wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:33 PM EST

PDB ID : 4V4V
EMDB ID : EMD-1056
Title : Structure of a pre-translocational E. coli ribosome obtained by fitting atomic models for RNA and protein components into cryo-EM map EMD-1056
Authors : Mitra, K.; Frank, J.
Deposited on : 2006-05-09
Resolution : 15.00 Å(reported)

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

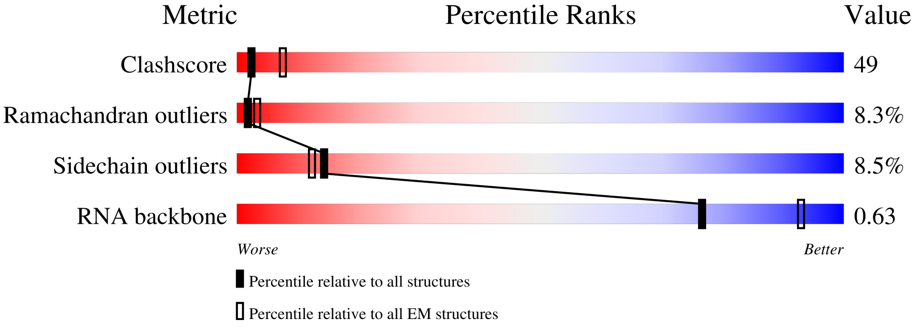
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance ⓘ

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

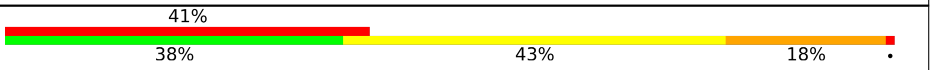
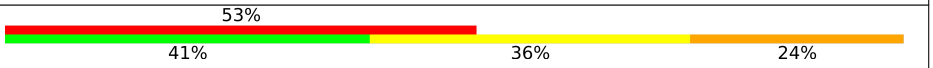
The reported resolution of this entry is 15.00 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AA	1488	
2	AU	76	
2	AV	76	
2	AW	76	
3	AB	236	
4	AC	206	
5	AD	204	

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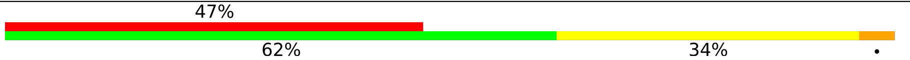
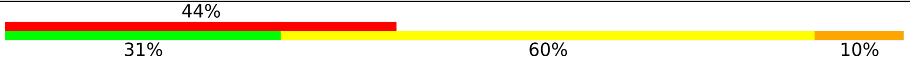
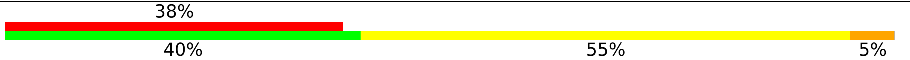
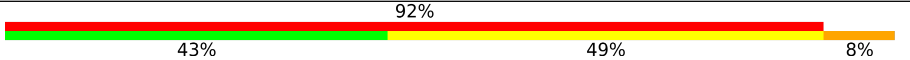
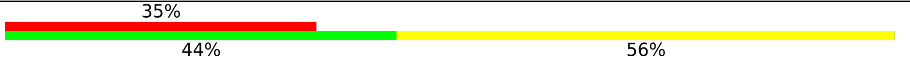
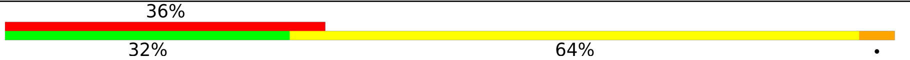
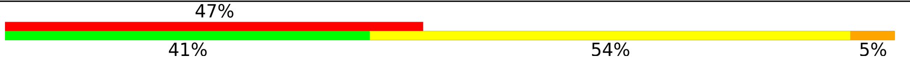
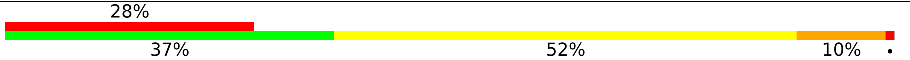
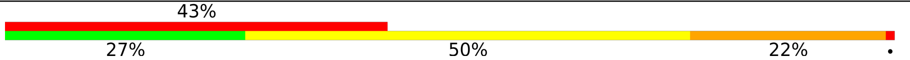
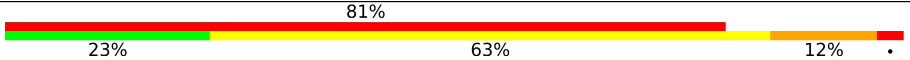
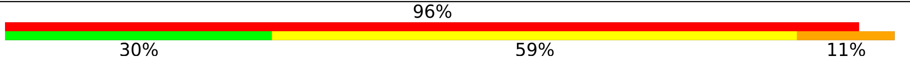
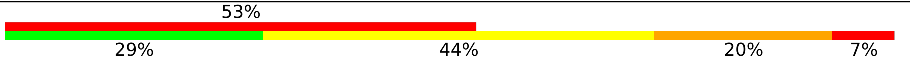
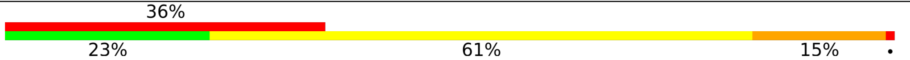
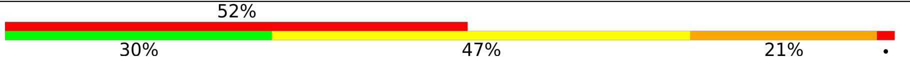
Mol	Chain	Length	Quality of chain
6	AE	148	67% 41% 55% • •
7	AF	95	51% 28% 65% 6%
8	AG	137	47% 62% 34% •
9	AH	127	52% 39% 58% •
10	AI	126	44% 31% 60% 10%
11	AJ	96	59% 31% 60% 7% •
12	AK	116	69% 43% 50% 7%
13	AL	101	38% 40% 55% 5%
14	AM	115	63% 51% 43% 5%
15	AN	61	92% 43% 49% 8%
16	AO	86	35% 44% 56%
17	AP	78	36% 32% 64% •
18	AQ	79	47% 41% 54% 5%
19	AR	69	70% 35% 64% •
20	AS	87	57% 45% 47% 7% •
21	AT	83	28% 37% 52% 10% •
22	B0	2740	43% 27% 50% 22% •
23	B9	108	50% 44% 38% 18%
24	B2	222	55% 41% 51% 7% •
25	B3	119	81% 23% 63% 12% •
25	B5	119	96% 30% 59% 11%
26	BA	227	53% 29% 44% 20% 7%
27	BB	209	53% 31% 62% 7%
28	BC	198	36% 23% 61% 15% •
29	BD	177	52% 30% 47% 21% •

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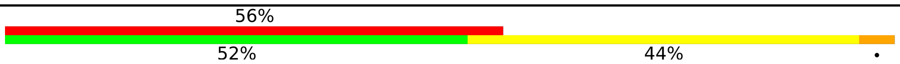
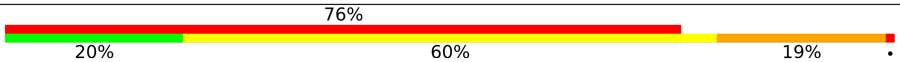
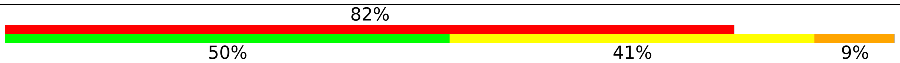
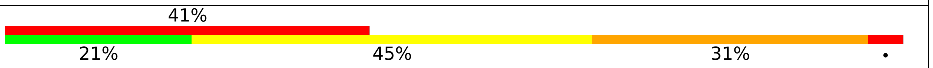
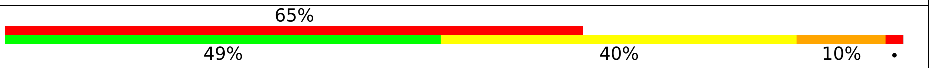
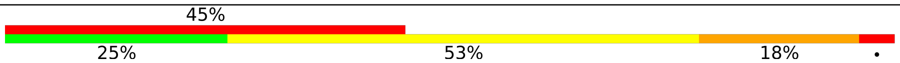
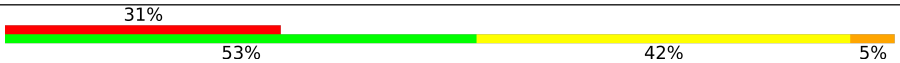
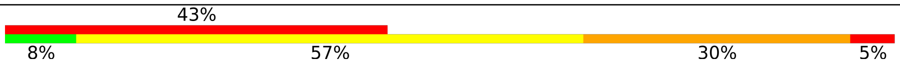
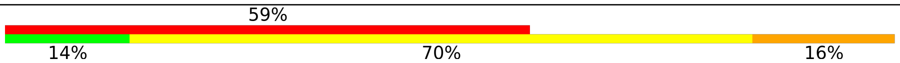
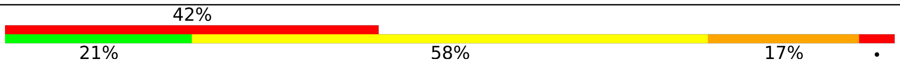
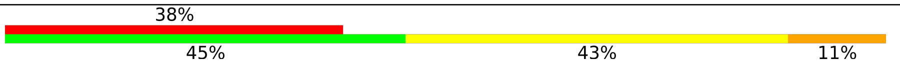
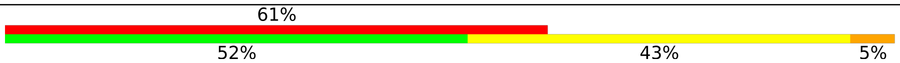
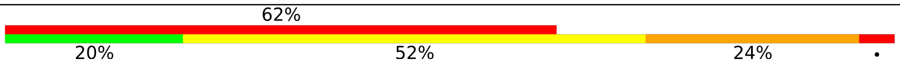
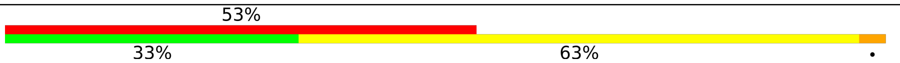
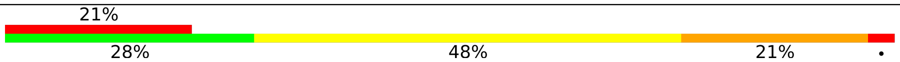
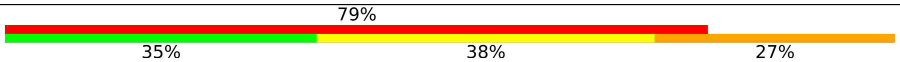
Mol	Chain	Length	Quality of chain
30	BE	167	
31	BF	149	
32	BG	139	
33	BH	142	
34	BI	122	
35	BJ	140	
36	BK	131	
37	BL	114	
38	BM	113	
39	BN	114	
40	BO	115	
41	BQ	106	
42	BR	92	
43	BS	99	
44	BT	94	
45	BU	84	
46	BW	60	
47	BX	56	
48	BZ	29	
49	B1	52	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 141668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1488	31924	14238	5854	10345	1487	0	0

