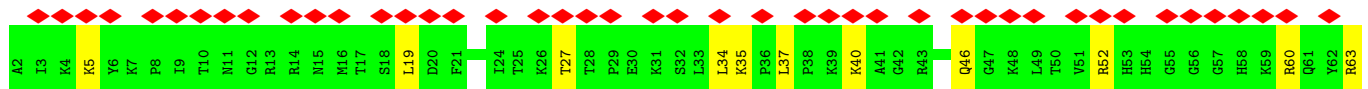
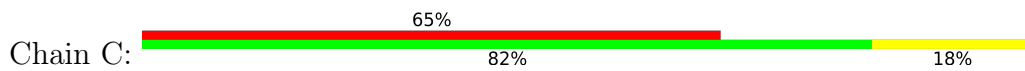


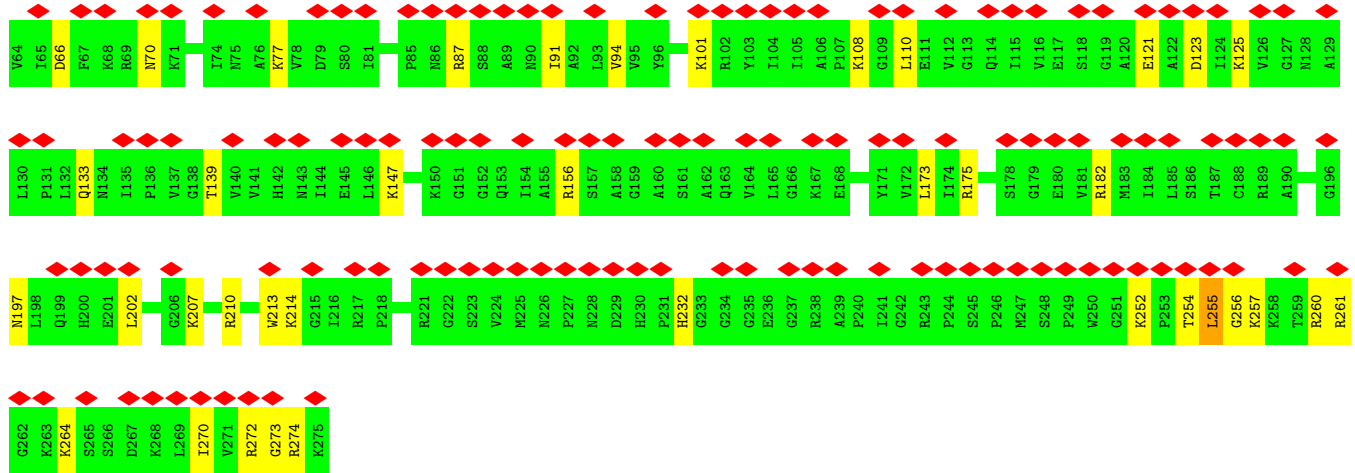


• Molecule 2: 5S ribosomal RNA

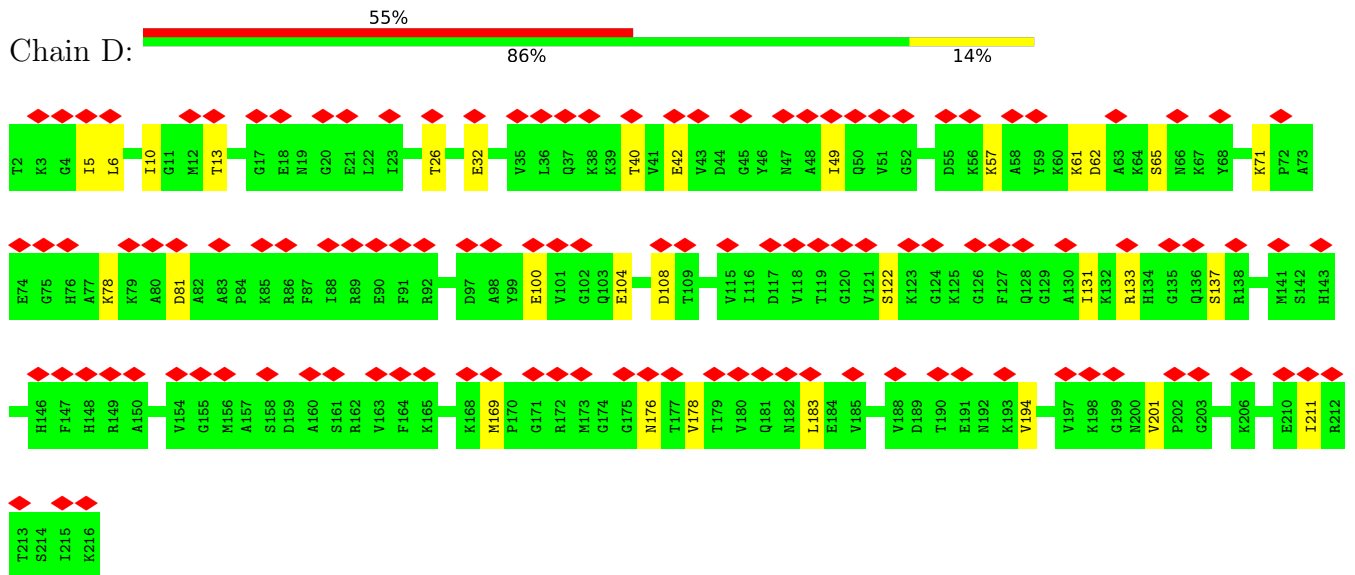


• Molecule 3: 50S ribosomal protein L2

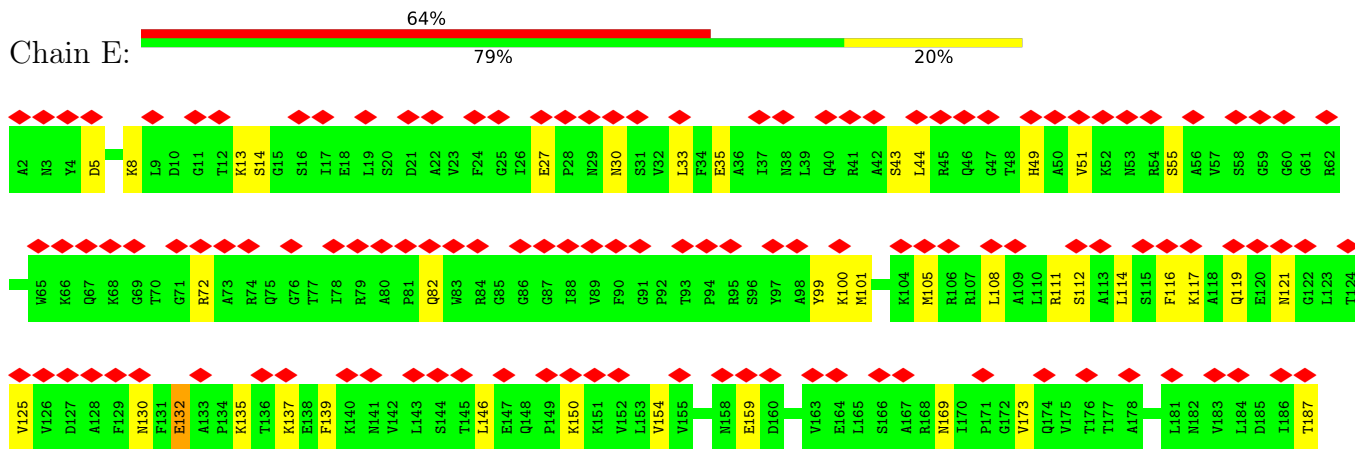


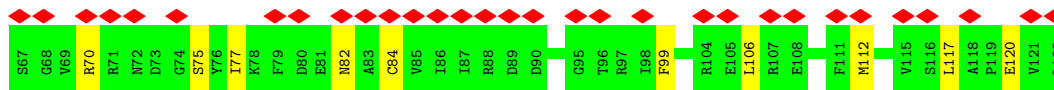
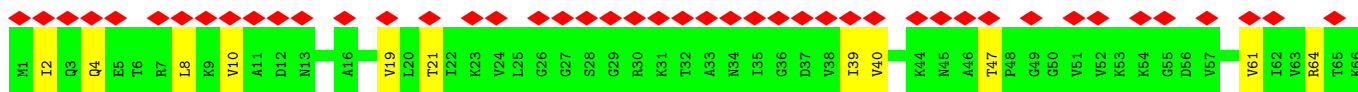


• Molecule 4: 50S ribosomal protein L3

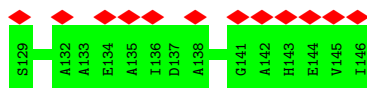
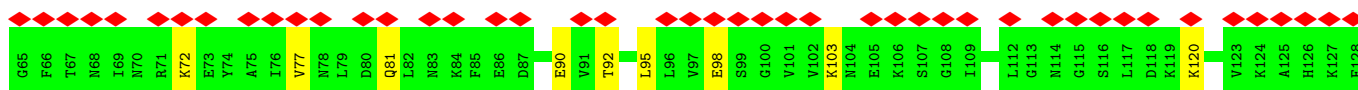
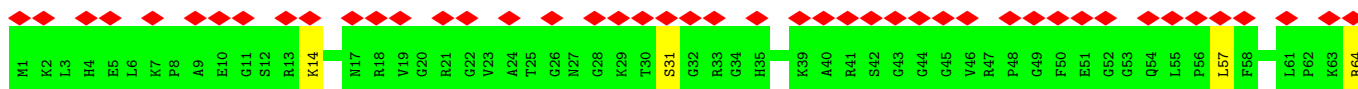
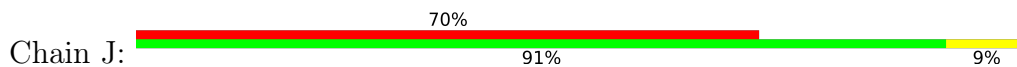


• Molecule 5: 50S ribosomal protein L4

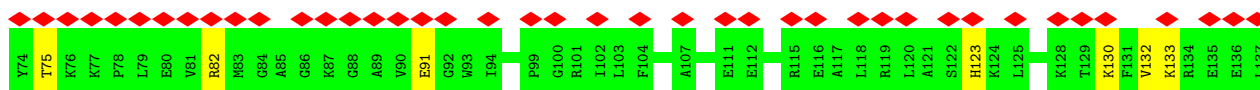
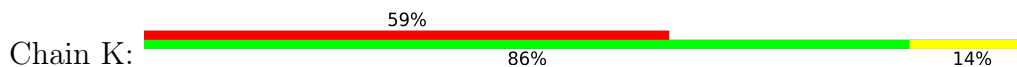




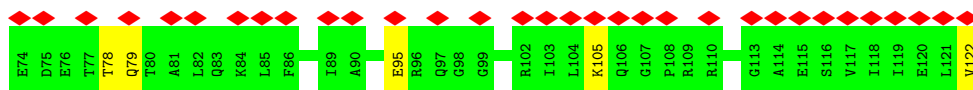
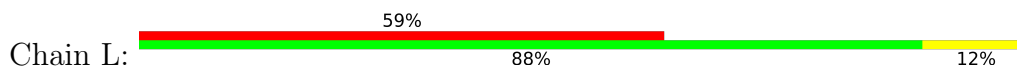
- Molecule 10: 50S ribosomal protein L15



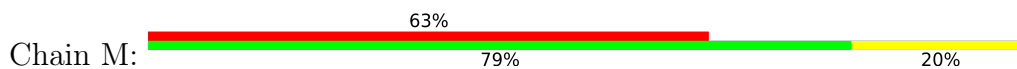
- Molecule 11: 50S ribosomal protein L16

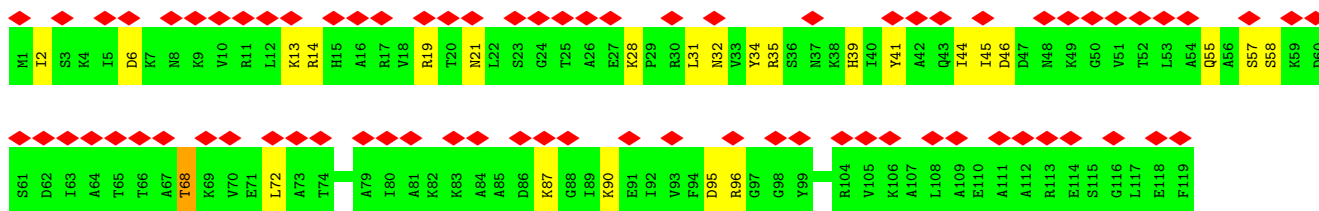


- Molecule 12: 50S ribosomal protein L17

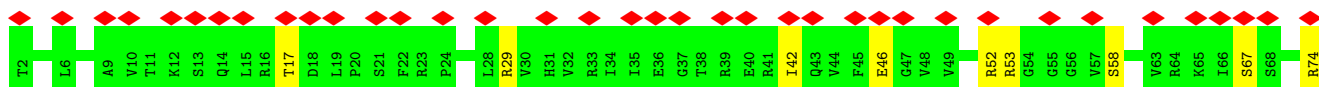
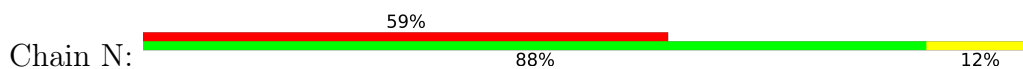


