



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:22 AM UTC

PDB ID : 7NWH / pdb_00007nwh
EMDB ID : EMD-12632
Title : Mammalian pre-termination 80S ribosome with eRF1 and eRF3 bound by Blasticidin S.
Authors : Powers, K.T.; Yadav, S.K.N.; Bufton, J.C.; Schaffitzel, C.
Deposited on : 2021-03-16
Resolution : 4.10 Å(reported)
Based on initial model : 5LZT

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:

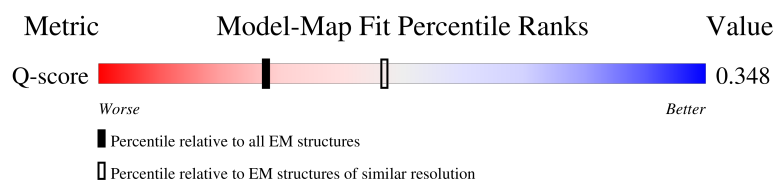
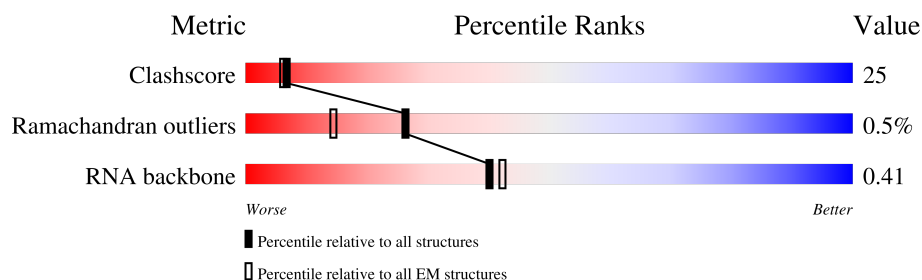
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.10 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	249	
2	C	378	
3	d	108	
4	DD	281	

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Mol	Chain	Length	Quality of chain
5	dd	56	
6	D	296	
7	e	129	
8	EE	263	
9	ee	133	
10	b	226	
11	E	291	
12	f	110	
13	FF	204	
14	ff	68	
15	F	249	
16	g	126	
17	BB	264	
18	GG	263	
19	gg	314	
20	G	242	
21	h	123	
22	HH	191	
23	hh	15	
24	bb	84	
25	H	190	
26	i	107	
27	II	208	
28	ii	437	
29	I	214	

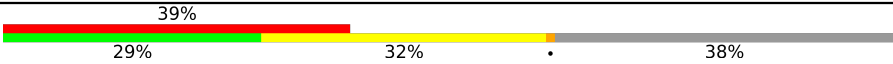
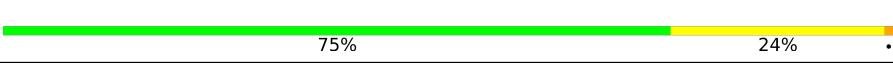
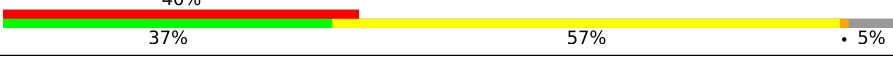
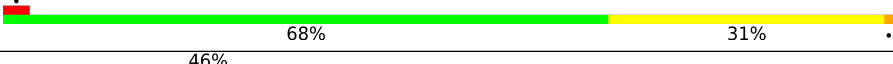
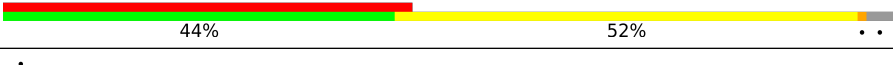
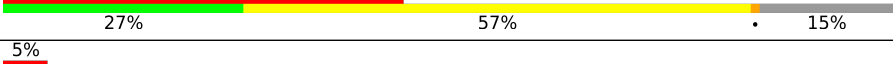
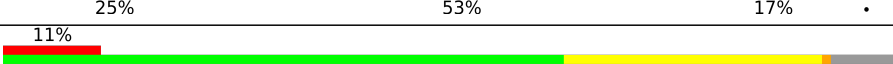
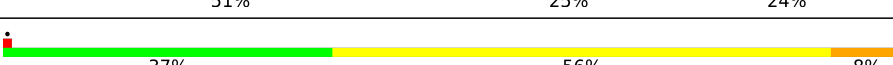
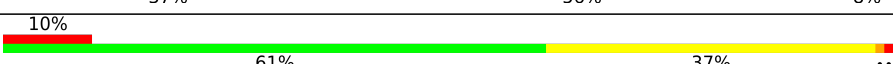
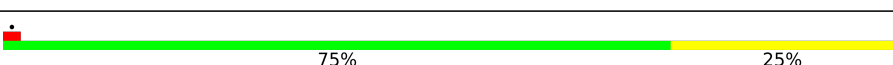
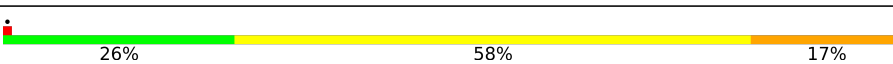
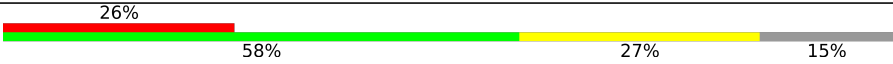
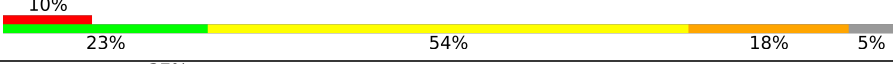
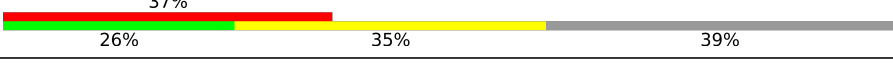
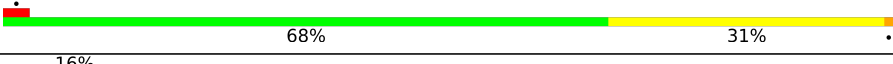
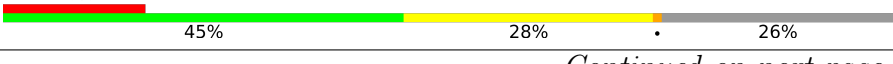
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Mol	Chain	Length	Quality of chain
30	j	97	
31	JJ	194	
32	jj	428	
33	J	176	
34	k	70	
35	KK	151	
36	L	211	
37	l	51	
38	LL	158	
39	M	218	
40	m	128	
41	MM	123	
42	N	204	
43	n	25	
44	NN	150	
45	O	203	
46	o	142	
47	OO	156	
48	P	199	
49	p	109	
50	PP	145	
51	Q	188	
52	r	137	
53	QQ	158	
54	R	196	

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Mol	Chain	Length	Quality of chain
55	s	318	
56	RR	145	
57	S	176	
58	t	196	
59	SS	152	
60	T	160	
61	TT	145	
62	U	128	
63	UU	118	
64	V	132	
65	VV	83	
66	W	134	
67	5	3705	
68	WW	139	
69	X	156	
70	7	120	
71	XX	142	
72	Y	134	
73	8	151	
74	YY	146	
75	Z	136	
76	9	1779	
77	ZZ	122	
78	a	147	
79	AA	295	

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Mol	Chain	Length	Quality of chain
80	aa	117	
81	B	402	
82	c	115	
83	CC	259	
84	cc	69	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	GCP	jj	700	-	-	X	-

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 385116 atoms, of which 165738 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	248	Total	C	H	N	O	S	0	0
			3891	1189	1993	389	314	6		

- Molecule 2 is a protein called uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	362	Total	C	H	N	O	S	0	0
			5936	1812	3053	577	480	14		

- Molecule 3 is a protein called eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	DD	228	Total	C	H	N	O	S	0	0
			3632	1126	1864	318	316	8		

- Molecule 5 is a protein called S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	dd	55	Total	C	H	N	O	S	0	0
			908	286	449	94	74	5		

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	D	293	Total	C	H	N	O	S	0	0
			4815	1512	2424	438	427	14		

- Molecule 7 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	e	128	Total	C	H	N	O	S	0	0
			2200	667	1147	216	165	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	EE	262	Total	C	H	N	O	S	0	0
			4253	1324	2177	386	358	8		

- Molecule 9 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	ee	55	Total	C	H	N	O	S	0	0
			935	274	492	97	71	1		

- Molecule 10 is a protein called eL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	b	104	Total	C	H	N	O	S	0	0
			1768	527	920	189	129	3		

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	216	Total	C	H	N	O	S	0	0
			3617	1115	1888	329	282	3		

- Molecule 12 is a protein called eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	f	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

- Molecule 13 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	FF	185	Total	C	H	N	O	S	0	0
			2993	921	1522	277	266	7		

- Molecule 14 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	ff	68	Total	C	H	N	O	S	0	0
			1120	351	565	103	94	7		

- Molecule 15 is a protein called uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	F	225	Total	C	H	N	O	S	0	0
			3870	1205	1995	358	303	9		

- Molecule 16 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	g	114	Total	C	H	N	O	S	0	0
			1905	566	999	187	147	6		

- Molecule 17 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	BB	213	Total	C	H	N	O	S	0	0
			3532	1098	1803	309	308	14		

- Molecule 18 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	GG	237	Total	C	H	N	O	S	0	0
			4005	1200	2082	387	329	7		

- Molecule 19 is a protein called Epididymis tissue sperm binding protein Li 3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	gg	313	Total	C	H	N	O	S	0	0
			4830	1535	2394	424	465	12		

- Molecule 20 is a protein called L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	233	Total	C	H	N	O	S	0	0
			3906	1199	2027	361	315	4		

- Molecule 21 is a protein called uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	h	122	Total	C	H	N	O	S	0	0
			2160	640	1147	204	168	1		

- Molecule 22 is a protein called S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	HH	185	Total	C	H	N	O	S	0	0
			3070	952	1582	271	264	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	hh	15	Total	C	H	N	O	P	0	0
			478	142	161	54	106	15		

- Molecule 24 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	bb	83	Total	C	H	N	O	S	0	0
			1323	408	672	121	115	7		

- Molecule 25 is a protein called L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	H	190	Total	C	H	N	O	S	0	0
			3113	954	1597	284	272	6		

- Molecule 26 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	i	102	Total	C	H	N	O	S	0	0
			1746	520	916	176	129	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	II	206	Total	C	H	N	O	S	0	0
			3459	1058	1773	332	291	5		

- Molecule 28 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	ii	419	Total	C	H	N	O	S	0	0
			6638	2104	3331	562	629	12		

- Molecule 29 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	I	205	Total	C	H	N	O	S	0	0
			3376	1056	1712	321	274	13		

- Molecule 30 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	j	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 31 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	JJ	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 32 is a protein called eRF3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	jj	428	Total	C	H	N	O	S	0	0
			6787	2144	3419	580	623	21		

- Molecule 33 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	J	170	Total	C	H	N	O	S	0	0
			2761	861	1399	254	241	6		

- Molecule 34 is a protein called L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	k	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 35 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	KK	96	Total	C	H	N	O	S	0	0
			1646	530	836	143	131	6		

- Molecule 36 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	L	210	Total	C	H	N	O	S	0	0
			3522	1065	1820	354	279	4		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	1	50	Total	C	H	N	O	S	0	0
			927	286	480	96	64	1		

- Molecule 38 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	LL	143	Total	C	H	N	O	S	0	0
			2425	749	1250	222	198	6		

- Molecule 39 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	M	138	Total	C	H	N	O	S	0	0
			2348	727	1211	221	182	7		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	m	52	Total	C	H	N	O	S	0	0
			894	266	465	90	67	6		

- Molecule 41 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	MM	117	Total	C	H	N	O	S	0	0
			1847	570	939	161	169	8		

- Molecule 42 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	N	203	Total	C	H	N	O	S	0	0
			3451	1072	1750	359	266	4		

- Molecule 43 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	25	Total	C	H	N	O	S	0	0
			525	145	286	64	27	3		

- Molecule 44 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	NN	149	Total	C	H	N	O	S	0	0
			2491	770	1289	228	203	1		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN UL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	O	199	Total	C	H	N	O	S	0	0
			3408	1051	1778	319	255	5		

- Molecule 46 is a protein called eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	o	104	Total	C	H	N	O	S	0	0
			1771	533	920	174	138	6		

- Molecule 47 is a protein called uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	OO	136	Total	C	H	N	O	S	0	0
			2055	621	1039	199	190	6		

- Molecule 48 is a protein called uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	P	153	Total	C	H	N	O	S	0	0
			2516	777	1274	241	215	9		

- Molecule 49 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	p	91	Total	C	H	N	O	S	0	0
			1466	445	758	136	120	7		

- Molecule 50 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	PP	120	Total	C	H	N	O	S	0	0
			2042	635	1045	187	168	7		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Q	187	Total	C	H	N	O	S	0	0
			3149	946	1634	315	250	4		

- Molecule 52 is a protein called eL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	r	124	Total	C	H	N	O	S	0	0
			2045	616	1051	205	167	6		

- Molecule 53 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	QQ	142	Total	C	H	N	O	S	0	0
			2323	717	1195	213	195	3		

- Molecule 54 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	R	180	Total	C	H	N	O	S	0	0
			3172	933	1664	328	238	9		

- Molecule 55 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	s	196	Total	C	H	N	O	S	0	0
			3071	959	1564	263	276	9		

- Molecule 56 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	RR	132	Total	C	H	N	O	S	0	0
			2189	670	1121	199	195	4		

- Molecule 57 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	S	176	Total	C	H	N	O	S	0	0
			2970	930	1508	285	236	11		

- Molecule 58 is a protein called uL12.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	t	153	Total	C	H	N	O	S	0	0
			2375	722	1215	218	217	3		

- Molecule 59 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	SS	144	Total	C	H	N	O	S	0	0
			2437	746	1247	241	202	1		

- Molecule 60 is a protein called eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	T	159	Total	C	H	N	O	S	0	0
			2665	823	1367	252	217	6		

- Molecule 61 is a protein called eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	TT	141	Total	C	H	N	O	S	0	0
			2229	688	1132	211	195	3		

- Molecule 62 is a protein called L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	U	99	Total	C	H	N	O	S	0	0
			1642	519	833	141	147	2		

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	UU	100	Total	C	H	N	O	S	0	0
			1657	498	862	152	141	4		

- Molecule 64 is a protein called eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	V	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 65 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	VV	83	Total	C	H	N	O	S	0	0
			1273	393	637	117	121	5		

- Molecule 66 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	W	106	Total	C	H	N	O	S	0	0
			1752	538	892	174	144	4		

- Molecule 67 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	5	3543	Total	C	H	N	O	P	0	0
			114361	33833	38389	13910	24686	3543		

- Molecule 68 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	WW	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 69 is a protein called uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	X	118	Total	C	H	N	O	S	0	0
			2007	618	1040	181	167	1		

- Molecule 70 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	7	120	Total	C	H	N	O	P	0	0
			3854	1141	1296	456	842	119		

- Molecule 71 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	XX	141	Total	C	H	N	O	S	0	0
			2263	693	1165	219	183	3		

- Molecule 72 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	Y	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 73 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	8	151	Total	C	H	N	O	P	0	0
			4837	1432	1629	564	1062	150		

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	YY	124	Total	C	H	N	O	S	0	0
			2094	640	1083	198	168	5		

- Molecule 75 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	Z	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 76 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	9	1698	Total	C	H	N	O	P	0	0
			54557	16180	18308	6508	11864	1697		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	ZZ	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

- Molecule 78 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	a	147	Total	C	H	N	O	S	0	0
			2372	734	1210	239	185	4		

- Molecule 79 is a protein called 40S_SA_C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	AA	217	Total	C	H	N	O	S	0	0
			3418	1086	1708	300	316	8		

- Molecule 80 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	aa	101	Total	C	H	N	O	S	0	0
			1678	507	864	170	132	5		

- Molecule 81 is a protein called uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	B	394	Total	C	H	N	O	S	0	0
			6482	2020	3310	597	542	13		

- Molecule 82 is a protein called eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	c	98	Total	C	H	N	O	S	0	0
			1555	481	794	134	140	6		

- Molecule 83 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	CC	221	Total	C	H	N	O	S	0	0
			3522	1111	1806	295	301	9		

- Molecule 84 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	cc	62	Total	C	H	N	O	S	0	0
			1002	297	514	97	92	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	5	HIS	ARG	conflict	UNP G1TIB4

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	dd	1	Total	Zn	0
			1	1	
85	ff	1	Total	Zn	0
			1	1	
85	g	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	aa	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

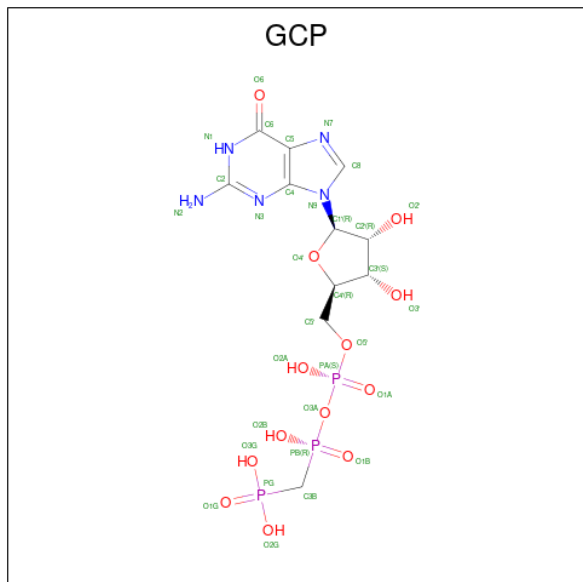
Mol	Chain	Residues	Atoms		AltConf
86	hh	2	Total	Mg	0
			2	2	
86	j	1	Total	Mg	0
			1	1	
86	jj	1	Total	Mg	0
			1	1	
86	o	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	5	189	Total	Mg	0
			189	189	
86	7	4	Total	Mg	0
			4	4	
86	8	10	Total	Mg	0
			10	10	
86	9	70	Total	Mg	0
			70	70	
86	a	1	Total	Mg	0
			1	1	

- Molecule 87 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
87	jj	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	

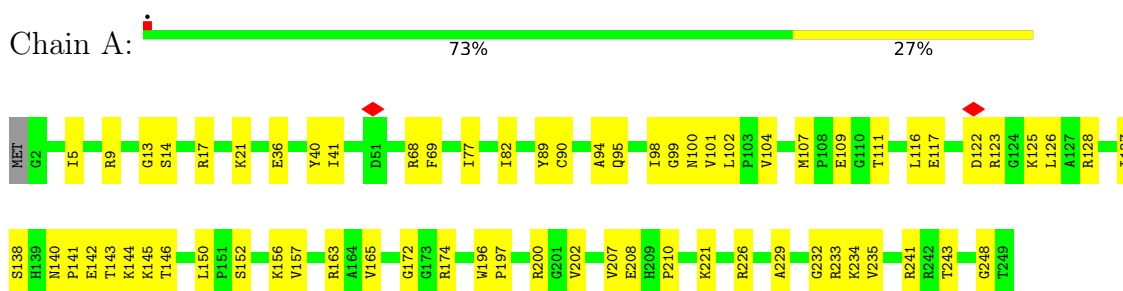
- Molecule 88 is BLASTICIDIN S (CCD ID: BLS) (formula: $C_{17}H_{26}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



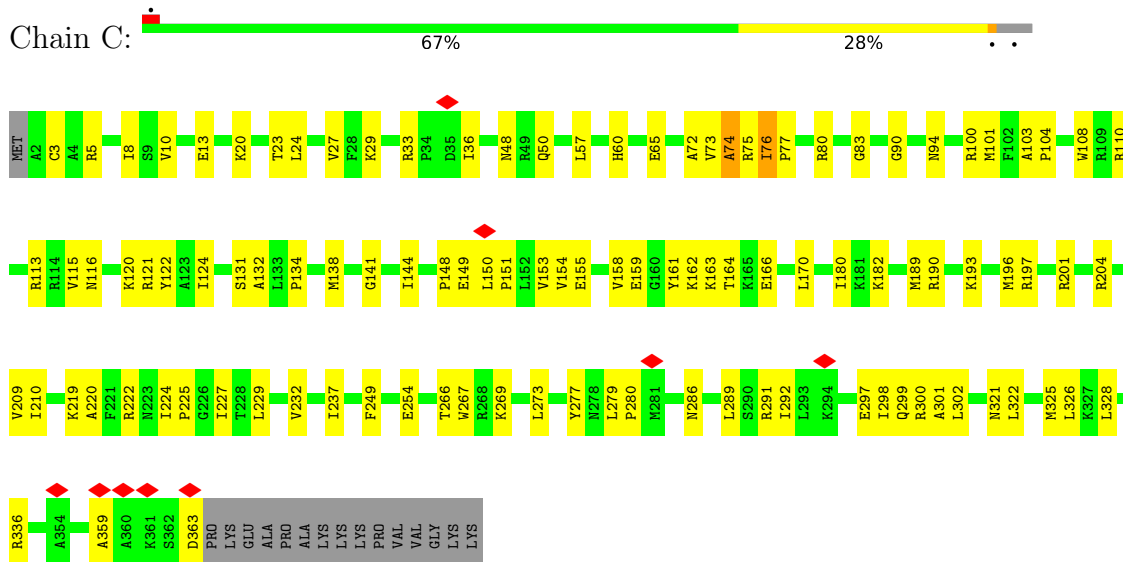
3 Residue-property plots [i](#)