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AU	76	1622	725	293	529	75	0	0
2	AV	76	1622	725	293	529	75	0	0
2	AW	76	1622	725	293	529	75	0	0

- Molecule 3 is a protein called 30S ribosomal subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	236	1847	1165	328	346	8	0	0

- Molecule 4 is a protein called 30S ribosomal subunit protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AC	206	1625	1028	305	289	3	0	0

- Molecule 5 is a protein called 30S ribosomal subunit protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AD	204	1638	1023	314	297	4	0	0

- Molecule 6 is a protein called 30S ribosomal subunit protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AE	148	1093	679	208	200	6	0	0

- Molecule 7 is a protein called 30S ribosomal subunit protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AF	95	784	495	143	140	6	0	0

- Molecule 8 is a protein called 30S ribosomal subunit protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AG	137	1079	671	204	200	4	0	0

- Molecule 9 is a protein called 30S ribosomal subunit protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AH	127	968	610	171	181	6	0	0

- Molecule 10 is a protein called 30S ribosomal subunit protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AI	126	1014	630	204	177	3	0	0

- Molecule 11 is a protein called 30S ribosomal subunit protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AJ	96	773	484	148	140	1	0	0

- Molecule 12 is a protein called 30S ribosomal subunit protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AK	116	870	535	173	159	3	0	0

- Molecule 13 is a protein called 30S ribosomal subunit protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AL	101	Total 787	C 486	N 159	O 138	S 4	0	0

- Molecule 14 is a protein called 30S ribosomal subunit protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AM	115	Total 892	C 552	N 179	O 158	S 3	0	0

- Molecule 15 is a protein called 30S ribosomal subunit protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AN	61	Total 500	C 310	N 108	O 80	S 2	0	0

- Molecule 16 is a protein called 30S ribosomal subunit protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AO	86	Total 697	C 430	N 139	O 127	S 1	0	0

- Molecule 17 is a protein called 30S ribosomal subunit protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AP	78	Total 622	C 390	N 122	O 109	S 1	0	0

- Molecule 18 is a protein called 30S ribosomal subunit protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AQ	79	Total 640	C 405	N 119	O 113	S 3	0	0

- Molecule 19 is a protein called 30S ribosomal subunit protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AR	69	Total 576	C 362	N 112	O 101	S 1	0	0

- Molecule 20 is a protein called 30S ribosomal subunit protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AS	87	695	443	132	118	2	0	0

- Molecule 21 is a protein called 30S ribosomal subunit protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AT	83	649	401	134	111	3	0	0

- Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	B0	2740	58824	26239	10826	19019	2740	0	0

- Molecule 23 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	B9	108	2310	1030	423	750	107	0	0

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	B2	222	1652	1031	301	314	6	0	0

- Molecule 25 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	B3	119	845	531	137	174	3	0	0
			Total	C	N	O	S		
25	B5	119	845	531	137	174	3	0	0

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BA	227	1733	1064	352	311	6	0	0

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BB	209	1565	979	288	294	4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BC	198	1531	960	280	287	4	0	0

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BD	177	1415	902	250	257	6	0	0

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BE	167	1253	789	228	234	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BF	149	1111	699	197	214	1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BG	139	1019	644	177	192	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BH	142	1129	714	212	199	4	0	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	122	Total	C	N	O	S	0	0
			939	588	180	166	5		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	140	Total	C	N	O	S	0	0
			1017	632	200	184	1		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	131	Total	C	N	O	S	0	0
			1036	661	200	171	4		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	114	Total	C	N	O	S	0	0
			908	564	184	156	4		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	BM	113	Total	C	N	O	0	0
			864	534	174	156		

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	115	Total	C	N	O	0	0
			937	598	190	149		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BQ	106	825	512	162	149	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BR	92	717	455	132	129	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	BS	99	762	480	143	139	0	0

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BT	94	753	479	137	134	3	0	0

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BU	84	634	391	129	113	1	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BW	60	495	305	96	92	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BX	56	435	272	84	77	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	BZ	29	234	145	47	42	0	0

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	B1	52	424	272	78	74	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: 16S ribosomal RNA

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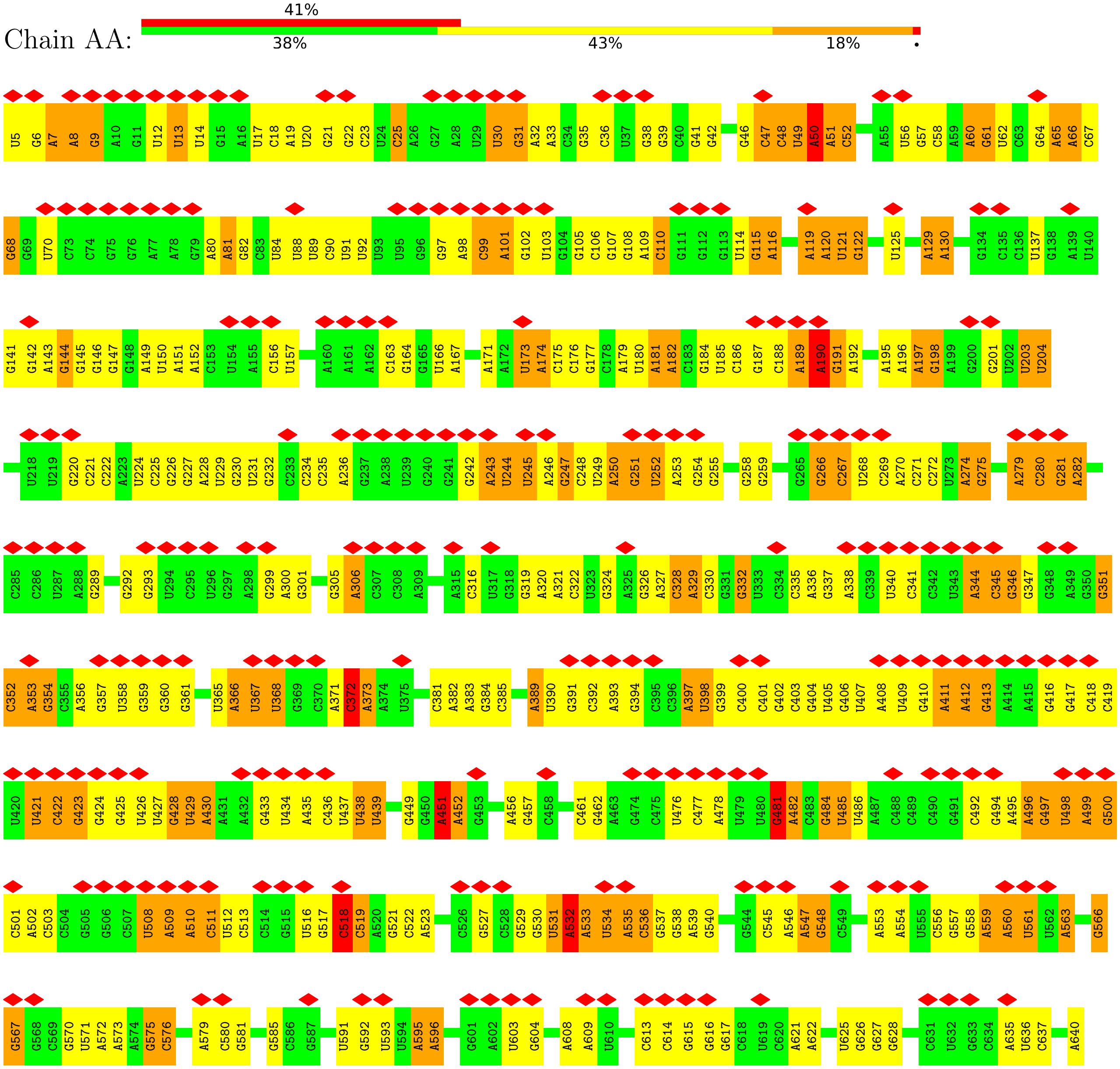

