



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 05:49 pm BST

PDB ID : 9QQL / pdb_00009qql
EMDB ID : EMD-53307
Title : Mouse RPS15 P131 Mutant Ribosome POST translocation state
Authors : Santo, P.E.; Astier, A.; Plisson-Chastang, C.
Deposited on : 2025-04-01
Resolution : 3.09 Å(reported)
Based on initial model : 7LS1

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

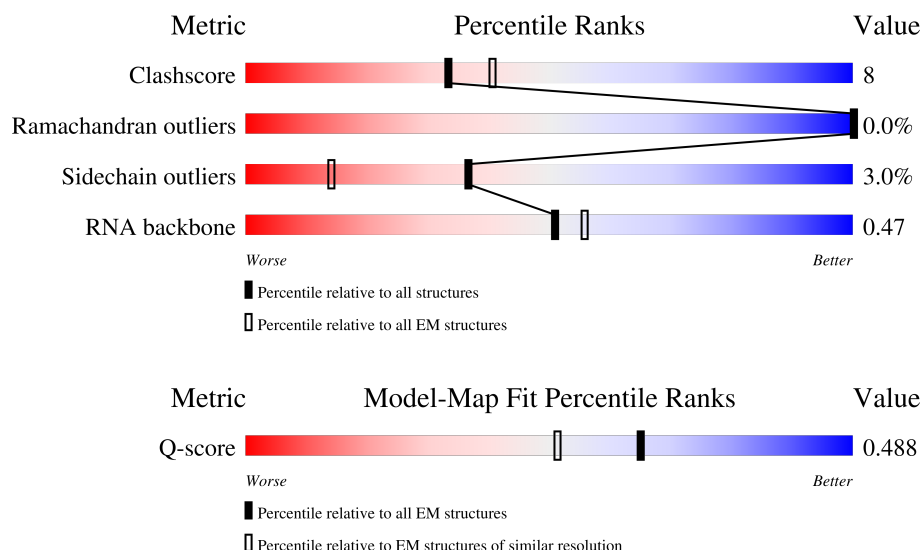
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.09 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14003 (2.59 - 3.59)

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

Mol	Chain	Length	Quality of chain
1	A1	270	6% 59% 23% 18%
2	A2	3615	18% 57% 36% 7%
3	A3	152	74% 58% 33% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B1	266	
5	B2	121	
6	B3	145	
7	Bv	76	
7	n2	76	
8	Bx	10	
9	C1	192	
10	C2	156	
11	C3	119	
12	D1	214	
13	D2	257	
14	D3	83	
15	E1	178	
16	E2	403	
17	E3	143	
18	F1	211	
19	F2	419	
20	F3	114	
21	G1	217	
22	G2	297	
23	G3	69	
24	H1	204	
25	H2	296	
26	H3	56	
27	I2	203	

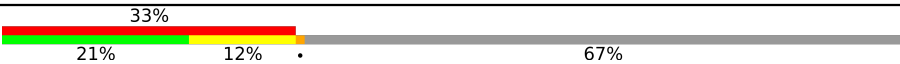
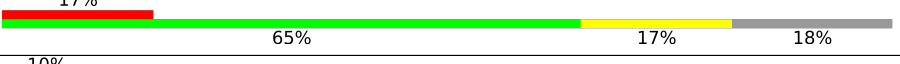
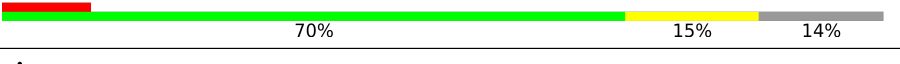
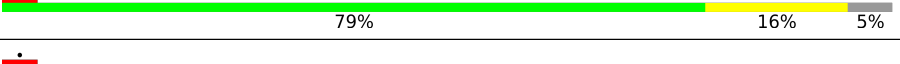
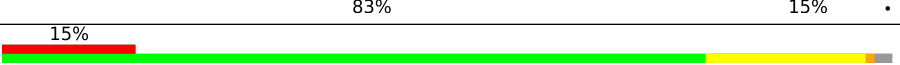
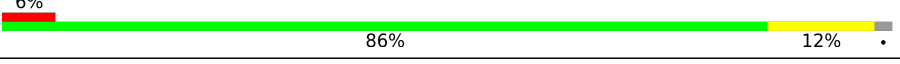
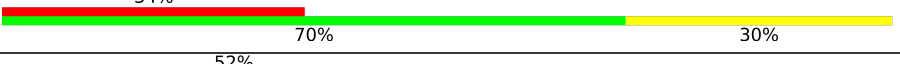
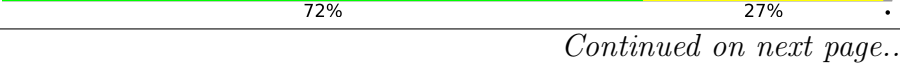
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	I3	317	
29	J2	184	
30	J3	293	
31	K2	188	
32	K3	249	
33	L1	217	
34	L2	196	
35	L3	194	
36	M2	176	
37	M3	132	
38	N2	160	
39	N3	151	
40	O2	128	
41	O3	151	
42	P2	140	
43	P3	130	
44	Q2	157	
45	Q3	133	
46	R2	156	
47	R3	125	
48	S2	145	
49	S3	84	
50	T2	136	
51	T3	133	
52	U2	148	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	U3	156	
54	V2	160	
55	W2	115	
56	X2	125	
57	Y2	135	
58	Z2	110	
59	a2	117	
60	b2	123	
61	c2	105	
62	d2	97	
63	e2	70	
64	f2	51	
65	g2	128	
66	h2	25	
67	i2	104	
68	j2	92	
69	k2	137	
70	m2	1635	
71	o2	295	
72	p2	264	
73	q2	243	
74	r2	263	
75	s2	204	
76	t2	194	
77	u2	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	v2	165	53% 35% 22% • 42%
79	w2	158	20% 68% 26% • 5%
80	x2	145	70% 54% 23% • 20%
81	y2	146	73% 63% 33% • •
82	z2	135	77% 75% 22% • •

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 213778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	222	Total	C	N	O	S	0	0
			1843	1185	353	297	8		

- Molecule 2 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	3615	Total	C	N	O	P	0	0
			77547	34568	14148	25217	3614		

- Molecule 3 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	140	Total	C	N	O	S	0	0
			1157	728	231	197	1		

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B1	223	Total	C	N	O	S	1	0
			1812	1156	351	301	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B2	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 6 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B3	141	Total	C	N	O	S	0	0
			1104	691	215	196	2		

- Molecule 7 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Bv	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		
7	n2	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 8 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Bx	10	Total	C	N	O	P	0	0
			200	90	20	80	10		

- Molecule 9 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	190	Total	C	N	O	S	0	0
			1519	956	284	273	6		

- Molecule 10 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C2	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 11 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C3	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D1	204	Total	C	N	O	S	0	0
			1656	1052	319	272	13		

- Molecule 13 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D2	251	Total	C	N	O	S	0	0
			1921	1204	393	318	6		

- Molecule 14 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D3	83	Total	C	N	O	S	0	0
			638	392	119	122	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E1	174	Total	C	N	O	S	0	0
			1397	880	260	251	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E2	402	Total	C	N	O	S	0	0
			3238	2060	609	555	14		

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E3	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 18 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F1	203	Total	C	N	O	S	0	0
			1643	1029	339	271	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F2	359	Total	C	N	O	S	0	0
			2867	1803	573	476	15		

- Molecule 20 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F3	98	Total	C	N	O	S	1	0
			789	491	164	129	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	?	-	ARG	deletion	UNP P62855

- Molecule 21 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G1	139	Total	C	N	O	S	0	0
			1143	732	221	183	7		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	G2	293	Total	C	N	O	S	0	0
			2389	1509	441	425	14		

- Molecule 23 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G3	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 24 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	H1	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 25 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	H2	221	Total	C	N	O	S	0	0
			1789	1145	342	298	4		

- Molecule 26 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H3	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

- Molecule 27 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I2	201	Total	C	N	O	S	0	0
			1640	1055	320	259	6		

- Molecule 28 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I3	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 29 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J2	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 30 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	J3	219	Total	C	N	O	S	0	0
			1700	1101	292	298	9		

- Molecule 31 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	K2	186	Total	C	N	O	S	0	0
			1511	946	313	248	4		

- Molecule 32 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K3	227	Total	C	N	O	S	0	0
			1840	1149	367	317	7		

- Molecule 33 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L1	161	Total	C	N	O	S	0	0
			1300	833	230	231	6		

- Molecule 34 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L2	179	Total	C	N	O	S	0	0
			1499	927	326	237	9		

- Molecule 35 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L3	184	Total	C	N	O	S	0	0
			1518	964	305	247	2		

- Molecule 36 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M2	175	Total	C	N	O	S	0	0
			1450	924	283	233	10		

- Molecule 37 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	M3	122	Total	C	N	O	S	0	0
			952	599	168	177	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M3	69	LEU	CYS	variant	UNP P63323

- Molecule 38 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N2	159	Total	C	N	O	S	0	0
			1299	824	252	217	6		

- Molecule 39 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N3	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O2	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	O3	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

- Molecule 42 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	P2	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 43 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	P3	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Q2	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 45 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Q3	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 47 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	R3	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 49 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S3	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 50 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 51 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	T3	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 52 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	U2	147	Total	C	N	O	S	0	0
			1164	736	239	185	4		

- Molecule 53 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U3	52	Total	C	N	O	S	0	0
			415	260	74	74	7		

- Molecule 54 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V2	117	Total	C	N	O	S	0	0
			945	596	198	146	5		

- Molecule 55 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W2	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 56 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 57 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y2	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 58 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Z2	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 59 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	a2	114	Total	C	N	O	S	0	0
			906	565	187	148	6		

- Molecule 60 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	b2	120	Total	C	N	O	S	0	0
			1001	634	201	165	1		

- Molecule 61 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	c2	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	d2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 63 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	e2	69	Total	C	N	O	S	0	0
			568	365	103	99	1		

- Molecule 64 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	f2	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 65 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	g2	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 66 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	h2	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 67 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	i2	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 68 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	j2	89	Total	C	N	O	S	0	0
			694	436	133	118	7		

- Molecule 69 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	k2	125	Total	C	N	O	S	0	0
			1001	621	207	168	5		

- Molecule 70 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	m2	1632	Total	C	N	O	P	0	0
			34879	15587	6261	11399	1632		

- Molecule 71 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	o2	214	Total	C	N	O	S	0	0
			1694	1077	297	312	8		

- Molecule 72 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	p2	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 73 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	q2	220	Total	C	N	O	S	0	0
			1711	1092	308	304	7		

- Molecule 74 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	r2	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 75 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	s2	183	Total	C	N	O	S	0	0
			1457	912	275	263	7		

- Molecule 76 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	t2	183	Total	C	N	O	S	0	0
			1278	822	243	213			

- Molecule 77 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	u2	206	Total	C	N	O	S	0	0
			1633	1025	322	281	5		

- Molecule 78 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	v2	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 79 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	w2	150	Total	C	N	O	S	0	0
			1220	776	228	210	6		

- Molecule 80 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	x2	116	Total	C	N	O	S	0	0
			959	610	178	164	7		

- Molecule 81 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	y2	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 82 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	z2	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
83	A2	82	Total	Mg	0
			82	82	
83	Bv	2	Total	Mg	0
			2	2	
83	H1	1	Total	Mg	0
			1	1	
83	J2	1	Total	Mg	0
			1	1	
83	P2	1	Total	Mg	0
			1	1	
83	d2	1	Total	Mg	0
			1	1	
83	m2	34	Total	Mg	0
			34	34	

- Molecule 84 is UNKNOWN (CCD ID: UNK) (formula: C₄H₉NO₂) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
84	A2	13	Total	C	N	O	0
			65	39	13	13	
84	Bv	1	Total	C	N	O	0
			5	3	1	1	
84	F2	3	Total	C	N	O	0
			15	9	3	3	
84	J2	1	Total	C	N	O	0
			5	3	1	1	
84	f2	4	Total	C	N	O	0
			20	12	4	4	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
85	F3	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

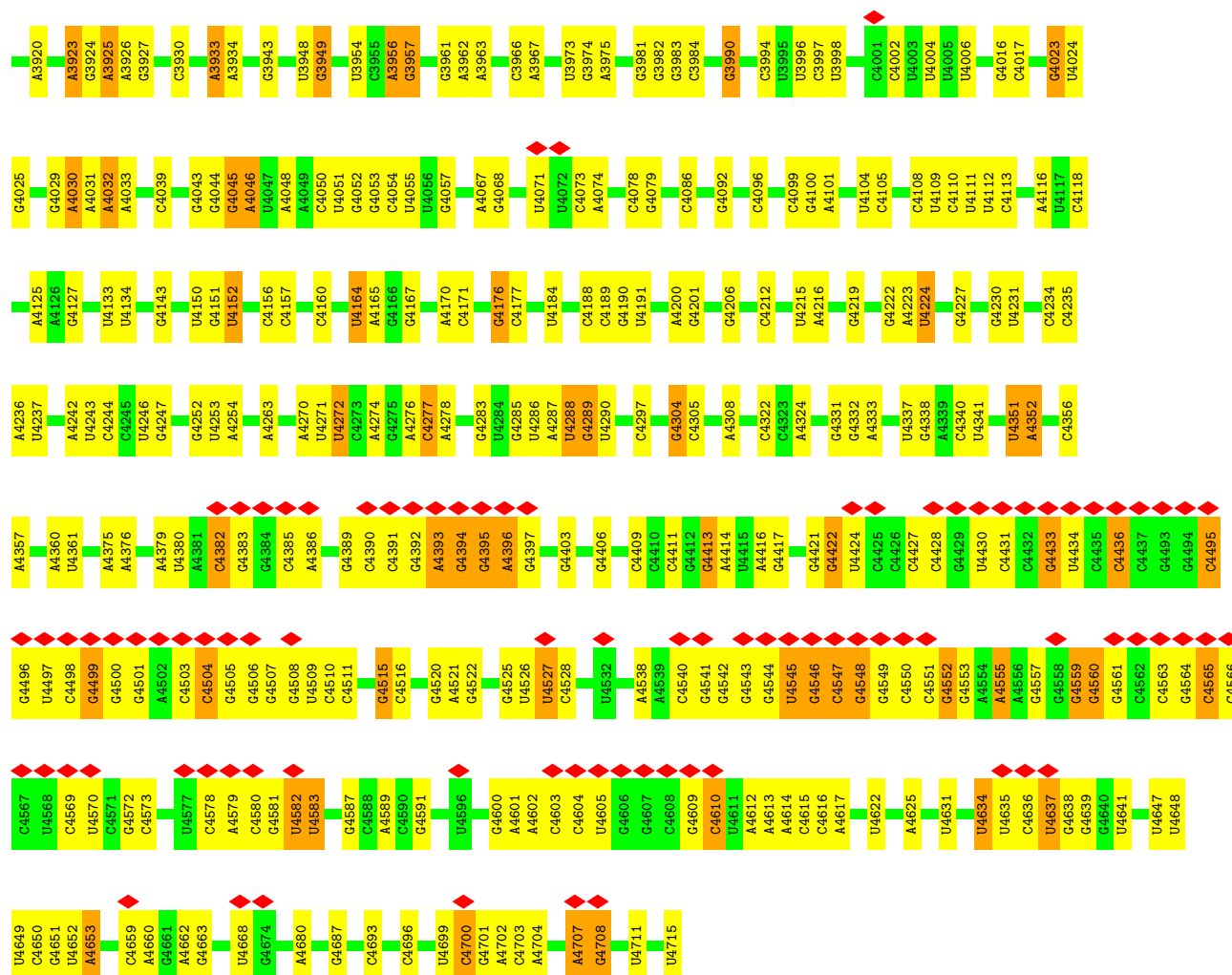
Mol	Chain	Residues	Atoms		AltConf
85	H3	1	Total 1	Zn 1	0
85	d2	1	Total 1	Zn 1	0
85	g2	1	Total 1	Zn 1	0
85	i2	1	Total 1	Zn 1	0
85	j2	1	Total 1	Zn 1	0

- Molecule 86 is water.

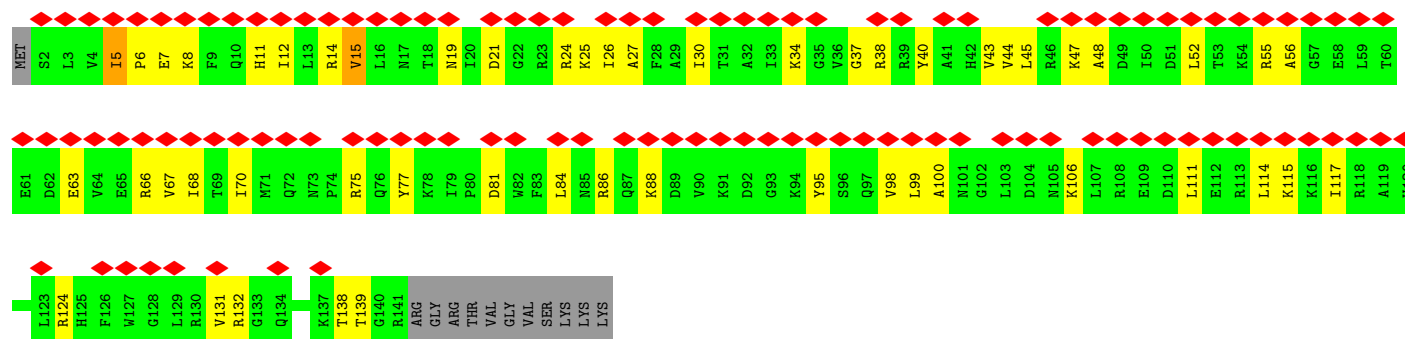
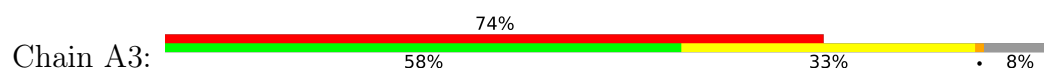
Mol	Chain	Residues	Atoms		AltConf
86	B1	1	Total 1	O 1	0



G3800	C3901	G3802	G3803	C3814	U3815	C3816	A3822	U3826	G3827	C3835	G3836	U3840	U3841	G3842	G3843	A3855	U3860	G3861	A3866	G3874	G3877	G3880	U3881	U3884	A3885	A3886	G3887	G3888	G3889	G3890	G3891	G3892	A3903	G3906	A3907	A3908	A3909	C3910	C3911	C3912	C3913	C3914	C3915	C3916	U3917															
U3716	U3717	U3718	U3719	U3720	U3721	G3726	G3734	A3735	G3736	G3737	C3738	G3739	G3743	G3744	G3745	G3746	G3747	G3748	G3749	C3750	C3751	C3752	G3758	G3759	C3760	U3761	C3762	U3763	C3764	C3765	C3766	U3767	U3768	C3769	U3770	G3771	G3772	C3776	A3777	A3778	G3781	U3782	C3783	C3784	G3785	U3786	U3787	C3788	C3789	G3790	G3796	C3797	U3798	G3799						
A3605	U3606	G3607	A3608	G3609	A3610	G3611	G3612	U3613	G3614	U3615	A3616	G3617	A3618	A3619	U3620	A3621	A3622	G3623	U3624	G3625	G3626	G3627	A3628	G3629	G3630	G3631	G3632	C3633	G3634	G3635	G3636	G3637	G3688	G3689	C3690	C3691	G3692	G3693	U3694	G3695	A3696	A3697	A3698	U3699	A3700	C3701	C3702	A3703	C3704	U3705	A3706	C3707	U3708	C3709	U3710	C3711	A3712	U3713	C3714	G3715
G3525	C3526	A3527	A3528	G3529	G3530	G3531	A3532	G3533	G3534	G3535	G3536	G3537	C3540	A3541	A3542	A3543	A3544	A3545	C3549	A3550	G3553	G3556	A3557	A3562	G3563	G3564	G3565	G3566	G3567	U3568	U3571	G3572	A3573	G3574	G3575	G3576	U3577	G3578	A3579	C3580	U3583	A3584	G3585	U3588	G3589	G3590	C3591	A3592	G3593	G3594	G3595	A3599	G3600	A3601	A3602	A3603	C3604			
A3416	C3417	U3418	A3419	U3420	G3421	A3422	C3423	U3424	U3425	G3426	U3427	U3428	U3429	A3430	A3431	G3432	G3433	A3440	A3441	U3442	C3447	U3452	C3453	C3466	G3467	U3470	A3471	A3472	A3473	U3474	G3475	U3476	G3479	U3494	G3495	U3496	C3499	U3504	A3505	C3506	U3507	A3508	A3512	A3517	A3518	A3523	G3524													
G3317	A3318	G3325	G3326	G3327	G3328	G3329	G3337	G3340	G3341	U3346	G3347	A3348	U3363	G3364	G3365	G3366	A3367	A3368	U3369	G3370	U3371	C3372	A3373	A3374	A3375	G3376	U3377	G3378	A3379	A3380	G3381	A3382	A3383	A3384	A3388	A3389	U3390	G3391	A3392	A3393	G3394	C3395	G3396	G3406	G3409	G3410	G3411	A3412	G3413	U3414	A3415									
A3416	C3417	U3418	A3419	U3420	G3421	A3422	C3423	U3424	U3425	G3426	U3427	U3428	U3429	A3430	A3431	G3432	G3433	A3440	A3441	U3442	C3447	U3452	C3453	C3466	G3467	U3470	A3471	A3472	A3473	U3474	G3475	U3476	G3479	U3494	G3495	U3496	C3499	U3504	A3505	C3506	U3507	A3508	A3512	A3517	A3518	A3523	G3524													
G3525	C3526	A3527	A3528	G3529	G3530	G3531	A3532	G3533	G3534	G3535	G3536	G3537	C3540	A3541	A3542	A3543	A3544	A3545	C3549	A3550	G3553	G3556	A3557	A3562	G3563	G3564	G3565	G3566	G3567	U3568	U3571	G3572	A3573	G3574	G3575	G3576	U3577	G3578	A3579	C3580	U3583	A3584	G3585	U3588	G3589	G3590	C3591	A3592	G3593	G3594	G3595	A3599	G3600	A3601	A3602	A3603	C3604			
A3605	U3606	G3607	A3608	G3609	A3610	G3611	G3612	U3613	G3614	U3615	A3616	G3617	A3618	A3619	U3620	A3621	A3622	G3623	U3624	G3625	G3626	G3627	A3628	G3629	G3630	G3631	G3632	C3633	G3634	G3635	G3636	G3637	G3688	G3689	C3690	C3691	G3692	G3693	U3694	G3695	A3696	A3697	A3698	U3699	A3700	C3701	C3702	A3703	C3704	U3705	A3706	C3707	U3708	C3709	U3710	C3711	A3712	U3713	C3714	G3715
U3716	U3717	U3718	U3719	U3720	U3721	G3726	G3734	A3735	G3736	G3737	C3738	G3739	G3743	G3744	G3745	G3746	G3747	G3748	G3749	C3750	C3751	C3752	G3758	G3759	C3760	U3761	C3762	U3763	C3764	C3765	C3766	U3767	U3768	C3769	U3770	G3771	G3772	C3776	A3777	A3778	G3781	U3782	C3783	C3784	G3785	U3786	U3787	C3788	C3789	G3790	G3796	C3797	U3798	G3799						
G3800	C3901	G3802	G3803	C3814	U3815	C3816	A3822	U3826	G3827	C3835	G3836	U3840	U3841	G3842	G3843	A3855	U3860	G3861	A3866	G3874	G3877	G3880	U3881	U3884	A3885	A3886	G3887	G3888	G3889	G3890	G3891	G3892	A3903	G3906	A3907	A3908	A3909	C3910	C3911	C3912	C3913	C3914	C3915	C3916	U3917															