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

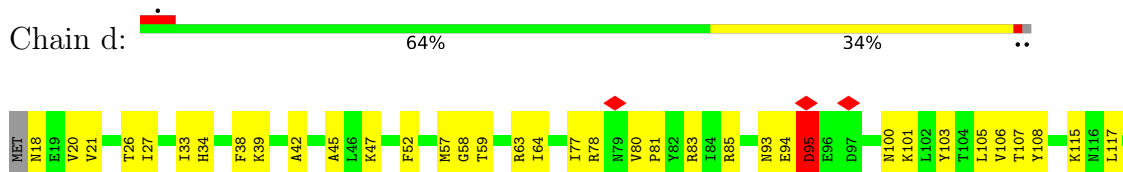
• Molecule 1: 60S ribosomal protein L8



• Molecule 2: uL4



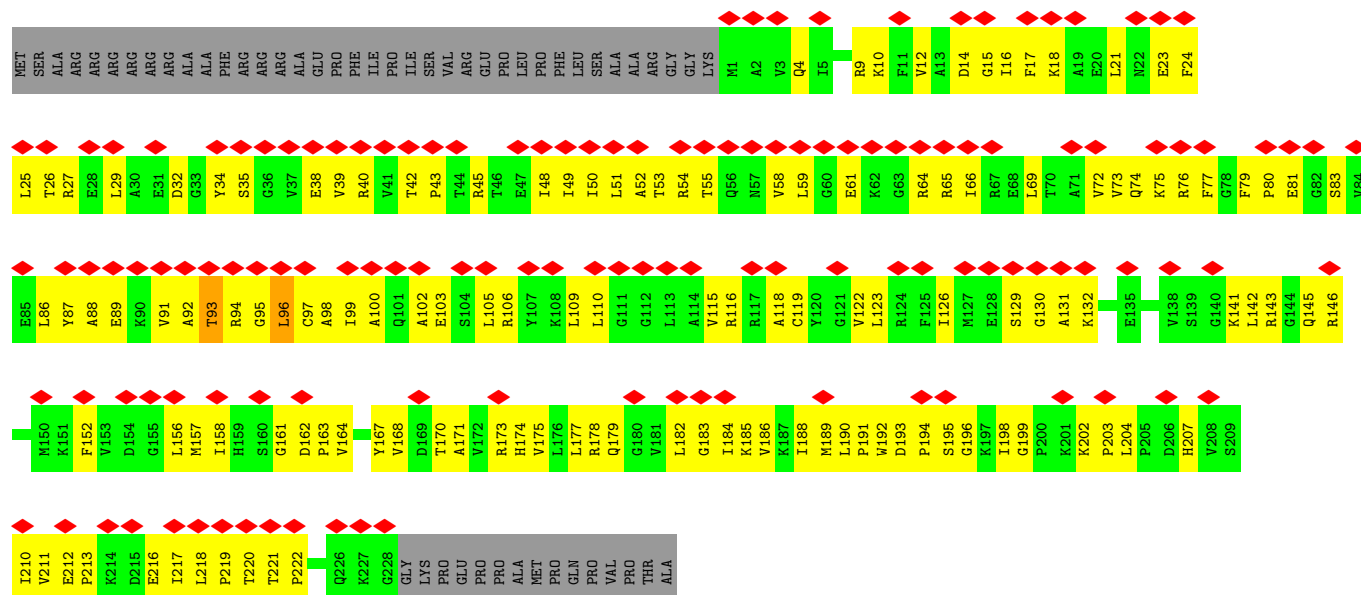
• Molecule 3: eL31



D123
E124

• Molecule 4: 40S ribosomal protein S3

Chain DD: 



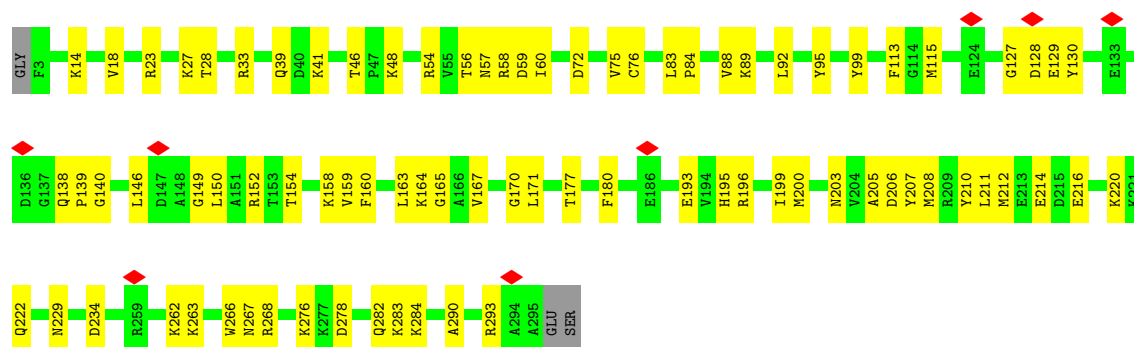
• Molecule 5: S29

Chain dd: 

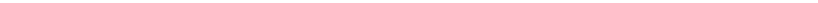


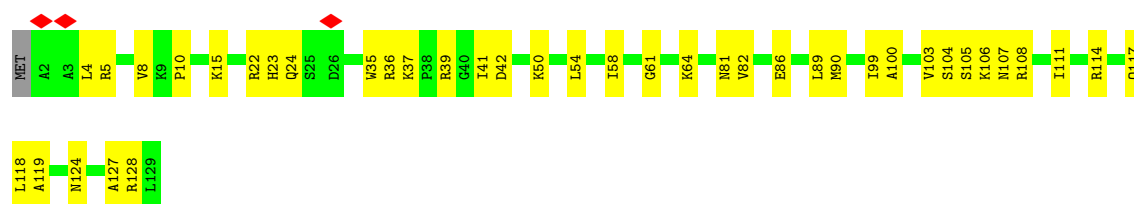
• Molecule 6: 60S ribosomal protein L5

Chain D: 



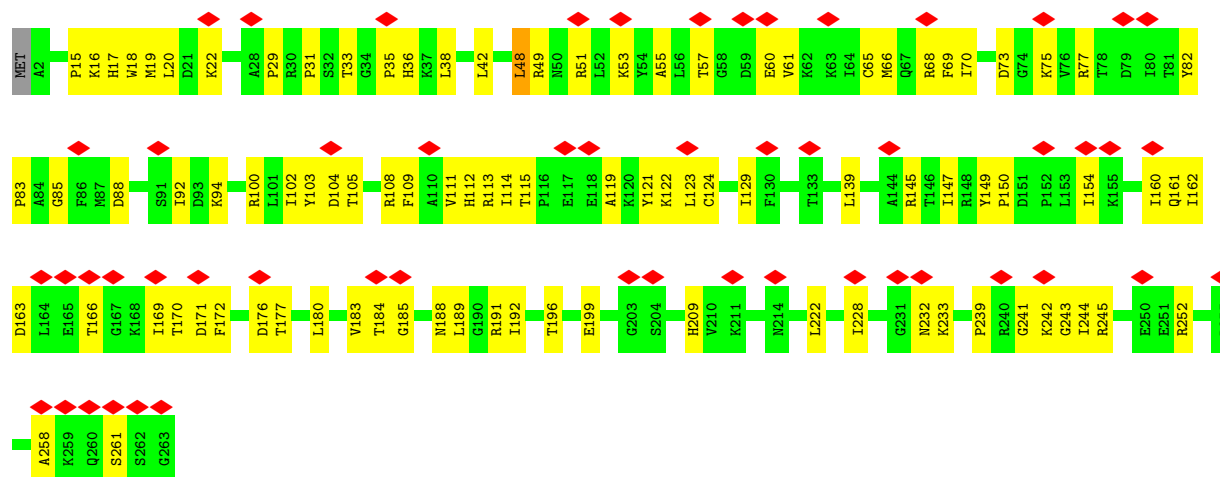
• Molecule 7: Ribosomal protein L32

Chain e:  68% 31%

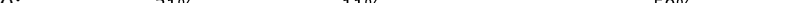


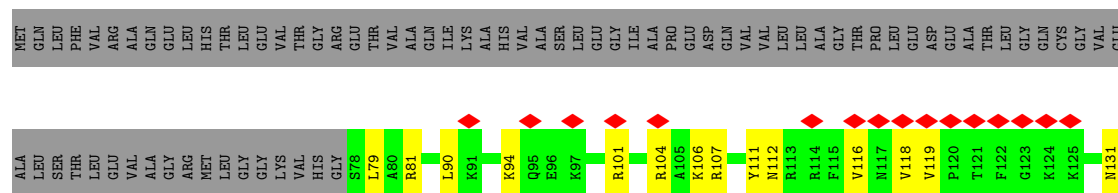
- Molecule 8: 40S ribosomal protein S4

Chain EE:

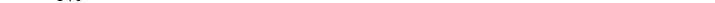


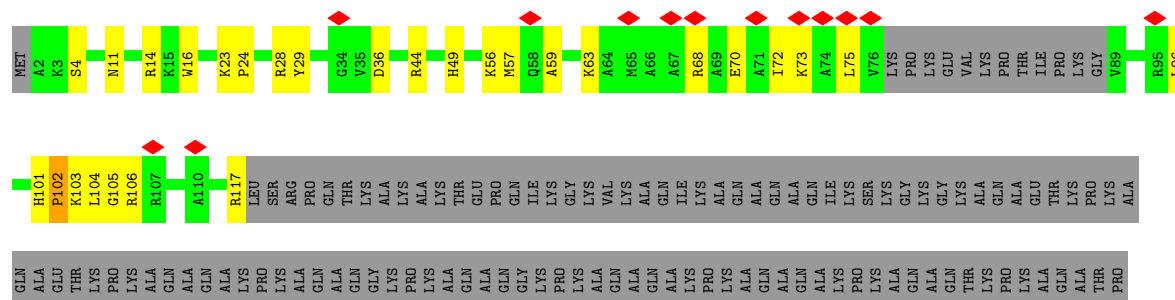
- Molecule 9: 40S ribosomal protein S30

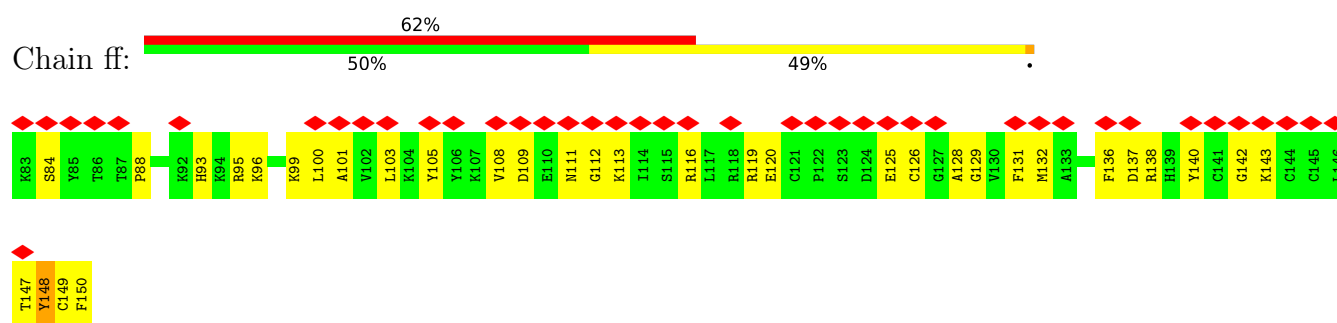
Chain ee: 



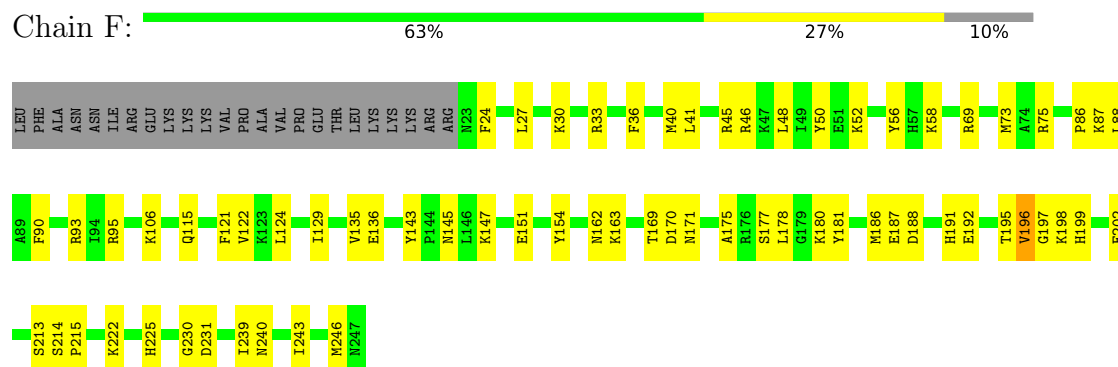
- Molecule 10: eL29

Chain b: 

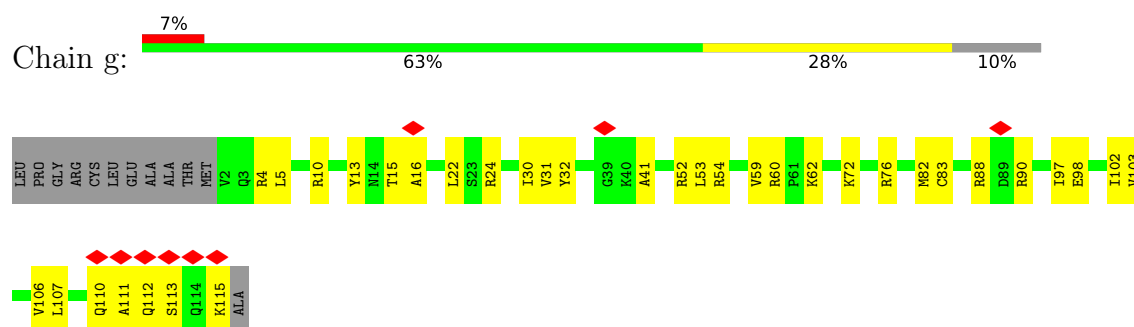




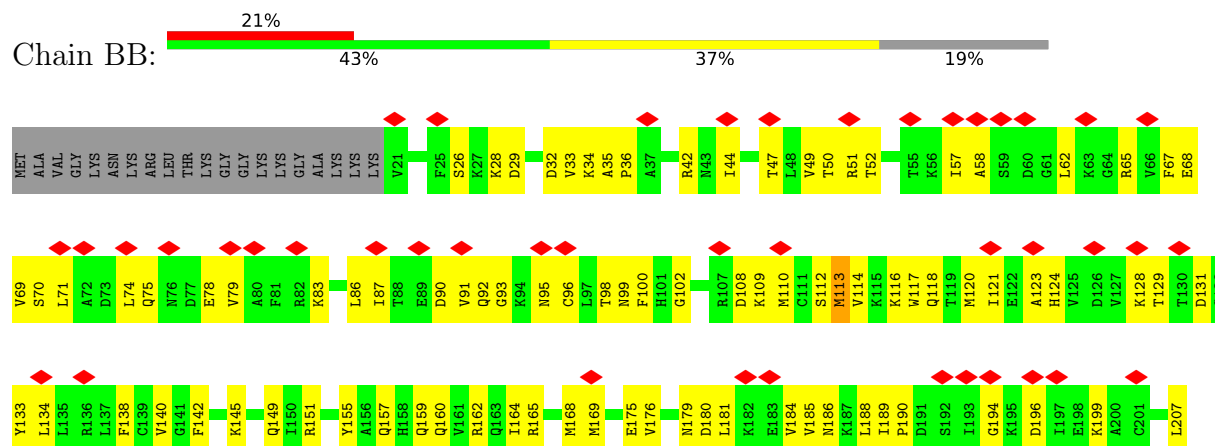
- Molecule 15: uL30

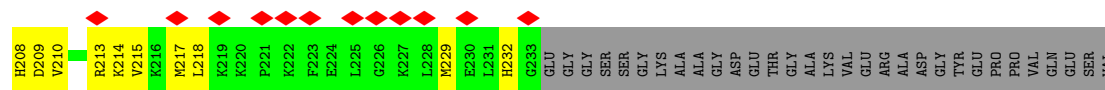


- Molecule 16: 60S ribosomal protein L34

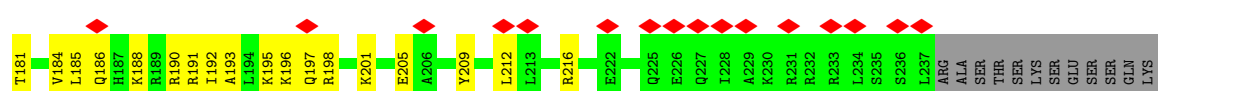
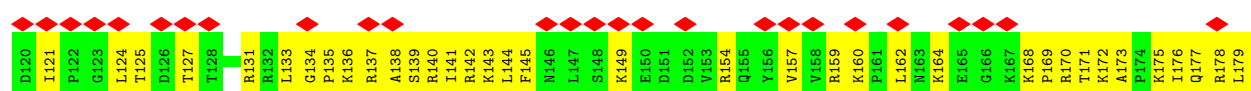
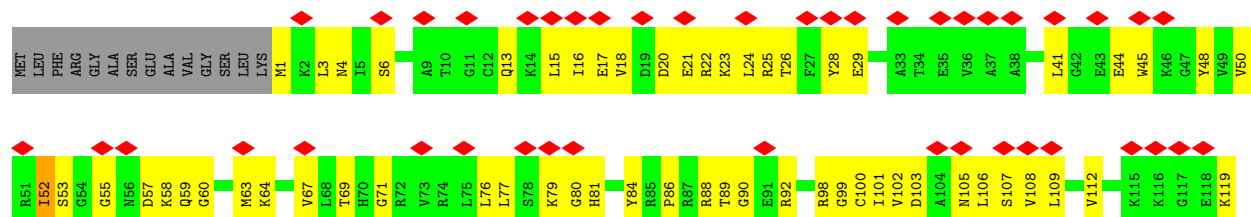


- Molecule 17: 40S ribosomal protein S3a

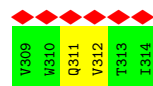
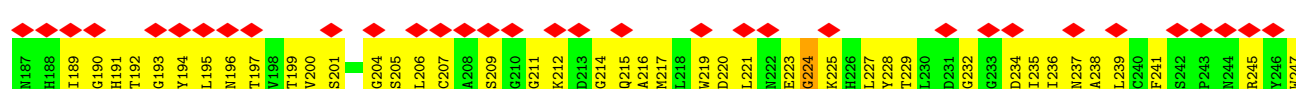
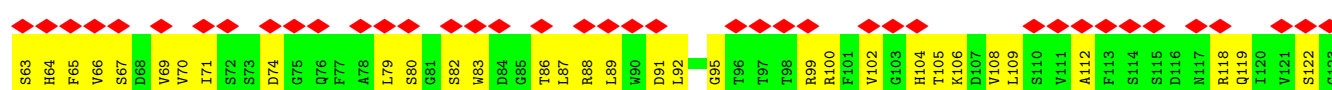




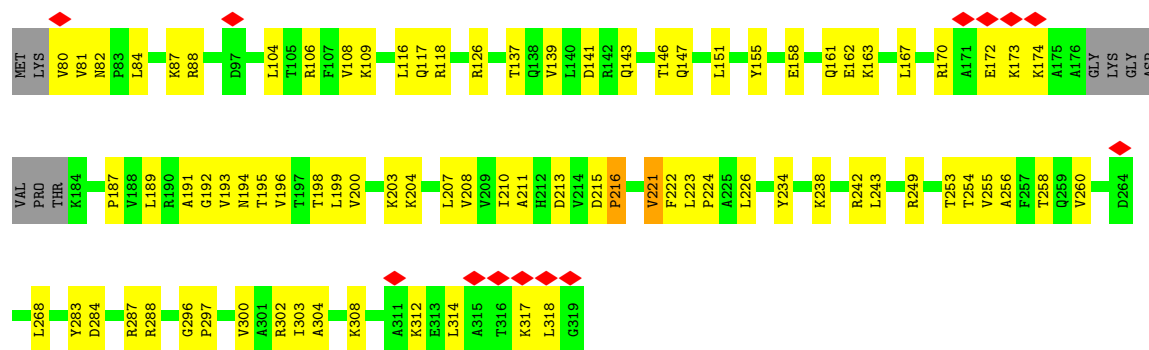
• Molecule 18: 40S ribosomal protein S6



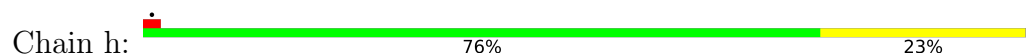
• Molecule 19: Epididymis tissue sperm binding protein Li 3a



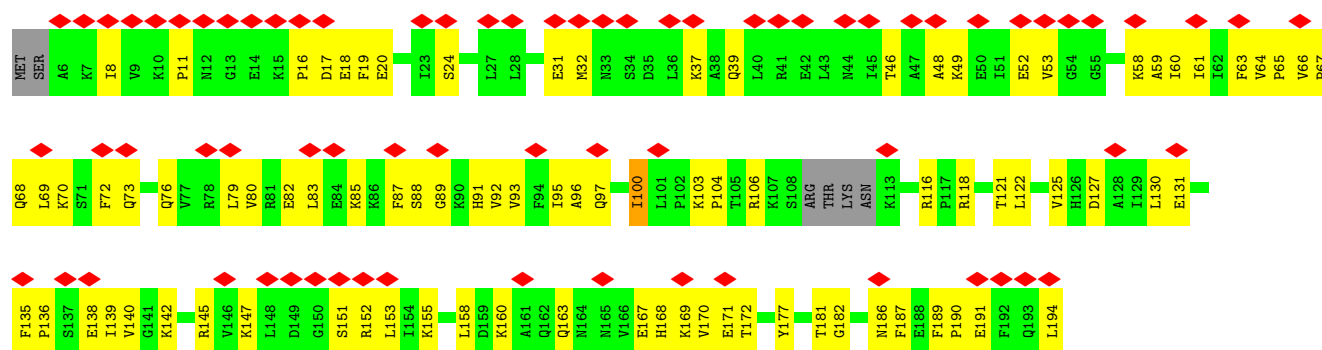
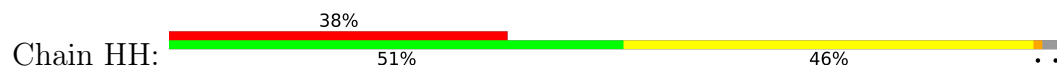
• Molecule 20: L7a



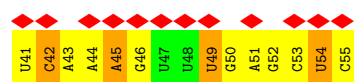
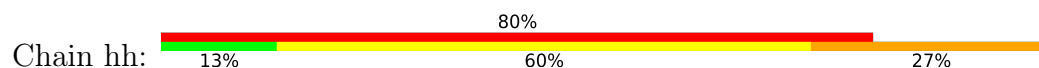
• Molecule 21: uL29



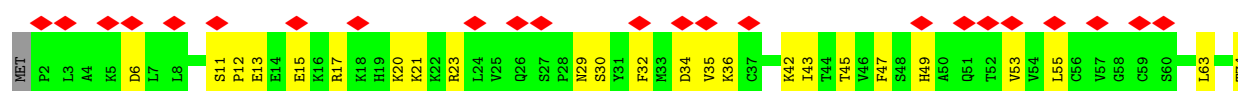
• Molecule 22: S7

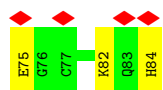


• Molecule 23: mRNA

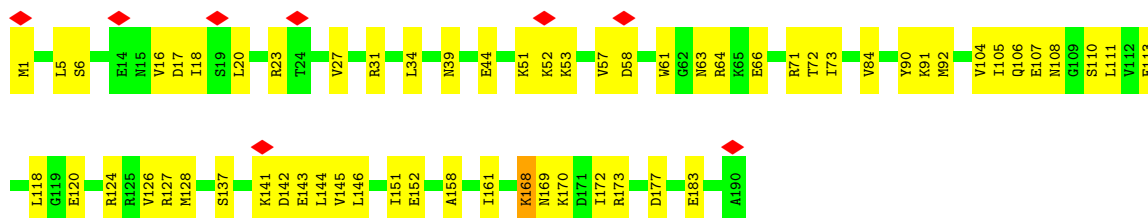


• Molecule 24: 40S ribosomal protein S27

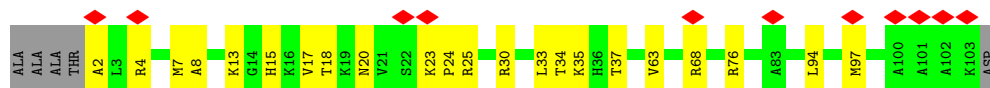
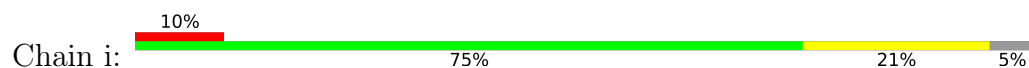