- Molecule 13: 50S ribosomal protein L18

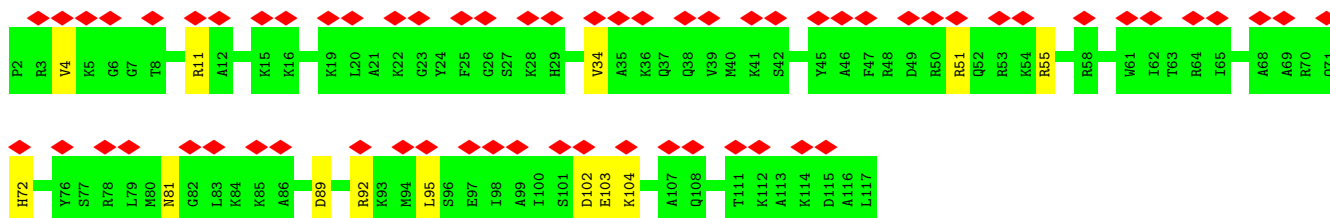
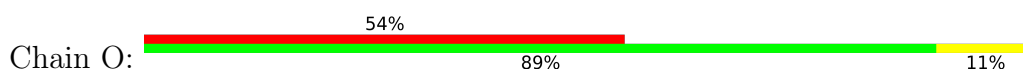




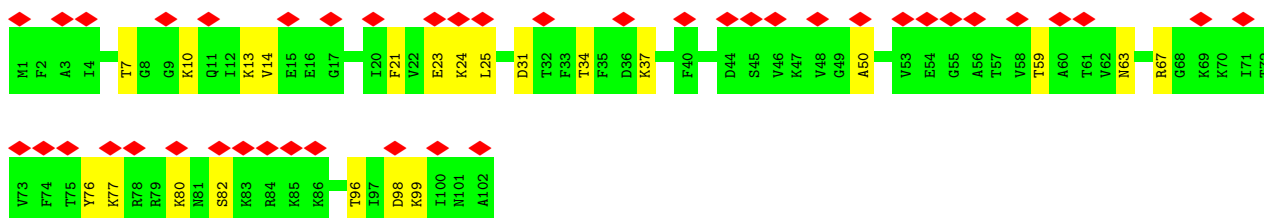
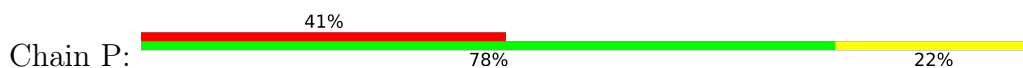
- Molecule 14: 50S ribosomal protein L19



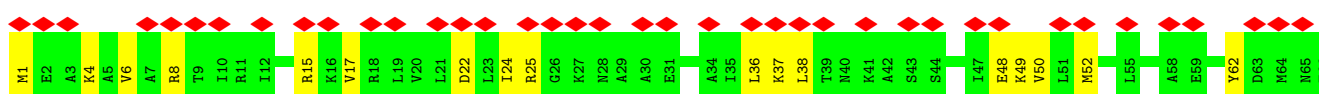
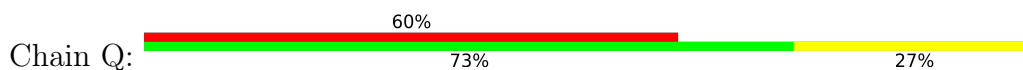
- Molecule 15: 50S ribosomal protein L20

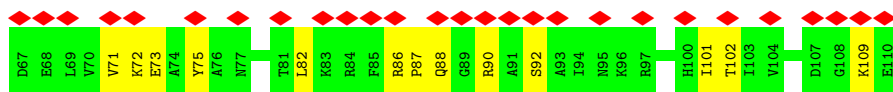


- Molecule 16: 50S ribosomal protein L21

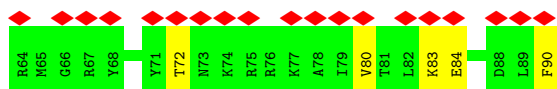
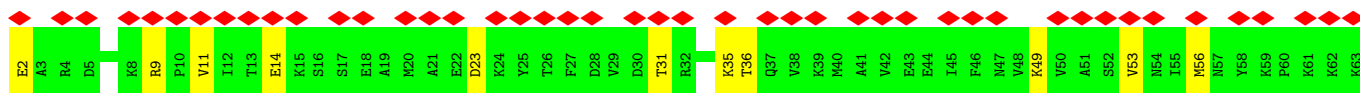
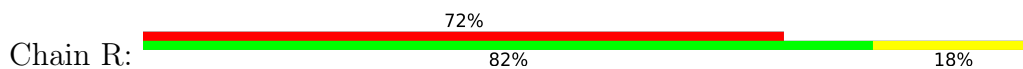


- Molecule 17: 50S ribosomal protein L22

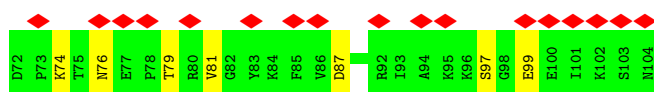
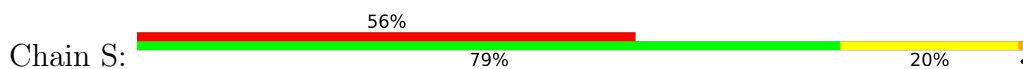




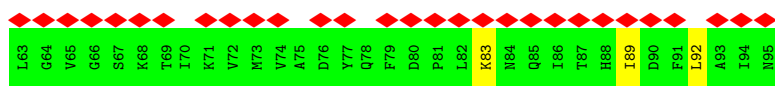
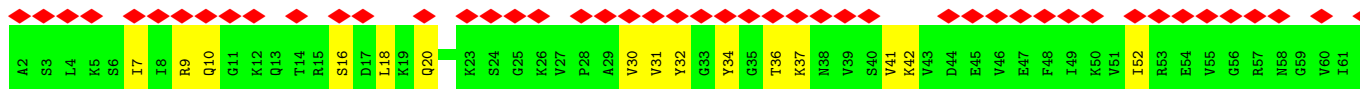
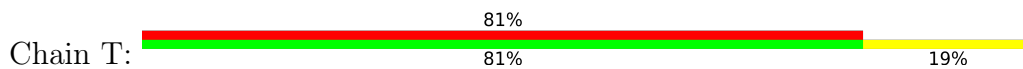
• Molecule 18: 50S ribosomal protein L23



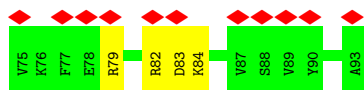
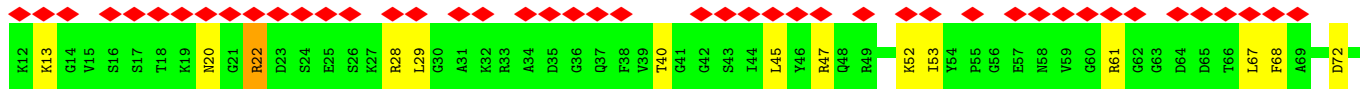
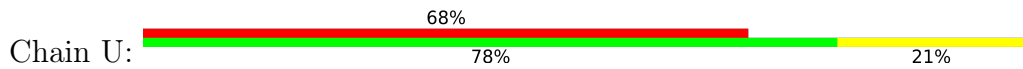
• Molecule 19: 50S ribosomal protein L24



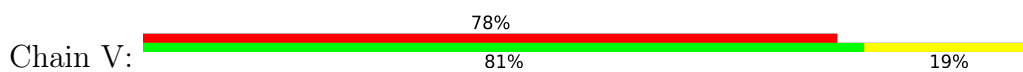
• Molecule 20: 50S ribosomal protein L25



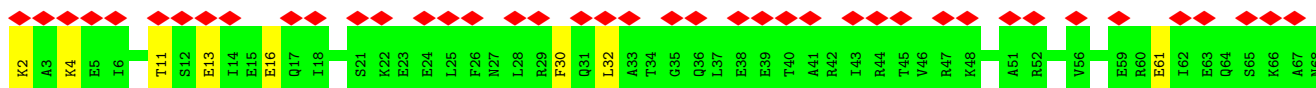
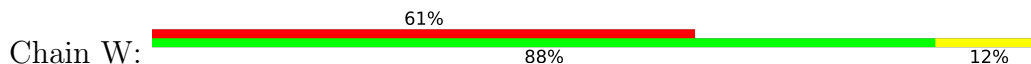
• Molecule 21: 50S ribosomal protein L27



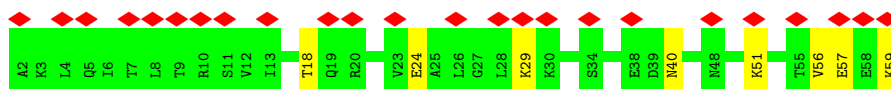
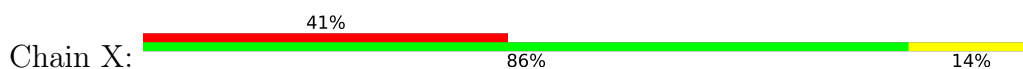
• Molecule 22: 50S ribosomal protein L28



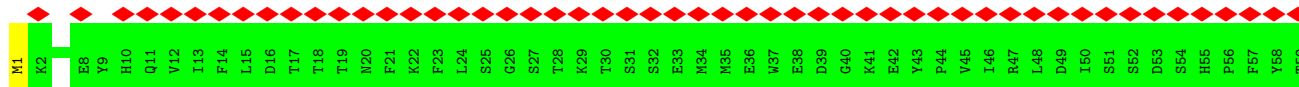
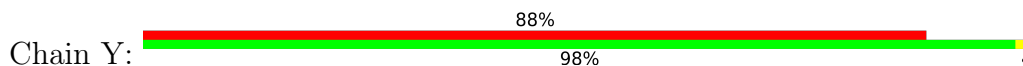
- Molecule 23: 50S ribosomal protein L29



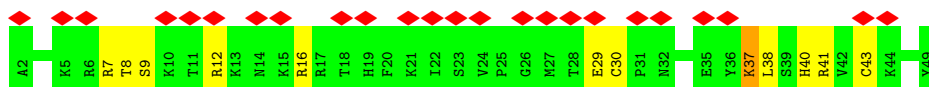
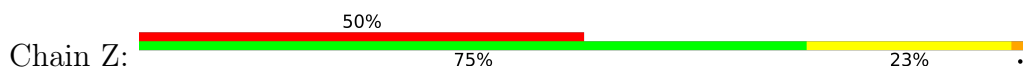
- Molecule 24: 50S ribosomal protein L30



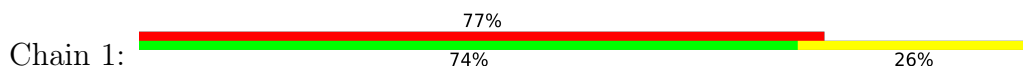
- Molecule 25: 50S ribosomal protein L31 type B



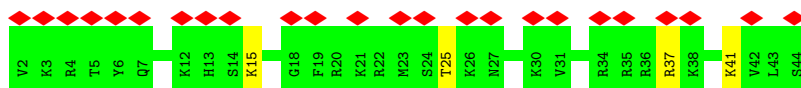
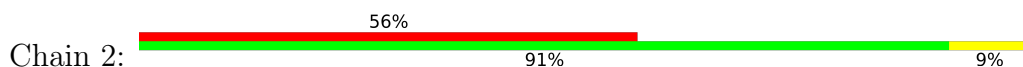
- Molecule 26: 50S ribosomal protein L32



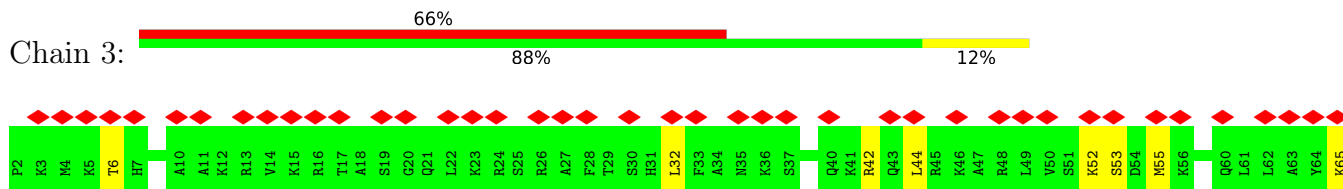
- Molecule 27: 50S ribosomal protein L33