• Molecule 3: Small ribosomal subunit protein uS13

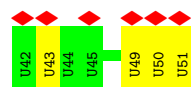


• Molecule 4: Large ribosomal subunit protein eL8

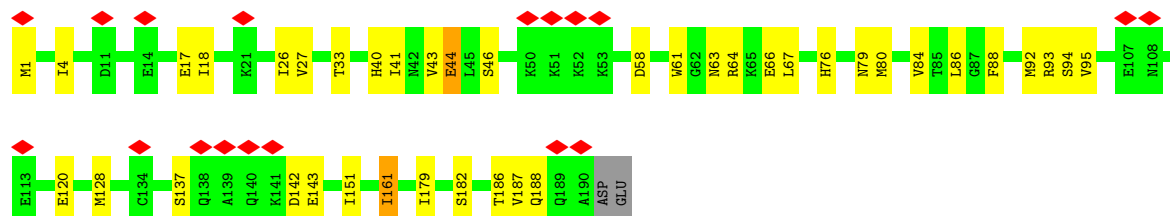
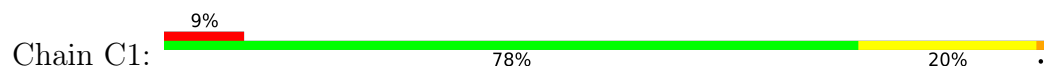




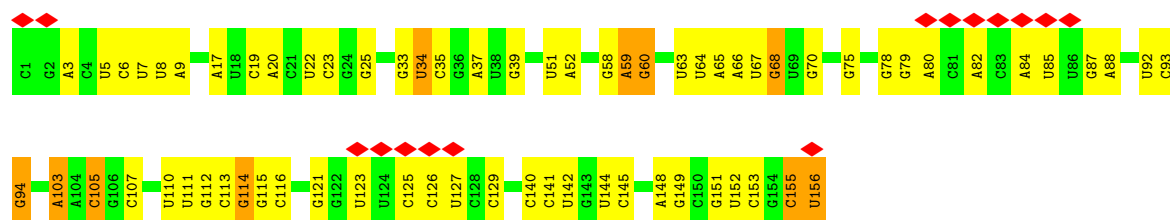
• Molecule 8: messenger RNA



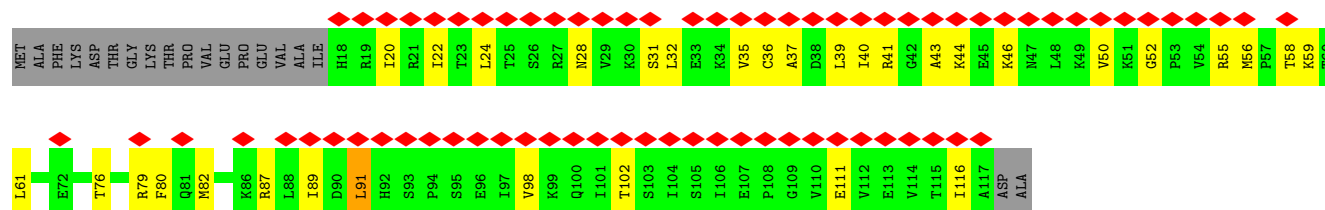
• Molecule 9: Large ribosomal subunit protein uL6



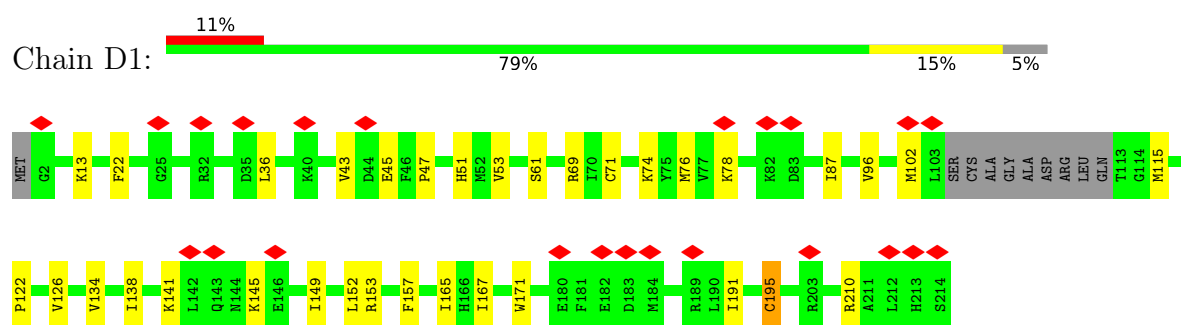
• Molecule 10: 5.8S ribosomal RNA



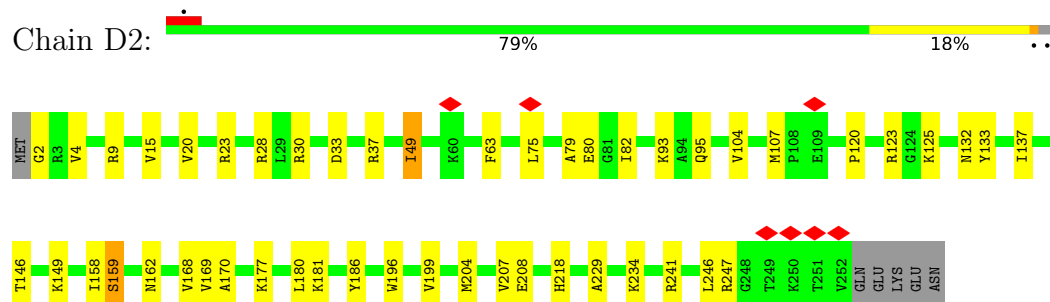
• Molecule 11: Small ribosomal subunit protein uS10



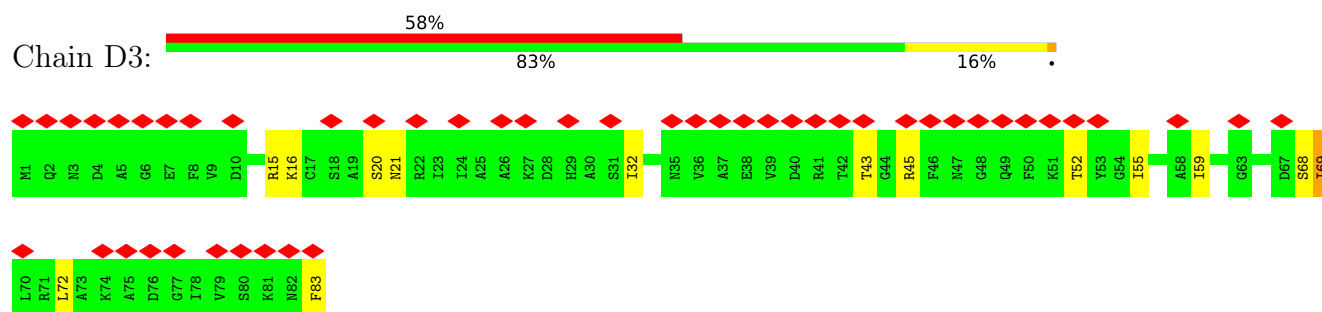
• Molecule 12: Large ribosomal subunit protein uL16



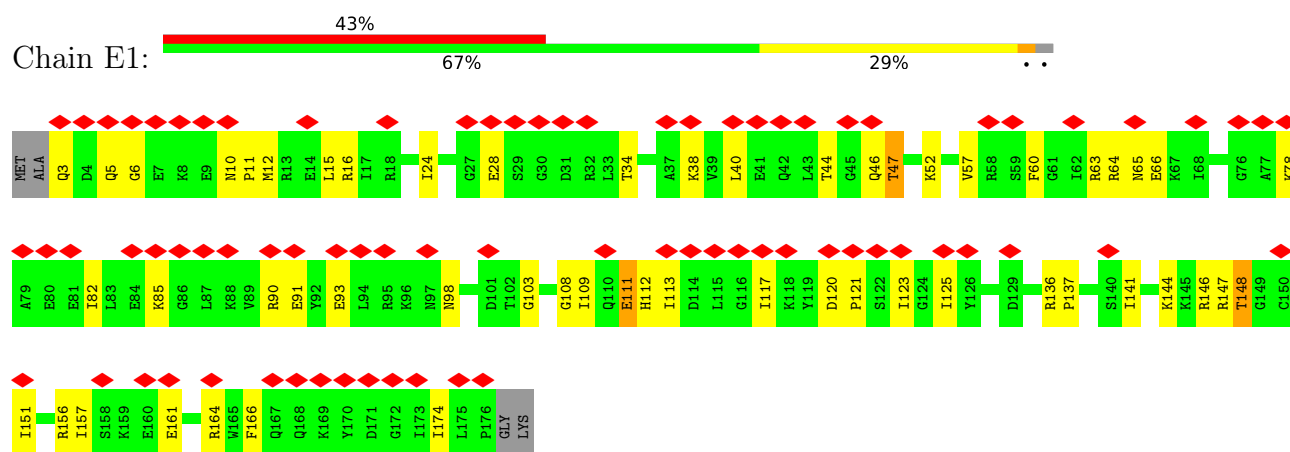
- Molecule 13: Large ribosomal subunit protein uL2



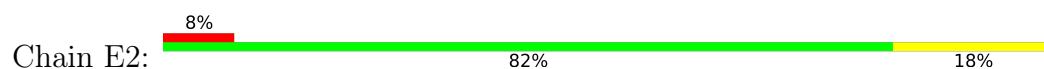
- Molecule 14: Small ribosomal subunit protein eS21

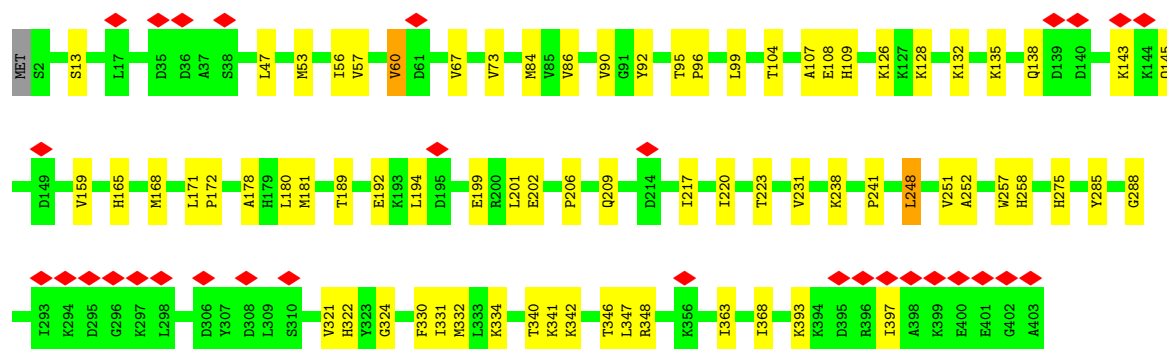


- Molecule 15: Large ribosomal subunit protein uL5

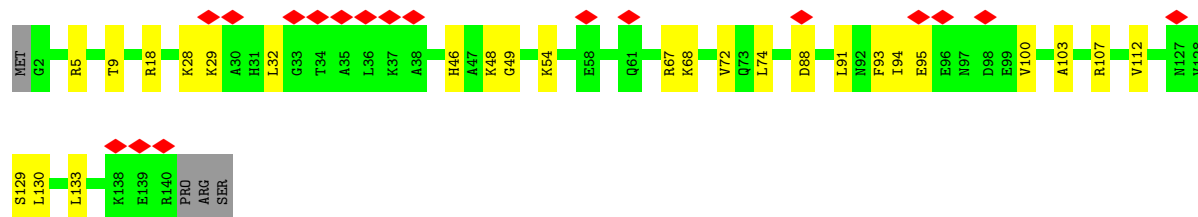
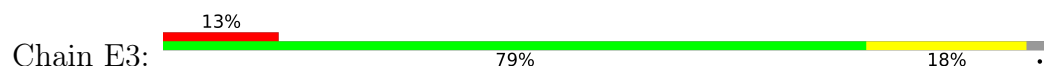


- Molecule 16: Large ribosomal subunit protein uL3

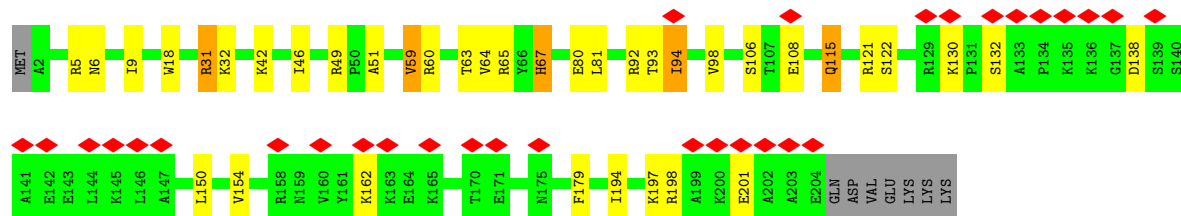
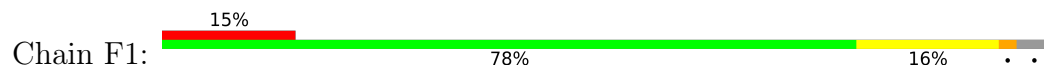




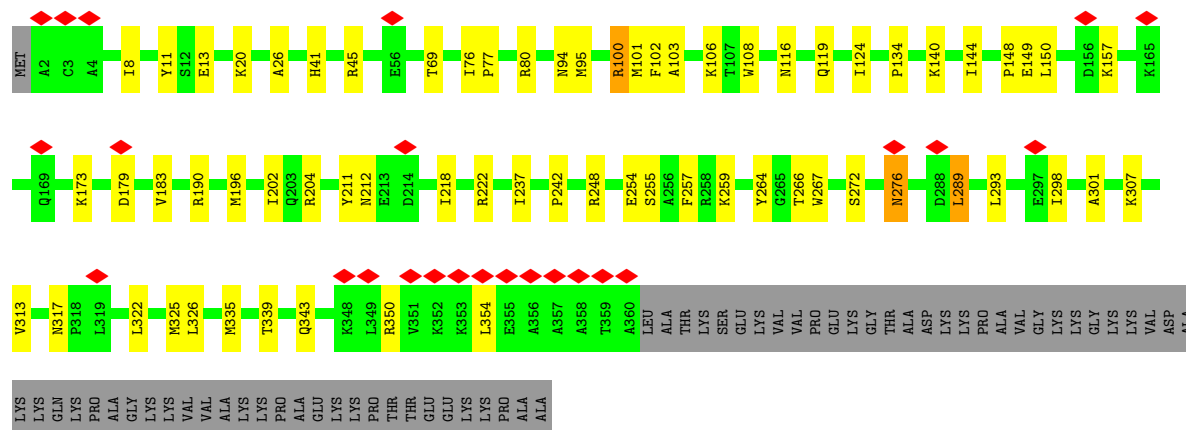
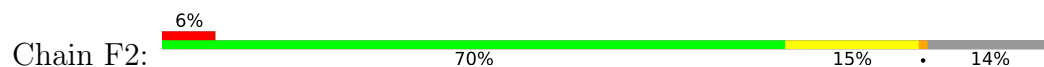
- Molecule 17: Small ribosomal subunit protein uS12

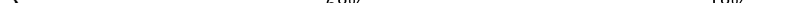


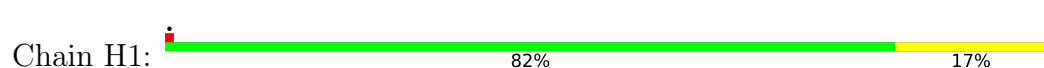
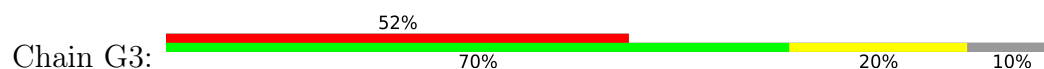
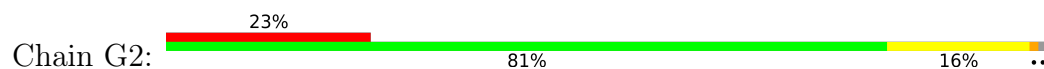
- Molecule 18: Large ribosomal subunit protein eL13



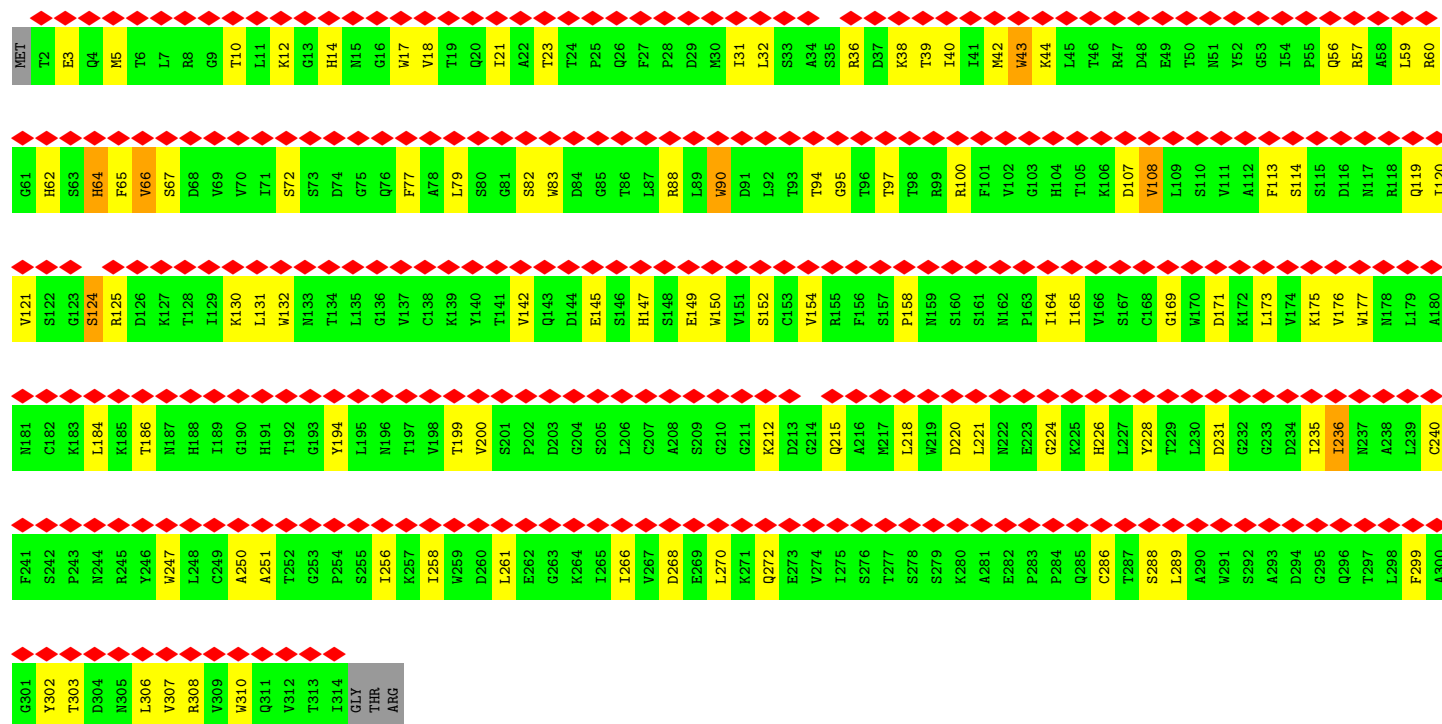
- Molecule 19: Large ribosomal subunit protein uL4



- Chain F3: 

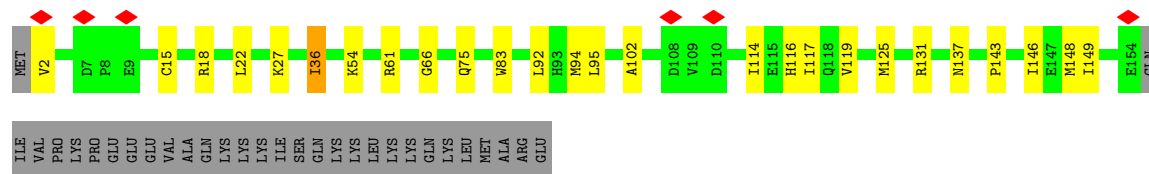






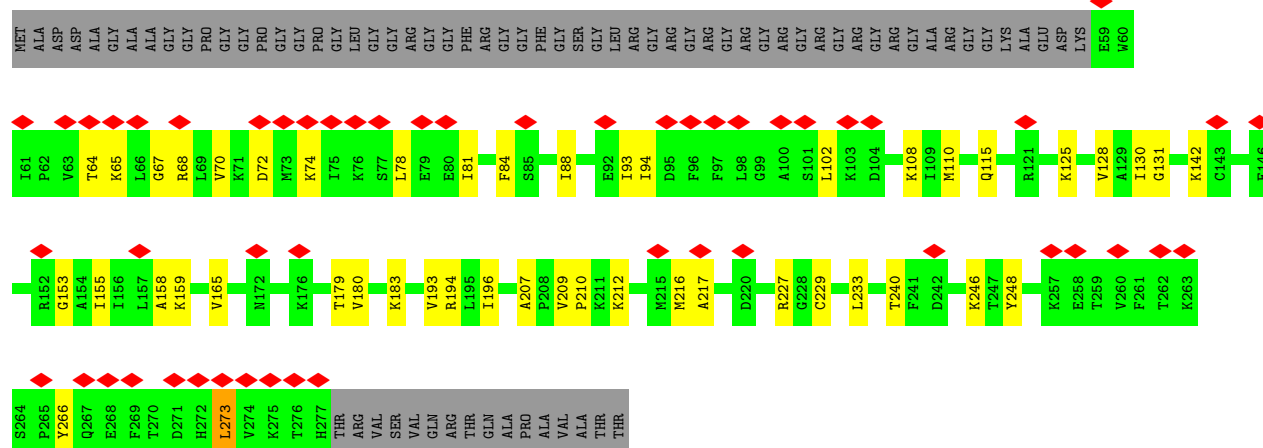
• Molecule 29: Large ribosomal subunit protein uL22

Chain J2: 69% 14% 17%

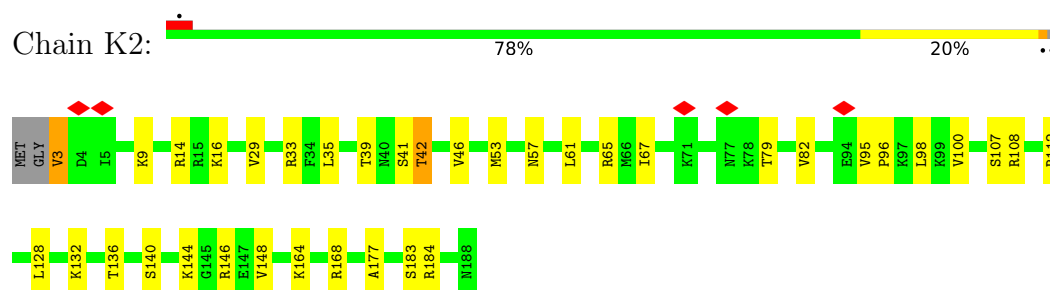


• Molecule 30: Small ribosomal subunit protein uS5

Chain J3: 59% 16% 25%



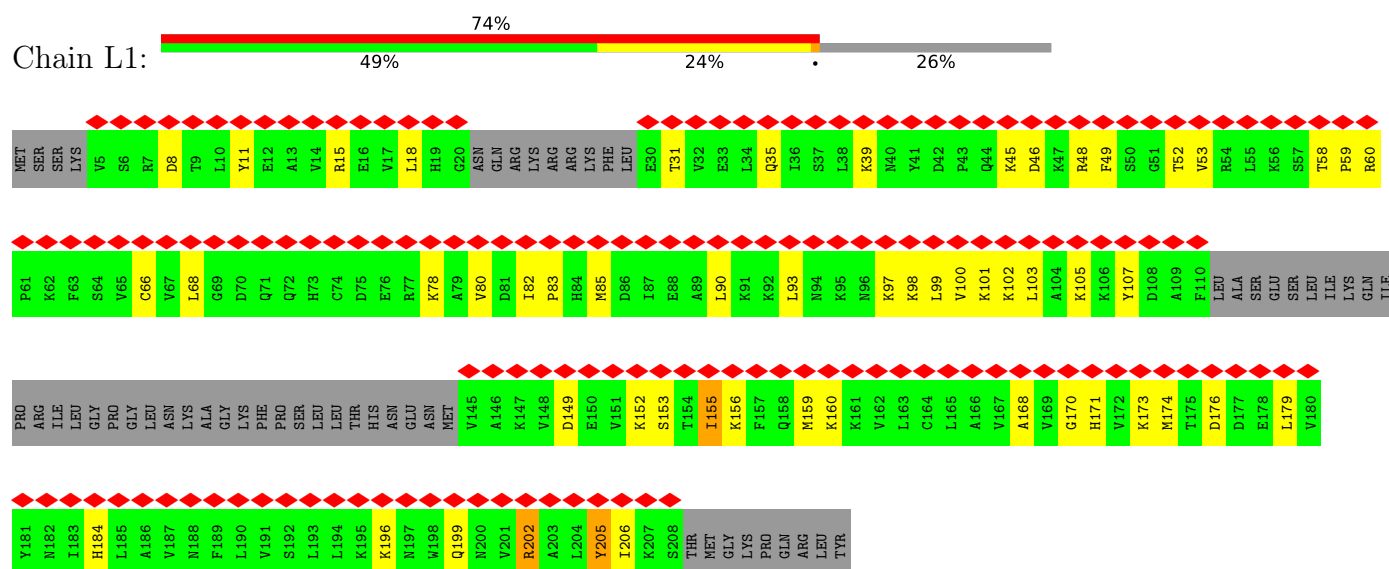
- Molecule 31: Large ribosomal subunit protein eL18