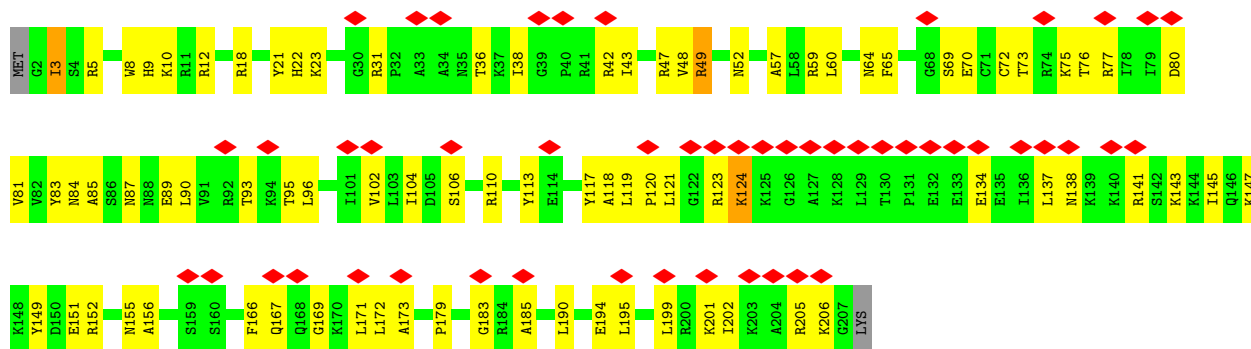
- Molecule 25: L9



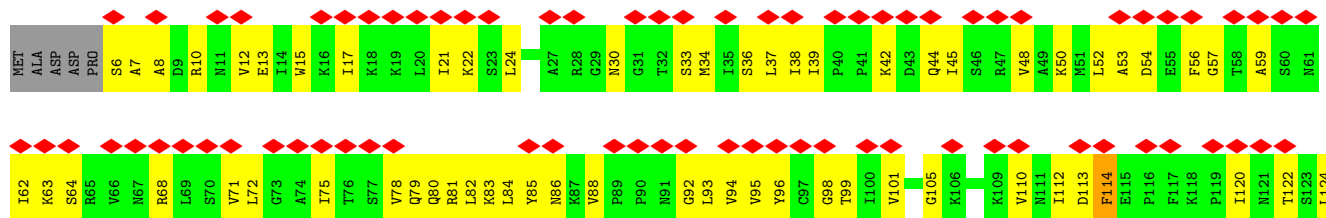
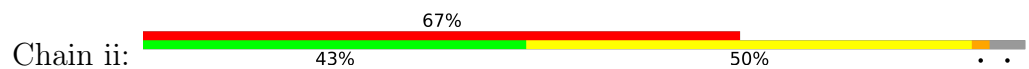
- Molecule 26: 60S ribosomal protein L36

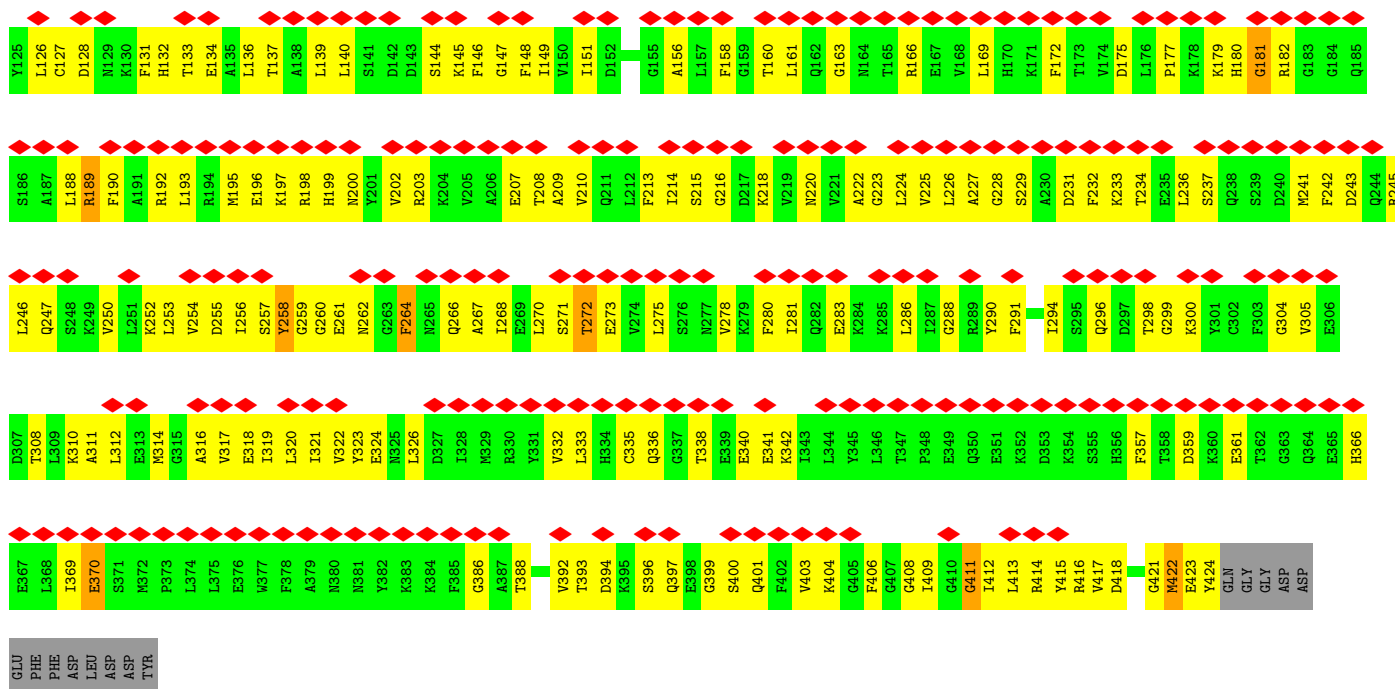


- Molecule 27: 40S ribosomal protein S8

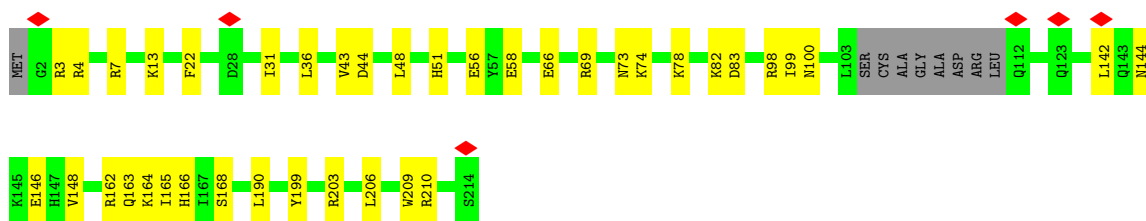
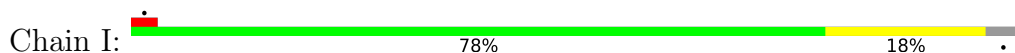


- Molecule 28: Eukaryotic peptide chain release factor subunit 1





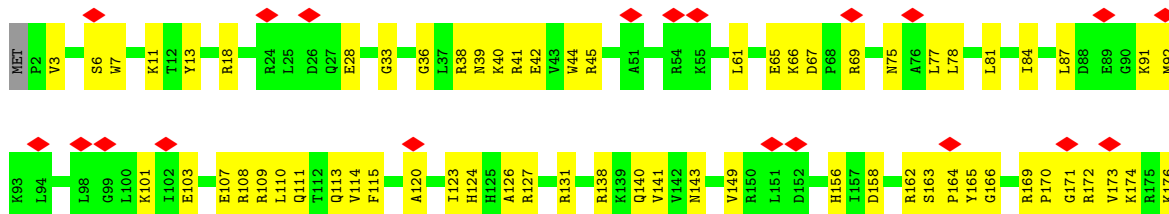
• Molecule 29: 60S ribosomal protein L10

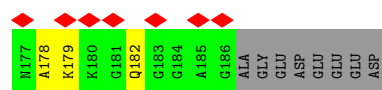


• Molecule 30: Ribosomal protein L37

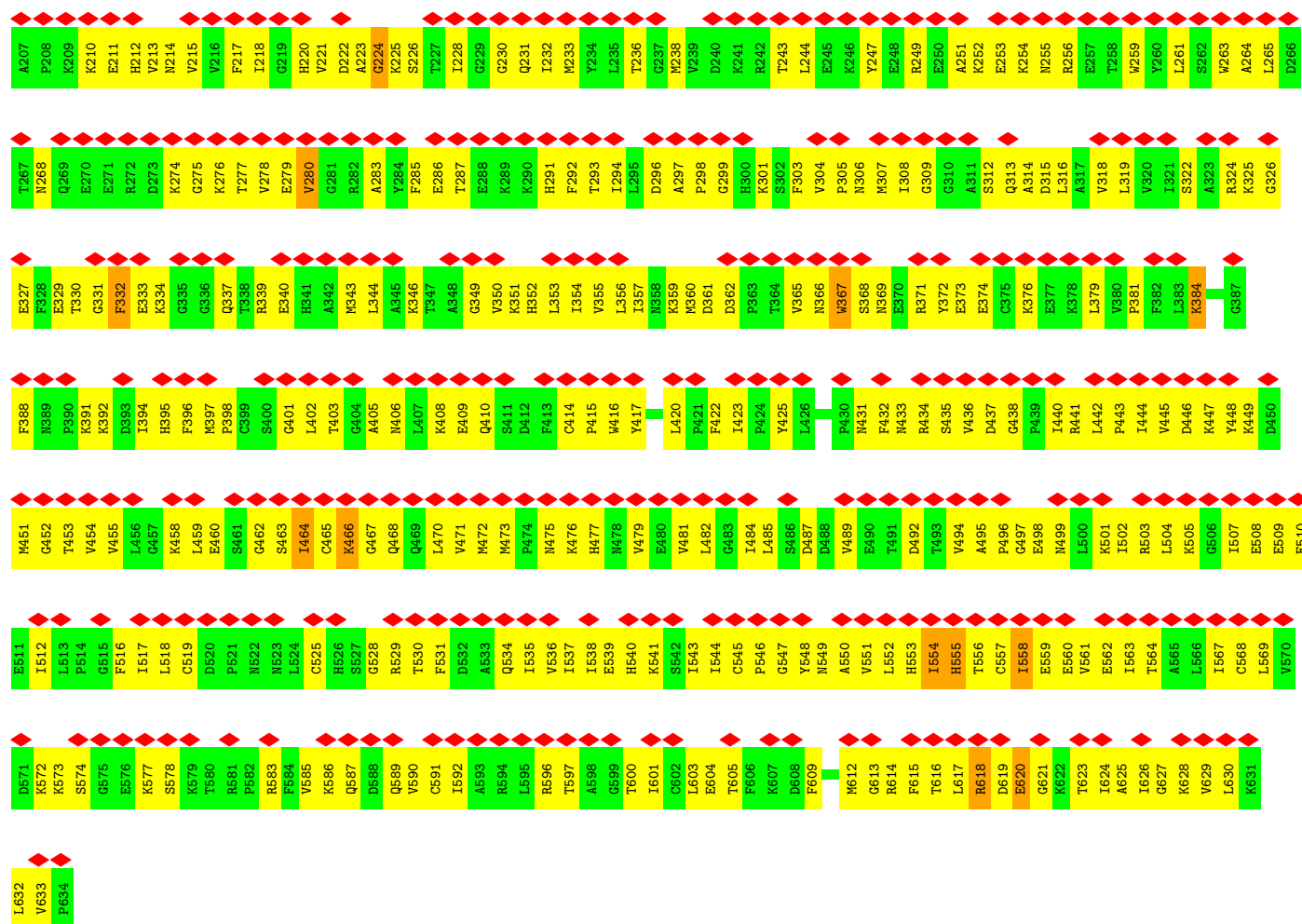
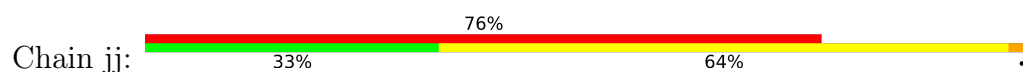


• Molecule 31: 40S ribosomal protein S9

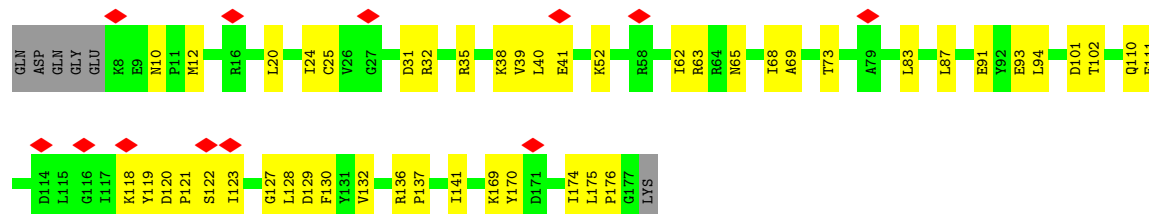




• Molecule 32: eRF3a

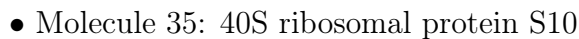


• Molecule 33: 60S ribosomal protein L11

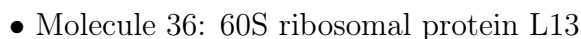


• Molecule 34: L38

Frequency	Percentage
Often	66%
Sometimes	33%



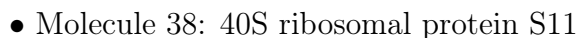
Response	Percentage
Yes	32%
No	23%
Don't know	38%
No opinion	36%



Frequency	Percentage
5%	5%
72%	72%
27%	27%



Category	Percentage
Very bad	6%
Bad	63%
Good	35%



Frequency	Percentage
Daily	14%
Often	50%
Sometimes	41%
Never	9%



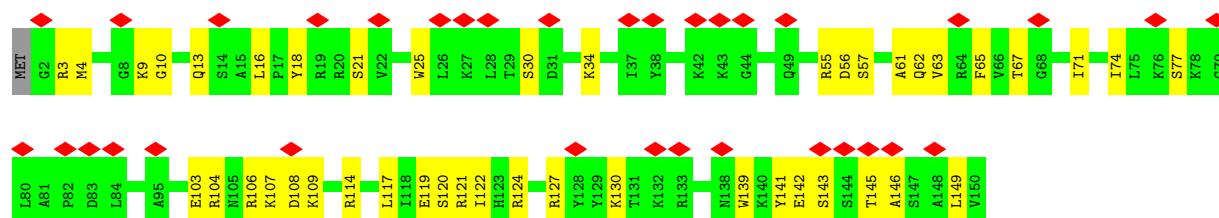




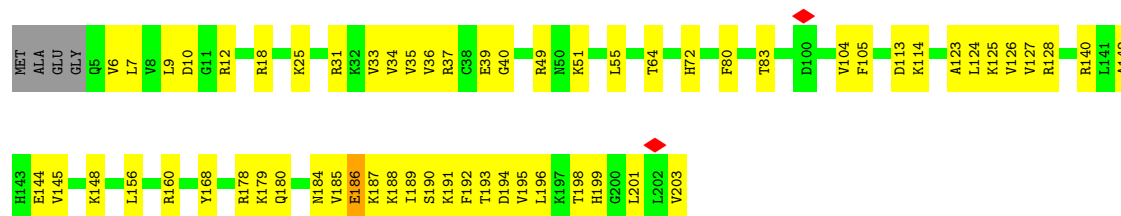
- Molecule 43: 60s ribosomal protein l41



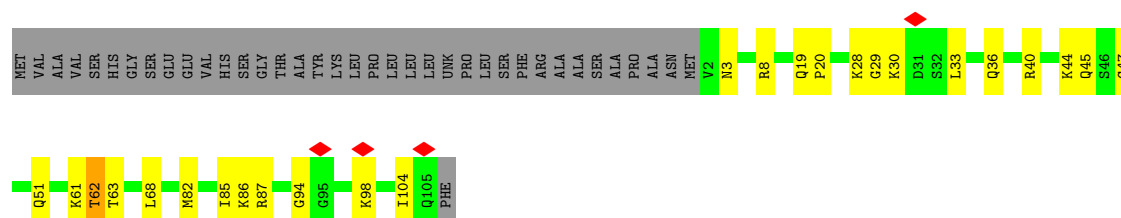
- Molecule 44: ribosomal protein uS15



- Molecule 45: 60S RIBOSOMAL PROTEIN UL13

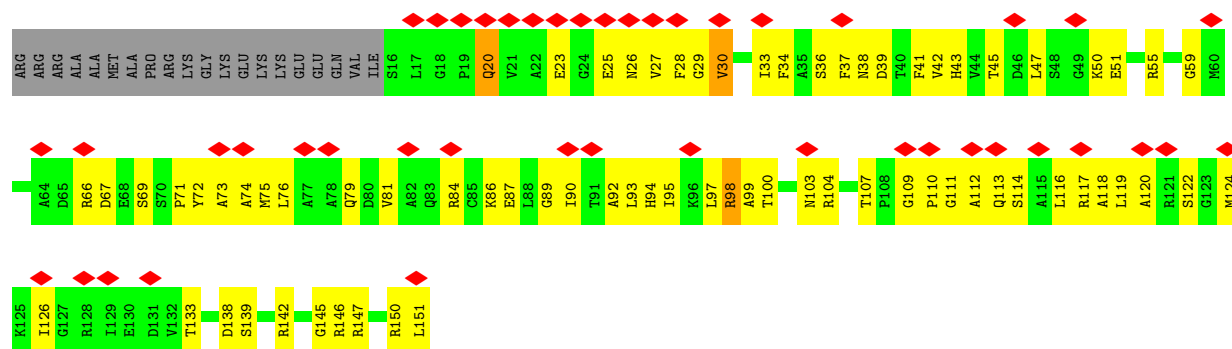


- Molecule 46: eL42

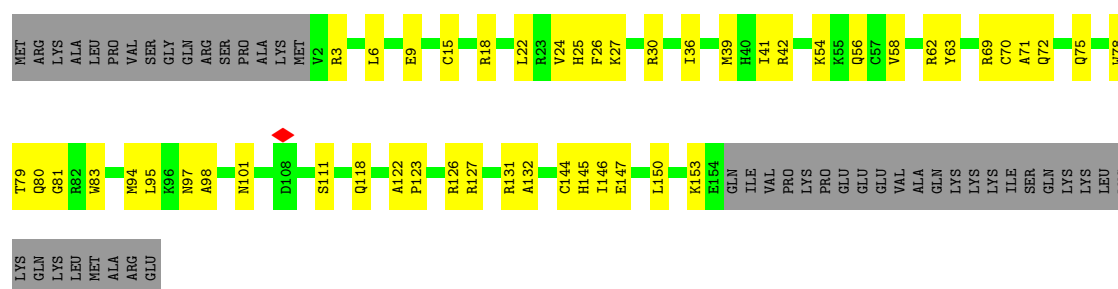


- Molecule 47: uS11





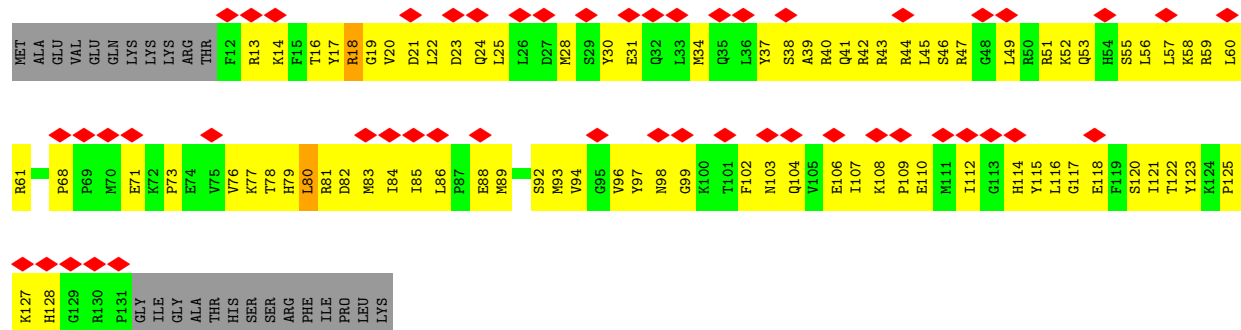
• Molecule 48: uL22



• Molecule 49: ribosomal protein eL43



• Molecule 50: 40S ribosomal protein uS19



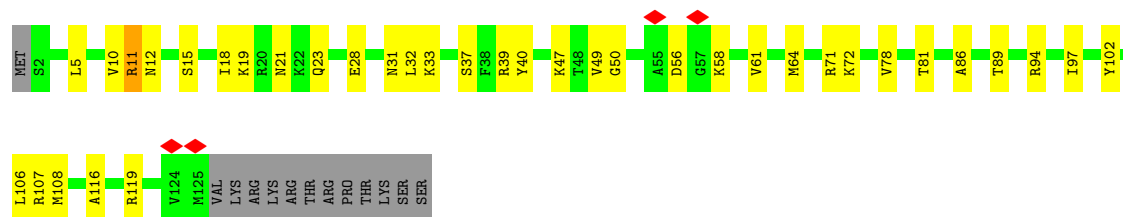
- Molecule 51: eL18

Chain Q: 

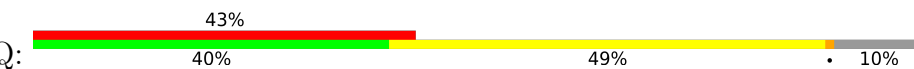


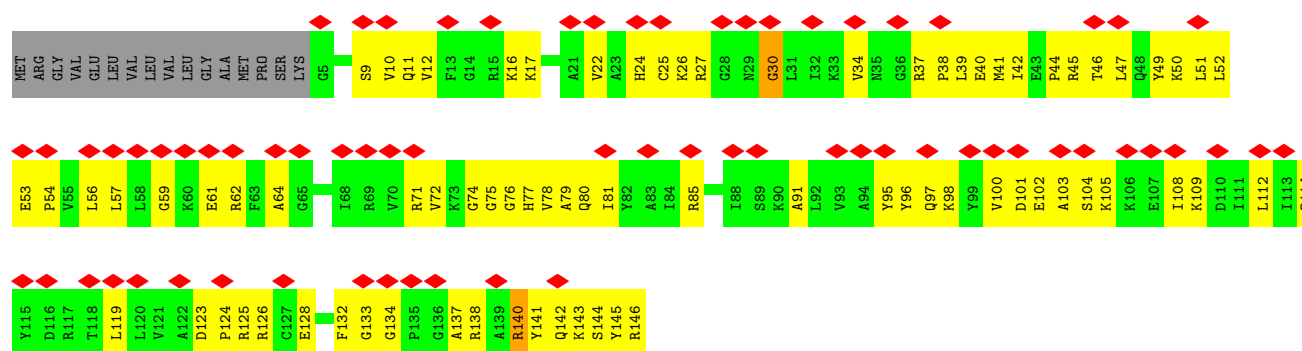
- Molecule 52: eL28

Chain r: 