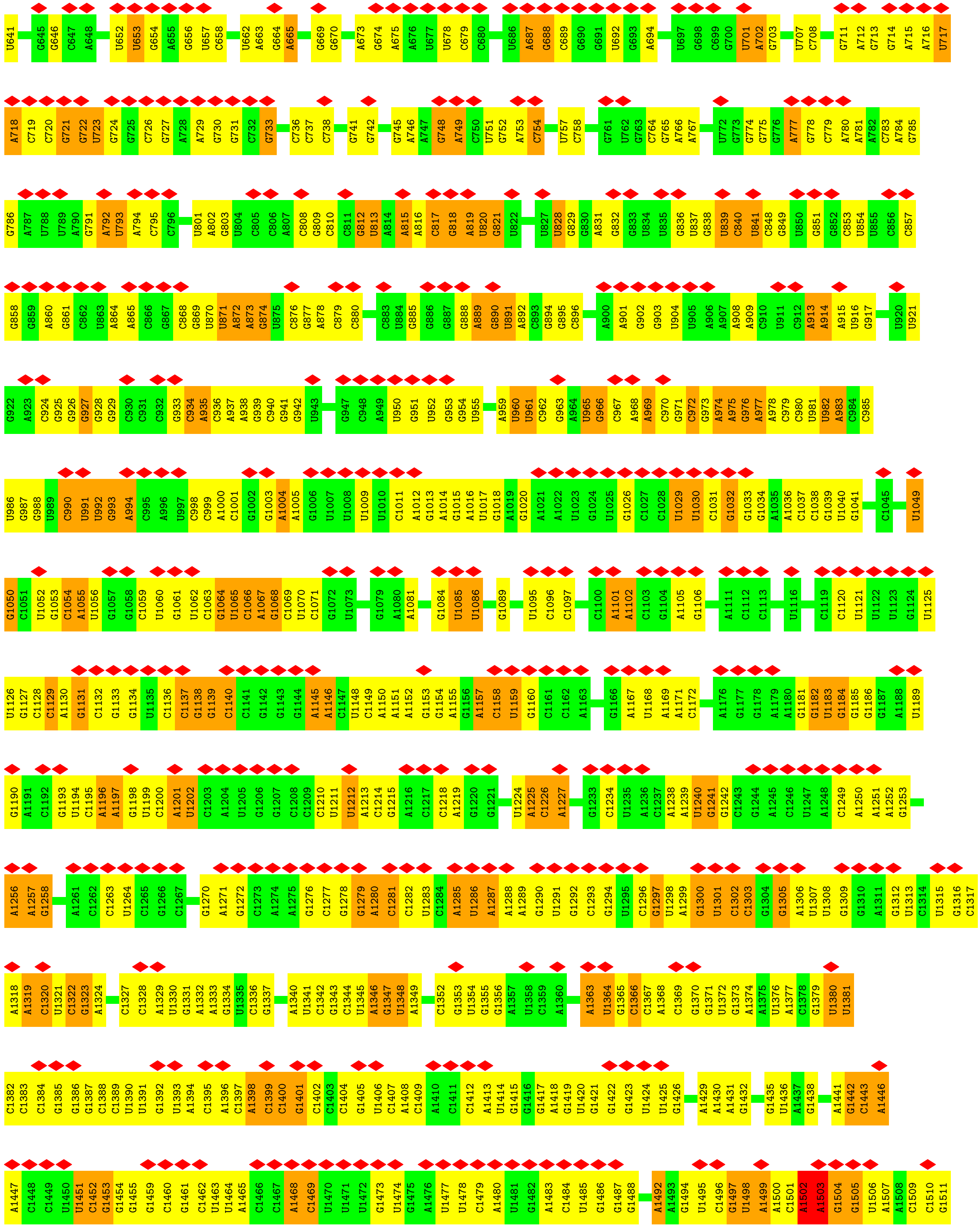
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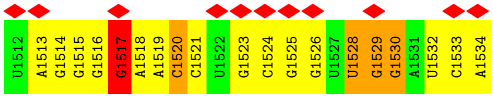

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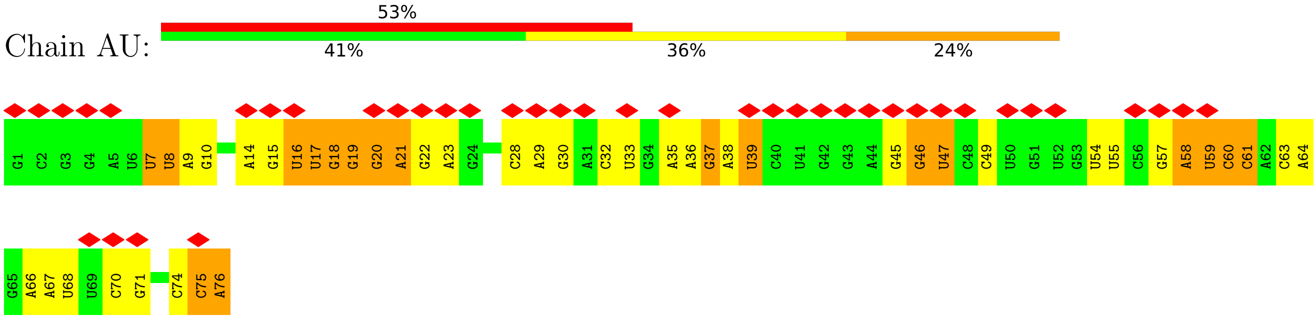

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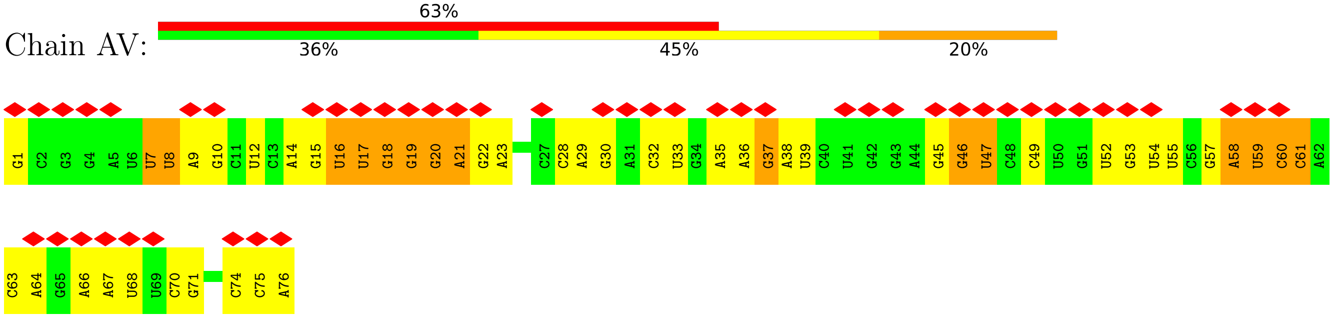
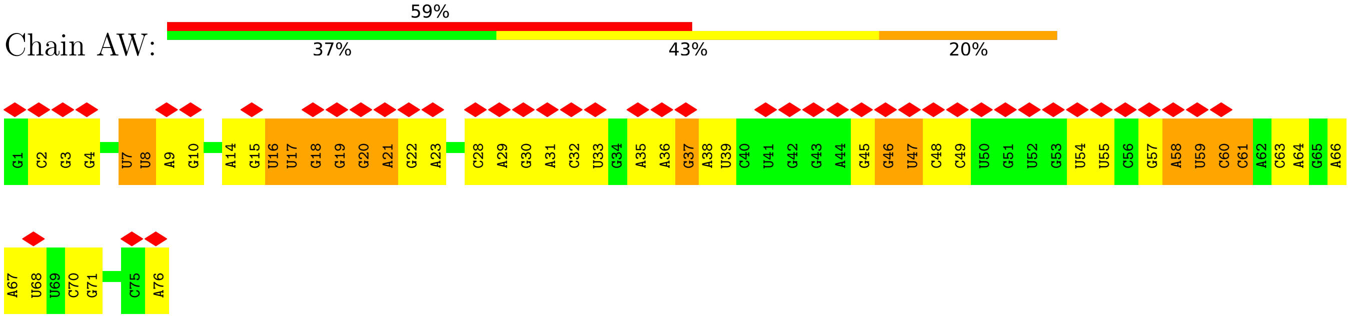
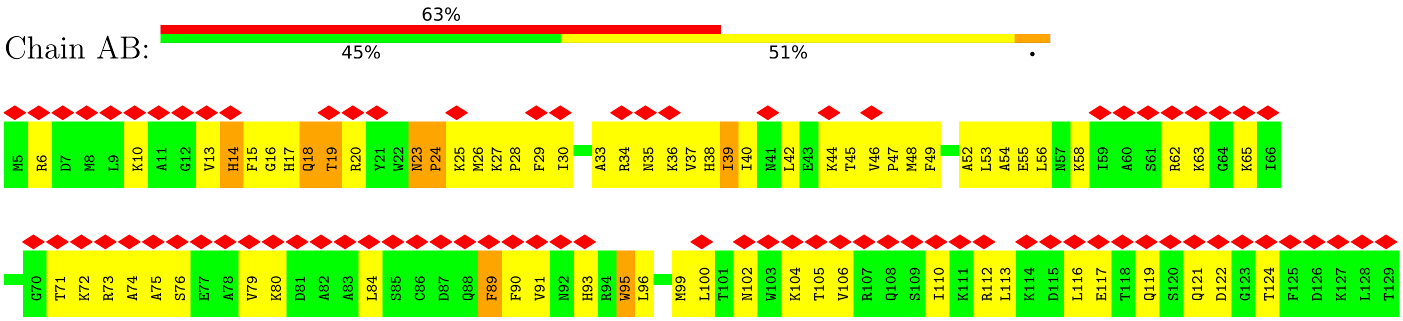
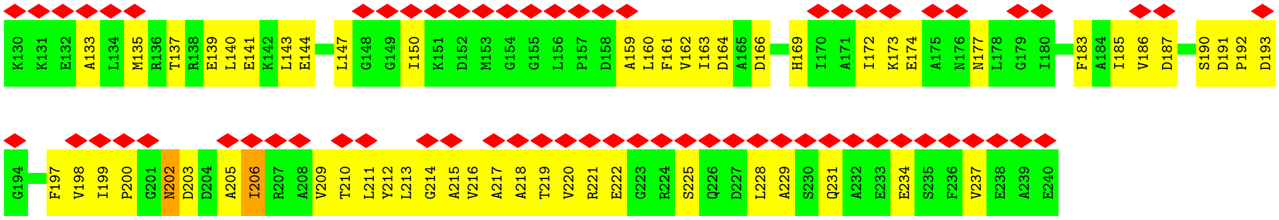