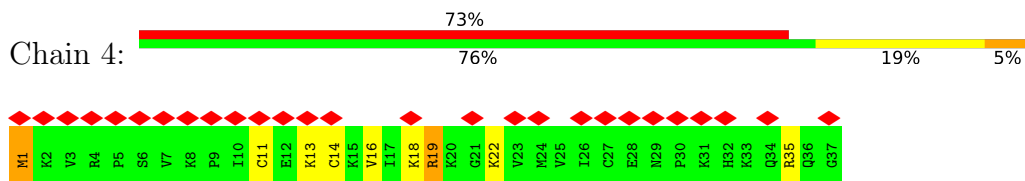
- Molecule 28: 50S ribosomal protein L34



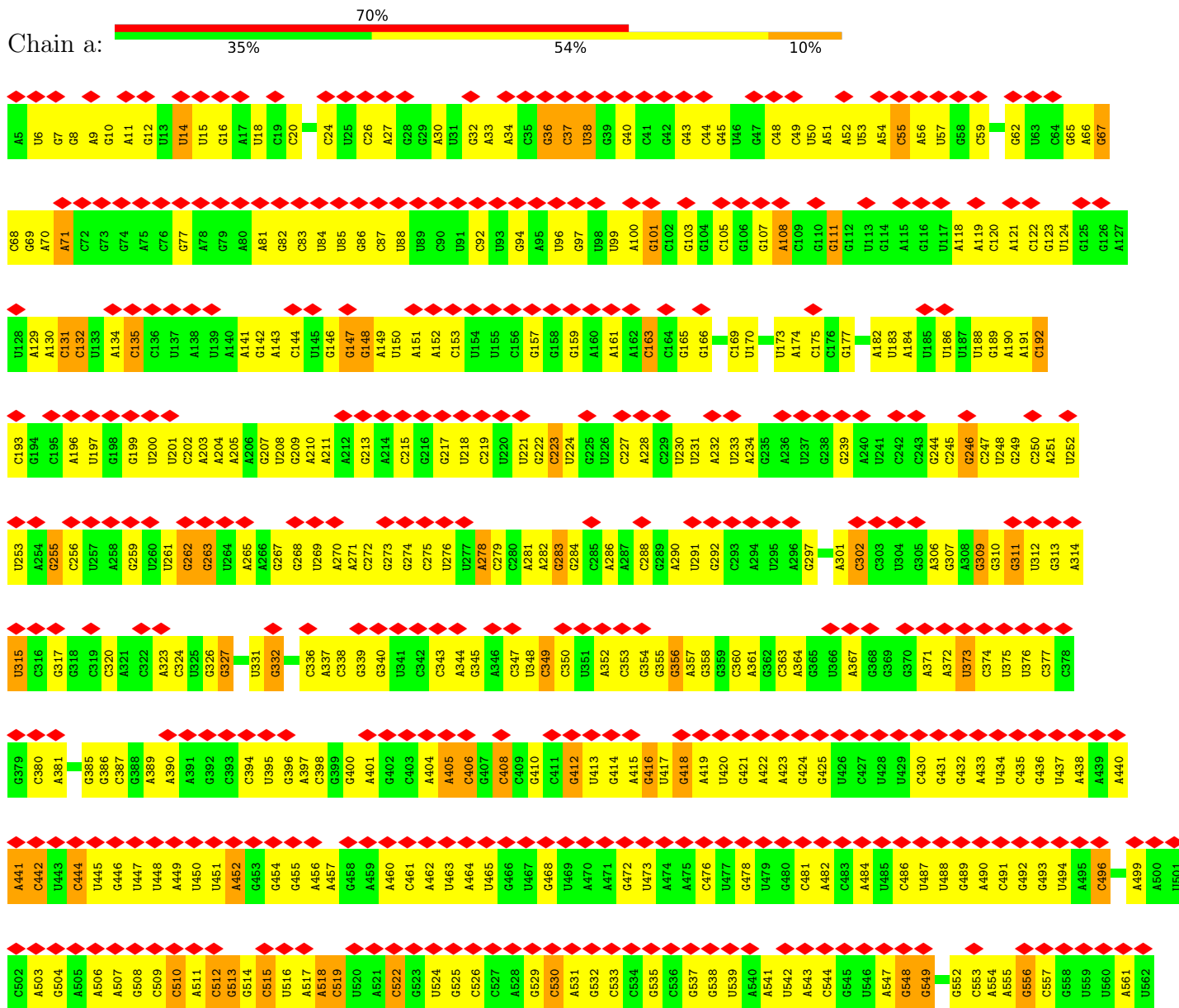
• Molecule 29: 50S ribosomal protein L35

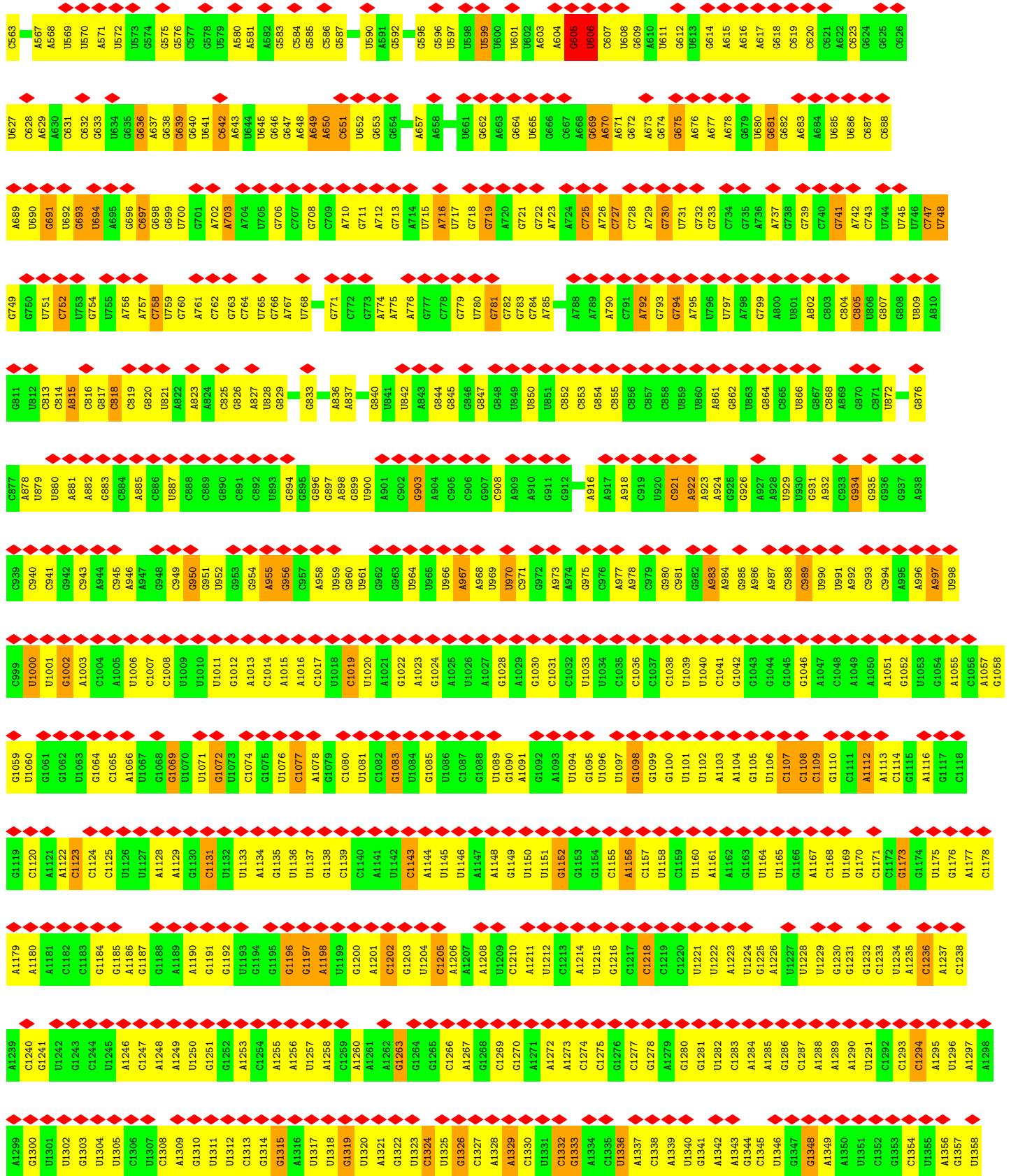


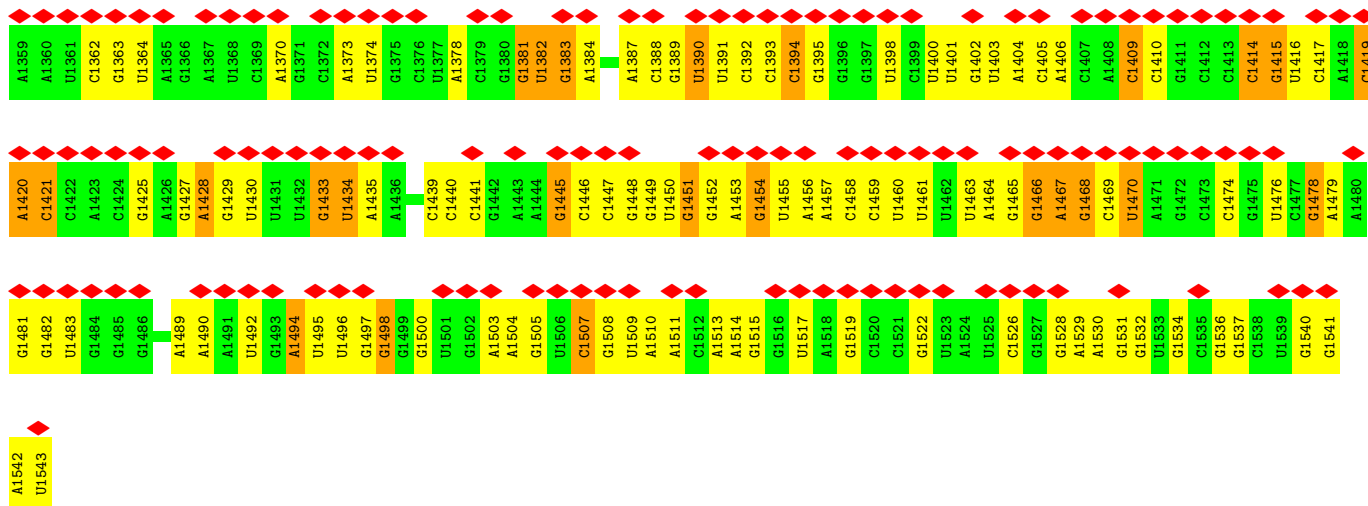
• Molecule 30: 50S ribosomal protein L36



