Full wwPDB EM Validation Report ⓘ

Dec 2, 2024 – 11:20 PM JST

PDB ID	:	8YLR
EMDB ID	:	EMD-38668
Title	:	State 6 (S6) of yeast 80S ribosome bound to 2 tRNAs and eEF2 and eEF3 during tranlocation
Authors	:	Cheng, J.; Wu, C.L.; Li, J.X.; Zhang, X.Z.
Deposited on	:	2024-03-06
Resolution	:	3.90 Å(reported)

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

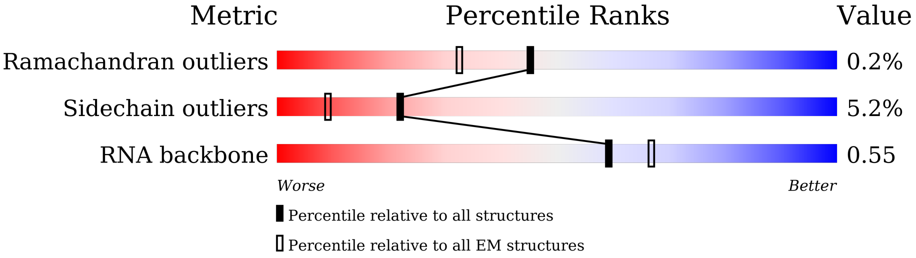
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

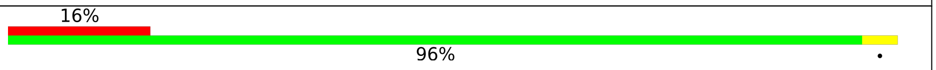
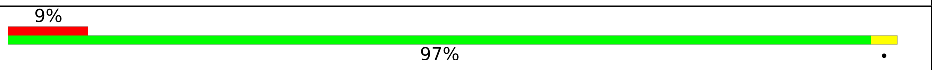
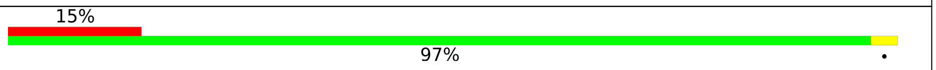
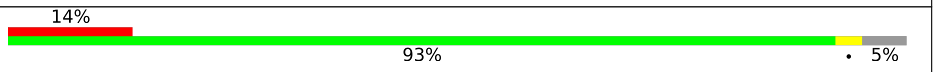
The reported resolution of this entry is 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	1799	
2	A	3394	
3	B	121	
4	C	158	
5	D	251	
6	F	361	
7	G	294	
8	H	175	

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Mol	Chain	Length	Quality of chain
9	I	223	9% 97% •
10	J	233	14% 97% •
11	K	191	12% 96% • •
12	L	218	22% 94% 6%
13	M	169	21% 94% 6%
14	N	193	11% 97% •
15	O	136	10% 98% •
16	P	203	16% 93% 7%
17	Q	197	11% 94% 6%
18	R	183	10% 96% •
19	S	185	13% 97% •
20	T	188	19% 97% •
21	U	171	8% 96% • •
22	V	159	12% 95% • •
23	W	100	20% 96% •
24	X	136	19% 97% •
25	Y	126	37% 97% •
26	Z	121	13% 96% •
27	a	125	8% 97% •
28	b	135	8% 98% •
29	c	148	10% 97% •
30	d	58	21% 93% 7%
31	e	96	15% 97% •
32	f	109	22% 97% •
33	g	127	17% 96% •

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Mol	Chain	Length	Quality of chain
34	h	106	9% 95% 5%
35	i	112	20% 93% 7%
36	j	119	12% 97% •
37	k	99	10% 96% •
38	l	81	10% 90% 10%
39	m	77	17% 94% 6%
40	n	50	24% 90% 10%
41	o	52	19% 90% 10%
42	p	25	20% 96% •
43	q	103	20% 93% 7%
44	r	91	18% 95% 5%
45	t	75	67% 77% 23%
45	u	75	23% 76% 23% •
46	v	1044	93% 92% • 6%
47	x	842	61% 95% 5%
48	SA	222	62% 95% 5%
49	SC	92	62% 89% 11%
50	SD	121	83% 98% •
51	SE	117	72% 91% 9%
52	SF	141	56% 95% • •
53	SH	145	52% 94% 6%
54	SI	143	59% 95% 5%
55	SJ	100	52% 98% •
56	SK	108	38% 52% 7% 41%
57	SM	53	36% 89% 11%

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Mol	Chain	Length	Quality of chain
58	SN	73	86% 96% •
59	SO	312	69% 96% •
60	SQ	232	63% 91% 6% •
61	SS	258	63% 95% 5%
62	ST	228	57% 94% 6%
63	SR	216	30% 96% •
64	SV	200	38% 88% 6% 6%
65	SW	184	38% 92% 5% •
66	SX	142	47% 90% 10%
67	SY	150	45% 95% 5%
68	SZ	127	61% 96% •
69	Sa	87	54% 93% 7%
70	Sb	129	39% 96% • •
71	Sc	144	55% 95% 5%
72	Sd	134	53% 95% 5%
73	Se	94	40% 98% •
74	Sf	81	52% 98% •
75	Sg	60	58% 93% 7%
76	SG	121	50% 93% 7%
77	SP	206	36% 95% 5%
78	SU	184	46% 93% 7%
79	SL	63	76% 89% 11%
80	SB	206	70% 94% 6%
81	E	386	15% 95% 5%

2 Entry composition ⓘ

There are 81 unique types of molecules in this entry. The entry contains 216620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3192	Total	C	N	O	P	0	0
			68278	30498	12313	22275	3192		

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	294	2351	1484	410	455	2	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein eL6B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	167	1307	843	234	230	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	222	1784	1151	324	308	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	22	ILE	THR	conflict	UNP P05737

- Molecule 10 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	233	1804	1151	323	327	3	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	191	1508	957	274	273	4	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	218	1764	1117	334	306	7	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein uL5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	169	1346	843	252	247	4	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein eL13A.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL14A.

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	203	1720	1077	361	281	1	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein uL13A.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	R	183	1416	879	284	253	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein eL18A.

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

- Molecule 20 is a protein called Large ribosomal subunit protein eL19A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	T	188	1515	932	323	260	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	171	1437	925	266	243	3	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein eL21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	159	1272	802	245	221	4	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein eL22A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	W	100	796	516	131	149	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL14A.

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

- Molecule 25 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	126	836	525	165	145	1	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	121	964	620	169	173	2	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein uL24A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 28 is a protein called Large ribosomal subunit protein eL27A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	d	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 32 is a protein called Large ribosomal subunit protein eL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 34 is a protein called Large ribosomal subunit protein eL33A.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL34A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	i	112	880	545	179	152	4	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	j	119	969	615	186	167	1	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein eL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	k	99	766	478	154	132	2	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein eL37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	l	81	645	393	141	106	5	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL40A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	o	52	410	254	86	65	5	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein eL41A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	p	25	229	139	62	27	1	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein eL42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	q	103	824	517	167	135	5	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein eL43A.

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

- Molecule 45 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
45	t	75	1605	716	297	517	75	0	0
			Total	C	N	O	P		
45	u	74	1584	706	292	512	74	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	10	A	G	conflict	GB 176433
u	10	A	G	conflict	GB 176433

- Molecule 46 is a protein called Elongation factor 3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	v	977	7476	4726	1295	1418	37	0	0

- Molecule 47 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	x	842	6559	4166	1124	1238	31	0	0

- Molecule 48 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	SA	222	1729	1098	312	313	6	0	0

- Molecule 49 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SC	92	752	487	122	141	2	0	0

- Molecule 50 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SD	121	875	551	153	169	2	0	0

- Molecule 51 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SE	117	916	583	171	155	7	0	0

- Molecule 52 is a protein called Small ribosomal subunit protein uS9A.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SH	145	1188	741	237	208	2	0	0

- Molecule 54 is a protein called Small ribosomal subunit protein eS19A.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SJ	100	Total 797	C 506	N 144	O 146	S 1	0	0

- Molecule 56 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	SK	64	Total 519	C 332	N 95	O 92	0	0

- Molecule 57 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SM	53	Total 442	C 274	N 92	O 72	S 4	0	0

- Molecule 58 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SN	73	Total 560	C 355	N 106	O 95	S 4	0	0

- Molecule 59 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SO	312	Total 2383	C 1514	N 409	O 452	S 8	0	0

- Molecule 60 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SQ	225	Total 1794	C 1137	N 329	O 324	S 4	0	0

- Molecule 61 is a protein called Small ribosomal subunit protein eS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	258	Total 2056	C 1308	N 387	O 358	S 3	0	0

- Molecule 62 is a protein called Small ribosomal subunit protein eS6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	ST	228	Total 1815	C 1138	N 351	O 323	S 3	0	0

- Molecule 63 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SR	216	Total 1626	C 1042	N 287	O 295	S 2	0	0

- Molecule 64 is a protein called Small ribosomal subunit protein eS8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SV	187	Total 1476	C 916	N 295	O 263	S 2	0	0

- Molecule 65 is a protein called Small ribosomal subunit protein uS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SW	178	Total 1441	C 913	N 278	O 249	S 1	0	0

- Molecule 66 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SX	142	Total 1142	C 733	N 217	O 189	S 3	0	0

- Molecule 67 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS11B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	SZ	127	891	545	182	163	1	0	0

- Molecule 69 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Sa	87	673	415	125	131	2	0	0

- Molecule 70 is a protein called Small ribosomal subunit protein uS8A.

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

- Molecule 71 is a protein called Small ribosomal subunit protein uS12A.

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

- Molecule 72 is a protein called Small ribosomal subunit protein eS24A.

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

- Molecule 73 is a protein called Small ribosomal subunit protein eS26A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Se	94	750	462	157	126	5	0	0

- Molecule 74 is a protein called Small ribosomal subunit protein eS27A.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sg	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 76 is a protein called Small ribosomal subunit protein eS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SG	121	Total	C	N	O	S	0	0
			961	599	182	178	2		

- Molecule 77 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SP	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 78 is a protein called Small ribosomal subunit protein eS7A.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	SU	184	Total	C	N	O	0	0
			1473	946	263	264		

- Molecule 79 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SL	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 80 is a protein called Small ribosomal subunit protein uS7.

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

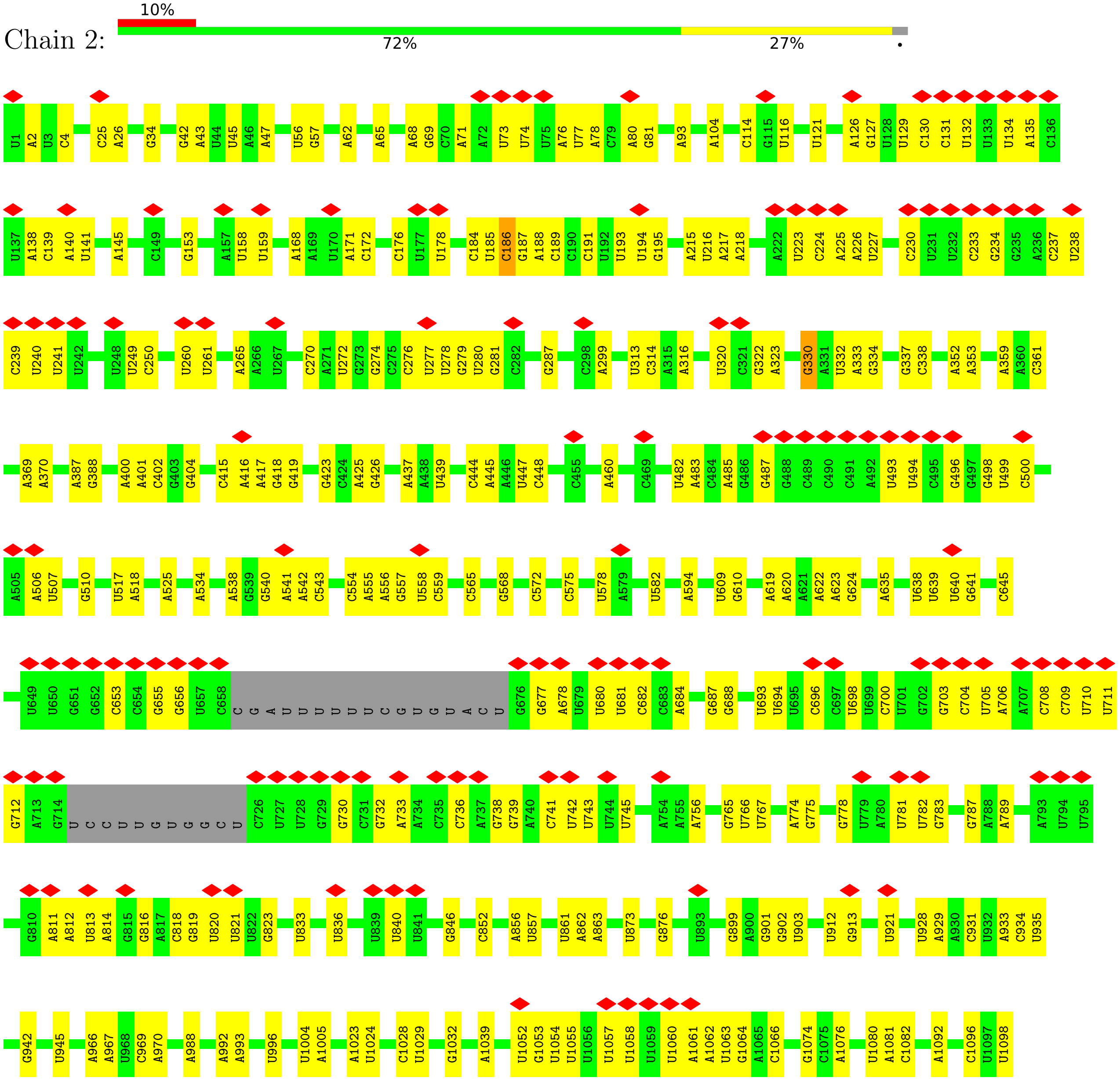
- Molecule 81 is a protein called Large ribosomal subunit protein uL3.

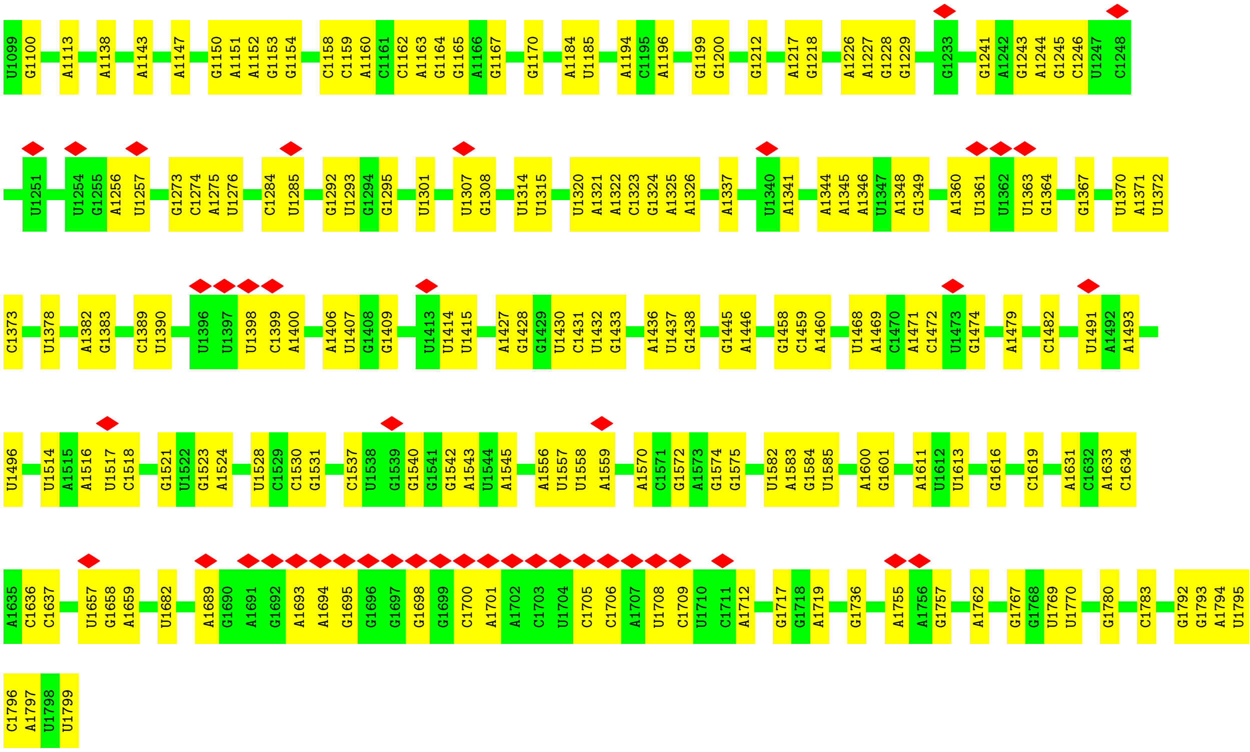
Mol	Chain	Residues	Atoms					AltConf	Trace
81	E	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

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.

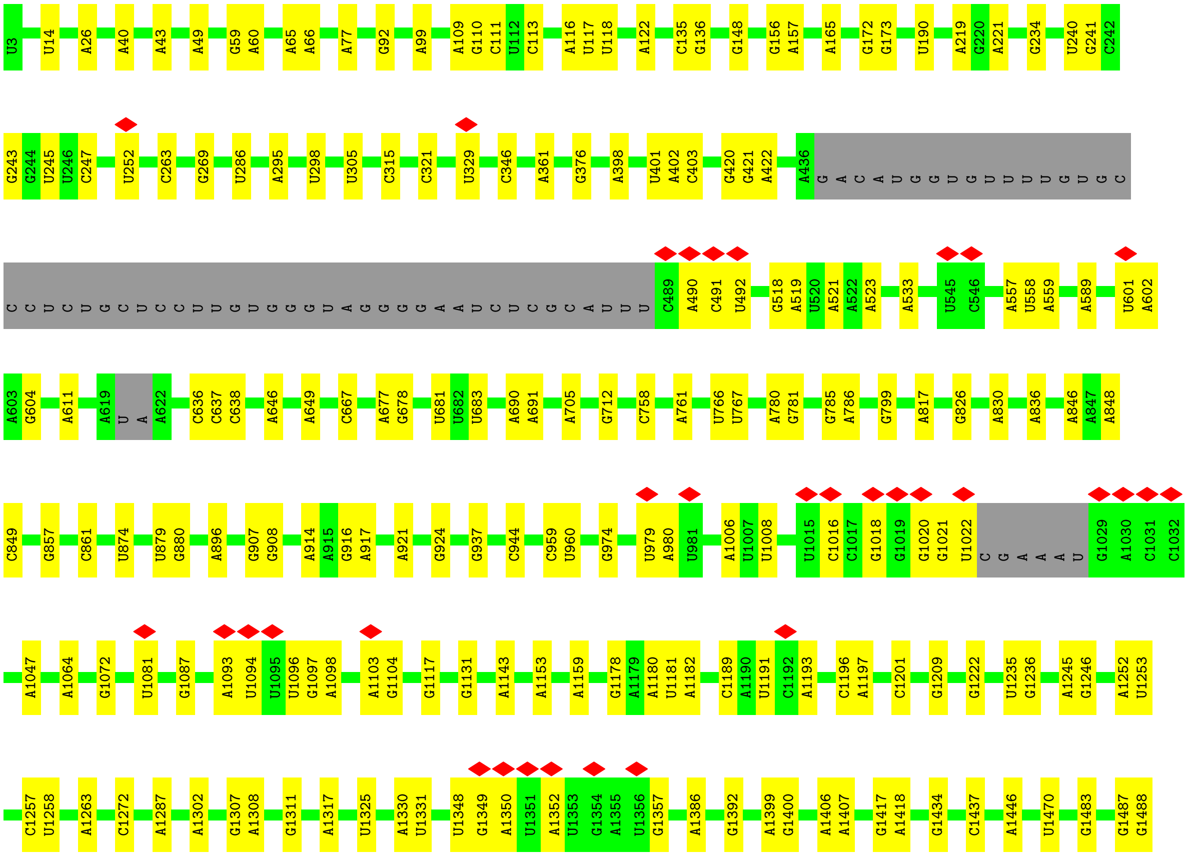
- Molecule 1: 18S rRNA

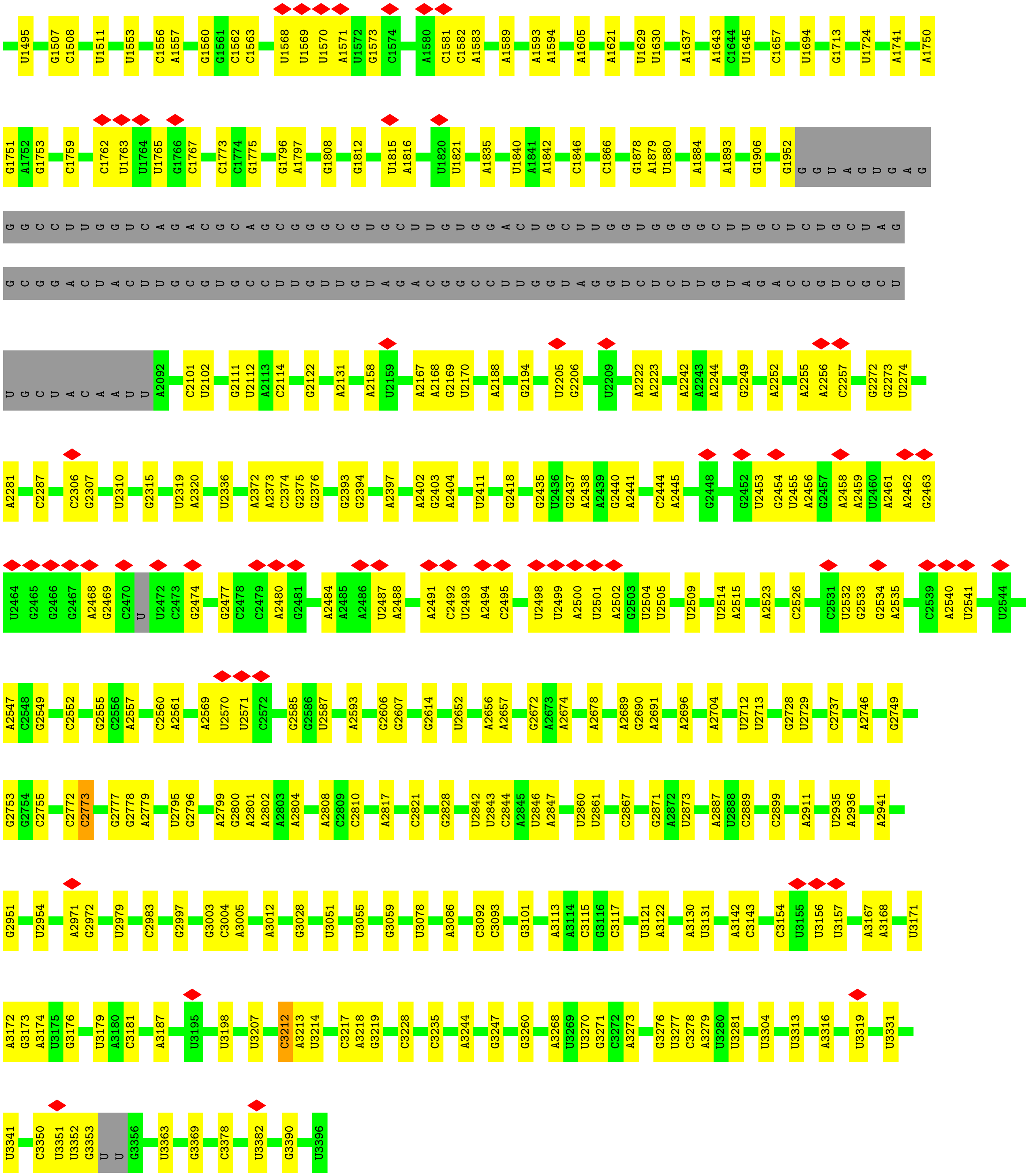




- Molecule 2: 25S rRNA

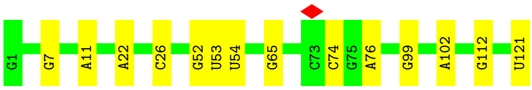
Chain A:





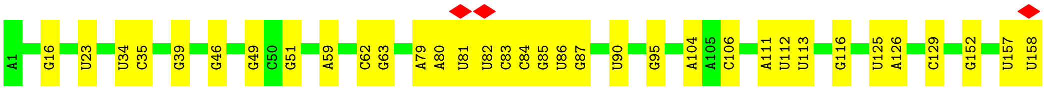
- Molecule 3: 5S rRNA

Chain B:

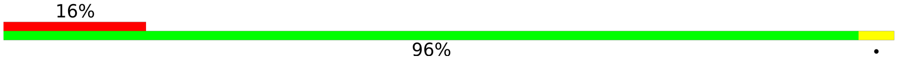
- Molecule 4: 5.8S rRNA

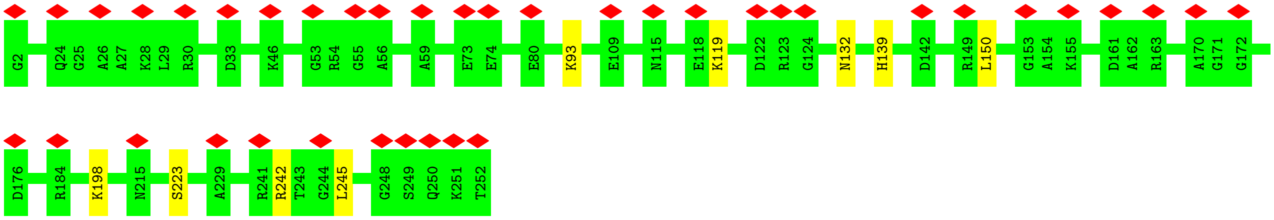
Chain C:



- Molecule 5: Large ribosomal subunit protein uL2A

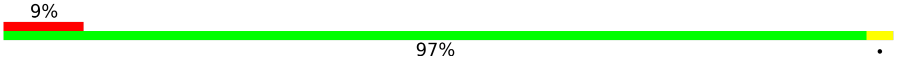
Chain D:

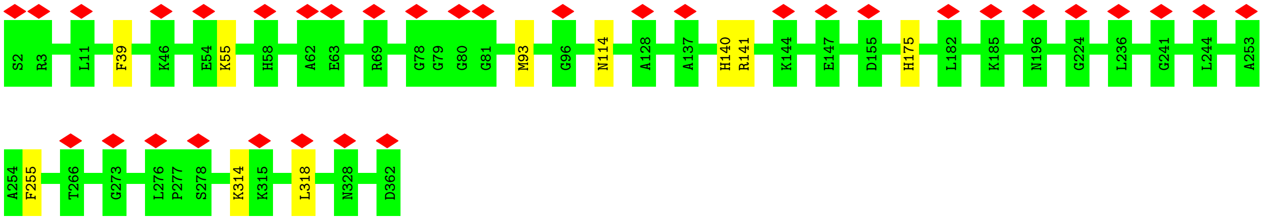




- Molecule 6: Large ribosomal subunit protein uL4A

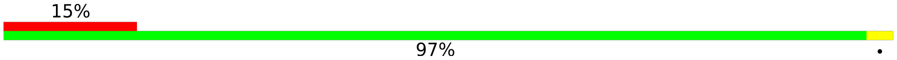
Chain F:

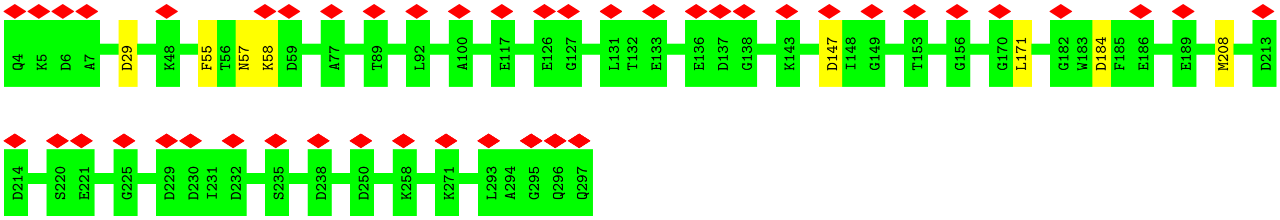




- Molecule 7: Large ribosomal subunit protein uL18

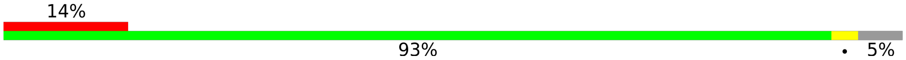
Chain G:

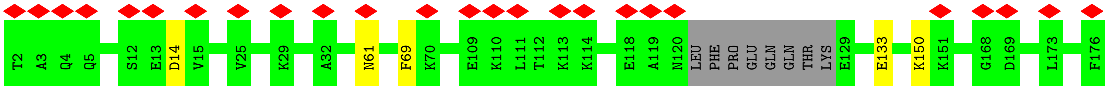




- Molecule 8: Large ribosomal subunit protein eL6B

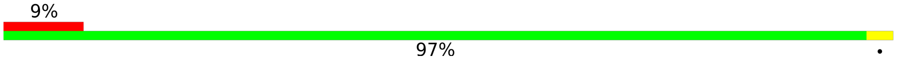
Chain H:

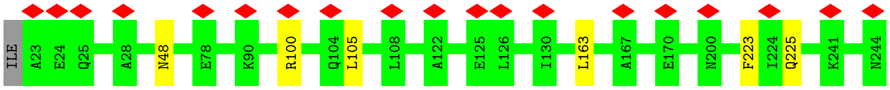




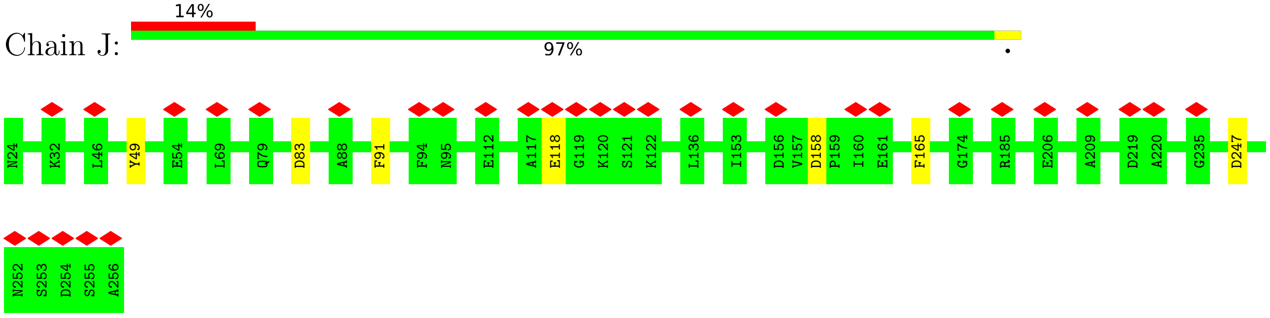
- Molecule 9: Large ribosomal subunit protein uL30A

Chain I:

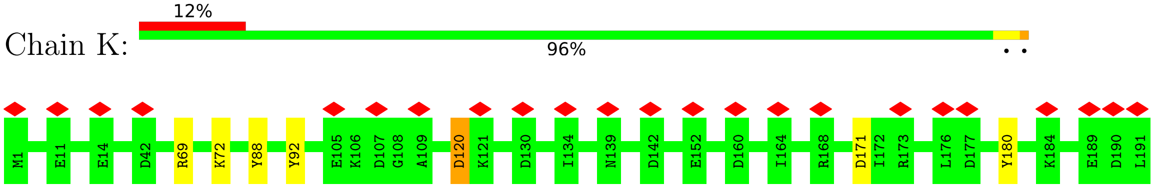




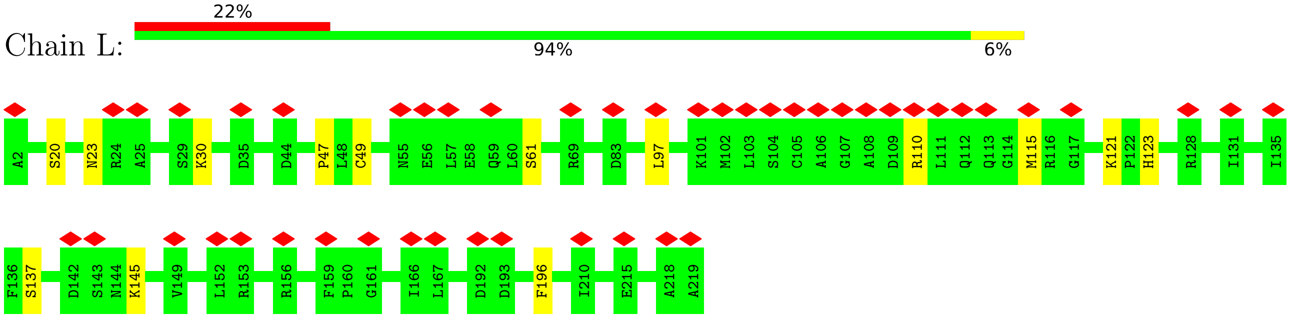
- Molecule 10: Large ribosomal subunit protein eL8A



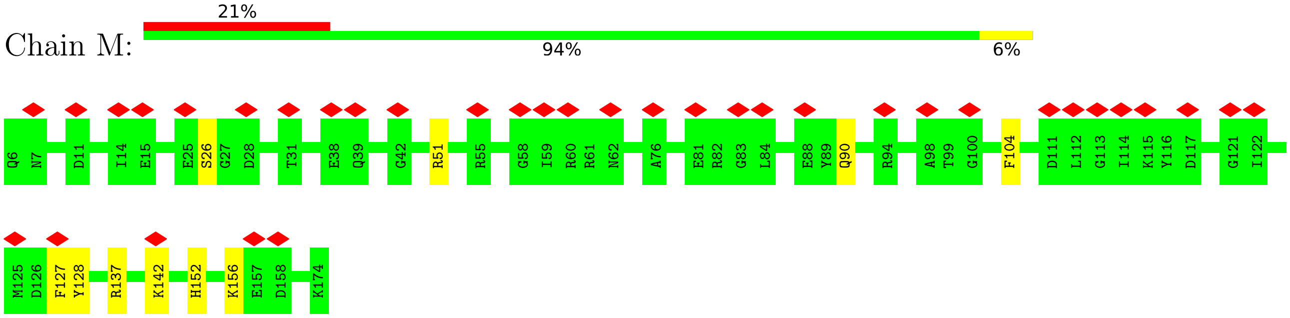
- Molecule 11: Large ribosomal subunit protein uL6A



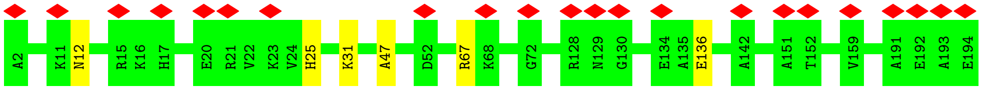
- Molecule 12: Large ribosomal subunit protein uL16



- Molecule 13: Large ribosomal subunit protein uL5B

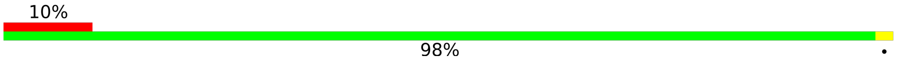


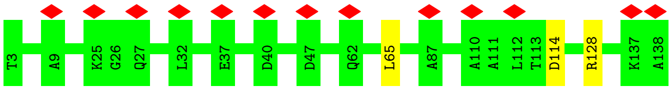
- Molecule 14: Large ribosomal subunit protein eL13A



- Molecule 15: Large ribosomal subunit protein eL14A

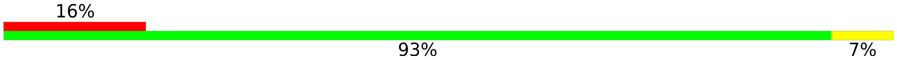
Chain O:

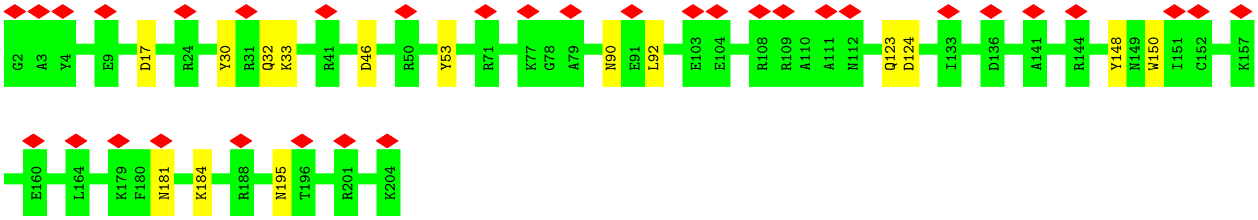




- Molecule 16: Large ribosomal subunit protein eL15A

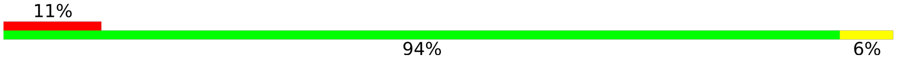
Chain P:

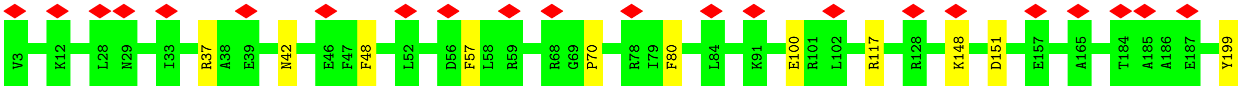




- Molecule 17: Large ribosomal subunit protein uL13A

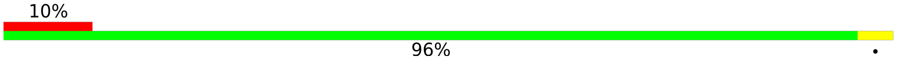
Chain Q:

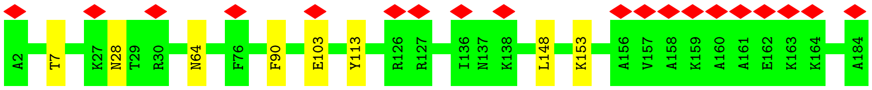




- Molecule 18: Large ribosomal subunit protein uL22A

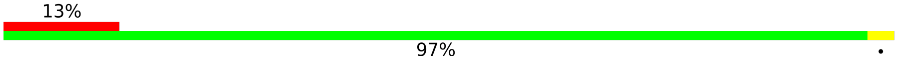
Chain R:

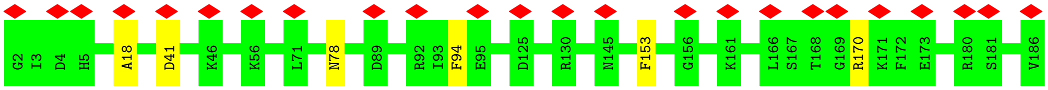




- Molecule 19: Large ribosomal subunit protein eL18A

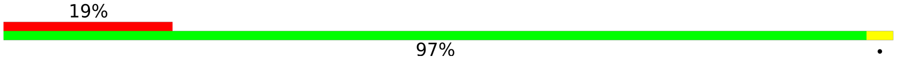
Chain S:

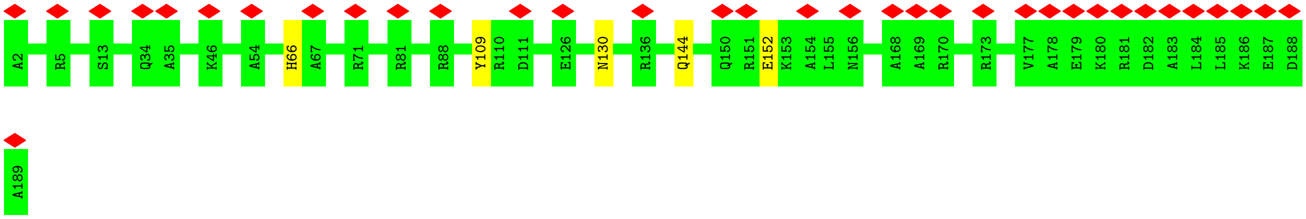




- Molecule 20: Large ribosomal subunit protein eL19A

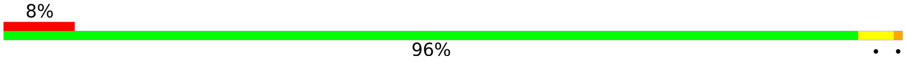
Chain T:

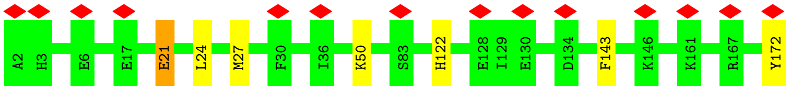




- Molecule 21: Large ribosomal subunit protein eL20A

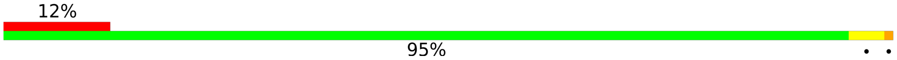
Chain U:

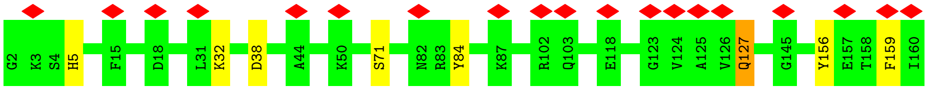




- Molecule 22: Large ribosomal subunit protein eL21A

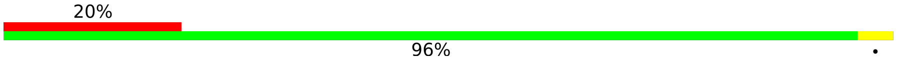
Chain V:

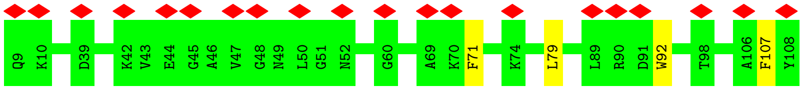




- Molecule 23: Large ribosomal subunit protein eL22A

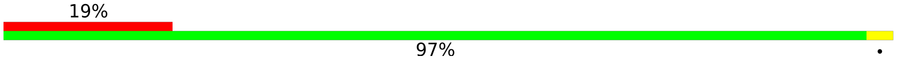
Chain W:

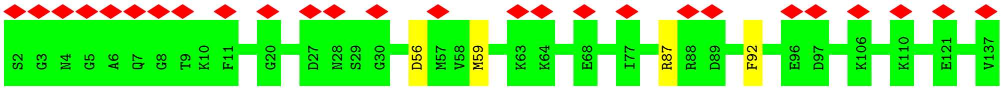




- Molecule 24: Large ribosomal subunit protein uL14A

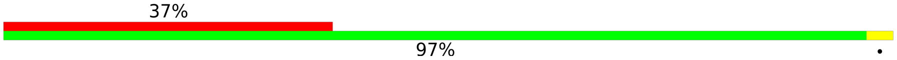
Chain X:



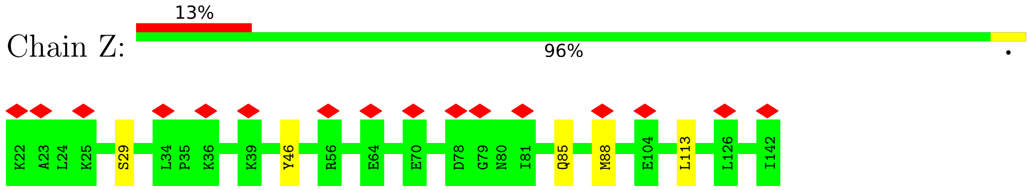


- Molecule 25: Large ribosomal subunit protein eL24A

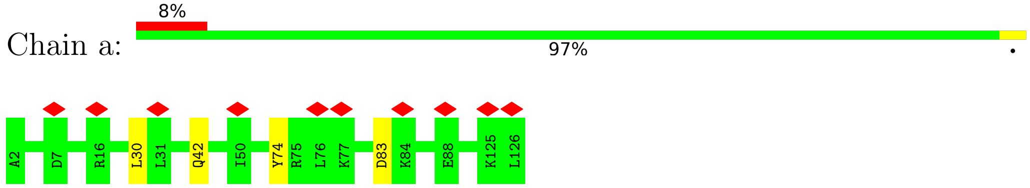
Chain Y:



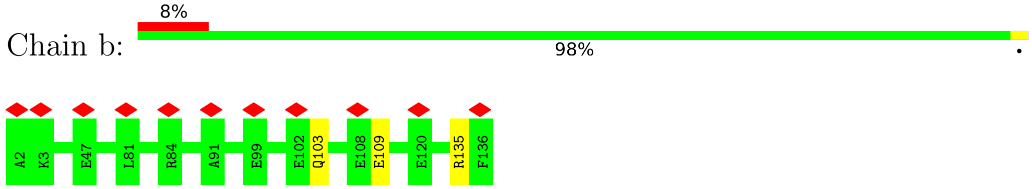
- Molecule 26: Large ribosomal subunit protein uL23



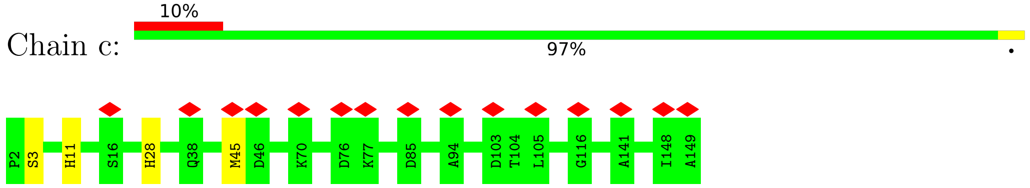
- Molecule 27: Large ribosomal subunit protein uL24A



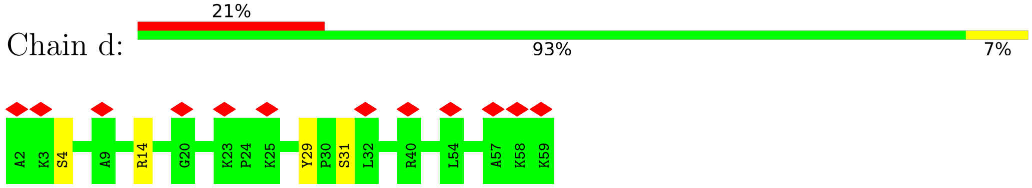
- Molecule 28: Large ribosomal subunit protein eL27A



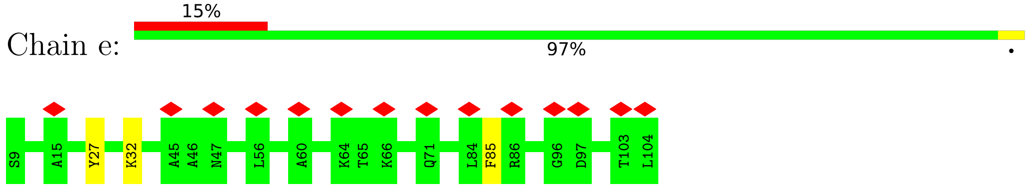
- Molecule 29: Large ribosomal subunit protein uL15



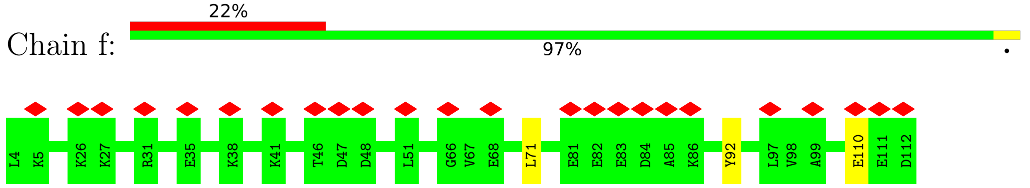
- Molecule 30: Large ribosomal subunit protein eL29



- Molecule 31: Large ribosomal subunit protein eL30

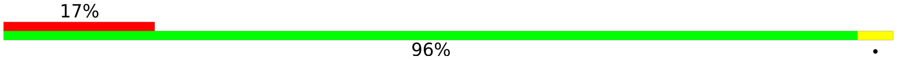


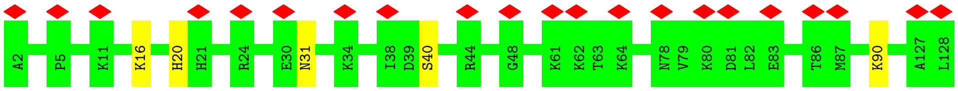
- Molecule 32: Large ribosomal subunit protein eL31A



- Molecule 33: Large ribosomal subunit protein eL32

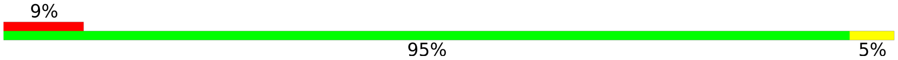
Chain g:

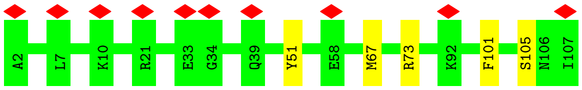




- Molecule 34: Large ribosomal subunit protein eL33A

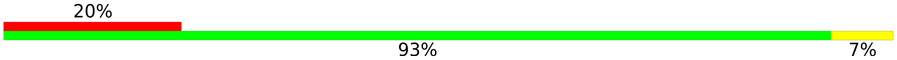
Chain h:

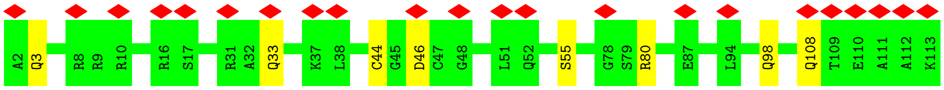




- Molecule 35: Large ribosomal subunit protein eL34A

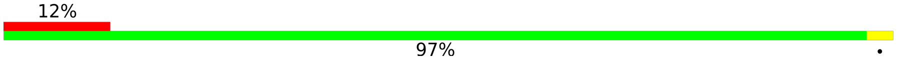
Chain i:

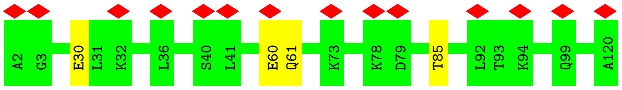




- Molecule 36: Large ribosomal subunit protein uL29A

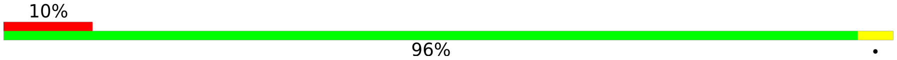
Chain j:

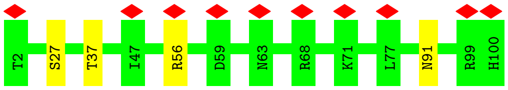




- Molecule 37: Large ribosomal subunit protein eL36A

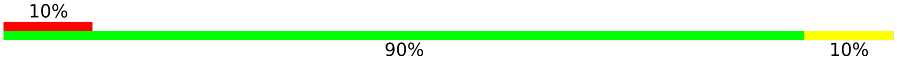
Chain k:

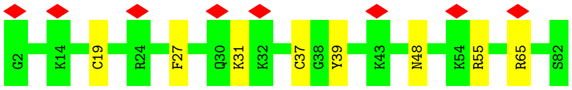




- Molecule 38: Large ribosomal subunit protein eL37A

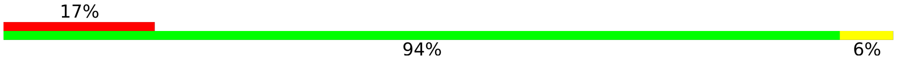
Chain l:

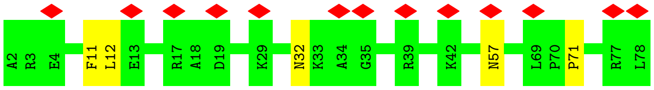




- Molecule 39: Large ribosomal subunit protein eL38

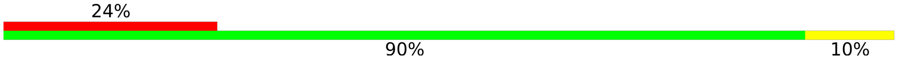
Chain m:

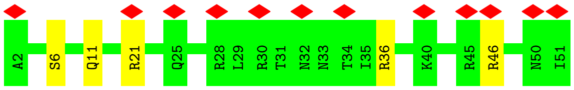




- Molecule 40: Large ribosomal subunit protein eL39

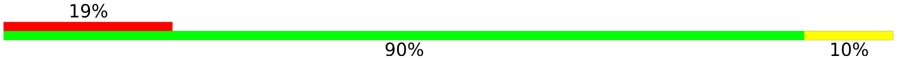
Chain n:

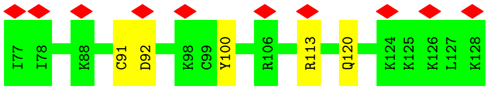




- Molecule 41: Large ribosomal subunit protein eL40A

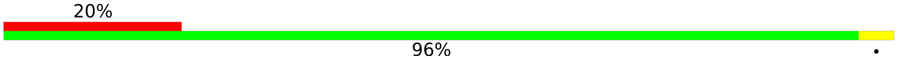
Chain o:

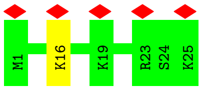




- Molecule 42: Large ribosomal subunit protein eL41A

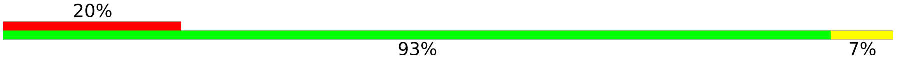
Chain p:

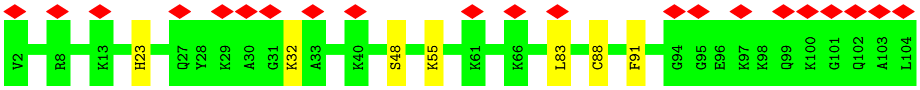




- Molecule 43: Large ribosomal subunit protein eL42A

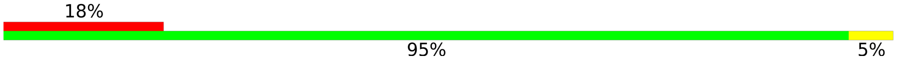
Chain q:

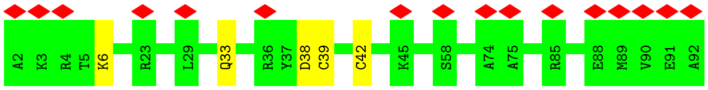




- Molecule 44: Large ribosomal subunit protein eL43A

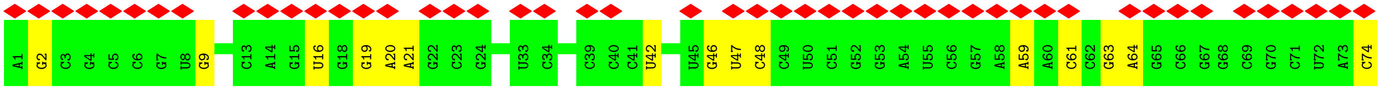
Chain r:





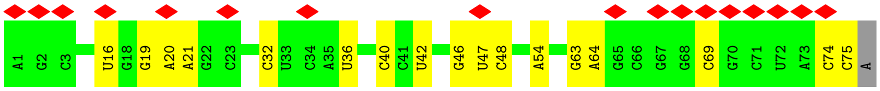
- Molecule 45: tRNA

Chain t:



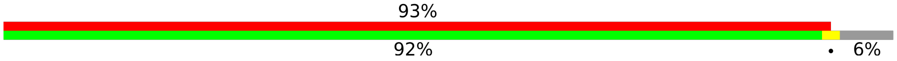
- Molecule 45: tRNA

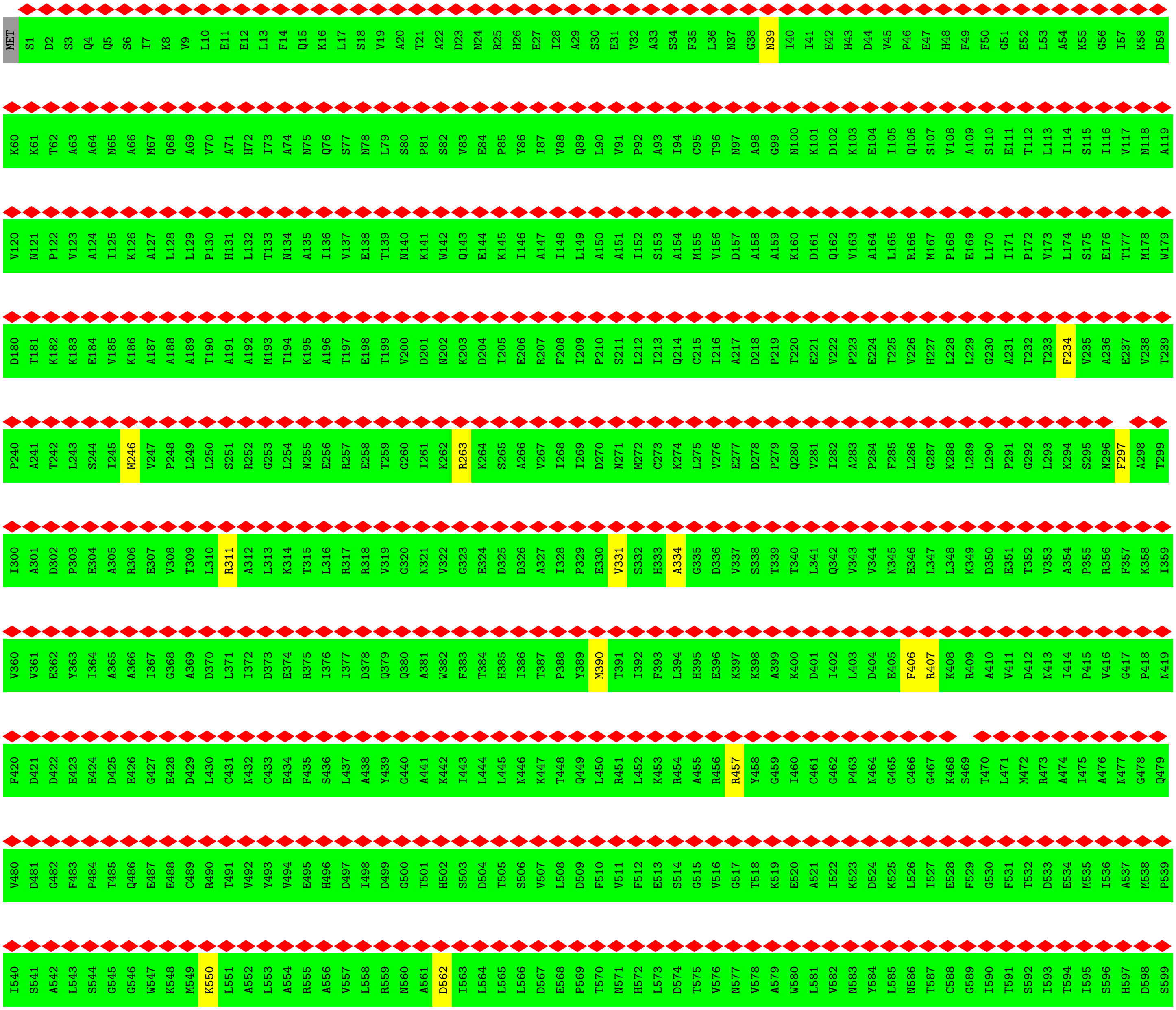
Chain u:

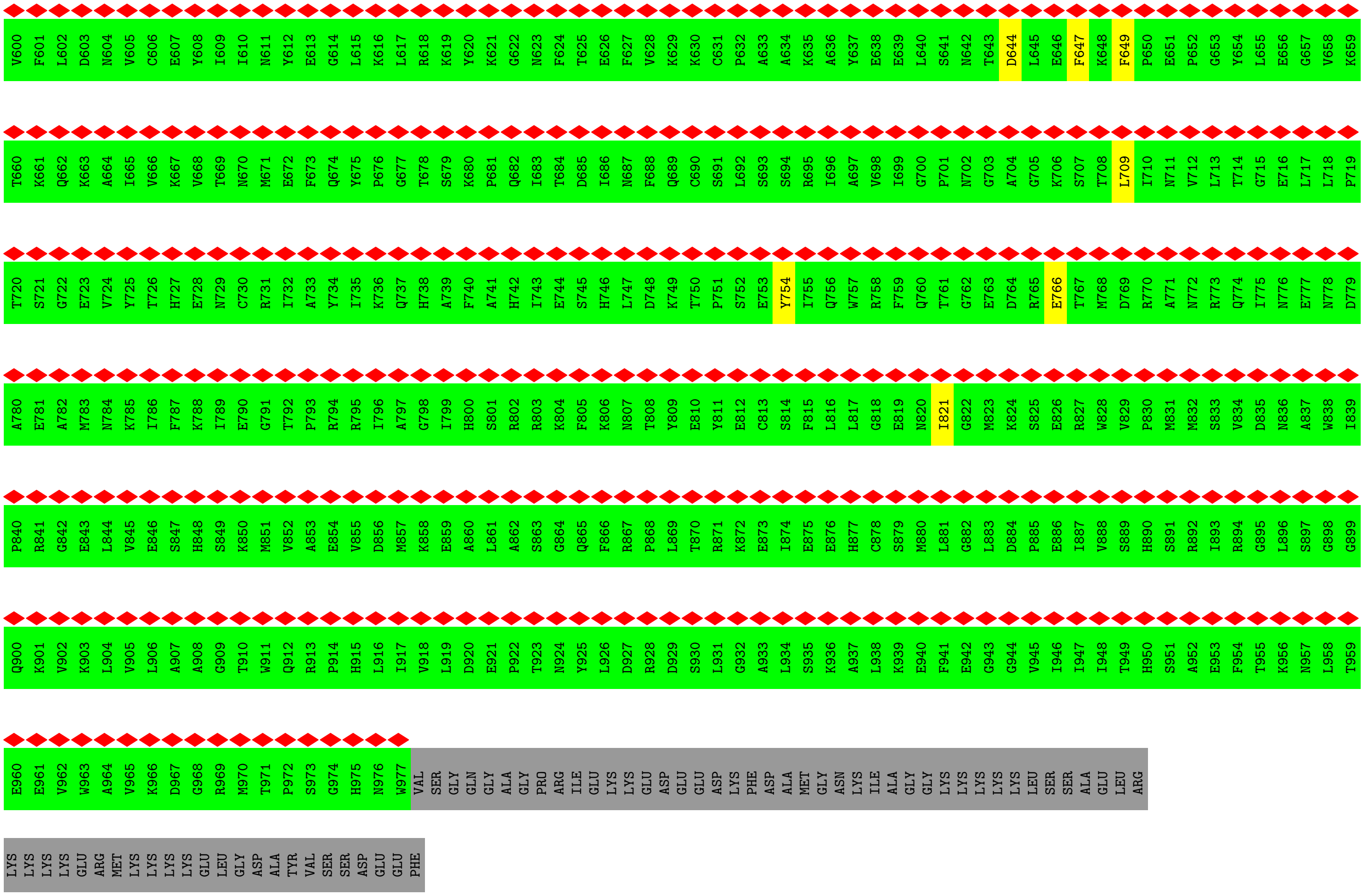


- Molecule 46: Elongation factor 3A

Chain v:

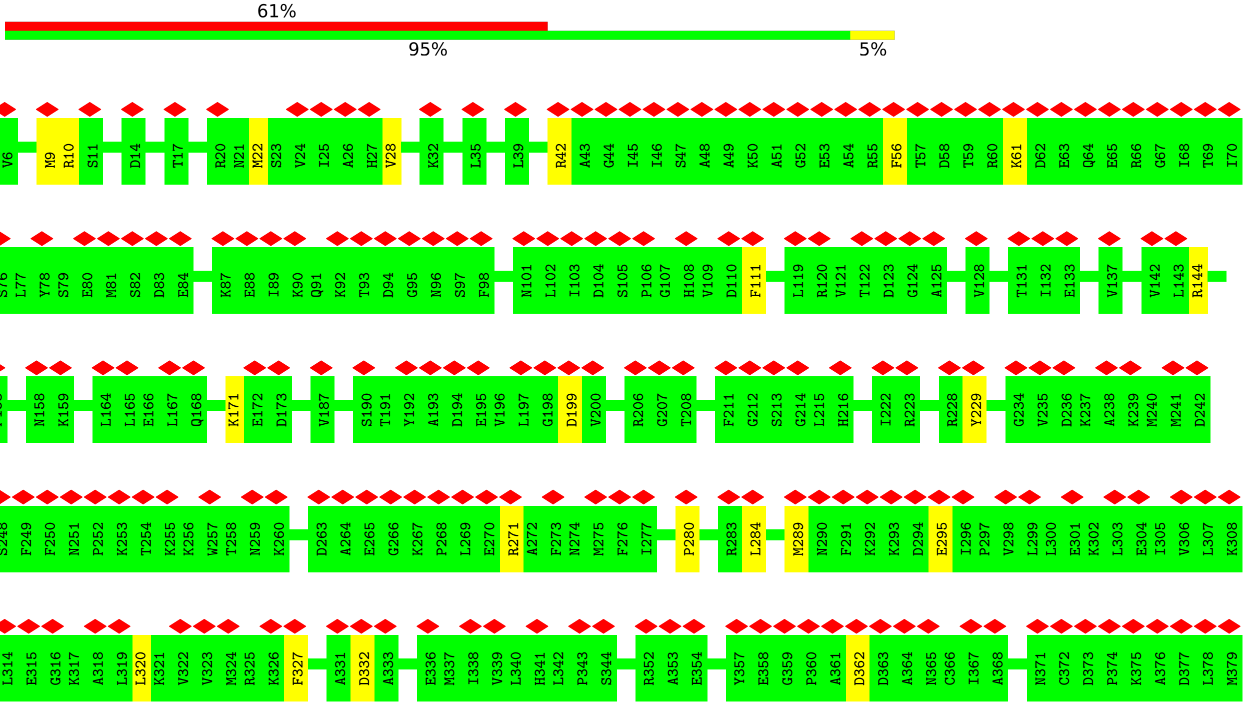


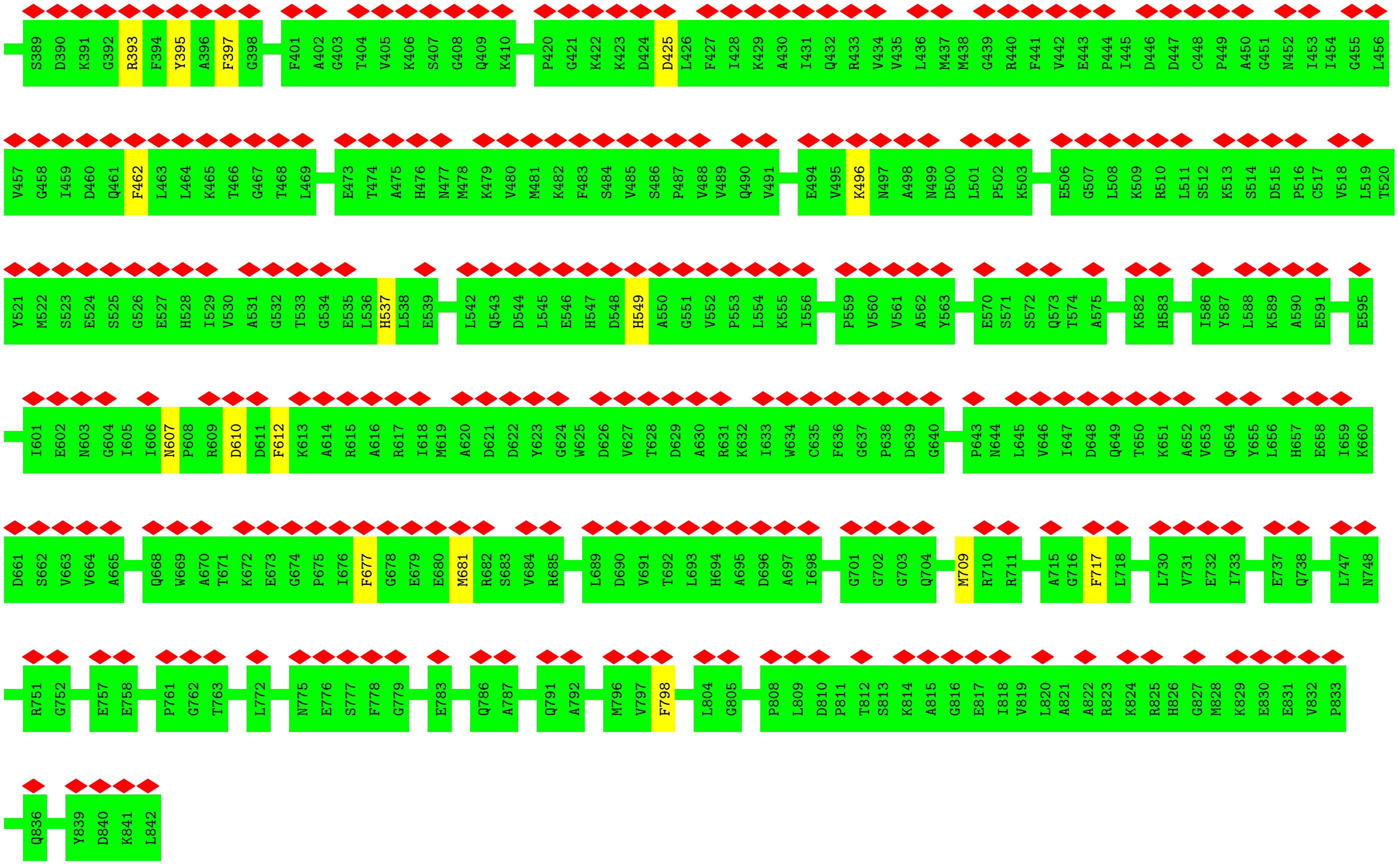




- Molecule 47: Elongation factor 2

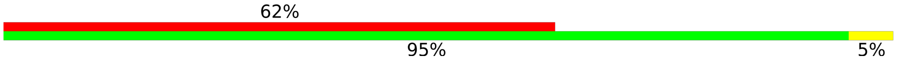
Chain x:

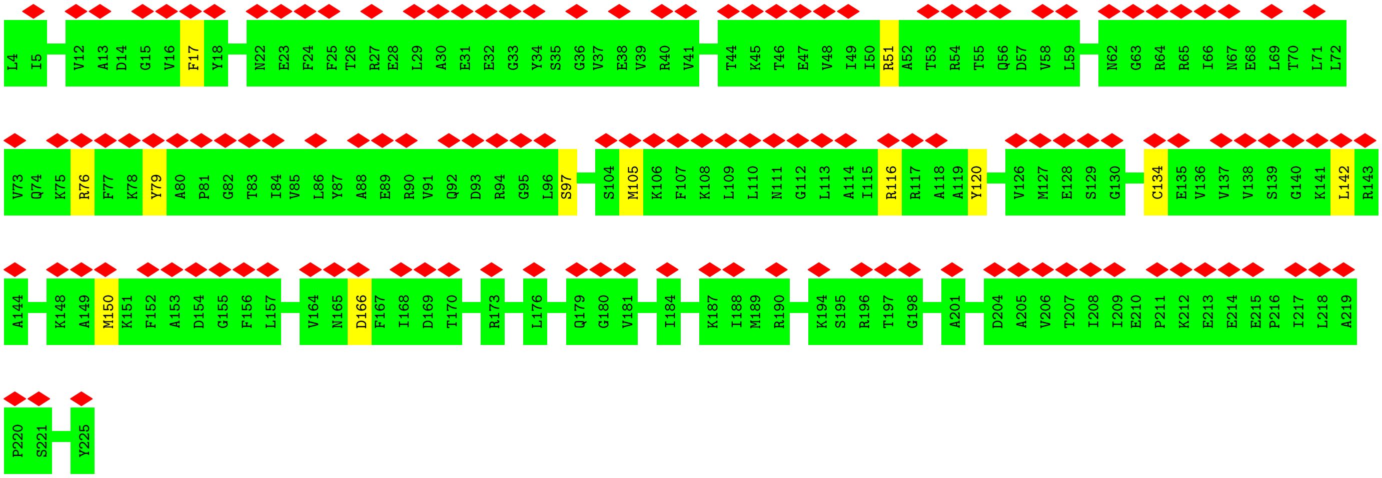




- Molecule 48: Small ribosomal subunit protein uS3

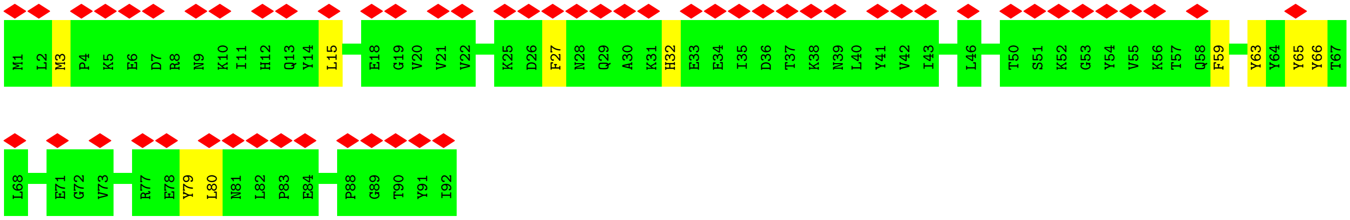
Chain SA:





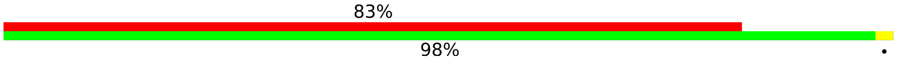
- Molecule 49: Small ribosomal subunit protein eS10A

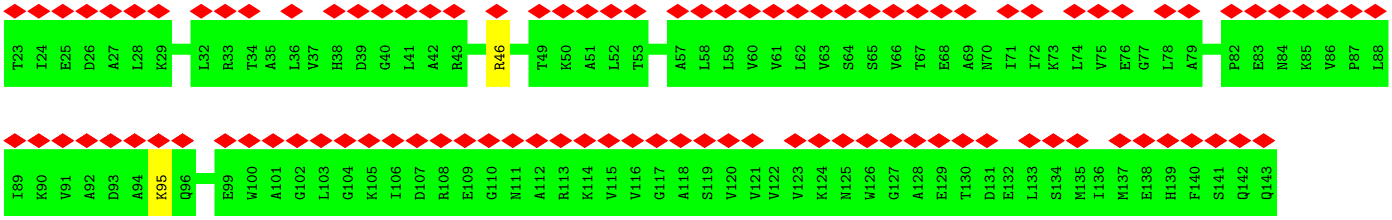
Chain SC:



- Molecule 50: Small ribosomal subunit protein eS12

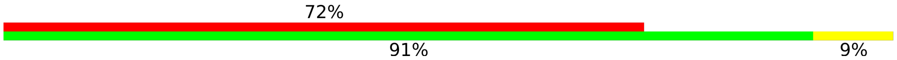
Chain SD:

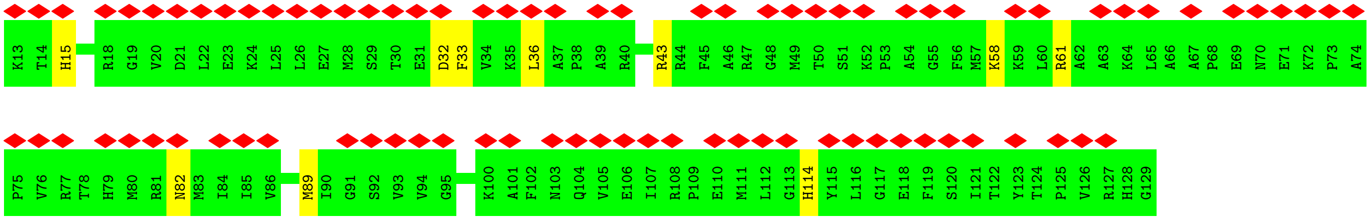




- Molecule 51: Small ribosomal subunit protein uS19

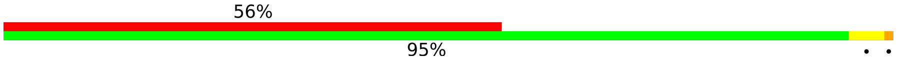
Chain SE:

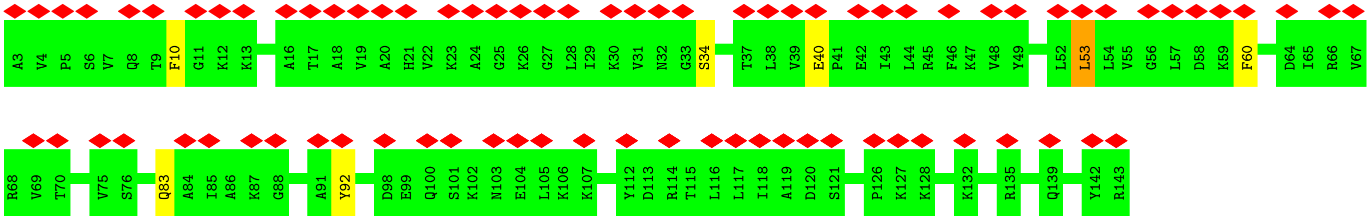




- Molecule 52: Small ribosomal subunit protein uS9A

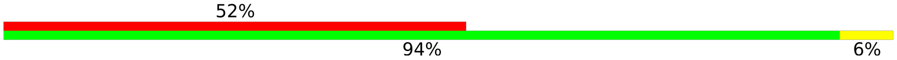
Chain SF:

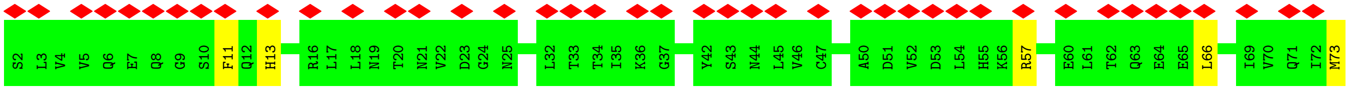


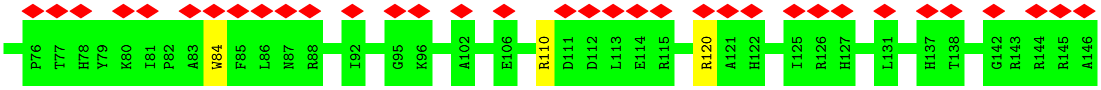


- Molecule 53: Small ribosomal subunit protein uS13A

Chain SH:

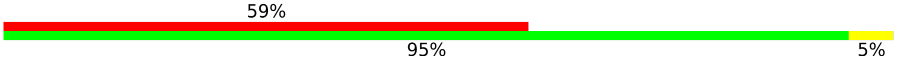


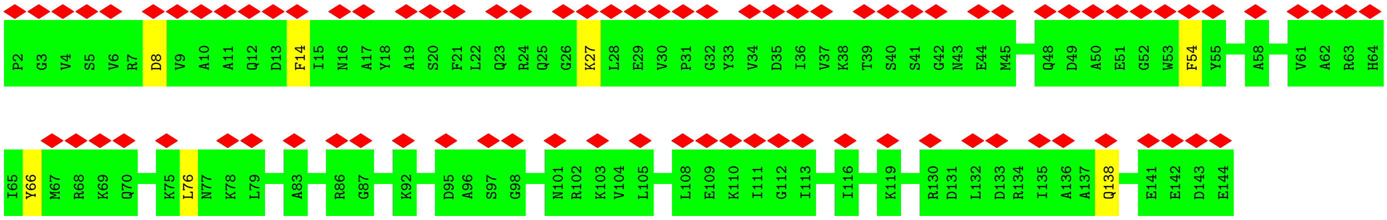




- Molecule 54: Small ribosomal subunit protein eS19A

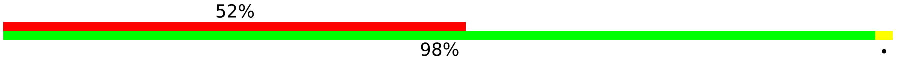
Chain SI:

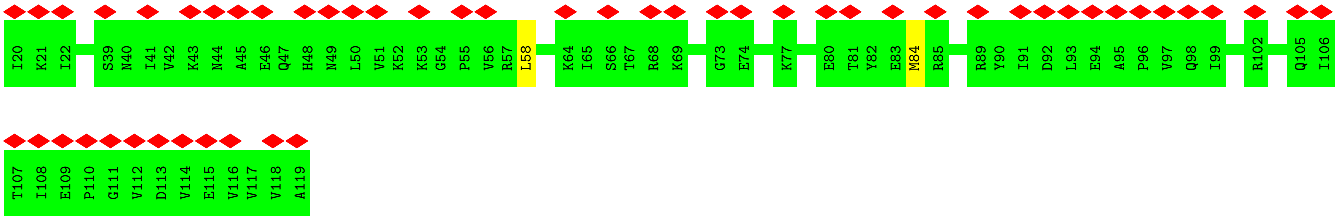




- Molecule 55: Small ribosomal subunit protein uS10

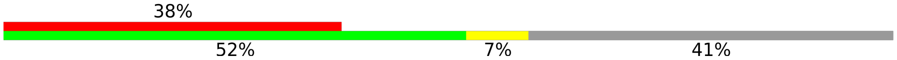
Chain SJ:

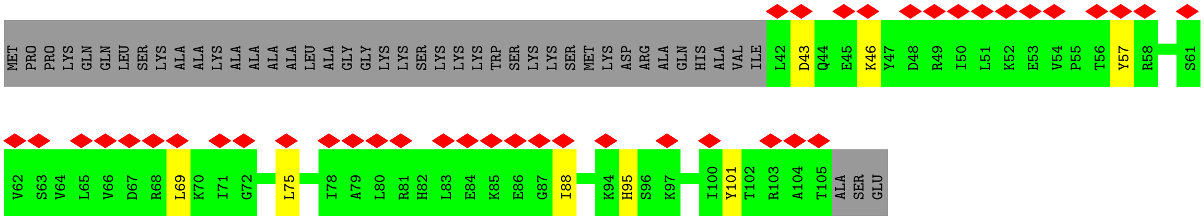




- Molecule 56: Small ribosomal subunit protein eS25A

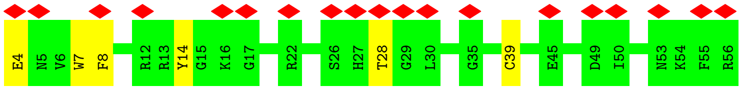
Chain SK:





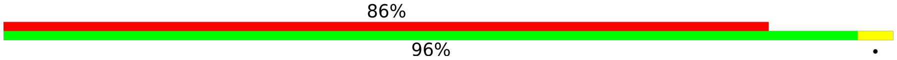
- Molecule 57: Small ribosomal subunit protein uS14A

