wwPDB EM Validation Summary Report (i)

Mar 15, 2026 – 02:10 AM UTC

PDB ID	:	8UR0 / pdb_00008ur0
EMDB ID	:	EMD-42479
Title	:	Escherichia coli transcription-translation coupled complex class B (TTC-B) containing RfaH bound to ops signal, NusA, mRNA with a 24 nt long spacer, and fMet-tRNAs in E-site and P-site of the ribosome
Authors	:	Molodtsov, V.; Wang, C.; Ebright, R.H.
Deposited on	:	2023-10-25
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

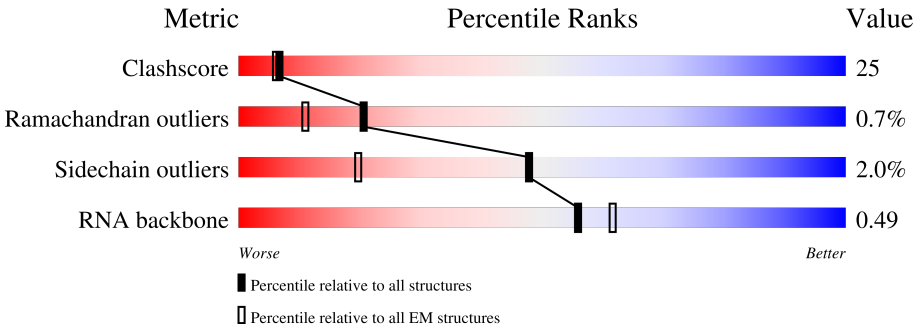
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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

Mol	Chain	Length	Quality of chain
1	0	103	36% 59% 41%
2	1	110	20% 59% 41%
3	2	100	5% 51% 42% · 6%
4	3	104	32% 65% 34% ·
5	4	94	23% 44% 56%
6	5	38	37% 55% 37% 8%
7	6	38	26% 63% 29% 8%

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Mol	Chain	Length	Quality of chain
8	7	41	12% 32% 49% 7% 10%
9	9	165	10% 20% 66% 10%
10	A	76	7% 16% 46% 38%
10	B	76	36% 17% 47% 36%
11	AA	1342	30% 81% 17%
12	AB	162	49% 20% 60% 15%
13	AC	329	40% 61% 6% 33%
13	AD	329	65% 75% 16% 9%
14	AE	1407	36% 78% 16% 5%
15	AF	91	47% 76% 14% 10%
16	AG	495	65% 31% 44% 22%
17	C	75	11% 35% 52% 12%
18	D	1542	12% 50% 43% 7%
19	E	87	30% 47% 52%
20	F	71	21% 41% 58%
21	G	241	12% 49% 42% 7%
22	H	557	11% 25% 20% 54%
23	I	233	5% 47% 41% 11%
24	J	206	67% 32%
25	K	167	10% 45% 46% 7%
26	L	135	34% 27% 47% 23%
27	M	179	34% 41% 42% 16%
28	N	130	12% 52% 48%
29	O	130	25% 49% 45%
30	P	103	47% 48%

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Mol	Chain	Length	Quality of chain
31	Q	129	19% 43% 45% 9%
32	R	124	18% 57% 40%
33	S	101	53% 46%
34	T	89	43% 42% 56%
35	U	82	5% 51% 49%
36	V	84	44% 42% 54% 5%
37	W	92	29% 54% 34% 10%
38	X	118	42% 57% 39%
39	Y	142	9% 33% 65%
40	Z	121	10% 9% 16% 75%
41	a	2904	14% 51% 42% 7%
42	b	85	24% 59% 31% 11%
43	c	78	42% 67% 32%
44	d	120	14% 64% 31% 5%
45	e	63	38% 46% 51%
46	f	59	25% 51% 47%
47	g	70	26% 40% 53% 6%
48	h	273	16% 63% 36%
49	i	57	42% 54% 44%
50	j	209	7% 56% 44%
51	k	55	24% 47% 47% 5%
52	l	201	32% 60% 40%
53	m	46	13% 57% 43%
54	n	179	22% 43% 55%
55	o	65	11% 58% 35% 5%

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Mol	Chain	Length	Quality of chain
56	p	177	20% 68% 31%
57	q	38	61% 39%
58	r	149	37% 68% 32%
59	s	142	6% 56% 43%
60	t	123	6% 46% 54%
61	u	144	26% 62% 37%
62	v	136	5% 47% 51%
63	w	127	9% 46% 45% 6%
64	x	117	39% 62% 37%
65	y	115	12% 63% 37%
66	z	118	12% 57% 42%

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
68	ZN	AE	1502	-	-	X	-

2 Entry composition (i)

There are 68 unique types of molecules in this entry. The entry contains 280292 atoms, of which 98639 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 Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA ops.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	35	Total	C	N	O	P	0	0
			726	342	141	208	35		

- Molecule 7 is a DNA chain called T DNA ops.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	35	Total	C	N	O	P	0	0
			703	336	117	215	35		

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	37	Total	C	N	O	P	0	0
			772	345	110	280	37		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site fMet-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2434	723	814	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 12 is a protein called Transcription antitermination protein RfaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	161	Total	C	N	O	S	0	0
			1286	828	222	232	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	299	Total	C	N	O	S	0	0
			2078	1287	378	407	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	1337	Total	C	N	O	S	0	0
			10404	6535	1856	1963	50		

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AG	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

- Molecule 18 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	D	1524	Total	C	H	N	O	P	0	0
			49126	14585	16423	6003	10591	1524		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 22 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 23 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 24 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 25 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 26 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 27 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 28 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 29 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 31 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 32 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 33 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 34 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 35 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 36 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 37 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 38 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 39 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 41 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 48 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	k	52	Total	C	H	N	O	0	0
			890	275	464	78	73		

- Molecule 52 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 58 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 59 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 60 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 61 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 62 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 63 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 64 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	x	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 65 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 66 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	z	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	AE	1	Total	Mg	0
			1	1	

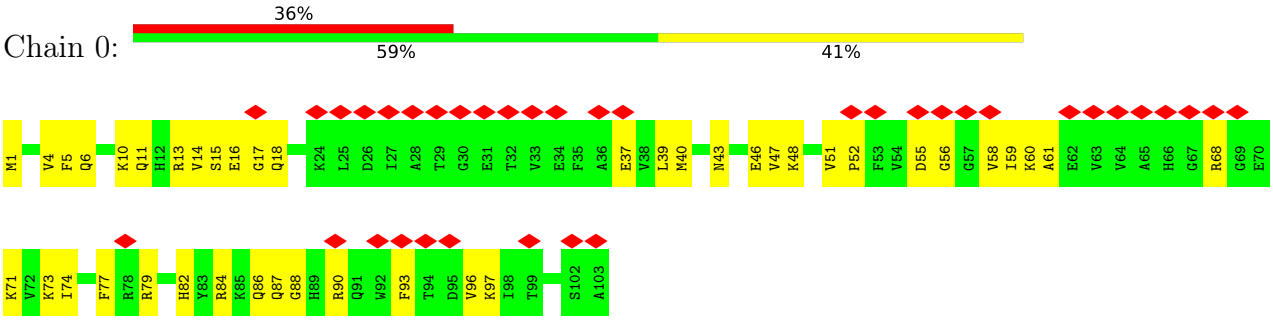
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	AE	2	Total	Zn	0
			2	2	

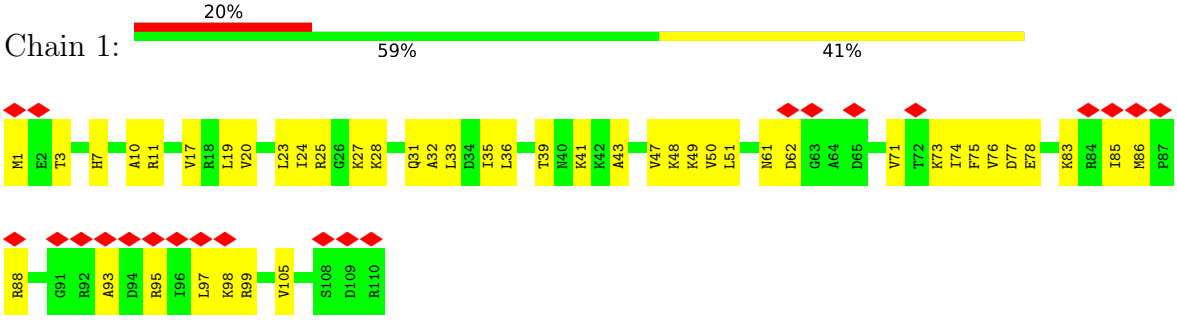
3 Residue-property plots (i)

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.

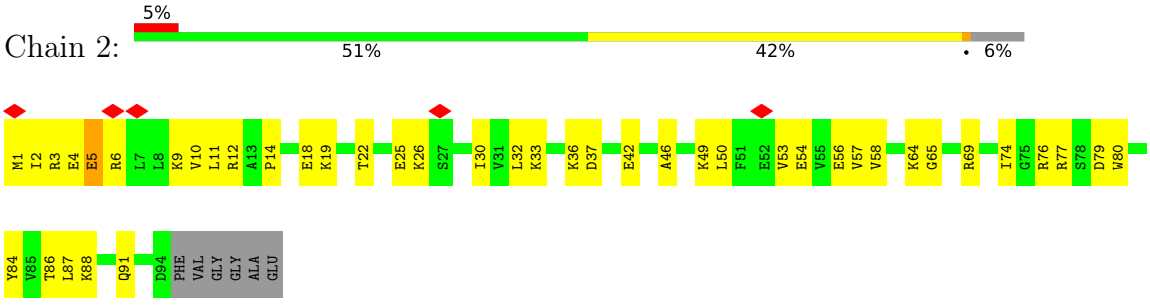
• Molecule 1: Ribosomal protein L21



• Molecule 2: 50S ribosomal protein L22

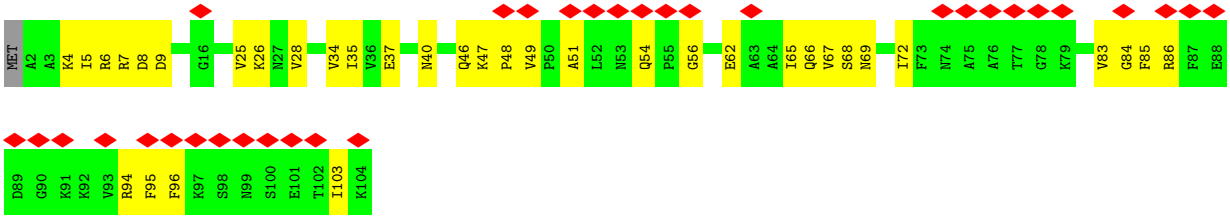


• Molecule 3: 50S ribosomal protein L23

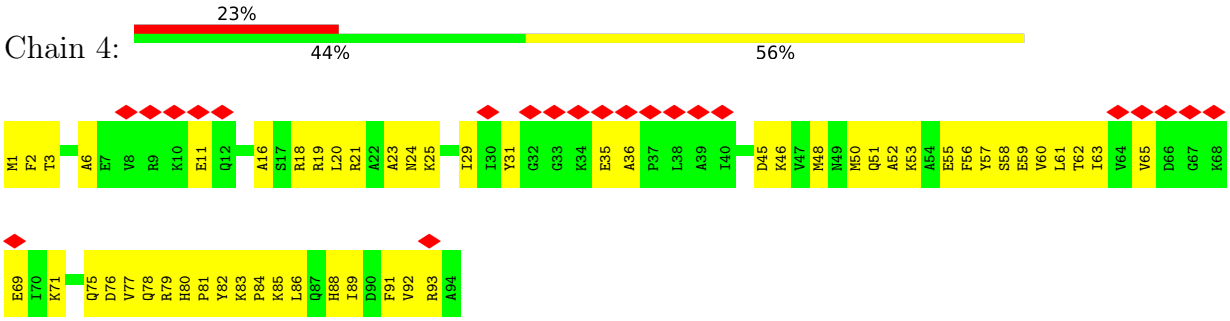


• Molecule 4: 50S ribosomal protein L24

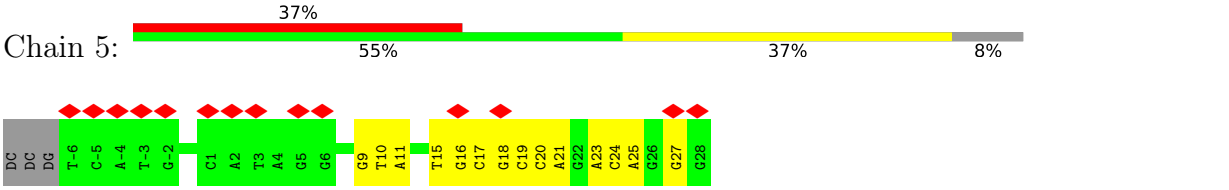




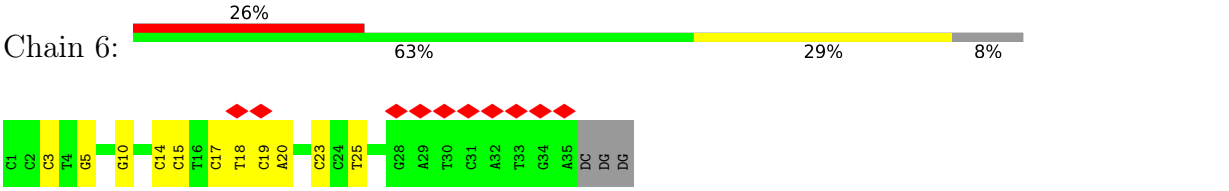
• Molecule 5: 50S ribosomal protein L25



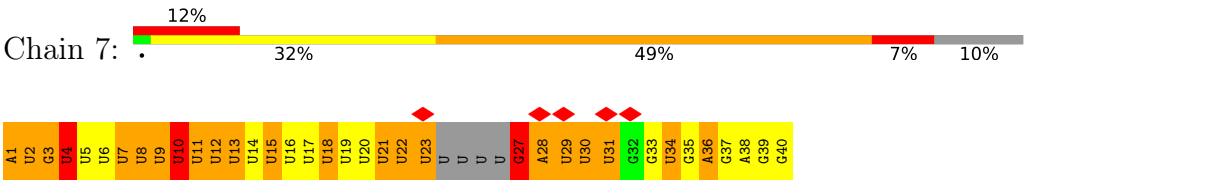
• Molecule 6: NT DNA ops



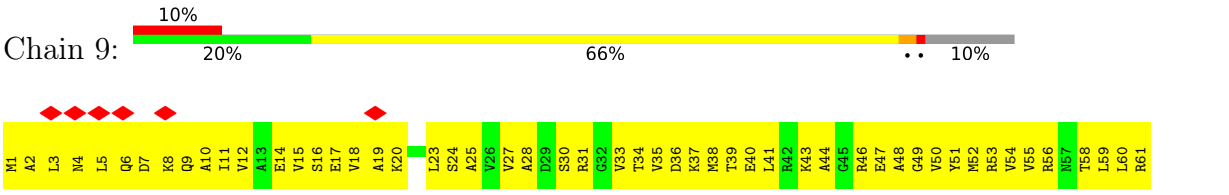
• Molecule 7: T DNA ops

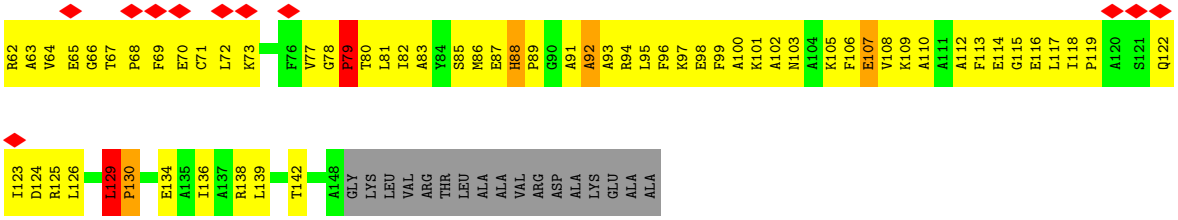


• Molecule 8: mRNA with 24 nt long spacer

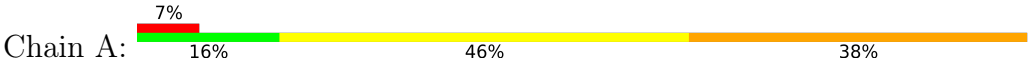


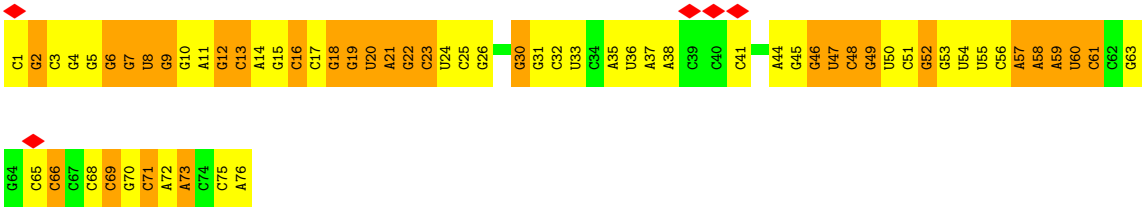
• Molecule 9: 50S ribosomal protein L10



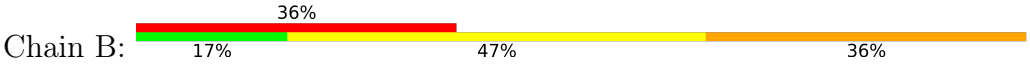


• Molecule 10: E-site and P-site fMet-tRNA



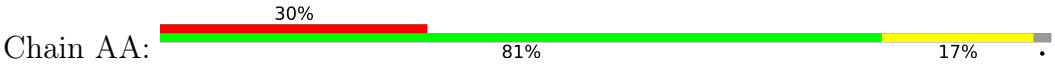


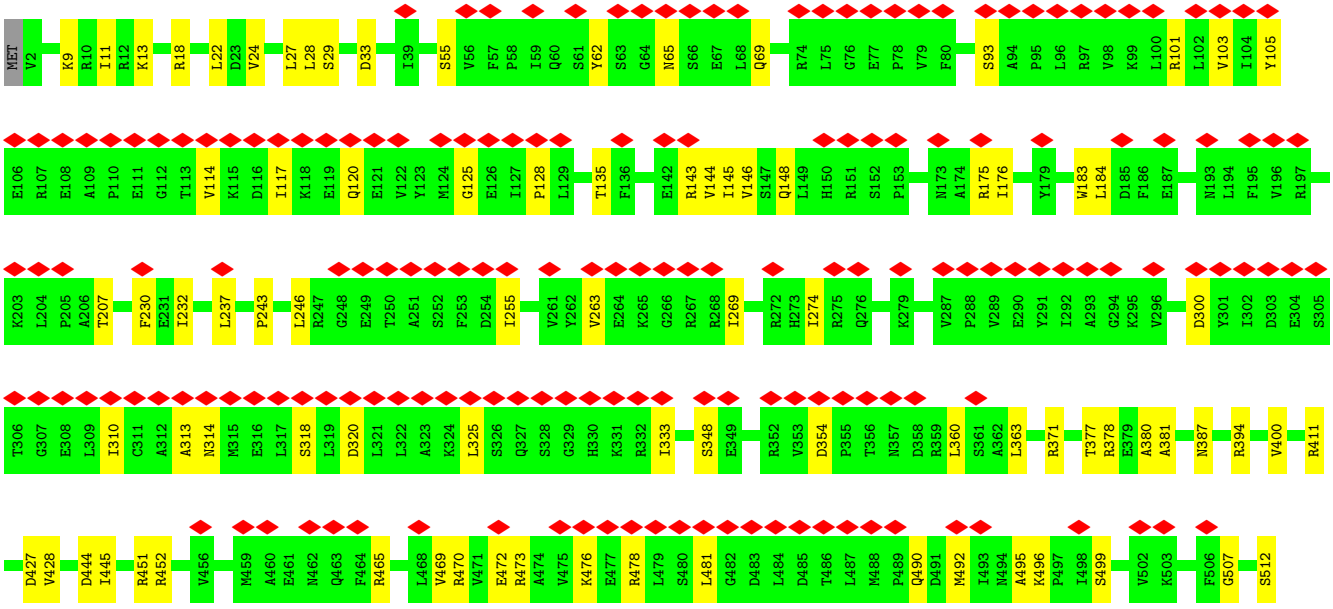
• Molecule 10: E-site and P-site fMet-tRNA