- Molecule 2: tRNA



- Molecule 3: 30S ribosomal subunit protein S2





- Molecule 4: 30S ribosomal subunit protein S3

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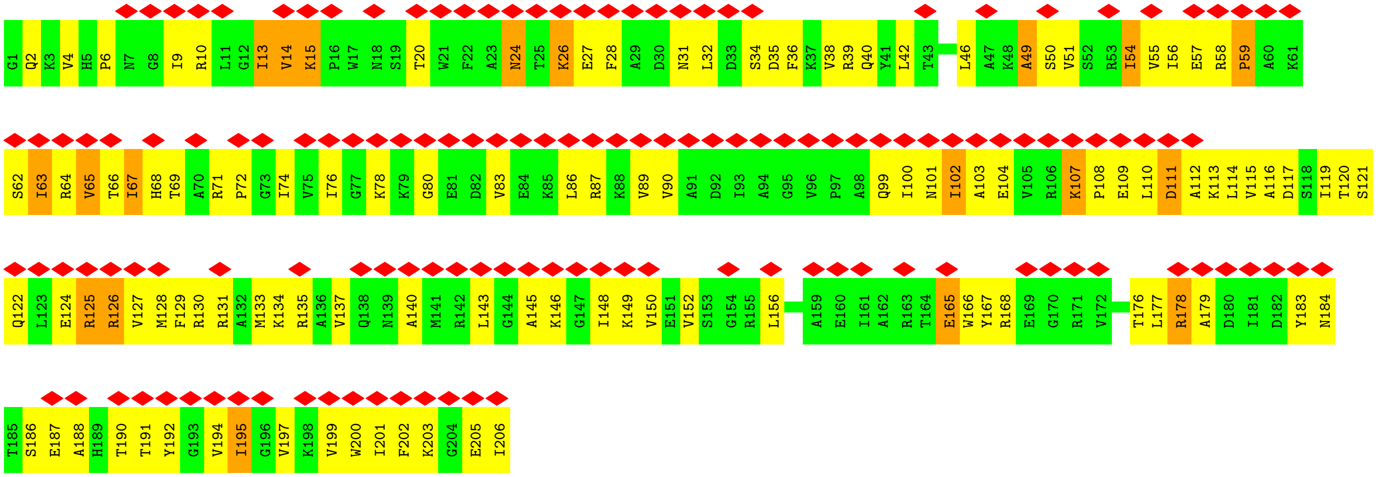
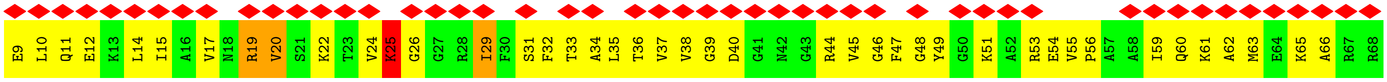


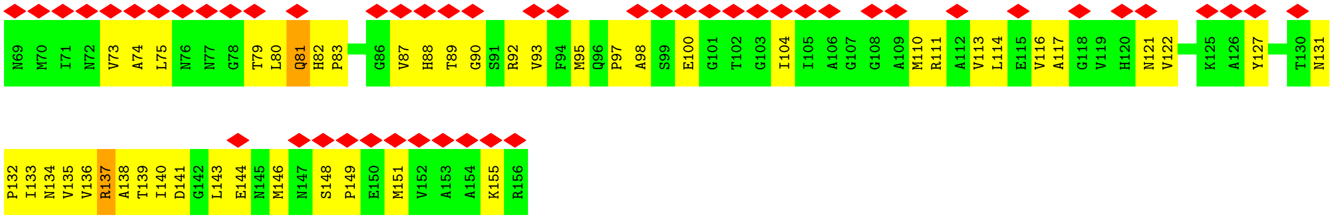
- Molecule 5: 30S ribosomal subunit protein S4

Chain AD:

- Molecule 6: 30S ribosomal subunit protein S5

Chain AE:





- Molecule 7: 30S ribosomal subunit protein S6

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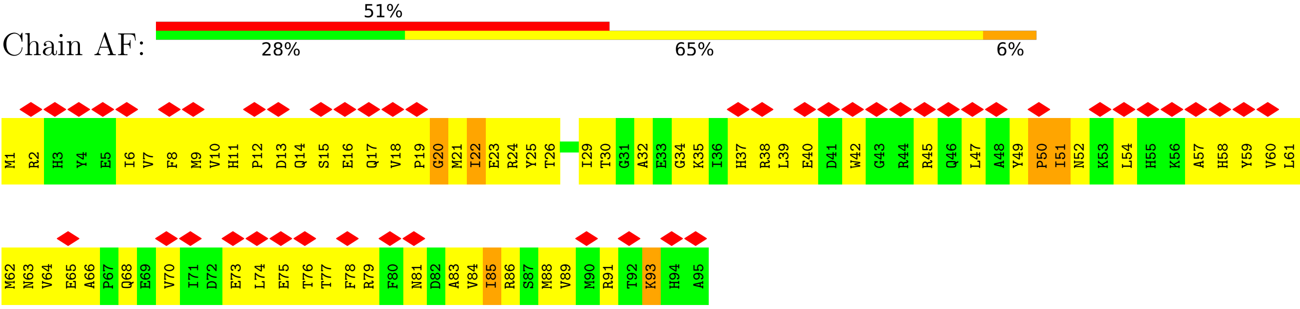

- Molecule 8: 30S ribosomal subunit protein S7

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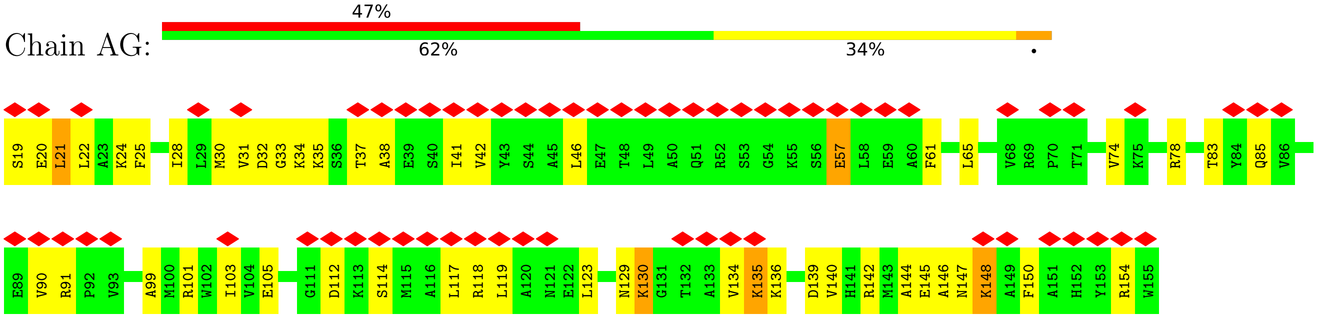

- Molecule 9: 30S ribosomal subunit protein S8

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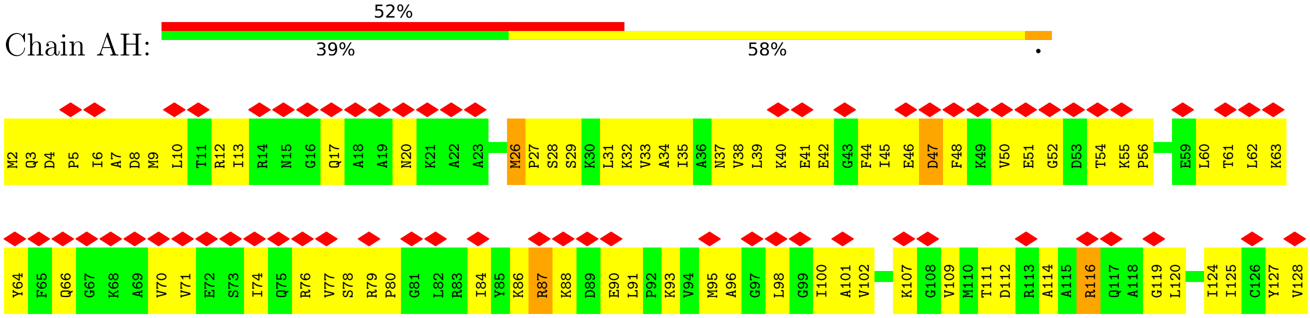

- Molecule 10: 30S ribosomal subunit protein S9

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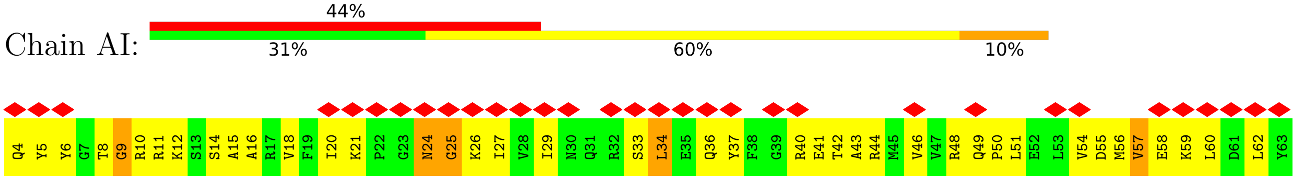

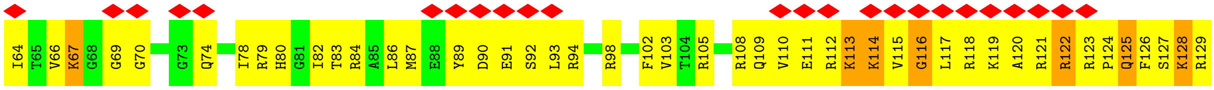

- Molecule 11: 30S ribosomal subunit protein S10

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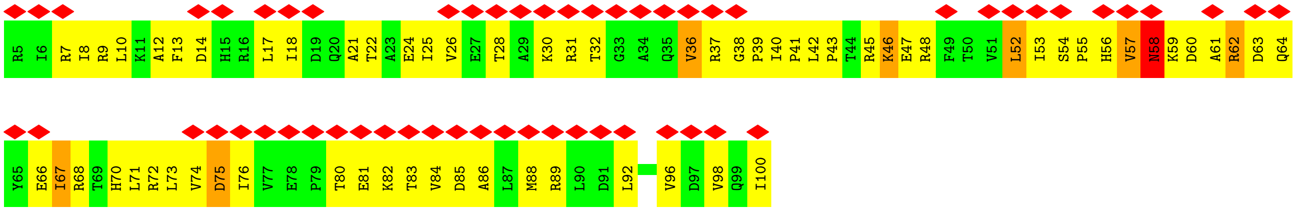