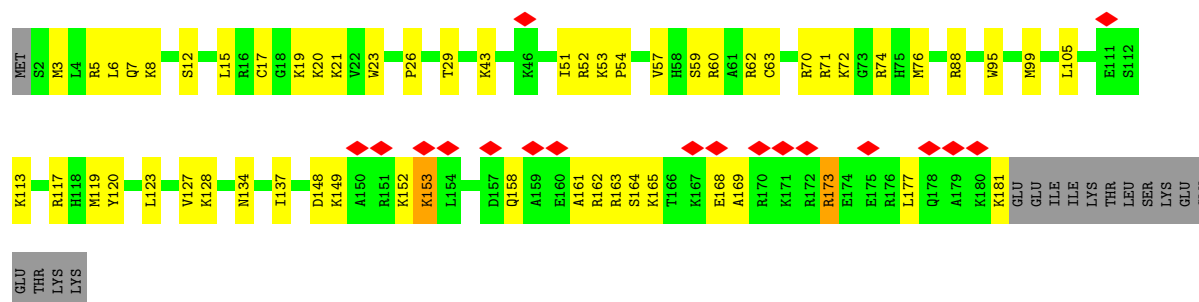
- Molecule 53: Ribosomal protein S16

Chain QQ: 

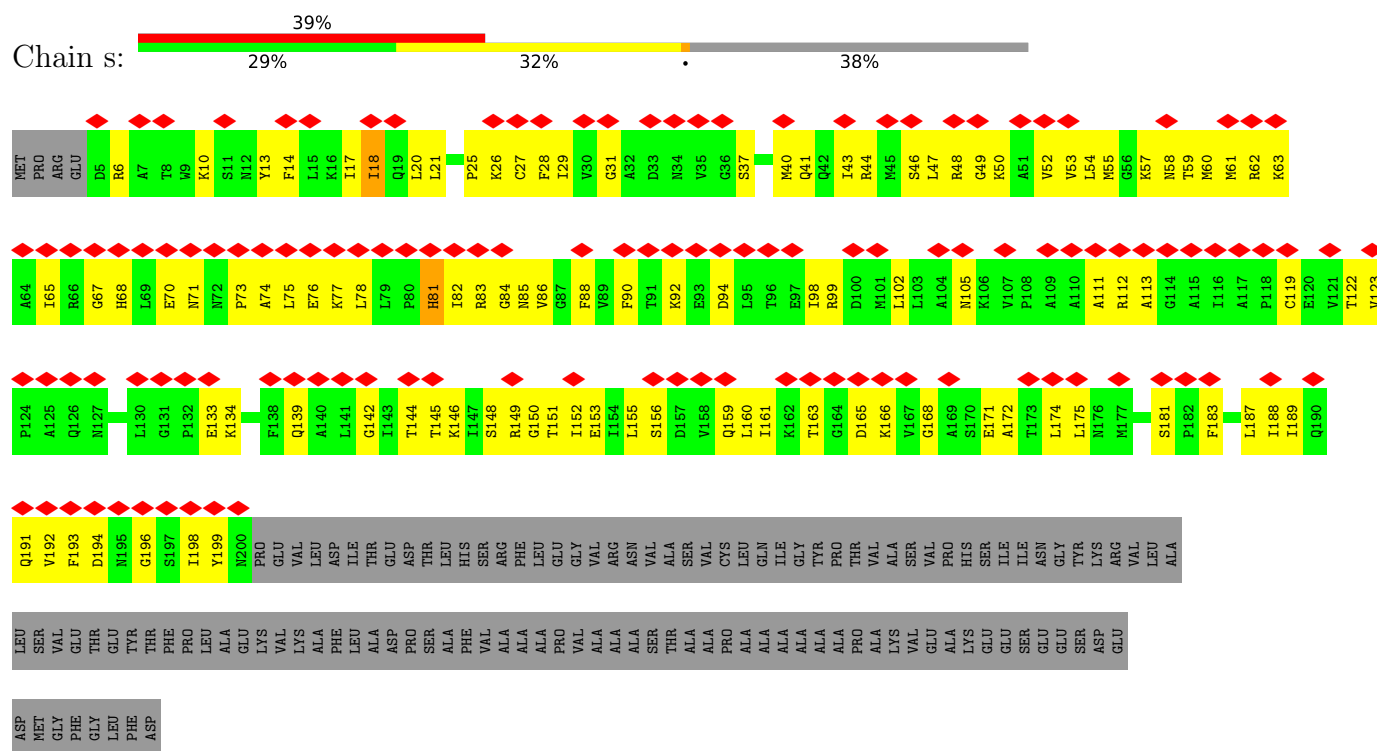


- Molecule 54: 60S ribosomal protein L19

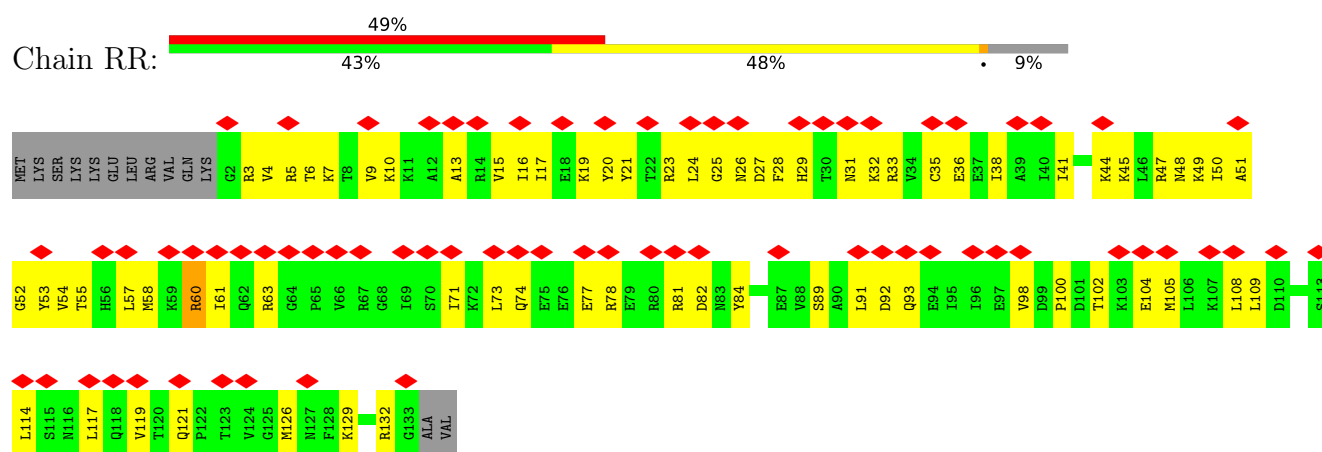
Chain R: 



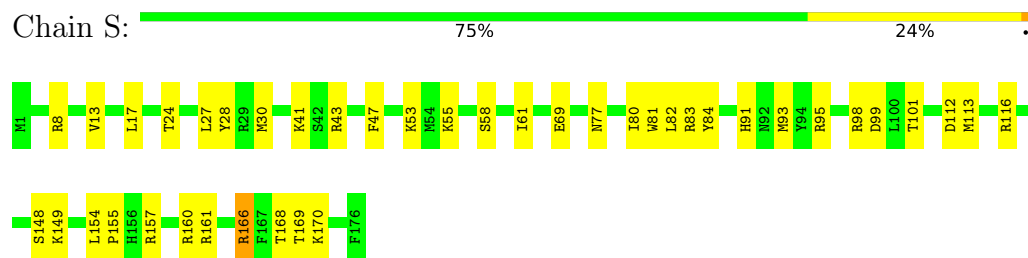
- Molecule 55: 60S acidic ribosomal protein P0



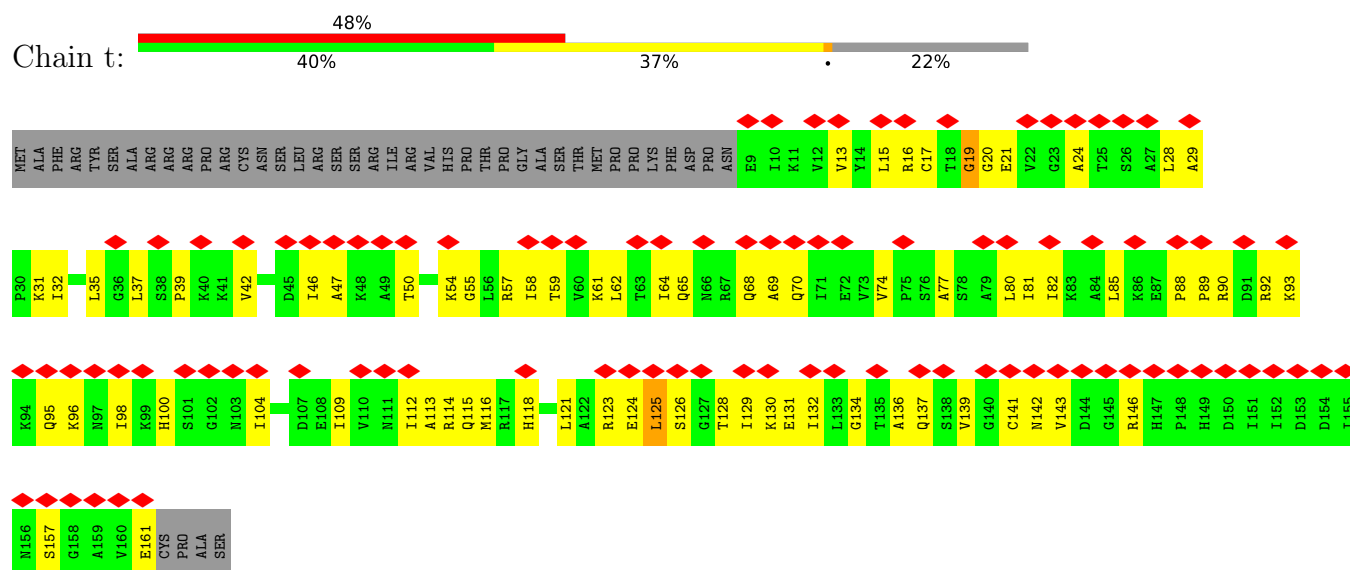
- Molecule 56: 40S ribosomal protein S17



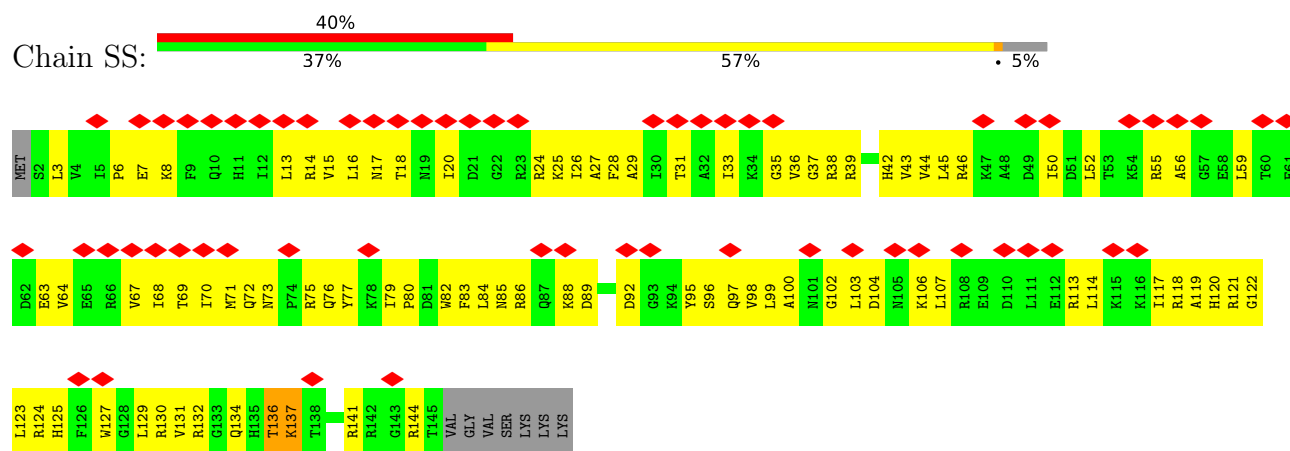
- Molecule 57: 60S ribosomal protein L18a



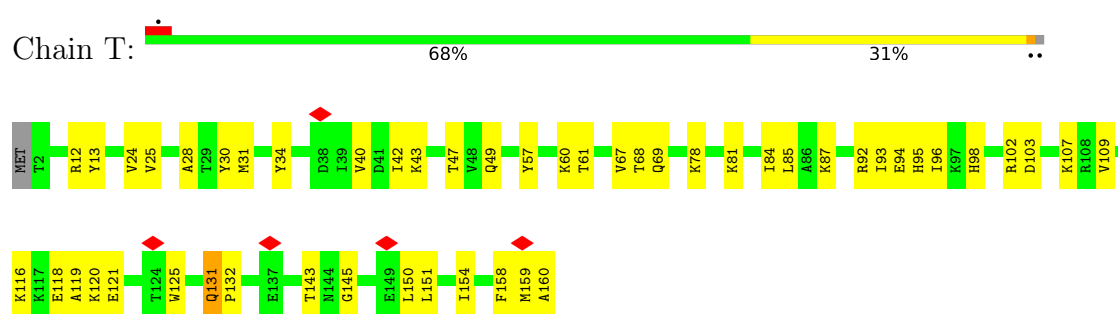
- Molecule 58: uL12



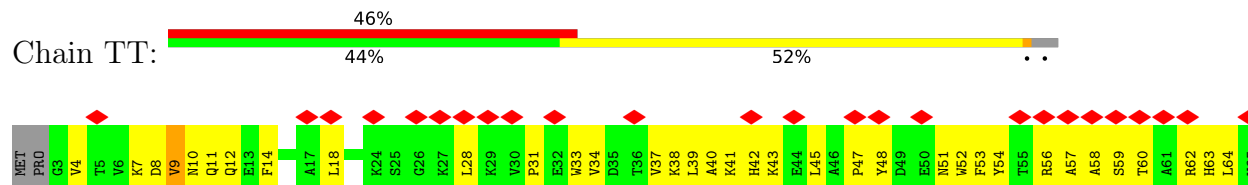
• Molecule 59: 40S ribosomal protein uS13



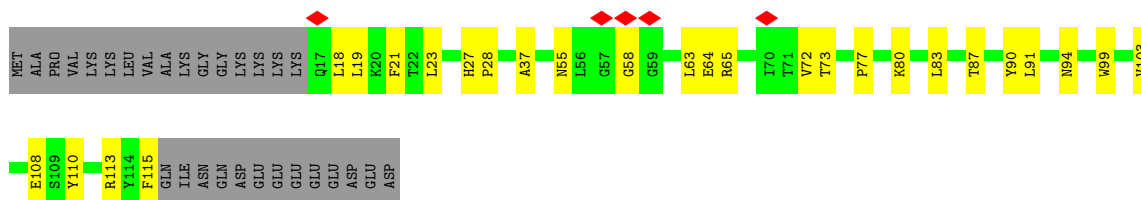
• Molecule 60: eL21



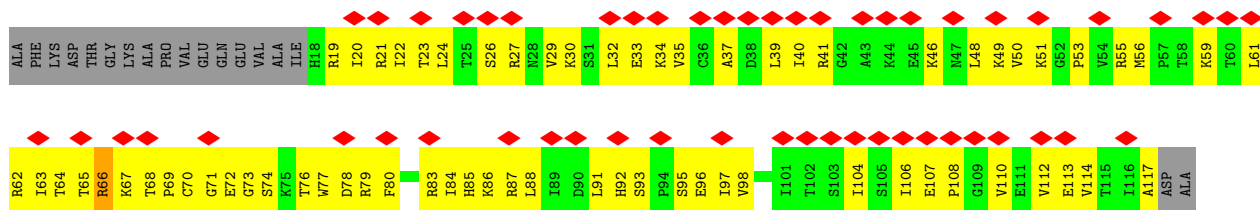
• Molecule 61: eS19



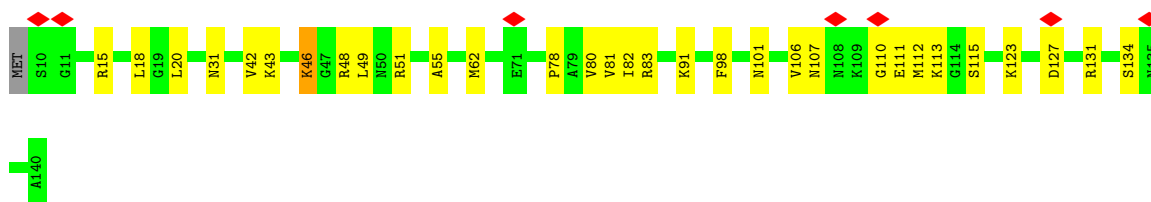
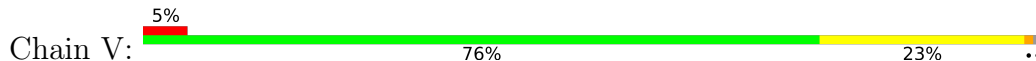
- Molecule 62: L22



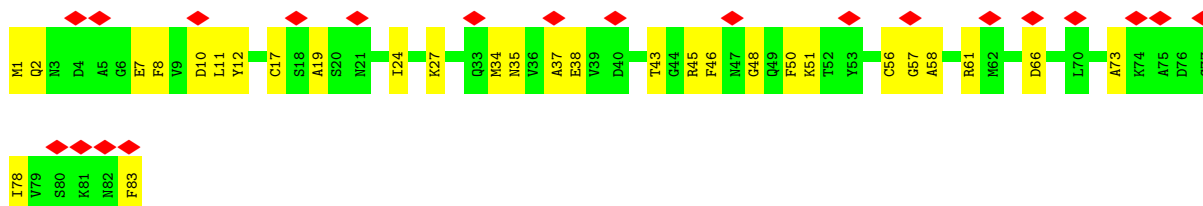
- Molecule 63: 40S ribosomal protein S20



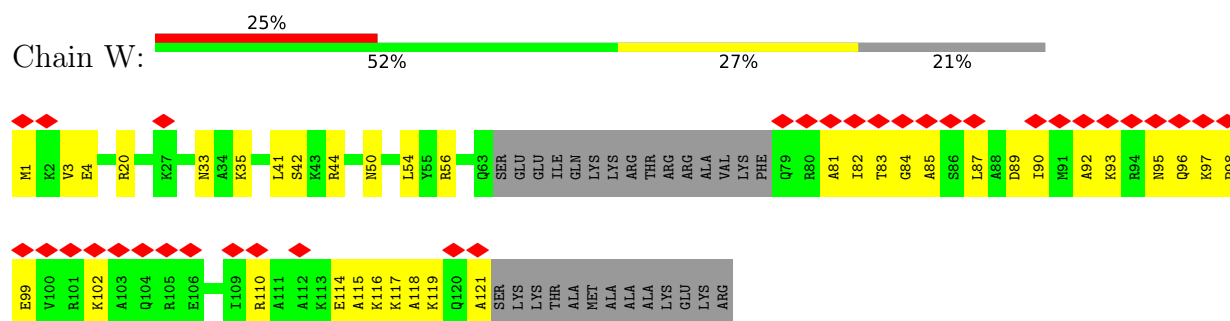
- Molecule 64: eL14



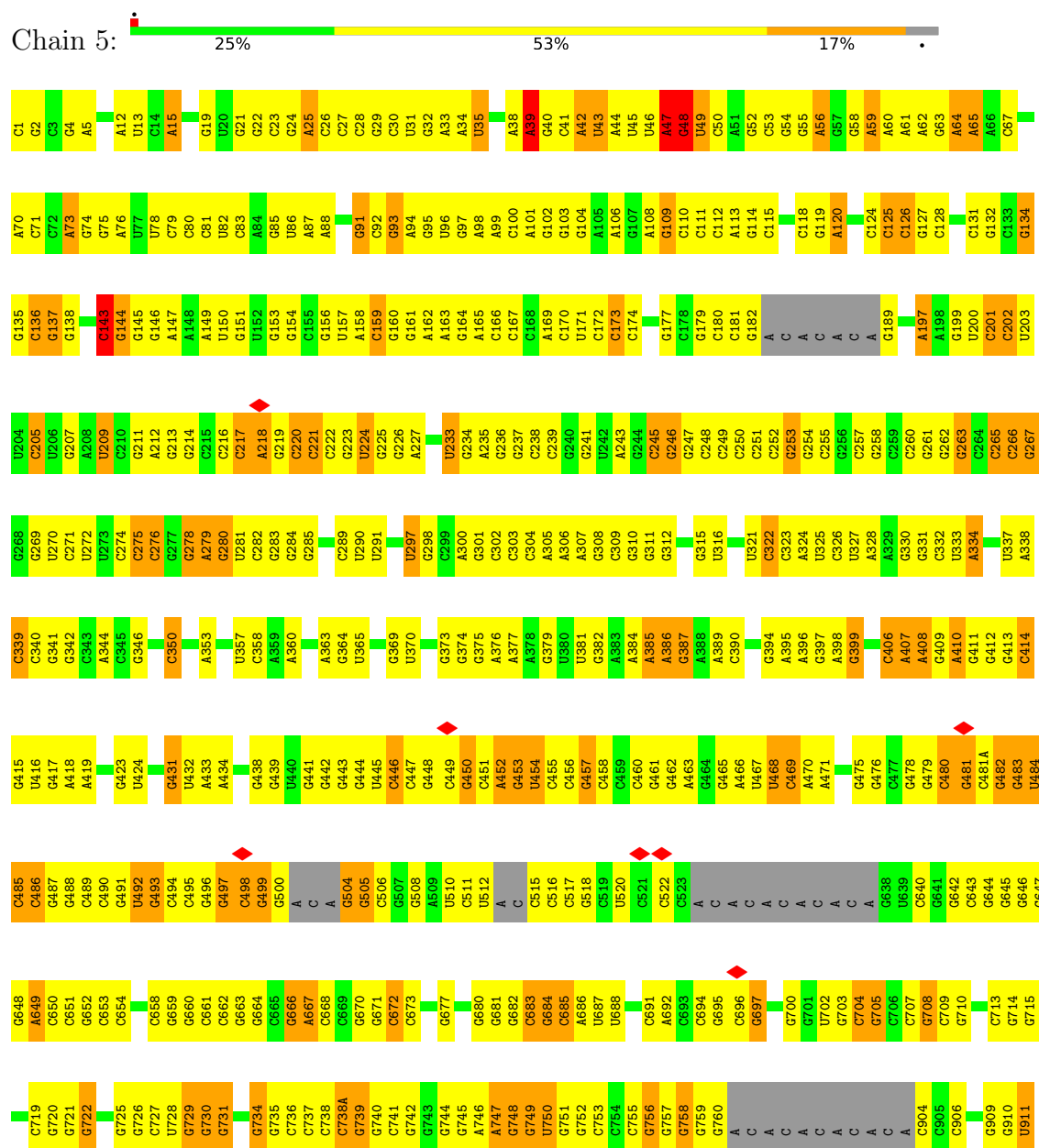
- Molecule 65: 40S ribosomal protein S21