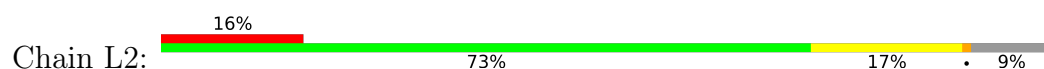
- Molecule 32: Small ribosomal subunit protein eS6

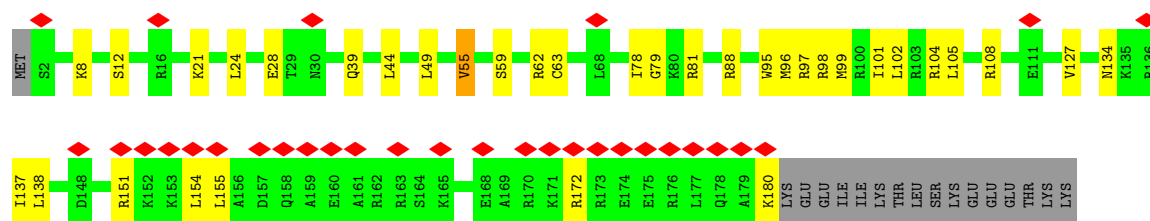


- Molecule 33: Large ribosomal subunit protein uL1

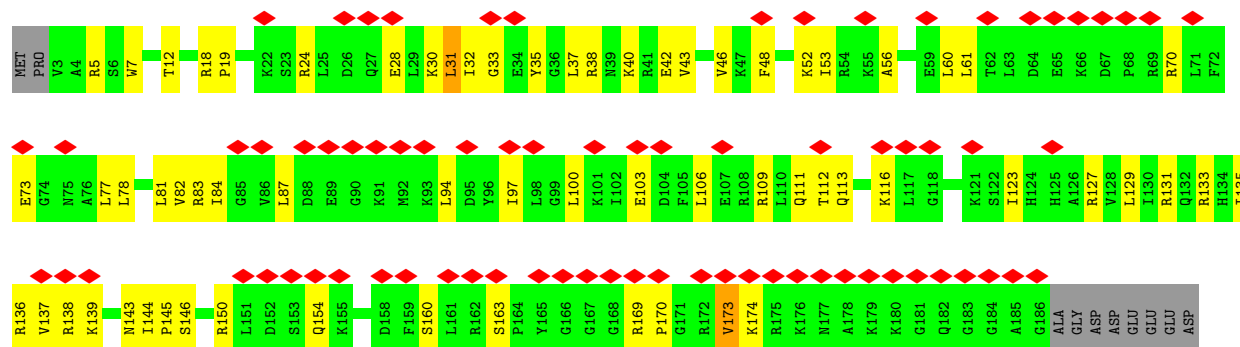
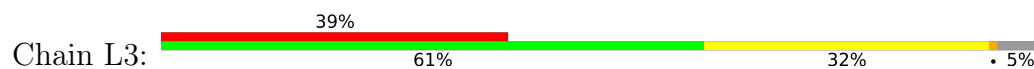


- Molecule 34: Large ribosomal subunit protein eL19

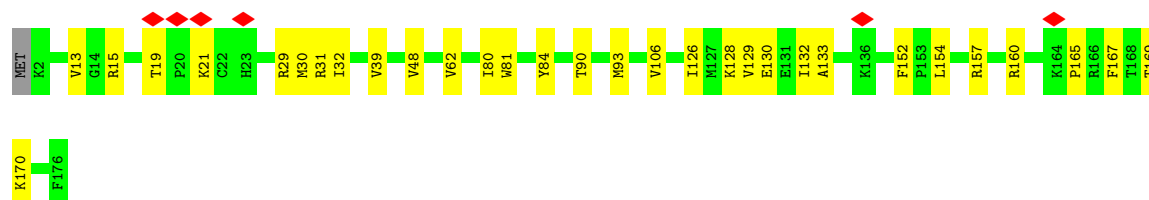
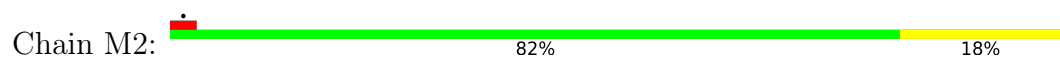




- Molecule 35: Small ribosomal subunit protein uS4



- Molecule 36: Large ribosomal subunit protein eL20

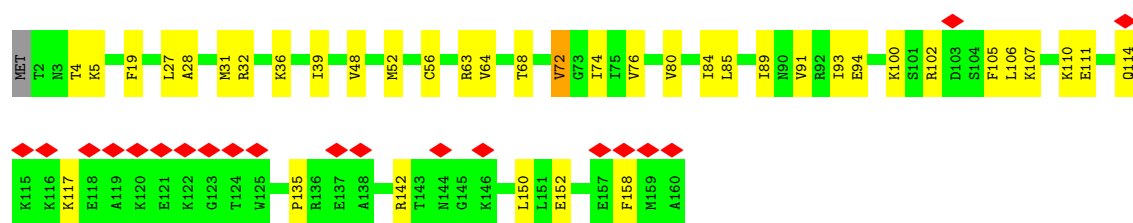


- Molecule 37: Small ribosomal subunit protein eS12



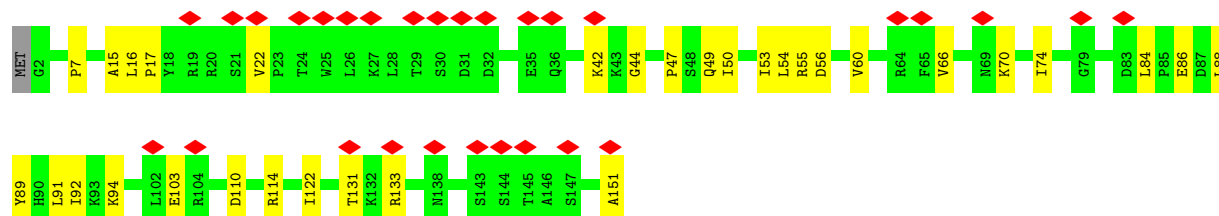
- Molecule 38: Large ribosomal subunit protein eL21

Chain N2: 



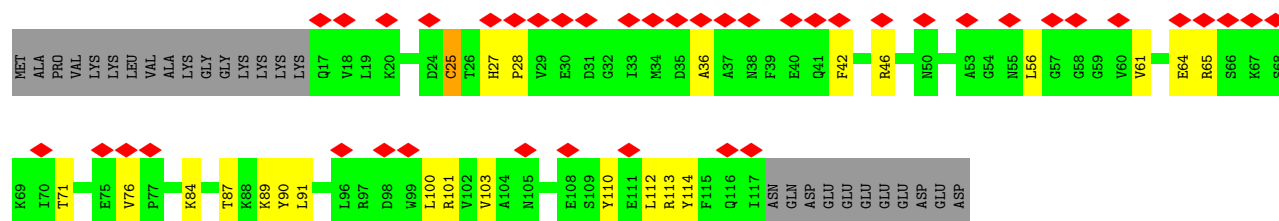
- Molecule 39: Small ribosomal subunit protein uS15

Chain N3: 



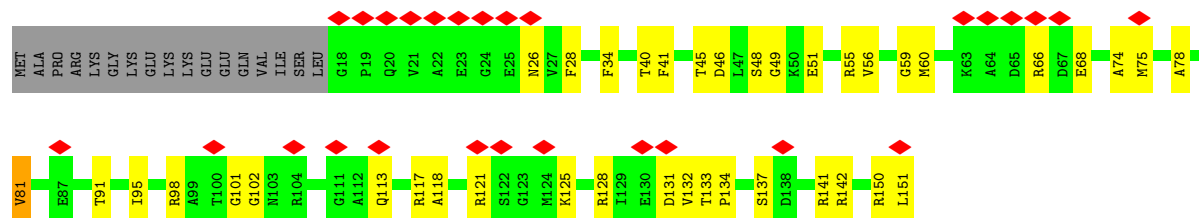
- Molecule 40: Large ribosomal subunit protein eL22

Chain O2: 



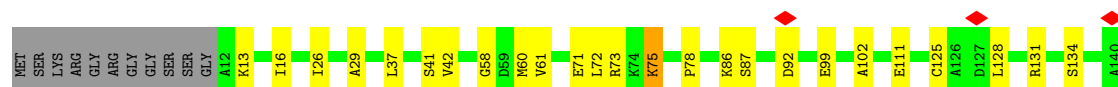
- Molecule 41: Small ribosomal subunit protein uS11

Chain O3: 

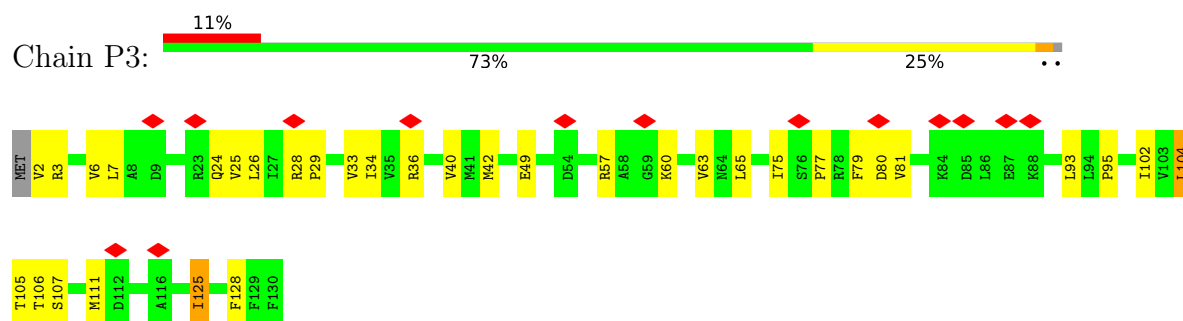


- Molecule 42: Large ribosomal subunit protein uL14

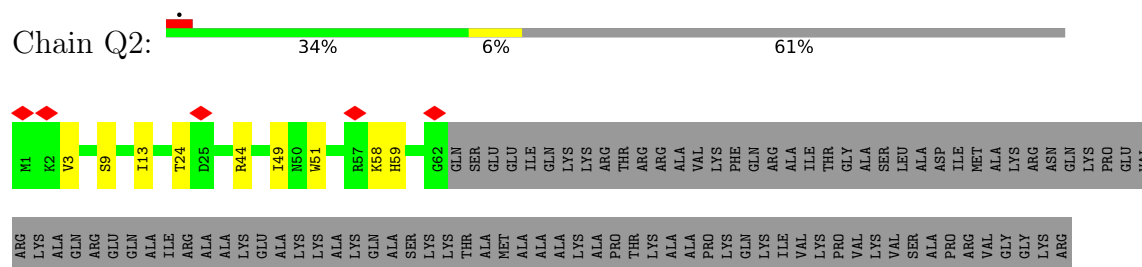
Chain P2: 



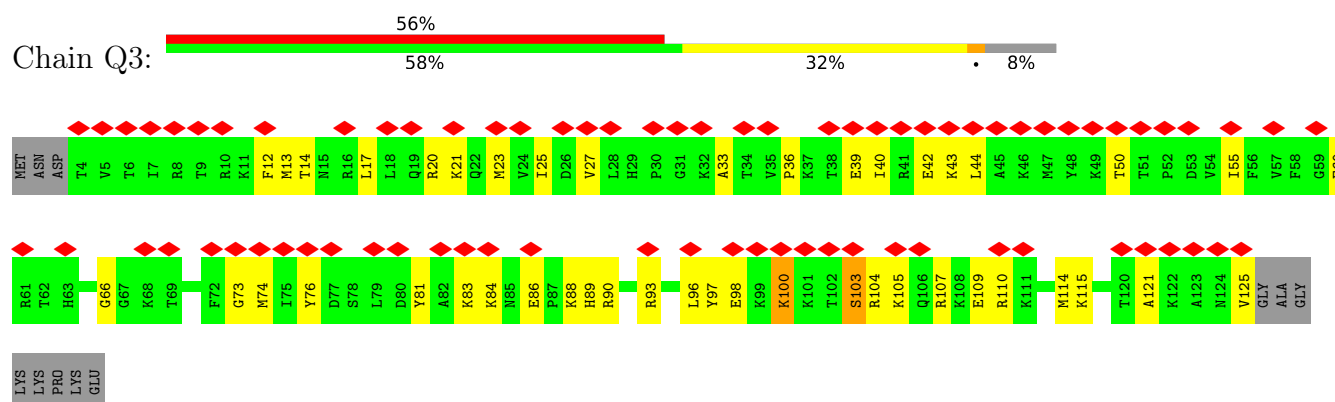
- Molecule 43: Small ribosomal subunit protein uS8



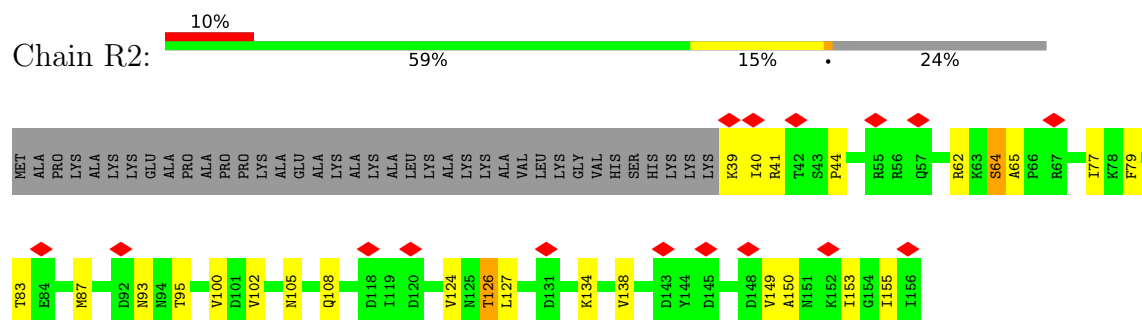
- Molecule 44: Large ribosomal subunit protein eL24



- Molecule 45: Small ribosomal subunit protein eS24

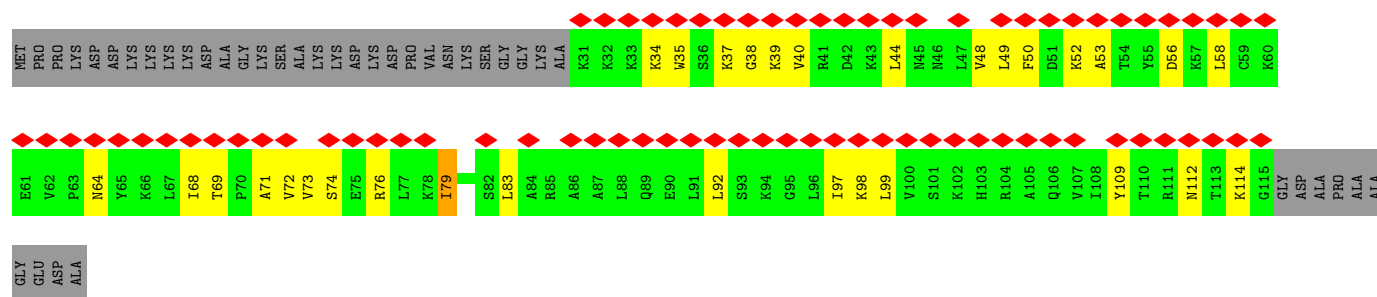


- Molecule 46: Large ribosomal subunit protein uL23

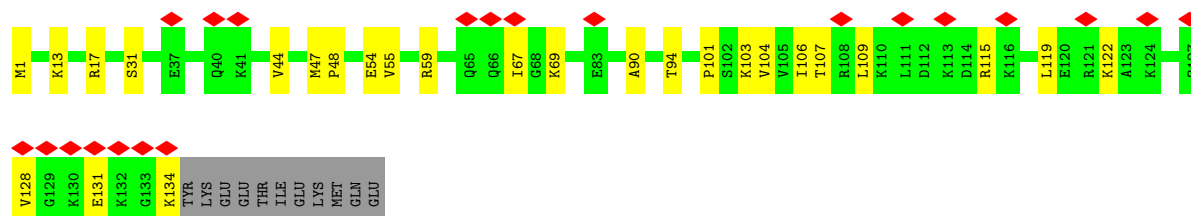
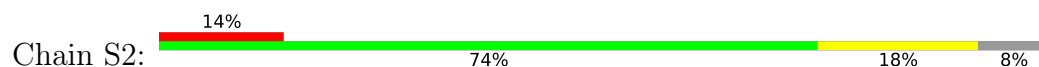


- Molecule 47: Small ribosomal subunit protein eS25

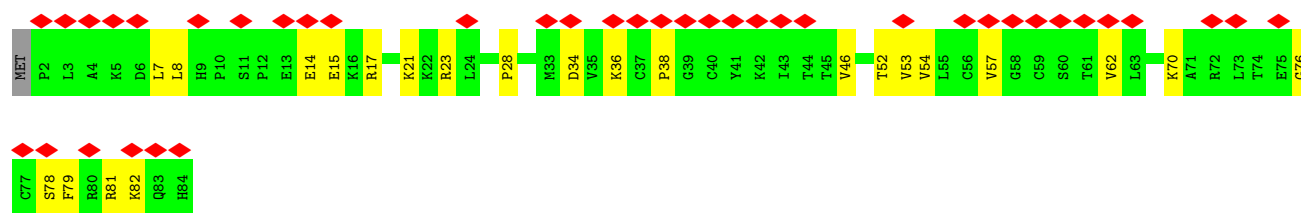




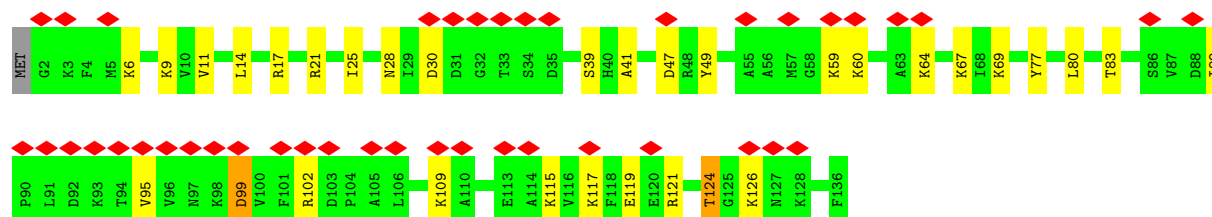
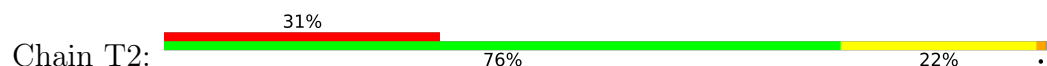
- Molecule 48: Large ribosomal subunit protein uL24



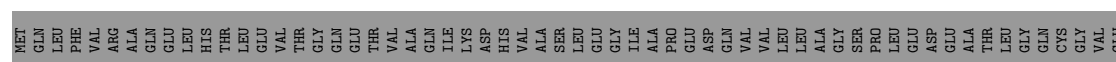
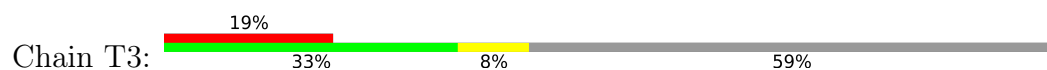
- Molecule 49: Small ribosomal subunit protein eS27

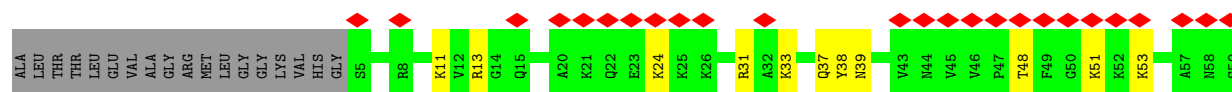


- Molecule 50: Large ribosomal subunit protein eL27

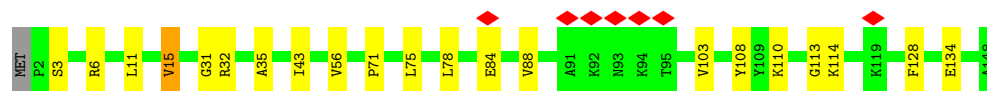
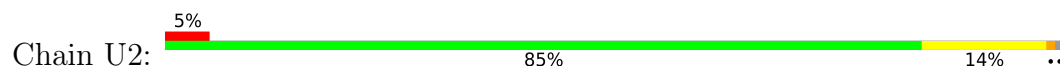


- Molecule 51: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

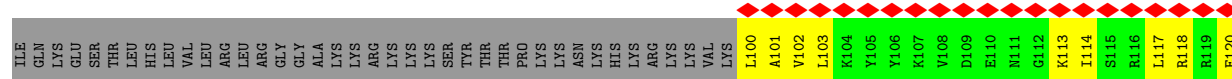
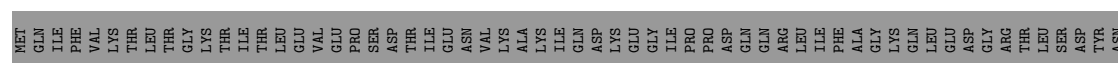




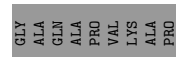
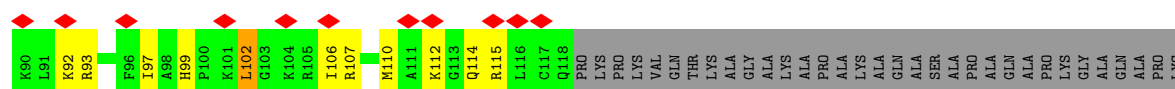
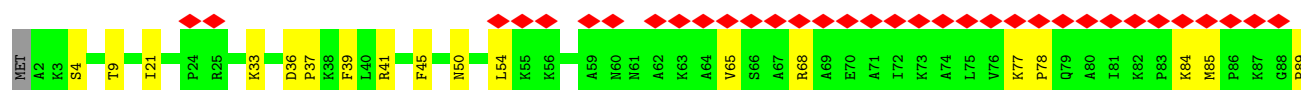
- Molecule 52: Large ribosomal subunit protein uL15



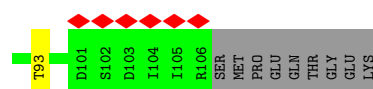
- Molecule 53: Ubiquitin-ribosomal protein eS31 fusion protein



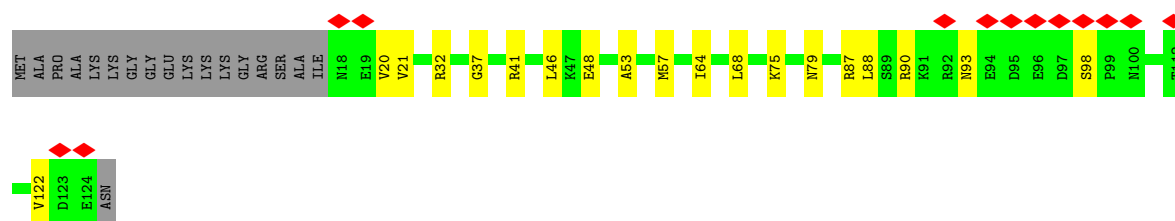
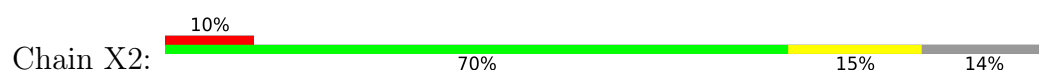
- Molecule 54: Large ribosomal subunit protein eL29



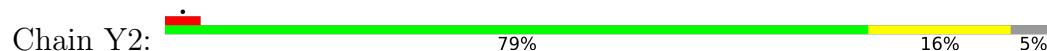
- Molecule 55: Large ribosomal subunit protein eL30