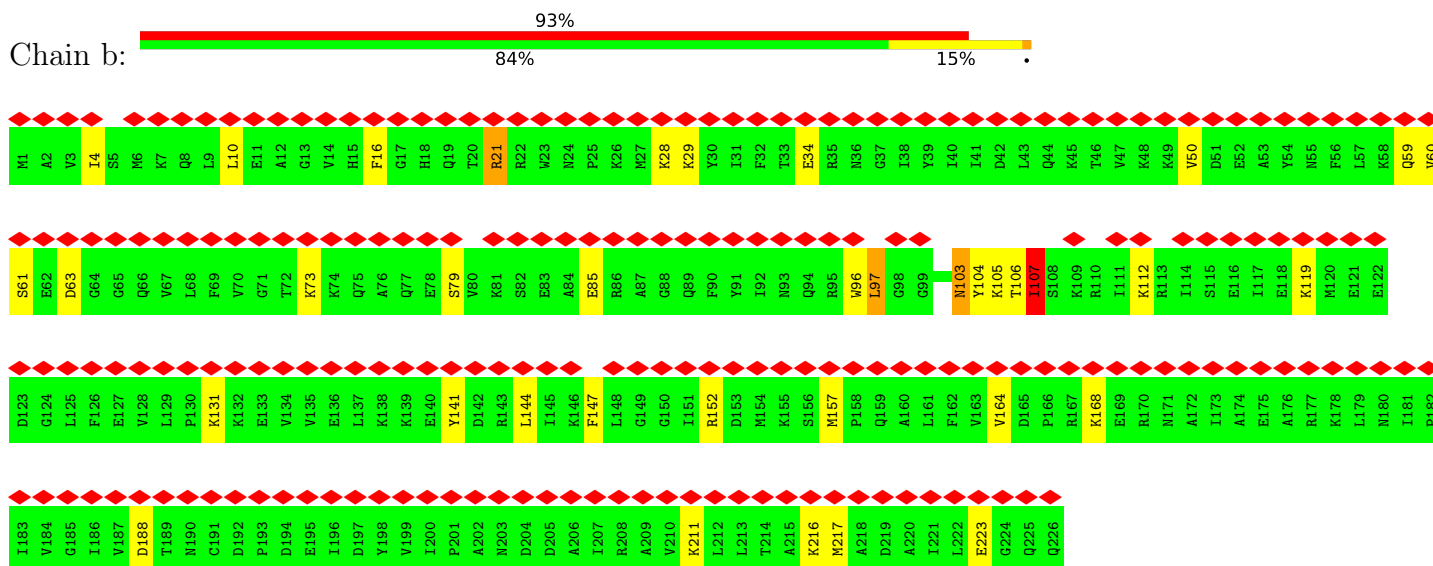
• Molecule 31: 16S ribosomal RNA







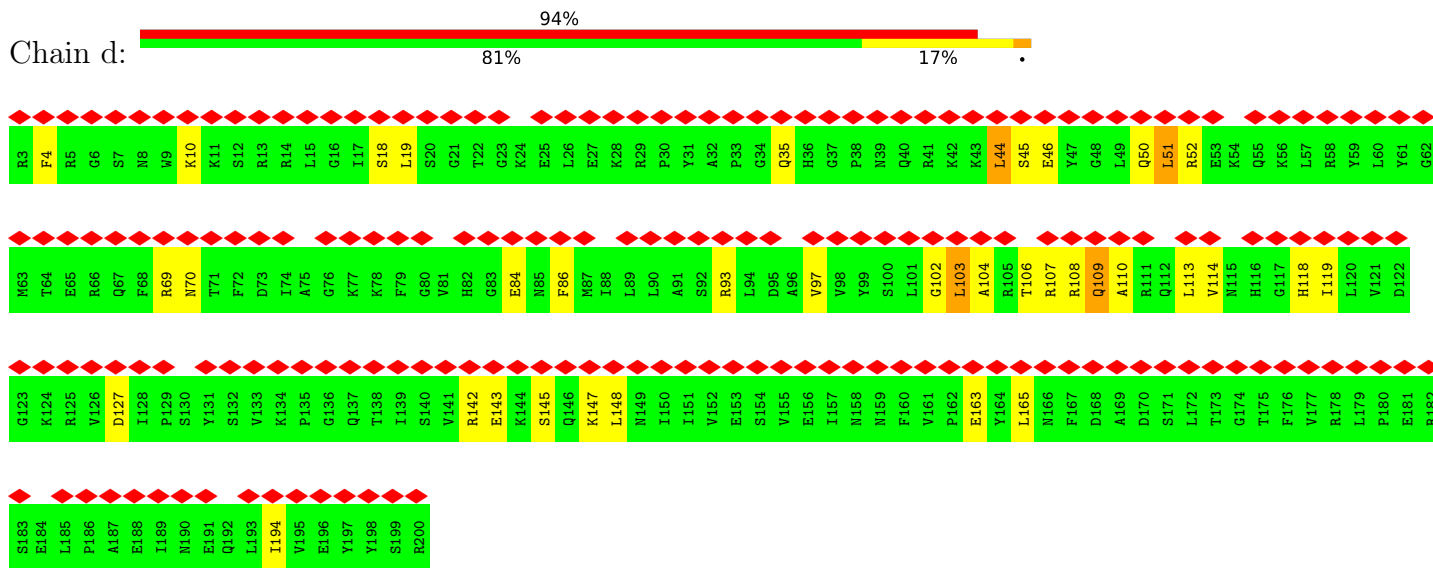
• Molecule 32: 30S ribosomal protein S2



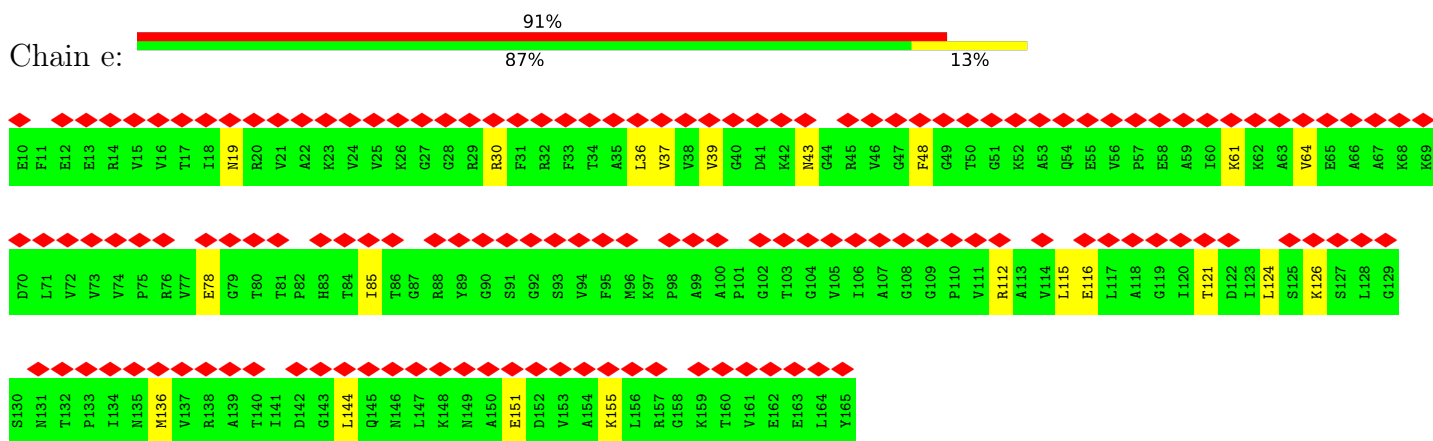
• Molecule 33: 30S ribosomal protein S3



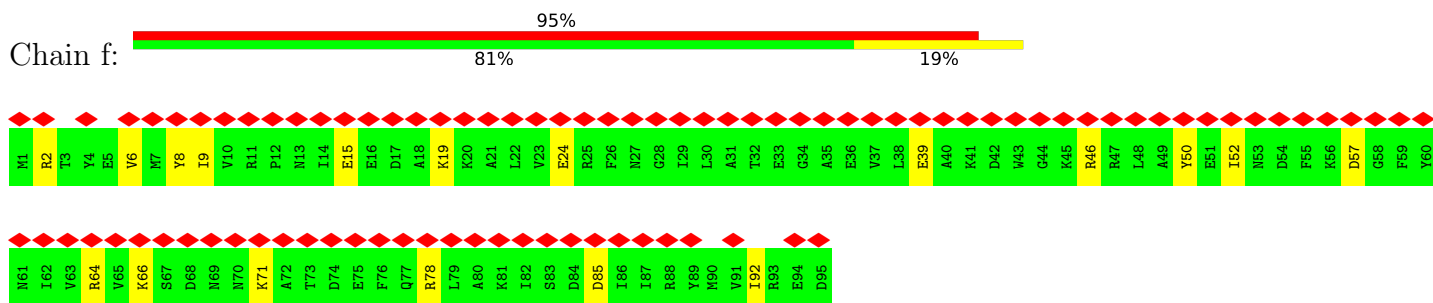
• Molecule 34: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S5

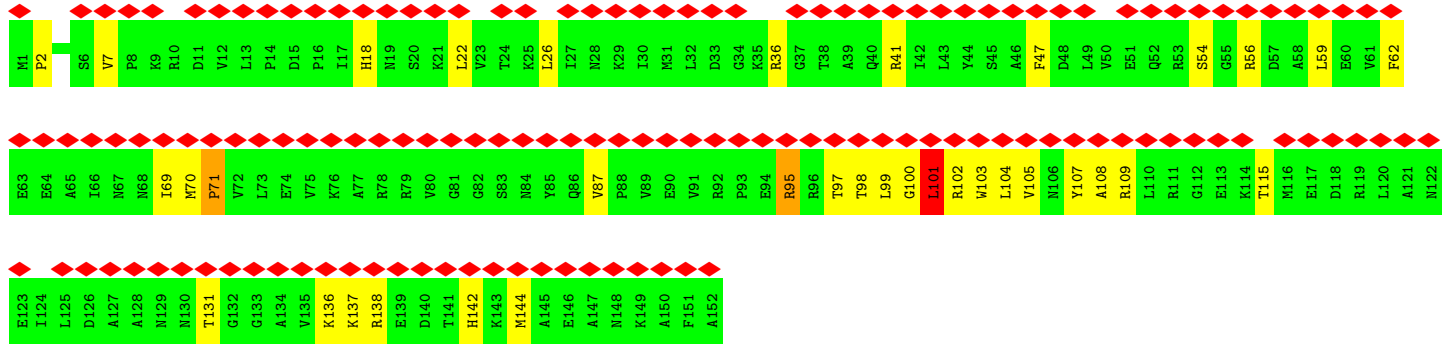


• Molecule 36: 30S ribosomal protein S6

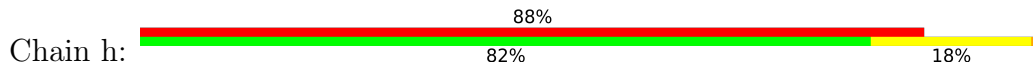


• Molecule 37: 30S ribosomal protein S7

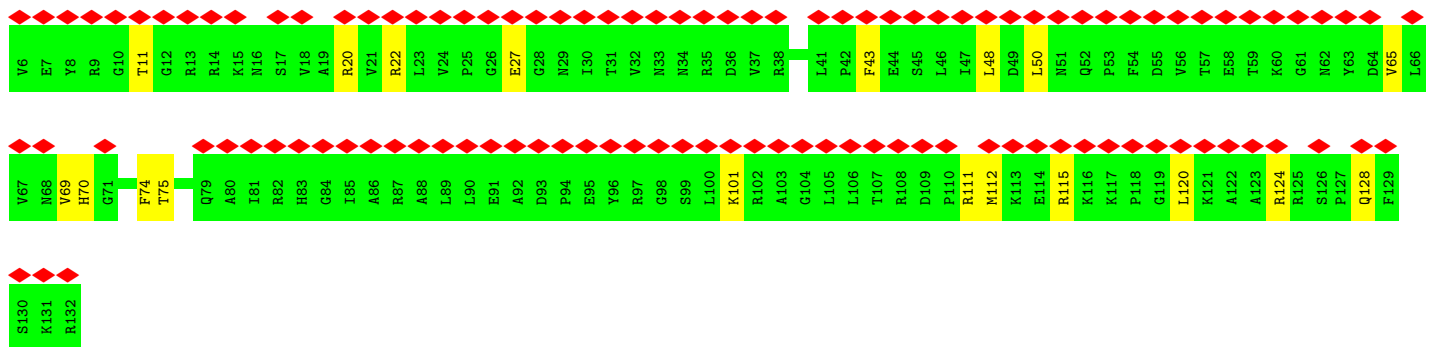
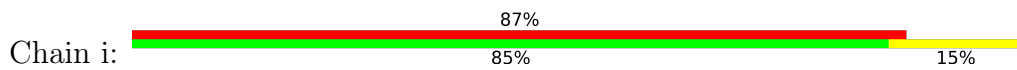




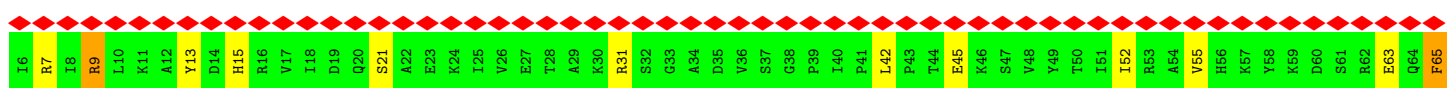
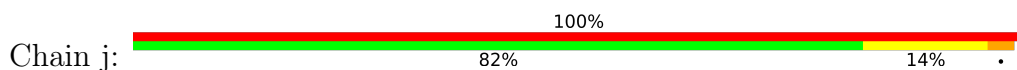
• Molecule 38: 30S ribosomal protein S8

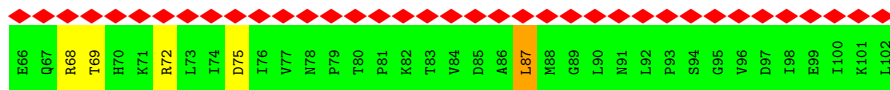


• Molecule 39: 30S ribosomal protein S9

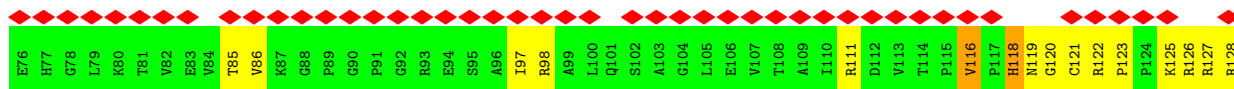
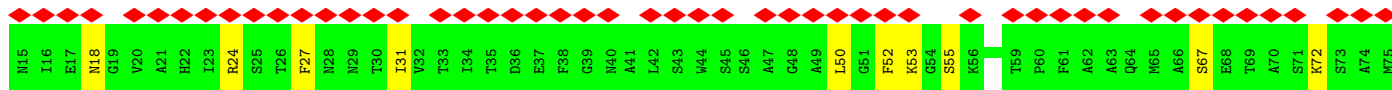
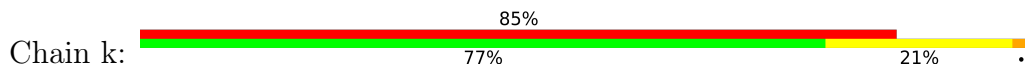