- Molecule 12: 30S ribosomal subunit protein S11

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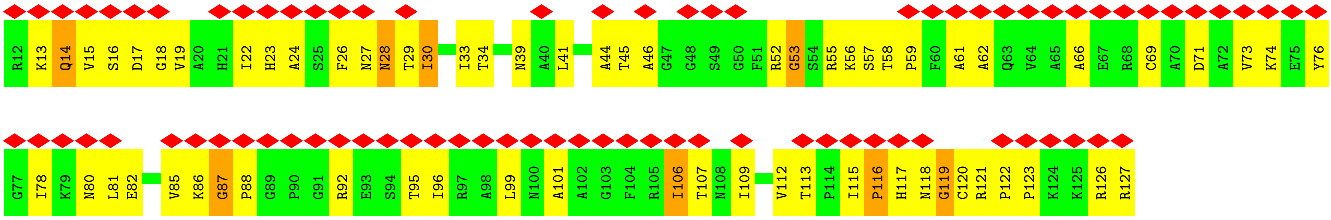
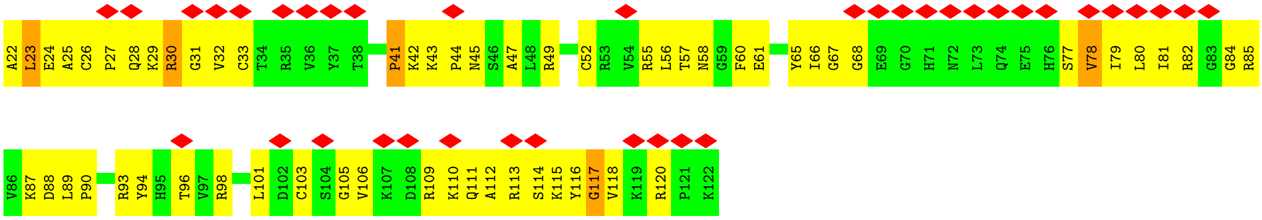


- Molecule 13: 30S ribosomal subunit protein S12

Chain AL:



- Molecule 14: 30S ribosomal subunit protein S13

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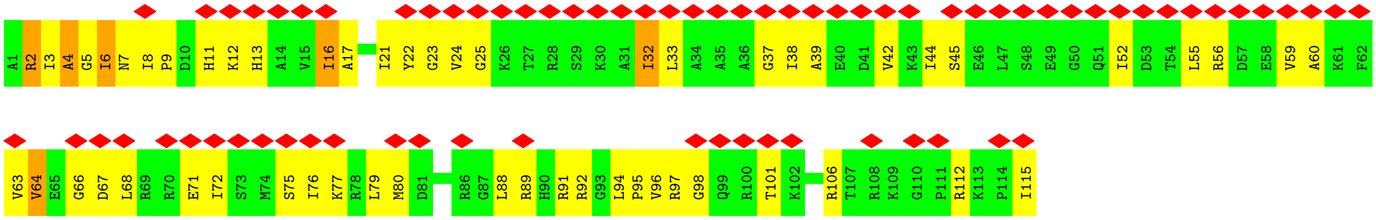
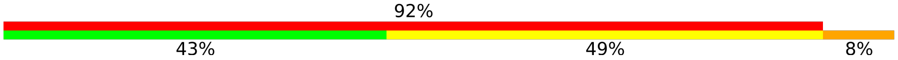
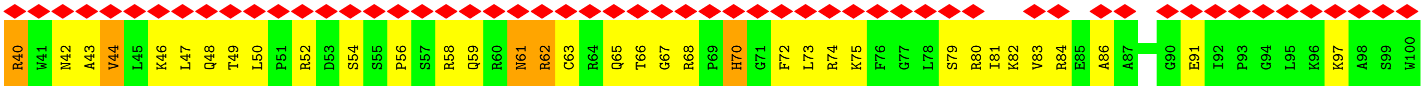


- Molecule 15: 30S ribosomal subunit protein S14

Chain AN:





- Molecule 16: 30S ribosomal subunit protein S15

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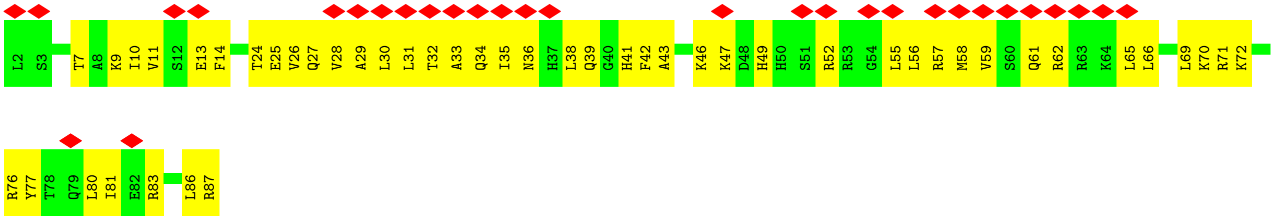

- Molecule 17: 30S ribosomal subunit protein S16

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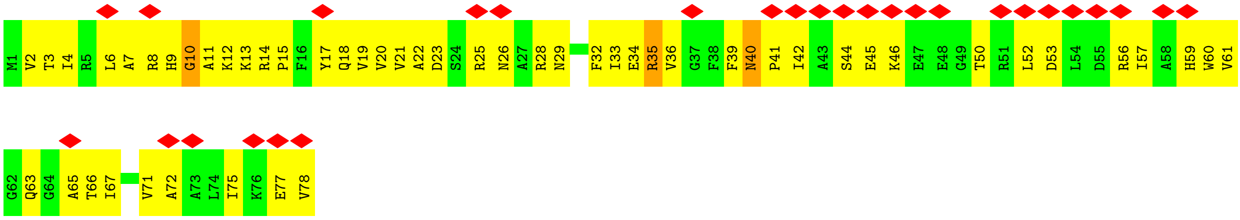

- Molecule 18: 30S ribosomal subunit protein S17

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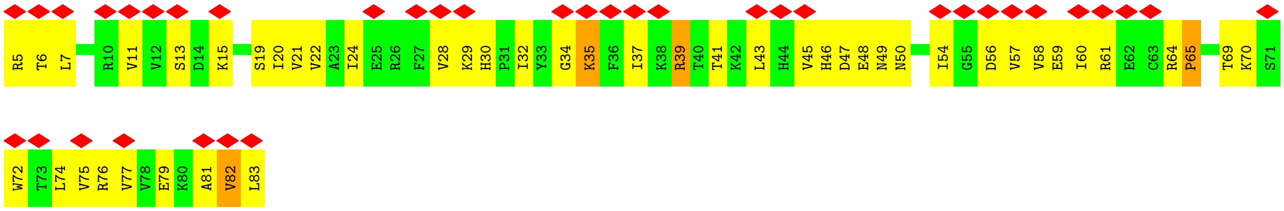

- Molecule 19: 30S ribosomal subunit protein S18

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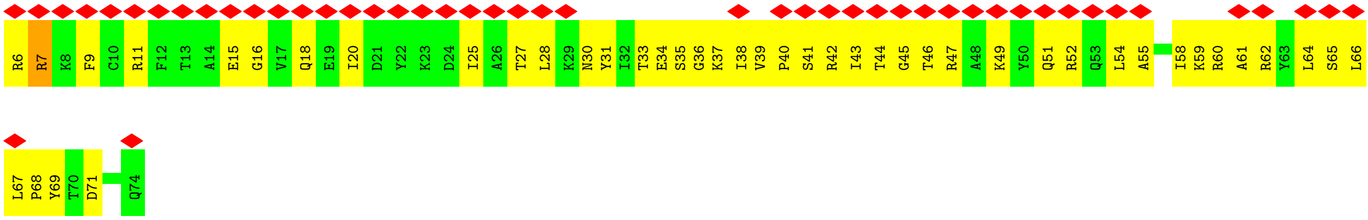
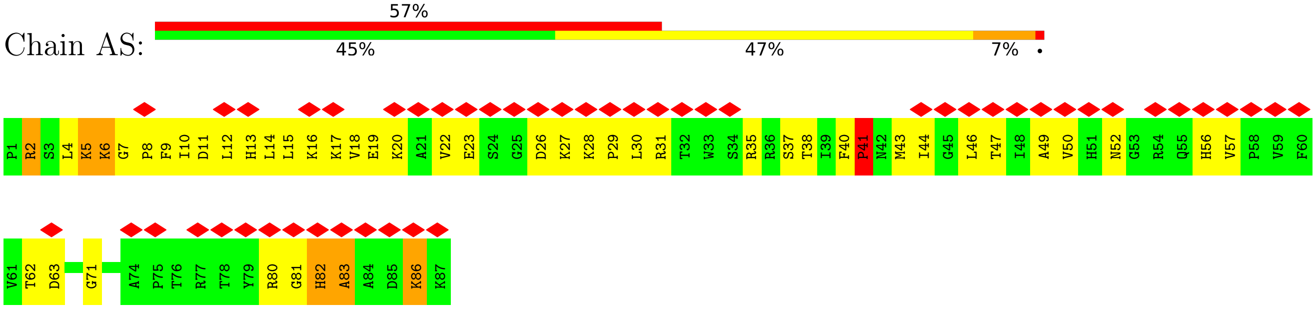
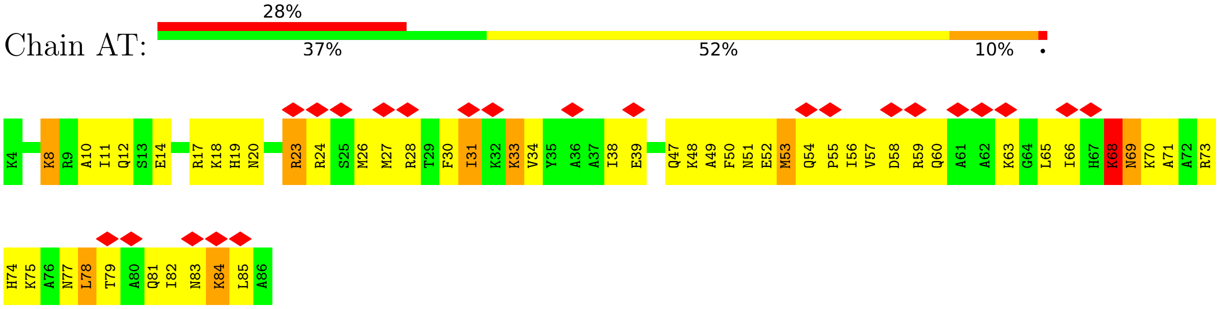