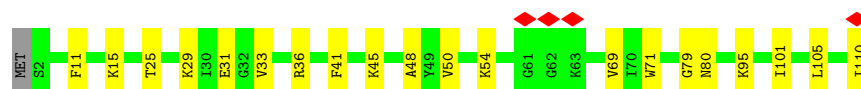
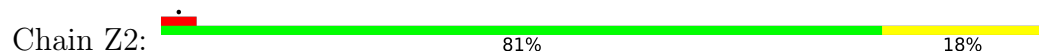
- Molecule 56: Large ribosomal subunit protein eL31



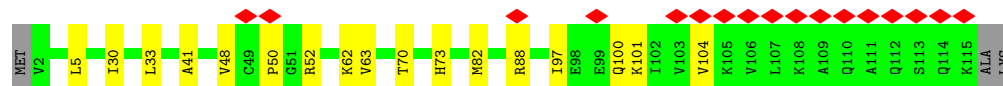
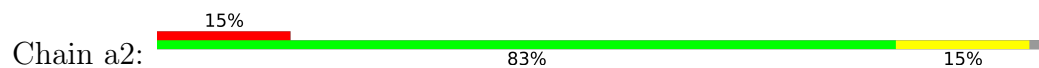
- Molecule 57: Large ribosomal subunit protein eL32



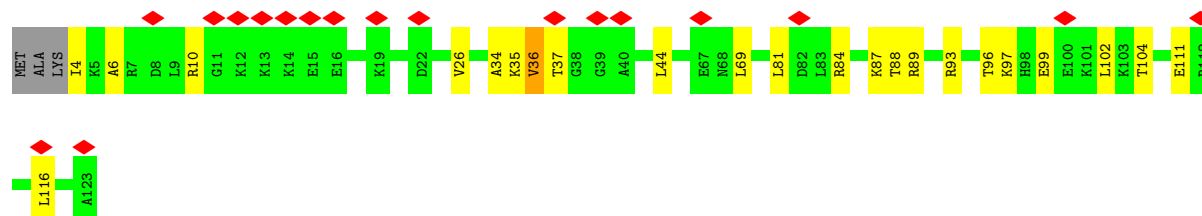
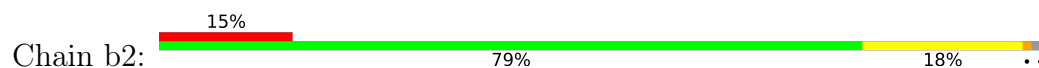
- Molecule 58: Large ribosomal subunit protein eL33



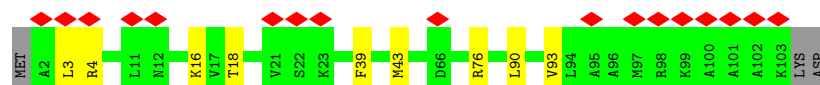
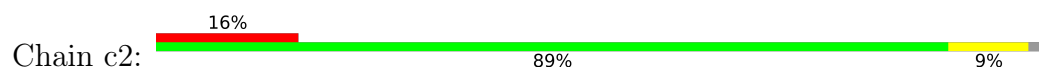
- Molecule 59: Large ribosomal subunit protein eL34



- Molecule 60: Large ribosomal subunit protein uL29

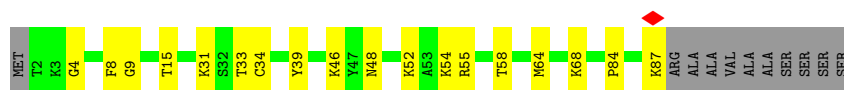


- Molecule 61: Large ribosomal subunit protein eL36



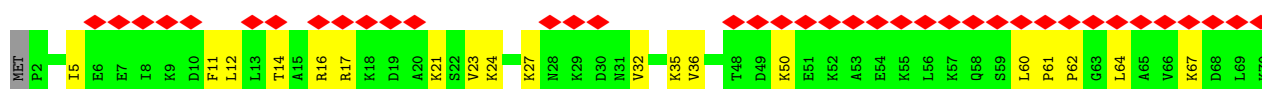
- Molecule 62: Large ribosomal subunit protein eL37

Chain d2: 



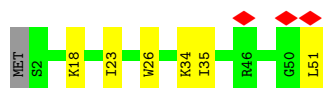
- Molecule 63: Large ribosomal subunit protein eL38

Chain e2: 



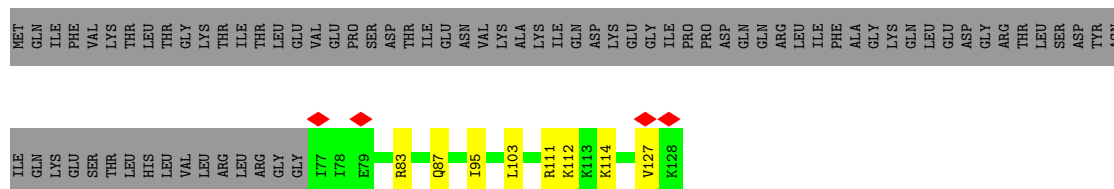
- Molecule 64: Large ribosomal subunit protein eL39

Chain f2: 



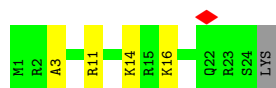
- Molecule 65: Ubiquitin-ribosomal protein eL40 fusion protein

Chain g2: 



- Molecule 66: 60S ribosomal protein L41

Chain h2: 

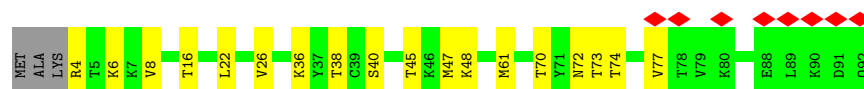
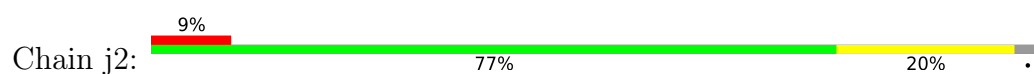


- Molecule 67: Large ribosomal subunit protein eL42

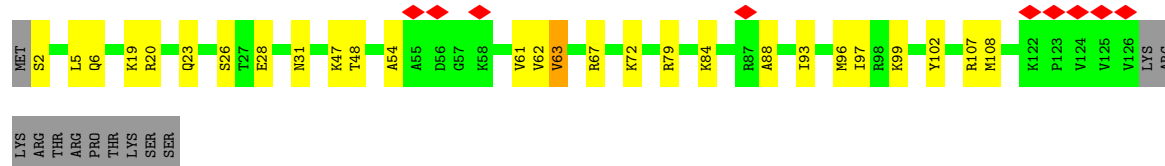
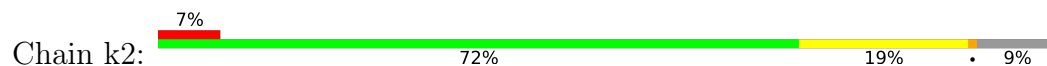
Chain i2: 



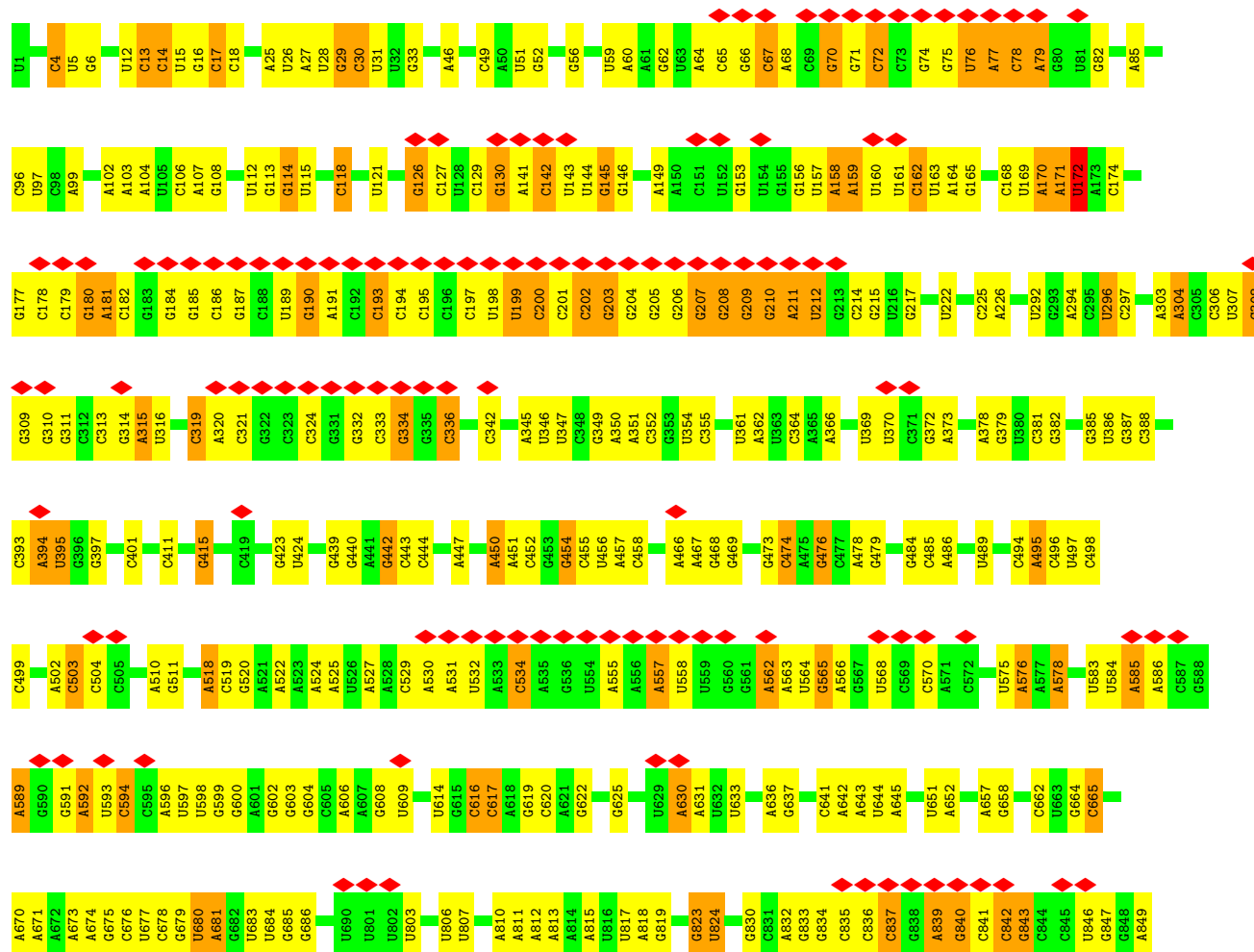
- Molecule 68: Large ribosomal subunit protein eL43

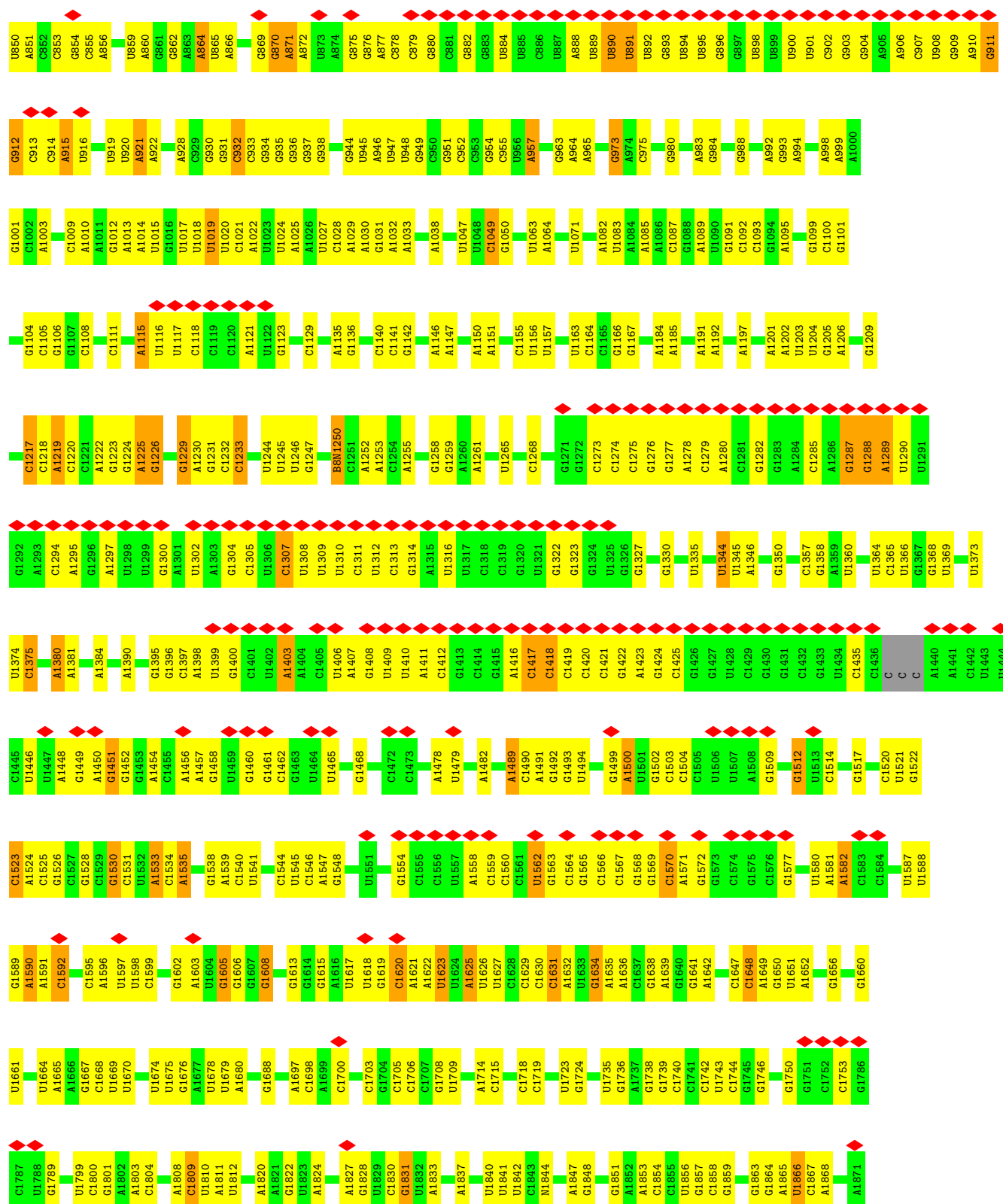


- Molecule 69: Large ribosomal subunit protein eL28

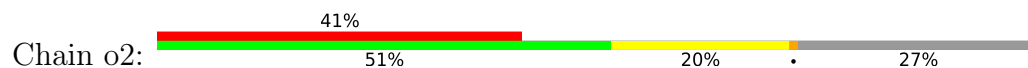


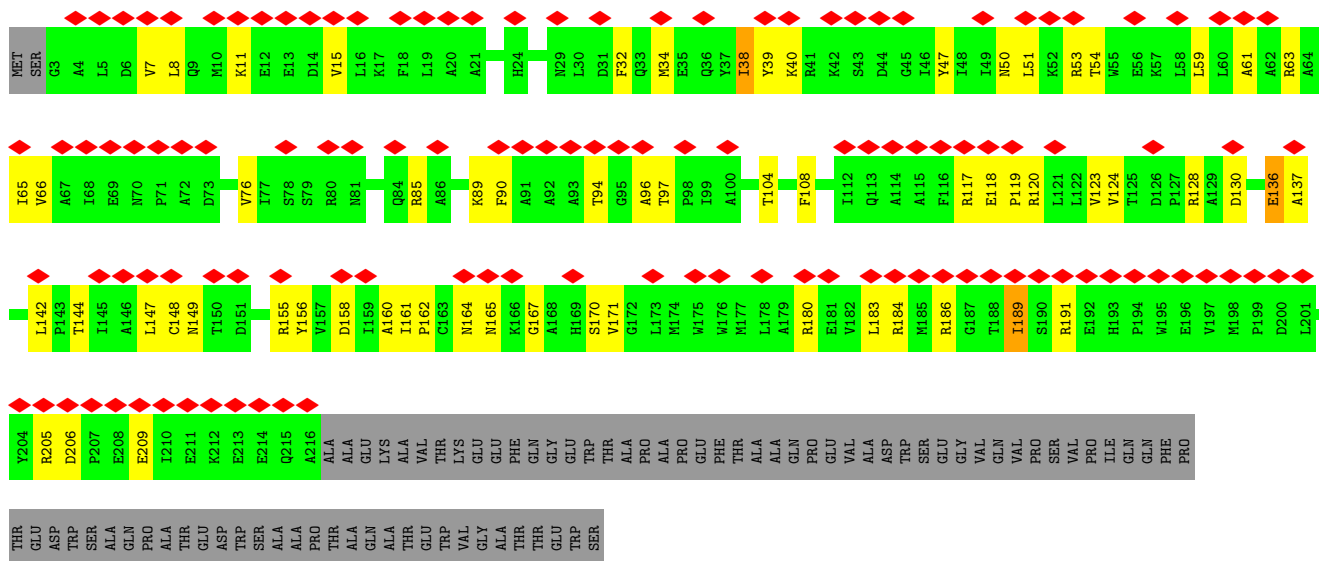
- Molecule 70: 18S ribosomal RNA



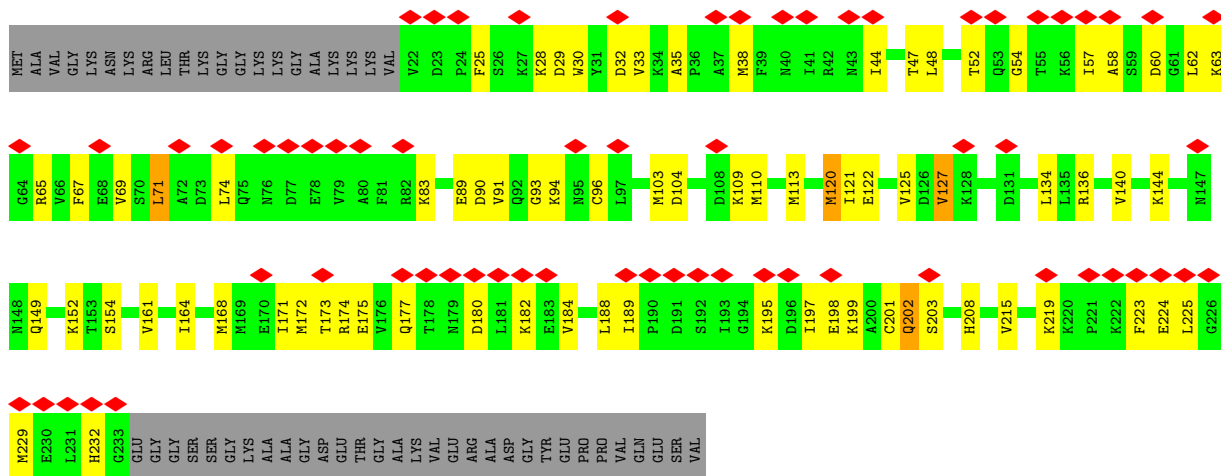


• Molecule 71: Small ribosomal subunit protein uS2

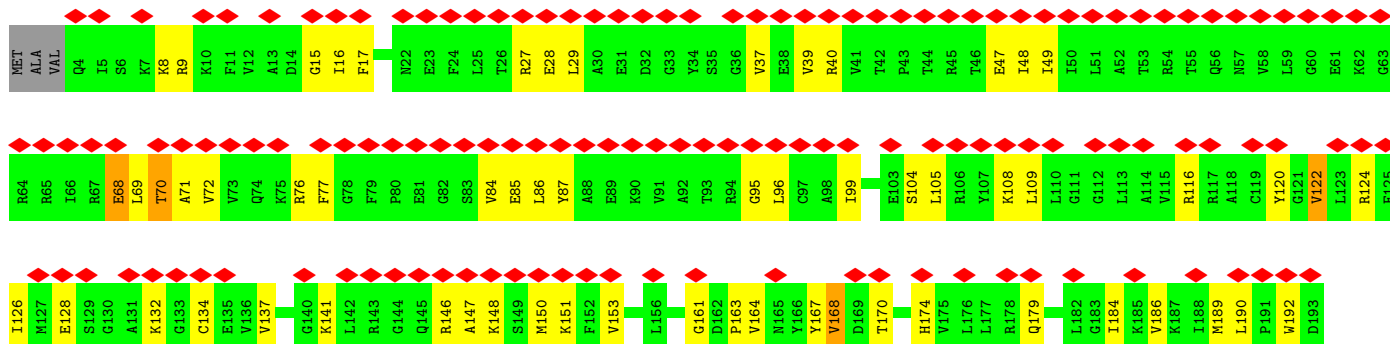


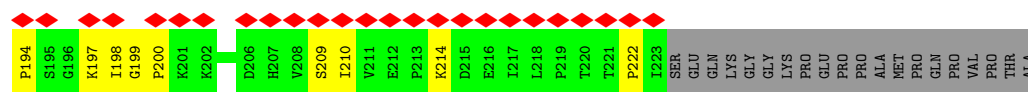


• Molecule 72: 40S ribosomal protein S3a

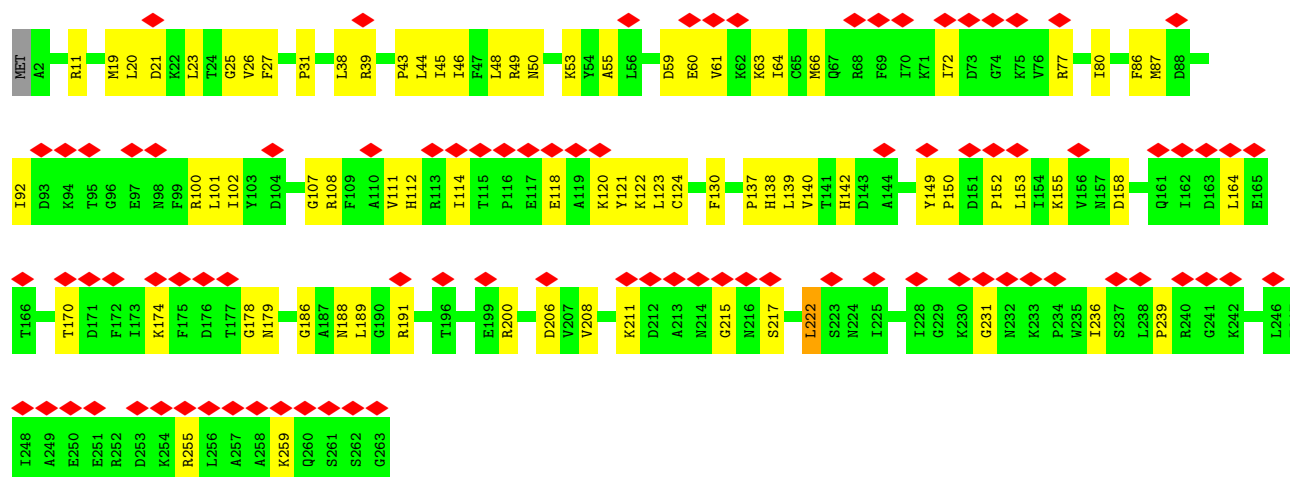


• Molecule 73: Small ribosomal subunit protein uS3

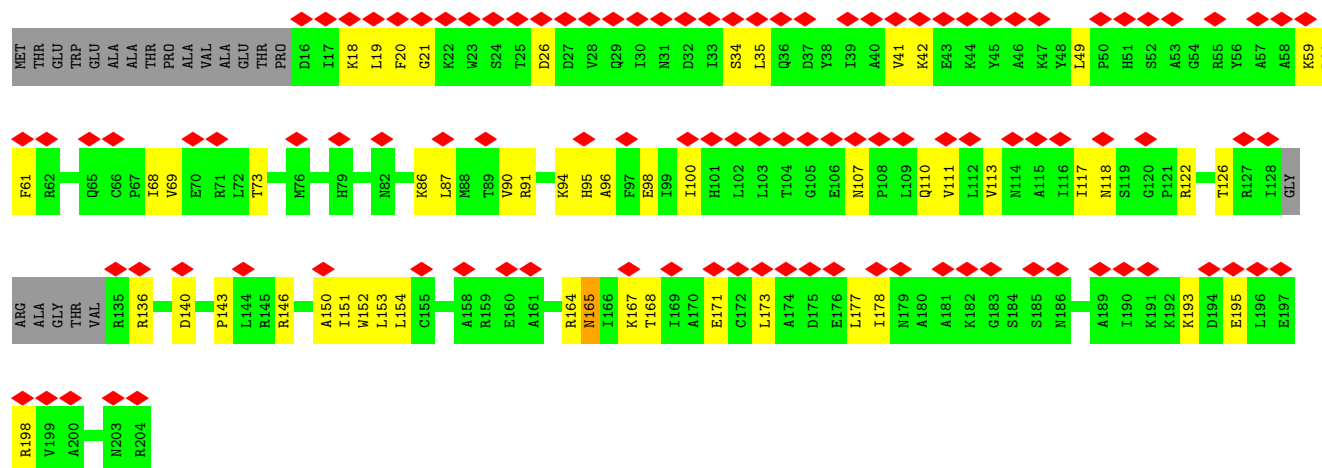




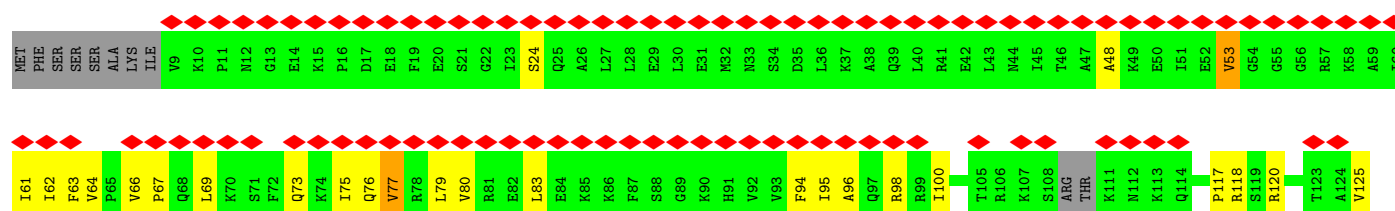
• Molecule 74: Small ribosomal subunit protein eS4