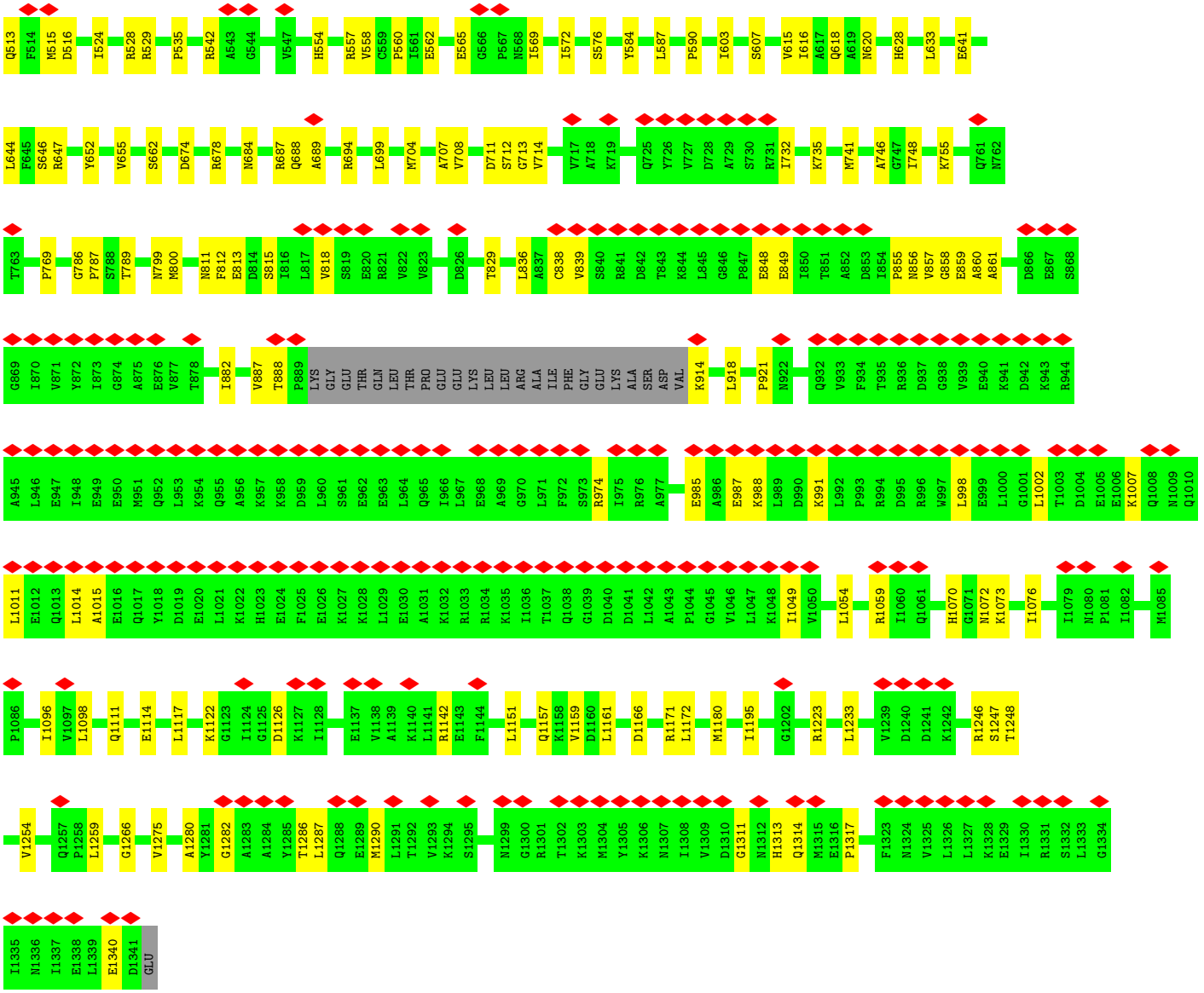




• Molecule 11: DNA-directed RNA polymerase subunit beta

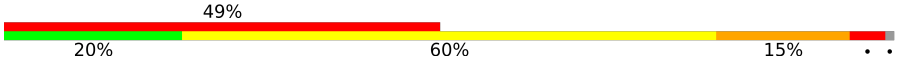


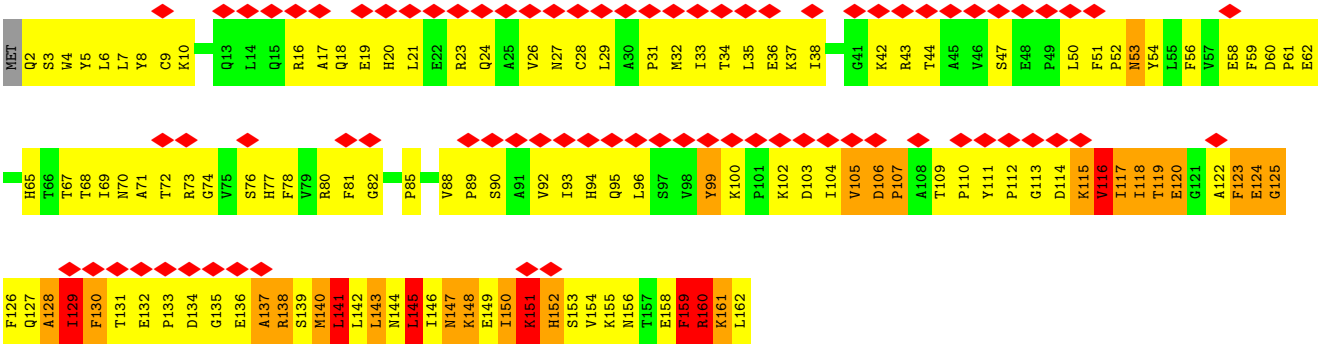




• Molecule 12: Transcription antitermination protein RfaH

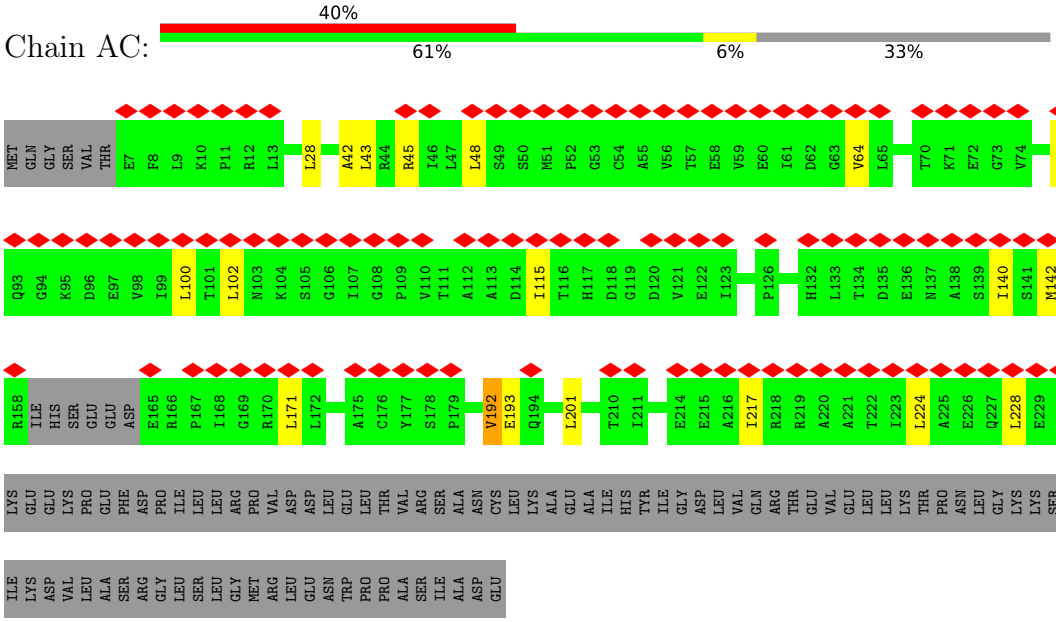
Chain AB:





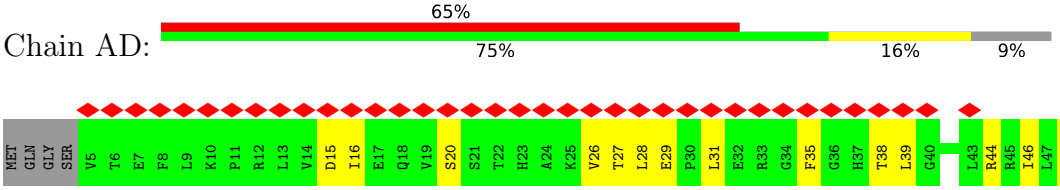
• Molecule 13: DNA-directed RNA polymerase subunit alpha

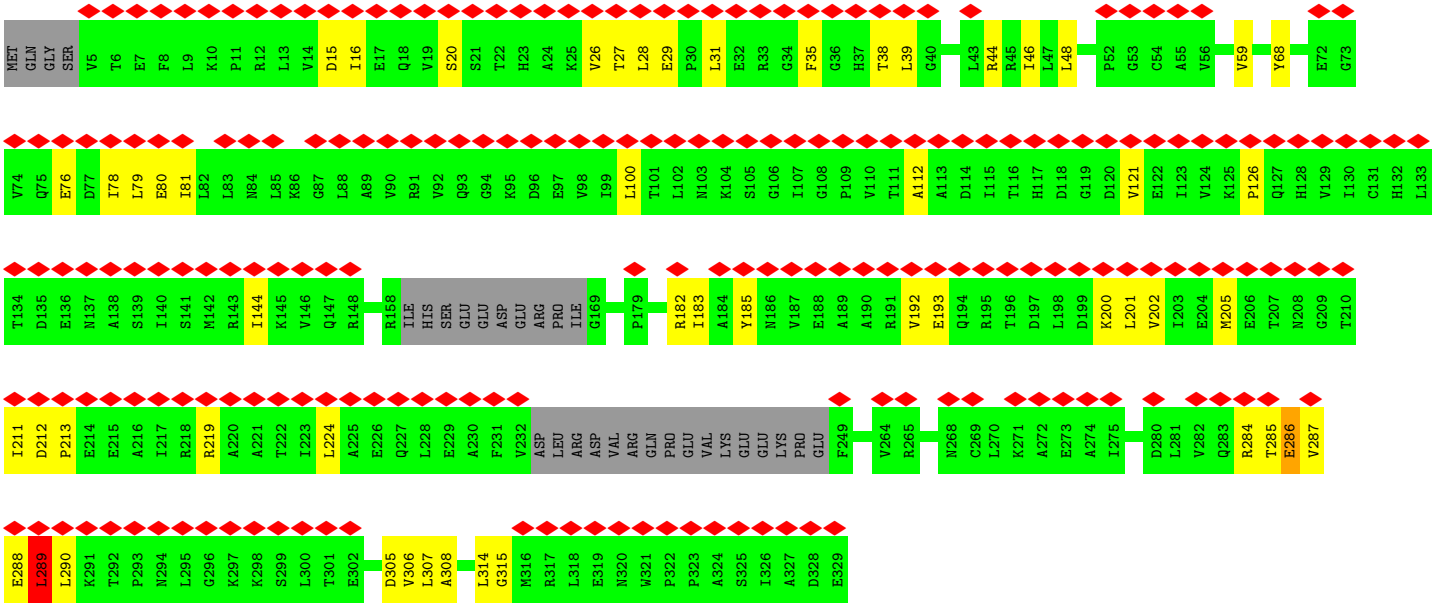
Chain AC:



• Molecule 13: DNA-directed RNA polymerase subunit alpha

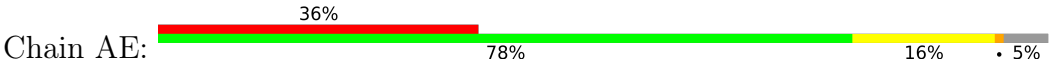
Chain AD:

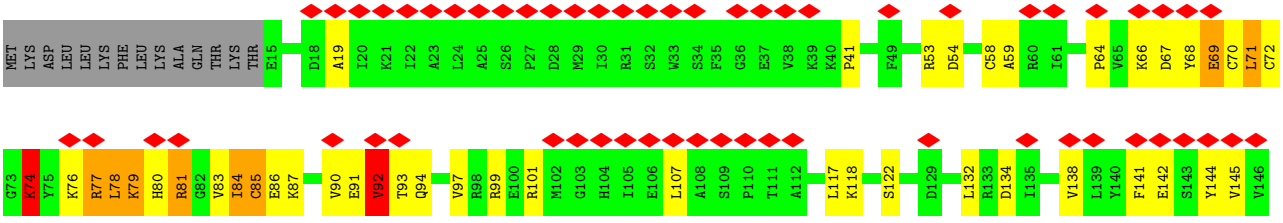


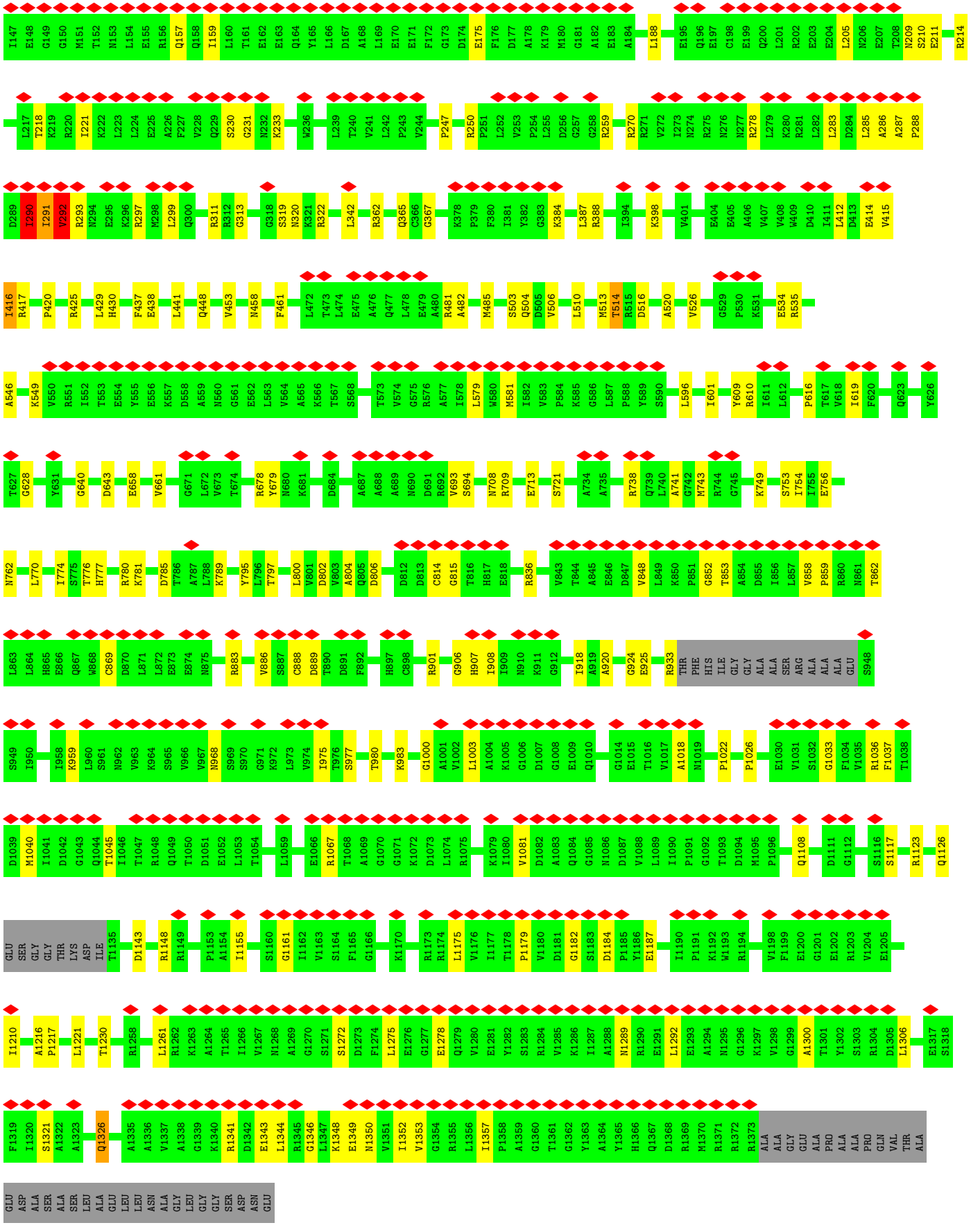


• Molecule 14: DNA-directed RNA polymerase subunit beta'

Chain AE:

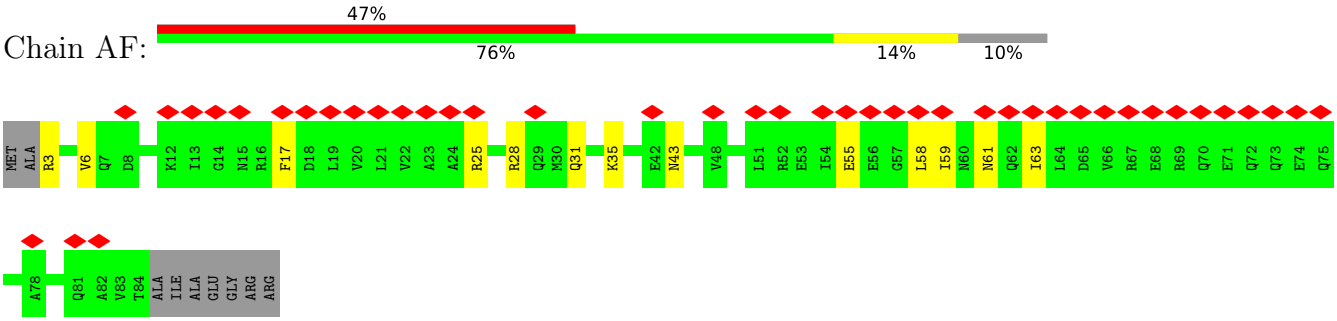





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L217 T218 K219 R220 I221 K222 L223 L224 E225 A226 F227 V228 Q229 S230 G231 N232 K233 W236 L239 T240 V241 L242 P243 V244 P247 R250 P251 L252 V253 P254 L255 D256 G257 G258 R259 R270 R271 V272 I273 N274 R275 N276 N277 R278 L279 K280 R281 L282 L283 D284 L285 A286 A287 P288
D289 I290 I291 V292 R293 N294 E295 K296 R297 M298 L299 Q300 R311 R312 G313 G318 S319 N320 K321 R322 L342 R362 Q365 C366 G367 K378 P379 F380 I381 Y382 G383 K384 L387 R388 I394 K398 V401 E404 E405 A406 V407 V408 W409 D410 I411 L412 D413 E414 V415
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GLU SER GLY GLY THR LYS ASP ILE T1135 D1143 R1148 R1149 P1153 A1154 I1155 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1170 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 I1190 P1191 K1192 W1193 R1194 V1198 F1199 E1200 G1201 E1202 R1203 V1204 E1205
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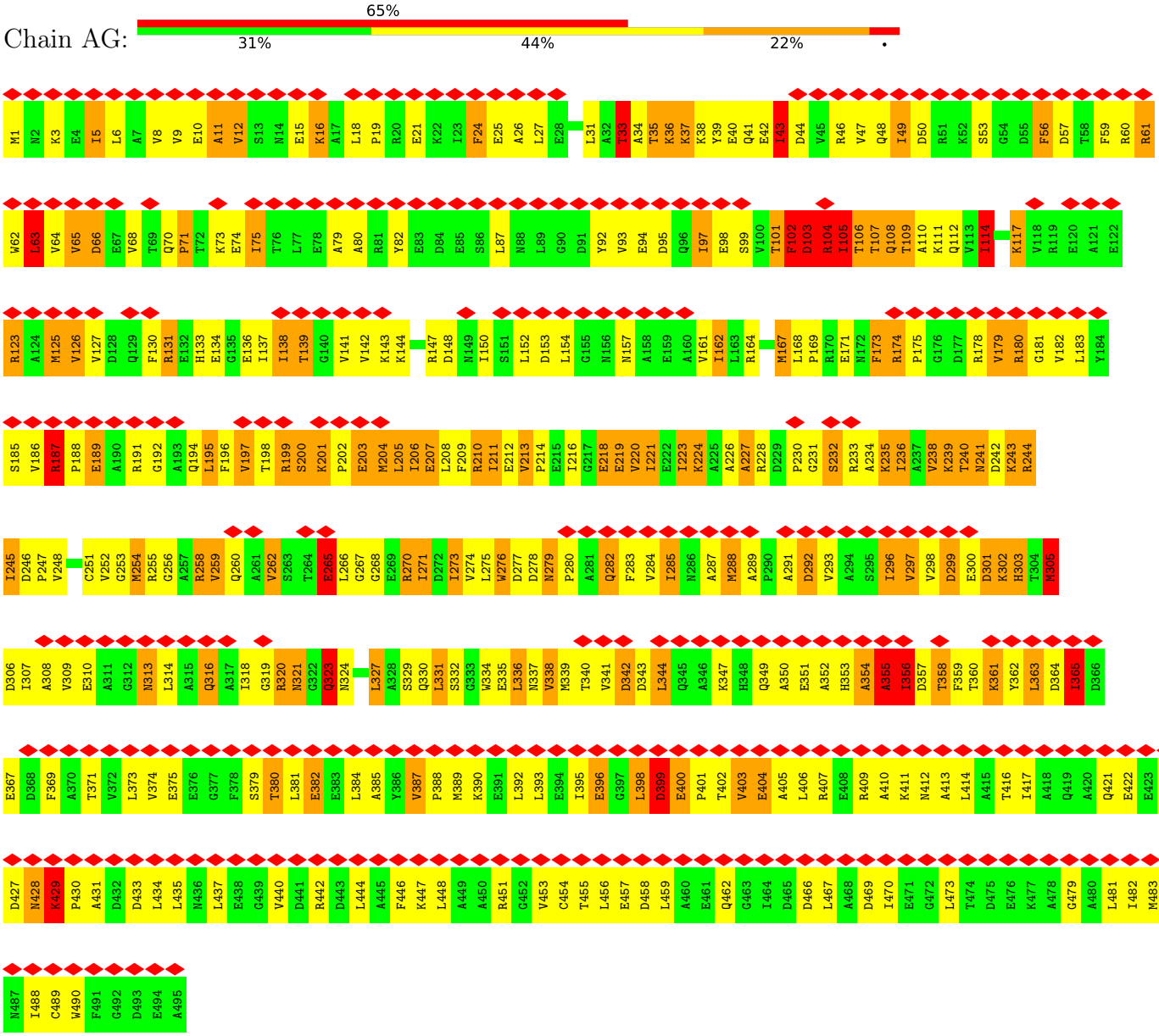
• Molecule 15: DNA-directed RNA polymerase subunit omega

Chain AF:



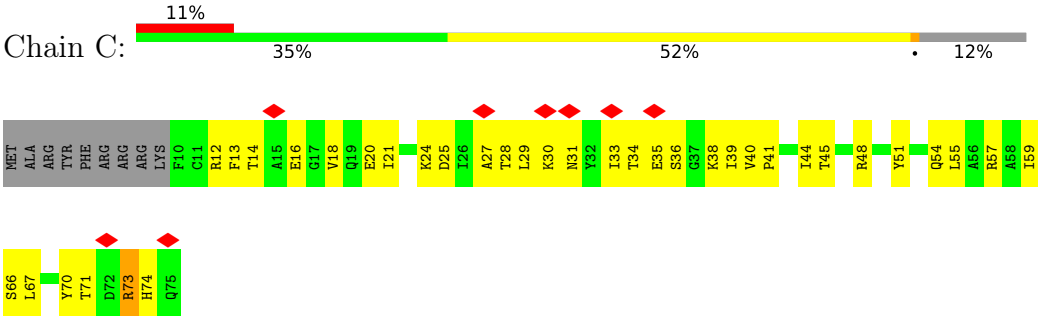
• Molecule 16: Transcription termination/antitermination protein NusA

Chain AG:



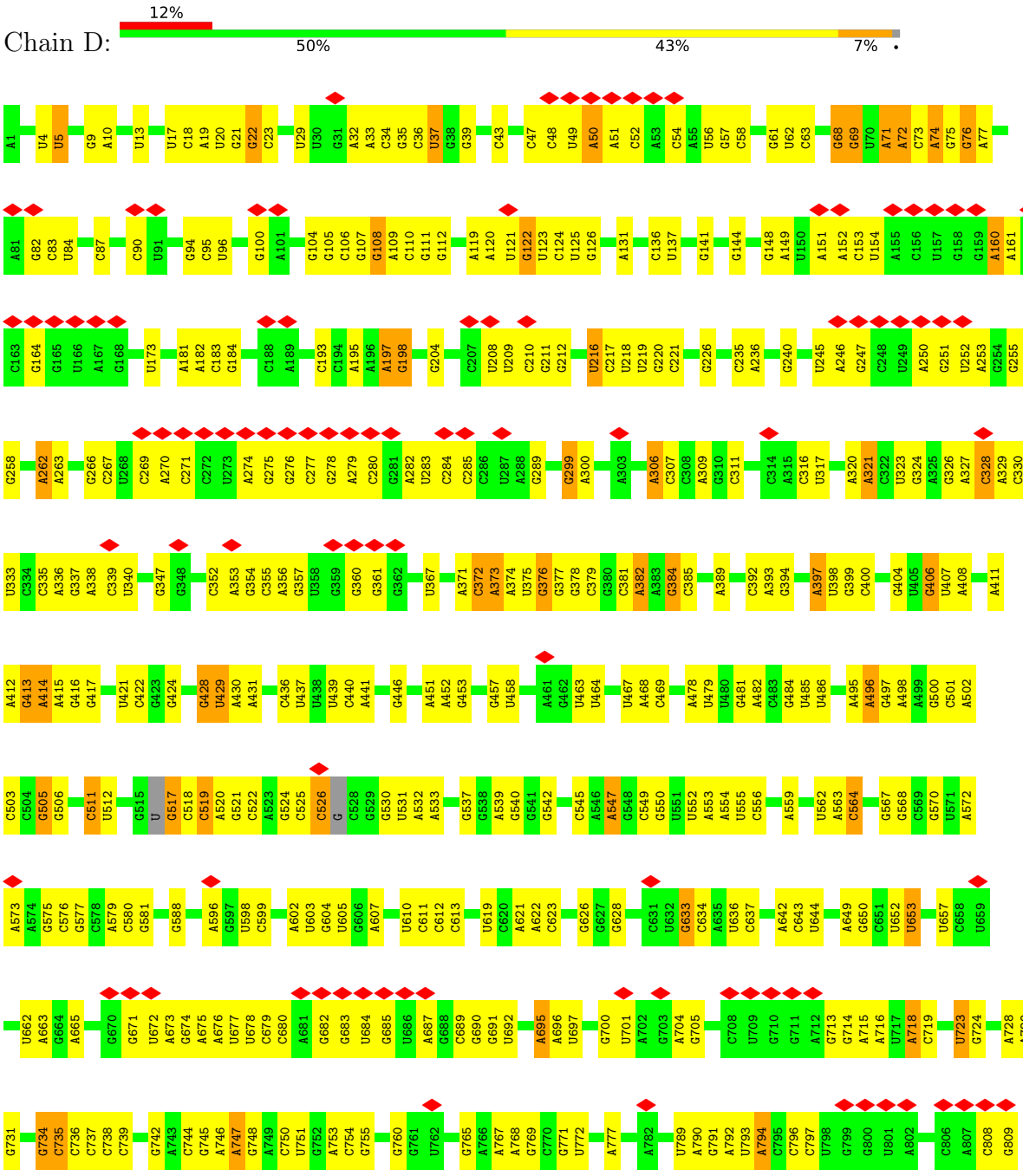
• Molecule 17: 30S ribosomal protein S18

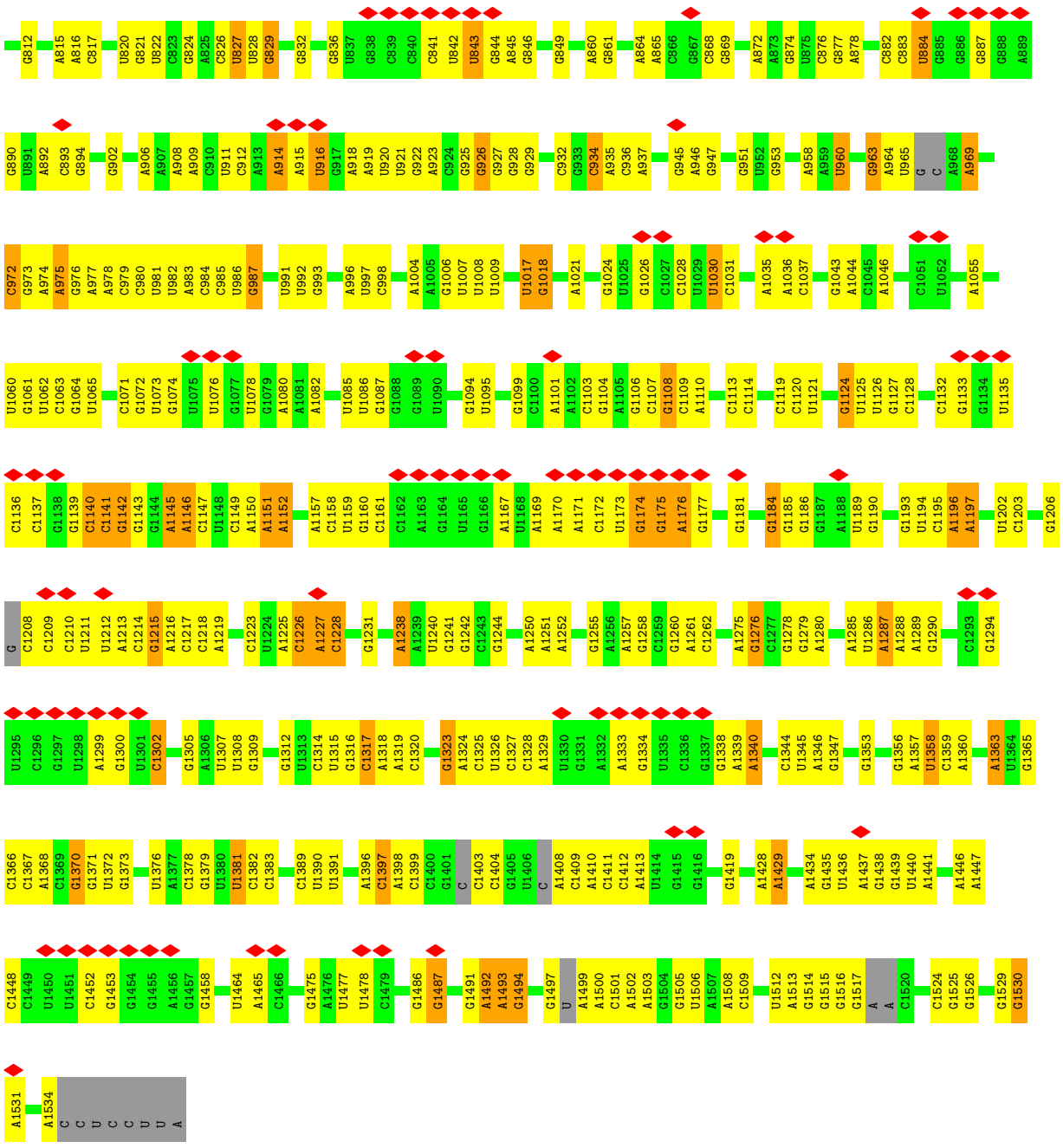
Chain C:



• Molecule 18: 16S rRNA

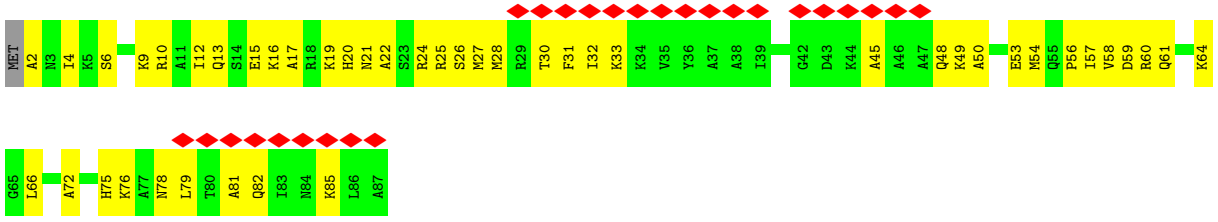
Chain D:





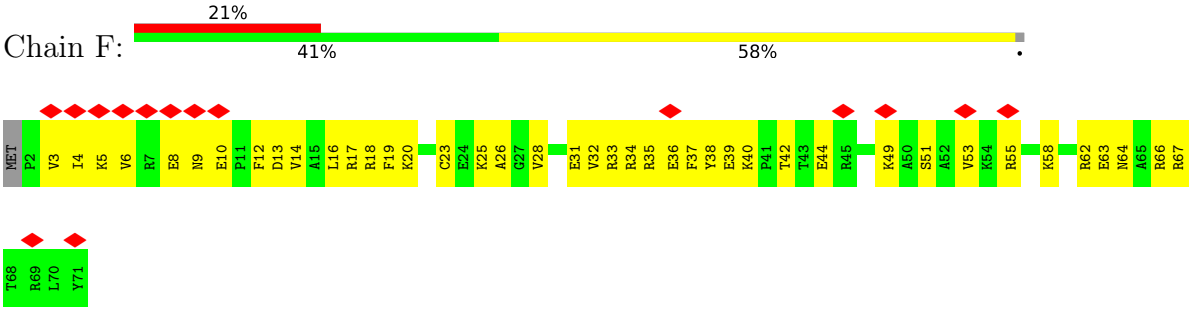
• Molecule 19: 30S ribosomal protein S20





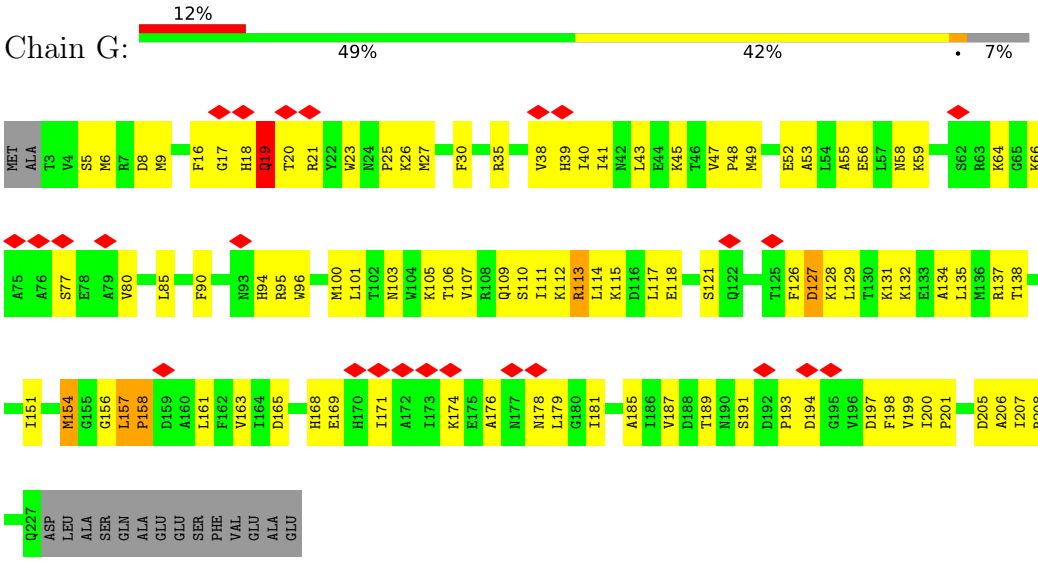
• Molecule 20: 30S ribosomal protein S21

Chain F:



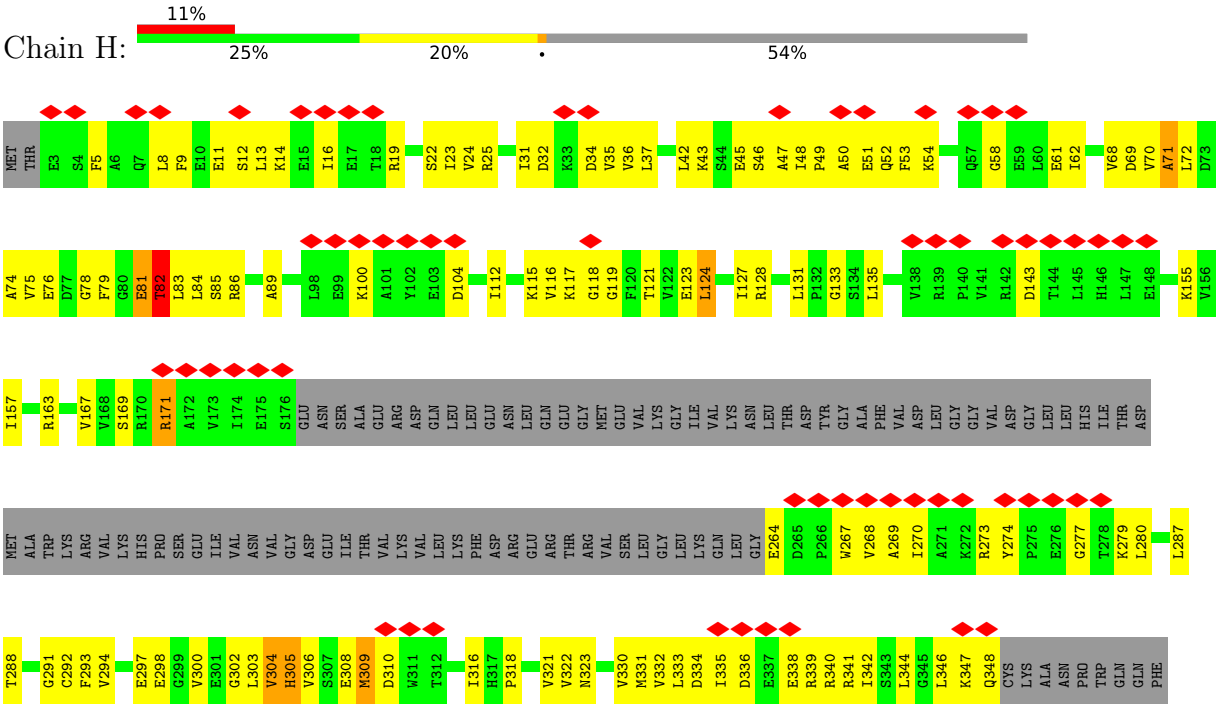
• Molecule 21: 30S ribosomal protein S2

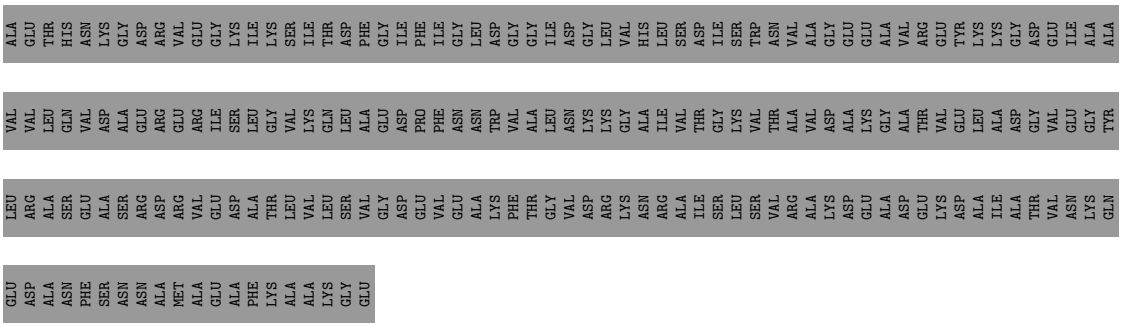
Chain G:



• Molecule 22: 30S ribosomal protein S1

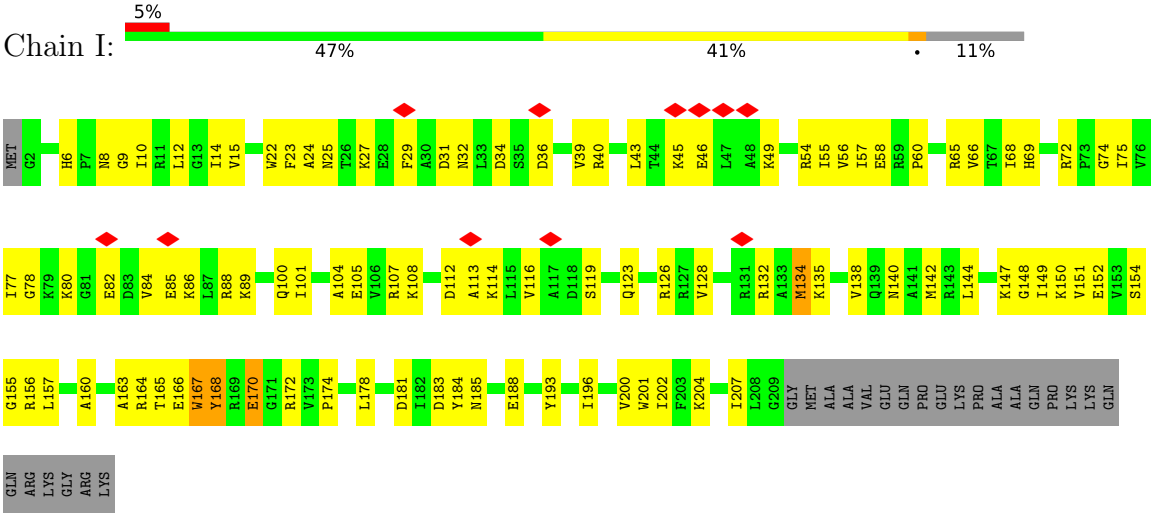
Chain H:





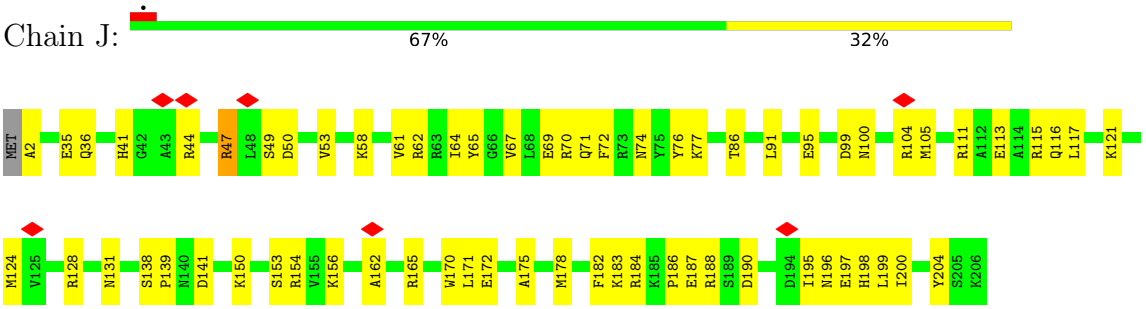
• Molecule 23: 30S ribosomal protein S3

Chain I:



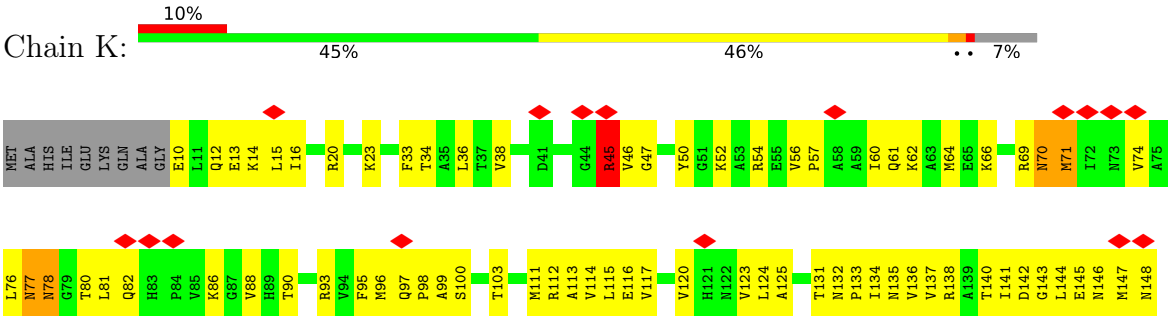
• Molecule 24: 30S ribosomal protein S4

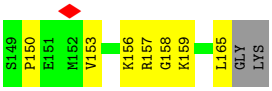
Chain J:



• Molecule 25: 30S ribosomal protein S5

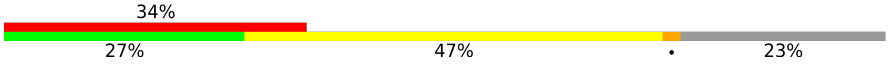
Chain K:

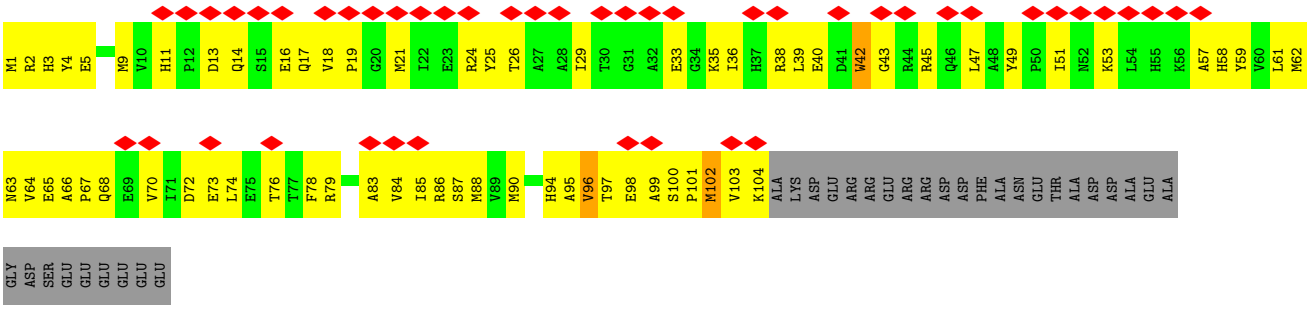




• Molecule 26: 30S ribosomal protein S6

Chain L:

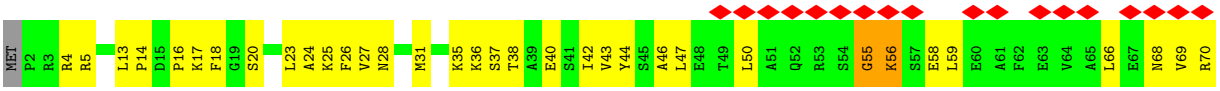




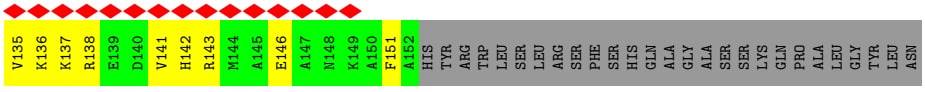
• Molecule 27: 30S ribosomal protein S7

Chain M:





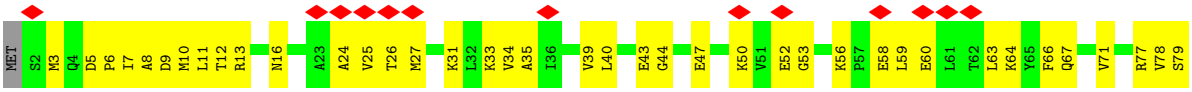


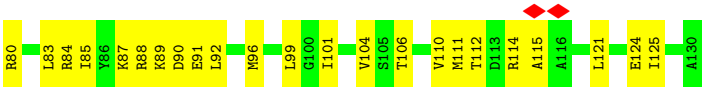


• Molecule 28: 30S ribosomal protein S8

Chain N:



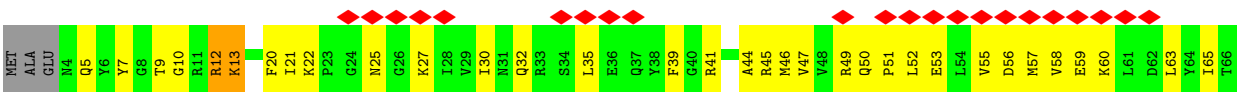


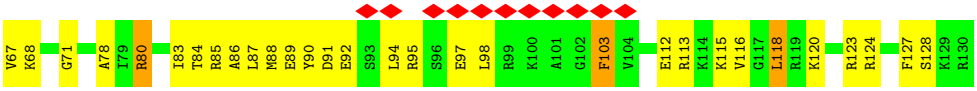


• Molecule 29: 30S ribosomal protein S9

Chain O:



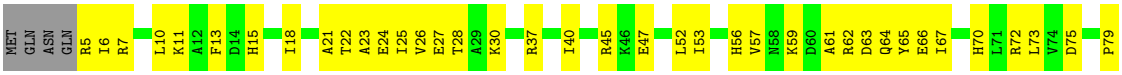


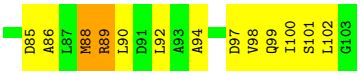


• Molecule 30: 30S ribosomal protein S10

Chain P:



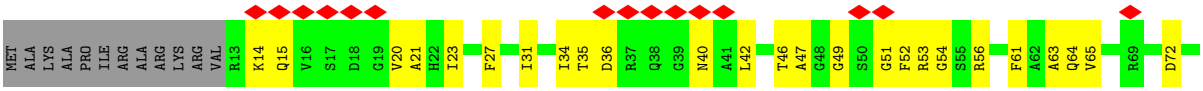


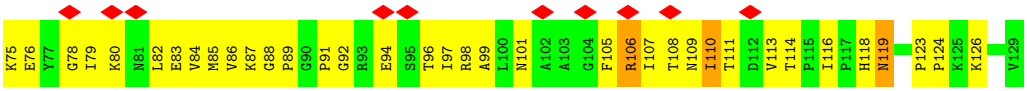


• Molecule 31: 30S ribosomal protein S11

Chain Q:



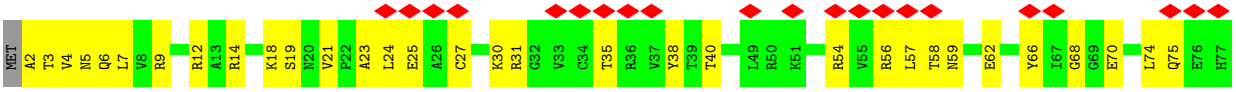


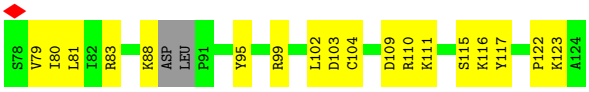


• Molecule 32: 30S ribosomal protein S12

Chain R:



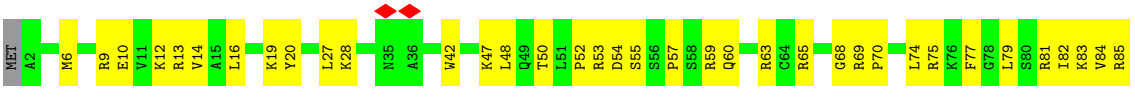


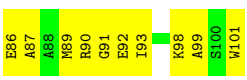


• Molecule 33: 30S ribosomal protein S14

Chain S:



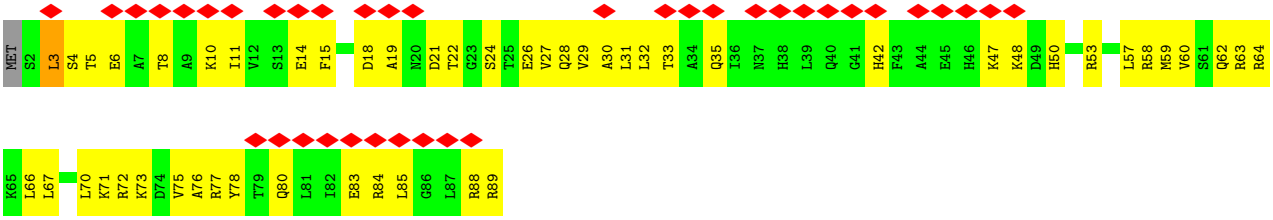




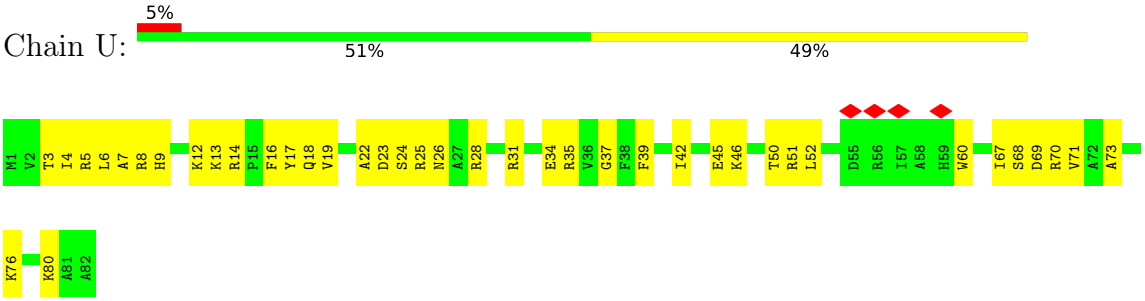
• Molecule 34: 30S ribosomal protein S15

Chain T:

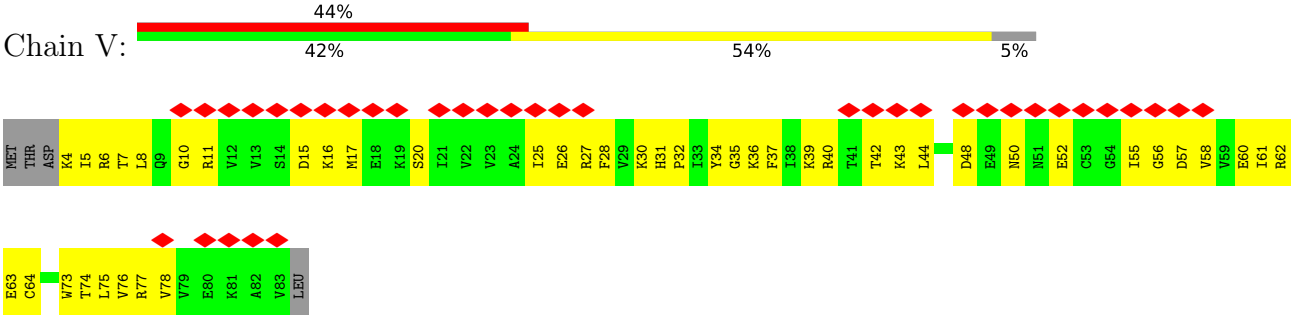




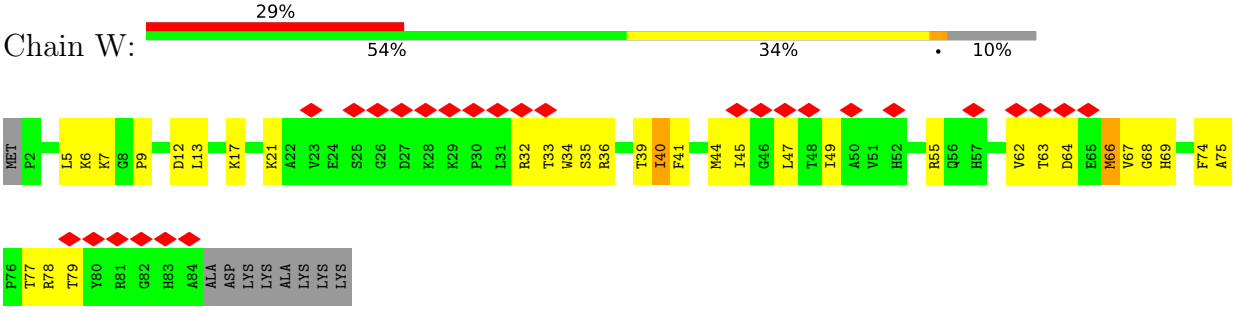
• Molecule 35: 30S ribosomal protein S16



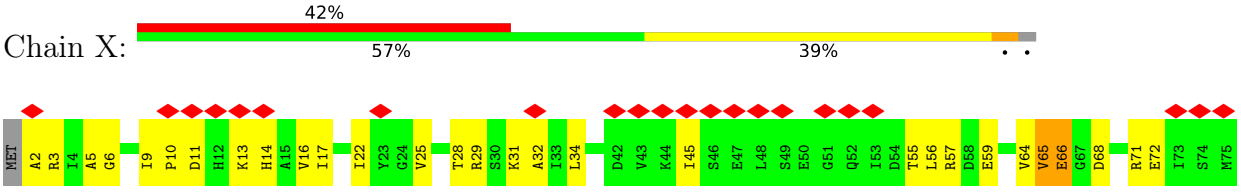
• Molecule 36: 30S ribosomal protein S17

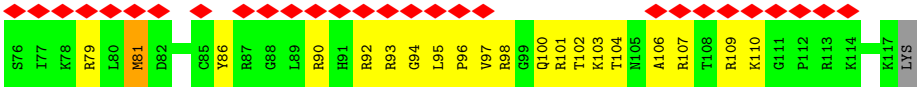


• Molecule 37: 30S ribosomal protein S19



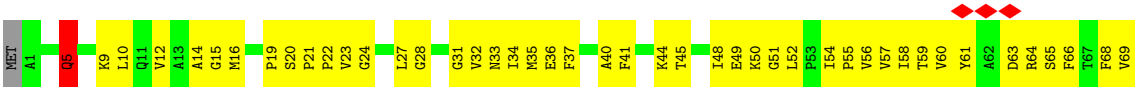
• Molecule 38: 30S ribosomal protein S13