- Molecule 66: 60S ribosomal protein L24-like protein



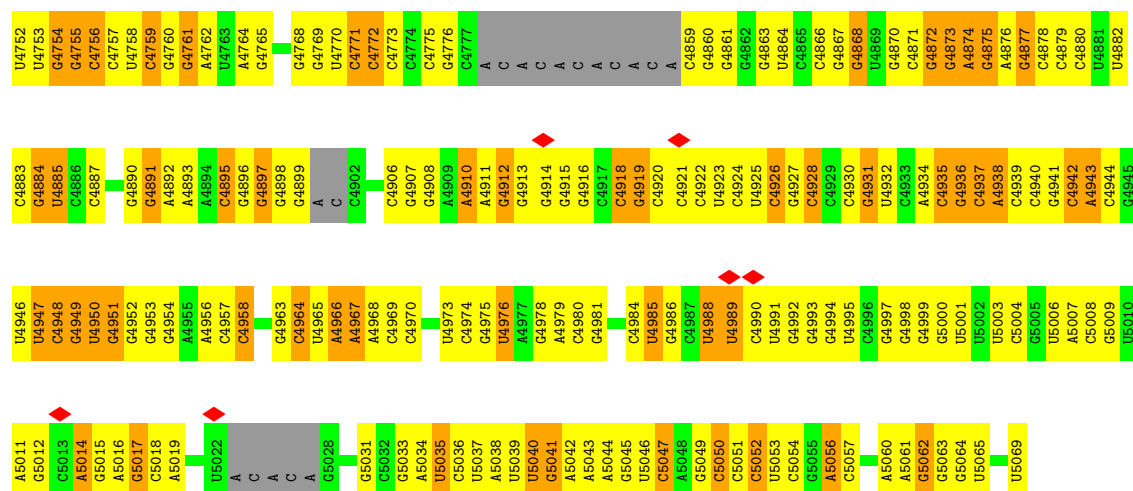
- Molecule 67: 28S Ribosomal RNA



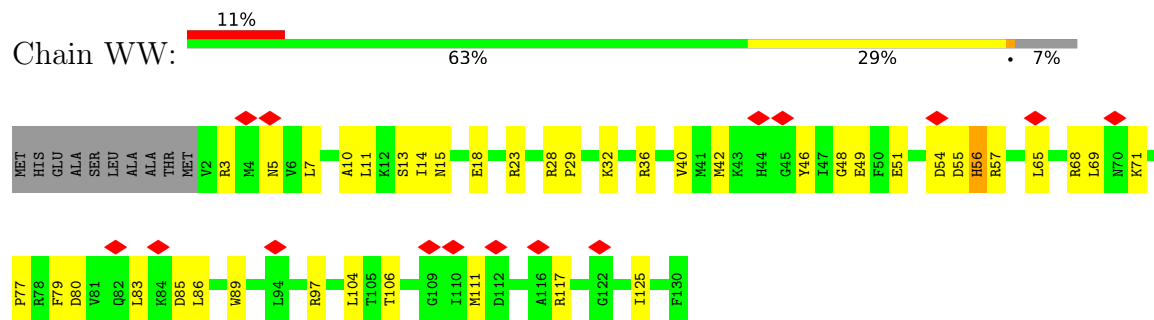
A1896	A1897	A1825	G1753	G1679	G1545	C1477	G1415	G1353	G1288	C1216	G1094	U971	G912
A1898	C1827	G1826	U1754	G1680	C1546	C1478	G1416	A1354	C1289	G1217	G1098	G971A	U913
A1899	C1828	C1755	C1755	G1681	A1547	G1479	C1417	G1355	G1290	G1218	C1099	C972	G914
C1900	G1829	U1756	U1757	A1683	G1549	C1481	A	U1356	G1291	G1219	C1100	C973	A915
C1901				U1684	G1550	G1482	C1418	G1358	C1292	C	A	C974	C916
C1902	G1833	G1760		G1685	C1551	C1483	G1419	G1359	G1293	A	C	G975	A917
C1903	U1834	G1761		G1618	G1552	C1484	G1419	G1360	A1294	A	C	G976	G918
G1904	G1835	C1762		U1620	G1553	C1485	A1420		U1295	C	A	C977	C919
U1905	G1836	C1763		U1621	A1554	C1486	G1421		U1296	C	A	C978	C920
U1906	A1837			U1622	G1555	G1487		C1363	U1297	A	A	C979	C921
				G1618	G1556	G1488	G1424	A	U1298	C	A	C981	G922A
				U1620	A1557	G1489	G1425	C	G1299	C	A	C982	G922B
				U1621	A1558	G1490	A1427	A	G1300	C	A	C983	C923
				U1622	G1559	G1491	U1428	C1368	U1302	A	A	C984	C924
				G1626	A1560	G1492	C1429	C1369	A1303		C	C985	C925
				G1628		G1493	C1430	G1370	C1304	G1233	G1169		G926
				C1629		U1494	C1431	A1371		G1234		C988	G927
				A1630		G1495	G1432	A1372	A1307	G1235	G1172	C989	C928
				A1631		G1496	A1433	A1373	C1308	C1236	C1173		A929
				A1632		A1497	G1434	G1374	C1309	C1237	G1174		G930
				A1633		G1498	G1435	C1375		A	A1175	G1066	C931
				A1634		C1499	G1436	C1376	C1313	C1238	C1176	G1067	A932
				C1635		U1500	C1437	G1377	C1314	C	C1177	G1068	C933
				U1636		C1501	U1438	C1378	C1315	C	G1178	G1069	C934
				A1637		G1502	U1440	C1379		C		G1070	A935
						A1503	C1441	C1380	C1318	G1244		C1071	G935A
						G1504	C1442	U1381	C1319	C1245	U1179	C1072	C936
						C1505	A1443	G1382		G1246	A	C	U937
						G1506	G1444	G1383	G1321	U1247	C	C	C938
						C1507	U1445	C1384	A1322		C	A	C939
						U1508	C1446	G1385	A1323		C	A	
						G1509	C1447	C1386	C1324		C	A	
						U1510	G1448	A1387	G1185		C	A	
						G1511	C1449	A1388	U1186		C	A	
						G1512	C1450	U1389	G1187		C	A	
						U1513	G1451	G1390			C	A	
						U1514	A1452	A1391	C1190		C	A	
						A1515	G1453		C1191		C	A	
						G1516	A1454	G1394	C1192		A	C946	
						U1517	G1455	U1395	G1193		C	G949	
						A1518	C1456	G1396	G1194		C	G1074	G950
						C1519	G1457	A1397	G1195		C	G1075	G951
						U1520	C1458	A1398	G1196		C	C1076	G952
						C1521	A1459		C1197		C	G1077	
						G1522		C1401	G1271		C	A1078	G955
						A1523	C1463	C1402	C1272		C	A1079	A956
						U1524	G1464	U1398	G1273		C	C1080	G957
						G1525	C1465	C1403	A1274		C	C1081	G958
						U1526	G1466	G1404	G1275		C	C1082	G959
						A1527	C1467	C1405	G1276		C	U1083	A960
						A1600	G1468	G1406	G1277		C	C1204	G961
						U1601	C1469	C1406A	C1278		C	G1205	G962
						U1602	G1470	C1406B	C1280		C	C1207	G963
						C1603	C1471	C1406C	G1281		C	G1208	A964
						U1671	U1471	C1411	G1282		C	A1087	G965
						G1604	C1472	G1411A	G1283		C	G1088	
						U1672	U1473	C1411B	G1284		C	G1089	G966
						U1676	C1474	C1411C	G1285		C	G1090	C967
						G1677	G1475	G1412	U1286		C	G1091	C968
						U1608	C1476		G1287		C	G1214	C969
						U1609	C1476				C	C1215	G970



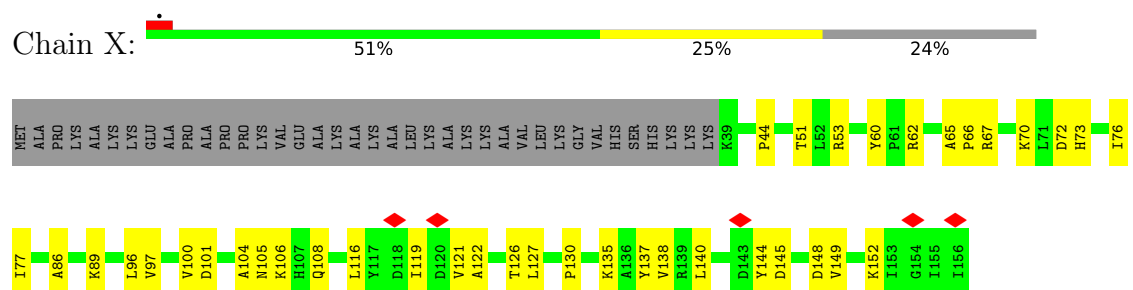




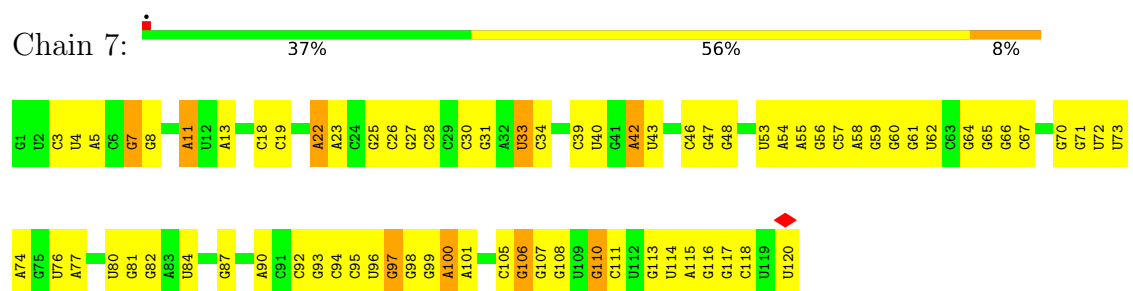
• Molecule 68: Ribosomal protein S15a



• Molecule 69: uL23

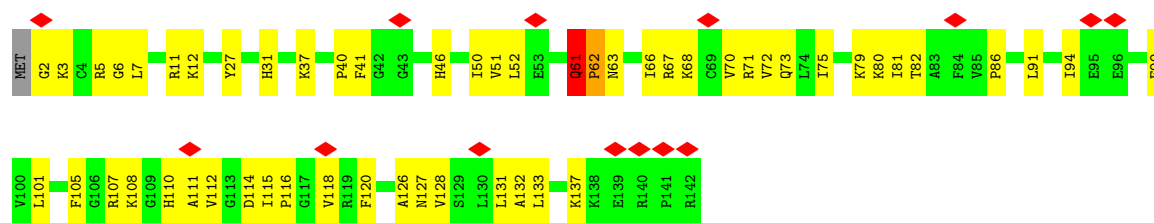


• Molecule 70: 5S Ribosomal RNA

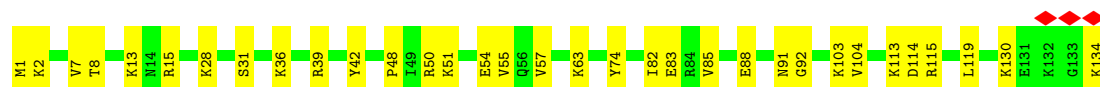
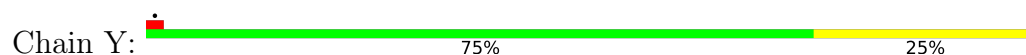


• Molecule 71: 40S ribosomal protein uS12

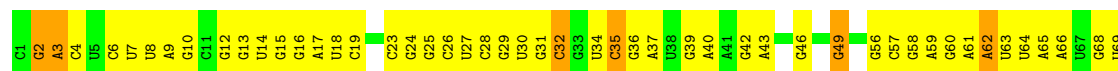




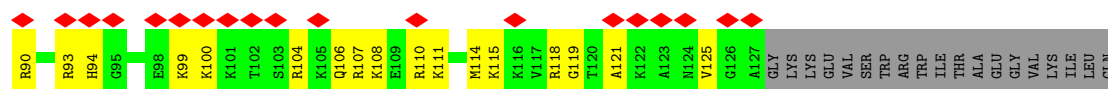
• Molecule 72: Ribosomal protein L26



• Molecule 73: 5.8S Ribosomal RNA



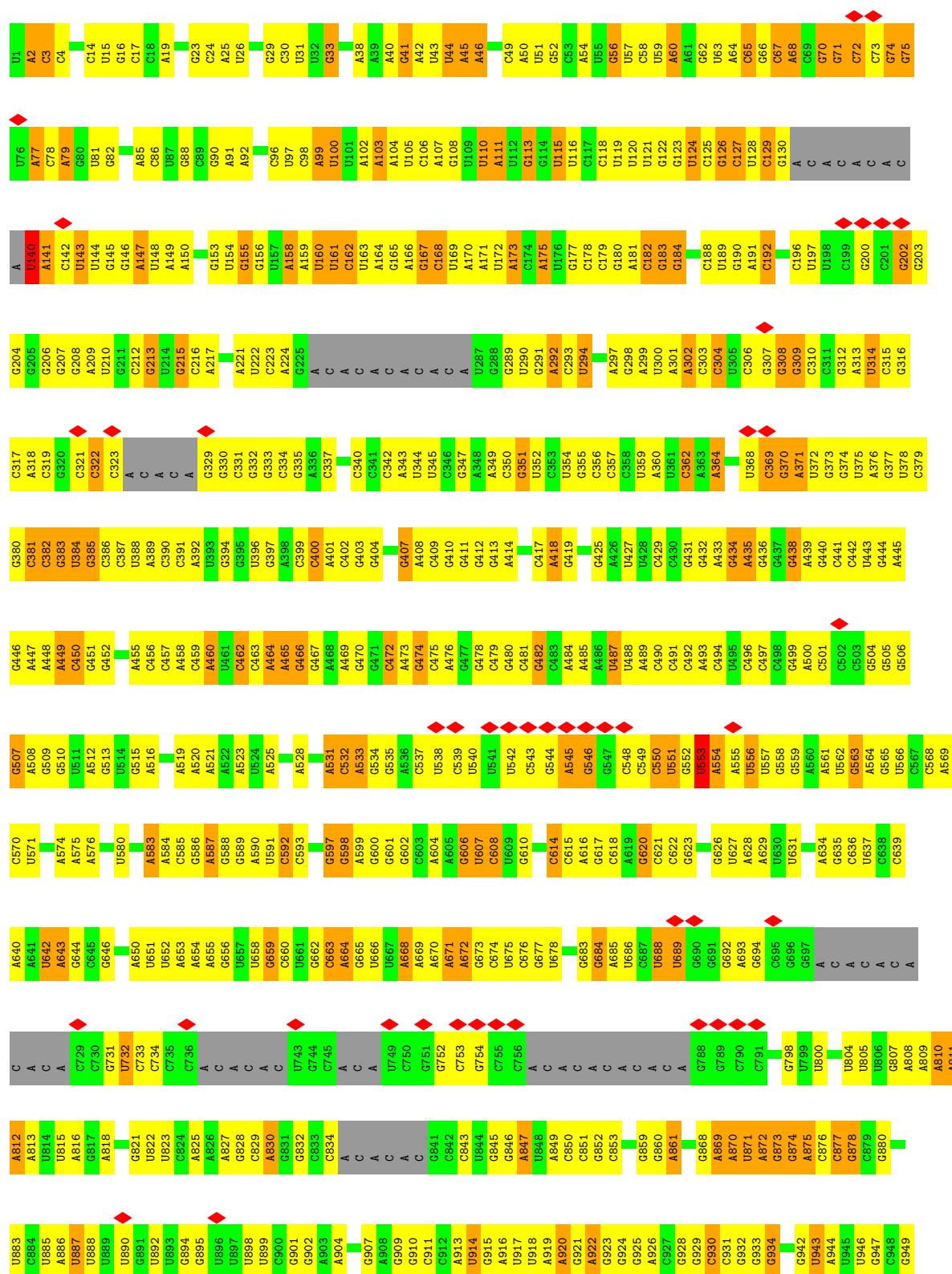
• Molecule 74: 40S ribosomal protein S24



• Molecule 75: 60S ribosomal protein L27



● Molecule 76: 18S Ribosomal RNA

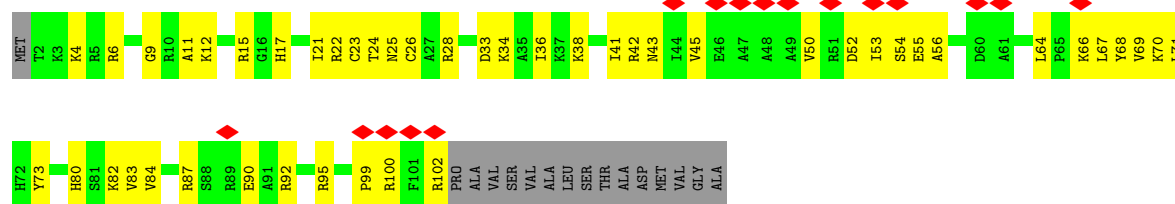




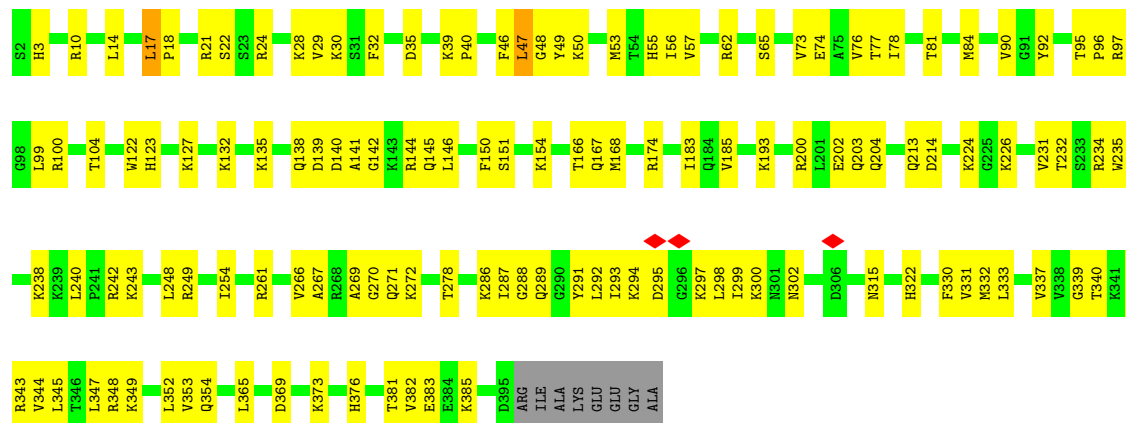


THR
THR
THR
GLU
TRP
SER

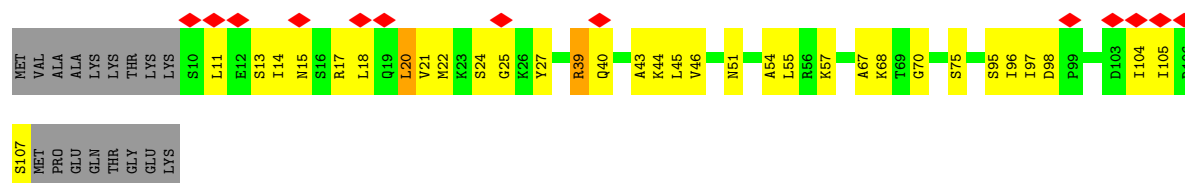
• Molecule 80: 40S ribosomal protein S26