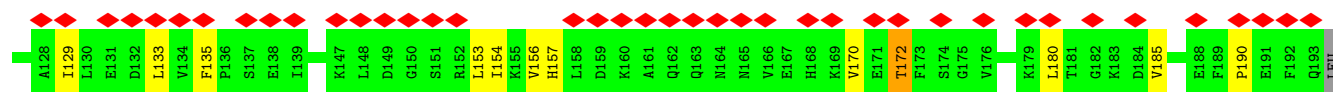


• Molecule 75: Small ribosomal subunit protein uS7

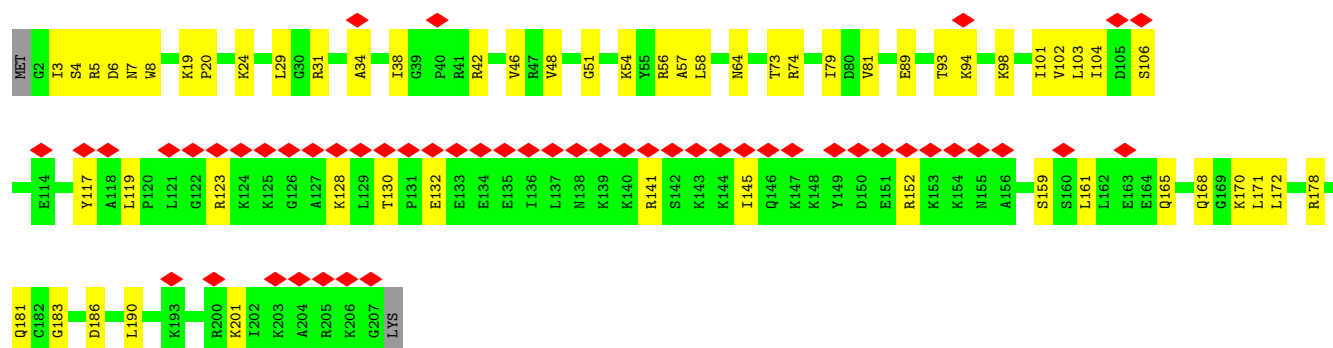
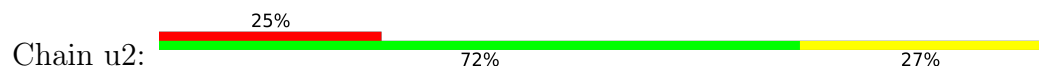


• Molecule 76: Small ribosomal subunit protein eS7

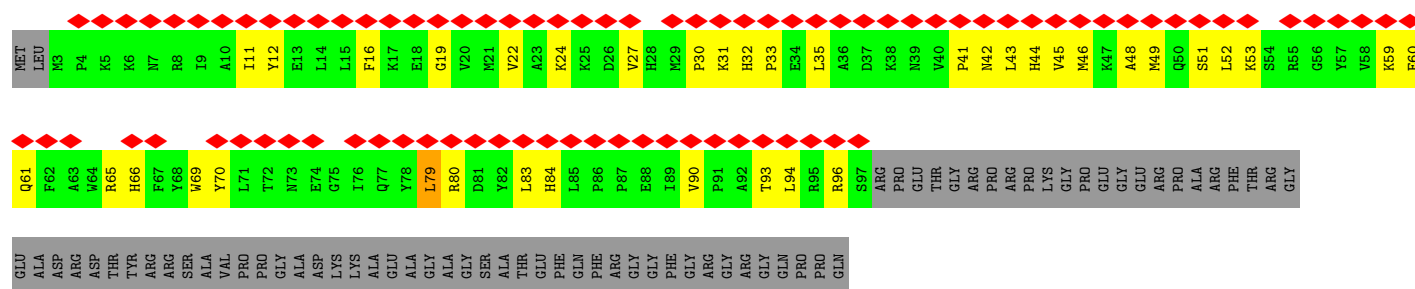
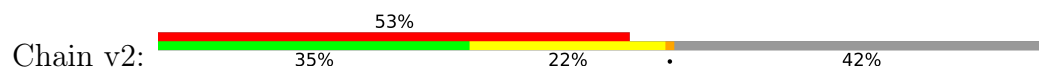




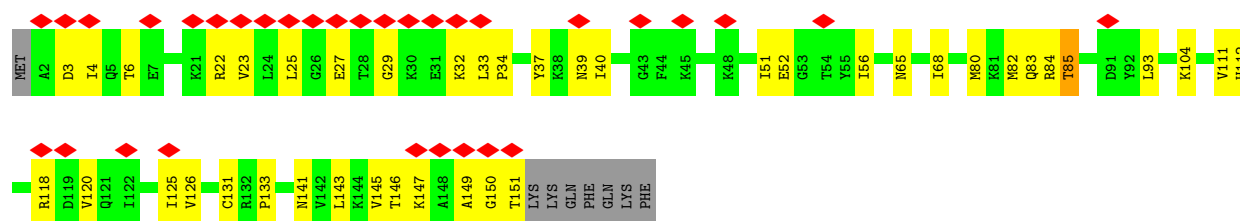
- Molecule 77: Small ribosomal subunit protein eS8



- Molecule 78: Small ribosomal subunit protein eS10



- Molecule 79: Small ribosomal subunit protein uS17

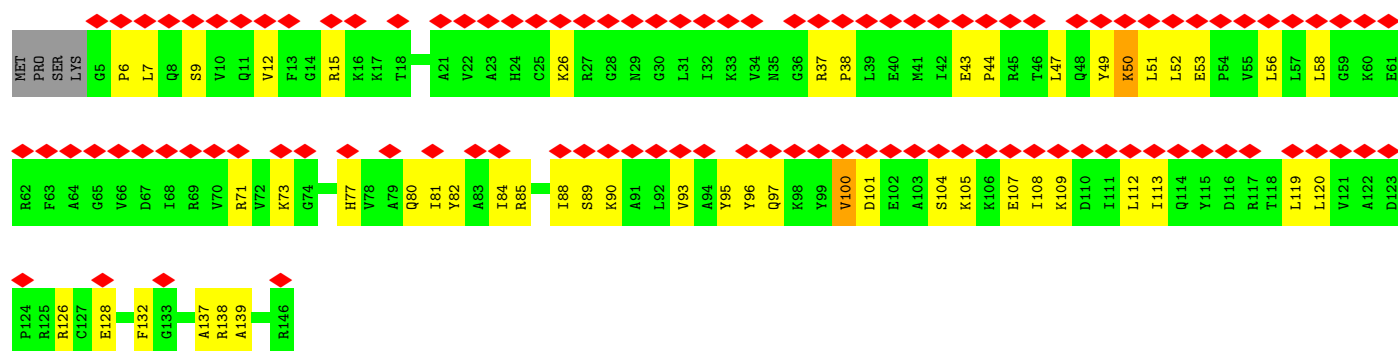
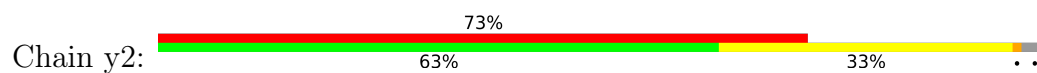


- Molecule 80: Small ribosomal subunit protein uS19

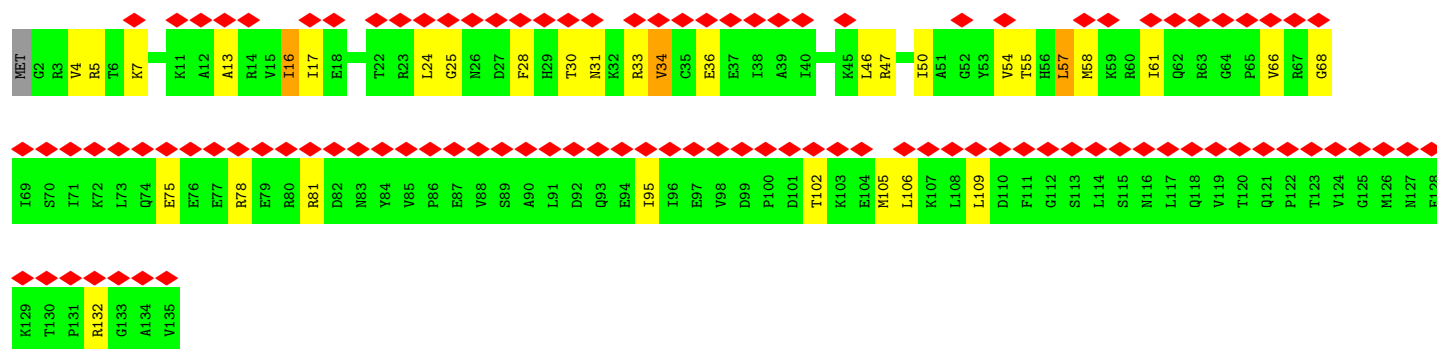
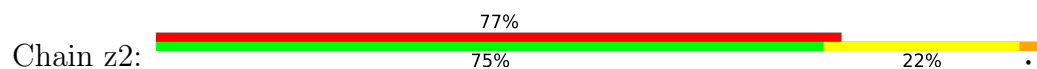




- Molecule 81: Small ribosomal subunit protein uS9



- Molecule 82: Small ribosomal subunit protein eS17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	100000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0285	Depositor
Map size (Å)	315.12, 315.12, 315.12	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 2MG, OMU, MG, OMC, 4AC, B8N, 5MC, B8T, A2M, UR3, OMG, 1MA, ZN

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	A1	0.26	0/1877	0.35	0/2502
2	A2	0.25	0/84889	0.31	1/132400 (0.0%)
3	A3	0.19	0/1175	0.49	0/1575
4	B1	0.22	0/1847	0.40	0/2486
5	B2	0.22	0/2836	0.26	0/4421
6	B3	0.18	0/1122	0.39	0/1503
7	Bv	0.14	0/1813	0.31	0/2823
7	n2	0.14	0/1813	0.31	0/2823
8	Bx	0.14	0/219	0.31	0/336
9	C1	0.22	0/1537	0.36	0/2065
10	C2	0.24	0/3675	0.30	0/5725
11	C3	0.18	0/805	0.42	0/1081
12	D1	0.22	0/1694	0.35	0/2261
13	D2	0.27	0/1959	0.39	0/2627
14	D3	0.18	0/645	0.43	0/863
15	E1	0.21	0/1420	0.47	0/1899
16	E2	0.24	0/3305	0.40	0/4422
17	E3	0.23	0/1097	0.42	0/1464
18	F1	0.26	0/1674	0.48	1/2241 (0.0%)
19	F2	0.24	0/2921	0.37	0/3921
20	F3	0.23	0/805	0.46	0/1079
21	G1	0.22	0/1165	0.39	0/1558
22	G2	0.21	0/2435	0.36	0/3260
23	G3	0.18	0/490	0.46	0/656
24	H1	0.27	0/1746	0.36	0/2338
25	H2	0.19	0/1822	0.37	0/2443
26	H3	0.20	0/466	0.52	0/618
27	I2	0.25	0/1670	0.38	0/2232
28	I3	0.17	0/2493	0.44	0/3394
29	J2	0.26	0/1268	0.42	0/1700
30	J3	0.21	0/1737	0.46	0/2348
31	K2	0.25	0/1535	0.37	0/2048

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	K3	0.19	0/1863	0.44	0/2481
33	L1	0.16	0/1318	0.44	0/1767
34	L2	0.21	0/1515	0.34	0/2002
35	L3	0.20	0/1542	0.41	0/2058
36	M2	0.25	0/1490	0.39	0/2000
37	M3	0.15	0/962	0.34	0/1289
38	N2	0.25	0/1327	0.37	0/1771
39	N3	0.19	0/1232	0.37	0/1656
40	O2	0.18	0/839	0.39	0/1126
41	O3	0.24	0/1015	0.45	0/1361
42	P2	0.26	0/983	0.47	1/1319 (0.1%)
43	P3	0.22	0/1051	0.42	0/1406
44	Q2	0.23	0/532	0.34	0/708
45	Q3	0.22	0/1019	0.53	0/1354
46	R2	0.22	0/984	0.39	0/1323
47	R3	0.18	0/691	0.46	0/922
48	S2	0.21	0/1132	0.33	0/1504
49	S3	0.22	0/665	0.54	0/891
50	T2	0.23	0/1130	0.39	0/1507
51	T3	0.21	0/443	0.35	0/582
52	U2	0.26	0/1193	0.36	0/1593
53	U3	0.24	0/424	0.67	0/566
54	V2	0.21	0/963	0.34	0/1275
55	W2	0.23	0/742	0.43	0/996
56	X2	0.24	0/903	0.36	0/1216
57	Y2	0.26	0/1071	0.37	0/1429
58	Z2	0.26	0/895	0.36	0/1198
59	a2	0.25	0/916	0.36	0/1221
60	b2	0.19	0/1009	0.34	0/1332
61	c2	0.18	0/843	0.31	0/1115
62	d2	0.27	0/720	0.46	0/952
63	e2	0.20	0/574	0.36	0/760
64	f2	0.24	0/454	0.33	0/599
65	g2	0.22	0/435	0.44	0/575
66	h2	0.24	0/231	0.33	0/294
67	i2	0.24	0/855	0.38	0/1128
68	j2	0.27	0/704	0.48	0/935
69	k2	0.23	0/1016	0.39	0/1363
70	m2	0.22	0/38207	0.30	0/59540
71	o2	0.19	0/1731	0.43	0/2352
72	p2	0.25	0/1749	0.54	0/2340
73	q2	0.22	0/1739	0.52	1/2342 (0.0%)
74	r2	0.22	0/2118	0.53	0/2849

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	s2	0.18	0/1477	0.40	0/1983
76	t2	0.19	0/1299	0.45	0/1767
77	u2	0.21	0/1662	0.45	0/2228
78	v2	0.20	0/824	0.46	0/1112
79	w2	0.28	0/1241	0.58	3/1662 (0.2%)
80	x2	0.18	0/977	0.47	0/1305
81	y2	0.23	0/1146	0.51	0/1534
82	z2	0.18	0/1094	0.46	0/1469
All	All	0.23	0/226900	0.35	7/333169 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	P2	92	ASP	N-CA-C	-6.42	103.46	113.02
18	F1	115	GLN	CB-CG-CD	6.41	123.49	112.60
73	q2	68	GLU	CA-CB-CG	6.39	126.87	114.10
79	w2	32	LYS	CA-C-N	6.38	129.22	120.67
79	w2	32	LYS	C-N-CA	6.38	129.22	120.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1843	0	1975	46	0
2	A2	77547	0	39263	852	0
3	A3	1157	0	1213	42	0
4	B1	1812	0	1947	44	0
5	B2	2538	0	1286	30	0
6	B3	1104	0	1139	38	0
7	Bv	1623	0	821	11	0
7	n2	1623	0	821	29	0
8	Bx	200	0	101	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C1	1519	0	1603	24	0
10	C2	3315	0	1685	39	0
11	C3	795	0	862	25	0
12	D1	1656	0	1706	24	0
13	D2	1921	0	2022	35	0
14	D3	638	0	635	10	0
15	E1	1397	0	1425	39	0
16	E2	3238	0	3380	50	0
17	E3	1080	0	1147	21	0
18	F1	1643	0	1750	23	0
19	F2	2867	0	3040	51	0
20	F3	789	0	841	23	0
21	G1	1143	0	1219	17	0
22	G2	2389	0	2420	37	0
23	G3	488	0	514	13	0
24	H1	1701	0	1749	28	0
25	H2	1789	0	1932	40	0
26	H3	455	0	445	16	0
27	I2	1640	0	1792	33	0
28	I3	2436	0	2393	81	0
29	J2	1242	0	1274	20	0
30	J3	1700	0	1786	32	0
31	K2	1511	0	1636	21	0
32	K3	1840	0	1989	63	0
33	L1	1300	0	1375	41	0
34	L2	1499	0	1651	25	0
35	L3	1518	0	1632	47	0
36	M2	1450	0	1488	19	0
37	M3	952	0	993	30	0
38	N2	1299	0	1368	29	0
39	N3	1208	0	1294	24	0
40	O2	825	0	850	20	0
41	O3	1002	0	1023	45	0
42	P2	969	0	1031	12	0
43	P3	1034	0	1080	24	0
44	Q2	519	0	533	5	0
45	Q3	1002	0	1075	34	0
46	R2	967	0	1040	18	0
47	R3	683	0	761	25	0
48	S2	1115	0	1205	16	0
49	S3	651	0	672	17	0
50	T2	1107	0	1182	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	T3	438	0	484	9	0
52	U2	1164	0	1213	14	0
53	U3	415	0	393	15	0
54	V2	945	0	1037	17	0
55	W2	732	0	769	13	0
56	X2	888	0	930	10	0
57	Y2	1053	0	1147	16	0
58	Z2	876	0	912	14	0
59	a2	906	0	997	13	0
60	b2	1001	0	1138	15	0
61	c2	832	0	917	7	0
62	d2	705	0	737	12	0
63	e2	568	0	635	13	0
64	f2	444	0	483	4	0
65	g2	429	0	465	4	0
66	h2	230	0	276	7	0
67	i2	842	0	912	11	0
68	j2	694	0	738	13	0
69	k2	1001	0	1066	16	0
70	m2	34879	0	17619	492	0
71	o2	1694	0	1696	44	0
72	p2	1722	0	1794	57	0
73	q2	1711	0	1805	59	0
74	r2	2076	0	2177	61	0
75	s2	1457	0	1508	38	0
76	t2	1278	0	1207	21	0
77	u2	1633	0	1666	40	0
78	v2	800	0	818	37	0
79	w2	1220	0	1289	36	0
80	x2	959	0	1004	30	0
81	y2	1128	0	1195	44	0
82	z2	1080	0	1135	20	0
83	A2	82	0	0	0	0
83	Bv	2	0	0	0	0
83	H1	1	0	0	0	0
83	J2	1	0	0	0	0
83	P2	1	0	0	0	0
83	d2	1	0	0	0	0
83	m2	34	0	0	0	0
84	A2	65	0	16	0	0
84	Bv	5	0	1	0	0
84	F2	15	0	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	J2	5	0	2	0	0
84	f2	20	0	8	0	0
85	F3	1	0	0	0	0
85	H3	1	0	0	0	0
85	d2	1	0	0	0	0
85	g2	1	0	0	0	0
85	i2	1	0	0	0	0
85	j2	1	0	0	0	0
86	B1	1	0	0	0	0
All	All	213778	0	158256	3073	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 3073 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:1374:G:N2	2:A2:1379:C:O2	1.95	1.00
70:m2:1290:U:H3	70:m2:1313:C:H42	1.10	0.99
2:A2:740:A:H62	2:A2:828:G:H21	0.97	0.94
70:m2:1409:U:H5''	81:y2:71:ARG:HH12	1.31	0.93
2:A2:1754:G:H4'	36:M2:93:MET:HG2	1.51	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	220/270 (82%)	213 (97%)	7 (3%)	0	100	100
3	A3	138/152 (91%)	133 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B1	220/266 (83%)	213 (97%)	7 (3%)	0	100	100
6	B3	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
9	C1	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
11	C3	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
12	D1	200/214 (94%)	191 (96%)	9 (4%)	0	100	100
13	D2	249/257 (97%)	241 (97%)	8 (3%)	0	100	100
14	D3	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
15	E1	172/178 (97%)	168 (98%)	4 (2%)	0	100	100
16	E2	400/403 (99%)	388 (97%)	12 (3%)	0	100	100
17	E3	137/143 (96%)	132 (96%)	5 (4%)	0	100	100
18	F1	201/211 (95%)	192 (96%)	9 (4%)	0	100	100
19	F2	357/419 (85%)	346 (97%)	11 (3%)	0	100	100
20	F3	97/114 (85%)	95 (98%)	2 (2%)	0	100	100
21	G1	137/217 (63%)	135 (98%)	2 (2%)	0	100	100
22	G2	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
23	G3	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
24	H1	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
25	H2	215/296 (73%)	207 (96%)	8 (4%)	0	100	100
26	H3	52/56 (93%)	47 (90%)	5 (10%)	0	100	100
27	I2	199/203 (98%)	193 (97%)	6 (3%)	0	100	100
28	I3	311/317 (98%)	296 (95%)	15 (5%)	0	100	100
29	J2	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
30	J3	217/293 (74%)	213 (98%)	4 (2%)	0	100	100
31	K2	184/188 (98%)	180 (98%)	4 (2%)	0	100	100
32	K3	225/249 (90%)	216 (96%)	9 (4%)	0	100	100
33	L1	155/217 (71%)	148 (96%)	7 (4%)	0	100	100
34	L2	177/196 (90%)	176 (99%)	1 (1%)	0	100	100
35	L3	182/194 (94%)	176 (97%)	6 (3%)	0	100	100
36	M2	173/176 (98%)	165 (95%)	8 (5%)	0	100	100
37	M3	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
38	N2	157/160 (98%)	153 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	N3	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
40	O2	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
41	O3	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
42	P2	127/140 (91%)	122 (96%)	5 (4%)	0	100	100
43	P3	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
44	Q2	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
45	Q3	120/133 (90%)	117 (98%)	3 (2%)	0	100	100
46	R2	116/156 (74%)	111 (96%)	5 (4%)	0	100	100
47	R3	83/125 (66%)	79 (95%)	4 (5%)	0	100	100
48	S2	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
49	S3	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
50	T2	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
51	T3	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
52	U2	145/148 (98%)	138 (95%)	7 (5%)	0	100	100
53	U3	50/156 (32%)	43 (86%)	7 (14%)	0	100	100
54	V2	115/160 (72%)	110 (96%)	5 (4%)	0	100	100
55	W2	92/115 (80%)	89 (97%)	3 (3%)	0	100	100
56	X2	105/125 (84%)	105 (100%)	0	0	100	100
57	Y2	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
58	Z2	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
59	a2	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
60	b2	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
61	c2	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
62	d2	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
63	e2	67/70 (96%)	67 (100%)	0	0	100	100
64	f2	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
65	g2	50/128 (39%)	50 (100%)	0	0	100	100
66	h2	22/25 (88%)	22 (100%)	0	0	100	100
67	i2	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
68	j2	87/92 (95%)	83 (95%)	4 (5%)	0	100	100
69	k2	123/137 (90%)	120 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	o2	212/295 (72%)	208 (98%)	4 (2%)	0	100	100
72	p2	210/264 (80%)	187 (89%)	23 (11%)	0	100	100
73	q2	218/243 (90%)	211 (97%)	7 (3%)	0	100	100
74	r2	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
75	s2	179/204 (88%)	172 (96%)	7 (4%)	0	100	100
76	t2	179/194 (92%)	164 (92%)	15 (8%)	0	100	100
77	u2	204/208 (98%)	189 (93%)	15 (7%)	0	100	100
78	v2	93/165 (56%)	92 (99%)	1 (1%)	0	100	100
79	w2	148/158 (94%)	136 (92%)	11 (7%)	1 (1%)	18	49
80	x2	114/145 (79%)	110 (96%)	4 (4%)	0	100	100
81	y2	140/146 (96%)	135 (96%)	5 (4%)	0	100	100
82	z2	132/135 (98%)	120 (91%)	12 (9%)	0	100	100
All	All	11256/13001 (87%)	10846 (96%)	409 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
79	w2	25	LEU