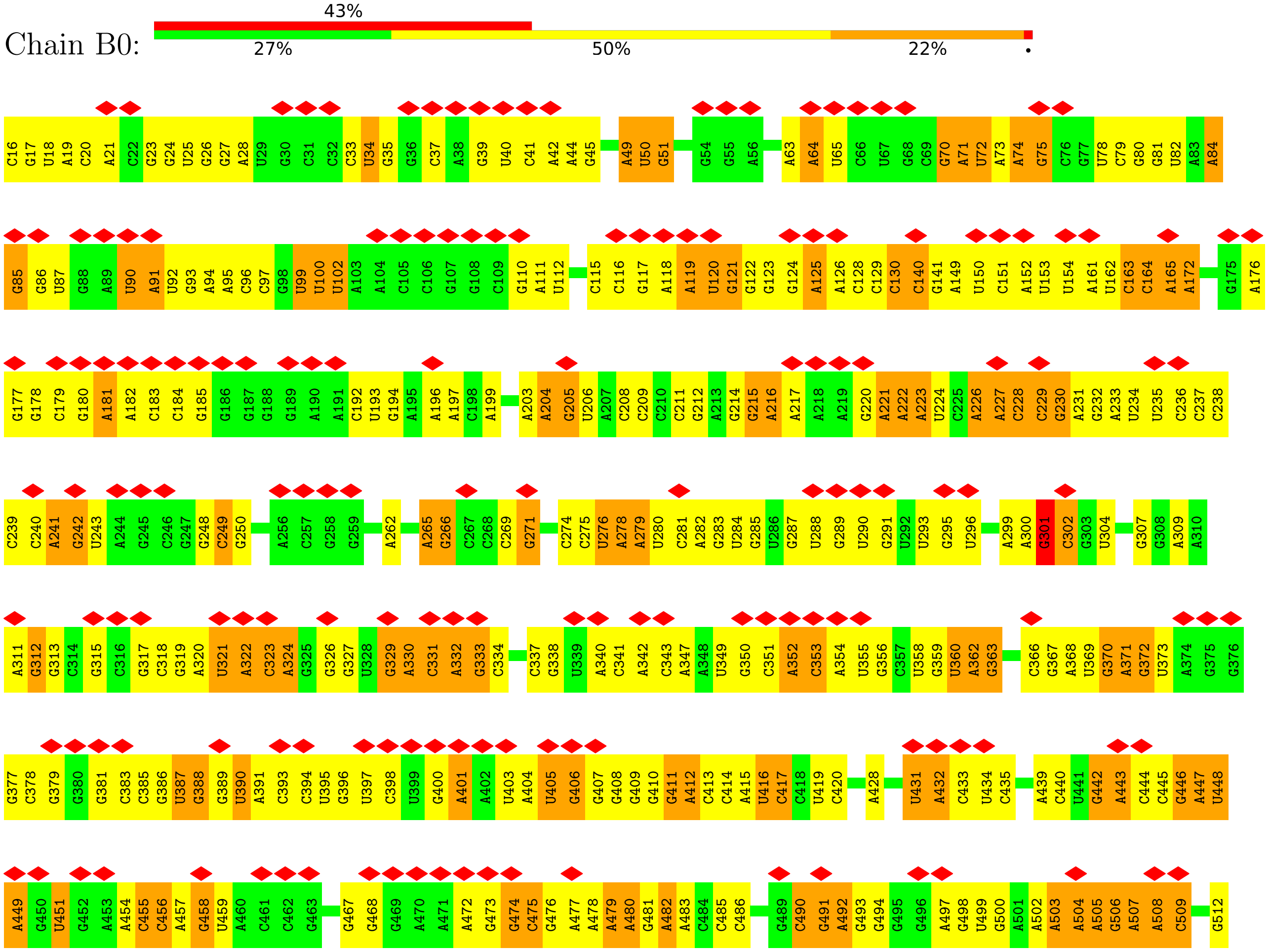
- Molecule 20: 30S ribosomal subunit protein S19