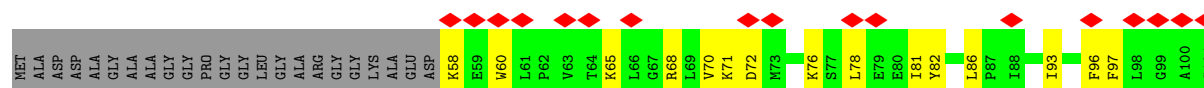
• Molecule 81: uL3

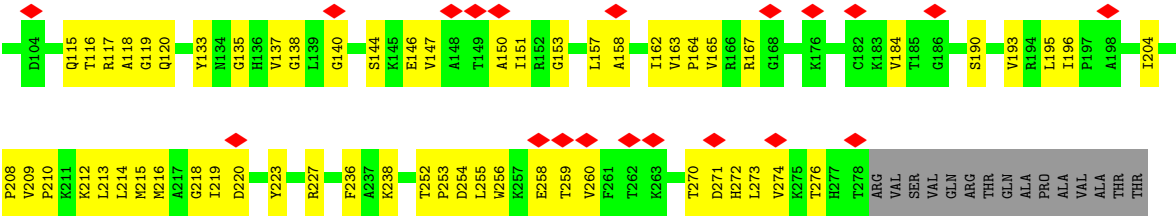


• Molecule 82: eL30

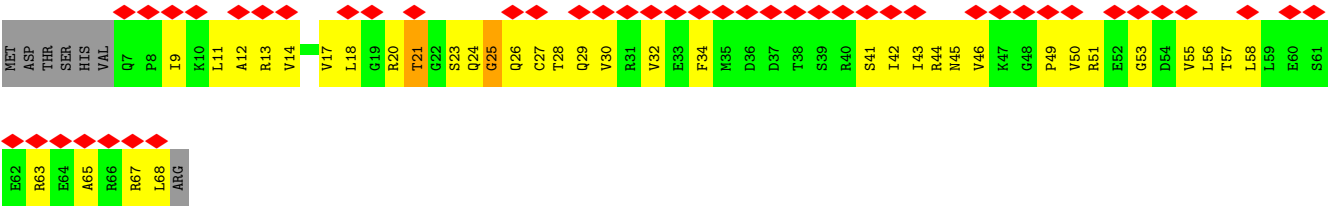


• Molecule 83: 40S ribosomal protein S2





• Molecule 84: 40S ribosomal protein S28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18937	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 ($e^-/\text{\AA}^2$)	41.92	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	79000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BLS, ZN, GCP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.03	0/1936	1.08	0/2596
2	C	1.06	0/2937	1.10	4/3946 (0.1%)
3	d	0.92	0/903	1.11	0/1216
4	DD	0.57	0/1796	1.11	3/2417 (0.1%)
5	dd	0.61	0/470	1.09	1/623 (0.2%)
6	D	0.77	0/2437	0.98	0/3264
7	e	1.11	0/1071	1.07	0/1429
8	EE	0.54	0/2118	0.98	1/2849 (0.0%)
9	ee	0.61	0/447	1.03	1/587 (0.2%)
10	b	0.85	0/861	1.03	0/1138
11	E	0.81	0/1762	1.03	1/2362 (0.0%)
12	f	1.06	1/895 (0.1%)	1.04	0/1198
13	FF	0.53	0/1492	1.05	1/2005 (0.0%)
14	ff	0.53	0/567	1.19	4/753 (0.5%)
15	F	1.11	0/1911	1.08	0/2549
16	g	0.88	0/916	1.06	0/1220
17	BB	0.55	0/1756	0.97	5/2350 (0.2%)
18	GG	0.53	0/1946	1.01	1/2590 (0.0%)
19	gg	0.45	0/2493	0.92	2/3394 (0.1%)
20	G	0.80	0/1910	1.03	1/2569 (0.0%)
21	h	0.88	0/1021	1.04	0/1348
22	HH	0.59	1/1510 (0.1%)	0.98	0/2022
23	hh	0.40	0/353	0.86	0/547
24	bb	0.53	0/665	0.91	0/891
25	H	0.87	0/1535	1.00	1/2063 (0.0%)
26	i	0.83	0/841	1.04	0/1112
27	II	0.57	0/1715	0.98	1/2287 (0.0%)
28	ii	0.55	0/3361	1.10	8/4519 (0.2%)
29	I	0.92	0/1702	1.03	1/2272 (0.0%)
30	j	1.02	0/720	1.12	1/952 (0.1%)
31	JJ	0.64	0/1550	0.92	0/2069
32	jj	0.53	0/3435	1.06	7/4633 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	J	0.73	0/1385	1.02	0/1852
34	k	0.78	0/575	0.98	0/761
35	KK	0.51	0/834	1.01	3/1125 (0.3%)
36	L	0.88	0/1733	1.07	1/2316 (0.0%)
37	l	0.93	0/459	1.07	0/608
38	LL	0.61	0/1195	0.95	0/1597
39	M	0.85	0/1158	1.06	0/1547
40	m	0.86	0/435	0.98	1/575 (0.2%)
41	MM	0.37	0/918	0.77	0/1233
42	N	1.06	0/1746	1.06	0/2338
43	n	0.72	0/240	1.40	1/305 (0.3%)
44	NN	0.61	0/1226	0.96	0/1649
45	O	1.07	0/1662	1.10	0/2222
46	o	0.79	0/864	1.11	1/1140 (0.1%)
47	OO	0.58	0/1029	1.06	3/1380 (0.2%)
48	P	1.00	0/1268	1.05	0/1700
49	p	0.92	0/718	1.00	0/953
50	PP	0.60	0/1017	1.10	1/1358 (0.1%)
51	Q	1.08	1/1539 (0.1%)	1.08	0/2054
52	r	0.95	0/1010	1.08	0/1354
53	QQ	0.53	0/1146	1.03	1/1534 (0.1%)
54	R	0.87	0/1524	1.09	5/2013 (0.2%)
55	s	0.54	0/1530	1.04	3/2064 (0.1%)
56	RR	0.54	0/1082	0.96	1/1452 (0.1%)
57	S	0.98	0/1501	1.00	1/2012 (0.0%)
58	t	0.72	1/1174 (0.1%)	1.03	0/1582
59	SS	0.57	0/1208	1.18	3/1618 (0.2%)
60	T	0.93	0/1326	1.08	2/1770 (0.1%)
61	TT	0.52	0/1115	0.97	1/1493 (0.1%)
62	U	0.71	0/823	0.99	0/1104
63	UU	0.64	0/805	1.18	4/1081 (0.4%)
64	V	1.04	0/993	1.02	2/1332 (0.2%)
65	VV	0.59	0/643	0.84	0/860
66	W	0.79	0/873	1.09	3/1158 (0.3%)
67	5	0.66	0/84975	0.81	24/132516 (0.0%)
68	WW	0.70	0/1051	0.94	0/1406
69	X	0.92	0/984	1.10	0/1323
70	7	0.61	0/2858	0.73	0/4455
71	XX	0.69	0/1116	0.96	0/1490
72	Y	0.93	0/1132	1.09	1/1504 (0.1%)
73	8	0.65	0/3581	0.79	0/5577
74	YY	0.50	0/1028	0.94	1/1366 (0.1%)
75	Z	0.81	0/1130	1.02	1/1507 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	9	0.47	0/40524	0.78	16/63134 (0.0%)
77	ZZ	0.49	0/604	1.00	0/810
78	a	1.09	0/1191	1.04	1/1590 (0.1%)
79	AA	0.58	0/1747	0.90	0/2374
80	aa	0.65	0/828	0.96	0/1109
81	B	0.95	0/3240	1.05	1/4339 (0.0%)
82	c	0.82	0/771	1.19	3/1034 (0.3%)
83	CC	0.68	0/1753	1.02	0/2369
84	cc	0.59	0/490	1.17	2/656 (0.3%)
All	All	0.69	4/234789 (0.0%)	0.90	131/343469 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
53	QQ	0	1
67	5	0	7
71	XX	0	1
76	9	0	1
79	AA	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	t	19	GLY	C-O	-18.00	1.14	1.24
12	f	29	LYS	CA-CB	-8.48	1.38	1.53
22	HH	100	ILE	C-N	6.01	1.46	1.33
51	Q	158	THR	C-N	-5.00	1.27	1.33

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	FF	19	LEU	N-CA-C	-9.13	92.04	108.02
32	jj	384	LYS	CB-CG-CD	8.13	129.99	111.30
47	OO	122	SER	N-CA-C	7.67	120.72	111.82
28	ii	260	GLY	N-CA-C	7.34	120.50	110.58
20	G	213	ASP	N-CA-C	7.07	122.69	111.81

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
67	5	1081	C	Sidechain
67	5	39	A	Sidechain
67	5	914	U	Sidechain
53	QQ	140	ARG	Peptide
3	d	95	ASP	Peptide

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	A	1898	1993	1993	64	0
2	C	2883	3053	3053	105	0
3	d	888	930	930	27	0
4	DD	1768	1864	1866	215	0
5	dd	459	449	450	73	0
6	D	2391	2424	2424	72	0
7	e	1053	1147	1147	36	0
8	EE	2076	2177	2177	77	0
9	ee	443	492	492	15	0
10	b	848	920	920	28	0
11	E	1729	1888	1887	84	0
12	f	876	912	912	32	0
13	FF	1471	1522	1522	148	0
14	ff	555	565	566	49	0
15	F	1875	1995	1995	60	0
16	g	906	999	1002	42	0
17	BB	1729	1803	1803	81	0
18	GG	1923	2082	2089	154	0
19	gg	2436	2394	2393	193	0
20	G	1879	2027	2027	72	0
21	h	1013	1147	1147	24	0
22	HH	1488	1582	1582	93	0
23	hh	317	161	161	17	0
24	bb	651	672	672	30	0
25	H	1516	1597	1597	45	0
26	i	830	916	916	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	II	1686	1773	1772	79	0
28	ii	3307	3331	3346	320	0
29	I	1664	1712	1712	31	0
30	j	705	737	738	24	0
31	JJ	1525	1640	1640	71	0
32	jj	3368	3419	3422	377	0
33	J	1362	1399	1399	52	0
34	k	569	637	637	21	0
35	KK	810	836	836	103	0
36	L	1702	1820	1820	61	0
37	l	447	480	480	14	0
38	LL	1175	1250	1249	58	0
39	M	1137	1211	1211	32	0
40	m	429	465	466	13	0
41	MM	908	939	939	55	0
42	N	1701	1750	1749	57	0
43	n	239	286	289	28	0
44	NN	1202	1289	1289	42	0
45	O	1630	1778	1778	53	0
46	o	851	920	923	24	0
47	OO	1016	1039	1039	77	0
48	P	1242	1274	1274	42	0
49	p	708	758	757	22	0
50	PP	997	1045	1045	165	0
51	Q	1515	1634	1634	49	0
52	r	994	1051	1051	38	0
53	QQ	1128	1195	1195	145	0
54	R	1508	1664	1664	60	0
55	s	1507	1564	1564	139	0
56	RR	1068	1121	1121	123	0
57	S	1462	1508	1508	37	0
58	t	1160	1215	1218	113	0
59	SS	1190	1247	1249	164	0
60	T	1298	1367	1366	42	0
61	TT	1097	1132	1132	123	0
62	U	809	833	833	21	0
63	UU	795	862	862	99	0
64	V	979	1039	1038	32	0
65	VV	636	637	637	26	0
66	W	860	892	903	38	0
67	5	75972	38389	38358	3068	0
68	WW	1034	1080	1080	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	X	967	1040	1040	33	0
70	7	2558	1296	1296	84	0
71	XX	1098	1165	1167	46	0
72	Y	1115	1205	1205	31	0
73	8	3208	1629	1629	163	0
74	YY	1011	1083	1083	43	0
75	Z	1107	1182	1182	49	0
76	9	36249	18308	18313	1912	0
77	ZZ	598	656	656	68	0
78	a	1162	1210	1209	43	0
79	AA	1710	1708	1708	75	0
80	aa	814	864	866	50	0
81	B	3172	3310	3310	123	0
82	c	761	794	794	39	0
83	CC	1716	1806	1806	65	0
84	cc	488	514	514	75	0
85	aa	1	0	0	0	0
85	dd	1	0	0	0	0
85	ff	1	0	0	0	0
85	g	1	0	0	0	0
85	j	1	0	0	0	0
85	m	1	0	0	0	0
85	o	1	0	0	0	0
85	p	1	0	0	0	0
86	5	189	0	0	0	0
86	7	4	0	0	0	0
86	8	10	0	0	0	0
86	9	70	0	0	0	0
86	P	1	0	0	0	0
86	V	1	0	0	0	0
86	a	1	0	0	0	0
86	hh	2	0	0	0	0
86	j	1	0	0	0	0
86	jj	1	0	0	0	0
86	o	1	0	0	0	0
87	jj	32	14	13	14	0
88	5	30	25	24	3	0
All	All	219378	165738	165761	9348	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 25.

The worst 5 of 9348 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)
88:5:5122:BLS:C1'	88:5:5122:BLS:O5'	1.65	1.41
67:5:4771:C:N3	67:5:4864:U:C4	2.12	1.17
76:9:1245:G:O2'	76:9:1492:U:OP1	1.61	1.15
76:9:1620:A:O2'	76:9:1624:U:OP2	1.65	1.14
19:gg:63:SER:OG	76:9:1396:A:O2'	1.64	1.13

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	A	246/249 (99%)	219 (89%)	27 (11%)	0	100	100
2	C	360/378 (95%)	335 (93%)	24 (7%)	1 (0%)	36	70
3	d	105/108 (97%)	90 (86%)	13 (12%)	2 (2%)	6	34
4	DD	226/281 (80%)	212 (94%)	13 (6%)	1 (0%)	30	65
5	dd	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
6	D	291/296 (98%)	273 (94%)	18 (6%)	0	100	100
7	e	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
8	EE	260/263 (99%)	244 (94%)	16 (6%)	0	100	100
9	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
10	b	100/226 (44%)	94 (94%)	5 (5%)	1 (1%)	12	46
11	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
12	f	107/110 (97%)	98 (92%)	7 (6%)	2 (2%)	6	34
13	FF	181/204 (89%)	164 (91%)	14 (8%)	3 (2%)	7	36
14	ff	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
15	F	223/249 (90%)	213 (96%)	9 (4%)	1 (0%)	30	65
16	g	112/126 (89%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	BB	211/264 (80%)	193 (92%)	18 (8%)	0	100	100
18	GG	235/263 (89%)	223 (95%)	12 (5%)	0	100	100
19	gg	311/314 (99%)	282 (91%)	27 (9%)	2 (1%)	21	58
20	G	229/242 (95%)	218 (95%)	9 (4%)	2 (1%)	14	49
21	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
22	HH	181/191 (95%)	173 (96%)	8 (4%)	0	100	100
24	bb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
25	H	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
26	i	100/107 (94%)	94 (94%)	6 (6%)	0	100	100
27	II	204/208 (98%)	188 (92%)	14 (7%)	2 (1%)	12	46
28	ii	417/437 (95%)	389 (93%)	24 (6%)	4 (1%)	12	46
29	I	201/214 (94%)	182 (90%)	19 (10%)	0	100	100
30	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
31	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
32	jj	426/428 (100%)	373 (88%)	46 (11%)	7 (2%)	7	37
33	J	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
34	k	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
35	KK	94/151 (62%)	88 (94%)	5 (5%)	1 (1%)	11	44
36	L	208/211 (99%)	192 (92%)	15 (7%)	1 (0%)	24	61
37	l	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
38	LL	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
39	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
40	m	50/128 (39%)	46 (92%)	4 (8%)	0	100	100
41	MM	115/123 (94%)	103 (90%)	12 (10%)	0	100	100
42	N	201/204 (98%)	186 (92%)	11 (6%)	4 (2%)	6	33
43	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
44	NN	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	18	55
45	O	197/203 (97%)	189 (96%)	7 (4%)	1 (0%)	24	61
46	o	102/142 (72%)	98 (96%)	4 (4%)	0	100	100
47	OO	134/156 (86%)	124 (92%)	8 (6%)	2 (2%)	8	39
48	P	151/199 (76%)	143 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	p	89/109 (82%)	82 (92%)	7 (8%)	0	100	100
50	PP	118/145 (81%)	104 (88%)	12 (10%)	2 (2%)	7	36
51	Q	185/188 (98%)	173 (94%)	11 (6%)	1 (0%)	24	61
52	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	16	52
53	QQ	140/158 (89%)	133 (95%)	6 (4%)	1 (1%)	18	55
54	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
55	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	12	46
56	RR	130/145 (90%)	121 (93%)	9 (7%)	0	100	100
57	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	7	36
58	t	151/196 (77%)	134 (89%)	16 (11%)	1 (1%)	18	55
59	SS	142/152 (93%)	137 (96%)	4 (3%)	1 (1%)	18	55
60	T	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
61	TT	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
62	U	97/128 (76%)	89 (92%)	8 (8%)	0	100	100
63	UU	98/118 (83%)	91 (93%)	7 (7%)	0	100	100
64	V	129/132 (98%)	119 (92%)	10 (8%)	0	100	100
65	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
66	W	102/134 (76%)	98 (96%)	4 (4%)	0	100	100
68	WW	127/139 (91%)	118 (93%)	7 (6%)	2 (2%)	7	37
69	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
71	XX	139/142 (98%)	125 (90%)	11 (8%)	3 (2%)	5	31
72	Y	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
74	YY	122/146 (84%)	115 (94%)	7 (6%)	0	100	100
75	Z	133/136 (98%)	125 (94%)	6 (4%)	2 (2%)	8	39
77	ZZ	73/122 (60%)	69 (94%)	4 (6%)	0	100	100
78	a	145/147 (99%)	129 (89%)	16 (11%)	0	100	100
79	AA	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	24	61
80	aa	99/117 (85%)	89 (90%)	9 (9%)	1 (1%)	12	46
81	B	392/402 (98%)	355 (91%)	35 (9%)	2 (0%)	24	61
82	c	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
83	CC	219/259 (85%)	205 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
All	All	12362/14087 (88%)	11478 (93%)	823 (7%)	61 (0%)	26	61

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	95	ASP
28	ii	272	THR
32	jj	466	LYS
32	jj	620	GLU
42	N	76	PRO

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	hh	14/15 (93%)	8 (57%)	0
67	5	3517/3705 (94%)	864 (24%)	155 (4%)
70	7	119/120 (99%)	14 (11%)	0
73	8	149/151 (98%)	34 (22%)	5 (3%)
76	9	1680/1779 (94%)	425 (25%)	66 (3%)
All	All	5479/5770 (94%)	1345 (24%)	226 (4%)

5 of 1345 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
23	hh	42	C
23	hh	43	A
23	hh	45	A
23	hh	46	G
23	hh	49	U

5 of 226 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
67	5	3625	G
76	9	1744	G

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Mol	Chain	Res	Type
67	5	4699	U
76	9	1679	A
76	9	1253	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 289 are monoatomic - leaving 2 for Mogul analysis.

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$
87	GCP	jj	700	-	32,34,34	3.10	12 (37%)	49,54,54	1.79	13 (26%)
88	BLS	5	5122	67	30,31,31	4.21	17 (56%)	30,43,43	1.61	6 (20%)

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
87	GCP	jj	700	-	-	5/19/38/38	0/3/3/3
88	BLS	5	5122	67	-	6/25/38/38	0/2/2/2

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	5	5122	BLS	O5'-C1'	11.79	1.65	1.42
88	5	5122	BLS	O5'-C5'	-9.89	1.24	1.43
87	jj	700	GCP	O4'-C1'	8.79	1.62	1.42
88	5	5122	BLS	C3'-C2'	7.35	1.55	1.33
88	5	5122	BLS	C4'-C5'	7.17	1.69	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	jj	700	GCP	C5-C4-N3	-5.80	119.16	128.39
87	jj	700	GCP	C2-N3-C4	4.84	120.63	112.30
88	5	5122	BLS	C8-C7-N6	4.82	122.84	116.25
87	jj	700	GCP	C2-N1-C6	-3.36	119.01	125.11
87	jj	700	GCP	PB-O3A-PA	-3.16	122.04	132.37

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	jj	700	GCP	PG-C3B-PB-O1B
87	jj	700	GCP	PG-C3B-PB-O2B
87	jj	700	GCP	PG-C3B-PB-O3A
87	jj	700	GCP	C5'-O5'-PA-O3A
87	jj	700	GCP	C5'-O5'-PA-O2A

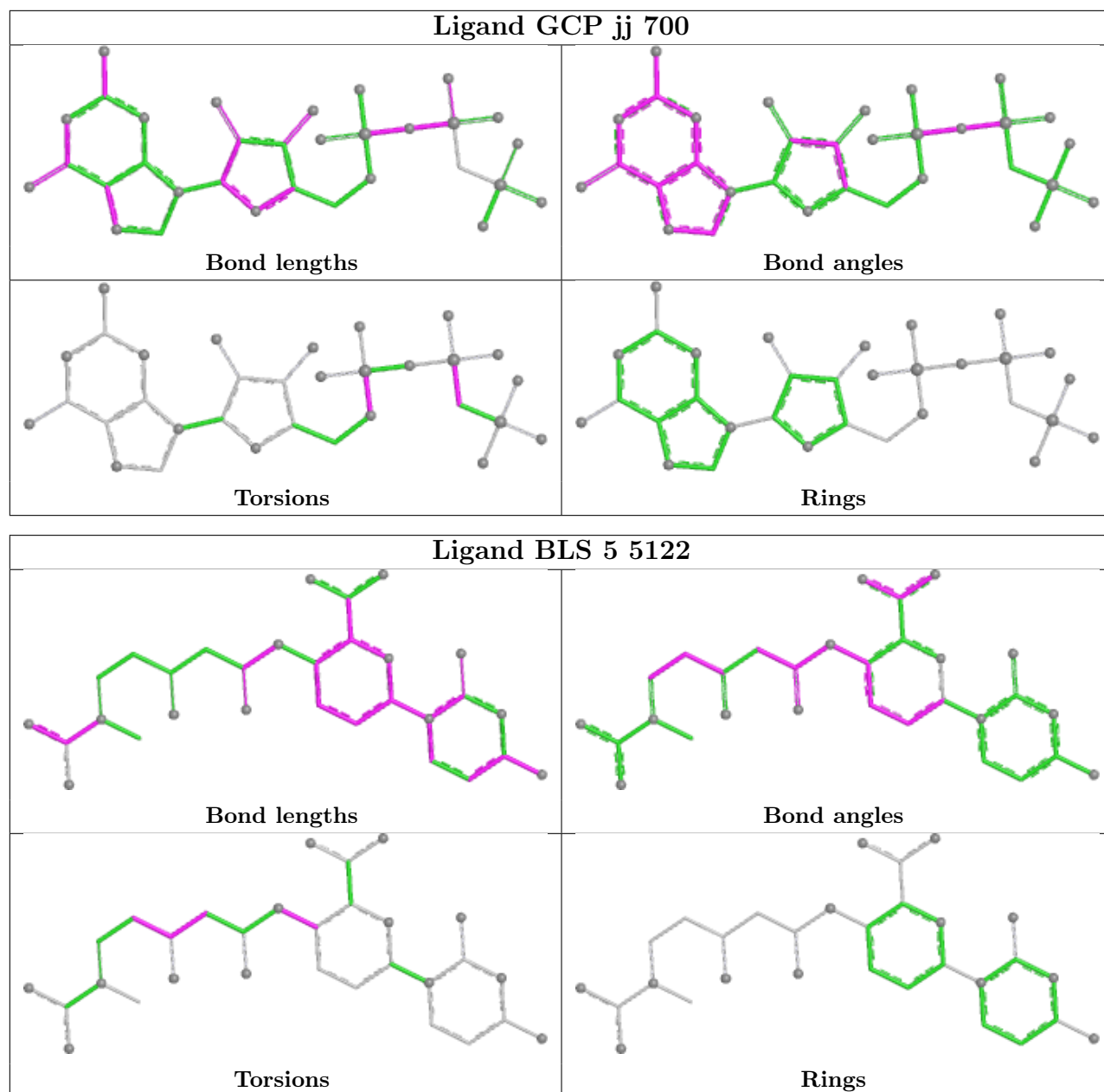
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	jj	700	GCP	14	0
88	5	5122	BLS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



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:

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Mol	Chain	Number of breaks
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Mol	Chain	Number of breaks
67	5	7
76	9	7
73	8	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	990:C	O3'	1064:G	P	17.61
1	5	1406(C):G	O3'	1411:C	P	17.48
1	8	79:G	O3'	85:U	P	15.70
1	5	4138:C	O3'	4146:G	P	15.08
1	9	322:C	O3'	323:C	P	9.57

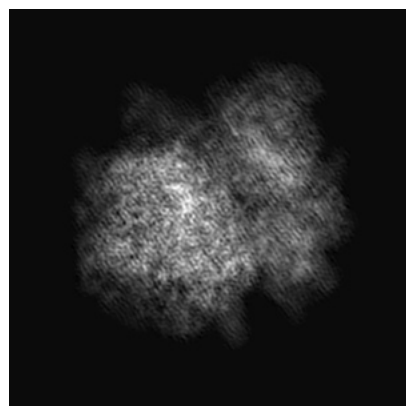
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12632. These allow visual inspection of the internal detail of the map and identification of artifacts.