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	
1	A1	193/234 (82%)	186 (96%)	7 (4%)	31	62
3	A3	122/132 (92%)	116 (95%)	6 (5%)	22	53
4	B1	193/223 (86%)	189 (98%)	4 (2%)	47	71
6	B3	112/115 (97%)	106 (95%)	6 (5%)	20	50
9	C1	169/171 (99%)	161 (95%)	8 (5%)	23	55
11	C3	92/107 (86%)	90 (98%)	2 (2%)	45	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D1	174/181 (96%)	171 (98%)	3 (2%)	53	74
13	D2	193/199 (97%)	188 (97%)	5 (3%)	40	68
14	D3	67/67 (100%)	65 (97%)	2 (3%)	36	65
15	E1	147/149 (99%)	141 (96%)	6 (4%)	27	59
16	E2	347/348 (100%)	340 (98%)	7 (2%)	48	72
17	E3	111/115 (96%)	110 (99%)	1 (1%)	70	80
18	F1	170/178 (96%)	158 (93%)	12 (7%)	13	41
19	F2	301/348 (86%)	295 (98%)	6 (2%)	48	72
20	F3	86/97 (89%)	85 (99%)	1 (1%)	63	78
21	G1	118/157 (75%)	116 (98%)	2 (2%)	53	74
22	G2	246/249 (99%)	243 (99%)	3 (1%)	63	78
23	G3	55/62 (89%)	54 (98%)	1 (2%)	51	73
24	H1	171/172 (99%)	169 (99%)	2 (1%)	63	78
25	H2	198/256 (77%)	195 (98%)	3 (2%)	57	75
26	H3	48/49 (98%)	47 (98%)	1 (2%)	47	71
27	I2	172/173 (99%)	164 (95%)	8 (5%)	23	55
28	I3	272/275 (99%)	261 (96%)	11 (4%)	28	60
29	J2	134/163 (82%)	132 (98%)	2 (2%)	57	75
30	J3	185/224 (83%)	181 (98%)	4 (2%)	45	71
31	K2	164/165 (99%)	157 (96%)	7 (4%)	26	57
32	K3	198/218 (91%)	195 (98%)	3 (2%)	57	75
33	L1	147/197 (75%)	143 (97%)	4 (3%)	39	67
34	L2	158/175 (90%)	153 (97%)	5 (3%)	34	64
35	L3	160/168 (95%)	155 (97%)	5 (3%)	35	64
36	M2	155/156 (99%)	150 (97%)	5 (3%)	34	64
37	M3	104/108 (96%)	101 (97%)	3 (3%)	37	66
38	N2	139/140 (99%)	133 (96%)	6 (4%)	26	57
39	N3	130/131 (99%)	126 (97%)	4 (3%)	35	64
40	O2	91/114 (80%)	89 (98%)	2 (2%)	45	71
41	O3	104/119 (87%)	103 (99%)	1 (1%)	68	79
42	P2	100/107 (94%)	95 (95%)	5 (5%)	22	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	P3	112/113 (99%)	107 (96%)	5 (4%)	24	56
44	Q2	54/126 (43%)	54 (100%)	0	100	100
45	Q3	107/115 (93%)	102 (95%)	5 (5%)	23	55
46	R2	106/133 (80%)	102 (96%)	4 (4%)	29	60
47	R3	75/103 (73%)	73 (97%)	2 (3%)	39	67
48	S2	124/135 (92%)	122 (98%)	2 (2%)	55	75
49	S3	75/76 (99%)	73 (97%)	2 (3%)	39	67
50	T2	117/118 (99%)	115 (98%)	2 (2%)	53	74
51	T3	45/106 (42%)	44 (98%)	1 (2%)	45	71
52	U2	120/121 (99%)	118 (98%)	2 (2%)	53	74
53	U3	45/140 (32%)	42 (93%)	3 (7%)	15	43
54	V2	98/124 (79%)	94 (96%)	4 (4%)	27	59
55	W2	79/97 (81%)	78 (99%)	1 (1%)	61	77
56	X2	98/110 (89%)	97 (99%)	1 (1%)	68	79
57	Y2	114/121 (94%)	112 (98%)	2 (2%)	51	73
58	Z2	88/89 (99%)	87 (99%)	1 (1%)	65	78
59	a2	98/100 (98%)	96 (98%)	2 (2%)	48	72
60	b2	108/110 (98%)	102 (94%)	6 (6%)	19	49
61	c2	86/89 (97%)	85 (99%)	1 (1%)	63	78
62	d2	73/80 (91%)	73 (100%)	0	100	100
63	e2	64/65 (98%)	63 (98%)	1 (2%)	55	75
64	f2	47/48 (98%)	45 (96%)	2 (4%)	26	57
65	g2	48/116 (41%)	47 (98%)	1 (2%)	47	71
66	h2	23/24 (96%)	23 (100%)	0	100	100
67	i2	91/92 (99%)	89 (98%)	2 (2%)	45	71
68	j2	73/75 (97%)	70 (96%)	3 (4%)	27	59
69	k2	109/121 (90%)	104 (95%)	5 (5%)	24	55
71	o2	179/242 (74%)	175 (98%)	4 (2%)	45	71
72	p2	193/229 (84%)	183 (95%)	10 (5%)	21	51
73	q2	184/202 (91%)	178 (97%)	6 (3%)	33	63
74	r2	224/225 (100%)	217 (97%)	7 (3%)	35	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	s2	156/170 (92%)	151 (97%)	5 (3%)	34	64
76	t2	110/174 (63%)	101 (92%)	9 (8%)	10	36
77	u2	165/180 (92%)	159 (96%)	6 (4%)	31	62
78	v2	86/136 (63%)	84 (98%)	2 (2%)	44	70
79	w2	134/142 (94%)	129 (96%)	5 (4%)	30	61
80	x2	105/130 (81%)	97 (92%)	8 (8%)	12	39
81	y2	117/121 (97%)	115 (98%)	2 (2%)	53	74
82	z2	120/121 (99%)	115 (96%)	5 (4%)	26	58
All	All	9776/11061 (88%)	9484 (97%)	292 (3%)	37	65

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	p2	120	MET
81	y2	100	VAL
73	q2	122	VAL
76	t2	153	LEU
28	I3	43	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
45	Q3	89	HIS
57	Y2	24	GLN
48	S2	18	HIS
54	V2	6	ASN
59	a2	114	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	C2	155/156 (99%)	32 (20%)	1 (0%)
2	A2	3593/3615 (99%)	741 (20%)	13 (0%)
5	B2	118/121 (97%)	8 (6%)	0
7	Bv	75/76 (98%)	20 (26%)	0
7	n2	75/76 (98%)	36 (48%)	0
70	m2	1624/1635 (99%)	402 (24%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Bx	9/10 (90%)	3 (33%)	0
All	All	5649/5689 (99%)	1242 (21%)	14 (0%)

5 of 1242 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A2	2	G
2	A2	5	A
2	A2	17	A
2	A2	21	G
2	A2	25	A

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A2	2430	G
2	A2	2463	U
10	C2	59	A
2	A2	4351	U
2	A2	4582	U

5.4 Non-standard residues in protein, DNA, RNA chains

108 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	1MA	A2	4067	2	21,25,26	0.32	0	31,37,40	0.47	0
70	OMU	m2	116	70	19,22,23	0.29	0	26,31,34	0.47	0
2	A2M	A2	2542	2	22,25,26	0.11	0	31,36,39	0.29	0
2	A2M	A2	1337	2	22,25,26	0.15	0	31,36,39	0.36	0
2	A2M	A2	2118	2,83	22,25,26	0.11	0	31,36,39	0.26	0
2	OMC	A2	3525	2	19,22,23	0.35	0	26,31,34	0.44	0
70	OMG	m2	511	83,70	23,26,27	0.33	0	33,38,41	0.44	0
2	A2M	A2	3374	2	22,25,26	0.12	0	31,36,39	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	A2	4188	2	19,22,23	0.37	0	26,31,34	0.47	0
2	OMG	A2	2119	2,83	23,26,27	0.36	0	33,38,41	0.40	0
2	A2M	A2	3486	2	22,25,26	0.11	0	31,36,39	0.37	0
2	OMG	A2	3848	2,7	23,26,27	0.35	0	33,38,41	0.35	0
2	OMC	A2	3497	2	19,22,23	0.33	0	26,31,34	0.37	0
2	OMG	A2	1438	2	23,26,27	0.28	0	33,38,41	0.37	0
70	PSU	m2	1083	70	18,21,22	0.70	1 (5%)	22,30,33	0.66	0
2	5MC	A2	4099	2	18,22,23	0.39	0	26,32,35	0.66	0
2	PSU	A2	4288	2	18,21,22	0.52	0	22,30,33	0.62	1 (4%)
2	OMG	A2	1335	2	23,26,27	0.38	0	33,38,41	0.42	0
2	PSU	A2	1490	2	18,21,22	0.92	1 (5%)	22,30,33	0.62	0
70	B8N	m2	1250	70	24,29,30	0.60	0	29,42,45	0.66	1 (3%)
2	OMC	A2	2177	2,83	19,22,23	0.31	0	26,31,34	0.39	0
2	A2M	A2	1137	2	22,25,26	0.12	0	31,36,39	0.22	0
2	A2M	A2	398	2	22,25,26	0.09	0	31,36,39	0.33	0
2	OMG	A2	2179	2	23,26,27	0.33	0	33,38,41	0.36	0
2	OMC	A2	2120	2	19,22,23	0.31	0	26,31,34	0.48	0
2	OMG	A2	4022	2	23,26,27	0.34	0	33,38,41	0.41	0
2	OMG	A2	3283	2	23,26,27	0.32	0	33,38,41	0.51	0
70	A2M	m2	99	83,70	22,25,26	0.10	0	31,36,39	0.45	0
2	A2M	A2	3481	2	22,25,26	0.10	0	31,36,39	0.30	0
2	OMG	A2	4289	2	23,26,27	0.38	0	33,38,41	0.44	0
2	OMG	A2	4146	2	23,26,27	0.36	0	33,38,41	0.42	0
2	A2M	A2	4175	2,83	22,25,26	0.12	0	31,36,39	0.42	0
70	A2M	m2	27	70	22,25,26	0.13	0	31,36,39	0.24	0
2	PSU	A2	2263	2	18,21,22	0.51	0	22,30,33	0.61	0
2	OMC	A2	2106	2	19,22,23	0.33	0	26,31,34	0.36	0
2	OMC	A2	2616	2	19,22,23	0.29	0	26,31,34	0.36	0
70	PSU	m2	824	70	18,21,22	0.61	1 (5%)	22,30,33	0.67	1 (4%)
2	PSU	A2	3420	2	18,21,22	0.42	0	22,30,33	0.48	0
70	OMU	m2	430	70	19,22,23	0.29	0	26,31,34	0.48	0
2	OMG	A2	4044	2	23,26,27	0.35	0	33,38,41	0.35	0
2	OMU	A2	3958	2	19,22,23	0.33	0	26,31,34	0.45	0
2	A2M	A2	2156	2	22,25,26	0.11	0	31,36,39	0.19	0
10	OMG	C2	75	10	23,26,27	0.30	0	33,38,41	0.39	0
70	B8T	m2	1339	70	19,22,23	0.40	0	26,31,34	0.39	0
2	OMG	A2	3400	2	23,26,27	0.31	0	33,38,41	0.39	0
70	PSU	m2	825	70	18,21,22	0.54	0	22,30,33	0.54	0
2	PSU	A2	4094	2	18,21,22	0.57	0	22,30,33	0.62	0
2	OMU	A2	3581	2	19,22,23	0.33	0	26,31,34	0.49	0
2	PSU	A2	1395	2	18,21,22	0.57	0	22,30,33	0.54	0
70	A2M	m2	1033	70	22,25,26	0.10	0	31,36,39	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	OMC	m2	1705	70	19,22,23	0.29	0	26,31,34	0.42	0
70	OMG	m2	603	70	23,26,27	0.31	0	33,38,41	0.35	0
2	2MG	A2	1330	2	23,26,27	0.35	0	32,38,41	0.39	0
2	A2M	A2	3380	2	22,25,26	0.10	0	31,36,39	0.34	0
70	OMG	m2	869	70	23,26,27	0.28	0	33,38,41	0.34	0
2	OMC	A2	3543	2	19,22,23	0.34	0	26,31,34	0.48	0
2	OMG	A2	3555	2,83	23,26,27	0.41	0	33,38,41	0.55	0
70	OMC	m2	174	70	19,22,23	0.33	0	26,31,34	0.50	0
2	OMG	A2	3880	2	23,26,27	0.32	0	33,38,41	0.54	0
70	OMC	m2	519	70	19,22,23	0.29	0	26,31,34	0.49	0
70	OMG	m2	685	70	23,26,27	0.33	0	33,38,41	0.57	0
70	PSU	m2	1245	70	18,21,22	0.49	0	22,30,33	0.60	0
2	OMC	A2	2559	2	19,22,23	0.32	0	26,31,34	0.36	0
2	PSU	A2	3945	2	18,21,22	0.55	0	22,30,33	0.55	0
70	A2M	m2	514	70	22,25,26	0.10	0	31,36,39	0.44	0
70	UR3	m2	1832	70	19,22,23	0.33	0	26,32,35	0.45	0
2	OMC	A2	1683	2,83	19,22,23	0.33	0	26,31,34	0.58	0
2	A2M	A2	4270	2	22,25,26	0.11	0	31,36,39	0.39	0
2	OMG	A2	1130	2	23,26,27	0.43	0	33,38,41	0.50	0
70	A2M	m2	486	70	22,25,26	0.10	0	31,36,39	0.18	0
2	OMG	A2	4275	2	23,26,27	0.36	0	33,38,41	0.49	0
70	OMG	m2	646	70	23,26,27	0.34	0	33,38,41	0.38	0
2	OMU	A2	2592	2	19,22,23	0.34	0	26,31,34	0.60	0
2	OMG	A2	4151	2	23,26,27	0.33	0	33,38,41	0.38	0
2	PSU	A2	1496	2	18,21,22	0.61	0	22,30,33	0.56	0
70	4AC	m2	1844	70	21,24,25	0.33	0	29,34,37	0.31	0
2	5MC	A2	3438	2,83	18,22,23	0.33	0	26,32,35	0.42	0
70	A2M	m2	578	70	22,25,26	0.14	0	31,36,39	0.29	0
2	OMC	A2	3464	2	19,22,23	0.33	0	26,31,34	0.37	0
2	PSU	A2	4280	2	18,21,22	0.56	0	22,30,33	0.55	0
2	A2M	A2	1140	2	22,25,26	0.11	0	31,36,39	0.19	0
2	A2M	A2	1347	2,83	22,25,26	0.11	0	31,36,39	0.57	0
70	A2M	m2	670	83,70	22,25,26	0.14	0	31,36,39	0.31	0
70	PSU	m2	614	70	18,21,22	0.59	1 (5%)	22,30,33	0.67	1 (4%)
2	OMU	A2	4150	2	19,22,23	0.31	0	26,31,34	0.42	0
70	OMU	m2	121	70	19,22,23	0.32	0	26,31,34	0.51	0
2	A2M	A2	4223	2	22,25,26	0.28	0	31,36,39	0.43	0
70	OMG	m2	1330	70	23,26,27	0.34	0	33,38,41	0.38	0
70	OMU	m2	172	70	19,22,23	0.26	0	26,31,34	0.63	1 (3%)
2	PSU	A2	3385	2	18,21,22	0.56	0	22,30,33	0.58	0
2	PSU	A2	4102	2,83	18,21,22	0.54	0	22,30,33	0.41	0
70	A2M	m2	1680	70	22,25,26	0.12	0	31,36,39	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	A2	1673	2	22,25,26	0.12	0	31,36,39	0.44	0
2	A2M	A2	3441	2	22,25,26	0.12	0	31,36,39	0.42	0
2	A2M	A2	2570	2	22,25,26	0.09	0	31,36,39	0.18	0
2	PSU	A2	4055	2	18,21,22	0.57	0	22,30,33	0.61	1 (4%)
2	OMU	A2	4272	2	19,22,23	0.43	0	26,31,34	0.64	0
70	OMG	m2	438	70	23,26,27	0.34	0	33,38,41	0.46	0
2	OMC	A2	2579	2	19,22,23	0.31	0	26,31,34	0.44	0
2	PSU	A2	4183	2	18,21,22	0.55	0	22,30,33	0.40	0
2	OMG	A2	3448	2	23,26,27	0.34	0	33,38,41	0.33	0
2	OMC	A2	4108	2	19,22,23	0.32	0	26,31,34	0.39	0
2	OMU	A2	3474	2	19,22,23	0.34	0	26,31,34	0.45	0
2	PSU	A2	4152	2	18,21,22	0.54	0	22,30,33	0.65	0
70	OMC	m2	355	70	19,22,23	0.32	0	26,31,34	0.40	0
2	OMC	A2	1154	2	19,22,23	0.32	0	26,31,34	0.42	0
2	OMC	A2	3357	2	19,22,23	0.29	0	26,31,34	0.47	0
2	PSU	A2	3371	2	18,21,22	0.57	0	22,30,33	0.59	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MA	A2	4067	2	-	0/7/25/26	0/3/3/3
70	OMU	m2	116	70	-	0/9/27/28	0/2/2/2
2	A2M	A2	2542	2	-	3/9/27/28	0/3/3/3
2	A2M	A2	1337	2	-	1/9/27/28	0/3/3/3
2	A2M	A2	2118	2,83	-	0/9/27/28	0/3/3/3
2	OMC	A2	3525	2	-	0/9/27/28	0/2/2/2
70	OMG	m2	511	83,70	-	0/9/27/28	0/3/3/3
2	A2M	A2	3374	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	4188	2	-	0/9/27/28	0/2/2/2
2	OMG	A2	2119	2,83	-	2/9/27/28	0/3/3/3
2	A2M	A2	3486	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	3848	2,7	-	0/9/27/28	0/3/3/3
2	OMC	A2	3497	2	-	0/9/27/28	0/2/2/2
2	OMG	A2	1438	2	-	3/9/27/28	0/3/3/3
70	PSU	m2	1083	70	-	1/7/25/26	0/2/2/2
2	5MC	A2	4099	2	-	3/7/25/26	0/2/2/2
2	PSU	A2	4288	2	-	4/7/25/26	0/2/2/2
2	OMG	A2	1335	2	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A2	1490	2	-	0/7/25/26	0/2/2/2
70	B8N	m2	1250	70	-	3/16/34/35	0/2/2/2
2	OMC	A2	2177	2,83	-	1/9/27/28	0/2/2/2
2	A2M	A2	1137	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	398	2	-	1/9/27/28	0/3/3/3
2	OMG	A2	2179	2	-	1/9/27/28	0/3/3/3
2	OMC	A2	2120	2	-	0/9/27/28	0/2/2/2
2	OMG	A2	4022	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	3283	2	-	0/9/27/28	0/3/3/3
70	A2M	m2	99	83,70	-	0/9/27/28	0/3/3/3
2	A2M	A2	3481	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	4289	2	-	3/9/27/28	0/3/3/3
2	OMG	A2	4146	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	4175	2,83	-	0/9/27/28	0/3/3/3
70	A2M	m2	27	70	-	0/9/27/28	0/3/3/3
2	PSU	A2	2263	2	-	0/7/25/26	0/2/2/2
2	OMC	A2	2106	2	-	4/9/27/28	0/2/2/2
2	OMC	A2	2616	2	-	0/9/27/28	0/2/2/2
70	PSU	m2	824	70	-	2/7/25/26	0/2/2/2
2	PSU	A2	3420	2	-	3/7/25/26	0/2/2/2
70	OMU	m2	430	70	-	4/9/27/28	0/2/2/2
2	OMG	A2	4044	2	-	0/9/27/28	0/3/3/3
2	OMU	A2	3958	2	-	0/9/27/28	0/2/2/2
2	A2M	A2	2156	2	-	0/9/27/28	0/3/3/3
10	OMG	C2	75	10	-	2/9/27/28	0/3/3/3
70	B8T	m2	1339	70	-	0/7/27/28	0/2/2/2
2	OMG	A2	3400	2	-	0/9/27/28	0/3/3/3
70	PSU	m2	825	70	-	0/7/25/26	0/2/2/2
2	PSU	A2	4094	2	-	0/7/25/26	0/2/2/2
2	OMU	A2	3581	2	-	1/9/27/28	0/2/2/2
2	PSU	A2	1395	2	-	0/7/25/26	0/2/2/2
70	A2M	m2	1033	70	-	0/9/27/28	0/3/3/3
70	OMC	m2	1705	70	-	0/9/27/28	0/2/2/2
70	OMG	m2	603	70	-	1/9/27/28	0/3/3/3
2	2MG	A2	1330	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	3380	2	-	1/9/27/28	0/3/3/3
70	OMG	m2	869	70	-	1/9/27/28	0/3/3/3
2	OMC	A2	3543	2	-	1/9/27/28	0/2/2/2
2	OMG	A2	3555	2,83	-	0/9/27/28	0/3/3/3
70	OMC	m2	174	70	-	3/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	A2	3880	2	-	0/9/27/28	0/3/3/3
70	OMC	m2	519	70	-	2/9/27/28	0/2/2/2
70	OMG	m2	685	70	-	2/9/27/28	0/3/3/3
70	PSU	m2	1245	70	-	2/7/25/26	0/2/2/2
2	OMC	A2	2559	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	3945	2	-	0/7/25/26	0/2/2/2
70	A2M	m2	514	70	-	0/9/27/28	0/3/3/3
70	UR3	m2	1832	70	-	2/7/25/26	0/2/2/2
2	OMC	A2	1683	2,83	-	0/9/27/28	0/2/2/2
2	A2M	A2	4270	2	-	0/9/27/28	0/3/3/3
2	OMG	A2	1130	2	-	1/9/27/28	0/3/3/3
70	A2M	m2	486	70	-	1/9/27/28	0/3/3/3
2	OMG	A2	4275	2	-	0/9/27/28	0/3/3/3
70	OMG	m2	646	70	-	3/9/27/28	0/3/3/3
2	OMU	A2	2592	2	-	0/9/27/28	0/2/2/2
2	OMG	A2	4151	2	-	2/9/27/28	0/3/3/3
2	PSU	A2	1496	2	-	0/7/25/26	0/2/2/2
70	4AC	m2	1844	70	-	0/11/29/30	0/2/2/2
2	5MC	A2	3438	2,83	-	0/7/25/26	0/2/2/2
70	A2M	m2	578	70	-	1/9/27/28	0/3/3/3
2	OMC	A2	3464	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	4280	2	-	0/7/25/26	0/2/2/2
2	A2M	A2	1140	2	-	3/9/27/28	0/3/3/3
2	A2M	A2	1347	2,83	-	3/9/27/28	0/3/3/3
70	A2M	m2	670	83,70	-	2/9/27/28	0/3/3/3
70	PSU	m2	614	70	-	0/7/25/26	0/2/2/2
2	OMU	A2	4150	2	-	0/9/27/28	0/2/2/2
70	OMU	m2	121	70	-	0/9/27/28	0/2/2/2
2	A2M	A2	4223	2	-	0/9/27/28	0/3/3/3
70	OMG	m2	1330	70	-	2/9/27/28	0/3/3/3
70	OMU	m2	172	70	-	3/9/27/28	0/2/2/2
2	PSU	A2	3385	2	-	1/7/25/26	0/2/2/2
2	PSU	A2	4102	2,83	-	3/7/25/26	0/2/2/2
70	A2M	m2	1680	70	-	1/9/27/28	0/3/3/3
2	A2M	A2	1673	2	-	0/9/27/28	0/3/3/3
2	A2M	A2	3441	2	-	4/9/27/28	0/3/3/3
2	A2M	A2	2570	2	-	0/9/27/28	0/3/3/3
2	PSU	A2	4055	2	-	0/7/25/26	0/2/2/2
2	OMU	A2	4272	2	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	OMG	m2	438	70	-	1/9/27/28	0/3/3/3
2	OMC	A2	2579	2	-	0/9/27/28	0/2/2/2
2	PSU	A2	4183	2	-	2/7/25/26	0/2/2/2
2	OMG	A2	3448	2	-	0/9/27/28	0/3/3/3
2	OMC	A2	4108	2	-	0/9/27/28	0/2/2/2
2	OMU	A2	3474	2	-	1/9/27/28	0/2/2/2
2	PSU	A2	4152	2	-	1/7/25/26	0/2/2/2
70	OMC	m2	355	70	-	1/9/27/28	0/2/2/2
2	OMC	A2	1154	2	-	0/9/27/28	0/2/2/2
2	OMC	A2	3357	2	-	4/9/27/28	0/2/2/2
2	PSU	A2	3371	2	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A2	1490	PSU	O4'-C1'	-3.35	1.39	1.43
70	m2	1083	PSU	O4'-C1'	-2.53	1.40	1.43
70	m2	824	PSU	O4'-C1'	-2.25	1.40	1.43
70	m2	614	PSU	O4'-C1'	-2.10	1.40	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	m2	172	OMU	O2'-C2'-C1'	2.44	113.84	109.08
70	m2	614	PSU	O4'-C1'-C2'	2.32	108.42	105.14
70	m2	824	PSU	O4'-C1'-C2'	2.28	108.36	105.14
2	A2	3371	PSU	O4'-C1'-C2'	2.08	108.08	105.14
70	m2	1250	B8N	O4'-C1'-C2'	2.05	108.03	105.14