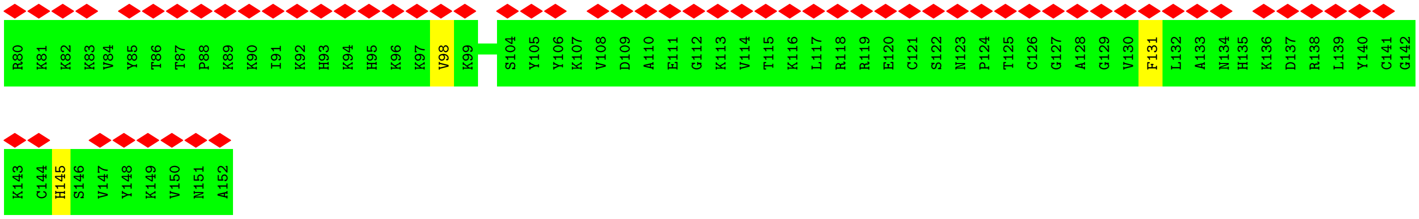
Chain SM:



- Molecule 58: Small ribosomal subunit protein eS31

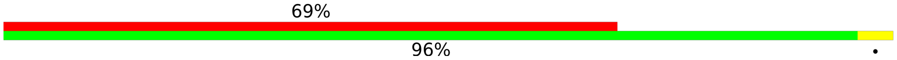
Chain SN:

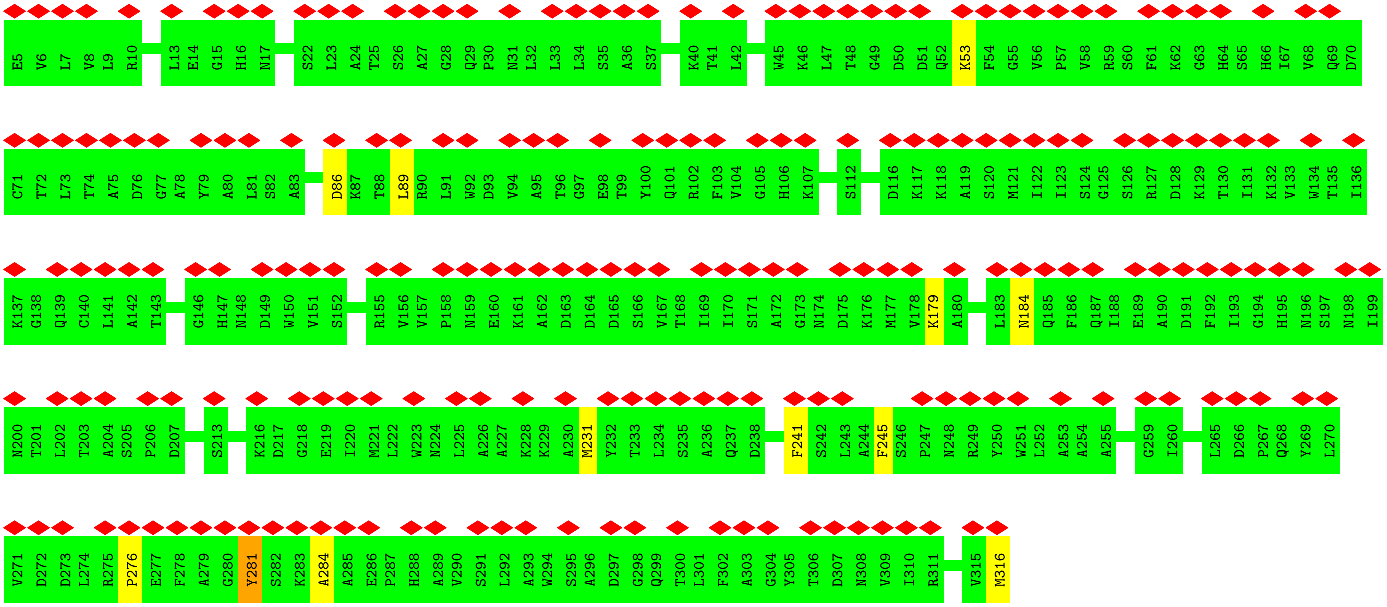




- Molecule 59: Small ribosomal subunit protein RACK1

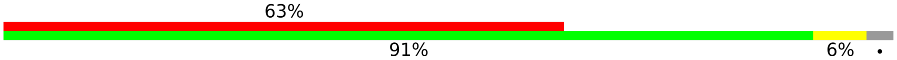
Chain SO:

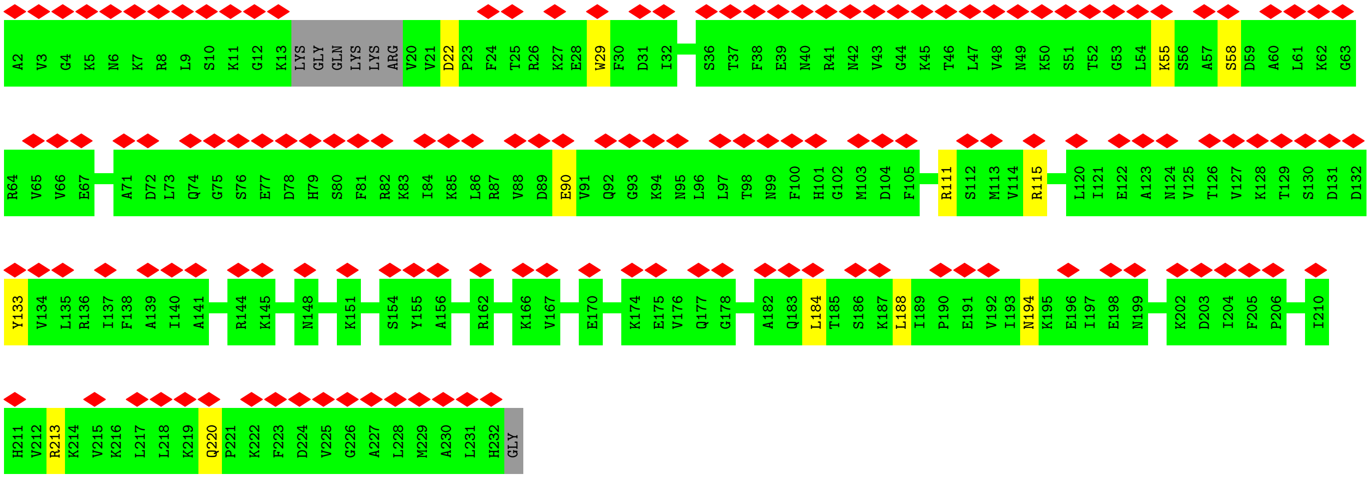




- Molecule 60: Small ribosomal subunit protein eS1A

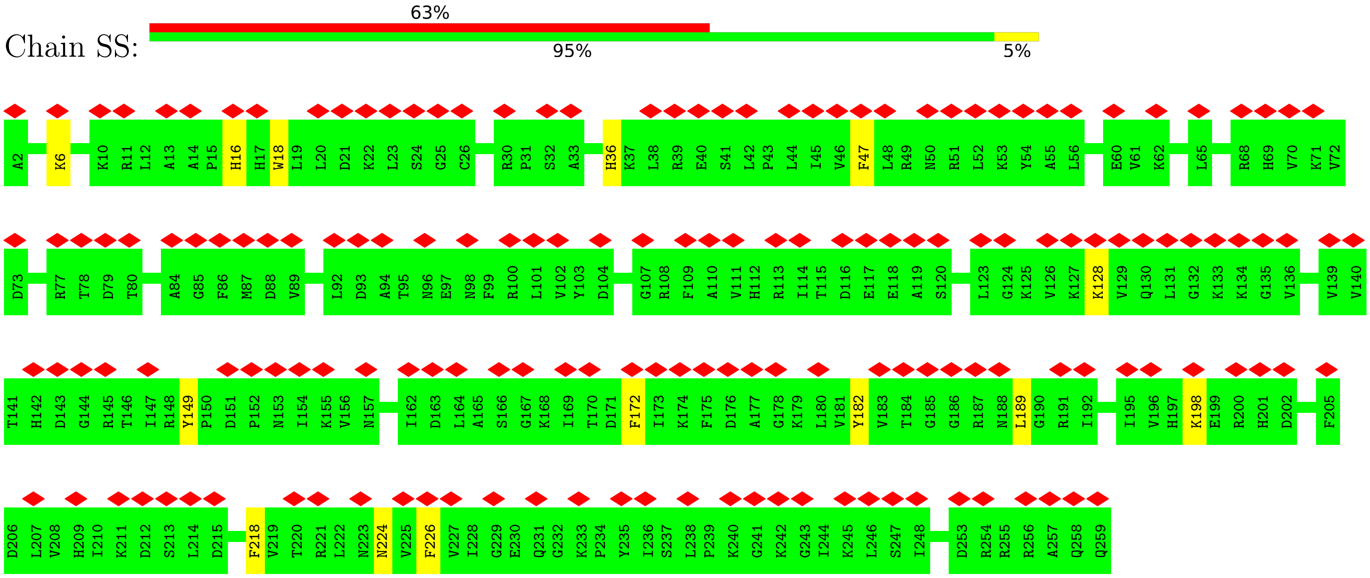
Chain SQ:





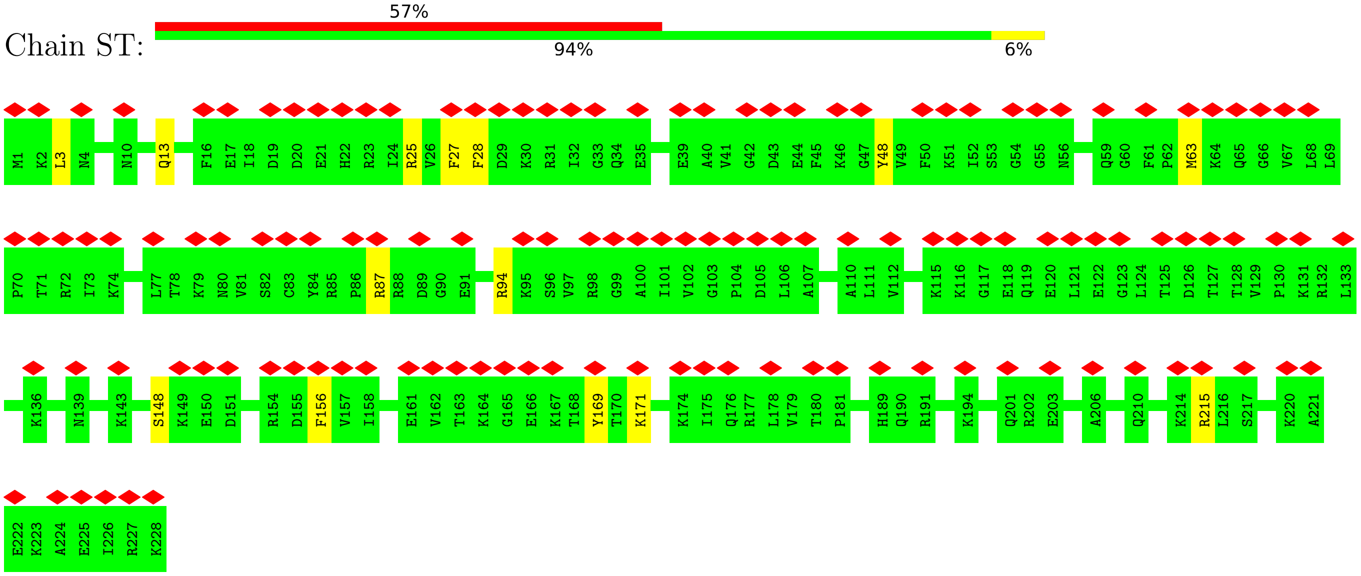
- Molecule 61: Small ribosomal subunit protein eS4A

Chain SS:



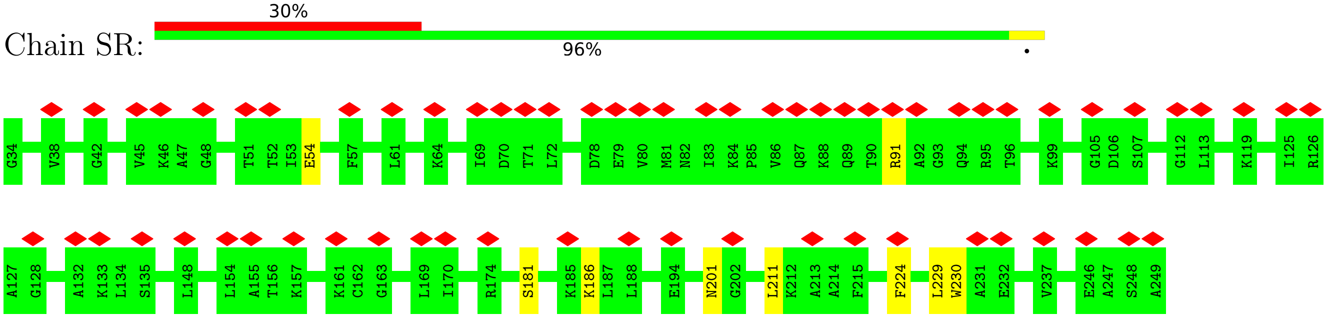
- Molecule 62: Small ribosomal subunit protein eS6A

Chain ST:



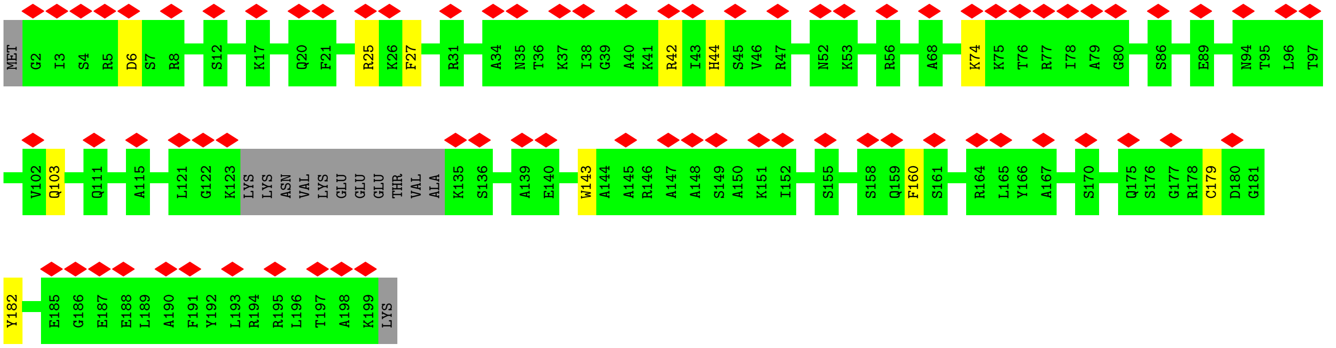
- Molecule 63: Small ribosomal subunit protein uS5

Chain SR:



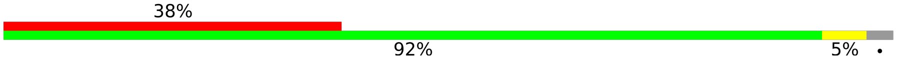
- Molecule 64: Small ribosomal subunit protein eS8A

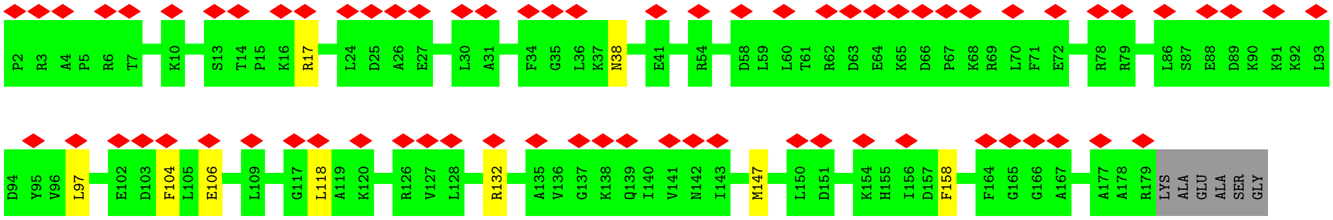
Chain SV:



- Molecule 65: Small ribosomal subunit protein uS4A

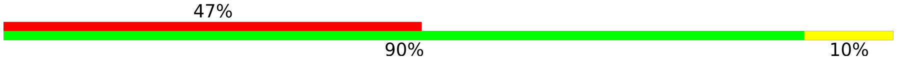
Chain SW:

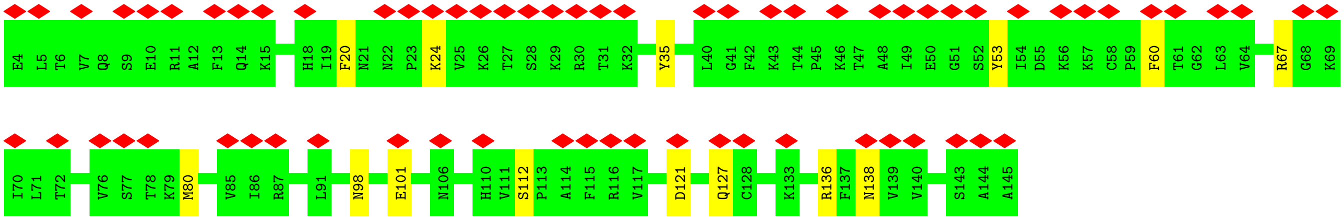




- Molecule 66: Small ribosomal subunit protein uS17A

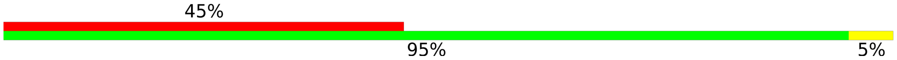
Chain SX:

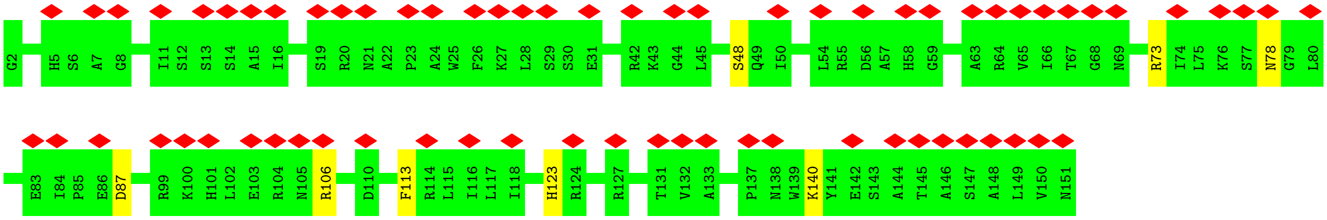




- Molecule 67: Small ribosomal subunit protein uS15

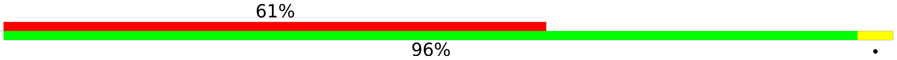
Chain SY:

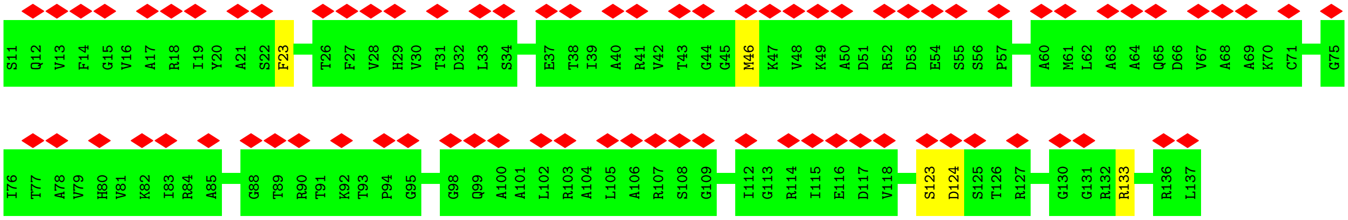




- Molecule 68: Small ribosomal subunit protein uS11B

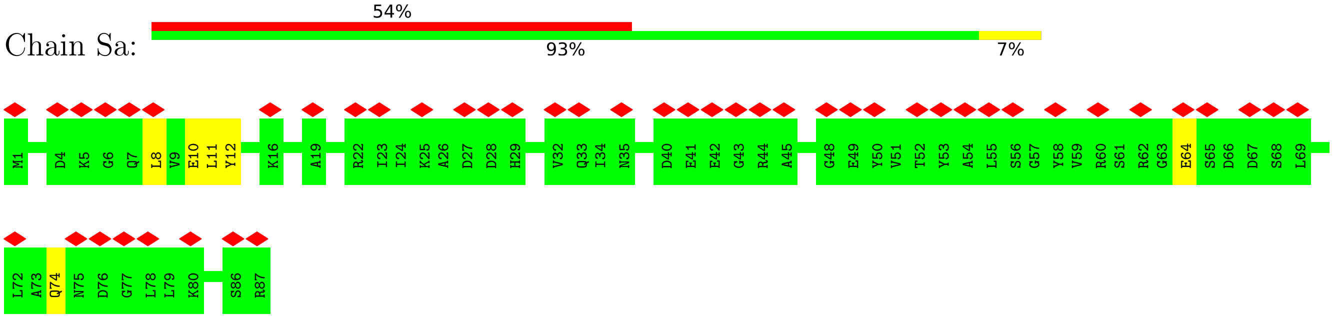
Chain SZ:





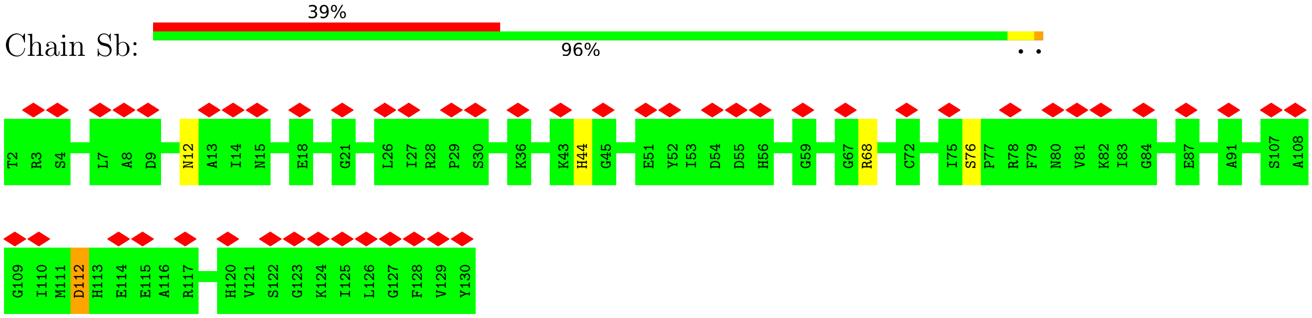
- Molecule 69: Small ribosomal subunit protein eS21A

Chain Sa:



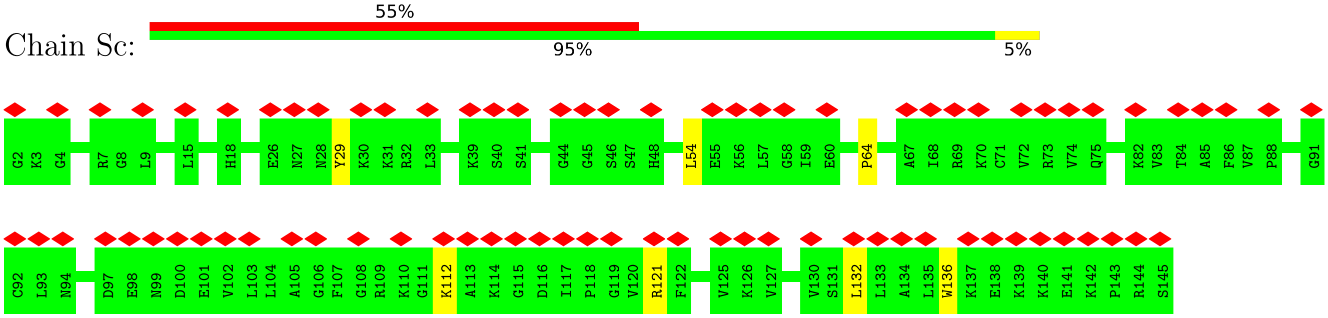
- Molecule 70: Small ribosomal subunit protein uS8A

Chain Sb:



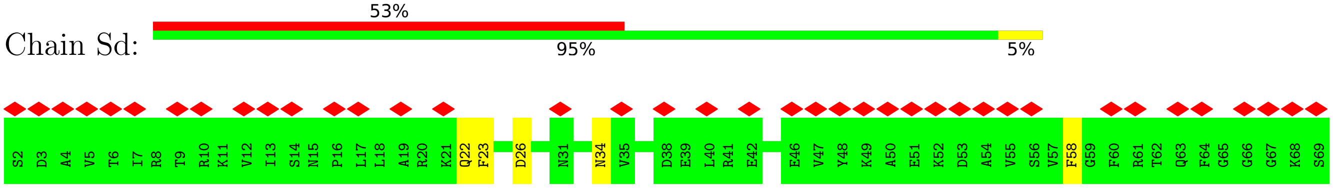
- Molecule 71: Small ribosomal subunit protein uS12A

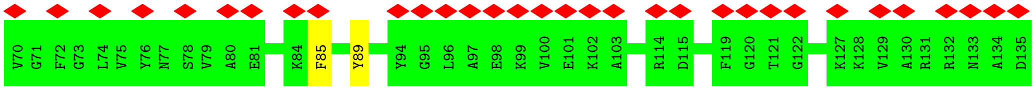
Chain Sc:



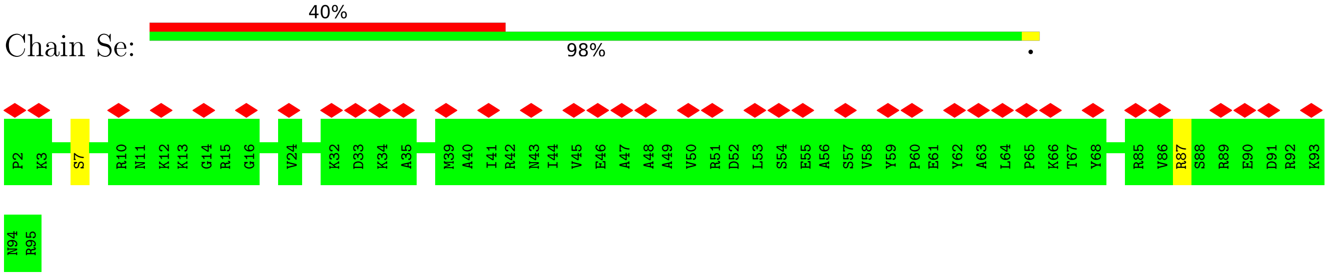
- Molecule 72: Small ribosomal subunit protein eS24A

Chain Sd:

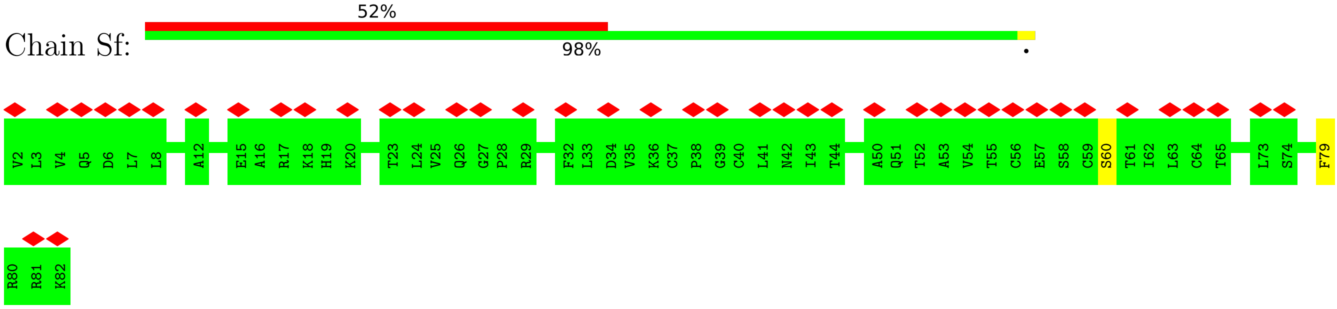




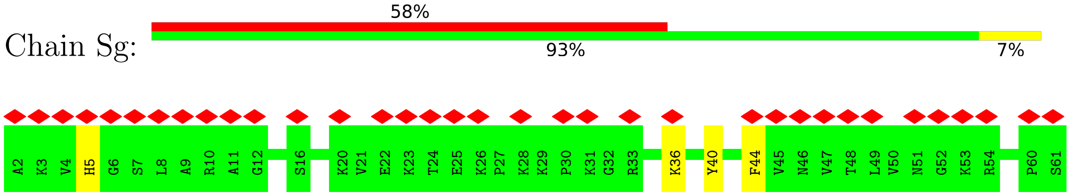
- Molecule 73: Small ribosomal subunit protein eS26A



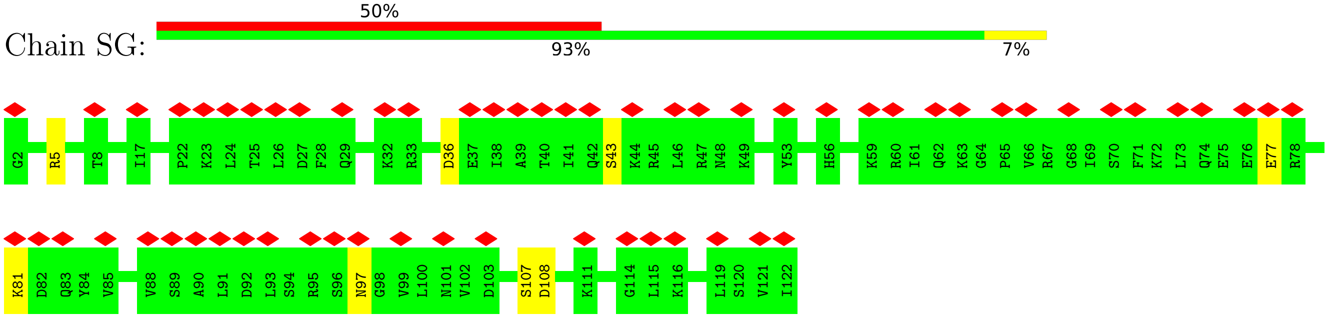
- Molecule 74: Small ribosomal subunit protein eS27A



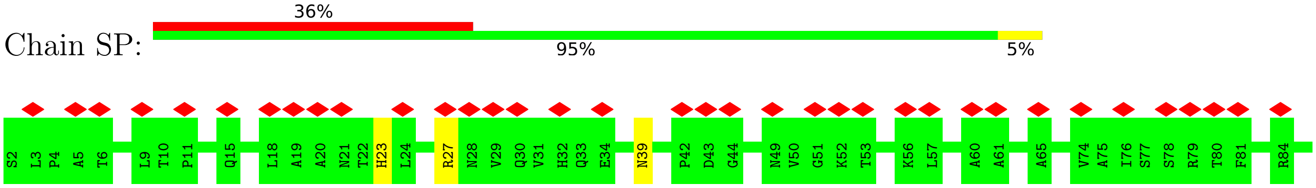
- Molecule 75: Small ribosomal subunit protein eS30A

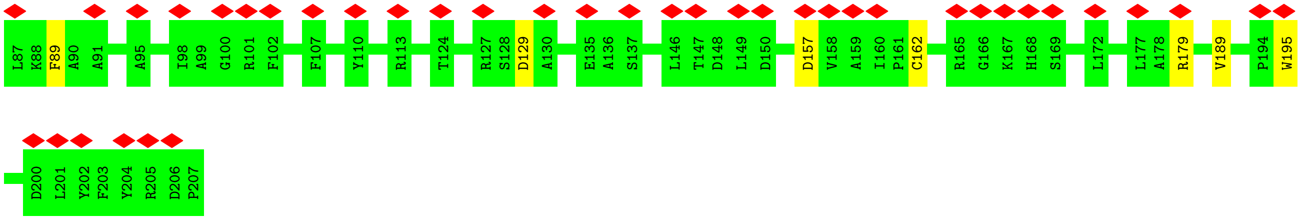


- Molecule 76: Small ribosomal subunit protein eS17A



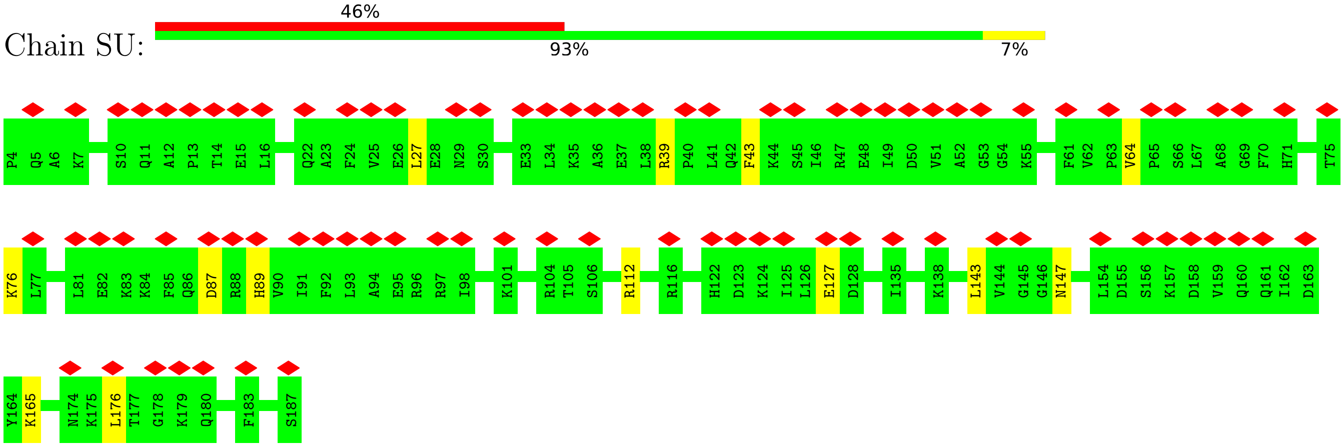
- Molecule 77: Small ribosomal subunit protein uS2A





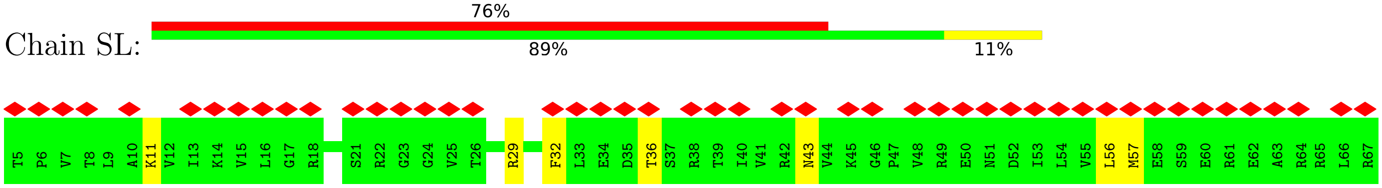
- Molecule 78: Small ribosomal subunit protein eS7A

Chain SU:



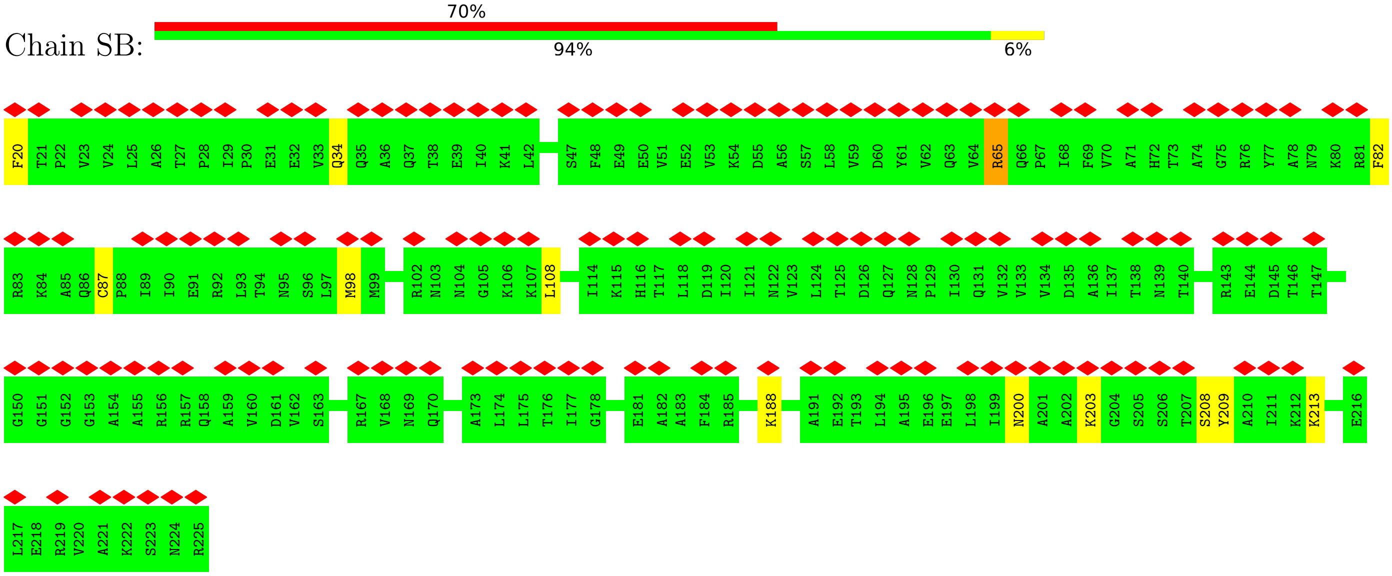
- Molecule 79: Small ribosomal subunit protein eS28A

Chain SL:

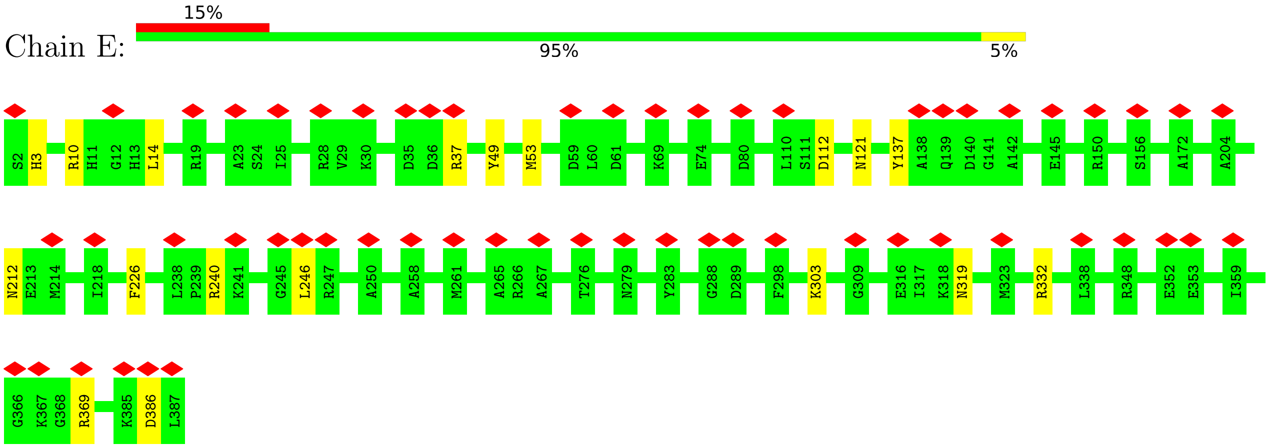


- Molecule 80: Small ribosomal subunit protein uS7

Chain SB:



- Molecule 81: Large ribosomal subunit protein uL3


Chain E:
15%
95%
5%
S2
H3
R10
H11
G12
H13
L14
R19
A23
S24
I25
R28
V29
K30
D35
D36
R37
Y49
M53
D59
L60
D61
K69
E74
D80
L110
S111
D112
N121
Y137
A138
Q139
D140
G141
A142
E145
R150
S156
A172
A204
N212
E213
M214
I218
F226
L238
P239
R240
K241
G245
L246
R247
A250
A258
M261
A265
R266
A267
T276
N279
Y283
G288
D289
F298
K303
G309
E316
I317
K318
N319
M323
R332
L338
R348
E352
E353
I359
G366
K367
G368
R369
K385
D386
L387

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.099	Depositor
Minimum map value	-0.558	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.26	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	2	0.18	0/42211	0.77	3/65773 (0.0%)
2	A	0.16	0/76425	0.74	7/119146 (0.0%)
3	B	0.15	0/2883	0.72	0/4491
4	C	0.17	0/3746	0.75	0/5832
5	D	0.26	0/1933	0.59	0/2598
6	F	0.25	0/2800	0.52	0/3790
7	G	0.25	0/2400	0.54	0/3239
8	H	0.25	0/1329	0.52	0/1794
9	I	0.25	0/1821	0.52	0/2451
10	J	0.26	0/1836	0.54	0/2481
11	K	0.25	0/1529	0.55	1/2060 (0.0%)
12	L	0.26	0/1801	0.58	0/2416
13	M	0.28	0/1367	0.65	0/1834
14	N	0.24	0/1568	0.57	0/2106
15	O	0.25	0/1068	0.55	0/1438
16	P	0.27	0/1757	0.64	0/2354
17	Q	0.27	0/1585	0.60	0/2128
18	R	0.26	0/1439	0.59	0/1938
19	S	0.25	0/1465	0.58	0/1965
20	T	0.26	0/1532	0.62	0/2043
21	U	0.26	0/1473	0.56	1/1980 (0.1%)
22	V	0.27	0/1296	0.60	1/1739 (0.1%)
23	W	0.26	0/812	0.57	1/1099 (0.1%)
24	X	0.26	0/1018	0.62	0/1369
25	Y	0.26	0/850	0.57	0/1152
26	Z	0.26	0/979	0.57	0/1321
27	a	0.25	0/995	0.60	0/1329
28	b	0.26	0/1106	0.54	0/1485
29	c	0.25	0/1200	0.55	0/1607
30	d	0.25	0/473	0.56	0/629
31	e	0.26	0/745	0.56	0/1001
32	f	0.28	0/890	0.63	0/1196
33	g	0.24	0/1034	0.53	0/1385
34	h	0.27	0/868	0.61	0/1168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	i	0.26	0/890	0.57	0/1189
36	j	0.27	0/978	0.63	1/1301 (0.1%)
37	k	0.25	0/772	0.54	0/1026
38	l	0.25	0/660	0.63	0/875
39	m	0.29	0/618	0.68	1/826 (0.1%)
40	n	0.34	0/443	0.73	0/588
41	o	0.25	0/416	0.62	0/553
42	p	0.26	0/230	0.82	0/296
43	q	0.26	0/836	0.54	0/1104
44	r	0.26	0/701	0.62	0/934
45	t	0.16	0/1795	0.75	0/2797
45	u	0.15	0/1771	0.77	0/2760
46	v	0.24	0/7611	0.50	0/10322
47	x	0.25	0/6685	0.54	2/9050 (0.0%)
48	SA	0.25	0/1754	0.57	0/2361
49	SC	0.27	0/769	0.63	0/1039
50	SD	0.23	0/883	0.51	0/1199
51	SE	0.26	0/936	0.60	0/1259
52	SF	0.26	0/1125	0.59	1/1510 (0.1%)
53	SH	0.24	0/1207	0.59	0/1623
54	SI	0.24	0/1130	0.54	0/1517
55	SJ	0.24	0/807	0.58	1/1091 (0.1%)
56	SK	0.27	0/526	0.66	0/706
57	SM	0.26	0/452	0.63	0/600
58	SN	0.27	0/571	0.61	0/768
59	SO	0.30	1/2436 (0.0%)	0.54	0/3318
60	SQ	0.25	0/1819	0.57	0/2442
61	SS	0.24	0/2097	0.55	0/2823
62	ST	0.24	0/1839	0.57	0/2460
63	SR	0.26	0/1656	0.59	1/2251 (0.0%)
64	SV	0.25	0/1501	0.57	0/2006
65	SW	0.25	0/1466	0.62	0/1966
66	SX	0.25	0/1168	0.57	0/1575
67	SY	0.24	0/1215	0.54	0/1638
68	SZ	0.24	0/901	0.58	0/1217
69	Sa	0.27	0/682	0.59	0/921
70	Sb	0.27	0/1038	0.63	1/1395 (0.1%)
71	Sc	0.25	0/1139	0.58	0/1518
72	Sd	0.25	0/1087	0.57	0/1449
73	Se	0.24	0/761	0.61	0/1016
74	Sf	0.25	0/620	0.55	0/838
75	Sg	0.24	0/480	0.54	0/639
76	SG	0.25	0/971	0.63	0/1303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
77	SP	0.26	0/1644	0.56	0/2249
78	SU	0.25	0/1498	0.56	0/2019
79	SL	0.31	0/499	0.77	0/670
80	SB	0.29	0/1629	0.70	1/2202 (0.0%)
81	E	0.24	0/3146	0.55	0/4228
All	All	0.21	1/232092 (0.0%)	0.68	23/339774 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	SO	281	TYR	C-N	5.73	1.47	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3212	C	N1-C2-O2	6.00	122.50	118.90
1	2	186	C	C2-N1-C1'	5.99	125.39	118.80
22	V	127	GLN	CA-CB-CG	5.95	126.50	113.40
2	A	2257	C	C2-N1-C1'	5.91	125.30	118.80
11	K	120	ASP	CB-CG-OD1	5.65	123.39	118.30
1	2	1706	C	N3-C2-O2	-5.62	117.97	121.90
63	SR	229	LEU	CA-CB-CG	5.61	128.20	115.30
1	2	330	G	N1-C6-O6	-5.60	116.54	119.90
39	m	71	PRO	CA-N-CD	-5.55	103.73	111.50
55	SJ	58	LEU	CA-CB-CG	5.55	128.07	115.30
23	W	79	LEU	CA-CB-CG	5.51	127.97	115.30
21	U	21	GLU	CA-CB-CG	5.49	125.48	113.40
80	SB	65	ARG	CA-CB-CG	5.44	125.37	113.40
2	A	2846	U	C2-N1-C1'	5.36	124.14	117.70
2	A	113	C	C2-N1-C1'	5.34	124.67	118.80
36	j	30	GLU	CA-CB-CG	5.30	125.07	113.40
52	SF	53	LEU	CA-CB-CG	5.26	127.40	115.30
47	x	284	LEU	CA-CB-CG	5.22	127.30	115.30
47	x	280	PRO	CA-N-CD	-5.17	104.27	111.50
2	A	2773	C	N1-C2-O2	5.16	122.00	118.90
2	A	1311	G	C5-C6-O6	5.12	131.67	128.60
70	Sb	112	ASP	CB-CG-OD1	5.11	122.90	118.30
2	A	2257	C	N1-C2-O2	5.03	121.92	118.90

There are no chirality outliers.

There are no planarity outliers.

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	
5	D	249/251 (99%)	227 (91%)	22 (9%)	0	100	100
6	F	359/361 (99%)	345 (96%)	14 (4%)	0	100	100
7	G	292/294 (99%)	279 (96%)	13 (4%)	0	100	100
8	H	163/175 (93%)	153 (94%)	10 (6%)	0	100	100
9	I	220/223 (99%)	209 (95%)	11 (5%)	0	100	100
10	J	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	30	65
11	K	189/191 (99%)	177 (94%)	12 (6%)	0	100	100
12	L	216/218 (99%)	194 (90%)	21 (10%)	1 (0%)	25	60
13	M	167/169 (99%)	154 (92%)	13 (8%)	0	100	100
14	N	191/193 (99%)	180 (94%)	9 (5%)	2 (1%)	13	46
15	O	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
16	P	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
17	Q	195/197 (99%)	190 (97%)	5 (3%)	0	100	100
18	R	181/183 (99%)	173 (96%)	8 (4%)	0	100	100
19	S	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	25	60
20	T	186/188 (99%)	185 (100%)	1 (0%)	0	100	100
21	U	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
22	V	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
23	W	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
24	X	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
25	Y	124/126 (98%)	108 (87%)	15 (12%)	1 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
27	a	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
28	b	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
29	c	146/148 (99%)	134 (92%)	12 (8%)	0	100	100
30	d	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	e	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
32	f	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
33	g	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
34	h	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
35	i	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
36	j	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
37	k	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
38	l	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
39	m	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
40	n	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
41	o	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
42	p	23/25 (92%)	23 (100%)	0	0	100	100
43	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
44	r	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
46	v	975/1044 (93%)	897 (92%)	75 (8%)	3 (0%)	37	70
47	x	840/842 (100%)	759 (90%)	79 (9%)	2 (0%)	44	75
48	SA	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
49	SC	90/92 (98%)	78 (87%)	12 (13%)	0	100	100
50	SD	119/121 (98%)	97 (82%)	22 (18%)	0	100	100
51	SE	115/117 (98%)	97 (84%)	18 (16%)	0	100	100
52	SF	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	19	54
53	SH	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
54	SI	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
55	SJ	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
56	SK	62/108 (57%)	57 (92%)	4 (6%)	1 (2%)	8	37
57	SM	51/53 (96%)	43 (84%)	8 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	SN	71/73 (97%)	47 (66%)	22 (31%)	2 (3%)	4	28
59	SO	310/312 (99%)	281 (91%)	26 (8%)	3 (1%)	13	46
60	SQ	221/232 (95%)	201 (91%)	20 (9%)	0	100	100
61	SS	256/258 (99%)	239 (93%)	17 (7%)	0	100	100
62	ST	226/228 (99%)	215 (95%)	10 (4%)	1 (0%)	30	65
63	SR	214/216 (99%)	197 (92%)	17 (8%)	0	100	100
64	SV	183/200 (92%)	178 (97%)	5 (3%)	0	100	100
65	SW	176/184 (96%)	166 (94%)	10 (6%)	0	100	100
66	SX	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
67	SY	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
68	SZ	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
69	Sa	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	11	43
70	Sb	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	51
71	Sc	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	19	54
72	Sd	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
73	Se	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
74	Sf	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
75	Sg	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
76	SG	119/121 (98%)	107 (90%)	12 (10%)	0	100	100
77	SP	204/206 (99%)	185 (91%)	17 (8%)	2 (1%)	13	46
78	SU	182/184 (99%)	173 (95%)	8 (4%)	1 (0%)	25	60
79	SL	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
80	SB	204/206 (99%)	178 (87%)	26 (13%)	0	100	100
81	E	384/386 (100%)	363 (94%)	21 (6%)	0	100	100
All	All	12767/13071 (98%)	11873 (93%)	869 (7%)	25 (0%)	45	75

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	158	ASP
25	Y	81	PRO
52	SF	40	GLU
56	SK	88	ILE
70	Sb	76	SER

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Mol	Chain	Res	Type
71	Sc	64	PRO
78	SU	64	VAL
47	x	677	PHE
59	SO	284	ALA
77	SP	39	ASN
77	SP	189	VAL
46	v	334	ALA
46	v	821	ILE
14	N	136	GLU
58	SN	145	HIS
62	ST	171	LYS
14	N	47	ALA
59	SO	281	TYR
69	Sa	10	GLU
12	L	47	PRO
46	v	331	VAL
58	SN	98	VAL
59	SO	276	PRO
19	S	18	ALA
47	x	28	VAL

5.3.2 Protein sidechains ⓘ

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	
5	D	190/193 (98%)	181 (95%)	9 (5%)	22	47
6	F	288/288 (100%)	278 (96%)	10 (4%)	31	54
7	G	241/243 (99%)	233 (97%)	8 (3%)	33	56
8	H	139/154 (90%)	134 (96%)	5 (4%)	30	54
9	I	186/187 (100%)	180 (97%)	6 (3%)	34	56
10	J	187/191 (98%)	181 (97%)	6 (3%)	34	56
11	K	168/171 (98%)	161 (96%)	7 (4%)	25	49
12	L	185/185 (100%)	172 (93%)	13 (7%)	12	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	145/147 (99%)	135 (93%)	10 (7%)	13	37
14	N	154/154 (100%)	150 (97%)	4 (3%)	41	61
15	O	107/107 (100%)	104 (97%)	3 (3%)	38	59
16	P	175/175 (100%)	160 (91%)	15 (9%)	8	31
17	Q	160/160 (100%)	149 (93%)	11 (7%)	13	37
18	R	138/145 (95%)	130 (94%)	8 (6%)	17	42
19	S	150/150 (100%)	145 (97%)	5 (3%)	33	56
20	T	152/153 (99%)	147 (97%)	5 (3%)	33	56
21	U	155/155 (100%)	148 (96%)	7 (4%)	23	48
22	V	135/136 (99%)	127 (94%)	8 (6%)	16	41
23	W	87/87 (100%)	84 (97%)	3 (3%)	32	55
24	X	104/104 (100%)	100 (96%)	4 (4%)	28	52
25	Y	56/108 (52%)	53 (95%)	3 (5%)	18	44
26	Z	104/105 (99%)	99 (95%)	5 (5%)	21	46
27	a	108/108 (100%)	104 (96%)	4 (4%)	29	53
28	b	112/115 (97%)	109 (97%)	3 (3%)	40	60
29	c	117/118 (99%)	113 (97%)	4 (3%)	32	55
30	d	46/46 (100%)	42 (91%)	4 (9%)	8	30
31	e	81/81 (100%)	78 (96%)	3 (4%)	29	53
32	f	92/96 (96%)	89 (97%)	3 (3%)	33	56
33	g	107/109 (98%)	102 (95%)	5 (5%)	22	47
34	h	90/90 (100%)	85 (94%)	5 (6%)	17	43
35	i	95/95 (100%)	87 (92%)	8 (8%)	9	32
36	j	104/104 (100%)	101 (97%)	3 (3%)	37	59
37	k	80/81 (99%)	76 (95%)	4 (5%)	20	45
38	l	67/67 (100%)	59 (88%)	8 (12%)	4	20
39	m	68/68 (100%)	64 (94%)	4 (6%)	16	41
40	n	45/45 (100%)	40 (89%)	5 (11%)	5	21
41	o	45/47 (96%)	40 (89%)	5 (11%)	5	21
42	p	22/23 (96%)	21 (96%)	1 (4%)	23	48
43	q	87/88 (99%)	80 (92%)	7 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	r	71/71 (100%)	66 (93%)	5 (7%)	12	36
46	v	789/890 (89%)	771 (98%)	18 (2%)	45	64
47	x	715/715 (100%)	679 (95%)	36 (5%)	20	45
48	SA	182/182 (100%)	170 (93%)	12 (7%)	14	38
49	SC	77/85 (91%)	67 (87%)	10 (13%)	3	18
50	SD	88/98 (90%)	86 (98%)	2 (2%)	45	64
51	SE	95/98 (97%)	85 (90%)	10 (10%)	5	22
52	SF	117/117 (100%)	111 (95%)	6 (5%)	20	45
53	SH	127/128 (99%)	119 (94%)	8 (6%)	15	40
54	SI	115/115 (100%)	108 (94%)	7 (6%)	15	41
55	SJ	93/93 (100%)	92 (99%)	1 (1%)	70	79
56	SK	57/89 (64%)	50 (88%)	7 (12%)	4	19
57	SM	47/47 (100%)	41 (87%)	6 (13%)	3	18
58	SN	57/64 (89%)	56 (98%)	1 (2%)	54	71
59	SO	250/257 (97%)	241 (96%)	9 (4%)	30	54
60	SQ	200/205 (98%)	187 (94%)	13 (6%)	14	39
61	SS	220/220 (100%)	206 (94%)	14 (6%)	14	39
62	ST	189/195 (97%)	176 (93%)	13 (7%)	13	37
63	SR	175/175 (100%)	167 (95%)	8 (5%)	23	47
64	SV	148/161 (92%)	137 (93%)	11 (7%)	11	35
65	SW	153/157 (98%)	144 (94%)	9 (6%)	16	41
66	SX	126/127 (99%)	112 (89%)	14 (11%)	5	21
67	SY	127/127 (100%)	119 (94%)	8 (6%)	15	40
68	SZ	81/96 (84%)	76 (94%)	5 (6%)	15	40
69	Sa	71/74 (96%)	66 (93%)	5 (7%)	12	36
70	Sb	110/110 (100%)	106 (96%)	4 (4%)	30	54
71	Sc	119/119 (100%)	113 (95%)	6 (5%)	20	45
72	Sd	112/112 (100%)	105 (94%)	7 (6%)	15	40
73	Se	81/81 (100%)	79 (98%)	2 (2%)	42	62
74	Sf	70/70 (100%)	68 (97%)	2 (3%)	37	59
75	Sg	50/51 (98%)	46 (92%)	4 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
76	SG	105/110 (96%)	97 (92%)	8 (8%)	11	34
77	SP	170/173 (98%)	162 (95%)	8 (5%)	22	47
78	SU	163/165 (99%)	151 (93%)	12 (7%)	11	35
79	SL	56/56 (100%)	49 (88%)	7 (12%)	3	18
80	SB	173/173 (100%)	160 (92%)	13 (8%)	11	34
81	E	320/322 (99%)	302 (94%)	18 (6%)	17	43
All	All	10671/11007 (97%)	10111 (95%)	560 (5%)	22	45