• Molecule 40: 30S ribosomal protein S10

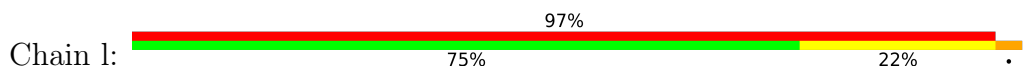




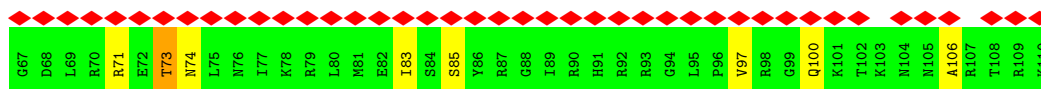
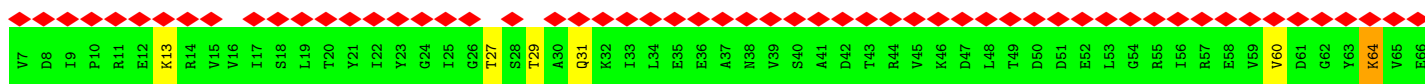
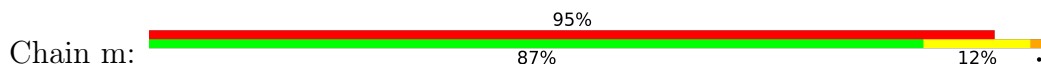
• Molecule 41: 30S ribosomal protein S11



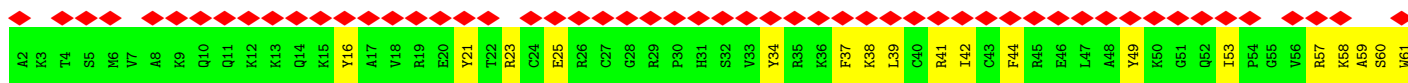
• Molecule 42: 30S ribosomal protein S12



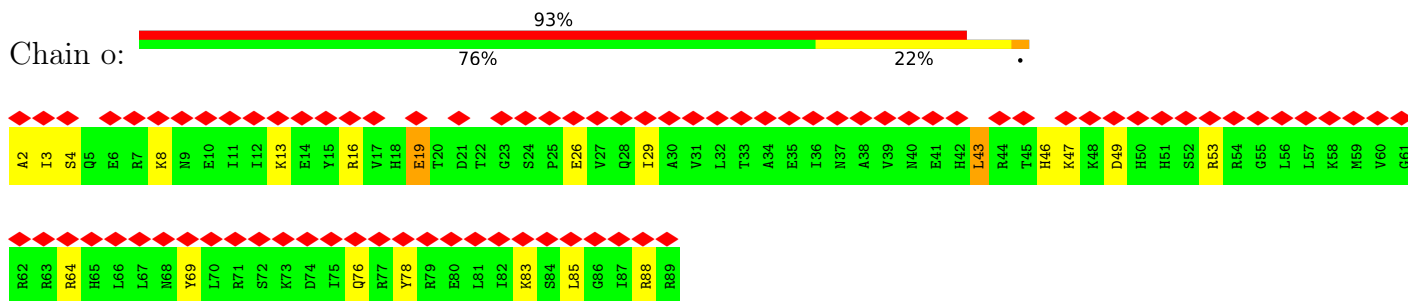
• Molecule 43: 30S ribosomal protein S13



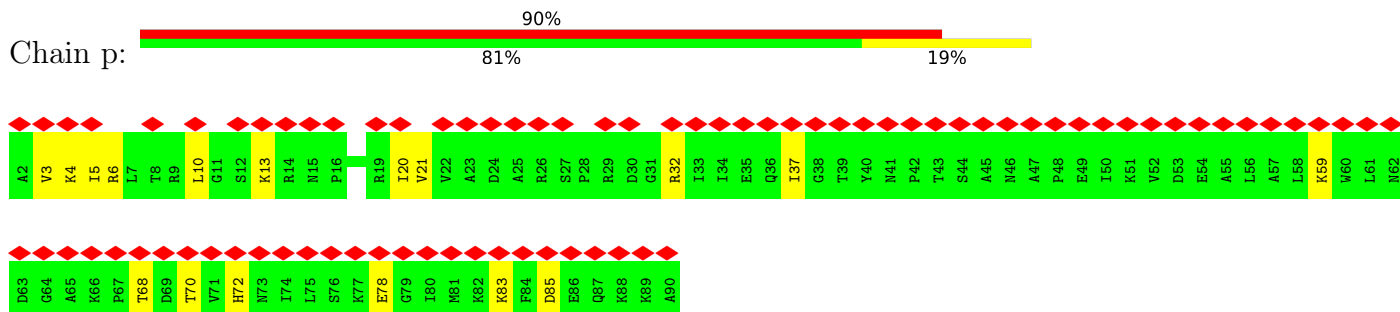
• Molecule 44: 30S ribosomal protein S14 type Z



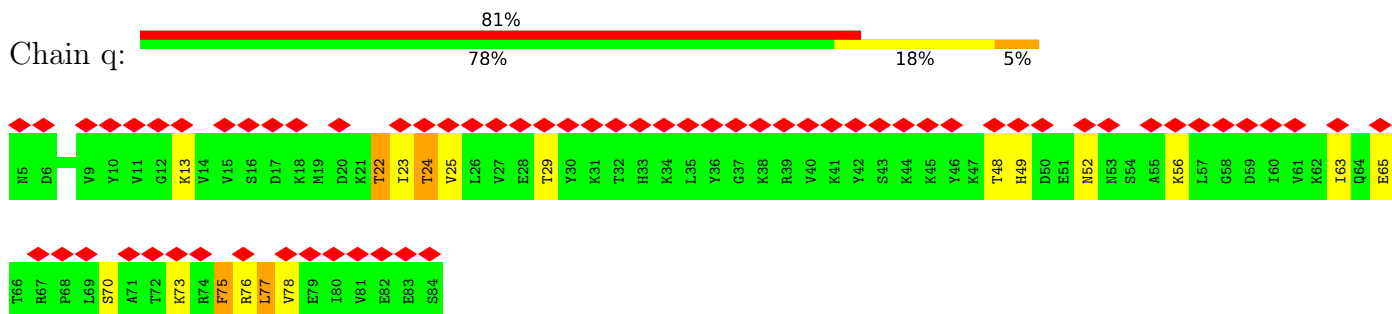
• Molecule 45: 30S ribosomal protein S15



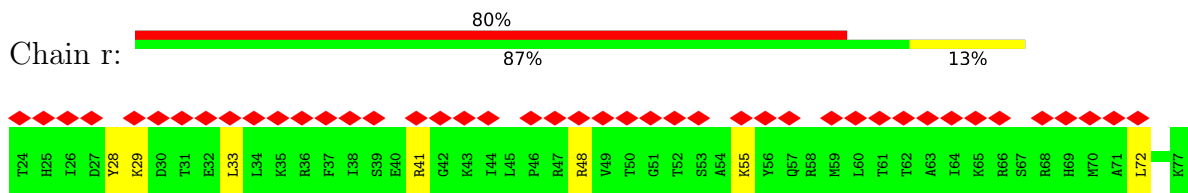
• Molecule 46: 30S ribosomal protein S16



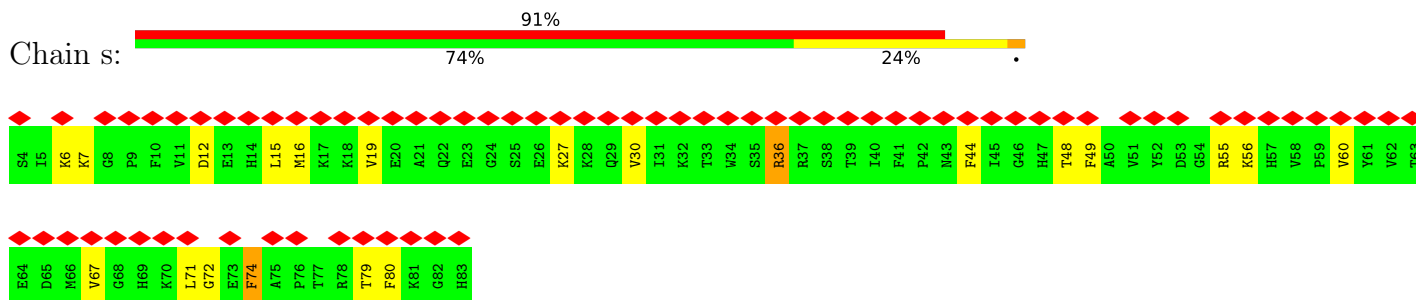
• Molecule 47: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S20

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.076	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (\AA)	430.4, 430.4, 430.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.076, 1.076, 1.076	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	1.69	183/69739 (0.3%)	1.60	1291/108751 (1.2%)
2	B	1.04	0/2733	1.42	26/4257 (0.6%)
3	C	0.61	0/2125	0.82	2/2853 (0.1%)
4	D	0.70	0/1651	0.70	1/2215 (0.0%)
5	E	0.69	1/1595 (0.1%)	0.74	0/2154
6	F	0.37	0/1339	0.66	0/1805
7	G	0.38	0/1281	0.66	0/1736
8	H	0.66	0/1165	0.71	0/1570
9	I	0.65	0/925	0.80	0/1242
10	J	0.62	0/1100	0.71	0/1467
11	K	2.44	1/1095 (0.1%)	0.78	1/1472 (0.1%)
12	L	0.59	0/936	0.79	0/1253
13	M	0.45	0/900	0.70	0/1205
14	N	0.65	0/901	0.74	0/1209
15	O	0.71	0/954	0.76	0/1264
16	P	0.72	0/800	0.76	0/1070
17	Q	0.65	0/845	0.80	0/1140
18	R	0.60	0/723	0.68	0/966
19	S	0.49	0/779	0.69	0/1043
20	T	0.39	0/730	0.64	0/981
21	U	0.66	0/628	0.81	1/833 (0.1%)
22	V	0.49	0/451	0.76	0/603
23	W	0.45	0/542	0.73	0/722
24	X	0.64	0/451	0.71	0/606
25	Y	0.31	0/378	0.57	0/521
26	Z	0.63	0/366	0.85	0/489
27	1	0.44	0/395	0.77	0/530
28	2	0.78	0/371	0.81	0/484
29	3	0.60	0/526	0.83	1/690 (0.1%)
30	4	0.50	0/298	0.88	1/392 (0.3%)
31	a	2.36	45/36913 (0.1%)	1.54	698/57564 (1.2%)
32	b	1.12	1/1846 (0.1%)	0.63	1/2477 (0.0%)
33	c	0.29	0/1523	0.65	0/2062
34	d	0.31	0/1526	0.69	1/2063 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	e	0.32	0/1159	0.63	0/1566
36	f	0.36	0/789	0.66	0/1060
37	g	0.39	0/1175	0.87	2/1584 (0.1%)
38	h	1.16	4/1037 (0.4%)	0.96	7/1392 (0.5%)
39	i	0.34	0/937	0.71	0/1269
40	j	0.33	0/764	0.76	0/1034
41	k	0.34	0/824	0.75	1/1119 (0.1%)
42	l	6.63	7/1054 (0.7%)	0.87	4/1415 (0.3%)
43	m	0.32	0/732	0.71	0/991
44	n	6.34	3/497 (0.6%)	1.03	4/662 (0.6%)
45	o	0.33	0/732	0.72	1/979 (0.1%)
46	p	0.33	0/705	0.65	0/952
47	q	0.35	0/629	0.81	1/849 (0.1%)
48	r	0.35	0/452	0.72	0/604
49	s	6.45	8/654 (1.2%)	1.28	11/879 (1.3%)
50	t	0.37	0/591	0.73	0/793
51	u	0.45	0/403	0.83	1/535 (0.2%)
52	v	0.33	0/1350	0.72	1/1812 (0.1%)
All	All	1.85	253/153014 (0.2%)	1.41	2057/229184 (0.9%)

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
3	C	0	5
5	E	0	1
6	F	0	2
7	G	0	1
8	H	0	4
11	K	0	3
12	L	0	1
13	M	0	1
16	P	0	2
19	S	0	1
26	Z	0	2
30	4	0	2
31	a	0	2
32	b	0	4
33	c	0	1
34	d	0	7

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	g	0	10
39	i	0	1
40	j	0	4
41	k	0	5
42	l	0	2
43	m	0	5
44	n	0	4
45	o	0	4
47	q	0	5
49	s	0	3
50	t	0	1
51	u	0	3
52	v	0	3
All	All	0	89

The worst 5 of 253 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	n	16	TYR	CB-CG	140.63	3.62	1.51
1	A	333	C	N1-C6	139.55	2.20	1.37
31	a	606	U	C2-N3	135.46	2.32	1.37
31	a	605	G	N3-C4	131.79	2.27	1.35
31	a	605	G	C2-N3	128.80	2.35	1.32

The worst 5 of 2057 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	G	C8-N9-C4	-101.80	65.68	106.40
1	A	393	G	N7-C8-N9	65.13	145.66	113.10
1	A	393	G	N9-C4-C5	52.43	126.37	105.40
1	A	393	G	N3-C4-C5	-40.30	108.45	128.60
31	a	605	G	C2-N3-C4	36.17	129.98	111.90

There are no chirality outliers.