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C2	75	OMG	O4'-C4'-C5'-O5'
10	C2	75	OMG	C3'-C4'-C5'-O5'
2	A2	398	A2M	C1'-C2'-O2'-CM'
2	A2	1140	A2M	O4'-C4'-C5'-O5'
2	A2	1140	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

52 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A2	4067	1MA	2	0
2	A2	2118	A2M	1	0
70	m2	511	OMG	5	0
2	A2	3374	A2M	1	0
2	A2	4188	OMC	1	0
2	A2	2119	OMG	1	0
2	A2	1438	OMG	2	0
2	A2	4099	5MC	2	0
2	A2	1490	PSU	1	0
2	A2	398	A2M	2	0
2	A2	2179	OMG	2	0
2	A2	2120	OMC	1	0
70	m2	99	A2M	1	0
2	A2	4289	OMG	2	0
70	m2	27	A2M	1	0
2	A2	2106	OMC	3	0
2	A2	3420	PSU	1	0
2	A2	4044	OMG	2	0
70	m2	1033	A2M	1	0
70	m2	1705	OMC	1	0
70	m2	603	OMG	2	0
2	A2	1330	2MG	1	0
2	A2	3380	A2M	1	0
70	m2	869	OMG	1	0
70	m2	174	OMC	2	0
2	A2	3880	OMG	1	0
70	m2	519	OMC	1	0
70	m2	685	OMG	1	0
2	A2	2559	OMC	2	0
2	A2	1683	OMC	2	0
2	A2	4270	A2M	1	0
2	A2	1130	OMG	1	0
70	m2	486	A2M	2	0
2	A2	1496	PSU	2	0
70	m2	1844	4AC	1	0
70	m2	578	A2M	1	0
2	A2	1140	A2M	1	0
2	A2	1347	A2M	2	0
2	A2	4150	OMU	1	0
70	m2	121	OMU	1	0
2	A2	4223	A2M	3	0
70	m2	172	OMU	1	0
70	m2	1680	A2M	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A2	1673	A2M	1	0
2	A2	2570	A2M	1	0
2	A2	4272	OMU	2	0
2	A2	4108	OMC	1	0
2	A2	3474	OMU	2	0
2	A2	4152	PSU	1	0
70	m2	355	OMC	2	0
2	A2	1154	OMC	2	0
2	A2	3371	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 150 ligands modelled in this entry, 128 are monoatomic and 22 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A2	21
70	m2	6

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m2	130:G	O3'	141:A	P	25.44
1	A2	1512:U	O3'	1521:A	P	24.55
1	A2	2658:G	O3'	3240:C	P	18.64
1	A2	891:C	O3'	917:G	P	18.18
1	m2	690:U	O3'	801:U	P	18.05

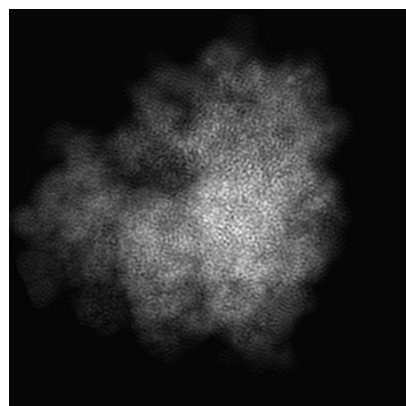
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53307. These allow visual inspection of the internal detail of the map and identification of artifacts.

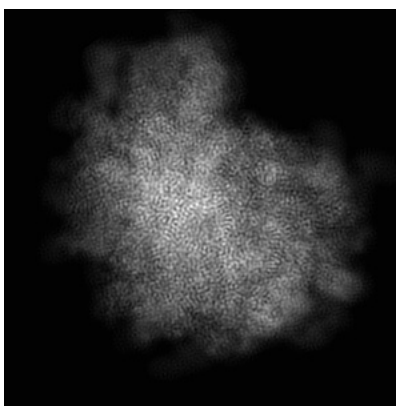
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

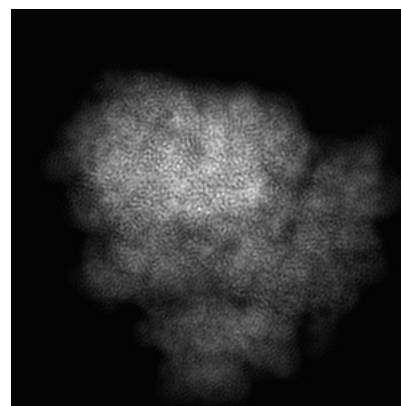
6.1.1 Primary map



X

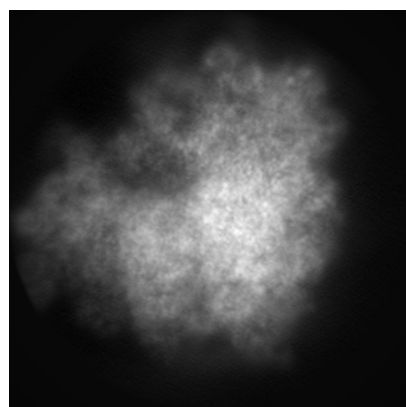


Y

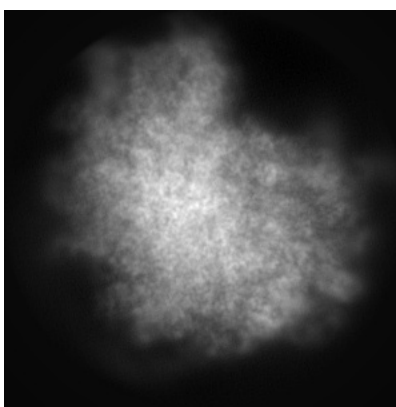


Z

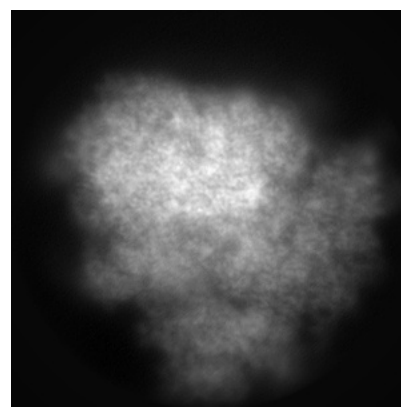
6.1.2 Raw map



X



Y

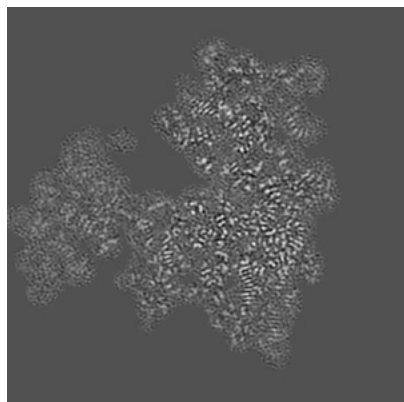


Z

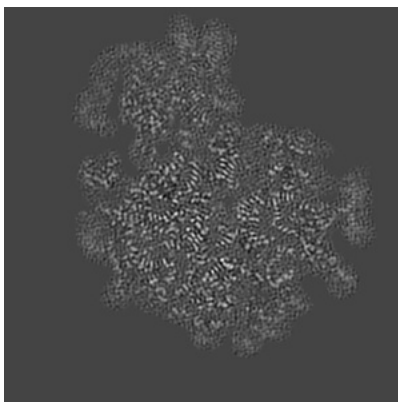
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

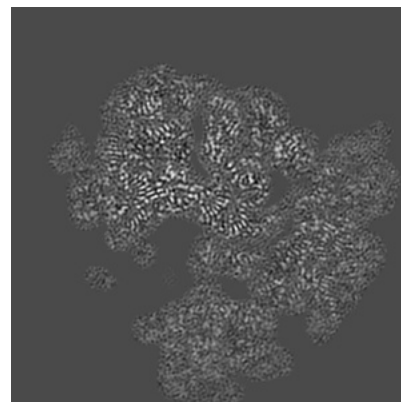
6.2.1 Primary map



X Index: 156

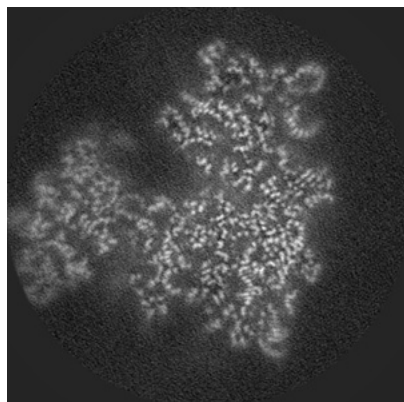


Y Index: 156

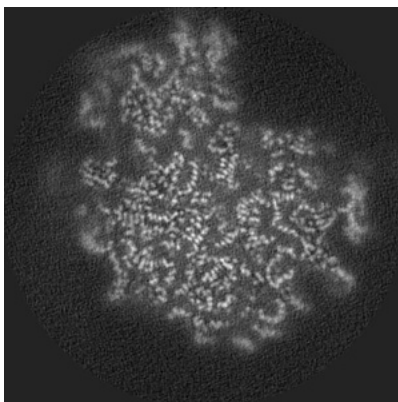


Z Index: 156

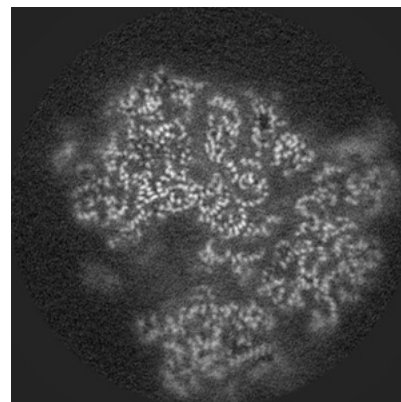
6.2.2 Raw map



X Index: 156



Y Index: 156

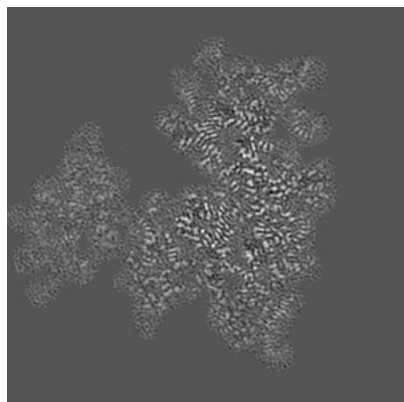


Z Index: 156

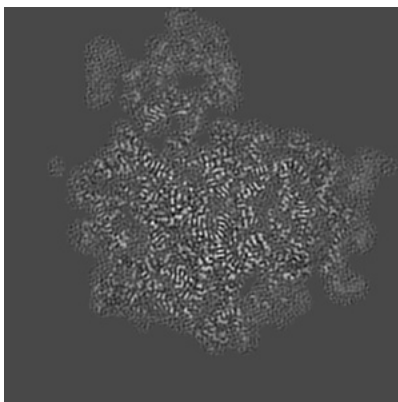
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

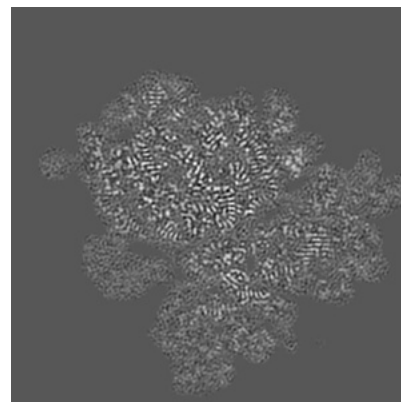
6.3.1 Primary map



X Index: 161

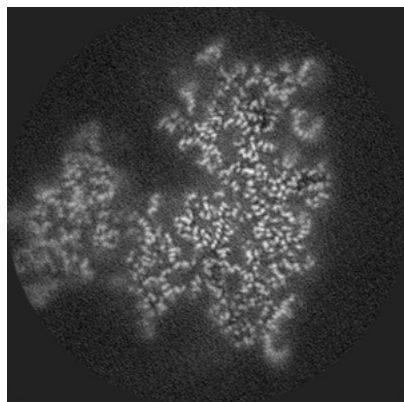


Y Index: 170

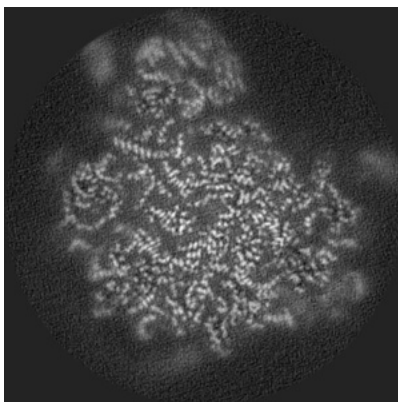


Z Index: 131

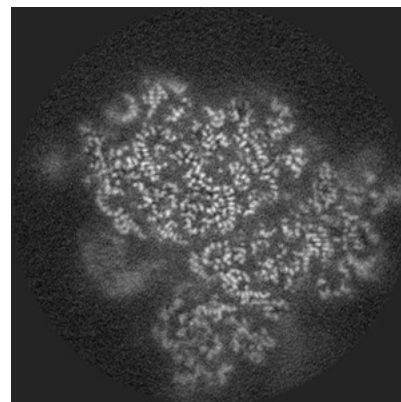
6.3.2 Raw map



X Index: 161



Y Index: 180

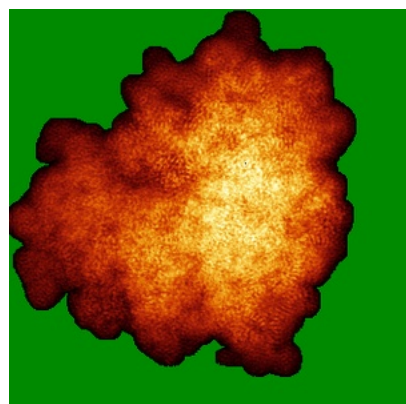


Z Index: 131

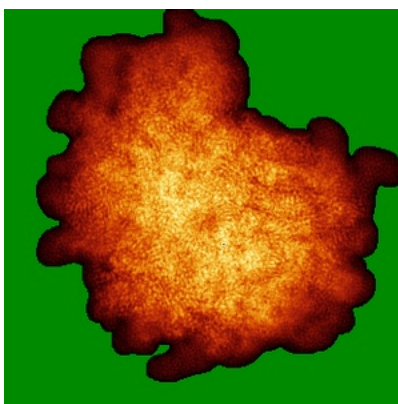
The images above show the largest variance slices of the map in three orthogonal directions.

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

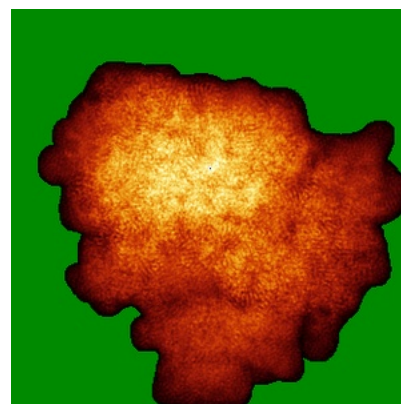
6.4.1 Primary map



X

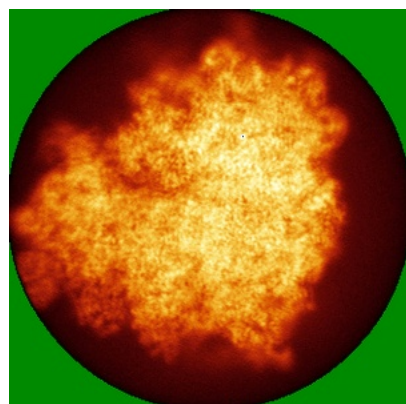


Y

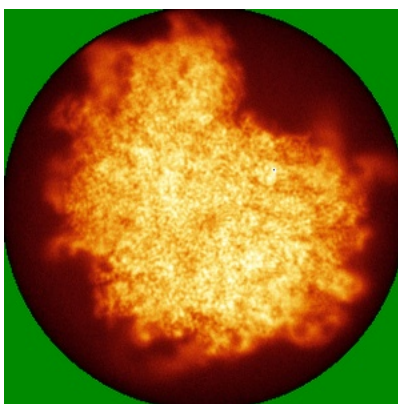


Z

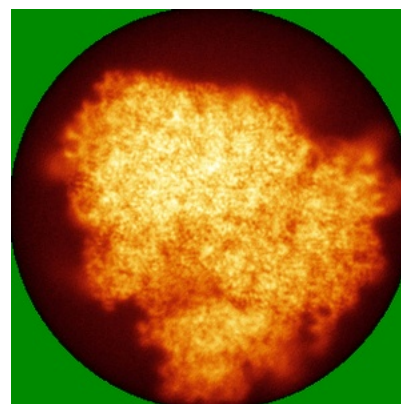
6.4.2 Raw map



X



Y

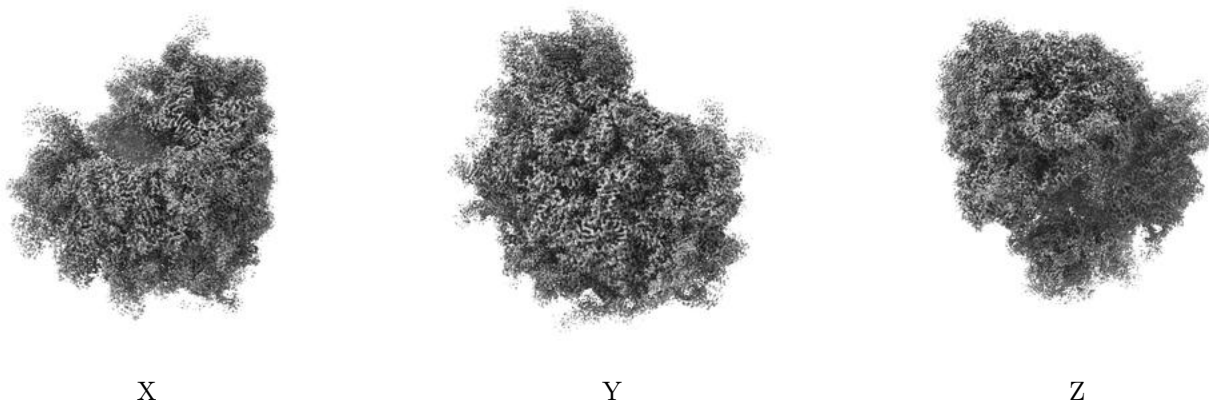


Z

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

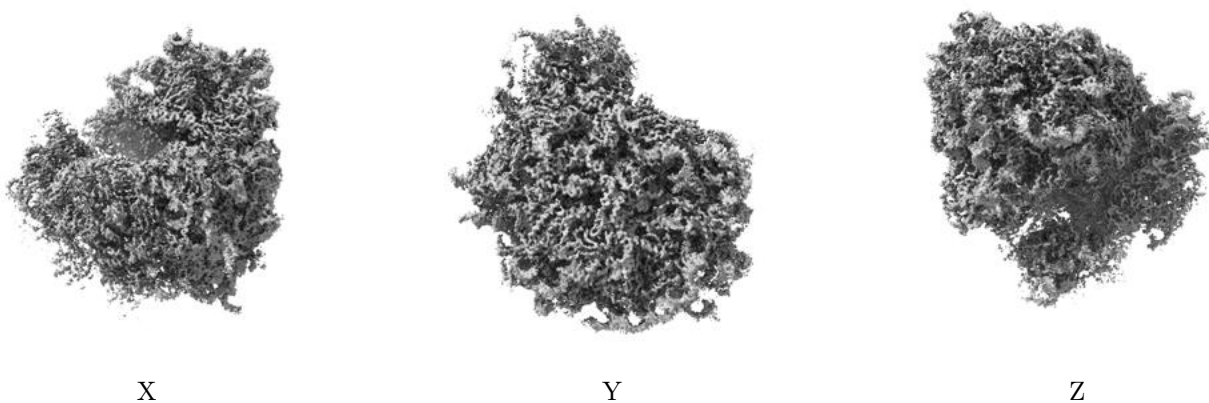
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0285. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

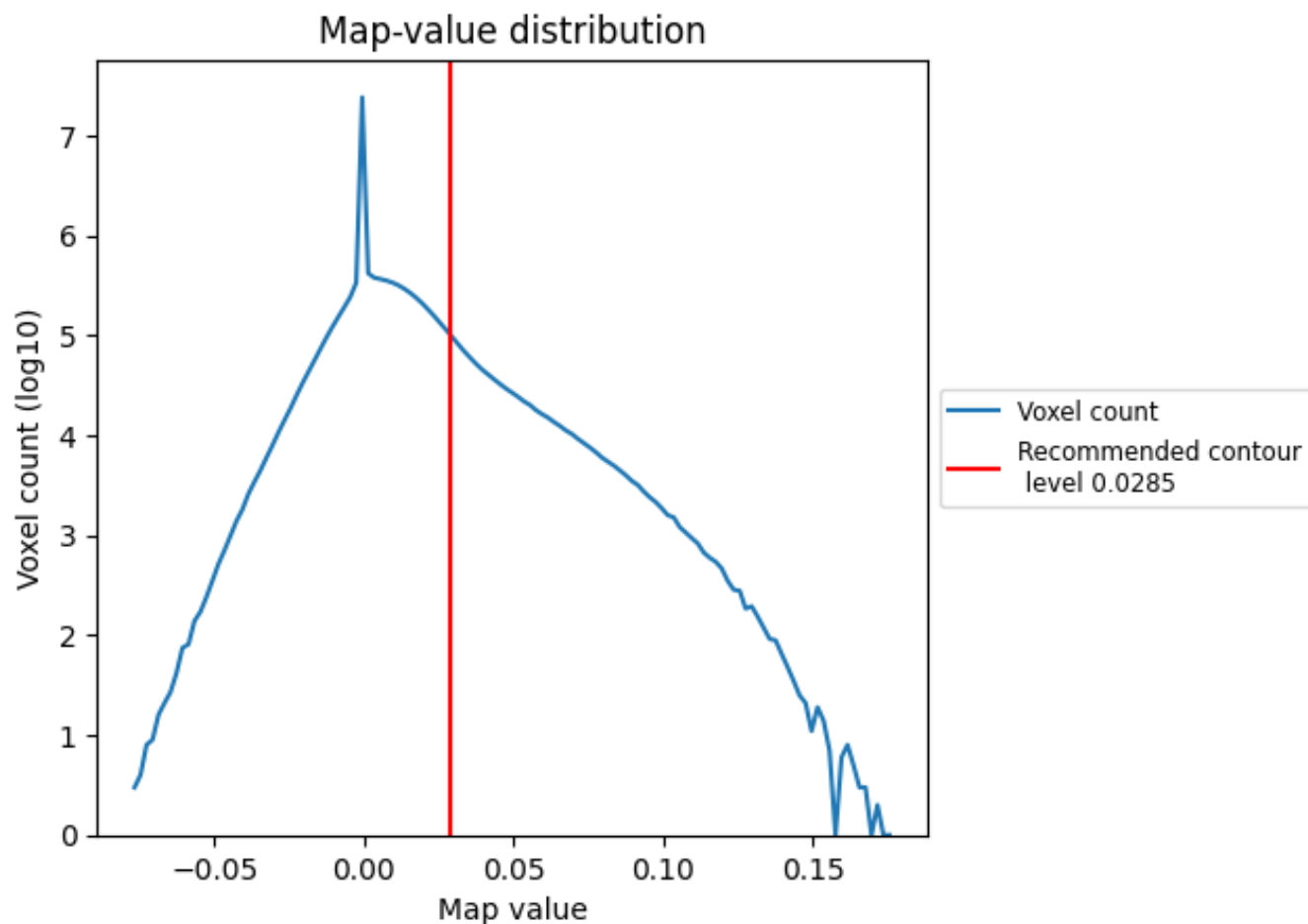
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