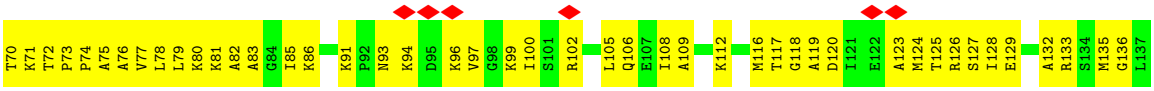


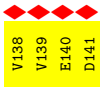


• Molecule 39: 50S ribosomal protein L11



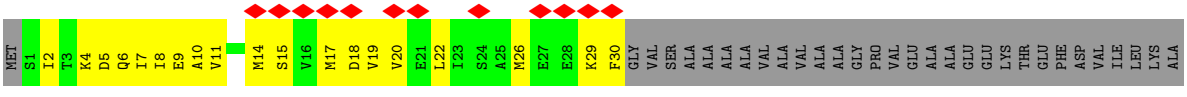






• Molecule 40: 50S ribosomal protein L7/L12



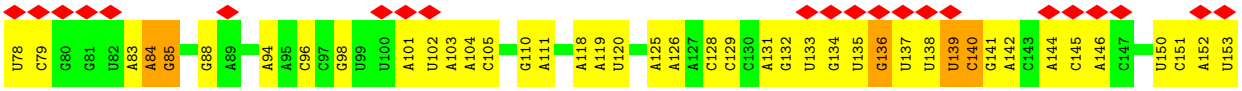


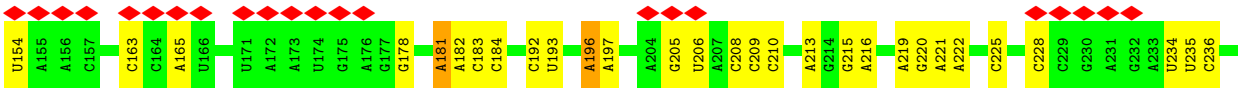


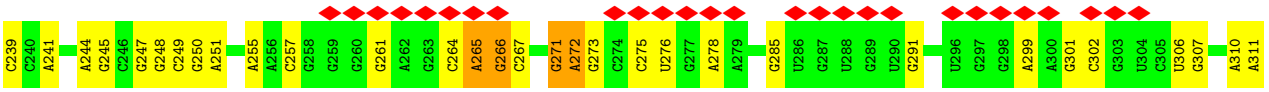
• Molecule 41: 23S rRNA

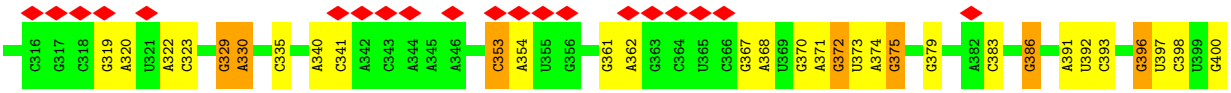


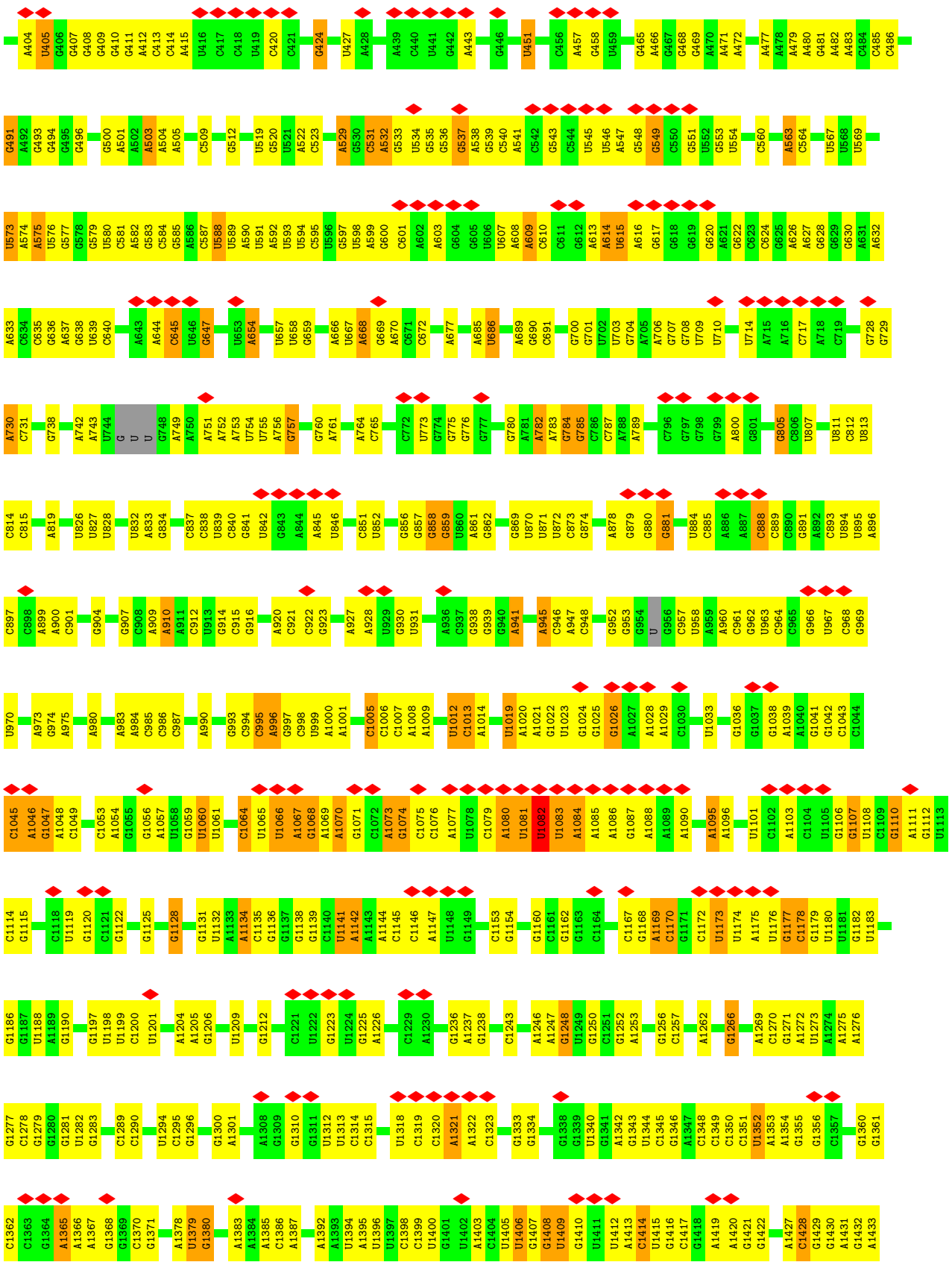


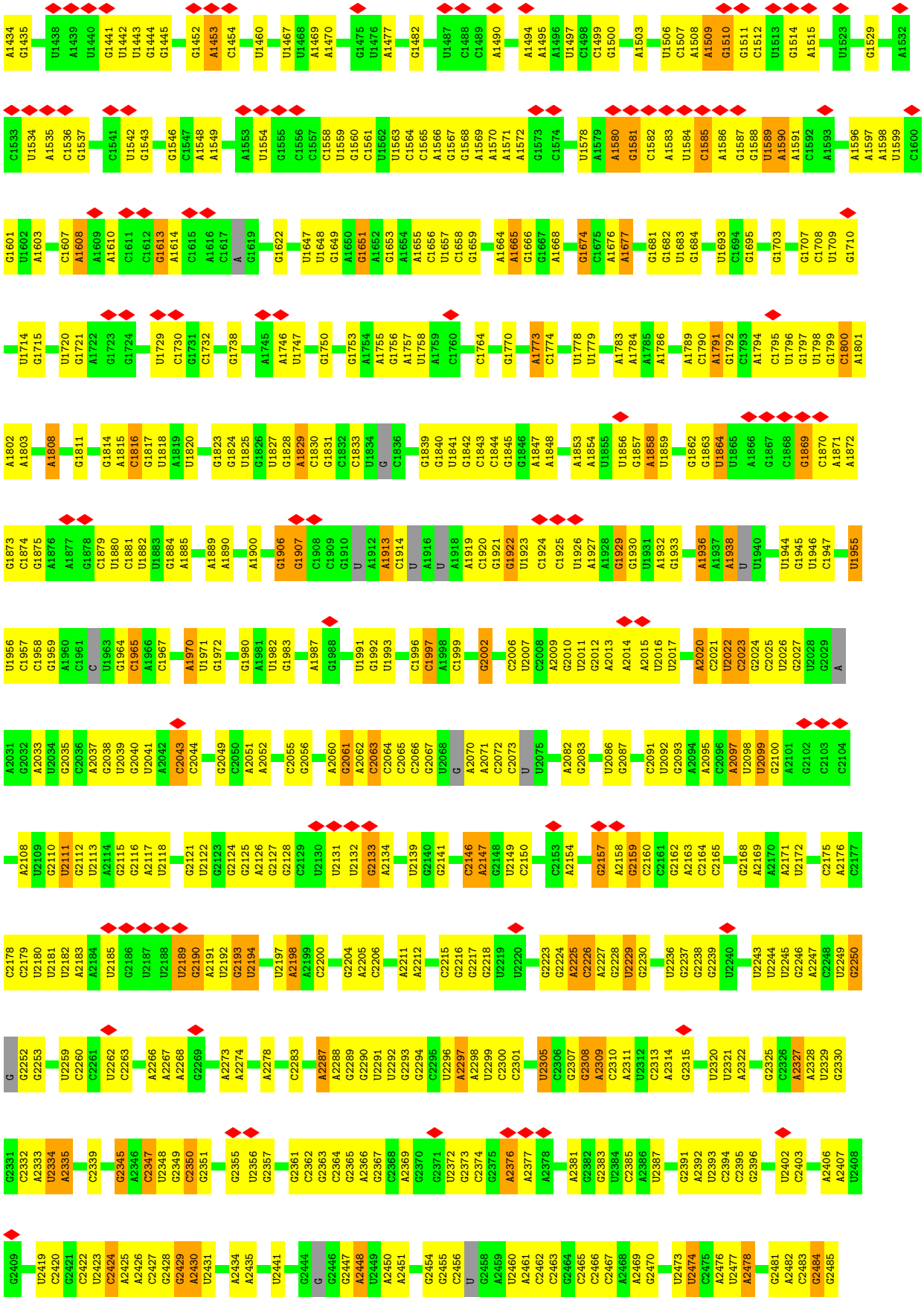


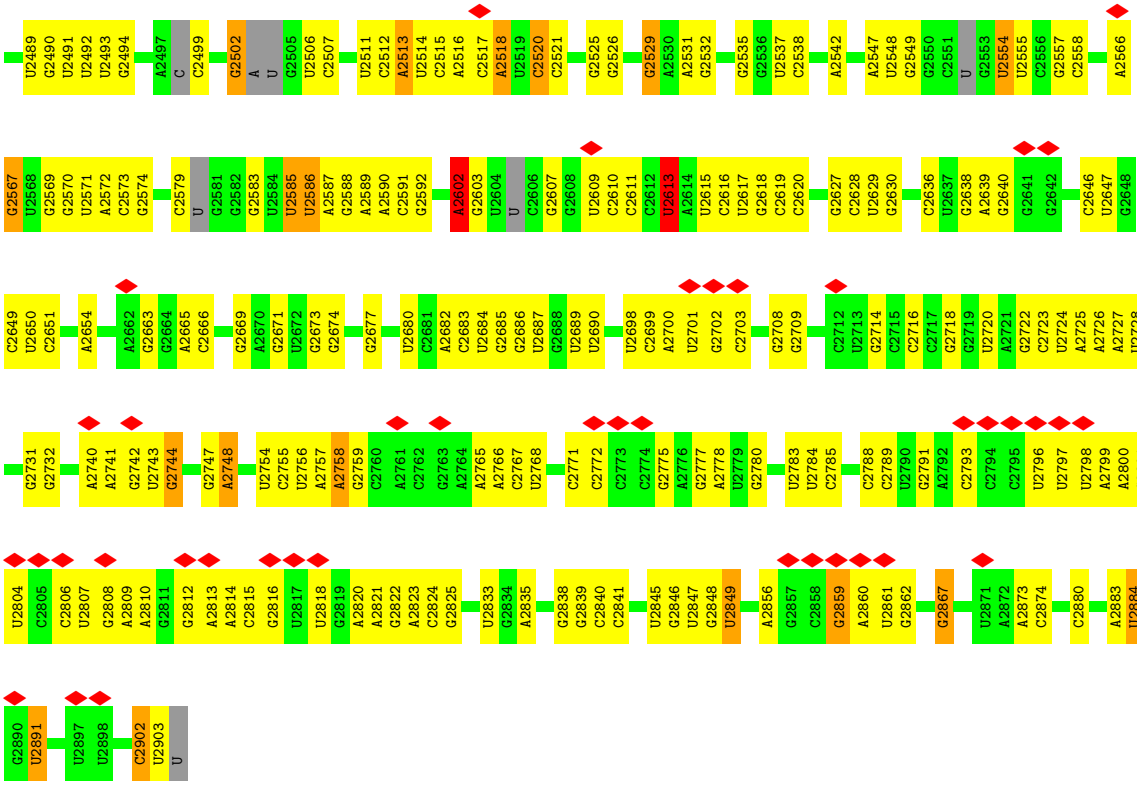







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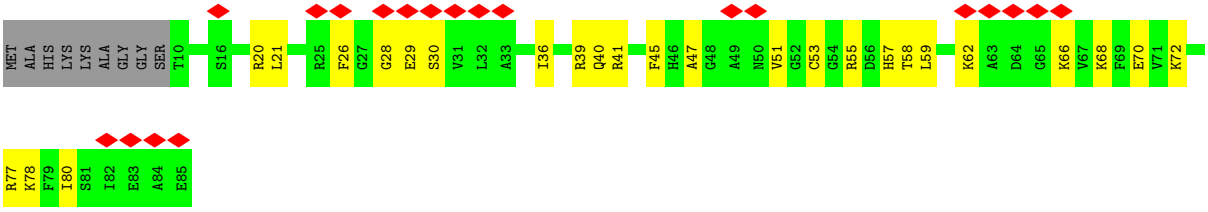

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• Molecule 42: 50S ribosomal protein L27

Chain b:

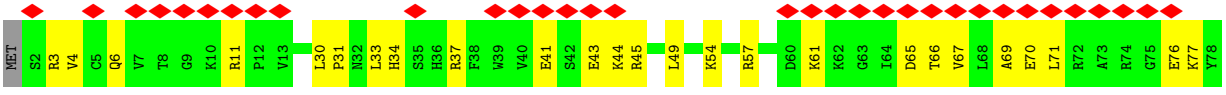




• Molecule 43: 50S ribosomal protein L28

Chain c:

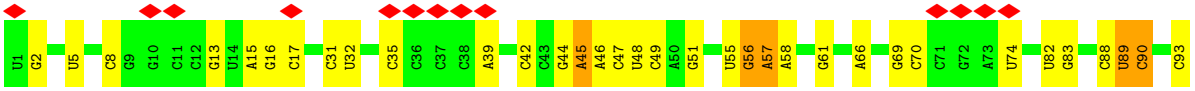


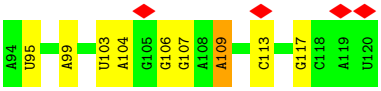


• Molecule 44: 5S rRNA

Chain d:



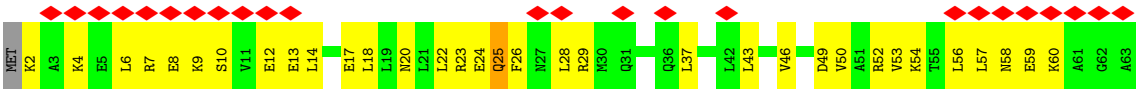




• Molecule 45: 50S ribosomal protein L29

Chain e:

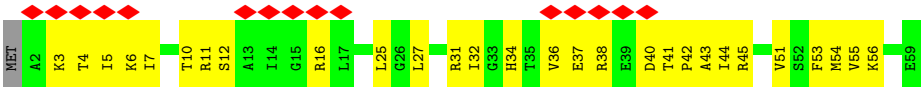




• Molecule 46: 50S ribosomal protein L30

Chain f:

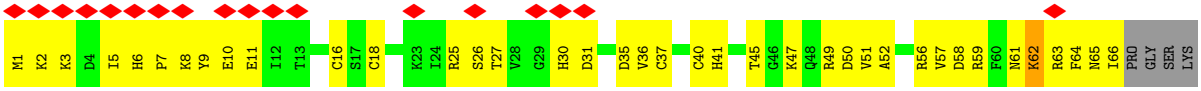




• Molecule 47: 50S ribosomal protein L31

Chain g:

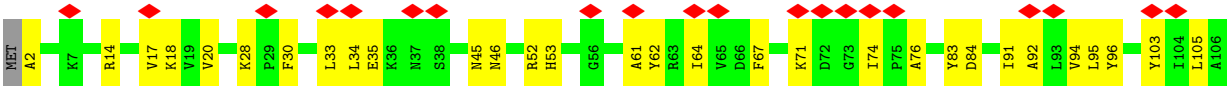


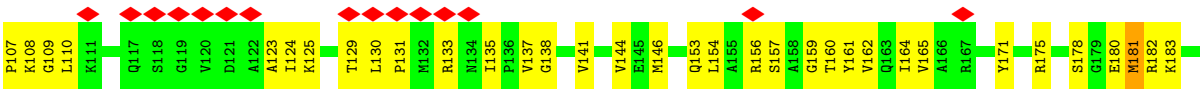


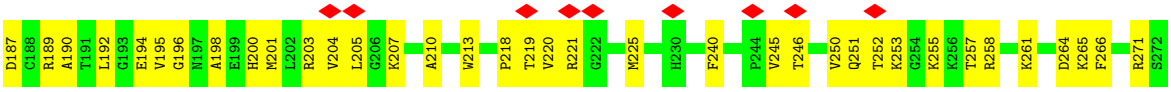
• Molecule 48: 50S ribosomal protein L2

Chain h:







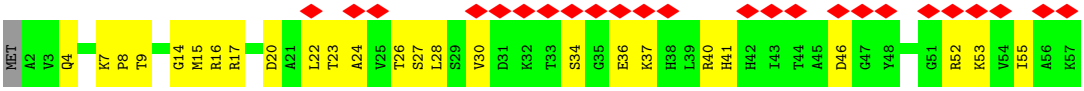




• Molecule 49: 50S ribosomal protein L32

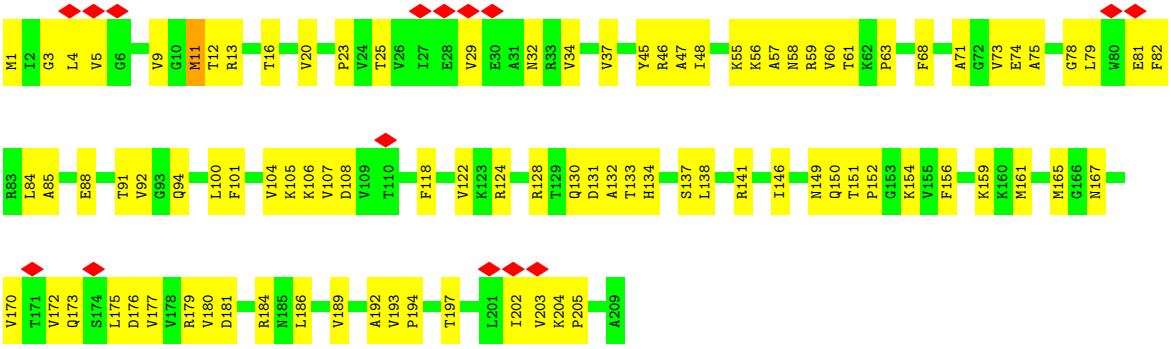
Chain i:





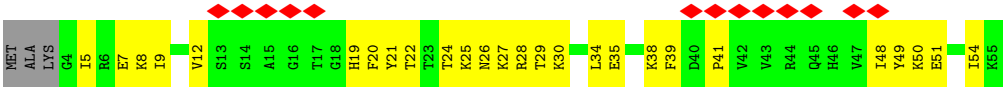
• Molecule 50: 50S ribosomal protein L3





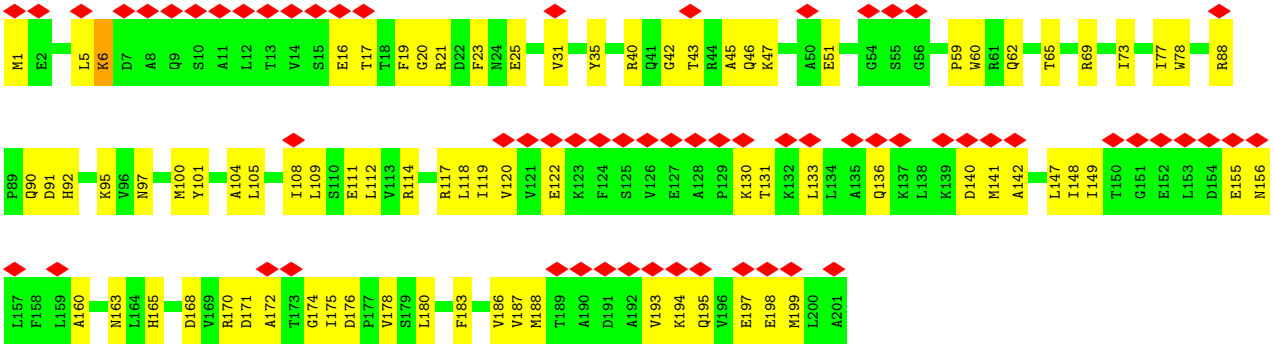
• Molecule 51: 50S ribosomal protein L33





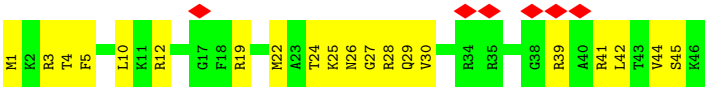
• Molecule 52: 50S ribosomal protein L4





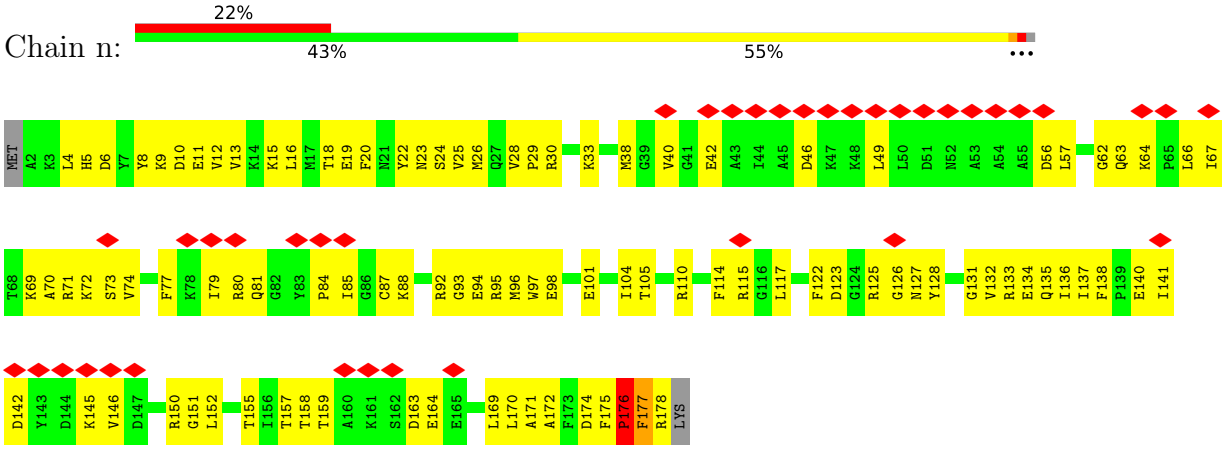
• Molecule 53: 50S ribosomal protein L34





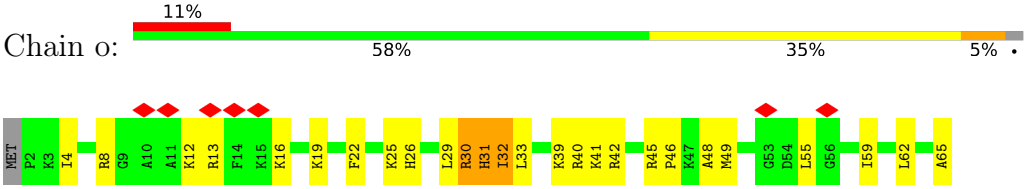
• Molecule 54: 50S ribosomal protein L5

Chain n:



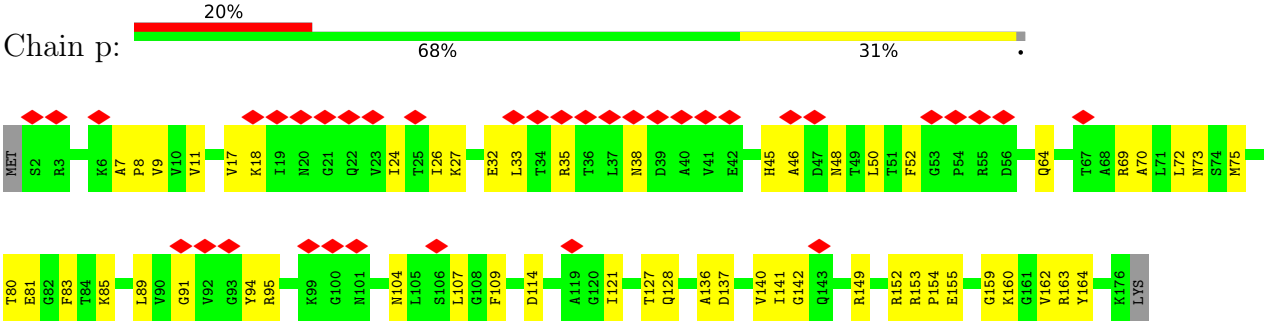
• Molecule 55: 50S ribosomal protein L35

Chain o:



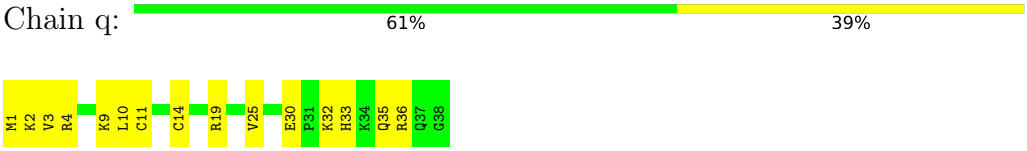
• Molecule 56: 50S ribosomal protein L6

Chain p:



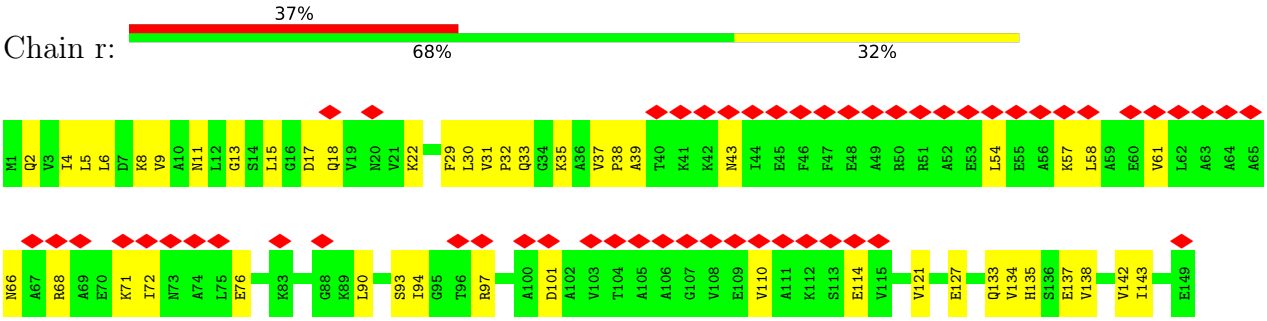
• Molecule 57: 50S ribosomal protein L36

Chain q:



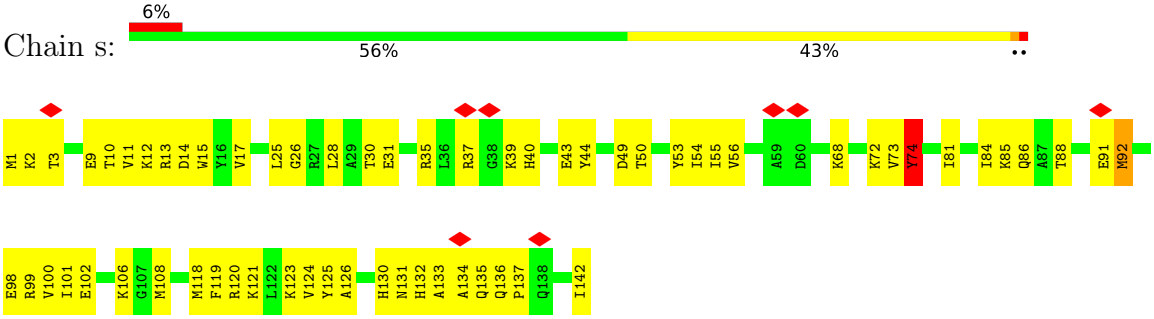
• Molecule 58: 50S ribosomal protein L9

Chain r:



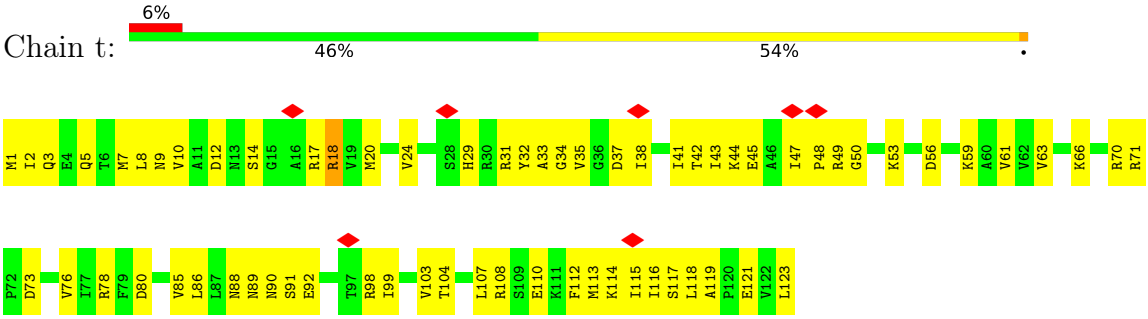
• Molecule 59: 50S ribosomal protein L13

Chain s:



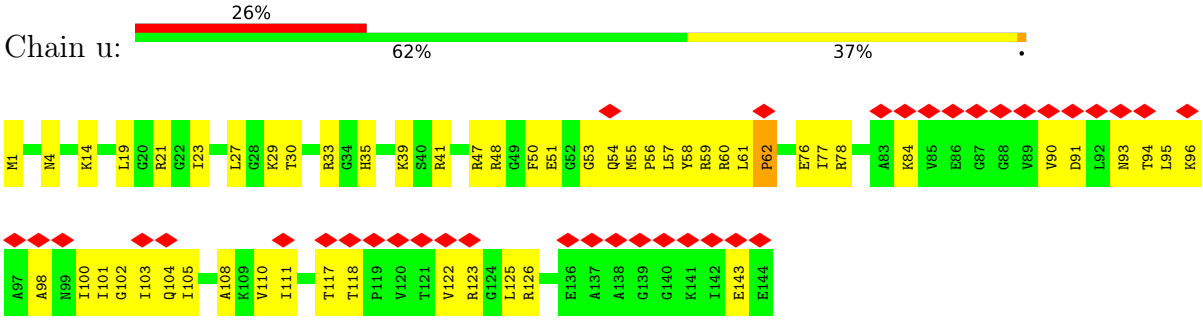
• Molecule 60: 50S ribosomal protein L14

Chain t:



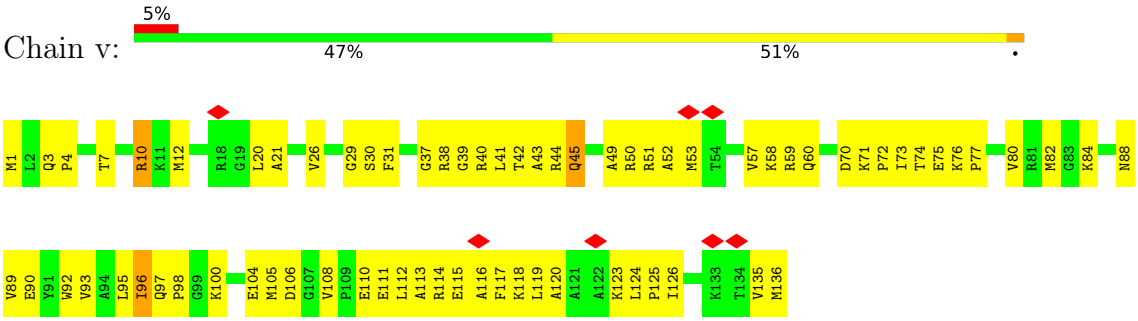
• Molecule 61: 50S ribosomal protein L15

Chain u:



• Molecule 62: 50S ribosomal protein L16

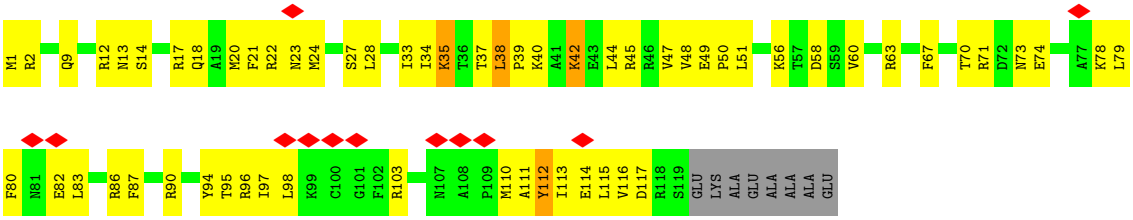
Chain v:



• Molecule 63: 50S ribosomal protein L17

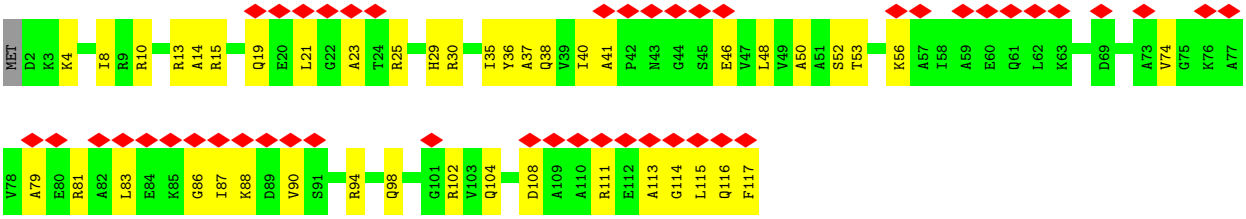
Chain w:





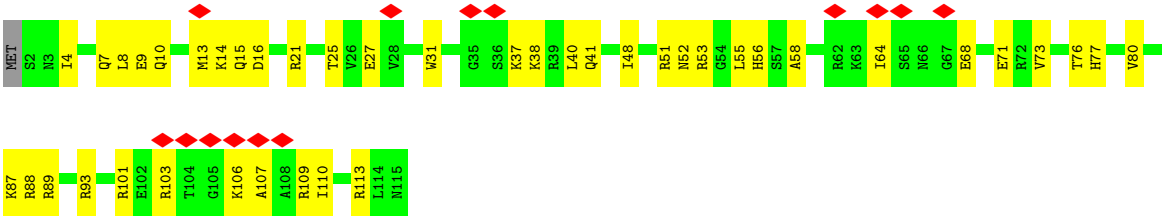
• Molecule 64: 50S ribosomal protein L18





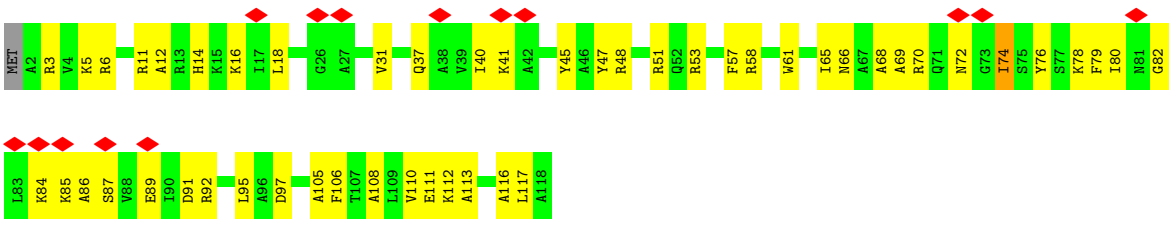
• Molecule 65: 50S ribosomal protein L19





• Molecule 66: 50S ribosomal protein L20





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14614	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0017	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0	0.42	0/829	0.51	0/1107
2	1	0.60	0/864	0.63	0/1156
3	2	0.55	1/752 (0.1%)	0.67	0/1005
4	3	0.35	0/796	0.49	0/1062
5	4	0.57	0/766	0.63	0/1025
6	5	0.56	0/816	0.78	0/1259
7	6	0.56	0/783	0.78	0/1203
8	7	0.56	2/856 (0.2%)	0.88	4/1326 (0.3%)
9	9	0.37	0/1131	0.74	2/1524 (0.1%)
10	A	0.27	0/1810	0.58	0/2821
10	B	0.27	0/1810	0.58	0/2821
11	AA	0.38	0/10547	0.62	0/14232
12	AB	0.61	0/1317	1.22	18/1786 (1.0%)
13	AC	0.38	0/1718	0.62	0/2328
13	AD	0.36	0/2096	0.69	3/2854 (0.1%)
14	AE	0.39	0/10561	0.64	7/14258 (0.0%)
15	AF	0.30	0/652	0.61	0/879
16	AG	0.97	5/3897 (0.1%)	1.40	48/5273 (0.9%)
17	C	0.67	0/553	0.81	1/743 (0.1%)
18	D	0.29	0/36610	0.41	9/57091 (0.0%)
19	E	0.61	0/675	0.72	0/895
20	F	0.53	0/597	0.61	0/792
21	G	0.68	5/1791 (0.3%)	0.79	8/2413 (0.3%)
22	H	0.38	0/1746	0.81	0/2382
23	I	0.57	1/1663 (0.1%)	0.68	4/2241 (0.2%)
24	J	0.46	0/1665	0.58	0/2227
25	K	0.71	2/1165 (0.2%)	0.81	5/1568 (0.3%)
26	L	0.68	1/867 (0.1%)	0.79	1/1171 (0.1%)
27	M	0.56	0/1195	0.69	2/1602 (0.1%)
28	N	0.50	0/989	0.58	0/1326
29	O	0.66	3/1034 (0.3%)	0.79	3/1375 (0.2%)
30	P	0.49	0/800	0.66	1/1082 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#\|Z\| >5	RMSZ	#\|Z\| >5
31	Q	0.72	2/893 (0.2%)	0.76	2/1205 (0.2%)
32	R	0.49	0/952	0.59	0/1274
33	S	0.53	0/817	0.61	0/1088
34	T	0.57	1/722 (0.1%)	0.68	0/964
35	U	0.41	0/659	0.53	0/884
36	V	0.48	0/657	0.63	0/881
37	W	0.56	1/680 (0.1%)	0.62	1/915 (0.1%)
38	X	0.45	0/909	0.72	1/1215 (0.1%)
39	Y	0.38	2/1046 (0.2%)	0.66	2/1410 (0.1%)
40	Z	0.12	0/227	0.40	0/304
41	a	0.30	0/69247	0.43	10/107985 (0.0%)
42	b	0.41	0/589	0.55	0/779
43	c	0.51	0/635	0.61	0/848
44	d	0.25	0/2872	0.37	0/4478
45	e	0.69	2/502 (0.4%)	0.65	1/667 (0.1%)
46	f	0.52	0/452	0.57	0/605
47	g	0.45	1/531 (0.2%)	0.64	0/709
48	h	0.49	1/2121 (0.0%)	0.58	1/2852 (0.0%)
49	i	0.41	0/450	0.55	0/599
50	j	0.51	0/1586	0.57	1/2134 (0.0%)
51	k	0.45	0/433	0.62	0/576
52	l	0.51	1/1571 (0.1%)	0.62	0/2113
53	m	0.45	0/380	0.56	0/498
54	n	0.46	0/1434	0.66	1/1926 (0.1%)
55	o	0.51	0/513	0.71	1/676 (0.1%)
56	p	0.41	0/1333	0.62	2/1805 (0.1%)
57	q	0.45	0/303	0.64	0/397
58	r	0.28	0/1122	0.48	0/1515
59	s	0.70	2/1152 (0.2%)	0.73	2/1551 (0.1%)
60	t	0.52	0/955	0.75	3/1279 (0.2%)
61	u	0.43	0/1062	0.59	0/1413
62	v	0.60	1/1093 (0.1%)	0.77	3/1460 (0.2%)
63	w	0.83	3/964 (0.3%)	0.80	3/1289 (0.2%)
64	x	0.34	0/902	0.50	0/1209
65	y	0.41	0/929	0.54	0/1242
66	z	0.61	2/960 (0.2%)	0.62	0/1278
All	All	0.41	39/195004 (0.0%)	0.56	150/286850 (0.1%)

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
9	9	0	3
12	AB	0	2
13	AC	0	1
13	AD	0	2
14	AE	0	4
16	AG	0	6
21	G	0	1
22	H	0	5
23	I	0	1
25	K	0	2
29	O	0	1
38	X	0	1
39	Y	0	1
54	n	0	1
55	o	0	1
59	s	0	1
61	u	0	2
All	All	0	35

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	AG	429	LYS	C-N	13.81	1.51	1.33
63	w	35	LYS	CE-NZ	-12.77	1.11	1.49
29	O	80	ARG	CD-NE	-10.52	1.31	1.46
63	w	42	LYS	CD-CE	-9.41	1.24	1.52
25	K	45	ARG	CG-CD	7.74	1.75	1.52

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AG	104	ARG	CA-C-N	17.91	154.21	121.97
16	AG	104	ARG	C-N-CA	17.91	154.21	121.97
16	AG	246	ASP	CA-C-N	14.51	137.97	119.84
16	AG	246	ASP	C-N-CA	14.51	137.97	119.84
16	AG	354	ALA	O-C-N	-13.68	107.32	122.09

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide

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Mol	Chain	Res	Type	Group
9	9	79	PRO	Peptide
9	9	92	ALA	Peptide
12	AB	140	MET	Peptide
12	AB	151	LYS	Peptide

5.2 Too-close contacts (i)

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	0	816	839	839	54	0
2	1	857	922	922	69	0
3	2	746	811	811	60	0
4	3	788	844	844	46	0
5	4	753	780	780	86	0
6	5	726	0	392	111	0
7	6	703	0	396	34	0
8	7	772	0	384	127	0
9	9	1117	0	1155	255	0
10	A	1620	826	827	108	0
10	B	1620	814	827	110	0
11	AA	10381	0	10389	267	0
12	AB	1286	0	1301	458	0
13	AC	1698	0	1718	12	0
13	AD	2078	0	1891	41	0
14	AE	10404	0	10623	285	0
15	AF	650	0	658	14	0
16	AG	3852	0	3827	820	0
17	C	544	559	560	107	0
18	D	32703	16423	16453	731	0
19	E	669	719	719	82	0
20	F	589	629	629	60	0
21	G	1760	1785	1787	181	0
22	H	1730	1454	1455	162	0
23	I	1636	1710	1710	157	0
24	J	1643	1707	1707	84	0
25	K	1152	1196	1196	135	0
26	L	848	846	846	105	0
27	M	1181	1235	1238	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	N	979	1031	1031	92	0
29	O	1022	1070	1070	93	0
30	P	790	831	831	139	0
31	Q	877	887	887	98	0
32	R	939	1001	1001	91	0
33	S	805	844	844	74	0
34	T	714	734	734	94	0
35	U	649	666	666	62	0
36	V	648	691	691	68	0
37	W	663	688	688	47	0
38	X	900	964	965	110	0
39	Y	1032	0	1088	215	0
40	Z	227	0	237	31	0
41	a	61841	31077	31120	1313	0
42	b	582	599	599	47	0
43	c	625	652	652	32	0
44	d	2569	1301	1301	44	0
45	e	501	531	531	46	0
46	f	448	488	488	39	0
47	g	522	520	520	68	0
48	h	2082	2154	2154	135	0
49	i	444	459	458	49	0
50	j	1565	1617	1616	122	0
51	k	426	464	464	42	0
52	l	1552	1619	1619	125	0
53	m	377	418	418	30	0
54	n	1410	1443	1444	157	0
55	o	504	572	572	52	0
56	p	1313	1358	1358	72	0
57	q	302	343	343	25	0
58	r	1111	1148	1148	54	0
59	s	1129	1162	1162	122	0
60	t	946	1023	1023	102	0
61	u	1053	1129	1129	79	0
62	v	1074	1157	1157	123	0
63	w	951	994	994	99	0
64	x	892	923	923	50	0
65	y	917	962	962	51	0
66	z	947	1020	1019	80	0
67	AE	1	0	0	0	0
68	AE	2	0	0	3	0
All	All	181653	98639	132791	7730	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 7730 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)
16:AG:425:LEU:CD2	16:AG:429:LYS:HE2	1.21	1.63
6:5:11:DA:C5'	12:AB:67:THR:HG22	1.20	1.61
14:AE:79:LYS:HA	14:AE:81:ARG:CZ	1.26	1.61
16:AG:219:GLU:HG2	21:G:156:GLY:CA	1.28	1.60
6:5:9:DG:H5"	11:AA:473:ARG:CB	1.29	1.58

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	0	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
2	1	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
3	2	92/100 (92%)	87 (95%)	5 (5%)	0	100	100
4	3	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
5	4	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
9	9	146/165 (88%)	101 (69%)	42 (29%)	3 (2%)	5	24
11	AA	1312/1342 (98%)	1197 (91%)	114 (9%)	1 (0%)	48	78
12	AB	159/162 (98%)	106 (67%)	42 (26%)	11 (7%)	1	6
13	AC	217/329 (66%)	204 (94%)	11 (5%)	2 (1%)	14	42
13	AD	293/329 (89%)	263 (90%)	27 (9%)	3 (1%)	12	40
14	AE	1331/1407 (95%)	1212 (91%)	113 (8%)	6 (0%)	24	54
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	AG	493/495 (100%)	376 (76%)	86 (17%)	31 (6%)	1 7
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100 100
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
20	F	68/71 (96%)	68 (100%)	0	0	100 100
21	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30 59
22	H	255/557 (46%)	182 (71%)	66 (26%)	7 (3%)	4 20
23	I	206/233 (88%)	193 (94%)	13 (6%)	0	100 100
24	J	203/206 (98%)	201 (99%)	2 (1%)	0	100 100
25	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	21 50
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	12 40
27	M	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	18 47
28	N	127/130 (98%)	123 (97%)	4 (3%)	0	100 100
29	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16 44
30	P	97/103 (94%)	89 (92%)	8 (8%)	0	100 100
31	Q	115/129 (89%)	107 (93%)	8 (7%)	0	100 100
32	R	117/124 (94%)	112 (96%)	5 (4%)	0	100 100
33	S	98/101 (97%)	97 (99%)	1 (1%)	0	100 100
34	T	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
35	U	80/82 (98%)	76 (95%)	4 (5%)	0	100 100
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100 100
37	W	81/92 (88%)	80 (99%)	1 (1%)	0	100 100
38	X	114/118 (97%)	103 (90%)	9 (8%)	2 (2%)	6 26
39	Y	139/142 (98%)	102 (73%)	37 (27%)	0	100 100
40	Z	28/121 (23%)	22 (79%)	6 (21%)	0	100 100
42	b	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100 100
45	e	60/63 (95%)	57 (95%)	3 (5%)	0	100 100
46	f	56/59 (95%)	52 (93%)	4 (7%)	0	100 100
47	g	64/70 (91%)	62 (97%)	2 (3%)	0	100 100
48	h	269/273 (98%)	255 (95%)	14 (5%)	0	100 100
49	i	54/57 (95%)	49 (91%)	5 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
51	k	50/55 (91%)	50 (100%)	0	0	100	100
52	l	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	n	175/179 (98%)	160 (91%)	14 (8%)	1 (1%)	21	50
55	o	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	7	29
56	p	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
57	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
58	r	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
59	s	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
60	t	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
61	u	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
62	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
63	w	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
64	x	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
65	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
66	z	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
All	All	10058/11053 (91%)	9180 (91%)	805 (8%)	73 (1%)	20	47

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	107	PRO
12	AB	125	GLY
12	AB	130	PHE
12	AB	137	ALA
12	AB	141	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	84/84 (100%)	84 (100%)	0	100 100
2	1	93/93 (100%)	93 (100%)	0	100 100
3	2	81/84 (96%)	81 (100%)	0	100 100
4	3	84/85 (99%)	84 (100%)	0	100 100
5	4	78/78 (100%)	78 (100%)	0	100 100
9	9	112/123 (91%)	112 (100%)	0	100 100
11	AA	1135/1157 (98%)	1130 (100%)	5 (0%)	84 83
12	AB	141/142 (99%)	122 (86%)	19 (14%)	4 15
13	AC	186/286 (65%)	186 (100%)	0	100 100
13	AD	185/286 (65%)	185 (100%)	0	100 100
14	AE	1122/1168 (96%)	1104 (98%)	18 (2%)	55 68
15	AF	70/75 (93%)	69 (99%)	1 (1%)	59 70
16	AG	409/409 (100%)	288 (70%)	121 (30%)	0 1
17	C	57/65 (88%)	57 (100%)	0	100 100
19	E	65/66 (98%)	65 (100%)	0	100 100
20	F	60/61 (98%)	60 (100%)	0	100 100
21	G	187/199 (94%)	187 (100%)	0	100 100
22	H	137/461 (30%)	137 (100%)	0	100 100
23	I	171/190 (90%)	171 (100%)	0	100 100
24	J	172/173 (99%)	171 (99%)	1 (1%)	78 80
25	K	119/126 (94%)	117 (98%)	2 (2%)	53 67
26	L	91/116 (78%)	91 (100%)	0	100 100
27	M	124/147 (84%)	124 (100%)	0	100 100
28	N	104/105 (99%)	104 (100%)	0	100 100
29	O	105/107 (98%)	105 (100%)	0	100 100
30	P	86/90 (96%)	85 (99%)	1 (1%)	63 72
31	Q	90/99 (91%)	90 (100%)	0	100 100
32	R	101/104 (97%)	101 (100%)	0	100 100
33	S	83/84 (99%)	83 (100%)	0	100 100
34	T	76/77 (99%)	76 (100%)	0	100 100
35	U	65/65 (100%)	65 (100%)	0	100 100
36	V	74/78 (95%)	74 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	W	72/79 (91%)	72 (100%)	0	100	100
38	X	94/96 (98%)	94 (100%)	0	100	100
39	Y	109/110 (99%)	109 (100%)	0	100	100
40	Z	26/85 (31%)	26 (100%)	0	100	100
42	b	58/63 (92%)	58 (100%)	0	100	100
43	c	67/68 (98%)	67 (100%)	0	100	100
45	e	54/55 (98%)	54 (100%)	0	100	100
46	f	48/49 (98%)	48 (100%)	0	100	100
47	g	59/62 (95%)	59 (100%)	0	100	100
48	h	216/218 (99%)	216 (100%)	0	100	100
49	i	47/48 (98%)	47 (100%)	0	100	100
50	j	164/164 (100%)	164 (100%)	0	100	100
51	k	47/49 (96%)	47 (100%)	0	100	100
52	l	165/165 (100%)	165 (100%)	0	100	100
53	m	38/38 (100%)	38 (100%)	0	100	100
54	n	148/150 (99%)	148 (100%)	0	100	100
55	o	51/52 (98%)	51 (100%)	0	100	100
56	p	136/138 (99%)	136 (100%)	0	100	100
57	q	34/34 (100%)	34 (100%)	0	100	100
58	r	114/114 (100%)	114 (100%)	0	100	100
59	s	116/116 (100%)	116 (100%)	0	100	100
60	t	104/104 (100%)	104 (100%)	0	100	100
61	u	103/103 (100%)	103 (100%)	0	100	100
62	v	109/109 (100%)	109 (100%)	0	100	100
63	w	99/103 (96%)	99 (100%)	0	100	100
64	x	86/87 (99%)	86 (100%)	0	100	100
65	y	99/100 (99%)	99 (100%)	0	100	100
66	z	89/90 (99%)	89 (100%)	0	100	100
All	All	8299/9132 (91%)	8131 (98%)	168 (2%)	48	65

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	AG	270	ARG
16	AG	337	ASN
16	AG	276	TRP
16	AG	303	HIS
16	AG	358	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
21	G	18	HIS
64	x	29	HIS
27	M	68	ASN
64	x	19	GLN
55	o	24	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	8 (10%)
10	B	75/76 (98%)	29 (38%)	8 (10%)
18	D	1514/1542 (98%)	290 (19%)	20 (1%)
41	a	2859/2904 (98%)	510 (17%)	0
44	d	119/120 (99%)	15 (12%)	0
8	7	36/41 (87%)	26 (72%)	5 (13%)
All	All	4678/4759 (98%)	899 (19%)	41 (0%)

5 of 899 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	3	G
8	7	4	U
8	7	5	U
8	7	7	U
8	7	8	U

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D	517	G
18	D	1213	A
18	D	991	U

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Mol	Chain	Res	Type
18	D	1196	A
18	D	1447	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 3 ligands modelled in this entry, 3 are monoatomic - 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)

There are no chain breaks in this entry.