5 of 89 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	173	LEU	Peptide
3	C	255	LEU	Peptide
3	C	257	LYS	Peptide
3	C	273	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	C	40	LYS	Peptide

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	
3	C	272/274 (99%)	215 (79%)	57 (21%)	0	100	100
4	D	213/215 (99%)	166 (78%)	47 (22%)	0	100	100
5	E	204/206 (99%)	175 (86%)	29 (14%)	0	100	100
6	F	173/175 (99%)	141 (82%)	32 (18%)	0	100	100
7	G	173/175 (99%)	140 (81%)	33 (19%)	0	100	100
8	H	143/145 (99%)	118 (82%)	25 (18%)	0	100	100
9	I	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
10	J	144/146 (99%)	124 (86%)	20 (14%)	0	100	100
11	K	135/137 (98%)	113 (84%)	22 (16%)	0	100	100
12	L	118/120 (98%)	101 (86%)	17 (14%)	0	100	100
13	M	117/119 (98%)	98 (84%)	19 (16%)	0	100	100
14	N	112/114 (98%)	94 (84%)	18 (16%)	0	100	100
15	O	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
16	P	100/102 (98%)	85 (85%)	15 (15%)	0	100	100
17	Q	108/110 (98%)	90 (83%)	17 (16%)	1 (1%)	17	57
18	R	87/89 (98%)	70 (80%)	17 (20%)	0	100	100
19	S	101/103 (98%)	82 (81%)	19 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
21	U	80/82 (98%)	70 (88%)	10 (12%)	0	100	100
22	V	56/58 (97%)	46 (82%)	10 (18%)	0	100	100
23	W	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
24	X	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
25	Y	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
26	Z	46/48 (96%)	29 (63%)	17 (37%)	0	100	100
27	1	45/47 (96%)	37 (82%)	8 (18%)	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	50 (81%)	12 (19%)	0	100	100
30	4	35/37 (95%)	21 (60%)	14 (40%)	0	100	100
32	b	224/226 (99%)	193 (86%)	31 (14%)	0	100	100
33	c	200/202 (99%)	161 (80%)	39 (20%)	0	100	100
34	d	196/198 (99%)	136 (69%)	59 (30%)	1 (0%)	29	67
35	e	154/156 (99%)	133 (86%)	21 (14%)	0	100	100
36	f	93/95 (98%)	75 (81%)	18 (19%)	0	100	100
37	g	149/152 (98%)	99 (66%)	50 (34%)	0	100	100
38	h	127/131 (97%)	98 (77%)	29 (23%)	0	100	100
39	i	125/127 (98%)	86 (69%)	39 (31%)	0	100	100
40	j	95/97 (98%)	59 (62%)	35 (37%)	1 (1%)	14	53
41	k	112/114 (98%)	81 (72%)	31 (28%)	0	100	100
42	l	133/135 (98%)	102 (77%)	29 (22%)	2 (2%)	10	47
43	m	100/104 (96%)	62 (62%)	38 (38%)	0	100	100
44	n	58/60 (97%)	36 (62%)	22 (38%)	0	100	100
45	o	86/88 (98%)	71 (83%)	15 (17%)	0	100	100
46	p	87/89 (98%)	68 (78%)	19 (22%)	0	100	100
47	q	78/80 (98%)	51 (65%)	27 (35%)	0	100	100
48	r	52/54 (96%)	43 (83%)	9 (17%)	0	100	100
49	s	78/80 (98%)	58 (74%)	20 (26%)	0	100	100
50	t	79/81 (98%)	59 (75%)	20 (25%)	0	100	100
51	u	50/52 (96%)	32 (64%)	18 (36%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	v	158/162 (98%)	117 (74%)	41 (26%)	0	100	100
All	All	5503/5608 (98%)	4369 (79%)	1129 (20%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	l	131	GLY
34	d	110	ALA
40	j	7	ARG
17	Q	87	PRO
42	l	135	PRO

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	
3	C	220/221 (100%)	177 (80%)	43 (20%)	1	9
4	D	173/173 (100%)	144 (83%)	29 (17%)	2	13
5	E	168/168 (100%)	126 (75%)	42 (25%)	0	4
6	F	141/154 (92%)	116 (82%)	25 (18%)	2	11
7	G	124/153 (81%)	101 (82%)	23 (18%)	1	10
8	H	122/123 (99%)	98 (80%)	24 (20%)	1	9
9	I	100/100 (100%)	79 (79%)	21 (21%)	1	7
10	J	109/112 (97%)	96 (88%)	13 (12%)	5	27
11	K	108/114 (95%)	93 (86%)	15 (14%)	3	22
12	L	96/101 (95%)	82 (85%)	14 (15%)	3	20
13	M	86/95 (90%)	61 (71%)	25 (29%)	0	3
14	N	93/100 (93%)	79 (85%)	14 (15%)	3	19
15	O	96/96 (100%)	83 (86%)	13 (14%)	4	23
16	P	84/86 (98%)	64 (76%)	20 (24%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	88/90 (98%)	59 (67%)	29 (33%)	0	2
18	R	78/80 (98%)	62 (80%)	16 (20%)	1	8
19	S	81/88 (92%)	59 (73%)	22 (27%)	0	3
20	T	78/82 (95%)	60 (77%)	18 (23%)	1	5
21	U	63/64 (98%)	45 (71%)	18 (29%)	0	3
22	V	44/49 (90%)	33 (75%)	11 (25%)	0	4
23	W	58/60 (97%)	50 (86%)	8 (14%)	3	22
24	X	52/52 (100%)	44 (85%)	8 (15%)	2	18
25	Y	23/56 (41%)	22 (96%)	1 (4%)	29	63
26	Z	35/44 (80%)	24 (69%)	11 (31%)	0	2
27	1	44/45 (98%)	32 (73%)	12 (27%)	0	3
28	2	39/39 (100%)	35 (90%)	4 (10%)	7	34
29	3	55/55 (100%)	48 (87%)	7 (13%)	4	24
30	4	35/35 (100%)	27 (77%)	8 (23%)	1	6
32	b	196/196 (100%)	160 (82%)	36 (18%)	1	10
33	c	138/164 (84%)	110 (80%)	28 (20%)	1	8
34	d	147/174 (84%)	114 (78%)	33 (22%)	1	6
35	e	118/122 (97%)	97 (82%)	21 (18%)	2	11
36	f	80/83 (96%)	62 (78%)	18 (22%)	1	6
37	g	118/128 (92%)	90 (76%)	28 (24%)	1	5
38	h	111/112 (99%)	88 (79%)	23 (21%)	1	8
39	i	86/105 (82%)	68 (79%)	18 (21%)	1	7
40	j	81/87 (93%)	66 (82%)	15 (18%)	1	10
41	k	82/90 (91%)	60 (73%)	22 (27%)	0	3
42	l	111/117 (95%)	80 (72%)	31 (28%)	0	3
43	m	62/92 (67%)	51 (82%)	11 (18%)	2	11
44	n	48/52 (92%)	35 (73%)	13 (27%)	0	3
45	o	77/80 (96%)	59 (77%)	18 (23%)	1	5
46	p	73/75 (97%)	56 (77%)	17 (23%)	1	5
47	q	65/75 (87%)	49 (75%)	16 (25%)	0	5
48	r	48/49 (98%)	41 (85%)	7 (15%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	s	67/70 (96%)	50 (75%)	17 (25%)	0	4
50	t	61/67 (91%)	49 (80%)	12 (20%)	1	9
51	u	40/48 (83%)	29 (72%)	11 (28%)	0	3
52	v	147/147 (100%)	115 (78%)	32 (22%)	1	6
All	All	4449/4768 (93%)	3528 (79%)	921 (21%)	3	8

5 of 921 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	l	5	VAL
51	u	38	TYR
34	d	103	LEU
50	t	79	MET
45	o	43	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
41	k	119	ASN
52	v	49	ASN
43	m	31	GLN
46	p	62	ASN
10	J	81	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2896/2905 (99%)	1223 (42%)	55 (1%)
2	B	114/115 (99%)	44 (38%)	0
31	a	1537/1539 (99%)	918 (59%)	0
All	All	4547/4559 (99%)	2185 (48%)	55 (1%)

5 of 2185 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	6	A
1	A	15	G

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Mol	Chain	Res	Type
1	A	28	A
1	A	34	U

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1108	C
1	A	1520	A
1	A	2816	C
1	A	2450	U
1	A	1190	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8
31	a	2
52	v	1
43	m	1
37	g	1

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Mol	Chain	Number of breaks
38	h	1
5	E	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	106:GLN	C	131:ILE	N	30.98
1	A	2207:U	O3'	2208:A	P	12.82
1	A	1939:A	O3'	1944:U	P	12.52
1	a	465:U	O3'	466:G	P	11.00
1	A	929:C	O3'	937:G	P	9.63

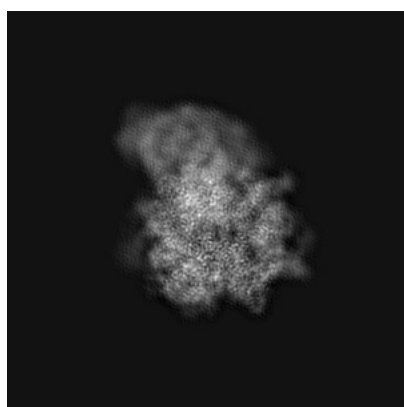
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10079. These allow visual inspection of the internal detail of the map and identification of artifacts.

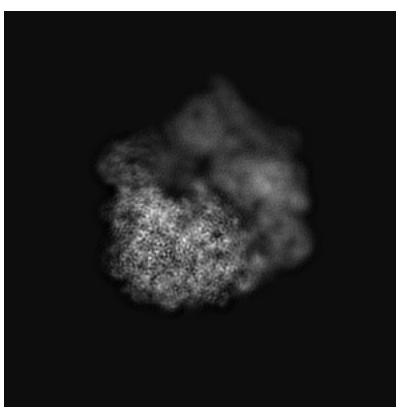
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

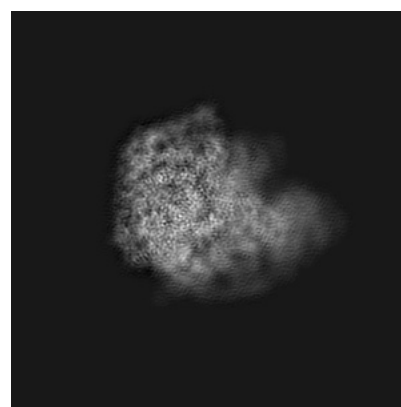
6.1.1 Primary map



X



Y

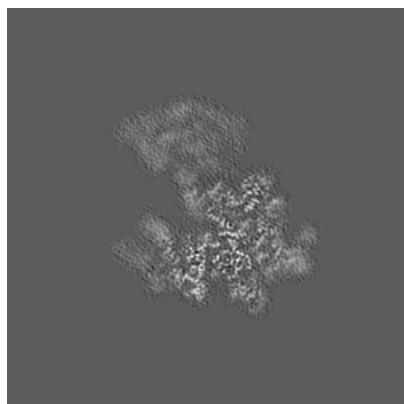


Z

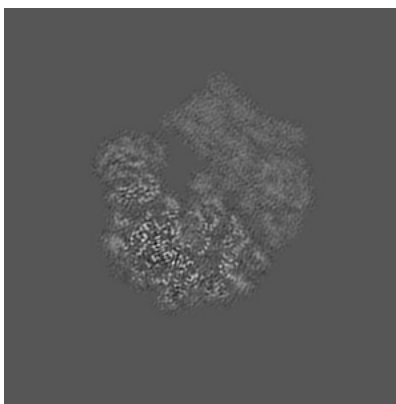
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