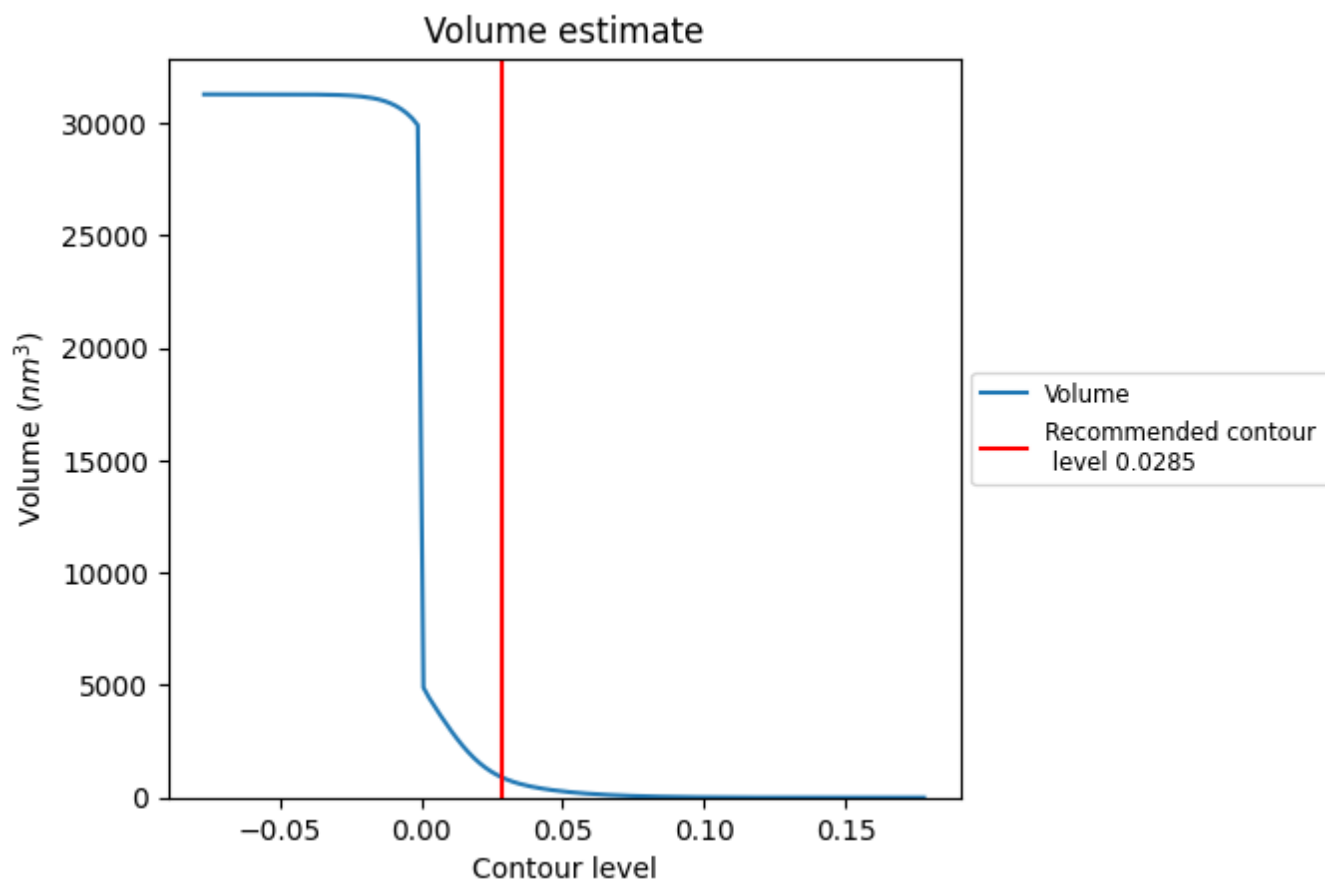
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

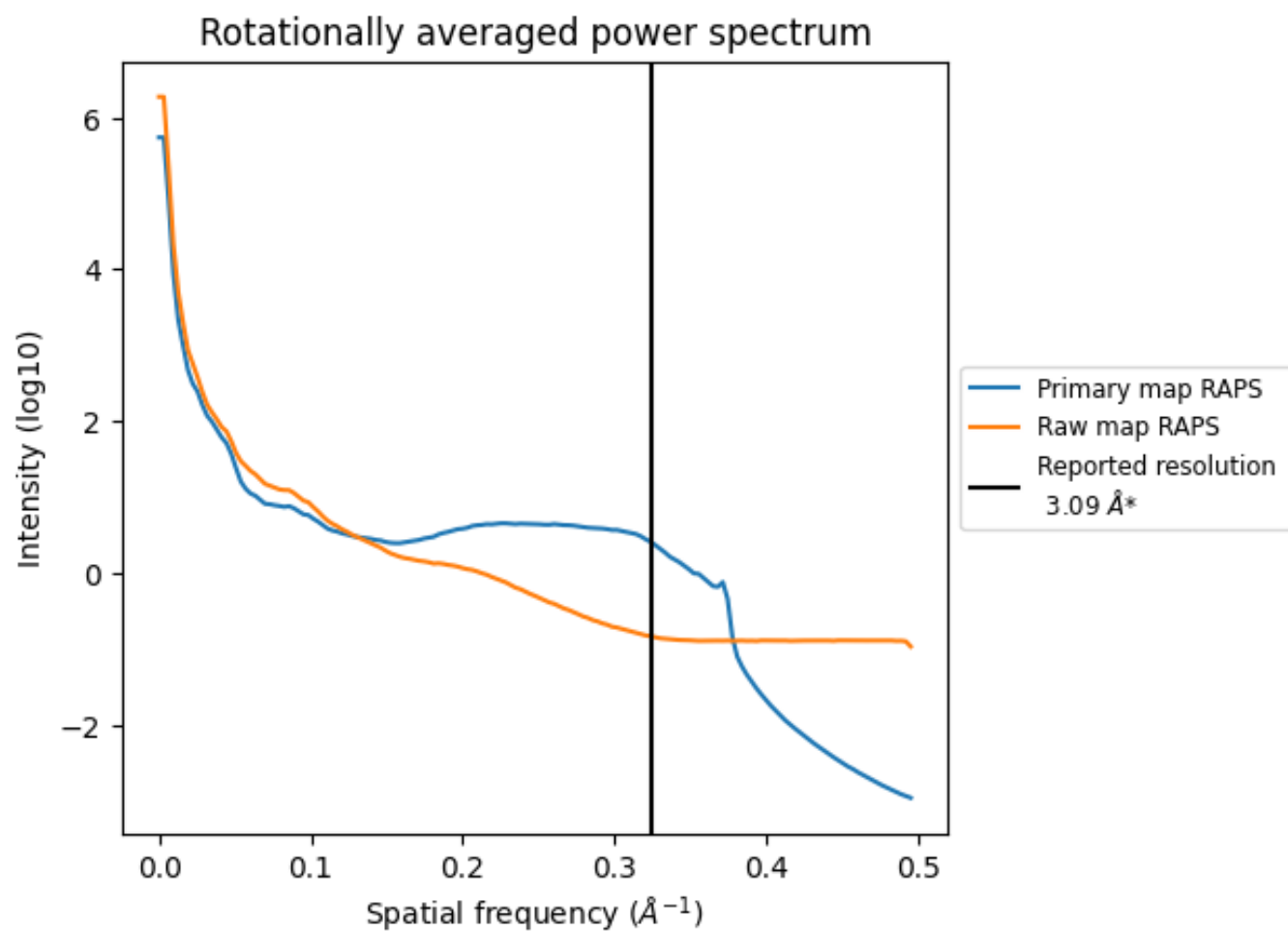
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 902 nm³; this corresponds to an approximate mass of 815 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 ⓘ

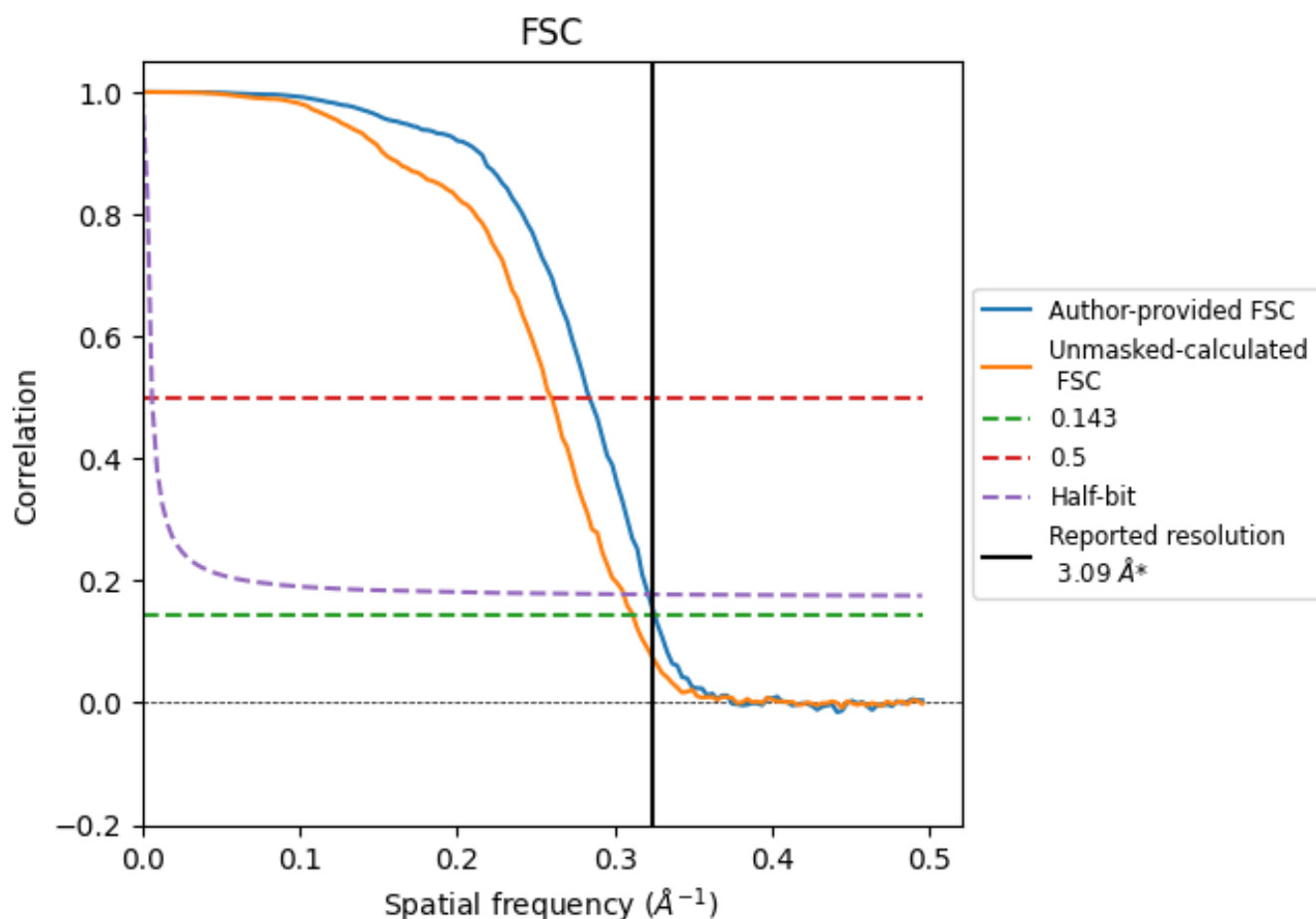


*Reported resolution corresponds to spatial frequency of $0.324 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.324 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

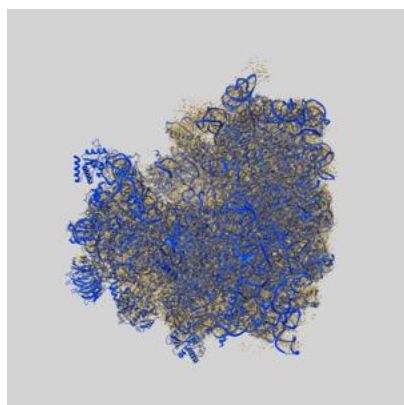
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.08	3.52	3.11
Unmasked-calculated*	3.21	3.85	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

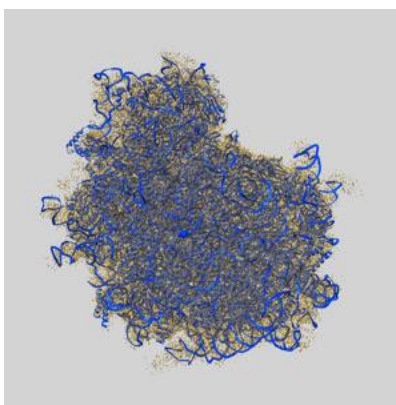
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53307 and PDB model 9QQL. Per-residue inclusion information can be found in section [3](#) on page [21](#).

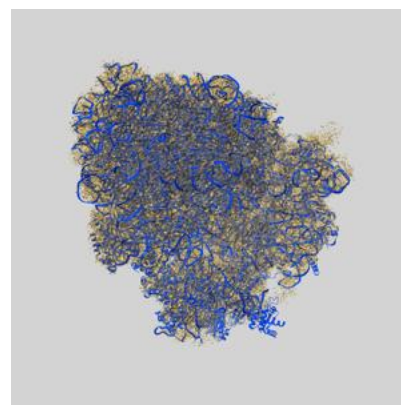
9.1 Map-model overlay [i](#)



X



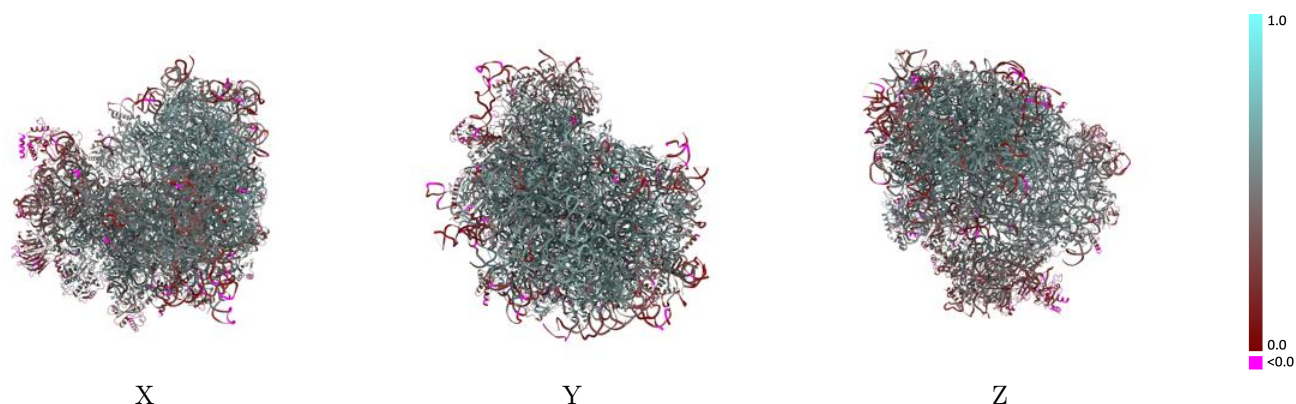
Y



Z

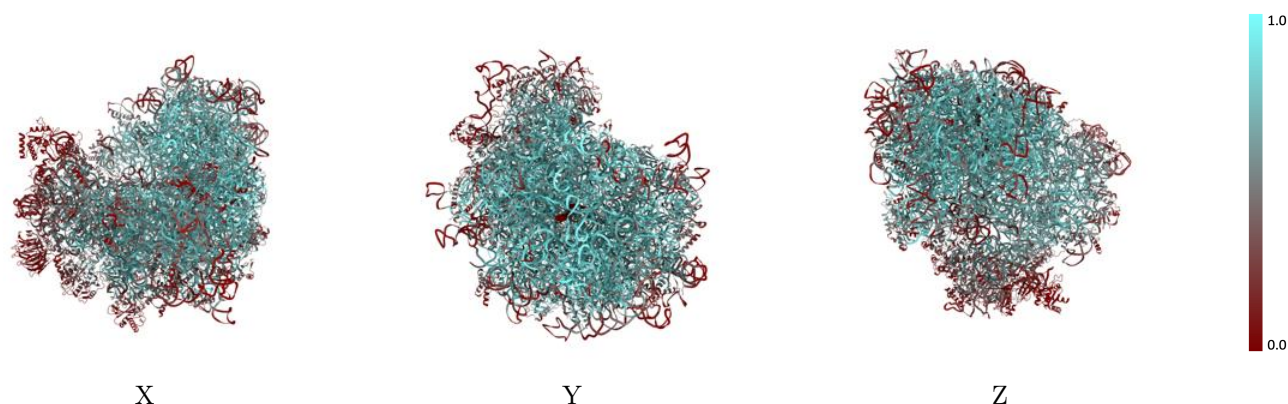
The images above show the 3D surface view of the map at the recommended contour level 0.0285 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



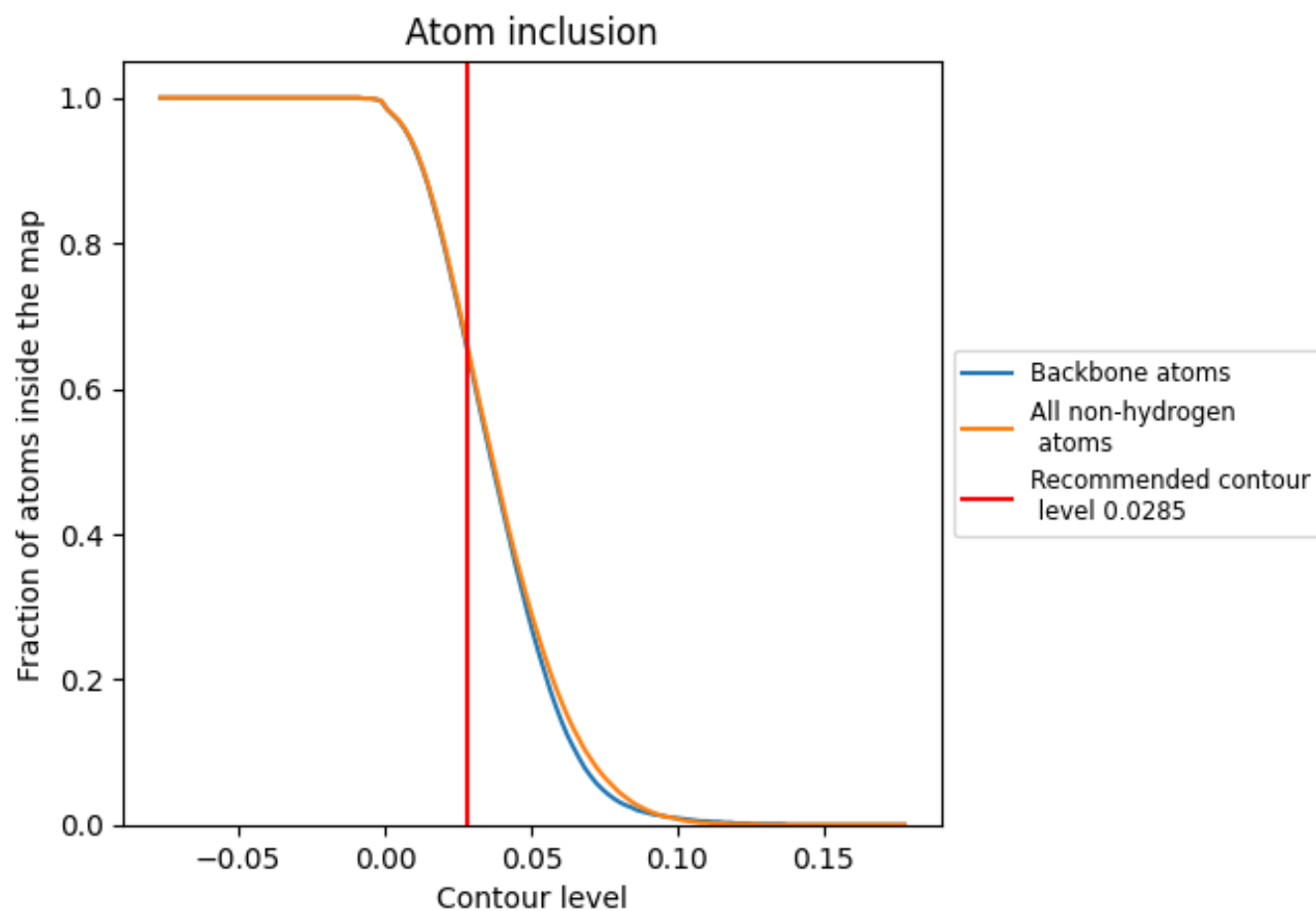
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0285).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.0285) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6530	 0.4880
A1	 0.7760	 0.5580
A2	 0.7540	 0.5080
A3	 0.2440	 0.3430
B1	 0.5550	 0.4560
B2	 0.8480	 0.5700
B3	 0.2840	 0.3660
Bv	 0.2800	 0.3410
Bx	 0.3000	 0.2900
C1	 0.6780	 0.5480
C2	 0.8210	 0.5400
C3	 0.2440	 0.3440
D1	 0.7320	 0.5430
D2	 0.8360	 0.5810
D3	 0.3730	 0.4440
E1	 0.4450	 0.4390
E2	 0.7600	 0.5640
E3	 0.6930	 0.5360
F1	 0.6790	 0.5230
F2	 0.7860	 0.5640
F3	 0.6610	 0.5240
G1	 0.6890	 0.5430
G2	 0.6070	 0.5080
G3	 0.3640	 0.3930
H1	 0.8730	 0.6030
H2	 0.5660	 0.4960
H3	 0.4540	 0.4210
I2	 0.7930	 0.5750
I3	 0.0640	 0.2400
J2	 0.8240	 0.5830
J3	 0.5720	 0.5130
K2	 0.8240	 0.5880
K3	 0.3230	 0.3830
L1	 0.0160	 0.1150
L2	 0.6880	 0.5100



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L3	0.4770	0.4500
M2	0.8050	0.5780
M3	0.0060	0.0970
N2	0.7250	0.5370
N3	0.6070	0.5070
O2	0.4810	0.4450
O3	0.6300	0.5040
P2	0.8070	0.5700
P3	0.6570	0.5260
Q2	0.7740	0.5610
Q3	0.3400	0.4180
R2	0.7090	0.5260
R3	0.1720	0.3040
S2	0.7010	0.5380
S3	0.4290	0.4260
T2	0.5660	0.4470
T3	0.4210	0.4090
U2	0.8130	0.5870
U3	0.0170	0.1410
V2	0.5270	0.4290
W2	0.6310	0.4900
X2	0.7130	0.5380
Y2	0.8210	0.5830
Z2	0.8530	0.5970
a2	0.7160	0.5040
b2	0.6760	0.5340
c2	0.6280	0.5100
d2	0.8620	0.5950
e2	0.4440	0.4160
f2	0.8010	0.5630
g2	0.7600	0.5520
h2	0.8180	0.5630
i2	0.7490	0.5630
j2	0.7530	0.5450
k2	0.7650	0.5580
m2	0.6740	0.4830
n2	0.1400	0.1790
o2	0.3830	0.4590
p2	0.5320	0.4770
q2	0.2700	0.3640
r2	0.4930	0.4760
s2	0.3900	0.4250

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
t2	 0.2620	 0.3650
u2	 0.5890	 0.4830
v2	 0.1620	 0.3260
w2	 0.6400	 0.4950
x2	 0.2150	 0.3400
y2	 0.3100	 0.3900
z2	 0.2300	 0.3550