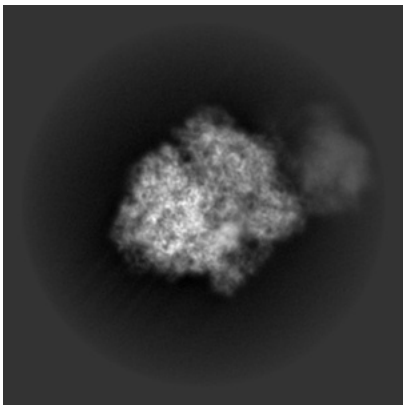
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42479. These allow visual inspection of the internal detail of the map and identification of artifacts.

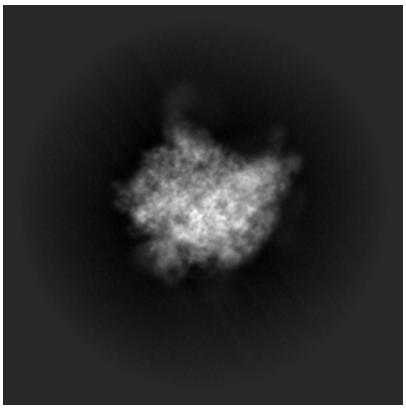
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

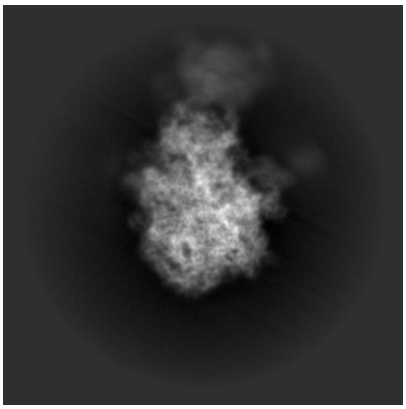
6.1.1 Primary map



X

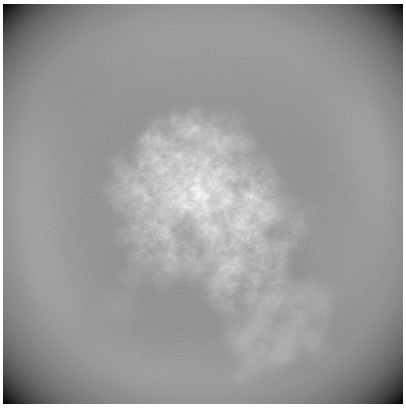


Y

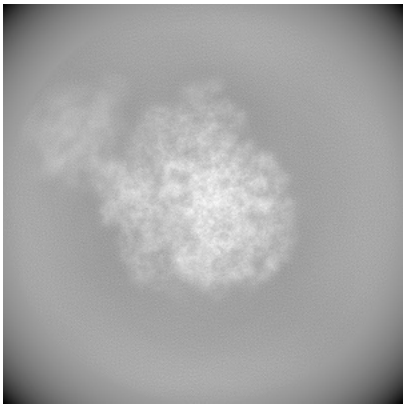


Z

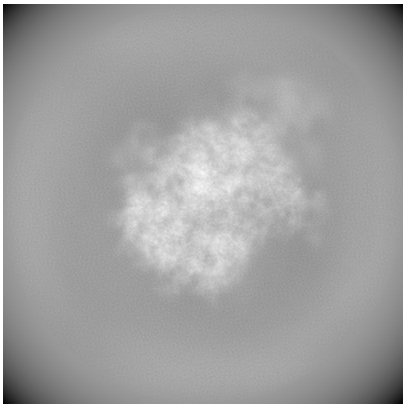
6.1.2 Raw map



X



Y

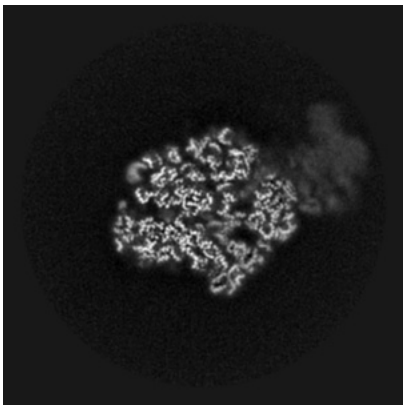


Z

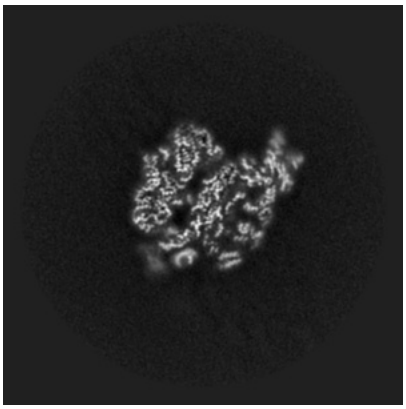
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

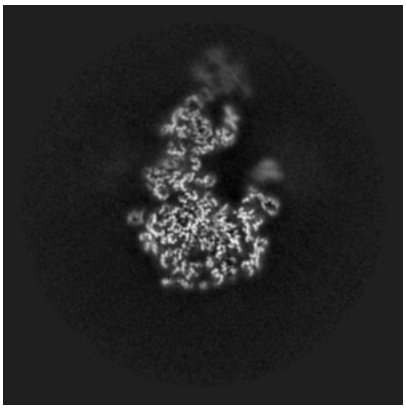
6.2.1 Primary map



X Index: 256

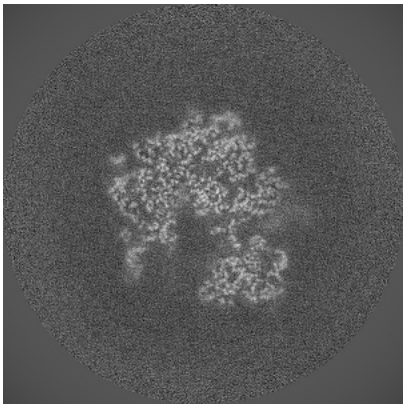


Y Index: 256

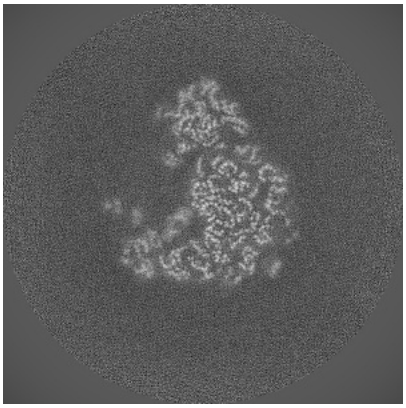


Z Index: 256

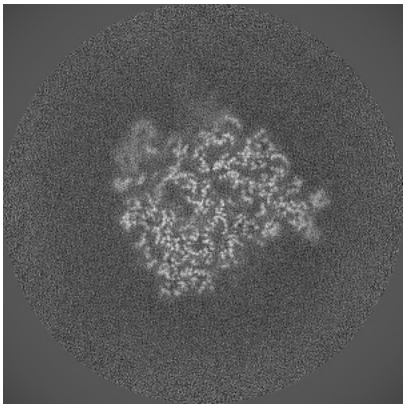
6.2.2 Raw map



X Index: 288



Y Index: 288

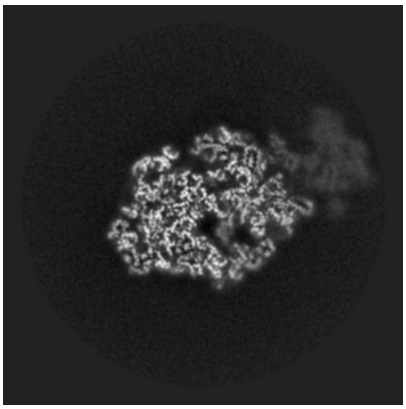


Z Index: 288

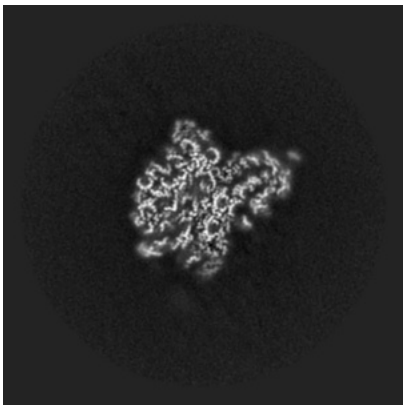
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

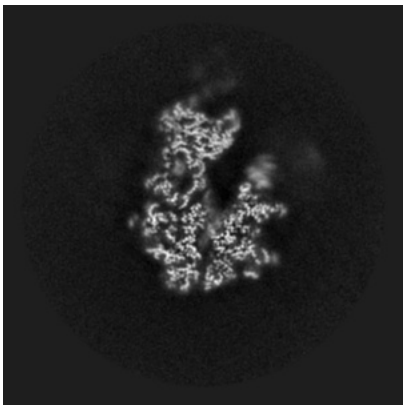
6.3.1 Primary map



X Index: 245

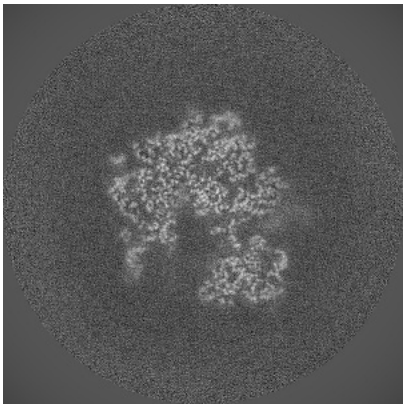


Y Index: 246

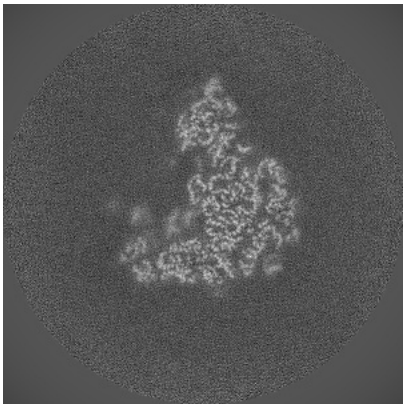


Z Index: 243

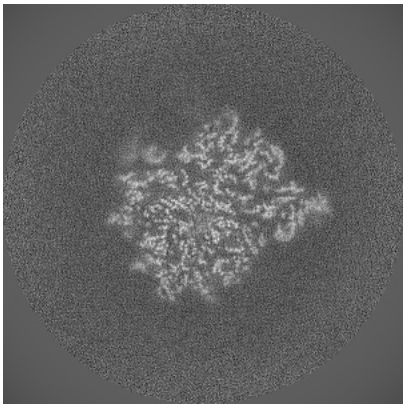
6.3.2 Raw map



X Index: 288



Y Index: 281

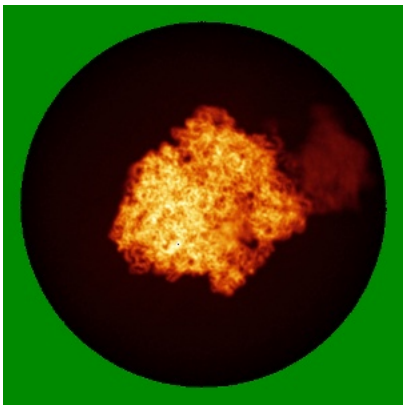


Z Index: 300

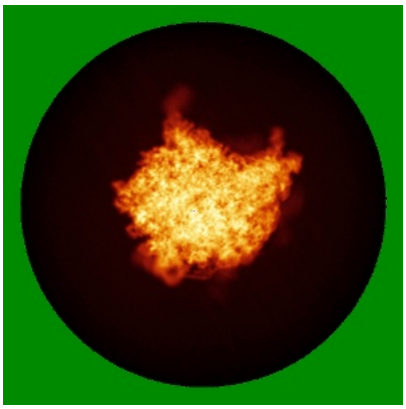
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

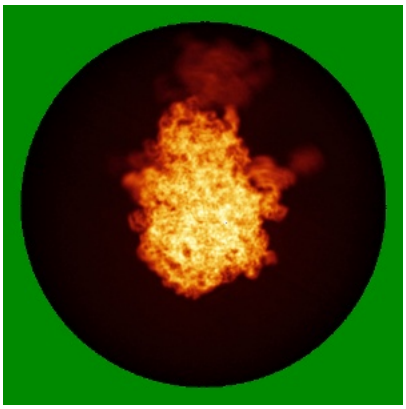
6.4.1 Primary map



X

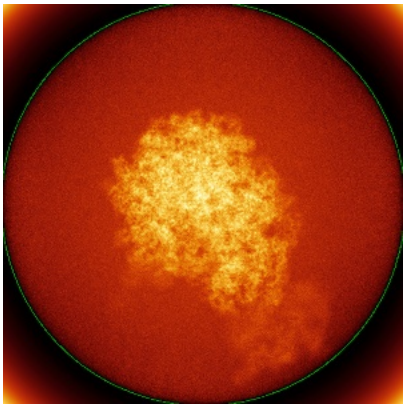


Y

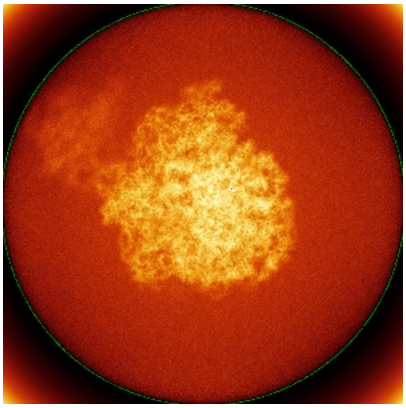


Z

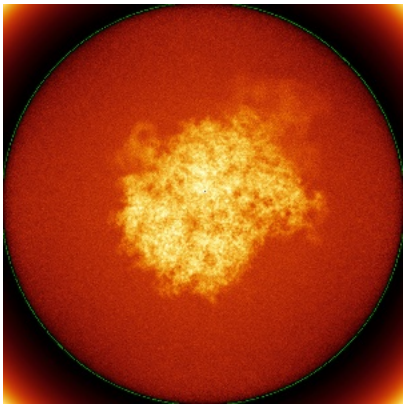
6.4.2 Raw map



X



Y

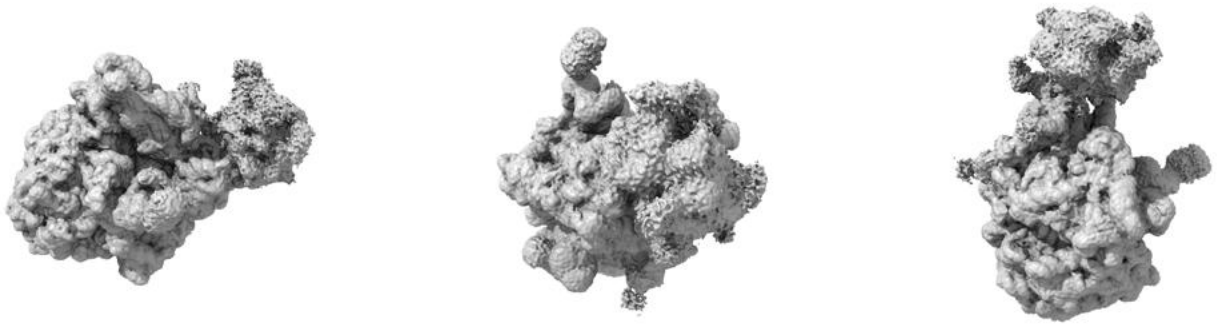


Z

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)

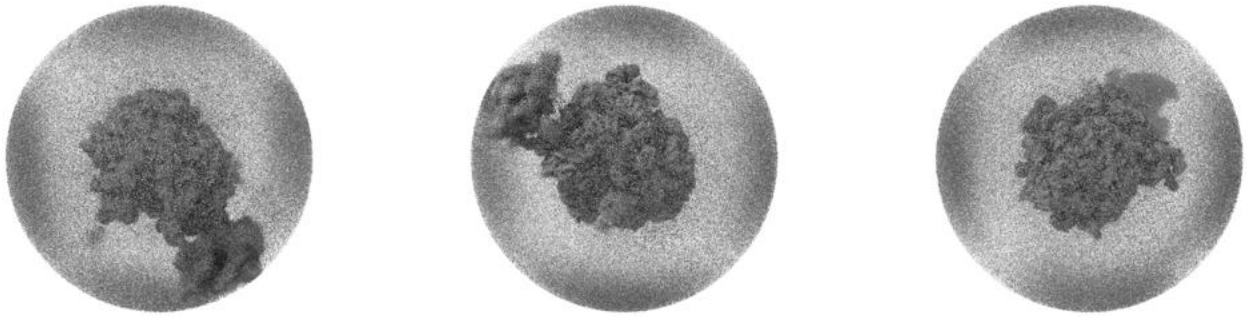
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

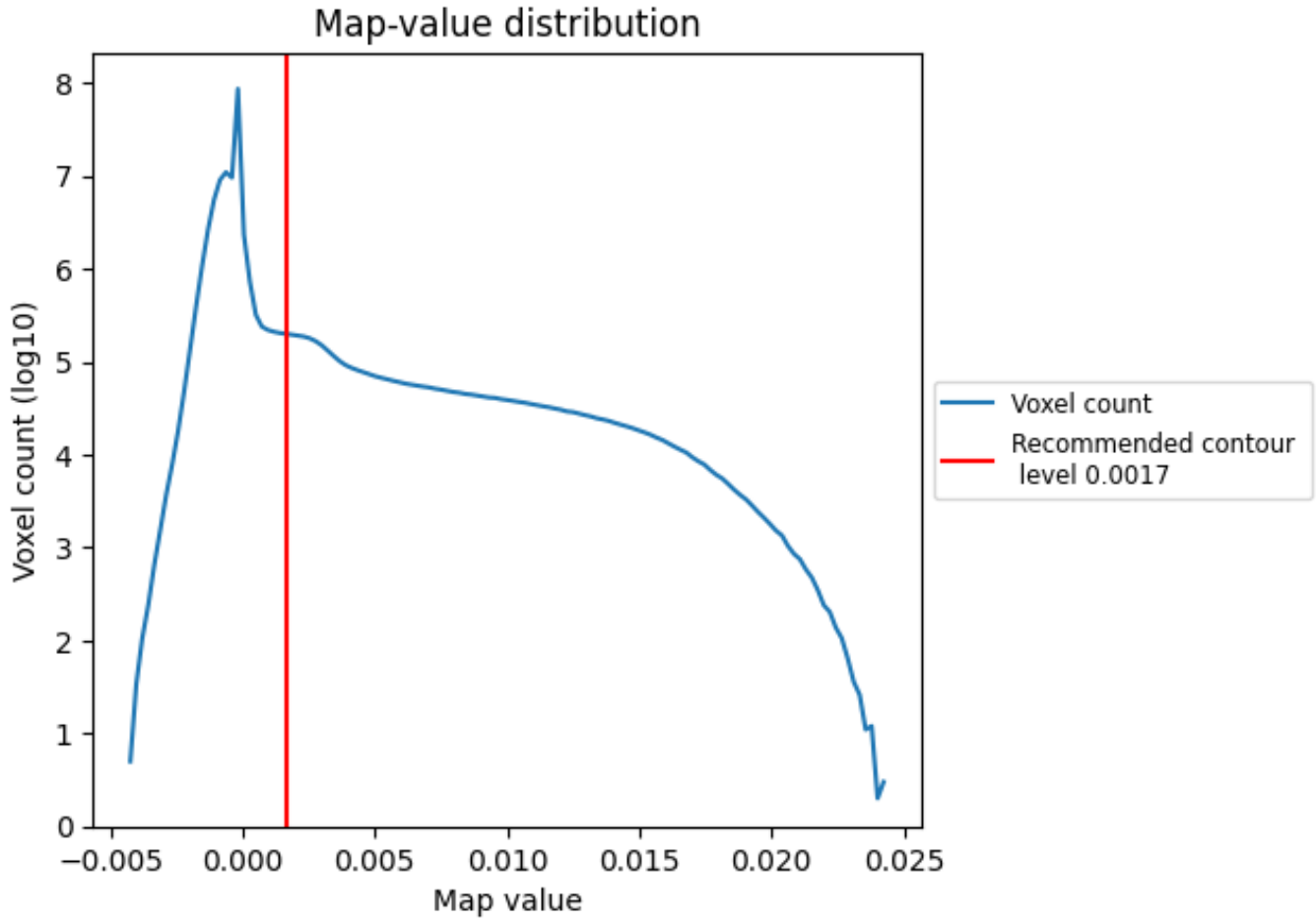
6.6 Mask visualisation (i)