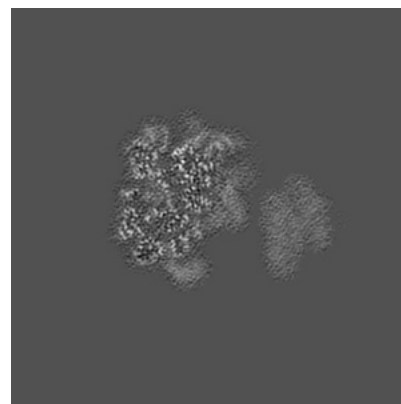
6.2.1 Primary map



X Index: 200



Y Index: 200

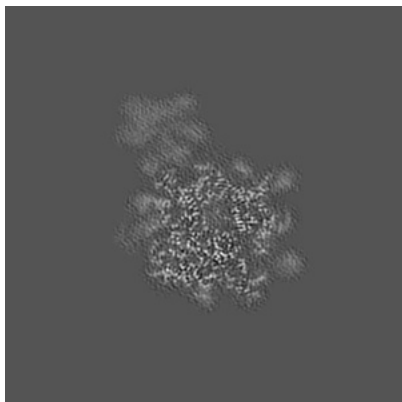


Z Index: 200

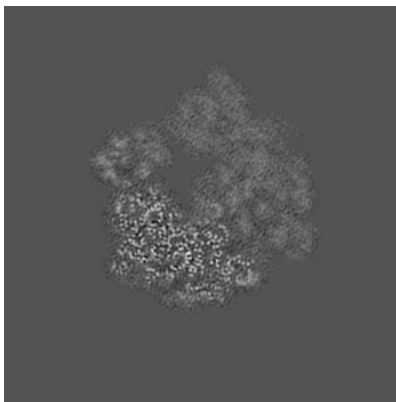
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

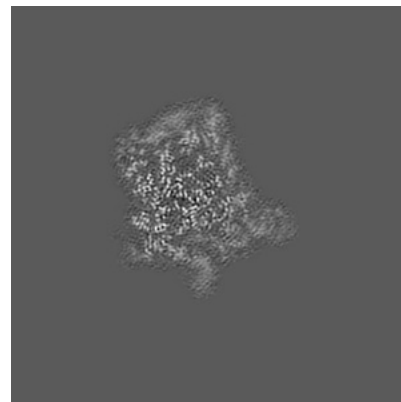
6.3.1 Primary map



X Index: 163



Y Index: 184

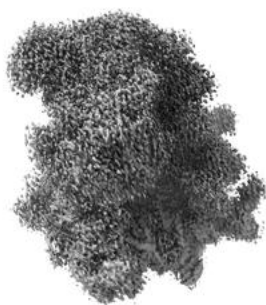


Z Index: 145

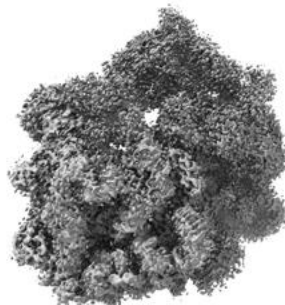
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

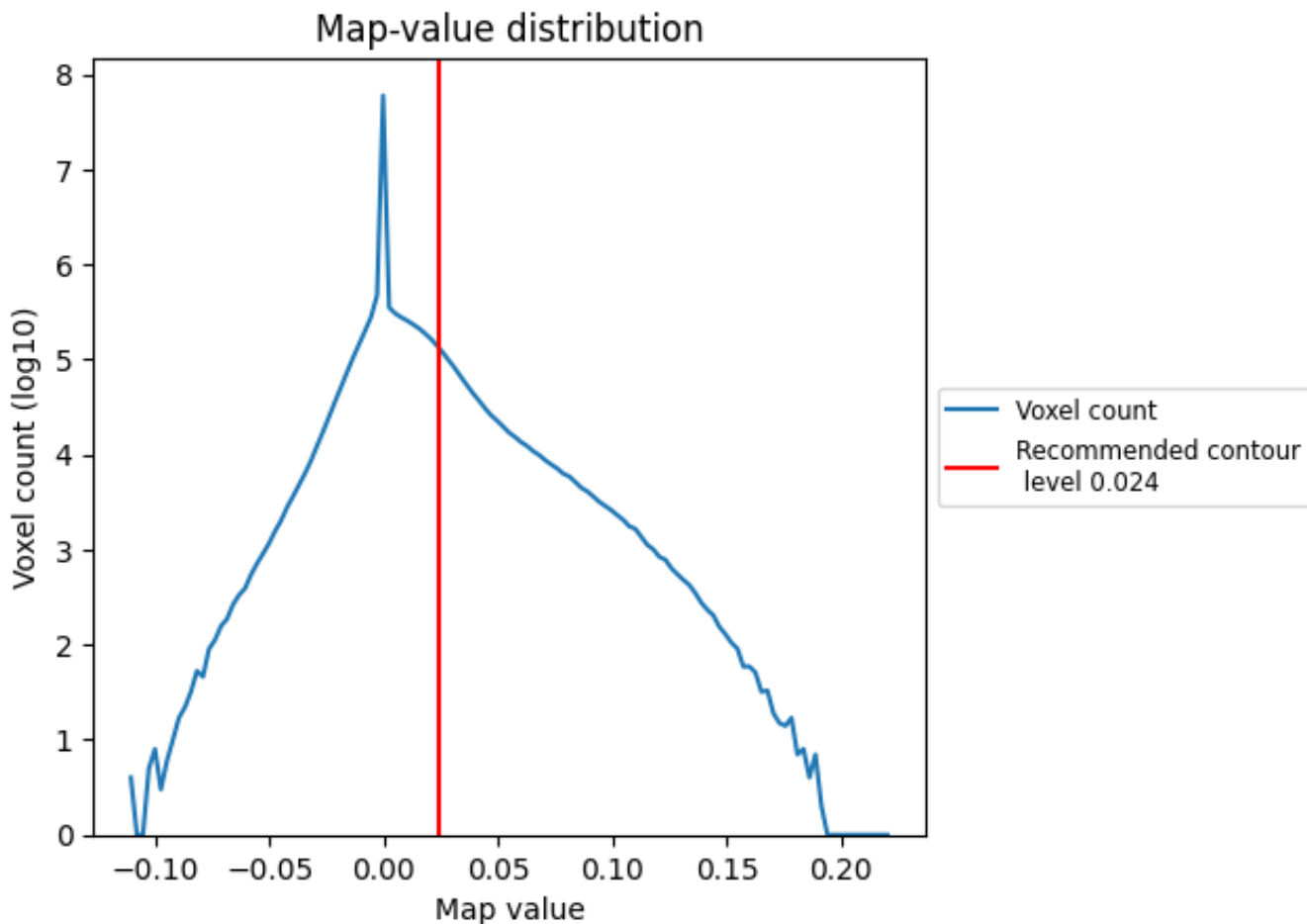
6.5 Mask visualisation

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

7 Map analysis [i](#)

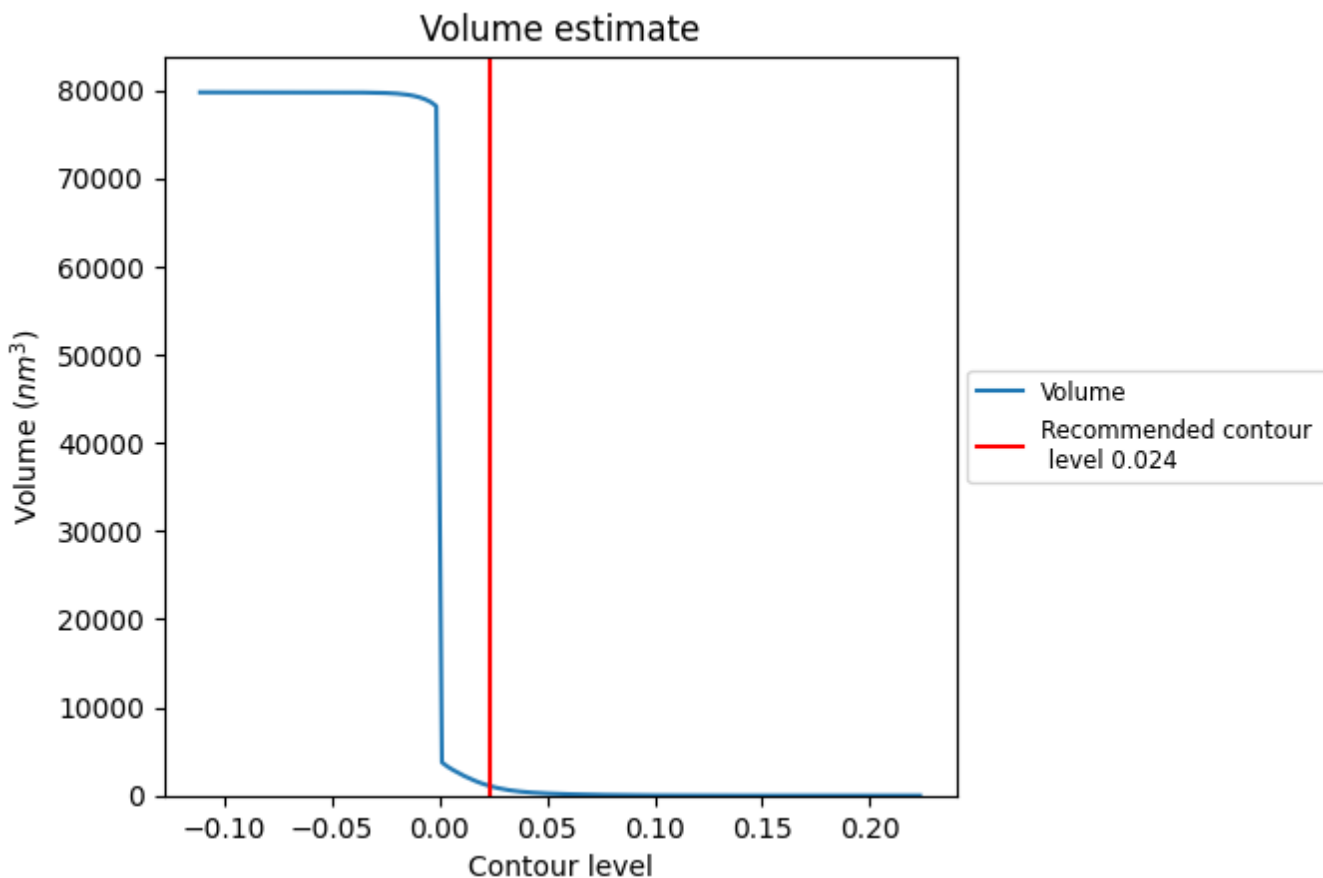
This section contains the results of statistical analysis of the map.

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.

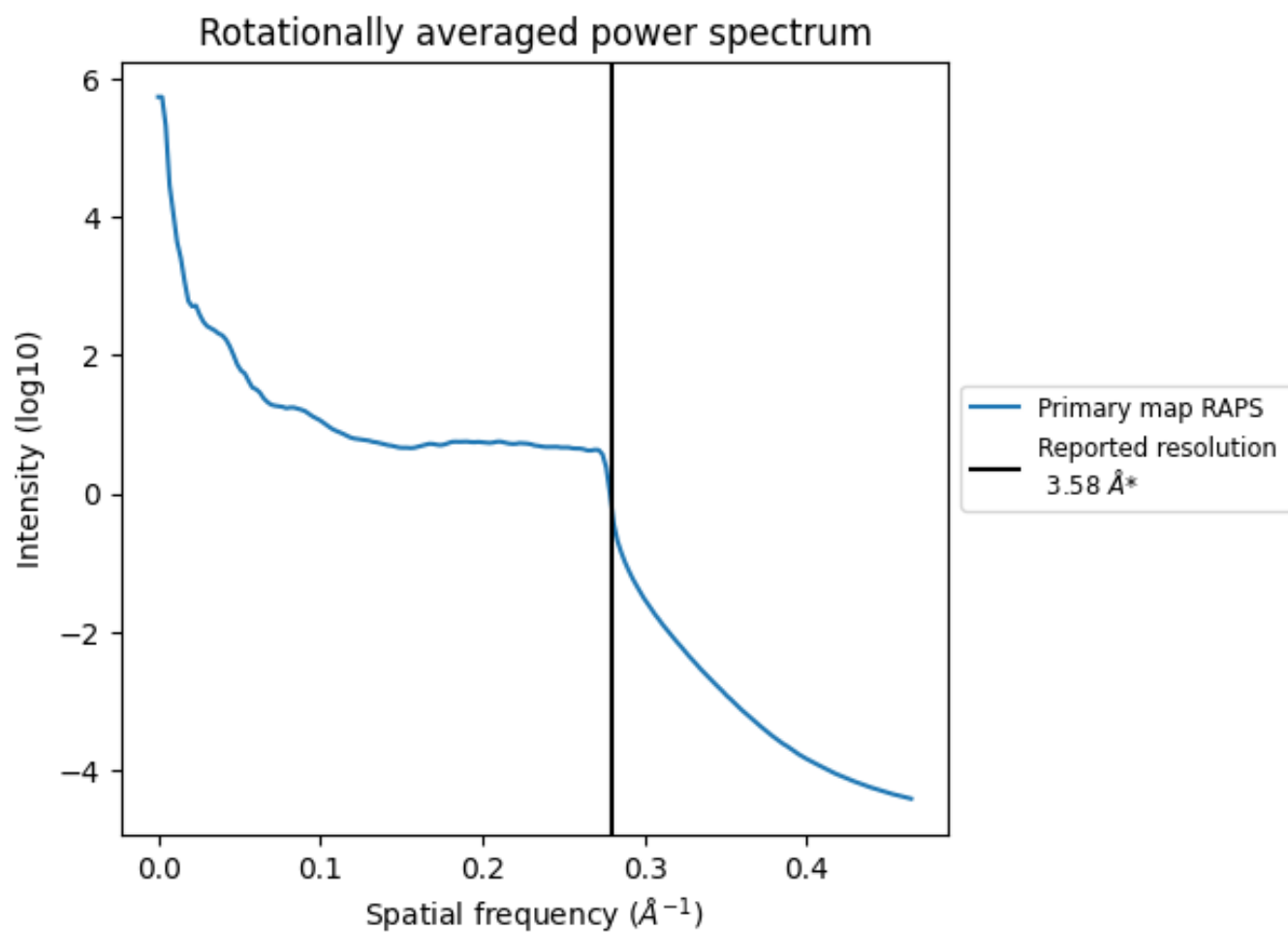
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1057 nm^3 ; this corresponds to an approximate mass of 955 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 0.279 Å⁻¹