All (560) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	93	LYS
5	D	119	LYS
5	D	132	ASN
5	D	139	HIS
5	D	150	LEU
5	D	198	LYS
5	D	223	SER
5	D	242	ARG
5	D	245	LEU
6	F	39	PHE
6	F	55	LYS
6	F	93	MET
6	F	114	ASN
6	F	140	HIS
6	F	141	ARG
6	F	175	HIS
6	F	255	PHE
6	F	314	LYS
6	F	318	LEU
7	G	29	ASP
7	G	55	PHE
7	G	57	ASN
7	G	58	LYS
7	G	147	ASP
7	G	171	LEU
7	G	184	ASP
7	G	208	MET
8	H	14	ASP
8	H	61	ASN

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Mol	Chain	Res	Type
8	H	69	PHE
8	H	133	GLU
8	H	150	LYS
9	I	48	ASN
9	I	100	ARG
9	I	105	LEU
9	I	163	LEU
9	I	223	PHE
9	I	225	GLN
10	J	49	TYR
10	J	83	ASP
10	J	91	PHE
10	J	118	GLU
10	J	165	PHE
10	J	247	ASP
11	K	69	ARG
11	K	72	LYS
11	K	88	TYR
11	K	92	TYR
11	K	120	ASP
11	K	171	ASP
11	K	180	TYR
12	L	20	SER
12	L	23	ASN
12	L	30	LYS
12	L	49	CYS
12	L	61	SER
12	L	97	LEU
12	L	110	ARG
12	L	115	MET
12	L	121	LYS
12	L	123	HIS
12	L	137	SER
12	L	145	LYS
12	L	196	PHE
13	M	26	SER
13	M	51	ARG
13	M	90	GLN
13	M	104	PHE
13	M	127	PHE
13	M	128	TYR
13	M	137	ARG

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Mol	Chain	Res	Type
13	M	142	LYS
13	M	152	HIS
13	M	156	LYS
14	N	12	ASN
14	N	25	HIS
14	N	31	LYS
14	N	67	ARG
15	O	65	LEU
15	O	114	ASP
15	O	128	ARG
16	P	17	ASP
16	P	30	TYR
16	P	32	GLN
16	P	33	LYS
16	P	46	ASP
16	P	53	TYR
16	P	90	ASN
16	P	92	LEU
16	P	123	GLN
16	P	124	ASP
16	P	148	TYR
16	P	150	TRP
16	P	181	ASN
16	P	184	LYS
16	P	195	ASN
17	Q	37[A]	ARG
17	Q	42[A]	ASN
17	Q	48[A]	PHE
17	Q	57[A]	PHE
17	Q	70[A]	PRO
17	Q	80[A]	PHE
17	Q	100[A]	GLU
17	Q	117[A]	ARG
17	Q	148[A]	LYS
17	Q	151[A]	ASP
17	Q	199[A]	TYR
18	R	7	THR
18	R	28	ASN
18	R	64	ASN
18	R	90	PHE
18	R	103	GLU
18	R	113	TYR

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Mol	Chain	Res	Type
18	R	148	LEU
18	R	153	LYS
19	S	41	ASP
19	S	78	ASN
19	S	94	PHE
19	S	153	PHE
19	S	170	ARG
20	T	66	HIS
20	T	109	TYR
20	T	130	ASN
20	T	144	GLN
20	T	152	GLU
21	U	21	GLU
21	U	24	LEU
21	U	27	MET
21	U	50	LYS
21	U	122	HIS
21	U	143	PHE
21	U	172	TYR
22	V	5	HIS
22	V	32	LYS
22	V	38	ASP
22	V	71	SER
22	V	84	TYR
22	V	127	GLN
22	V	156	TYR
22	V	159	PHE
23	W	71	PHE
23	W	92	TRP
23	W	107	PHE
24	X	56	ASP
24	X	59	MET
24	X	87	ARG
24	X	92	PHE
25	Y	21	PHE
25	Y	33	ASN
25	Y	42	GLN
26	Z	29	SER
26	Z	46	TYR
26	Z	85	GLN
26	Z	88	MET
26	Z	113	LEU

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Mol	Chain	Res	Type
27	a	30	LEU
27	a	42	GLN
27	a	74	TYR
27	a	83	ASP
28	b	103	GLN
28	b	109	GLU
28	b	135	ARG
29	c	3	SER
29	c	11	HIS
29	c	28	HIS
29	c	45	MET
30	d	4	SER
30	d	14	ARG
30	d	29	TYR
30	d	31	SER
31	e	27	TYR
31	e	32	LYS
31	e	85	PHE
32	f	71	LEU
32	f	92	TYR
32	f	110	GLU
33	g	16	LYS
33	g	20	HIS
33	g	31	ASN
33	g	40	SER
33	g	90	LYS
34	h	51	TYR
34	h	67	MET
34	h	73	ARG
34	h	101	PHE
34	h	105	SER
35	i	3	GLN
35	i	33	GLN
35	i	44	CYS
35	i	46	ASP
35	i	55	SER
35	i	80	ARG
35	i	98	GLN
35	i	108	GLN
36	j	60	GLU
36	j	61	GLN
36	j	85	THR

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Mol	Chain	Res	Type
37	k	27	SER
37	k	37	THR
37	k	56	ARG
37	k	91	ASN
38	l	19	CYS
38	l	27	PHE
38	l	31	LYS
38	l	37	CYS
38	l	39	TYR
38	l	48	ASN
38	l	55	ARG
38	l	65	ARG
39	m	11	PHE
39	m	12	LEU
39	m	32	ASN
39	m	57	ASN
40	n	6	SER
40	n	11	GLN
40	n	21	ARG
40	n	36	ARG
40	n	46	ARG
41	o	91	CYS
41	o	92	ASP
41	o	100	TYR
41	o	113	ARG
41	o	120	GLN
42	p	16	LYS
43	q	23	HIS
43	q	32	LYS
43	q	48	SER
43	q	55	LYS
43	q	83	LEU
43	q	88	CYS
43	q	91	PHE
44	r	6	LYS
44	r	33	GLN
44	r	38	ASP
44	r	39	CYS
44	r	42	CYS
46	v	39	ASN
46	v	234	PHE
46	v	246	MET

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Mol	Chain	Res	Type
46	v	263	ARG
46	v	297	PHE
46	v	311	ARG
46	v	390	MET
46	v	406	PHE
46	v	407	ARG
46	v	457	ARG
46	v	550	LYS
46	v	562	ASP
46	v	644	ASP
46	v	647	PHE
46	v	649	PHE
46	v	709	LEU
46	v	754	TYR
46	v	766	GLU
47	x	1	MET
47	x	9	MET
47	x	10	ARG
47	x	22	MET
47	x	42	ARG
47	x	56	PHE
47	x	61	LYS
47	x	111	PHE
47	x	144	ARG
47	x	150	ARG
47	x	171	LYS
47	x	199	ASP
47	x	229	TYR
47	x	243	ARG
47	x	271	ARG
47	x	289	MET
47	x	295	GLU
47	x	320	LEU
47	x	327	PHE
47	x	332	ASP
47	x	362	ASP
47	x	393	ARG
47	x	395	TYR
47	x	397	PHE
47	x	425	ASP
47	x	462	PHE
47	x	496	LYS

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Mol	Chain	Res	Type
47	x	537	HIS
47	x	549	HIS
47	x	607	ASN
47	x	610	ASP
47	x	612	PHE
47	x	681	MET
47	x	709	MET
47	x	717	PHE
47	x	798	PHE
48	SA	17	PHE
48	SA	51	ARG
48	SA	76	ARG
48	SA	79	TYR
48	SA	97	SER
48	SA	105	MET
48	SA	116	ARG
48	SA	120	TYR
48	SA	134	CYS
48	SA	142	LEU
48	SA	150	MET
48	SA	166	ASP
49	SC	3	MET
49	SC	15	LEU
49	SC	27	PHE
49	SC	32	HIS
49	SC	59	PHE
49	SC	63	TYR
49	SC	65	TYR
49	SC	66	TYR
49	SC	79	TYR
49	SC	80	LEU
50	SD	46	ARG
50	SD	95	LYS
51	SE	15	HIS
51	SE	32	ASP
51	SE	33	PHE
51	SE	36	LEU
51	SE	43	ARG
51	SE	58	LYS
51	SE	61	ARG
51	SE	82	ASN
51	SE	89	MET

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Mol	Chain	Res	Type
51	SE	114	HIS
52	SF	10	PHE
52	SF	34	SER
52	SF	53	LEU
52	SF	60	PHE
52	SF	83	GLN
52	SF	92	TYR
53	SH	11	PHE
53	SH	13	HIS
53	SH	57	ARG
53	SH	66	LEU
53	SH	73	MET
53	SH	84	TRP
53	SH	110	ARG
53	SH	120	ARG
54	SI	8	ASP
54	SI	14	PHE
54	SI	27	LYS
54	SI	54	PHE
54	SI	66	TYR
54	SI	76	LEU
54	SI	138	GLN
55	SJ	84	MET
56	SK	43	ASP
56	SK	46	LYS
56	SK	57	TYR
56	SK	69	LEU
56	SK	75	LEU
56	SK	95	HIS
56	SK	101	TYR
57	SM	4	GLU
57	SM	7	TRP
57	SM	8	PHE
57	SM	14	TYR
57	SM	28	THR
57	SM	39	CYS
58	SN	131	PHE
59	SO	53	LYS
59	SO	86	ASP
59	SO	89	LEU
59	SO	179	LYS
59	SO	184	ASN

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Mol	Chain	Res	Type
59	SO	231	MET
59	SO	241	PHE
59	SO	245	PHE
59	SO	316	MET
60	SQ	22	ASP
60	SQ	29	TRP
60	SQ	55	LYS
60	SQ	58	SER
60	SQ	90	GLU
60	SQ	111	ARG
60	SQ	115	ARG
60	SQ	133	TYR
60	SQ	184	LEU
60	SQ	188	LEU
60	SQ	194	ASN
60	SQ	213	ARG
60	SQ	220	GLN
61	SS	6	LYS
61	SS	16	HIS
61	SS	18	TRP
61	SS	36	HIS
61	SS	47	PHE
61	SS	128	LYS
61	SS	149	TYR
61	SS	172	PHE
61	SS	182	TYR
61	SS	189	LEU
61	SS	198	LYS
61	SS	218	PHE
61	SS	224	ASN
61	SS	226	PHE
62	ST	3	LEU
62	ST	13	GLN
62	ST	25	ARG
62	ST	27	PHE
62	ST	28	PHE
62	ST	48	TYR
62	ST	63	MET
62	ST	87	ARG
62	ST	94	ARG
62	ST	148	SER
62	ST	156	PHE

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Mol	Chain	Res	Type
62	ST	169	TYR
62	ST	215	ARG
63	SR	54	GLU
63	SR	91	ARG
63	SR	181	SER
63	SR	186	LYS
63	SR	201	ASN
63	SR	211	LEU
63	SR	224	PHE
63	SR	230	TRP
64	SV	6	ASP
64	SV	25	ARG
64	SV	27	PHE
64	SV	42	ARG
64	SV	44	HIS
64	SV	74	LYS
64	SV	103	GLN
64	SV	143	TRP
64	SV	160	PHE
64	SV	179	CYS
64	SV	182	TYR
65	SW	17	ARG
65	SW	38	ASN
65	SW	97	LEU
65	SW	104	PHE
65	SW	106	GLU
65	SW	118	LEU
65	SW	132	ARG
65	SW	147	MET
65	SW	158	PHE
66	SX	20	PHE
66	SX	24	LYS
66	SX	35	TYR
66	SX	53	TYR
66	SX	60	PHE
66	SX	67	ARG
66	SX	80	MET
66	SX	98	ASN
66	SX	101	GLU
66	SX	112	SER
66	SX	121	ASP
66	SX	127	GLN

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Mol	Chain	Res	Type
66	SX	136	ARG
66	SX	138	ASN
67	SY	48	SER
67	SY	73	ARG
67	SY	78	ASN
67	SY	87	ASP
67	SY	106	ARG
67	SY	113	PHE
67	SY	123	HIS
67	SY	140	LYS
68	SZ	23	PHE
68	SZ	46	MET
68	SZ	123	SER
68	SZ	124	ASP
68	SZ	133	ARG
69	Sa	8	LEU
69	Sa	11	LEU
69	Sa	12	TYR
69	Sa	64	GLU
69	Sa	74	GLN
70	Sb	12	ASN
70	Sb	44	HIS
70	Sb	68	ARG
70	Sb	112	ASP
71	Sc	29	TYR
71	Sc	54	LEU
71	Sc	112	LYS
71	Sc	121	ARG
71	Sc	132	LEU
71	Sc	136	TRP
72	Sd	22	GLN
72	Sd	23	PHE
72	Sd	26	ASP
72	Sd	34	ASN
72	Sd	58	PHE
72	Sd	85	PHE
72	Sd	89	TYR
73	Se	7	SER
73	Se	87	ARG
74	Sf	60	SER
74	Sf	79	PHE
75	Sg	5	HIS

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Mol	Chain	Res	Type
75	Sg	36	LYS
75	Sg	40	TYR
75	Sg	44	PHE
76	SG	5	ARG
76	SG	36	ASP
76	SG	43	SER
76	SG	77	GLU
76	SG	81	LYS
76	SG	97	ASN
76	SG	107	SER
76	SG	108	ASP
77	SP	23	HIS
77	SP	27	ARG
77	SP	89	PHE
77	SP	129	ASP
77	SP	157	ASP
77	SP	162	CYS
77	SP	179	ARG
77	SP	195	TRP
78	SU	27	LEU
78	SU	39	ARG
78	SU	43	PHE
78	SU	76	LYS
78	SU	87	ASP
78	SU	89	HIS
78	SU	112	ARG
78	SU	127	GLU
78	SU	143	LEU
78	SU	147	ASN
78	SU	165	LYS
78	SU	176	LEU
79	SL	11	LYS
79	SL	29	ARG
79	SL	32	PHE
79	SL	36	THR
79	SL	43	ASN
79	SL	56	LEU
79	SL	57	MET
80	SB	20	PHE
80	SB	34	GLN
80	SB	65	ARG
80	SB	82	PHE

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Mol	Chain	Res	Type
80	SB	87	CYS
80	SB	98	MET
80	SB	108	LEU
80	SB	188	LYS
80	SB	200	ASN
80	SB	203	LYS
80	SB	208	SER
80	SB	209	TYR
80	SB	213	LYS
81	E	3	HIS
81	E	10	ARG
81	E	14	LEU
81	E	37	ARG
81	E	49	TYR
81	E	53	MET
81	E	112	ASP
81	E	121	ASN
81	E	137	TYR
81	E	212	ASN
81	E	226	PHE
81	E	240	ARG
81	E	246	LEU
81	E	303	LYS
81	E	319	ASN
81	E	332	ARG
81	E	369	ARG
81	E	386	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	237	GLN
11	K	9	GLN
11	K	100	ASN
12	L	59	GLN
12	L	208	ASN
13	M	47	GLN
14	N	114	GLN
16	P	112	ASN
16	P	194	GLN
18	R	116	HIS
24	X	81	GLN

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Mol	Chain	Res	Type
25	Y	32	GLN
28	b	79	HIS
28	b	128	GLN
38	l	28	HIS
38	l	30	GLN
38	l	76	ASN
46	v	26	HIS
46	v	97	ASN
46	v	271	ASN
47	x	168	GLN
47	x	668	GLN
48	SA	174	HIS
49	SC	58	GLN
52	SF	77	GLN
52	SF	93	HIS
54	SI	25	GLN
56	SK	95	HIS
58	SN	123	ASN
59	SO	31	ASN
59	SO	200	ASN
59	SO	314	GLN
60	SQ	148	ASN
60	SQ	149	GLN
61	SS	69	HIS
62	ST	4	ASN
65	SW	110	GLN
67	SY	105	ASN
69	Sa	21	ASN
71	Sc	48	HIS
71	Sc	63	GLN
77	SP	131	GLN
80	SB	37	GLN
80	SB	104	ASN
80	SB	158	GLN
80	SB	169	ASN
81	E	269	GLN
81	E	319	ASN

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Mol	**Chain**	**Analysed**	**Backbone Outliers**	**Pucker Outliers**

Mol	**Chain**	**Analysed**	**Backbone Outliers**	**Pucker Outliers**
1	2	1768/1799 (98%)	471 (26%)	37 (2%)
2	A	3185/3394 (93%)	498 (15%)	6 (0%)
3	B	120/121 (99%)	14 (11%)	1 (0%)
4	C	157/158 (99%)	33 (21%)	1 (0%)
45	t	74/75 (98%)	17 (22%)	0
45	u	73/75 (97%)	17 (23%)	0
All	All	5377/5622 (95%)	1050 (19%)	45 (0%)

All (1050) RNA backbone outliers are listed below:

Mol	**Chain**	**Res**	**Type**
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	47	A
1	2	56	U
1	2	57	G
1	2	62	A
1	2	65	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	73	U
1	2	74	U
1	2	76	A
1	2	77	U
1	2	78	A
1	2	80	A
1	2	81	G
1	2	93	A
1	2	104	A
1	2	114	C
1	2	116	U
1	2	121	U
1	2	126	A
1	2	127	G

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Mol	Chain	Res	Type
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	134	U
1	2	135	A
1	2	138	A
1	2	140	A
1	2	141	U
1	2	145	A
1	2	153	G
1	2	158	U
1	2	159	U
1	2	168	A
1	2	171	A
1	2	172	C
1	2	176	C
1	2	178	U
1	2	184	C
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	189	C
1	2	191	C
1	2	193	U
1	2	194	U
1	2	195	G
1	2	215	A
1	2	216	U
1	2	217	A
1	2	218	A
1	2	223	U
1	2	225	A
1	2	226	A
1	2	227	U
1	2	230	C
1	2	233	C
1	2	234	G
1	2	238	U
1	2	239	C
1	2	240	U

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Mol	Chain	Res	Type
1	2	241	U
1	2	249	U
1	2	250	C
1	2	260	U
1	2	261	U
1	2	265	A
1	2	270	C
1	2	272	U
1	2	274	G
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	287	G
1	2	299	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	320	U
1	2	322	G
1	2	323	A
1	2	330	G
1	2	332	U
1	2	333	A
1	2	334	G
1	2	337	G
1	2	338	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C
1	2	369	A
1	2	370	A
1	2	387	A
1	2	388	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	415	C

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Mol	Chain	Res	Type
1	2	416	A
1	2	417	A
1	2	418	G
1	2	419	G
1	2	423	G
1	2	425	A
1	2	426	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	445	A
1	2	447	U
1	2	448	C
1	2	460	A
1	2	482	U
1	2	483	A
1	2	485	A
1	2	487	G
1	2	493	U
1	2	494	U
1	2	496	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	506	A
1	2	507	U
1	2	510	G
1	2	517	U
1	2	518	A
1	2	525	A
1	2	534	A
1	2	538	A
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	554	C
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C

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Mol	Chain	Res	Type
1	2	565	C
1	2	568	G
1	2	572	C
1	2	575	C
1	2	578	U
1	2	582	U
1	2	594	A
1	2	609	U
1	2	610	G
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	635	A
1	2	638	U
1	2	639	U
1	2	640	U
1	2	641	G
1	2	645	C
1	2	653	C
1	2	655	G
1	2	656	G
1	2	677	G
1	2	678	A
1	2	680	U
1	2	681	U
1	2	682	C
1	2	684	A
1	2	687	G
1	2	688	G
1	2	693	U
1	2	694	U
1	2	696	C
1	2	698	U
1	2	700	C
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	708	C
1	2	709	C

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Mol	Chain	Res	Type
1	2	710	U
1	2	711	U
1	2	712	G
1	2	730	G
1	2	732	G
1	2	733	A
1	2	736	C
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	745	U
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	781	U
1	2	782	U
1	2	783	G
1	2	787	G
1	2	789	A
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	816	G
1	2	818	C
1	2	820	U
1	2	821	U
1	2	823	G
1	2	833	U
1	2	836	U
1	2	840	U
1	2	846	G
1	2	852	C
1	2	856	A
1	2	857	U
1	2	861	U

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Mol	Chain	Res	Type
1	2	862	A
1	2	863	A
1	2	873	U
1	2	876	G
1	2	899	G
1	2	901	G
1	2	902	G
1	2	903	U
1	2	912	U
1	2	913	G
1	2	921	U
1	2	929	A
1	2	931	C
1	2	933	A
1	2	934	C
1	2	935	U
1	2	942	G
1	2	945	U
1	2	966	A
1	2	967	A
1	2	969	C
1	2	970	A
1	2	988	A
1	2	992	A
1	2	993	A
1	2	996	U
1	2	1004	U
1	2	1005	A
1	2	1024	U
1	2	1028	C
1	2	1029	U
1	2	1032	G
1	2	1039	A
1	2	1052	U
1	2	1053	G
1	2	1054	U
1	2	1055	U
1	2	1057	U
1	2	1058	U
1	2	1060	U
1	2	1061	A
1	2	1062	A

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Mol	Chain	Res	Type
1	2	1063	U
1	2	1064	G
1	2	1066	C
1	2	1074	G
1	2	1076	A
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1092	A
1	2	1096	C
1	2	1098	U
1	2	1100	G
1	2	1113	A
1	2	1138	A
1	2	1143	A
1	2	1147	A
1	2	1150	G
1	2	1151	A
1	2	1152	A
1	2	1153	G
1	2	1154	G
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1162	C
1	2	1163	A
1	2	1164	G
1	2	1165	G
1	2	1167	G
1	2	1170	G
1	2	1184	A
1	2	1185	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1212	G
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G

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Mol	Chain	Res	Type
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1256	A
1	2	1257	U
1	2	1274	C
1	2	1275	A
1	2	1276	U
1	2	1284	C
1	2	1285	U
1	2	1292	G
1	2	1293	U
1	2	1295	G
1	2	1301	U
1	2	1307	U
1	2	1308	G
1	2	1314	U
1	2	1315	U
1	2	1320	U
1	2	1321	A
1	2	1322	A
1	2	1323	C
1	2	1324	G
1	2	1325	A
1	2	1326	A
1	2	1337	A
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1349	G
1	2	1360	A
1	2	1361	U
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U

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Mol	Chain	Res	Type
1	2	1373	C
1	2	1378	U
1	2	1382	A
1	2	1383	G
1	2	1389	C
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1406	A
1	2	1407	U
1	2	1409	G
1	2	1414	U
1	2	1415	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1436	A
1	2	1437	U
1	2	1438	G
1	2	1445	G
1	2	1446	A
1	2	1458	G
1	2	1459	C
1	2	1460	A
1	2	1468	U
1	2	1469	A
1	2	1471	A
1	2	1472	C
1	2	1474	G
1	2	1479	A
1	2	1482	C
1	2	1491	U
1	2	1493	A
1	2	1496	U
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G

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Mol	Chain	Res	Type
1	2	1523	G
1	2	1524	A
1	2	1528	U
1	2	1530	C
1	2	1531	G
1	2	1537	C
1	2	1540	G
1	2	1542	G
1	2	1543	A
1	2	1545	A
1	2	1556	A
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1570	A
1	2	1572	G
1	2	1574	G
1	2	1575	G
1	2	1582	U
1	2	1583	A
1	2	1585	U
1	2	1600	A
1	2	1601	G
1	2	1611	A
1	2	1613	U
1	2	1616	G
1	2	1619	C
1	2	1631	A
1	2	1634	C
1	2	1637	C
1	2	1657	U
1	2	1658	G
1	2	1659	A
1	2	1682	U
1	2	1689	A
1	2	1693	A
1	2	1694	A
1	2	1695	G
1	2	1698	G
1	2	1700	C
1	2	1701	A
1	2	1705	C

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Mol	Chain	Res	Type
1	2	1708	U
1	2	1709	C
1	2	1712	A
1	2	1717	G
1	2	1719	A
1	2	1736	G
1	2	1755	A
1	2	1757	G
1	2	1762	A
1	2	1767	G
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
1	2	1797	A
1	2	1799	U
2	A	14	U
2	A	26	A
2	A	40	A
2	A	43	A
2	A	49	A
2	A	59	G
2	A	60	A
2	A	65	A
2	A	66	A
2	A	77	A
2	A	92	G
2	A	99	A
2	A	109	A
2	A	110	G
2	A	111	C
2	A	116	A
2	A	117	U
2	A	118	U
2	A	122	A
2	A	135	C
2	A	136	G

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Mol	Chain	Res	Type
2	A	148	G
2	A	156	G
2	A	157	A
2	A	165	A
2	A	172	G
2	A	173	G
2	A	190	U
2	A	219	A
2	A	221	A
2	A	234	G
2	A	240	U
2	A	241	G
2	A	243	G
2	A	245	U
2	A	247	C
2	A	252	U
2	A	263	C
2	A	269	G
2	A	286	U
2	A	295	A
2	A	298	U
2	A	305	U
2	A	315	C
2	A	321	C
2	A	329	U
2	A	346	C
2	A	361	A
2	A	376	G
2	A	398	A
2	A	401	U
2	A	402	A
2	A	403	C
2	A	420	G
2	A	421	G
2	A	422	A
2	A	490	A
2	A	491	C
2	A	492	U
2	A	518	G
2	A	519	A
2	A	521	A
2	A	523	A

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Mol	Chain	Res	Type
2	A	533	A
2	A	557	A
2	A	558	U
2	A	559	A
2	A	589	A
2	A	601	U
2	A	602	A
2	A	604	G
2	A	611	A
2	A	636	C
2	A	637	C
2	A	638	C
2	A	646	A
2	A	649	A
2	A	667	C
2	A	677	A
2	A	678	G
2	A	681	U
2	A	683	U
2	A	690	A
2	A	691	A
2	A	705	A
2	A	712	G
2	A	758	C
2	A	761	A
2	A	766	U
2	A	767	U
2	A	780	A
2	A	781	G
2	A	785	G
2	A	786	A
2	A	799	G
2	A	817	A
2	A	826	G
2	A	830	A
2	A	836	A
2	A	846	A
2	A	848	A
2	A	849	C
2	A	857	G
2	A	861	C
2	A	874	U