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

7 Map analysis

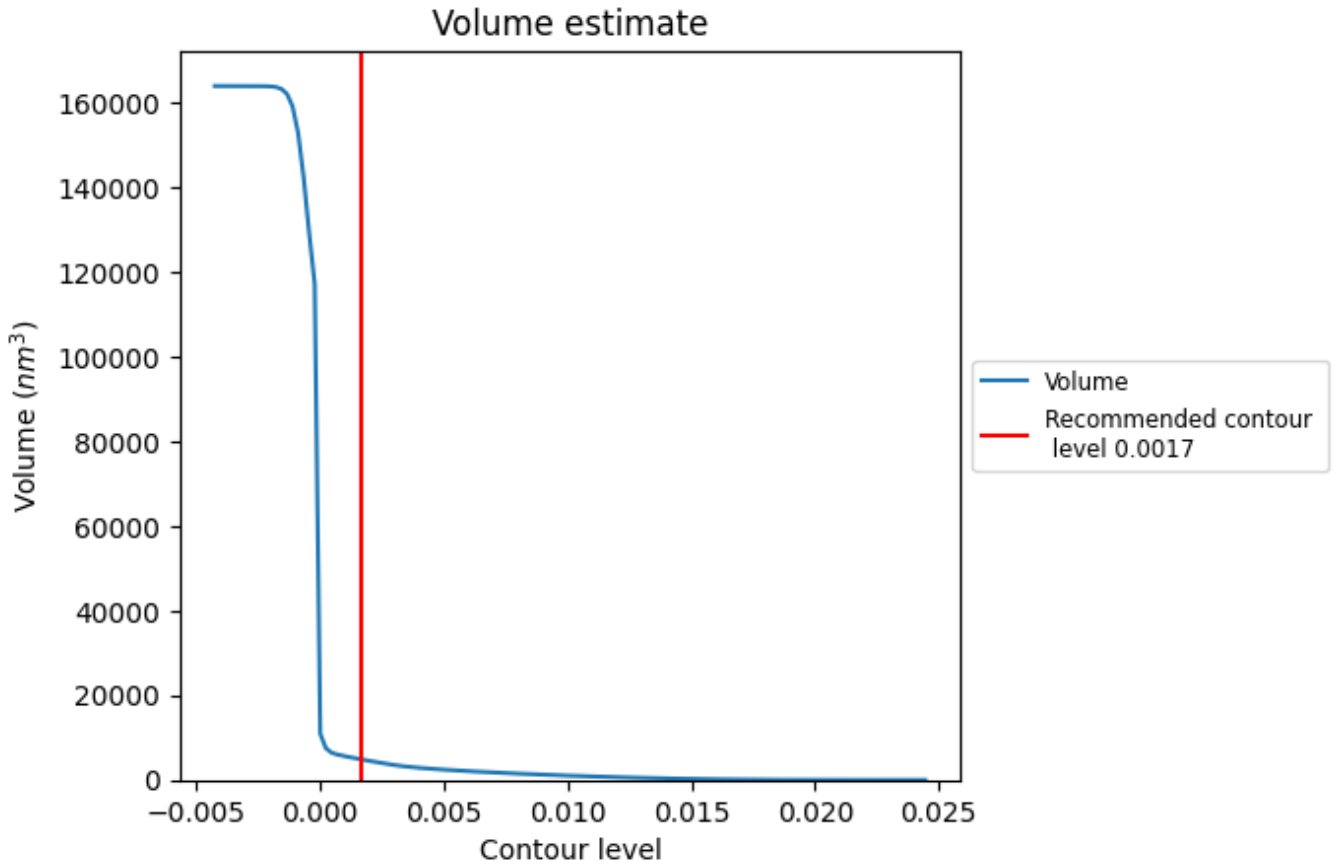
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

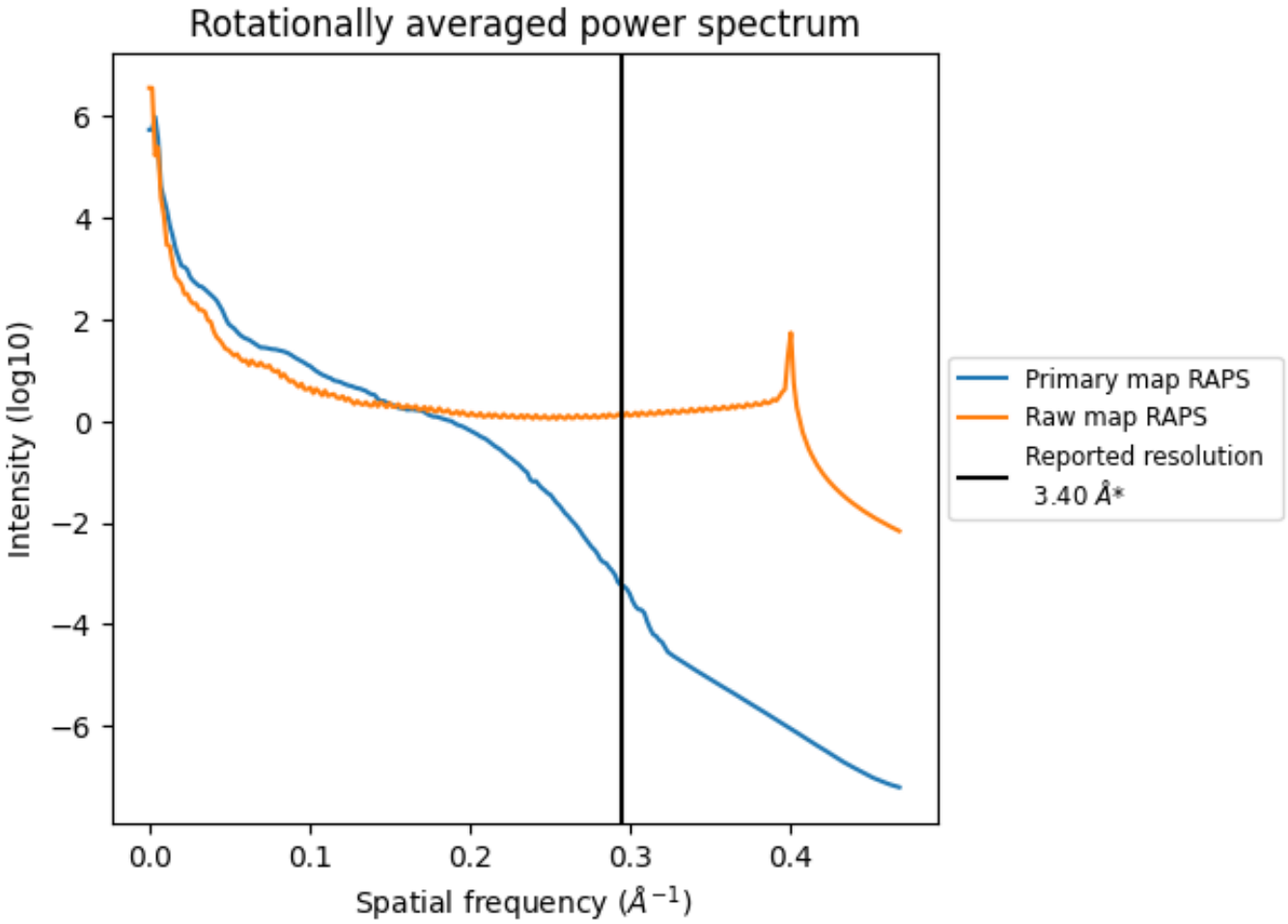
7.2 Volume estimate (i)



The volume at the recommended contour level is 4832 nm^3; this corresponds to an approximate mass of 4365 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

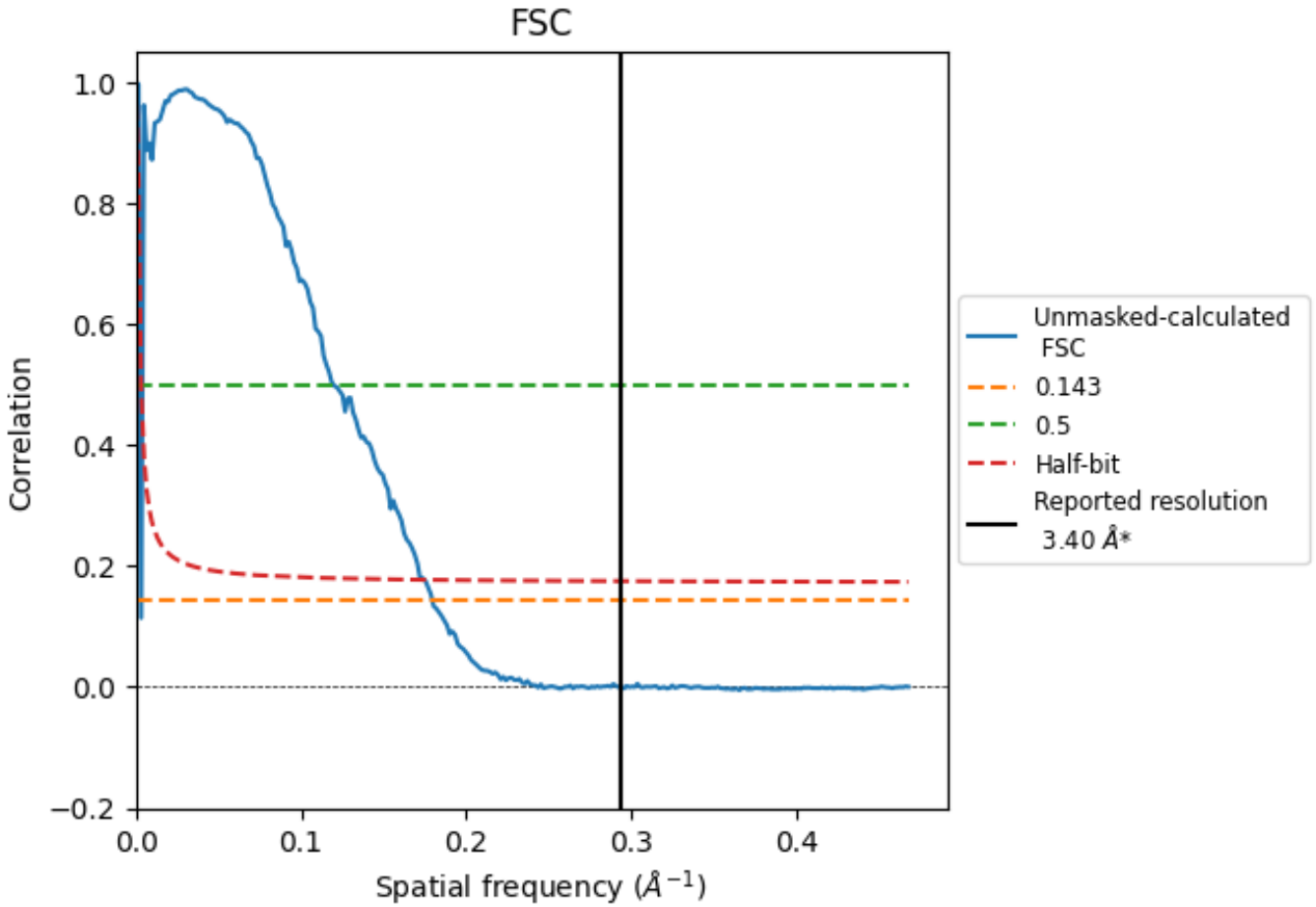


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

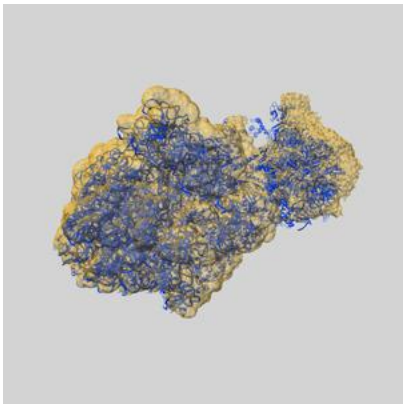
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	312.50	400.00	476.19

*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 312.50 differs from the reported value 3.4 by more than 10 %

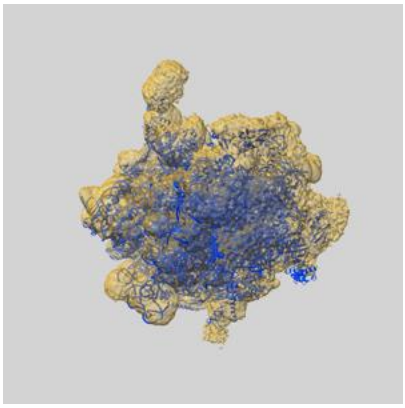
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42479 and PDB model 8UR0. Per-residue inclusion information can be found in section 3 on page 17.

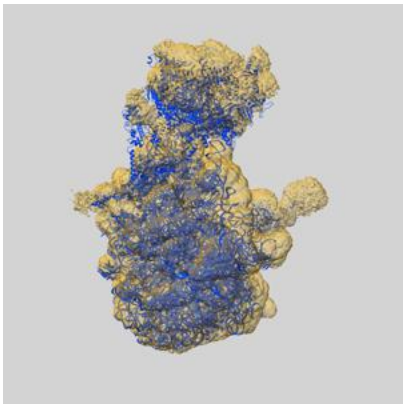
9.1 Map-model overlay



X



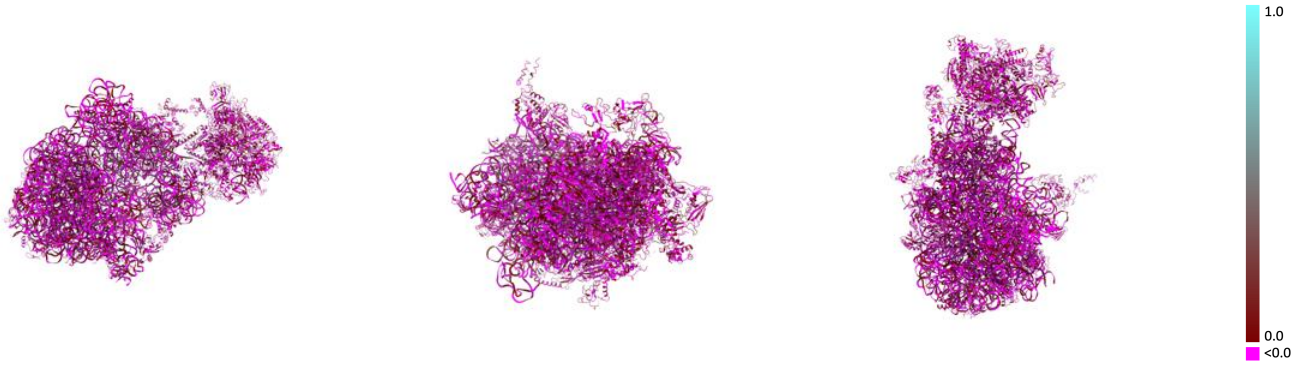
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

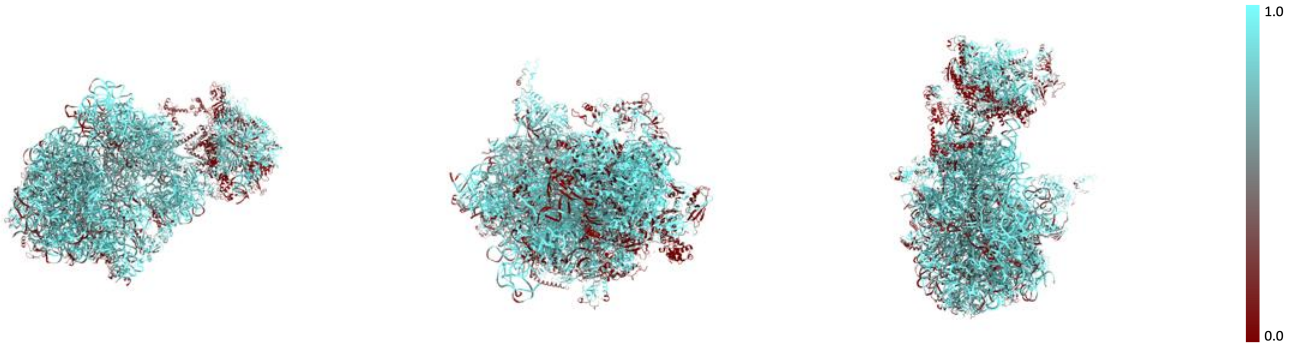
9.2 Q-score mapped to coordinate model



X Y Z

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

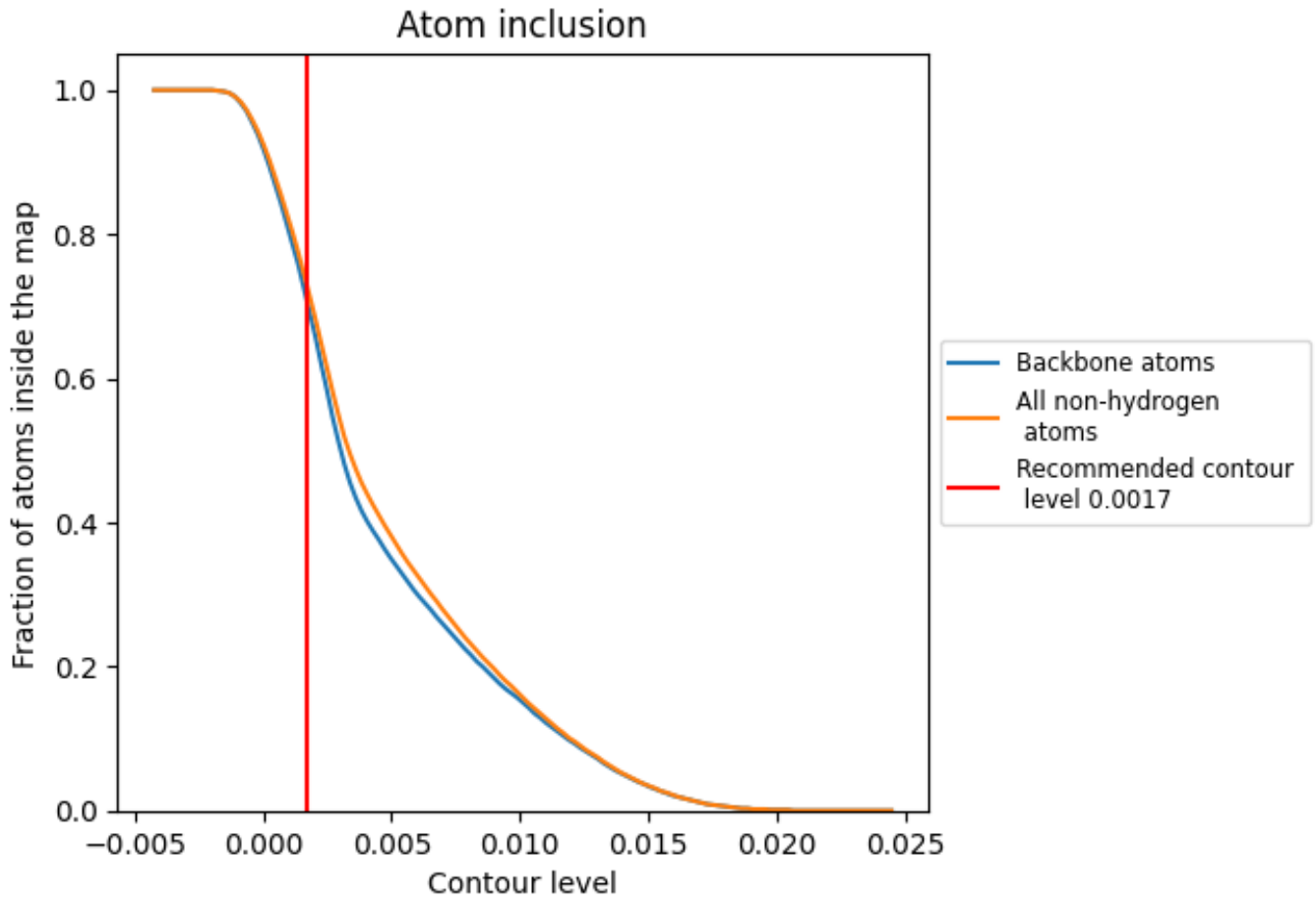
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0017).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 73% 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 (0.0017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	-0.0190
0	0.5720	0.0060
1	0.7340	-0.0160
2	0.8780	-0.0080
3	0.6240	-0.0180
4	0.7520	-0.0120
5	0.5790	0.0040
6	0.6440	-0.0190
7	0.7970	-0.0060
9	0.8550	0.0110
A	0.8820	0.0170
AA	0.6580	-0.0020
AB	0.4930	-0.0040
AC	0.3820	0.0060
AD	0.2530	0.0050
AE	0.5830	0.0040
AF	0.3960	0.0070
AG	0.3200	-0.0070
B	0.5800	-0.0370
C	0.8030	-0.0220
D	0.8270	-0.0270
E	0.6650	-0.0280
F	0.7530	-0.0110
G	0.8500	-0.0090
H	0.7140	-0.0020
I	0.9130	-0.0060
J	0.9270	-0.0050
K	0.8540	-0.0240
L	0.5150	-0.0420
M	0.5780	-0.0190
N	0.8520	-0.0460
O	0.6890	-0.0110
P	0.9690	-0.0120
Q	0.7580	-0.0340
R	0.7520	0.0040



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Chain	Atom inclusion	Q-score
S	0.9690	-0.0360
T	0.5220	-0.0290
U	0.9070	-0.0210
V	0.5650	-0.0180
W	0.6630	-0.0130
X	0.5350	-0.0430
Y	0.8710	0.0130
Z	0.5680	-0.0100
a	0.7970	-0.0270
b	0.7170	-0.0100
c	0.5320	-0.0370
d	0.8140	-0.0140
e	0.5670	-0.0580
f	0.6950	0.0120
g	0.6670	-0.0170
h	0.7890	-0.0330
i	0.5790	-0.0310
j	0.8850	-0.0290
k	0.7110	-0.0250
l	0.6330	-0.0120
m	0.8540	-0.0420
n	0.7420	-0.0340
o	0.8660	-0.0390
p	0.7650	-0.0170
q	0.9900	0.0020
r	0.6030	0.0110
s	0.8790	-0.0200
t	0.8830	-0.0030
u	0.6950	-0.0270
v	0.9090	-0.0390
w	0.8580	-0.0180
x	0.5550	-0.0090
y	0.8480	-0.0460
z	0.8470	-0.0100