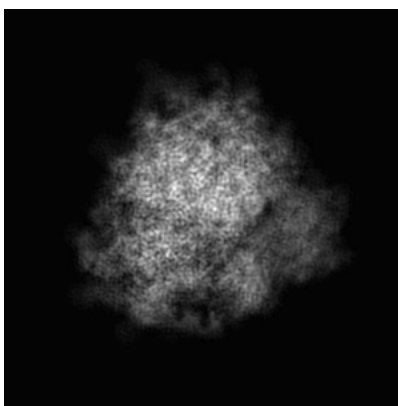
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

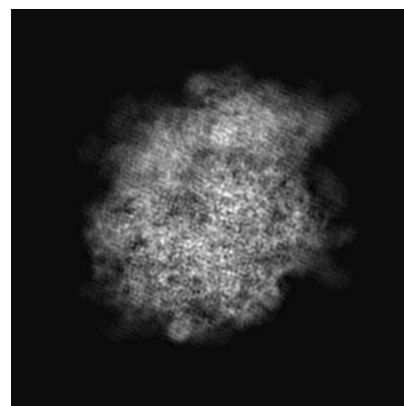
6.1.1 Primary map



X

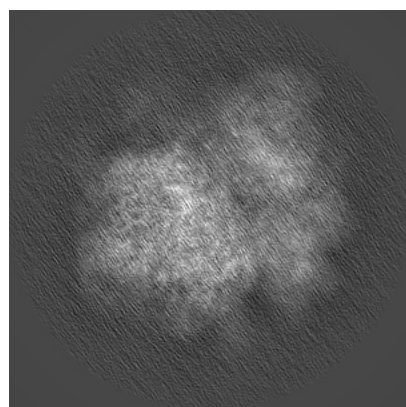


Y

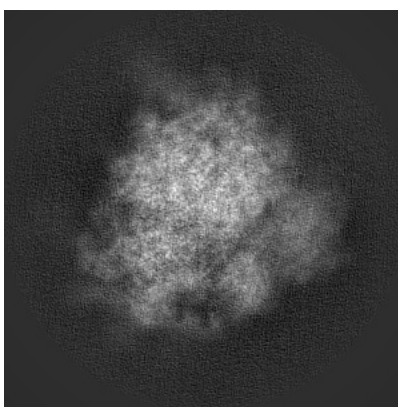


Z

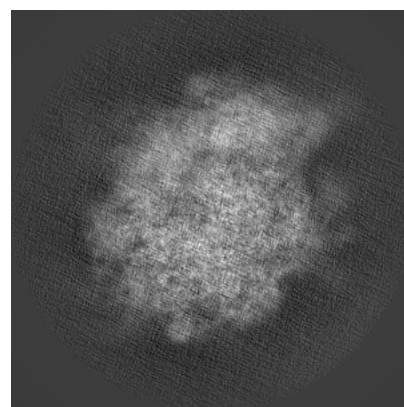
6.1.2 Raw map



X



Y

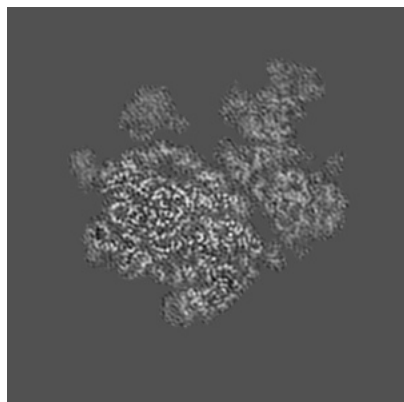


Z

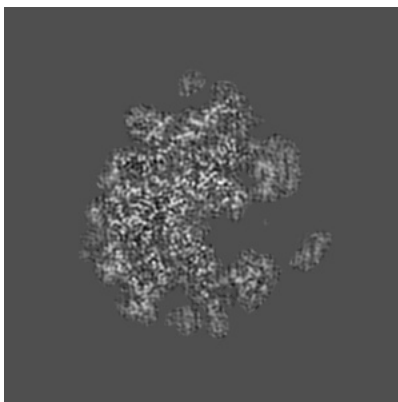
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

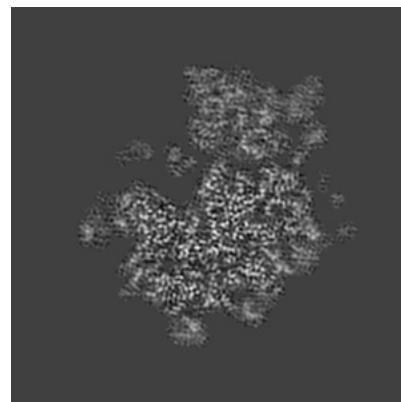
6.2.1 Primary map



X Index: 150

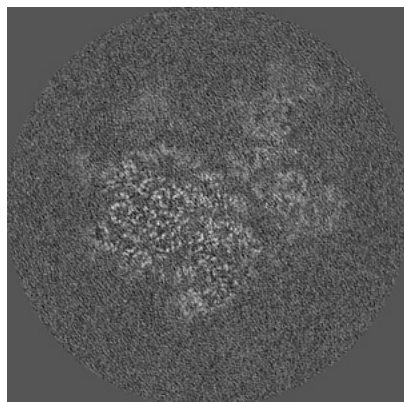


Y Index: 150

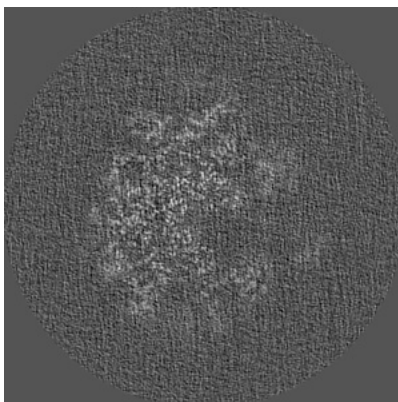


Z Index: 150

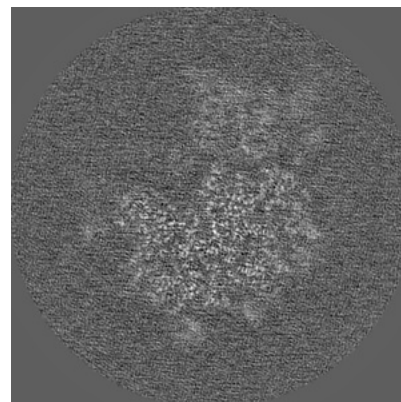
6.2.2 Raw map



X Index: 150



Y Index: 150

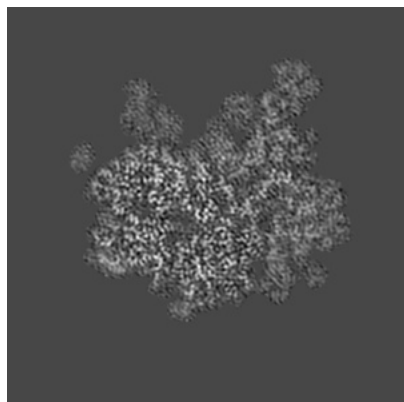


Z Index: 150

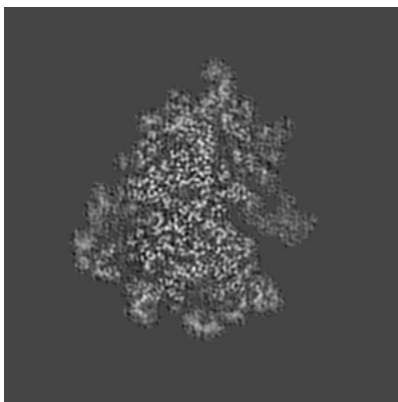
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

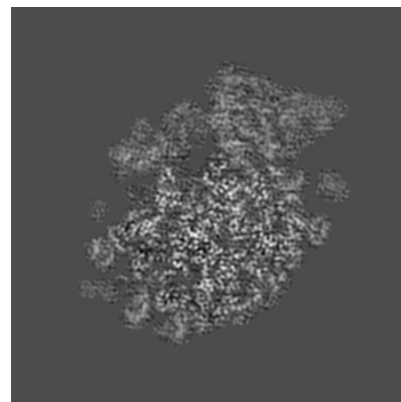
6.3.1 Primary map



X Index: 158

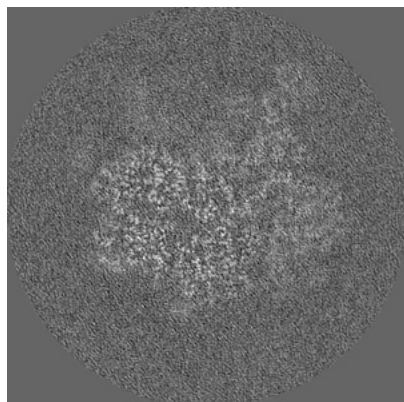


Y Index: 130

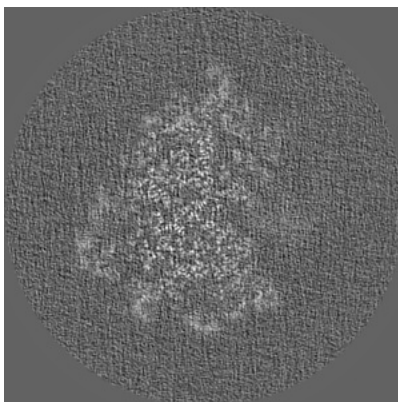


Z Index: 128

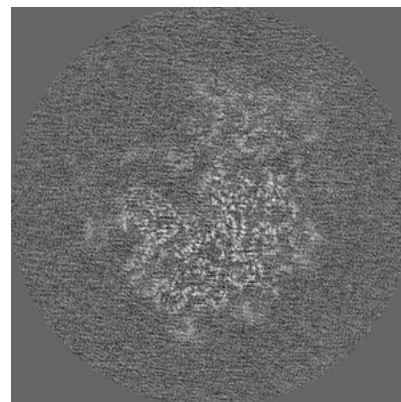
6.3.2 Raw map



X Index: 158



Y Index: 130

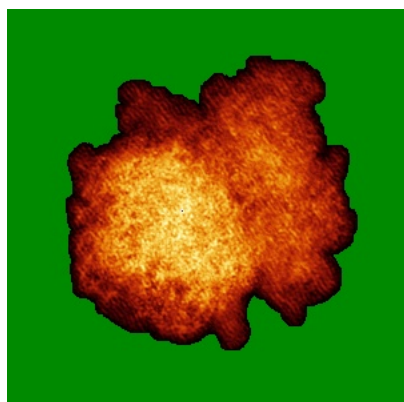


Z Index: 148

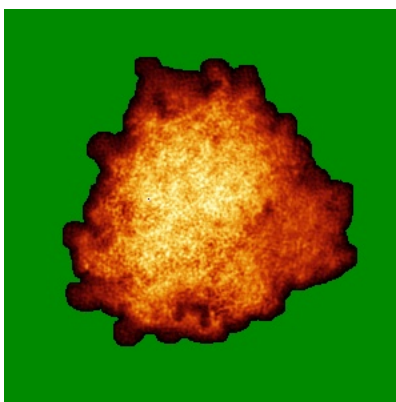
The images above show the largest variance slices of the map in three orthogonal directions.

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

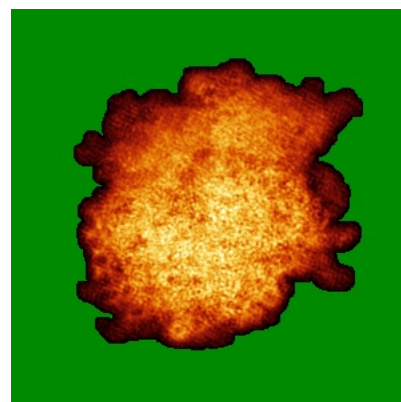
6.4.1 Primary map



X

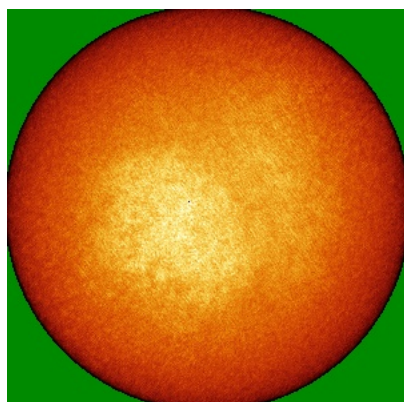


Y

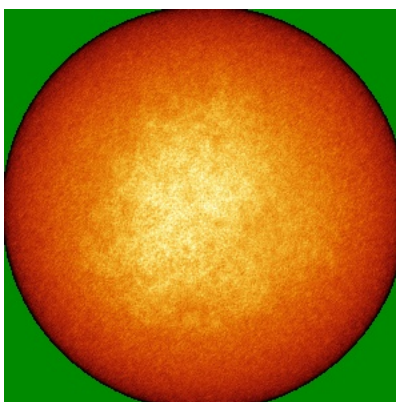


Z

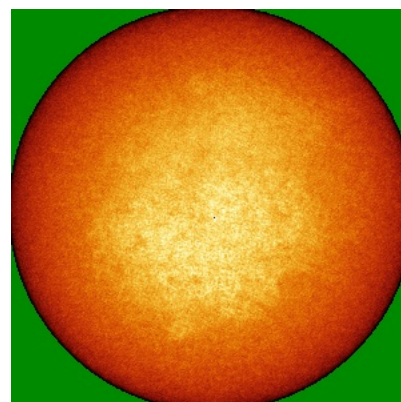
6.4.2 Raw map



X



Y

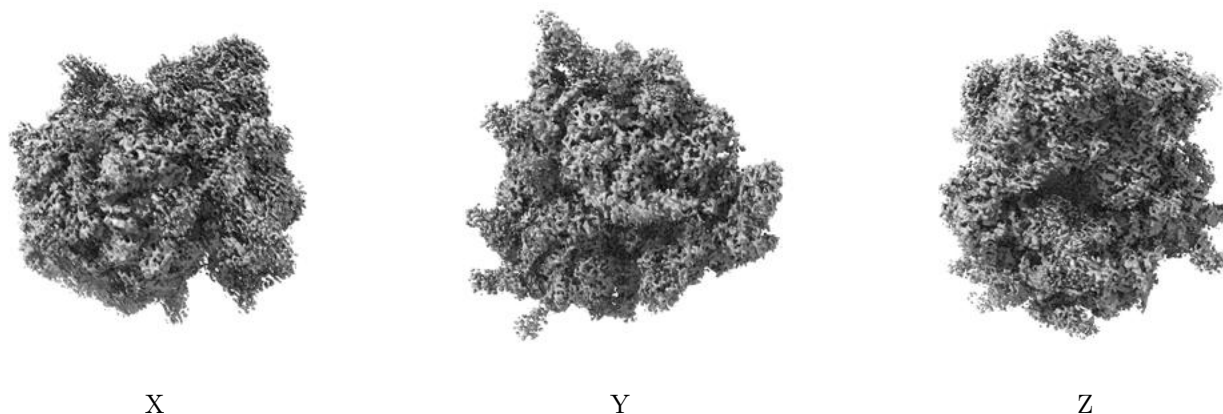


Z

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.

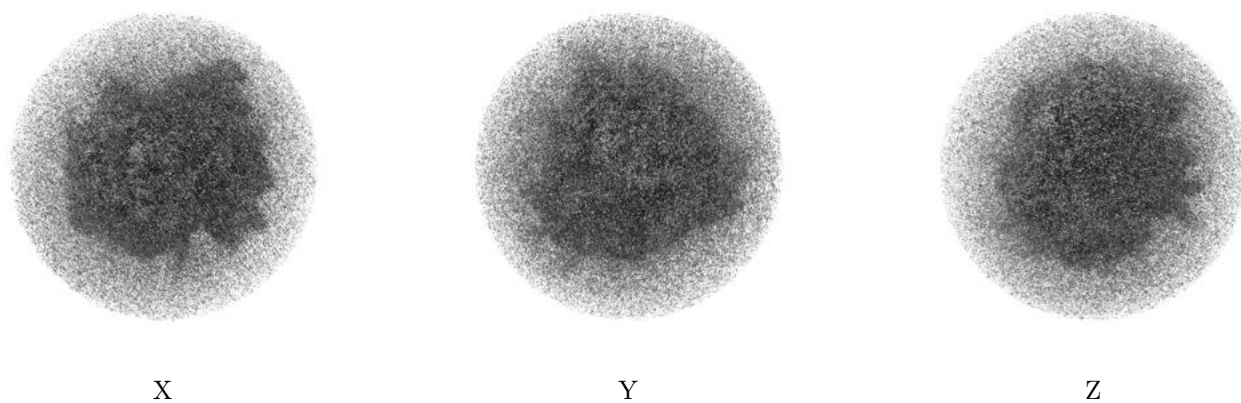
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

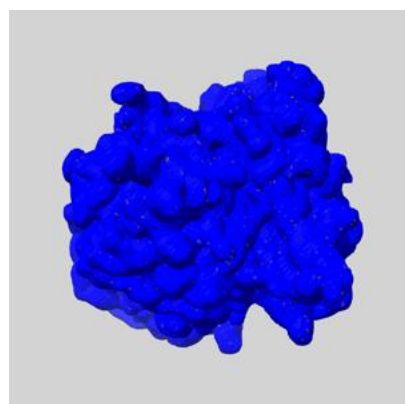
6.6 Mask visualisation [i](#)

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

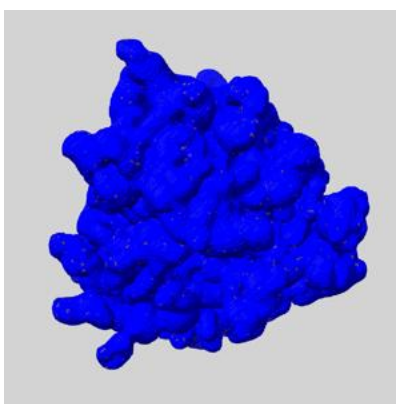
A mask typically either:

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

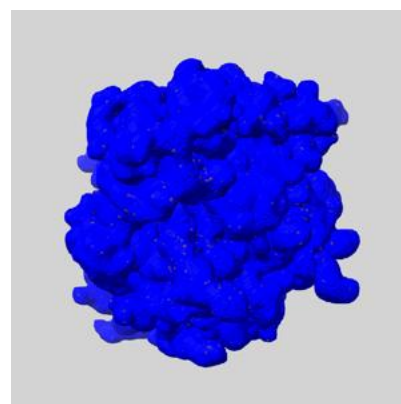
6.6.1 emd_12632_msk_1.map [i](#)



X



Y

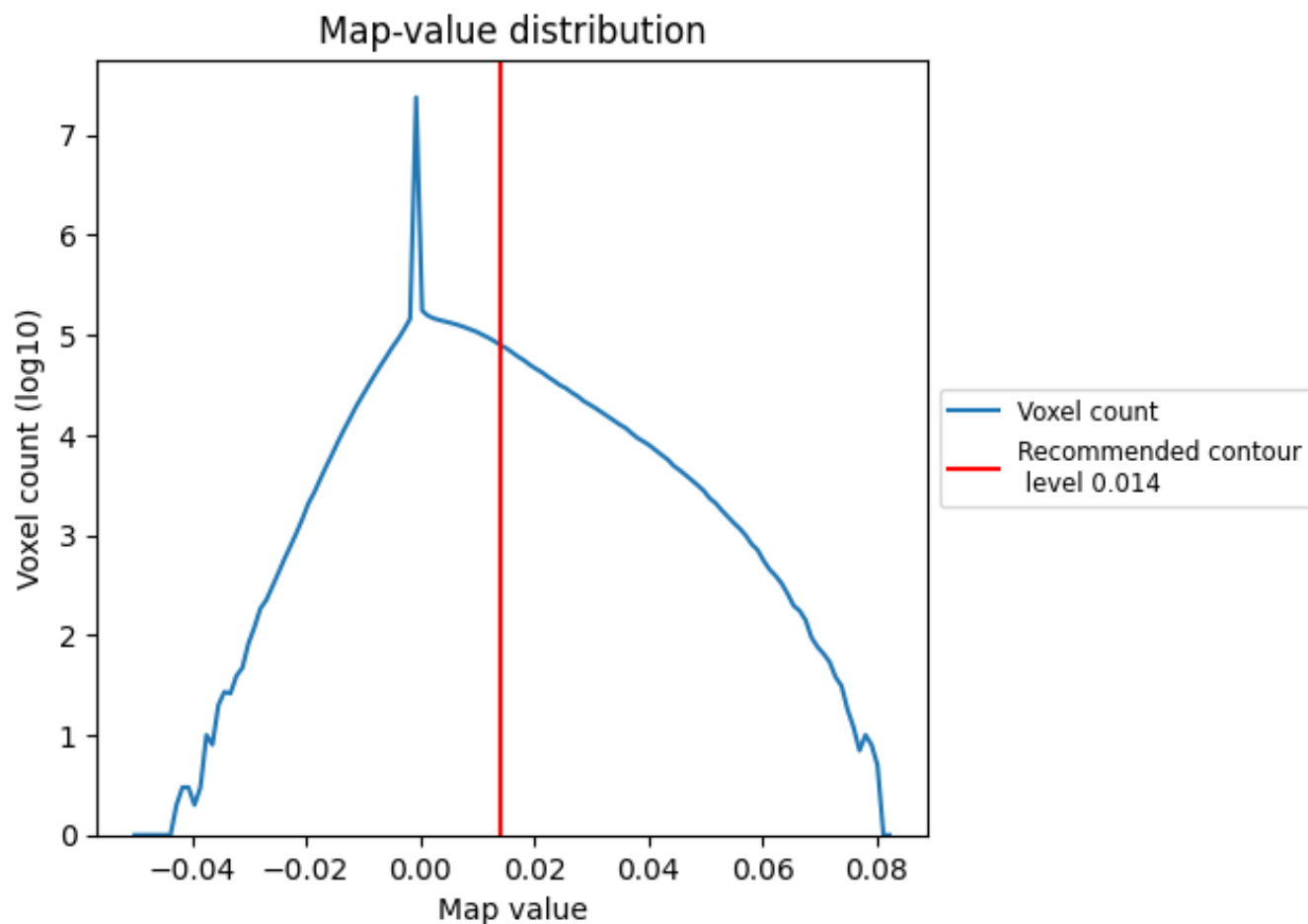


Z

7 Map analysis [i](#)

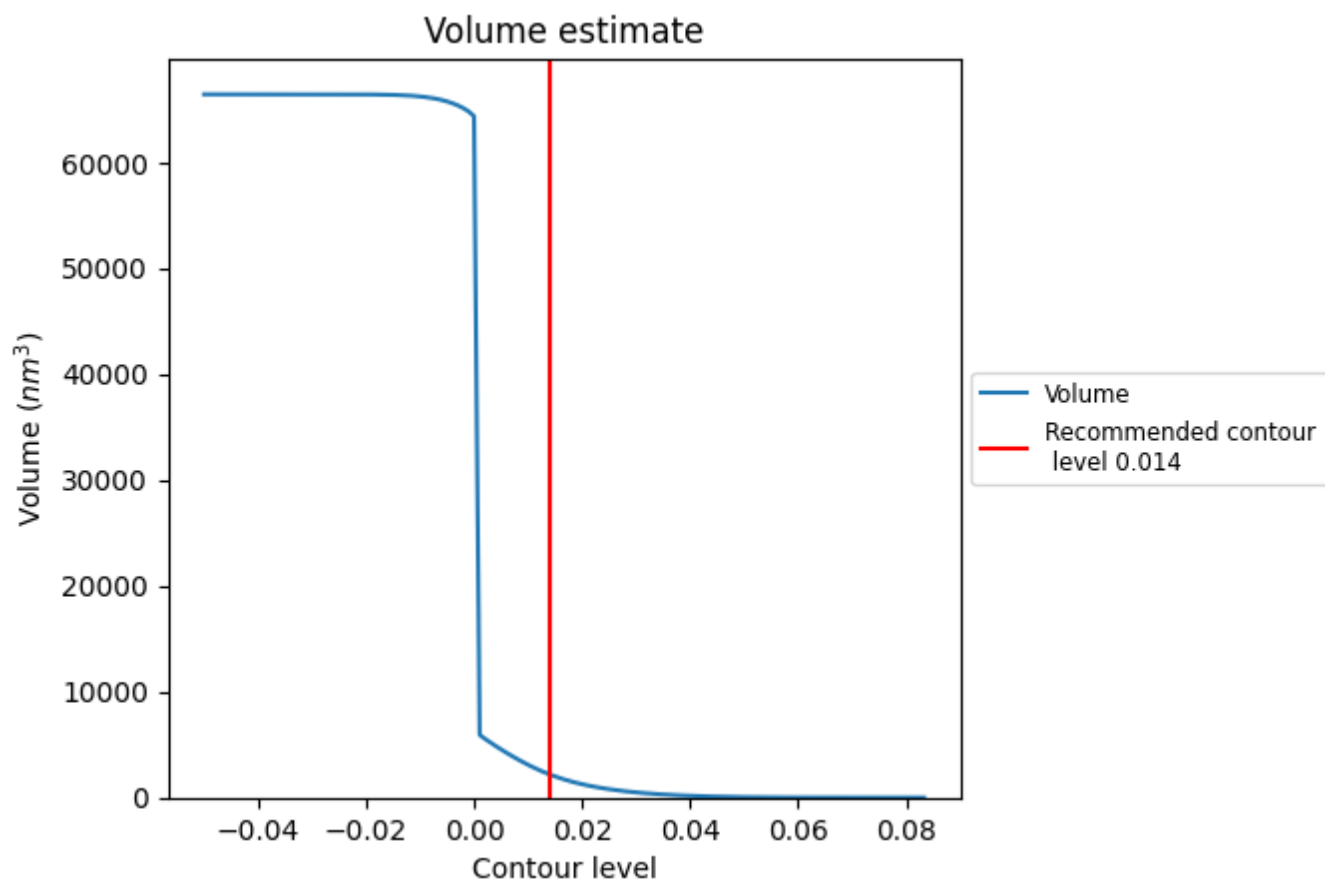
This section contains the results of statistical analysis of the map.