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Mol	Chain	Res	Type
2	A	879	U
2	A	880	G
2	A	896	A
2	A	907	G
2	A	908	G
2	A	914	A
2	A	916	G
2	A	917	A
2	A	921	A
2	A	924	G
2	A	937	G
2	A	944	C
2	A	959	C
2	A	960	U
2	A	974	G
2	A	979	U
2	A	980	A
2	A	1006	A
2	A	1008	U
2	A	1016	C
2	A	1018	G
2	A	1020	G
2	A	1021	G
2	A	1022	U
2	A	1047	A
2	A	1064	A
2	A	1072	G
2	A	1081	U
2	A	1087	G
2	A	1093	A
2	A	1094	U
2	A	1096	U
2	A	1097	G
2	A	1098	A
2	A	1103	A
2	A	1104	G
2	A	1117	G
2	A	1131	G
2	A	1143	A
2	A	1153	A
2	A	1159	A
2	A	1178	G

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Mol	Chain	Res	Type
2	A	1180	A
2	A	1181	U
2	A	1182	A
2	A	1189	C
2	A	1191	U
2	A	1193	A
2	A	1196	C
2	A	1197	A
2	A	1201	C
2	A	1209	G
2	A	1222	G
2	A	1235	U
2	A	1236	G
2	A	1245	A
2	A	1246	G
2	A	1252	A
2	A	1253	U
2	A	1257	C
2	A	1258	U
2	A	1263	A
2	A	1272	C
2	A	1287	A
2	A	1302	A
2	A	1307	G
2	A	1308	A
2	A	1317	A
2	A	1325	U
2	A	1330	A
2	A	1331	U
2	A	1348	U
2	A	1349	G
2	A	1350	A
2	A	1352	A
2	A	1357	G
2	A	1386	A
2	A	1392	G
2	A	1399	A
2	A	1400	G
2	A	1406	A
2	A	1407	A
2	A	1417	G
2	A	1418	A

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Mol	Chain	Res	Type
2	A	1434	G
2	A	1437	C
2	A	1446	A
2	A	1470	U
2	A	1483	G
2	A	1487	G
2	A	1488	G
2	A	1495	U
2	A	1507	G
2	A	1508	C
2	A	1511	U
2	A	1553	U
2	A	1556	C
2	A	1557	A
2	A	1560	G
2	A	1562	C
2	A	1563	C
2	A	1568	U
2	A	1569	U
2	A	1570	U
2	A	1571	A
2	A	1573	G
2	A	1581	C
2	A	1582	C
2	A	1583	A
2	A	1589	A
2	A	1593	A
2	A	1594	A
2	A	1605	A
2	A	1621	A
2	A	1629	U
2	A	1630	U
2	A	1637	A
2	A	1643	A
2	A	1645	U
2	A	1657	C
2	A	1694	U
2	A	1713	G
2	A	1724	U
2	A	1741	A
2	A	1750	A
2	A	1751	G

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Mol	Chain	Res	Type
2	A	1753	G
2	A	1759	C
2	A	1762	C
2	A	1763	U
2	A	1765	U
2	A	1767	C
2	A	1773	C
2	A	1775	G
2	A	1796	G
2	A	1797	A
2	A	1808	G
2	A	1812	G
2	A	1815	U
2	A	1816	A
2	A	1821	U
2	A	1835	A
2	A	1840	U
2	A	1842	A
2	A	1846	C
2	A	1866	C
2	A	1878	G
2	A	1879	A
2	A	1880	U
2	A	1884	A
2	A	1893	A
2	A	1906	G
2	A	1952	G
2	A	2101	C
2	A	2102	U
2	A	2111	G
2	A	2112	U
2	A	2114	C
2	A	2122	G
2	A	2131	A
2	A	2158	A
2	A	2167	A
2	A	2169	G
2	A	2170	U
2	A	2188	A
2	A	2194	G
2	A	2205	U
2	A	2206	G

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Mol	Chain	Res	Type
2	A	2222	A
2	A	2223	A
2	A	2242	A
2	A	2244	A
2	A	2249	G
2	A	2252	A
2	A	2255	A
2	A	2256	A
2	A	2272	G
2	A	2273	G
2	A	2274	U
2	A	2281	A
2	A	2287	C
2	A	2306	C
2	A	2307	G
2	A	2310	U
2	A	2315	G
2	A	2319	U
2	A	2320	A
2	A	2336	U
2	A	2372	A
2	A	2373	A
2	A	2374	C
2	A	2375	G
2	A	2376	G
2	A	2393	G
2	A	2394	G
2	A	2397	A
2	A	2402	A
2	A	2403	G
2	A	2404	A
2	A	2411	U
2	A	2418	G
2	A	2435	G
2	A	2437	G
2	A	2438	A
2	A	2440	G
2	A	2441	A
2	A	2444	C
2	A	2445	A
2	A	2453	U
2	A	2454	G

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Mol	Chain	Res	Type
2	A	2455	U
2	A	2456	A
2	A	2458	A
2	A	2459	A
2	A	2461	A
2	A	2462	A
2	A	2463	G
2	A	2468	A
2	A	2469	G
2	A	2474	G
2	A	2477	G
2	A	2480	A
2	A	2484	A
2	A	2487	U
2	A	2488	A
2	A	2491	A
2	A	2492	C
2	A	2493	U
2	A	2494	A
2	A	2495	C
2	A	2498	U
2	A	2499	U
2	A	2500	A
2	A	2501	U
2	A	2502	A
2	A	2504	U
2	A	2505	U
2	A	2509	U
2	A	2514	U
2	A	2515	A
2	A	2523	A
2	A	2526	C
2	A	2532	U
2	A	2533	G
2	A	2534	G
2	A	2535	A
2	A	2540	A
2	A	2541	U
2	A	2547	A
2	A	2549	G
2	A	2552	C
2	A	2555	G

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Mol	Chain	Res	Type
2	A	2557	A
2	A	2560	C
2	A	2561	A
2	A	2569	A
2	A	2570	U
2	A	2571	U
2	A	2585	G
2	A	2587	U
2	A	2593	A
2	A	2606	G
2	A	2607	G
2	A	2614	G
2	A	2652	U
2	A	2656	A
2	A	2657	A
2	A	2672	G
2	A	2674	A
2	A	2678	A
2	A	2689	A
2	A	2690	G
2	A	2691	A
2	A	2696	A
2	A	2704	A
2	A	2712	U
2	A	2713	U
2	A	2728	G
2	A	2729	U
2	A	2737	C
2	A	2746	A
2	A	2749	G
2	A	2753	G
2	A	2755	C
2	A	2772	C
2	A	2773	C
2	A	2777	G
2	A	2778	G
2	A	2779	A
2	A	2795	U
2	A	2796	G
2	A	2799	A
2	A	2800	G
2	A	2801	A

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Mol	Chain	Res	Type
2	A	2802	A
2	A	2804	A
2	A	2808	A
2	A	2810	C
2	A	2817	A
2	A	2821	C
2	A	2828	G
2	A	2843	U
2	A	2844	C
2	A	2847	A
2	A	2860	U
2	A	2861	U
2	A	2867	C
2	A	2871	G
2	A	2873	U
2	A	2887	A
2	A	2889	C
2	A	2899	C
2	A	2911	A
2	A	2935	U
2	A	2936	A
2	A	2941	A
2	A	2951	G
2	A	2954	U
2	A	2971	A
2	A	2972	G
2	A	2979	U
2	A	2983	C
2	A	2997	G
2	A	3003	G
2	A	3005	A
2	A	3012	A
2	A	3028	G
2	A	3051	U
2	A	3055	U
2	A	3059	G
2	A	3078	U
2	A	3086	A
2	A	3092	C
2	A	3093	C
2	A	3101	G
2	A	3113	A

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Mol	Chain	Res	Type
2	A	3115	C
2	A	3117	C
2	A	3122	A
2	A	3130	A
2	A	3131	U
2	A	3142	A
2	A	3143	C
2	A	3154	C
2	A	3156	U
2	A	3157	U
2	A	3167	A
2	A	3168	A
2	A	3171	U
2	A	3172	A
2	A	3173	G
2	A	3174	A
2	A	3176	G
2	A	3179	U
2	A	3181	C
2	A	3187	A
2	A	3198	U
2	A	3207	U
2	A	3212	C
2	A	3213	A
2	A	3214	U
2	A	3217	C
2	A	3218	A
2	A	3219	G
2	A	3228	C
2	A	3235	C
2	A	3244	A
2	A	3247	G
2	A	3260	G
2	A	3268	A
2	A	3270	U
2	A	3271	G
2	A	3273	A
2	A	3276	G
2	A	3277	U
2	A	3278	C
2	A	3279	A
2	A	3281	U

Continued on next page...

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Mol	Chain	Res	Type
2	A	3304	U
2	A	3313	U
2	A	3316	A
2	A	3319	U
2	A	3331	U
2	A	3341	U
2	A	3350	C
2	A	3351	U
2	A	3352	U
2	A	3353	G
2	A	3363	U
2	A	3369	G
2	A	3378	C
2	A	3382	U
2	A	3390	G
3	B	7	G
3	B	11	A
3	B	22	A
3	B	26	C
3	B	52	G
3	B	53	U
3	B	54	U
3	B	65	G
3	B	74	C
3	B	76	A
3	B	99	G
3	B	102	A
3	B	112	G
3	B	121	U
4	C	16	G
4	C	23	U
4	C	34	U
4	C	35	C
4	C	39	G
4	C	46	G
4	C	49	G
4	C	51	G
4	C	59	A
4	C	62	C
4	C	63	G
4	C	79	A
4	C	80	A

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Mol	Chain	Res	Type
4	C	81	U
4	C	82	U
4	C	83	C
4	C	84	C
4	C	86	U
4	C	87	G
4	C	90	U
4	C	95	G
4	C	104	A
4	C	106	C
4	C	111	A
4	C	112	U
4	C	113	U
4	C	116	G
4	C	125	U
4	C	126	A
4	C	129	C
4	C	152	G
4	C	157	U
4	C	158	U
45	t	2	G
45	t	9	G
45	t	16	U
45	t	19	G
45	t	20	A
45	t	21	A
45	t	42	U
45	t	46	G
45	t	47	U
45	t	48	C
45	t	59	A
45	t	61	C
45	t	63	G
45	t	64	A
45	t	74	C
45	t	75	C
45	t	76	A
45	u	16	U
45	u	19	G
45	u	20	A
45	u	21	A
45	u	32	C

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Mol	Chain	Res	Type
45	u	36	U
45	u	40	C
45	u	42	U
45	u	46	G
45	u	47	U
45	u	48	C
45	u	54	A
45	u	63	G
45	u	64	A
45	u	69	C
45	u	74	C
45	u	75	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	68	A
1	2	77	U
1	2	139	C
1	2	215	A
1	2	224	C
1	2	237	C
1	2	322	G
1	2	352	A
1	2	387	A
1	2	400	A
1	2	447	U
1	2	541	A
1	2	555	A
1	2	609	U
1	2	639	U
1	2	705	U
1	2	711	U
1	2	819	G
1	2	912	U
1	2	928	U
1	2	1023	A
1	2	1226	A
1	2	1245	G
1	2	1256	A
1	2	1273	G
1	2	1274	C

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Mol	Chain	Res	Type
1	2	1321	A
1	2	1323	C
1	2	1344	A
1	2	1382	A
1	2	1430	U
1	2	1471	A
1	2	1557	U
1	2	1584	G
1	2	1633	A
1	2	1636	C
1	2	1657	U
2	A	1562	C
2	A	2168	A
2	A	2533	G
2	A	2842	U
2	A	3004	C
2	A	3121	U
3	B	52	G
4	C	85	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

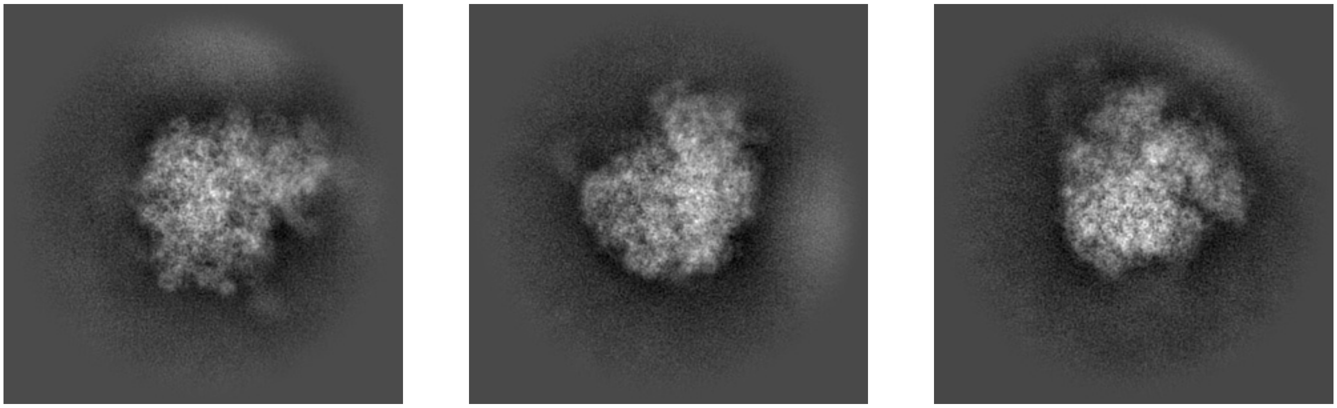
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-38668. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

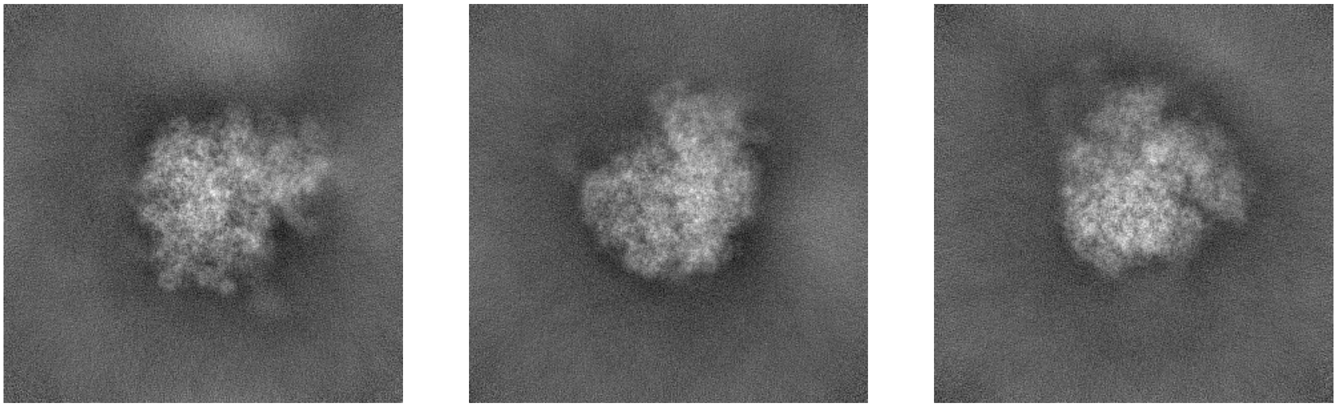
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

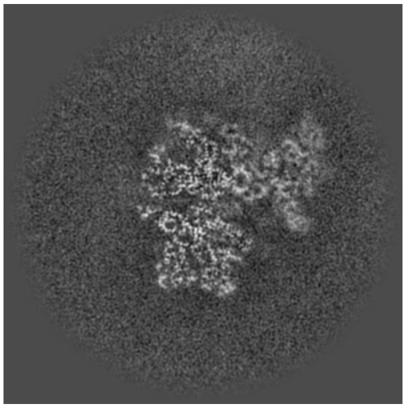


X Y Z

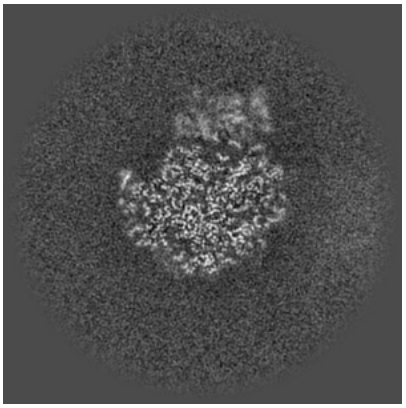
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

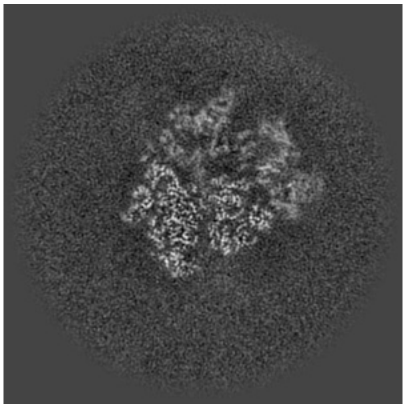
6.2.1 Primary map



X Index: 200

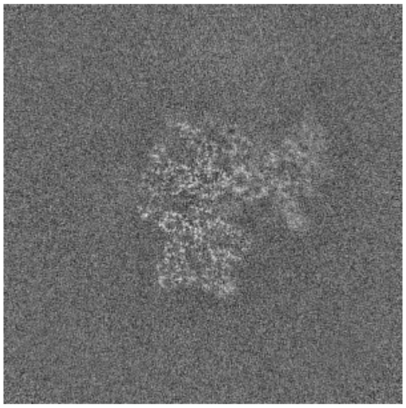


Y Index: 200

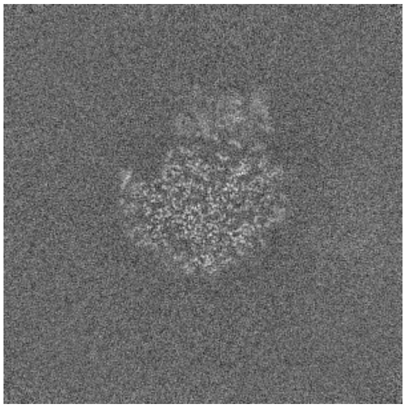


Z Index: 200

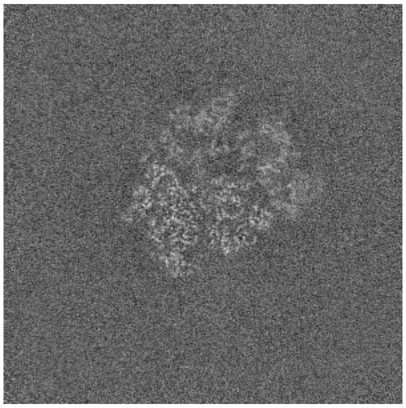
6.2.2 Raw map



X Index: 200



Y Index: 200

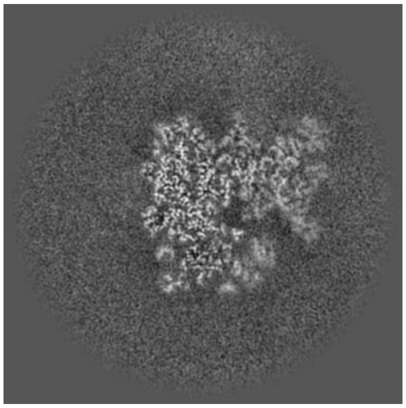


Z Index: 200

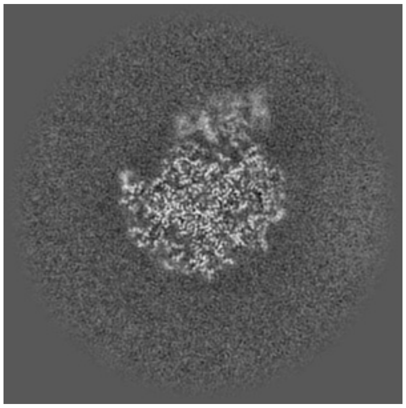
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

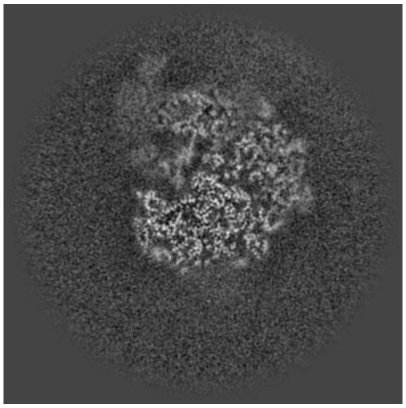
6.3.1 Primary map



X Index: 213

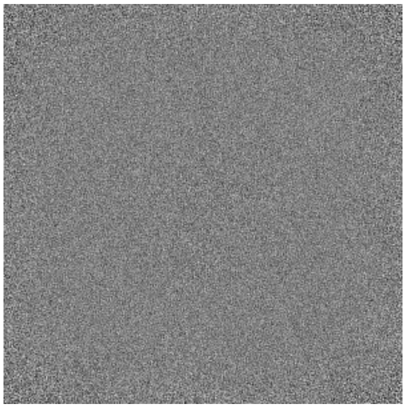


Y Index: 198

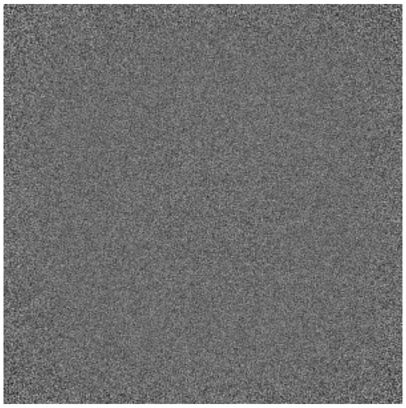


Z Index: 223

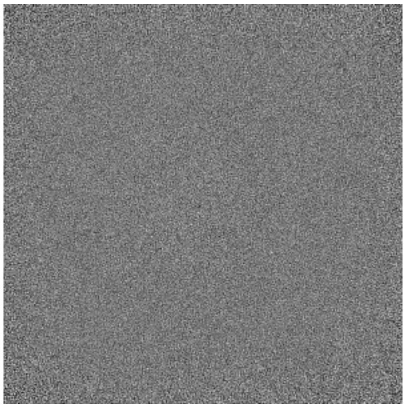
6.3.2 Raw map



X Index: 0



Y Index: 0

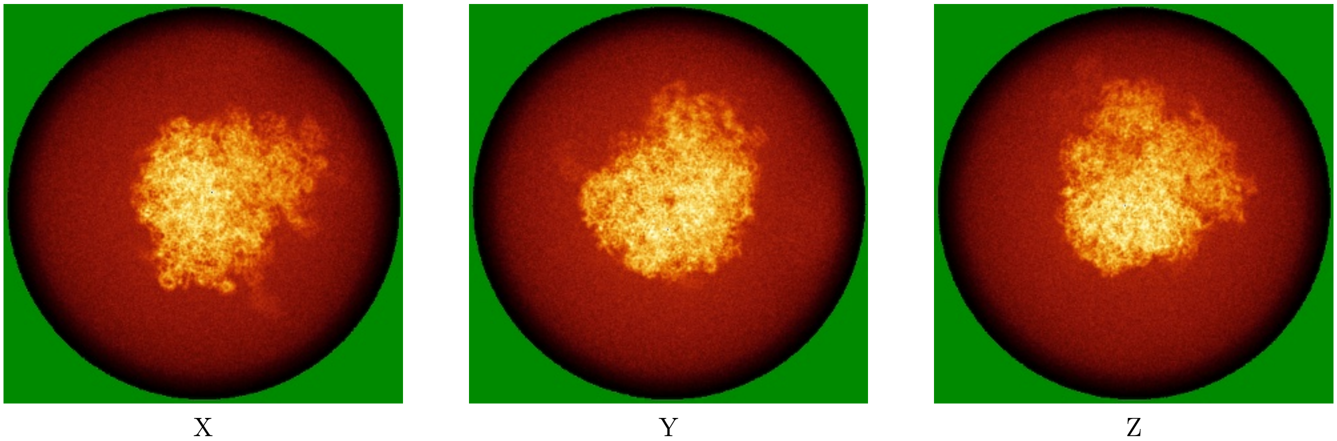


Z Index: 0

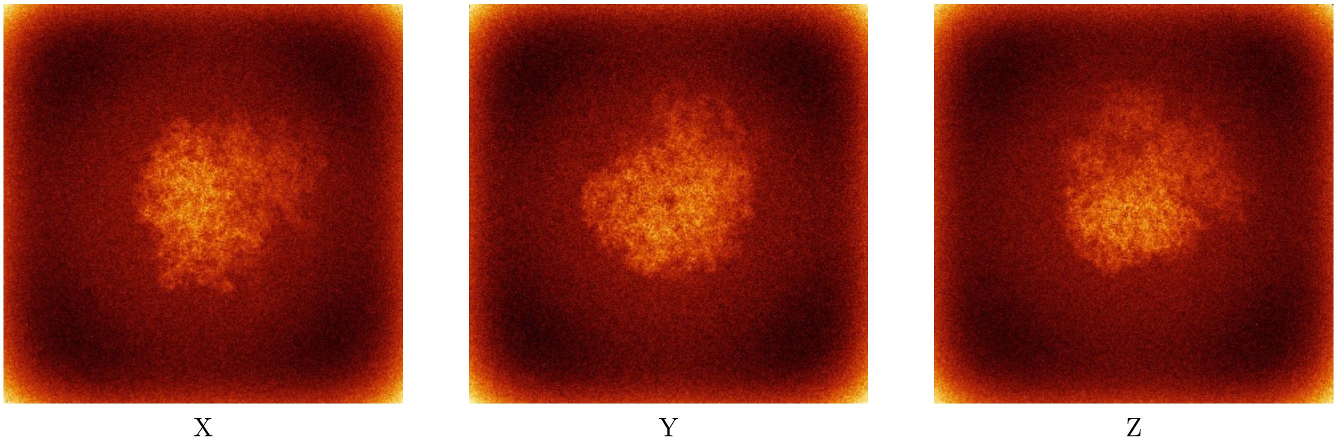
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map


X Y Z

6.4.2 Raw map


X Y Z

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

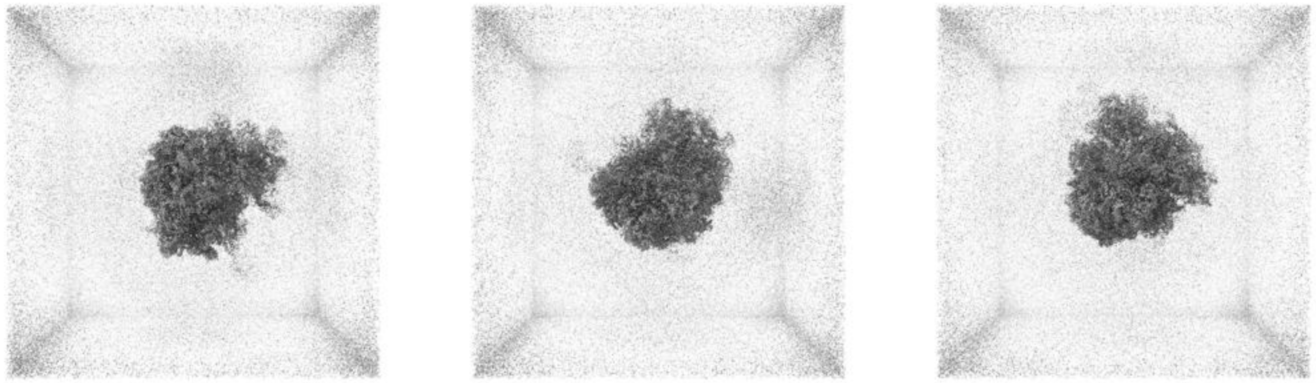
6.5 Orthogonal surface views

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

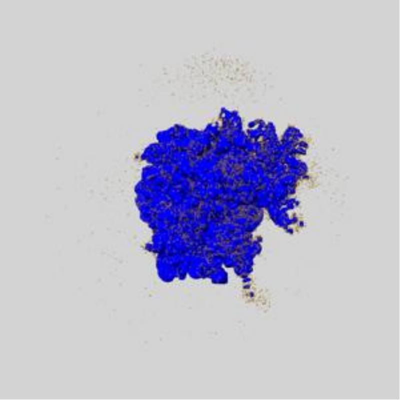
6.6 Mask visualisation

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

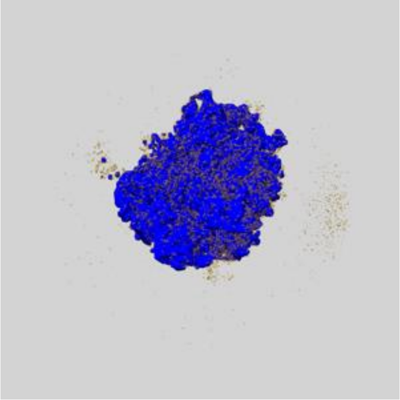
A mask typically either:

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

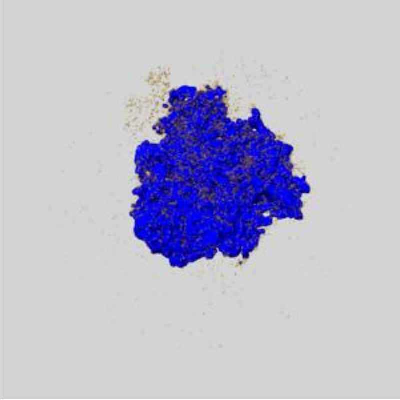
6.6.1 emd_38668_msk_1.map



X



Y

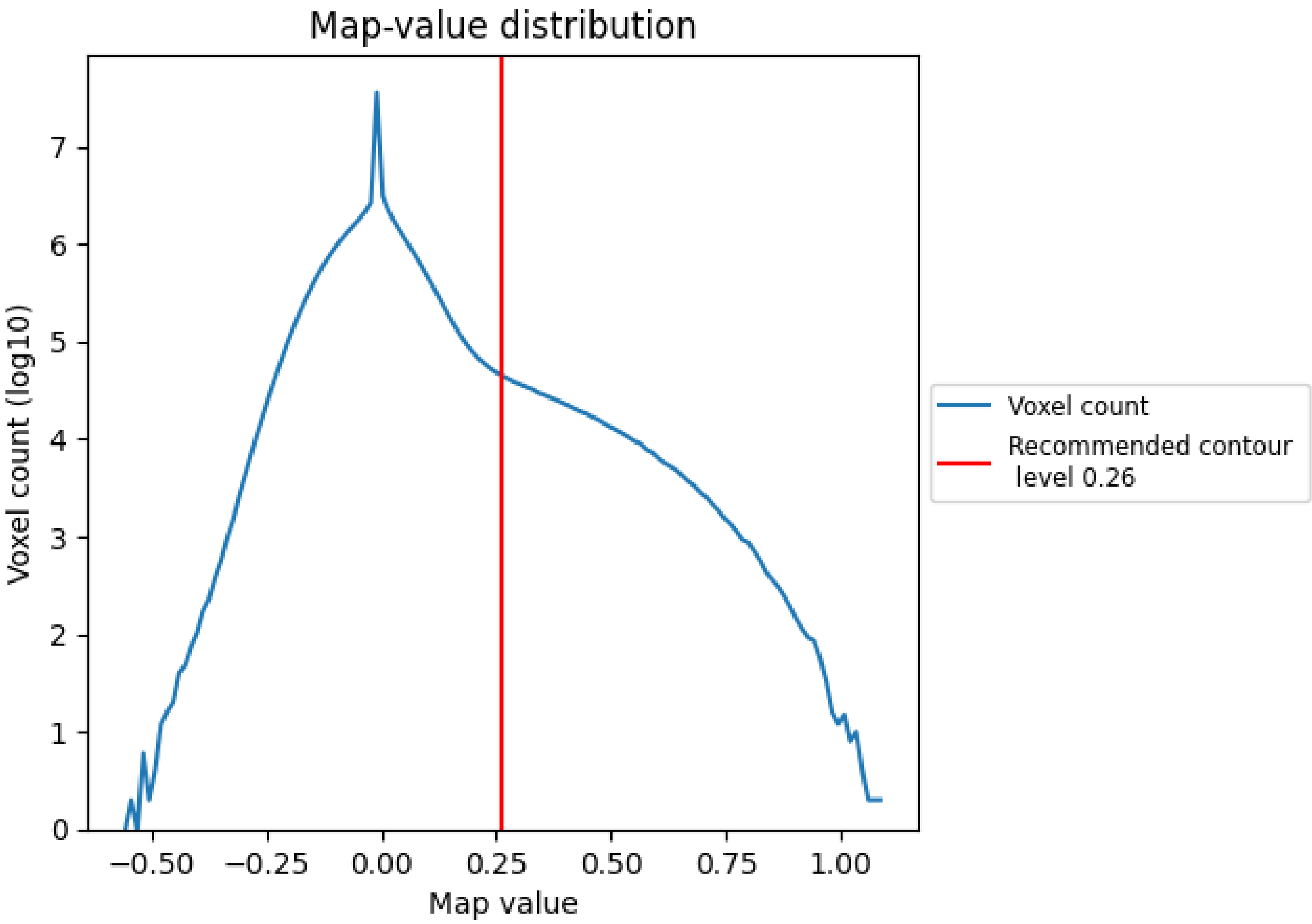


Z

7 Map analysis ⓘ

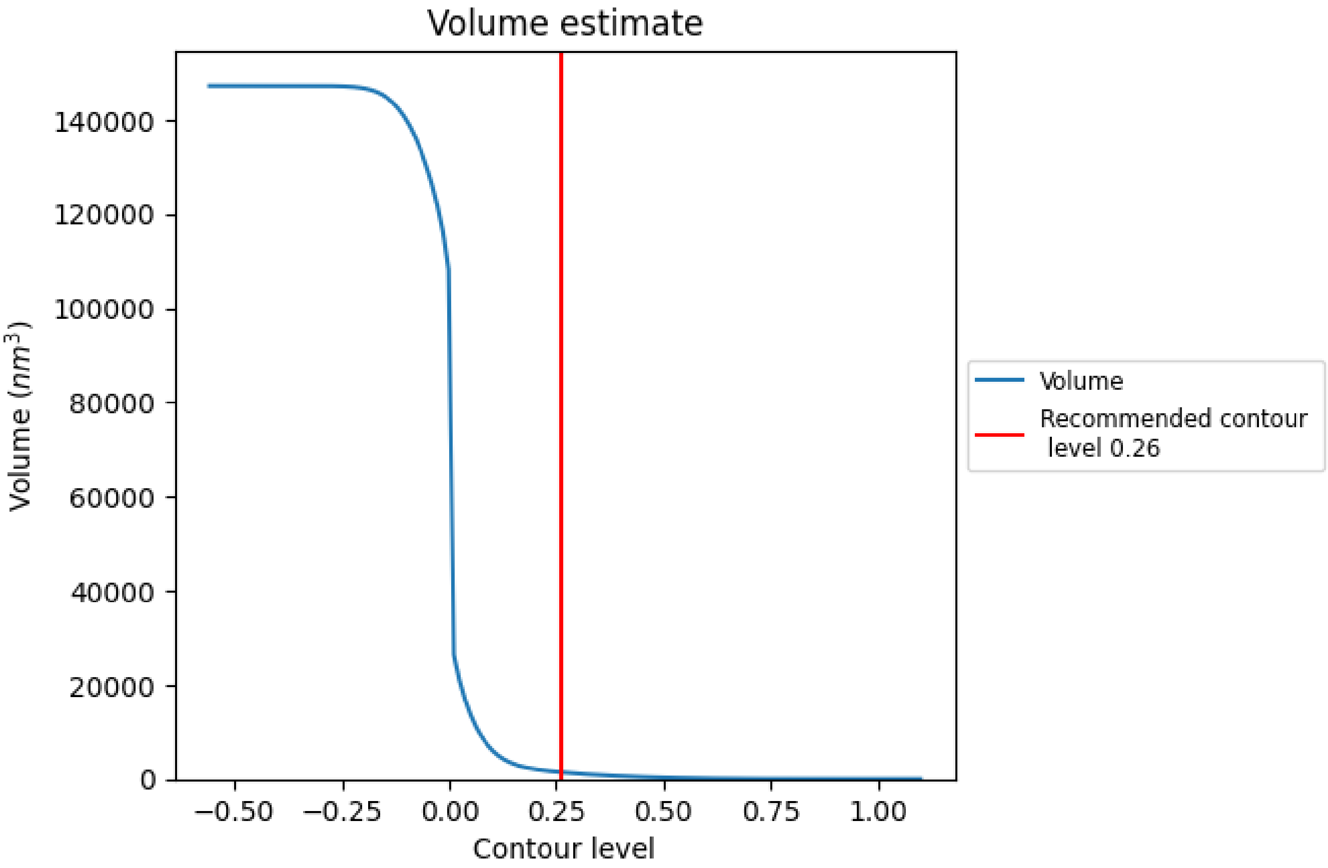
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

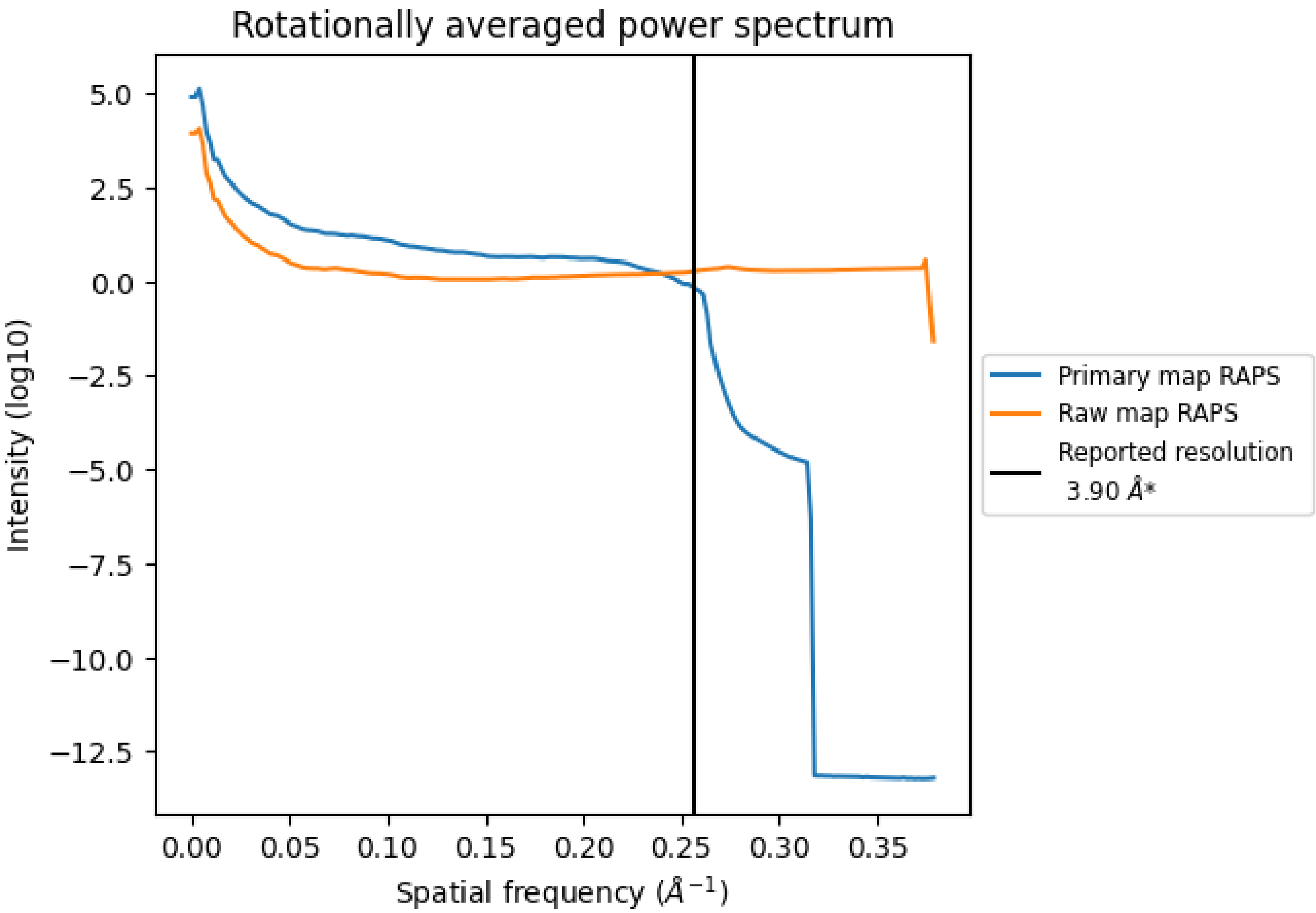
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1459 nm^3; this corresponds to an approximate mass of 1318 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 ⓘ

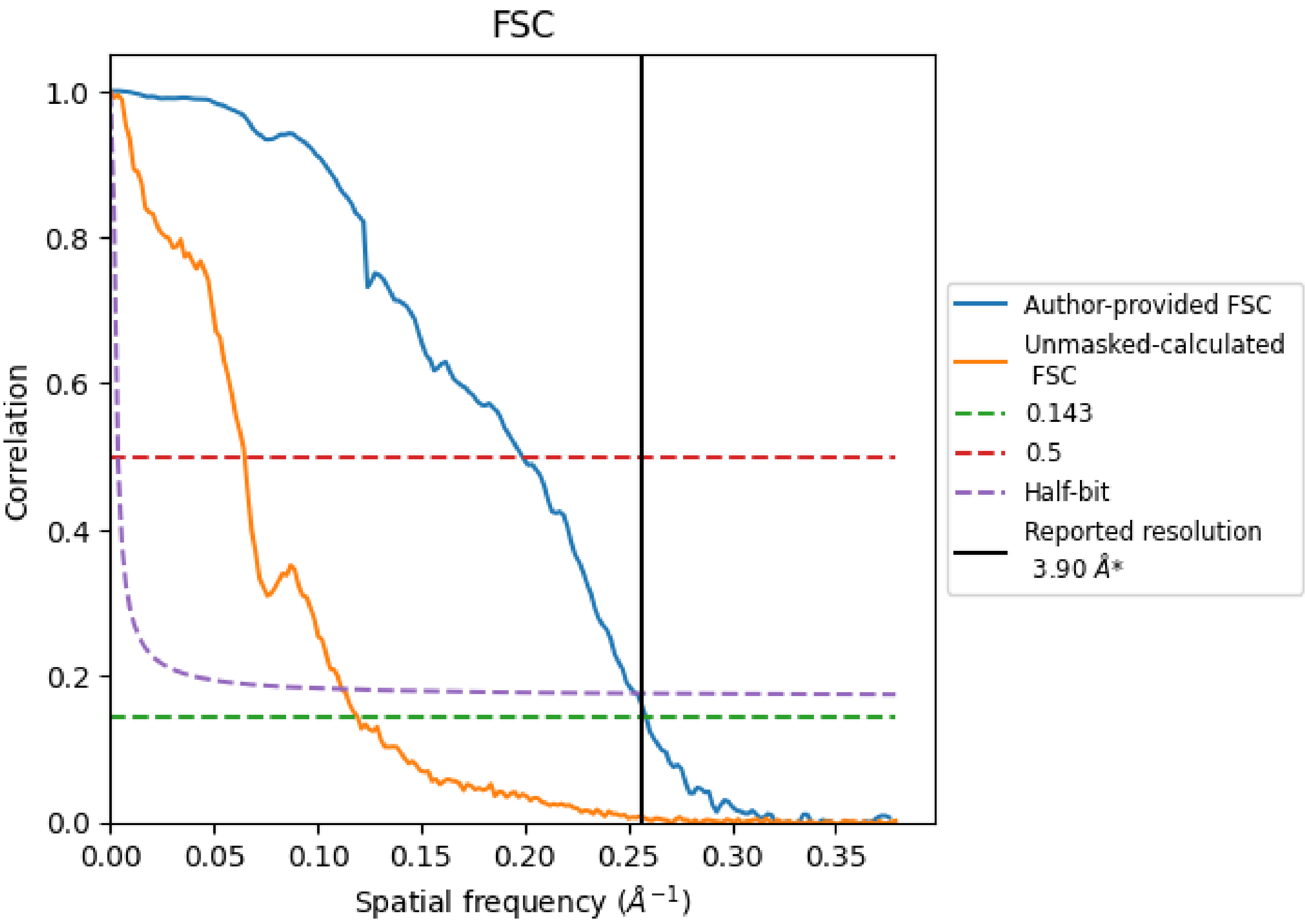


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

8.2 Resolution estimates ⓘ

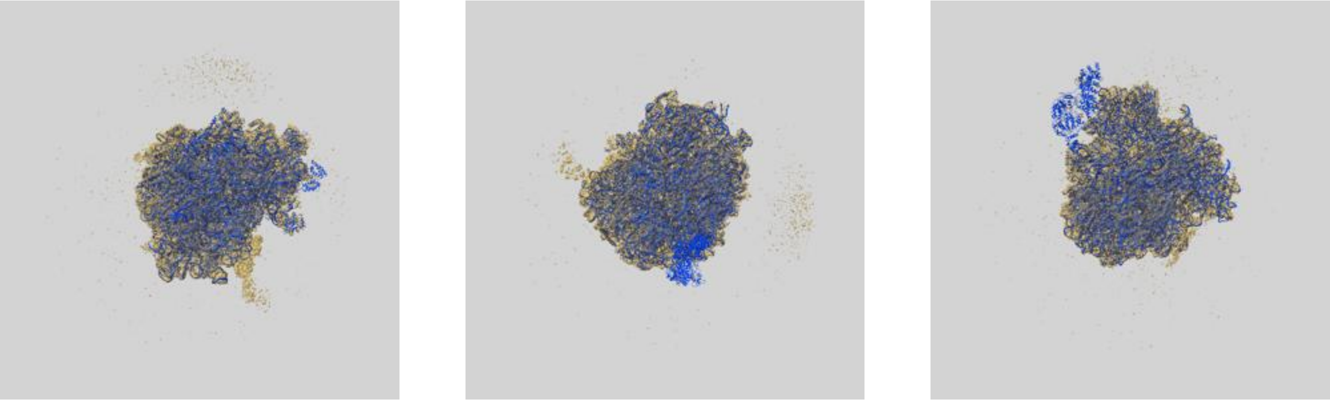
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.87	5.03	3.94
Unmasked-calculated*	8.38	15.43	8.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.38 differs from the reported value 3.9 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38668 and PDB model 8YLR. Per-residue inclusion information can be found in section 3 on page 18.

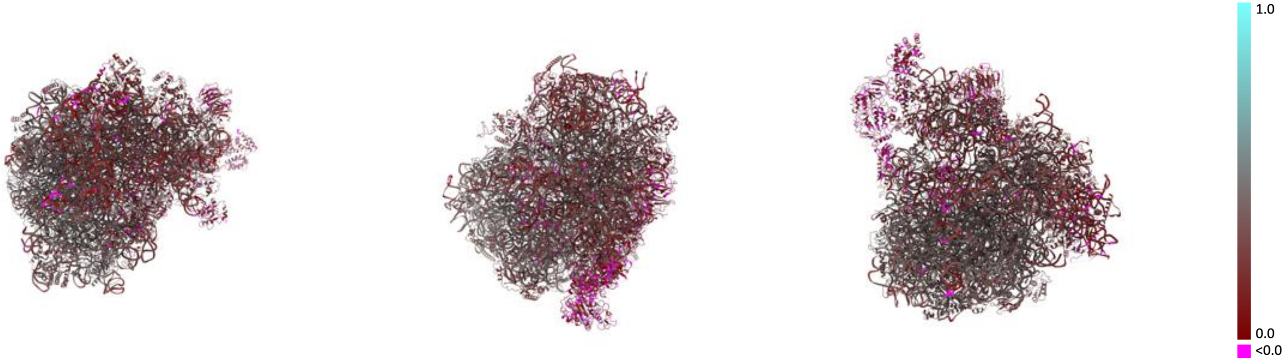
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

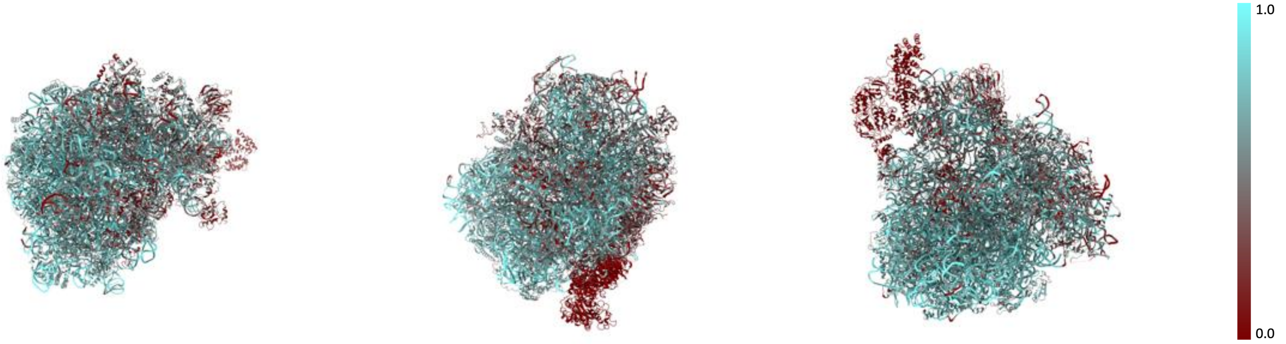
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

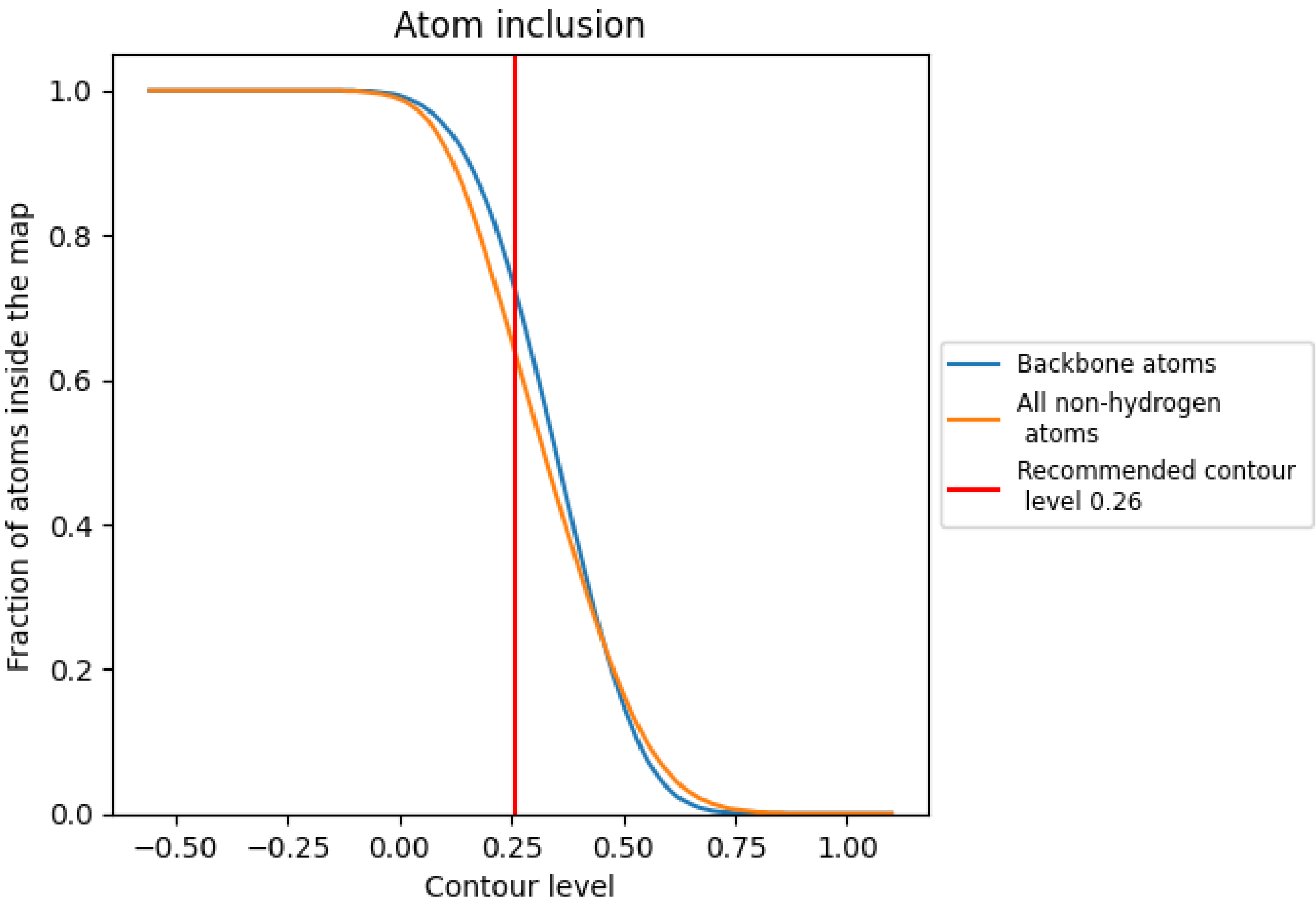
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.26).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 63% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.3220
2	0.7110	0.2750
A	0.8340	0.3660
B	0.8880	0.3710
C	0.8560	0.3830
D	0.5970	0.4190
E	0.6230	0.4050
F	0.6420	0.4070
G	0.6070	0.3380
H	0.6120	0.3760
I	0.6340	0.3800
J	0.6100	0.3630
K	0.6110	0.3740
L	0.5790	0.3590
M	0.5670	0.3110
N	0.6560	0.3950
O	0.6760	0.3830
P	0.6000	0.4110
Q	0.6350	0.3810
R	0.6110	0.3970
S	0.6150	0.4060
SA	0.3540	0.2780
SB	0.2940	0.2160
SC	0.3540	0.2490
SD	0.1790	0.1680
SE	0.2990	0.2650
SF	0.3580	0.2740
SG	0.4030	0.2290
SH	0.3650	0.2750
SI	0.3640	0.2550
SJ	0.3590	0.2840
SK	0.3100	0.2490
SL	0.2310	0.2190
SM	0.5080	0.3250
SN	0.1830	0.1620

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Chain	Atom inclusion	Q-score
SO	0.2870	0.1660
SP	0.4620	0.2770
SQ	0.3390	0.1880
SR	0.5150	0.3340
SS	0.3370	0.2550
ST	0.3780	0.2630
SU	0.4060	0.2690
SV	0.4540	0.3050
SW	0.4490	0.2830
SX	0.4080	0.3340
SY	0.4270	0.2890
SZ	0.3710	0.2060
Sa	0.4380	0.3040
Sb	0.4660	0.3200
Sc	0.3890	0.3270
Sd	0.3750	0.2260
Se	0.4670	0.3080
Sf	0.3990	0.2590
Sg	0.3620	0.2940
T	0.5950	0.3570
U	0.6280	0.4110
V	0.6020	0.4050
W	0.5770	0.3500
X	0.5640	0.3990
Y	0.5040	0.3160
Z	0.6200	0.3940
a	0.6440	0.3990
b	0.6230	0.3730
c	0.6590	0.4210
d	0.5800	0.3880
e	0.6040	0.3540
f	0.5710	0.3990
g	0.5860	0.4090
h	0.6630	0.4090
i	0.5560	0.4000
j	0.6290	0.3680
k	0.6390	0.3840
l	0.6380	0.4280
m	0.5780	0.3790
n	0.5450	0.3880
o	0.6060	0.4040
p	0.5430	0.3630

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Chain	Atom inclusion	Q-score
q	0.5640	0.4190
r	0.5770	0.3850
t	0.2710	0.1440
u	0.5570	0.1940
v	0.0150	0.1270
x	0.3320	0.2630