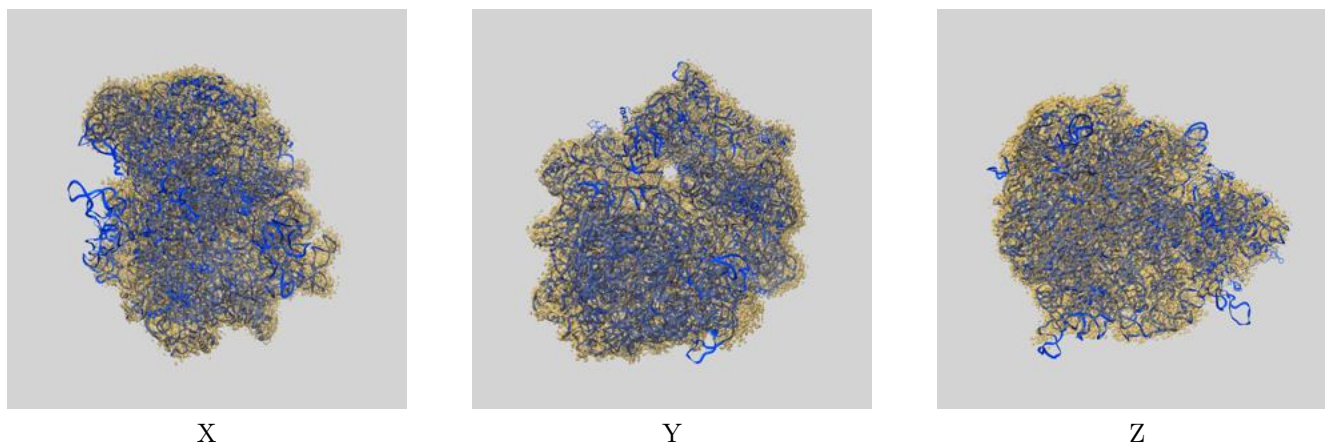
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

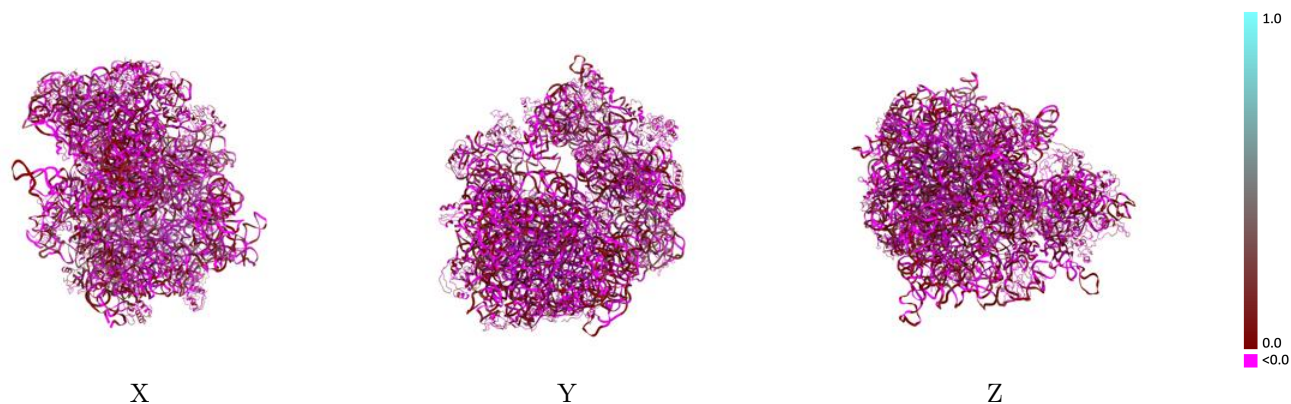
This section contains information regarding the fit between EMDB map EMD-10079 and PDB model 6S13. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



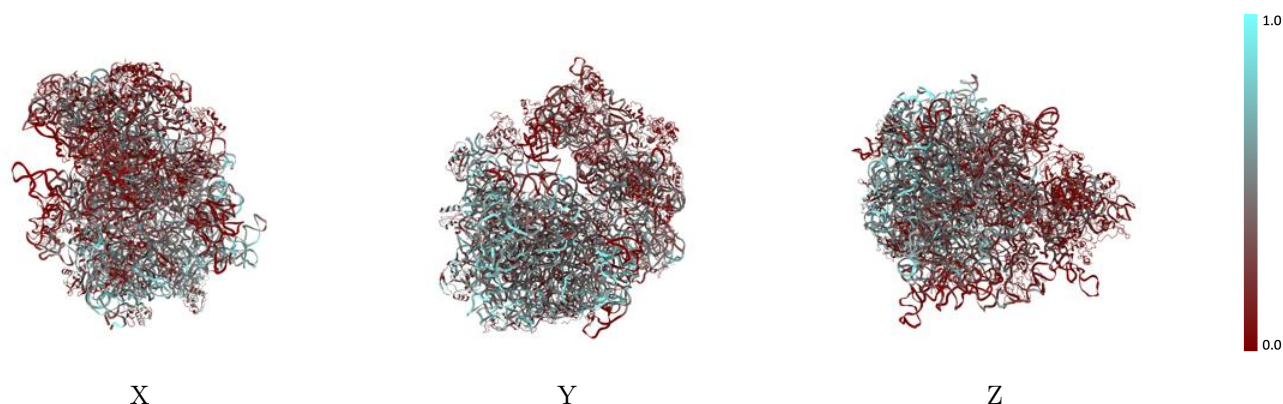
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



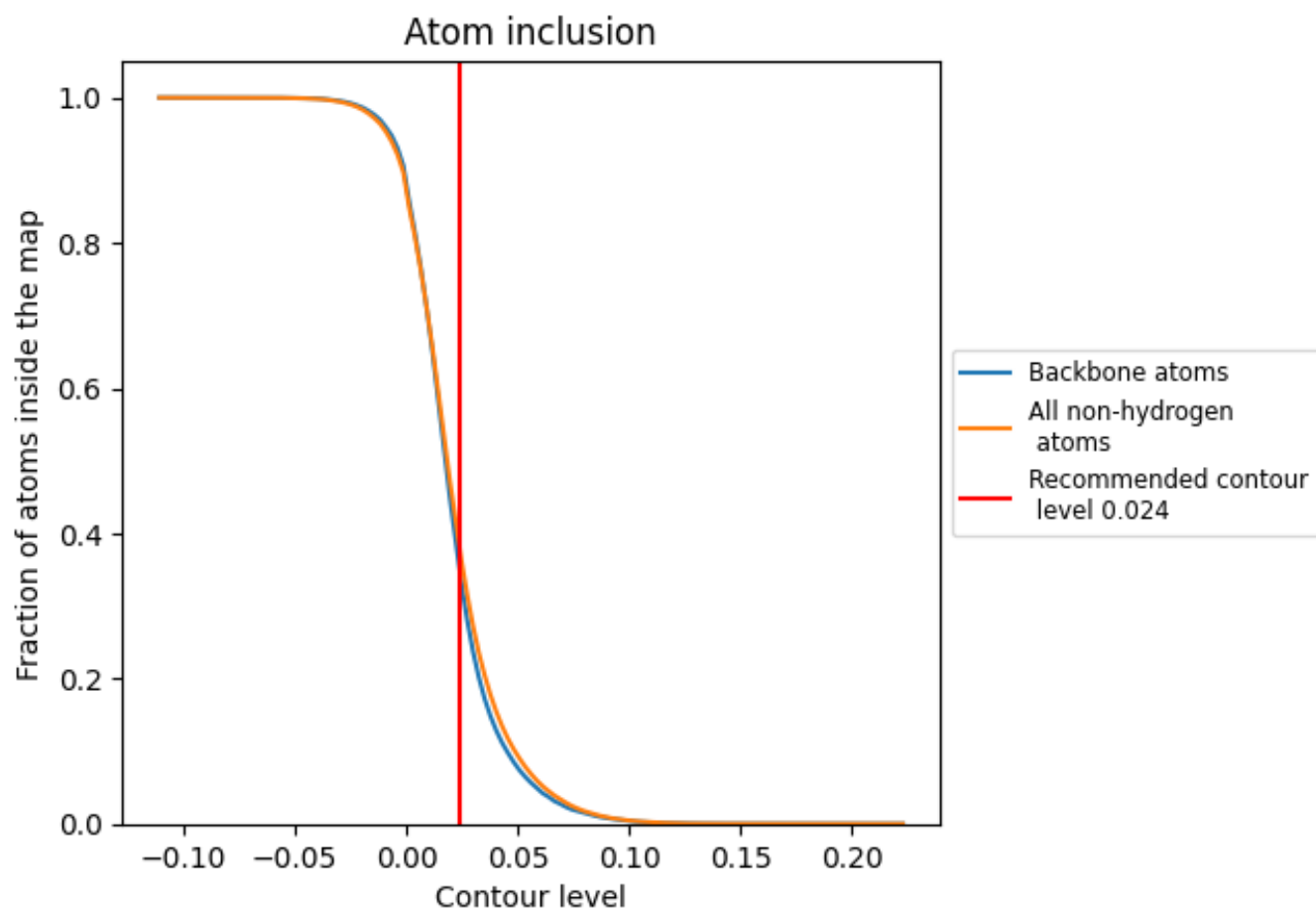
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 35% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





































The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3784	 0.0000
1	 0.2293	 -0.0040
2	 0.3497	 -0.0540
3	 0.3127	 -0.0380
4	 0.2976	 -0.0180
A	 0.4742	 -0.0050
B	 0.5730	 0.0480
C	 0.2989	 -0.0630
D	 0.3768	 -0.0010
E	 0.3472	 -0.0200
F	 0.1908	 0.0070
G	 0.0866	 0.0210
H	 0.4270	 0.0400
I	 0.3464	 -0.0150
J	 0.2963	 -0.0570
K	 0.3748	 0.0310
L	 0.3726	 -0.0090
M	 0.3257	 0.0230
N	 0.3690	 0.0090
O	 0.4070	 -0.0140
P	 0.4679	 0.0640
Q	 0.3611	 0.0150
R	 0.3147	 -0.0280
S	 0.3775	 0.0320
T	 0.2116	 0.0450
U	 0.2736	 -0.0630
V	 0.2564	 -0.0090
W	 0.3752	 0.0050
X	 0.4444	 0.0470
Y	 0.1304	 0.0480
Z	 0.4467	 0.0150
a	 0.3059	 0.0100
b	 0.0942	 -0.0110
c	 0.0956	 0.0130
d	 0.1575	 0.0010



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Chain	Atom inclusion	Q-score
e	 0.1374	 -0.0050
f	 0.0995	 -0.0310
g	 0.1184	 0.0080
h	 0.1735	 0.0040
i	 0.1862	 0.0240
j	 0.0682	 -0.0030
k	 0.1957	 -0.0190
l	 0.0587	 0.0220
m	 0.1018	 -0.0340
n	 0.1545	 -0.0110
o	 0.1236	 -0.0240
p	 0.1846	 0.0060
q	 0.2294	 -0.0070
r	 0.2196	 -0.0020
s	 0.1340	 -0.0130
t	 0.1201	 -0.0030
u	 0.1835	 0.0260
v	 0.0602	 0.0240