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.

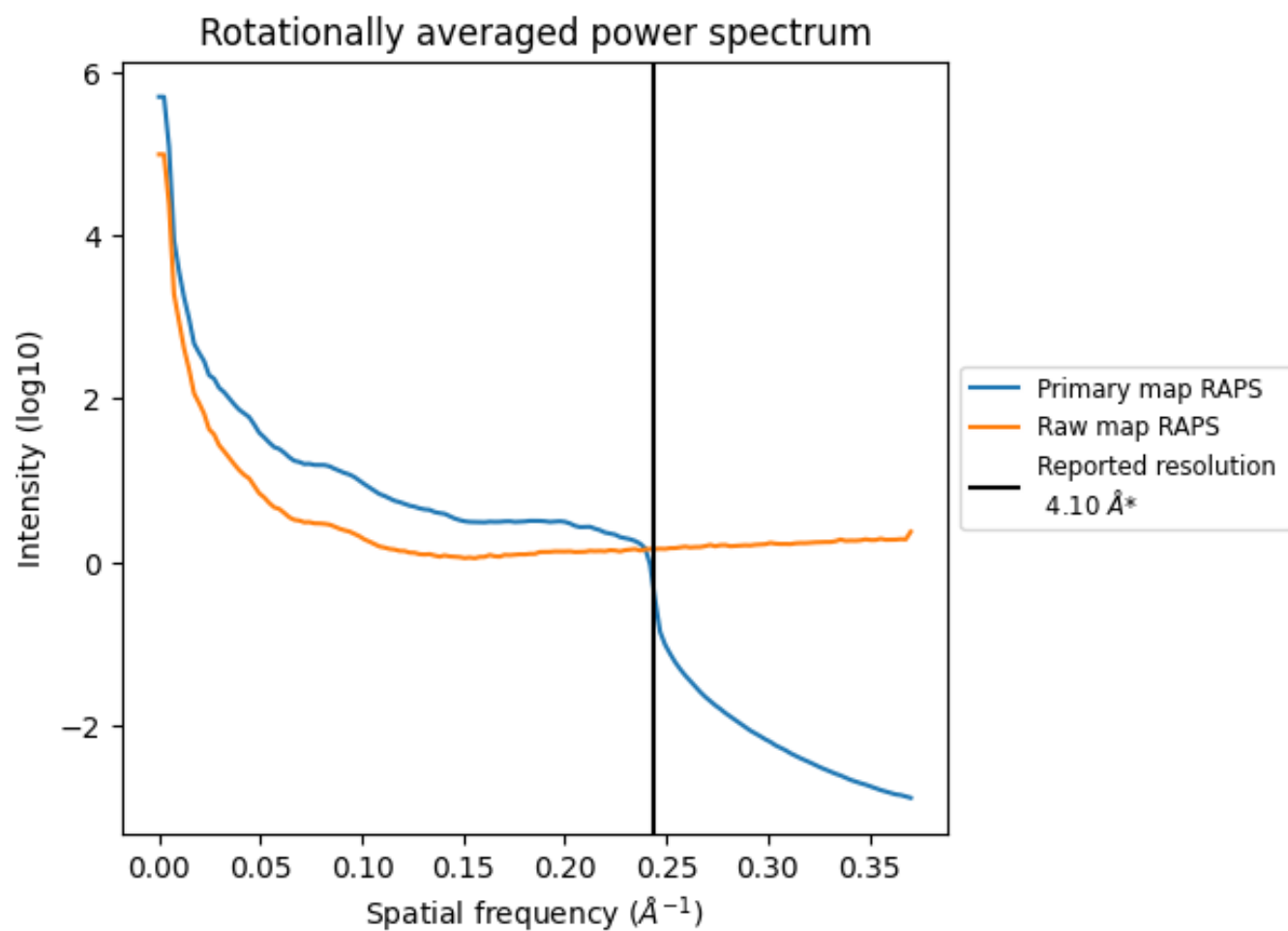
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2180 nm³; this corresponds to an approximate mass of 1970 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 ⓘ

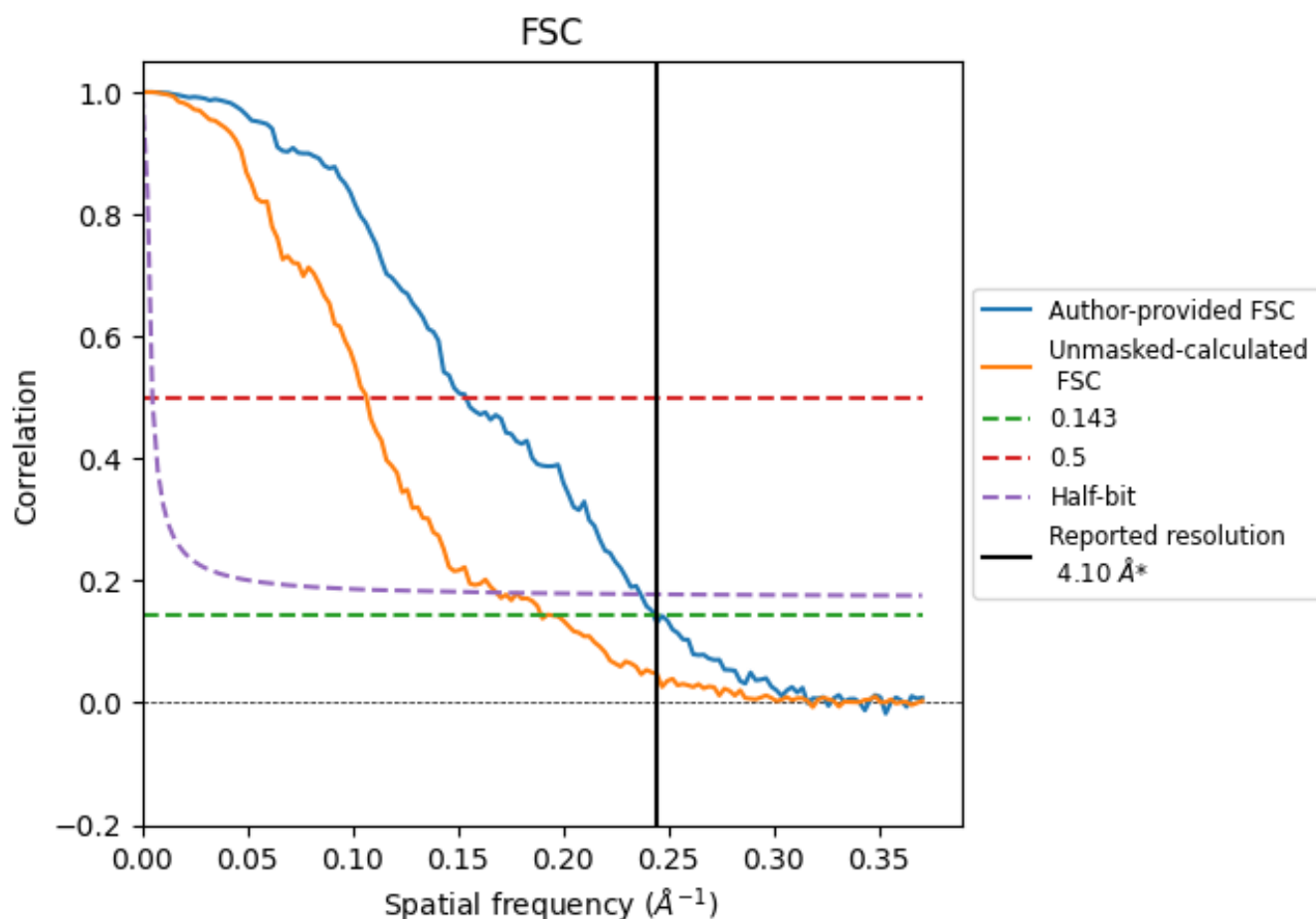


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

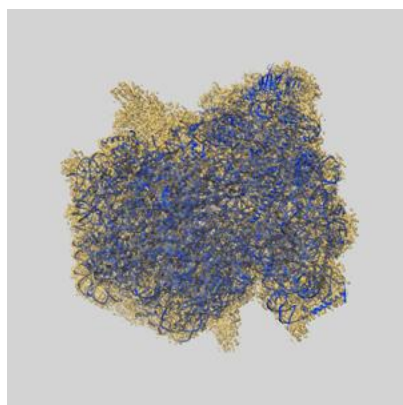
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	6.51	4.22
Unmasked-calculated*	5.28	9.40	5.94

*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 5.28 differs from the reported value 4.1 by more than 10 %

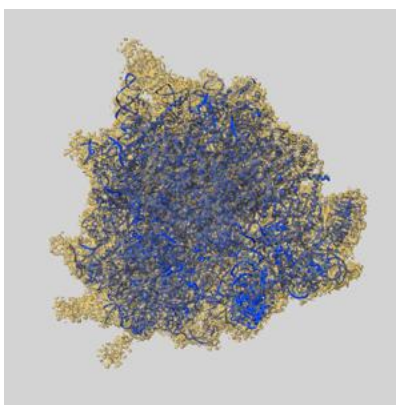
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12632 and PDB model 7NWH. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

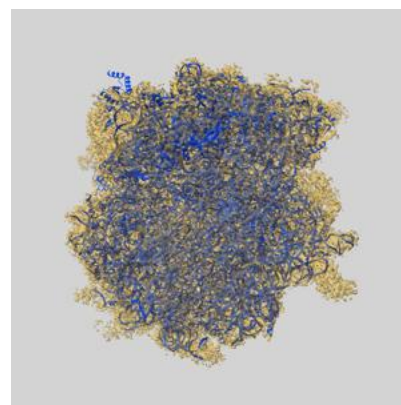
9.1 Map-model overlay [i](#)



X



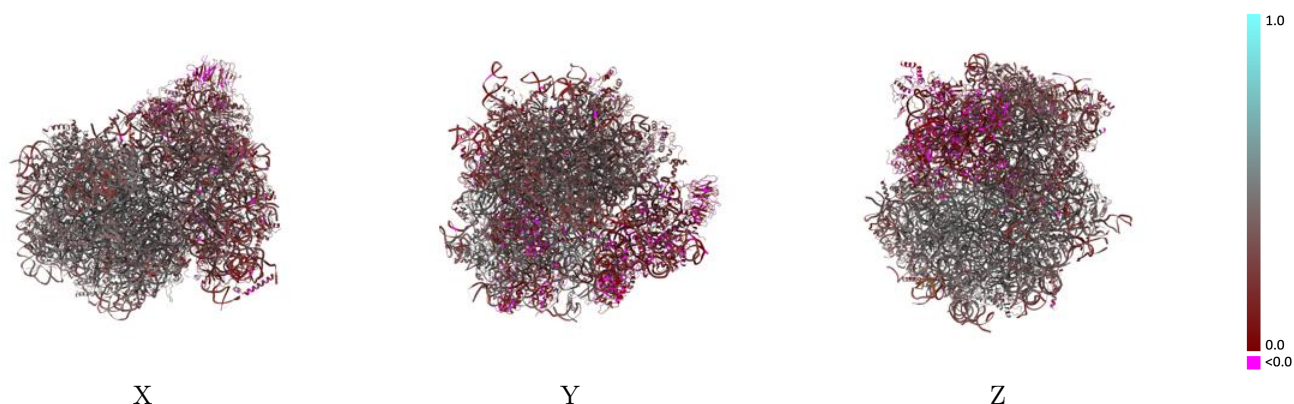
Y



Z

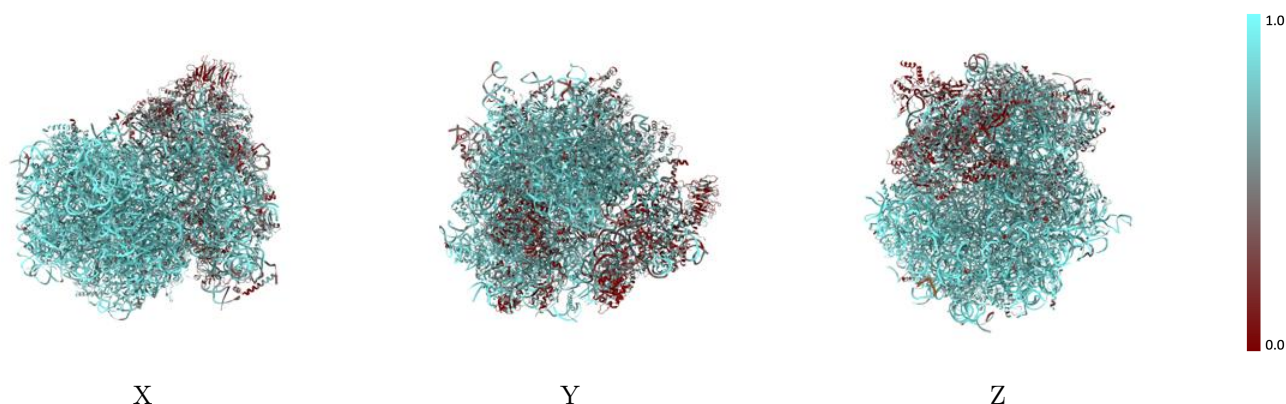
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



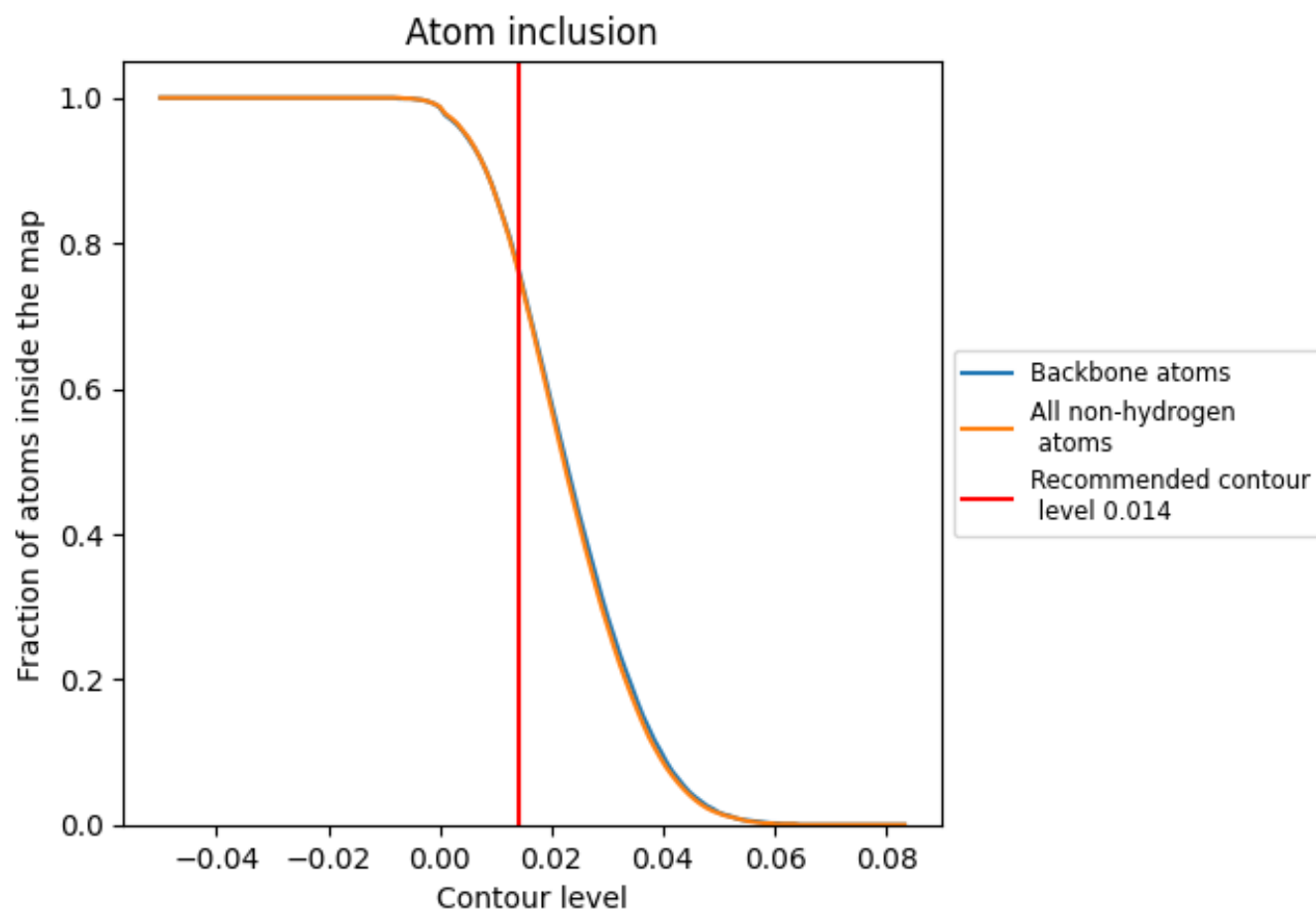
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.3480
5	 0.9280	 0.3970
7	 0.9630	 0.4130
8	 0.9480	 0.4100
9	 0.7790	 0.2790
A	 0.8120	 0.4540
AA	 0.6060	 0.3260
B	 0.8010	 0.4370
BB	 0.5570	 0.2980
C	 0.8140	 0.4440
CC	 0.6570	 0.3580
D	 0.7990	 0.3880
DD	 0.3700	 0.2000
E	 0.8020	 0.4100
EE	 0.6000	 0.3260
F	 0.8010	 0.4240
FF	 0.3400	 0.1590
G	 0.7540	 0.3880
GG	 0.5020	 0.2420
H	 0.7740	 0.4150
HH	 0.4890	 0.2780
I	 0.8050	 0.4320
II	 0.5820	 0.3030
J	 0.7540	 0.3480
JJ	 0.6530	 0.3220
KK	 0.3990	 0.1850
L	 0.7750	 0.4060
LL	 0.6600	 0.3600
M	 0.8090	 0.4130
MM	 0.0810	 0.0870
N	 0.8450	 0.4470
NN	 0.6130	 0.3210
O	 0.8190	 0.4320
OO	 0.5510	 0.2680
P	 0.8260	 0.4440



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Chain	Atom inclusion	Q-score
PP	 0.4930	 0.1590
Q	 0.8020	 0.4370
QQ	 0.4360	 0.1810
R	 0.7500	 0.3910
RR	 0.4000	 0.2170
S	 0.8210	 0.4420
SS	 0.4810	 0.1830
T	 0.7980	 0.4440
TT	 0.4500	 0.1640
U	 0.7380	 0.3510
UU	 0.4080	 0.1710
V	 0.7720	 0.4530
VV	 0.6000	 0.3340
W	 0.5700	 0.3100
WW	 0.6480	 0.3580
X	 0.8060	 0.4180
XX	 0.7280	 0.3910
Y	 0.8090	 0.4200
YY	 0.5400	 0.2790
Z	 0.7930	 0.3830
ZZ	 0.3690	 0.1690
a	 0.8220	 0.4490
aa	 0.6620	 0.3430
b	 0.7220	 0.3870
bb	 0.5540	 0.3160
c	 0.6940	 0.3420
cc	 0.2750	 0.1690
d	 0.7780	 0.4200
dd	 0.4500	 0.1990
e	 0.8270	 0.4580
ee	 0.5920	 0.3220
f	 0.8470	 0.4600
ff	 0.3460	 0.2120
g	 0.7800	 0.4170
gg	 0.2730	 0.1370
h	 0.8020	 0.3970
hh	 0.2130	 0.1730
i	 0.7710	 0.3880
ii	 0.2780	 0.1660
j	 0.8740	 0.4480
jj	 0.2420	 0.1590
k	 0.7400	 0.3890

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Chain	Atom inclusion	Q-score
l	 0.8360	 0.4370
m	 0.8150	 0.4180
n	 0.6280	 0.3300
o	 0.7790	 0.4390
p	 0.7940	 0.4420
r	 0.8020	 0.4280
s	 0.3250	 0.1490
t	 0.3160	 0.1860