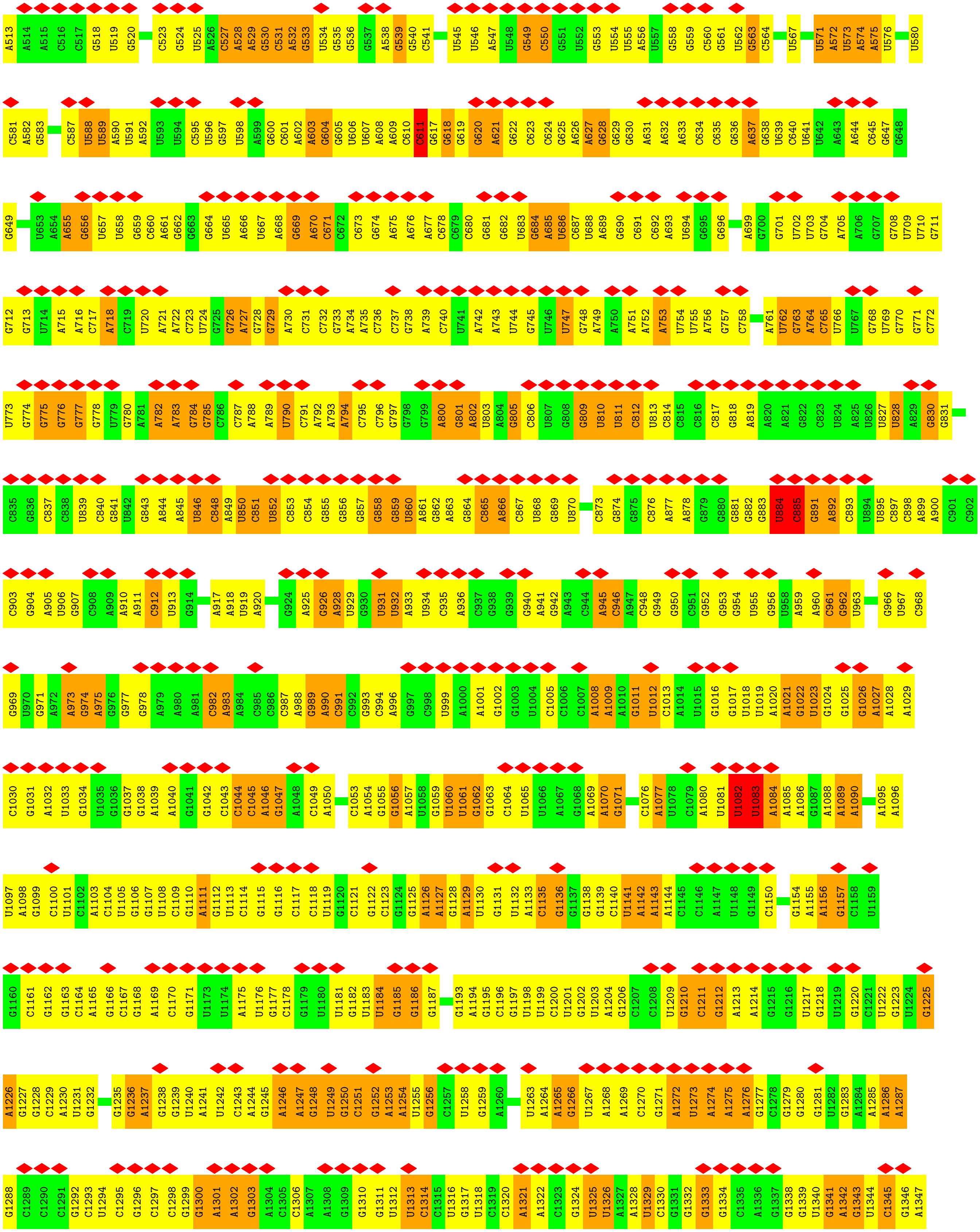


- Molecule 21: 30S ribosomal subunit protein S20



- Molecule 22: 23S ribosomal RNA

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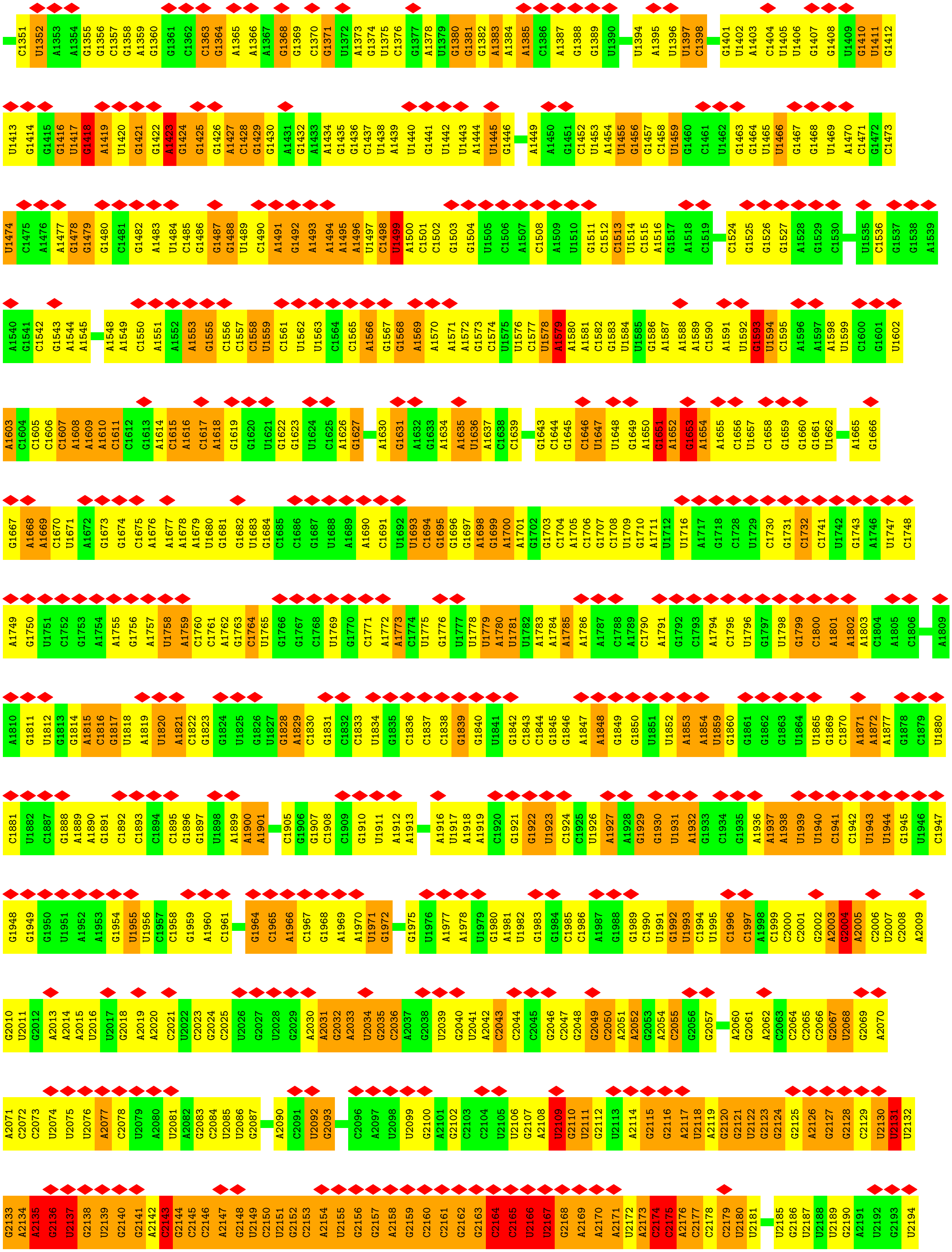
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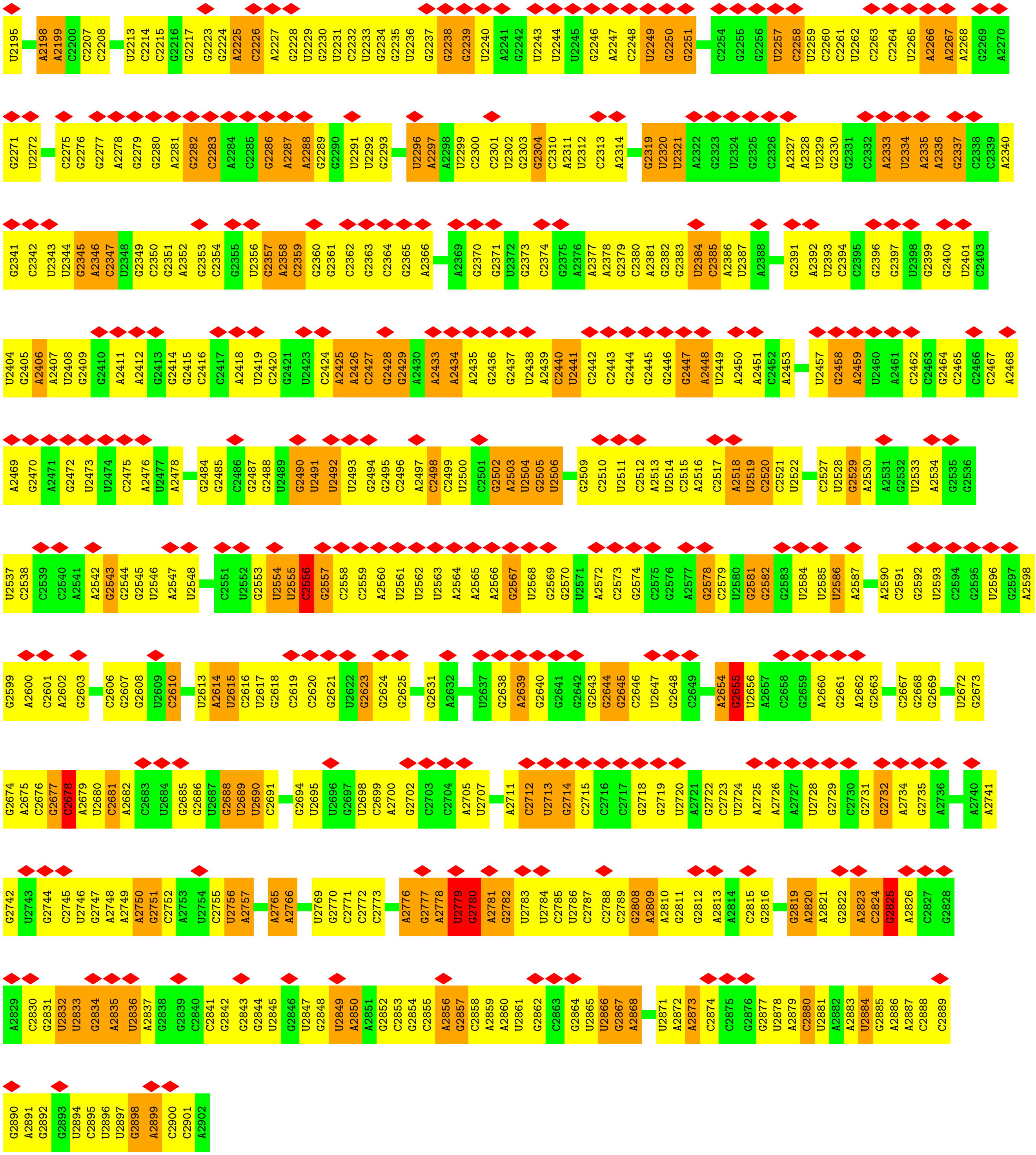
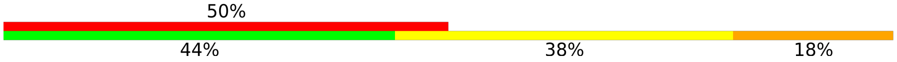
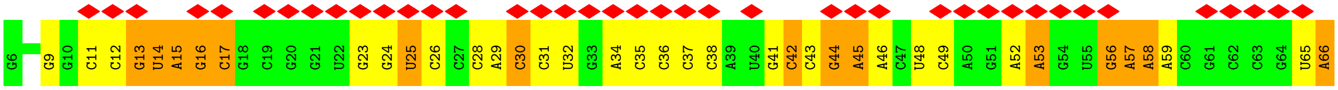
G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 G2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2185 G2186 U2187 U2188 U2189 G2190 A2191 U2192 G2193 U2194

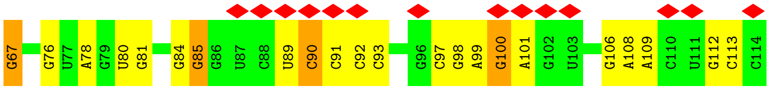


- Molecule 23: 5S ribosomal RNA

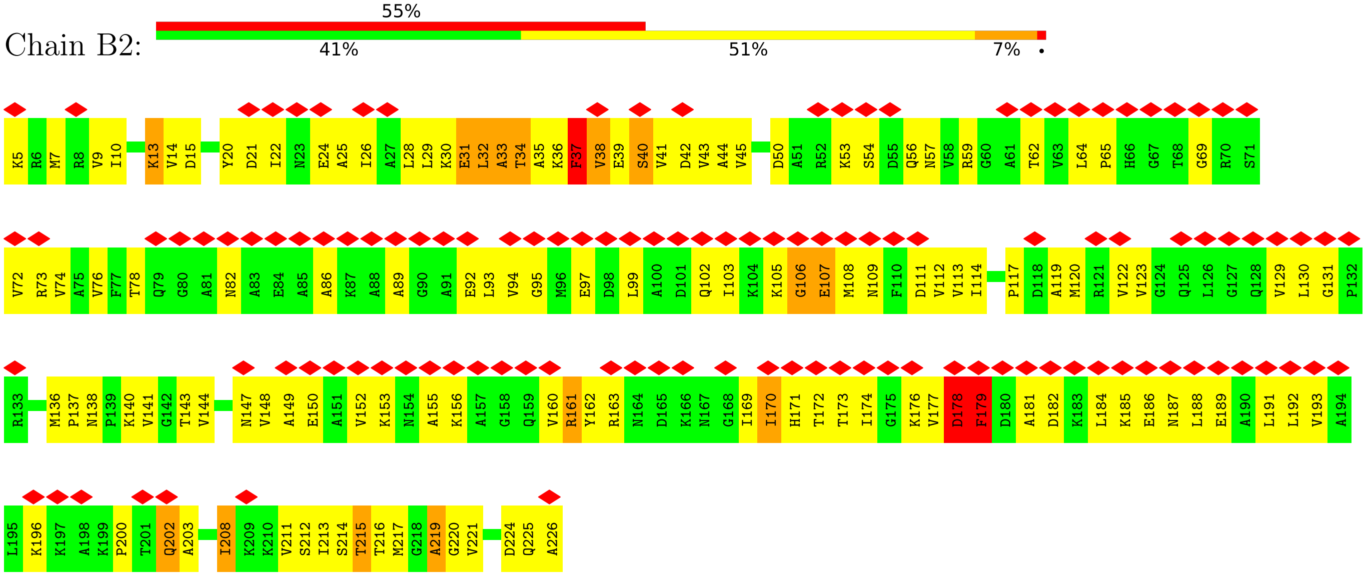
Chain B9:



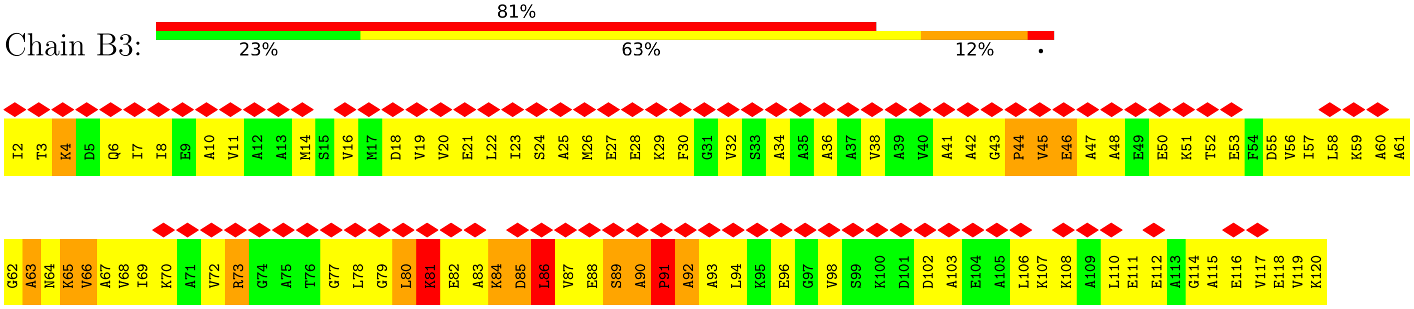




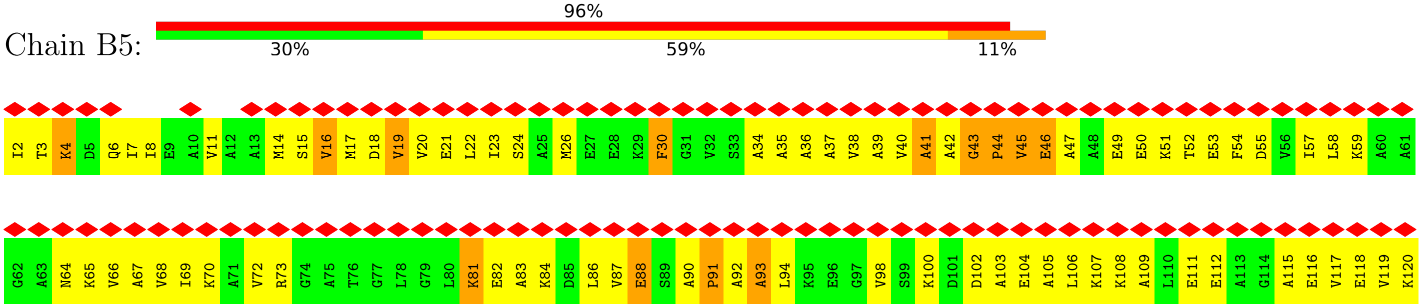
• Molecule 24: 50S ribosomal protein L1



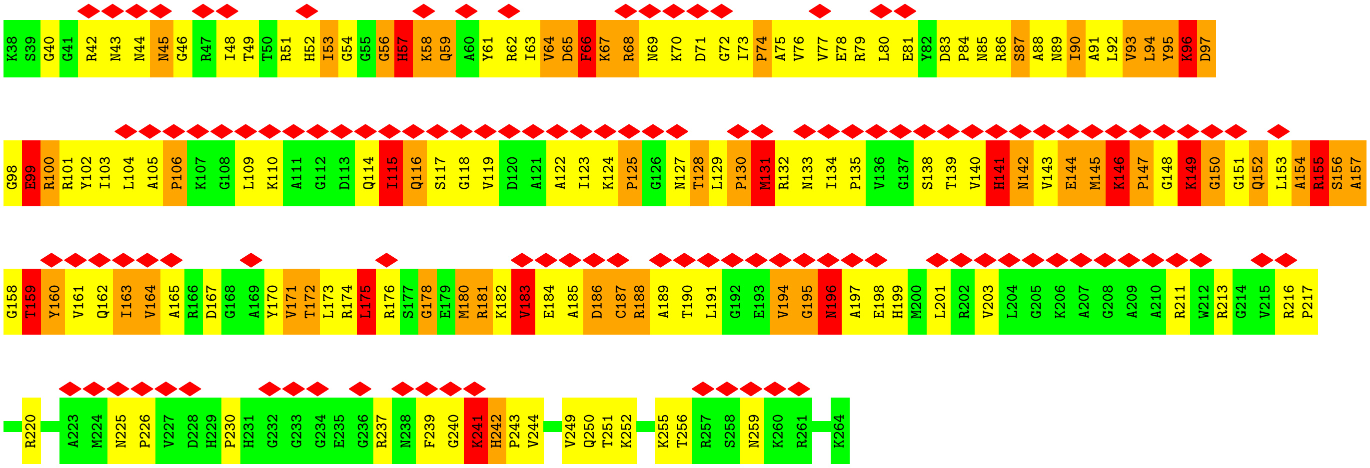
• Molecule 25: 50S ribosomal protein L7/L12



• Molecule 25: 50S ribosomal protein L7/L12

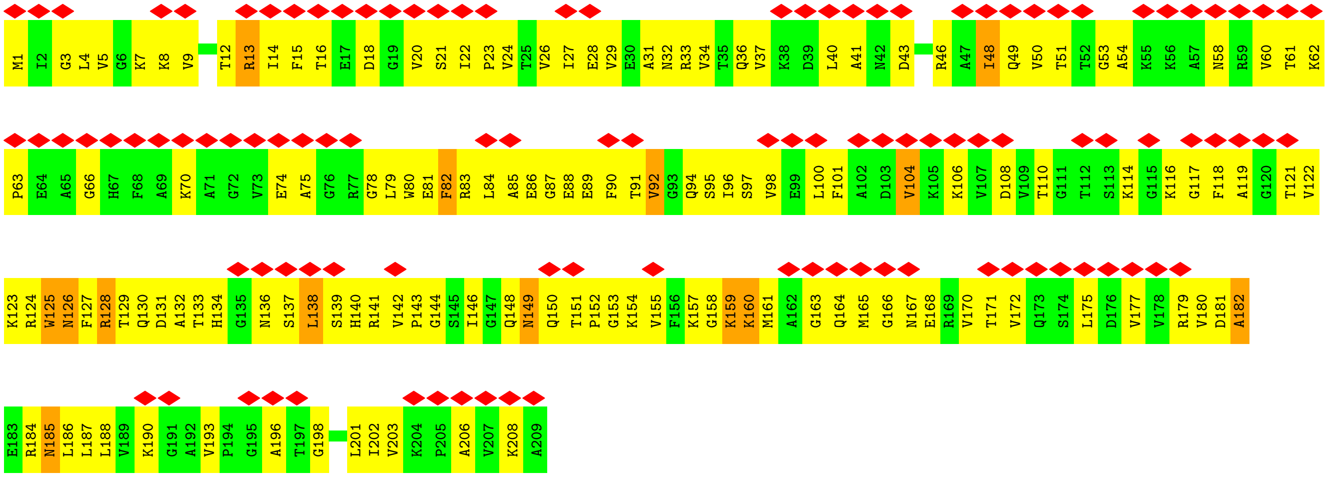


• Molecule 26: 50S ribosomal protein L2



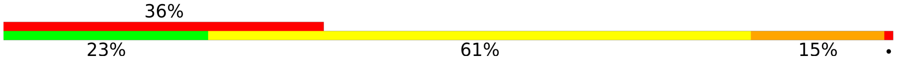
- Molecule 27: 50S ribosomal protein L3

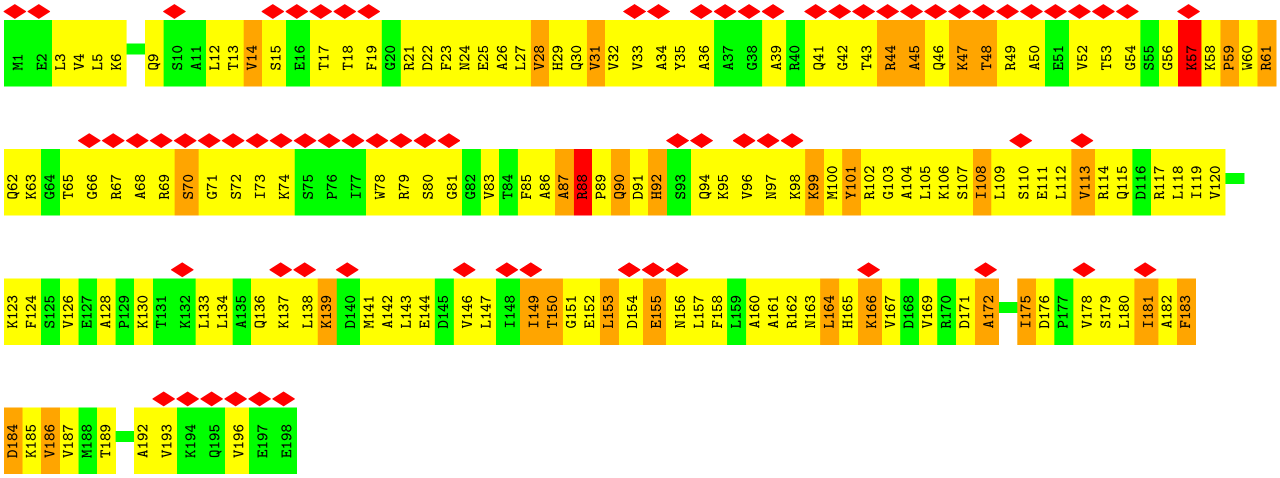
Chain BB:



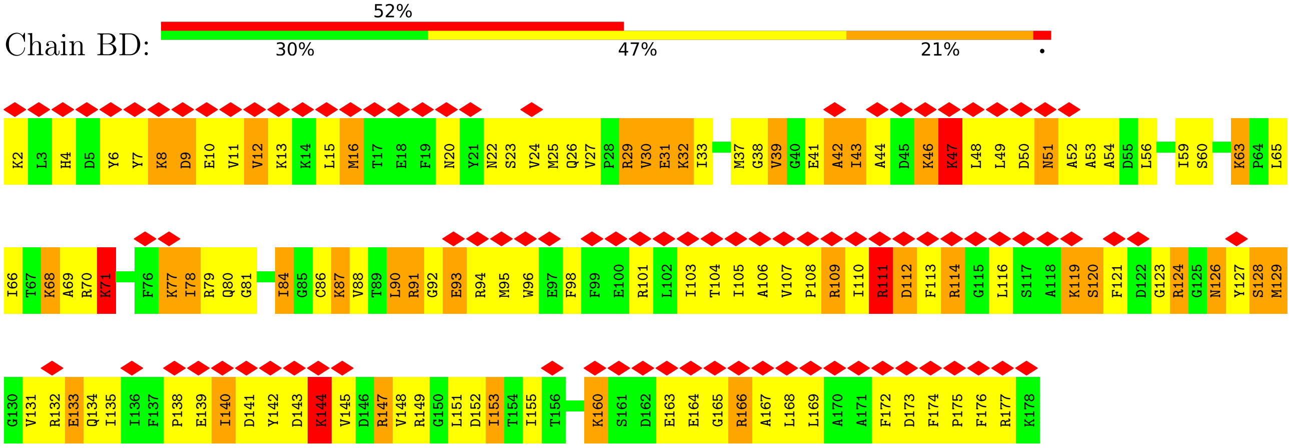
- Molecule 28: 50S ribosomal protein L4

Chain BC:

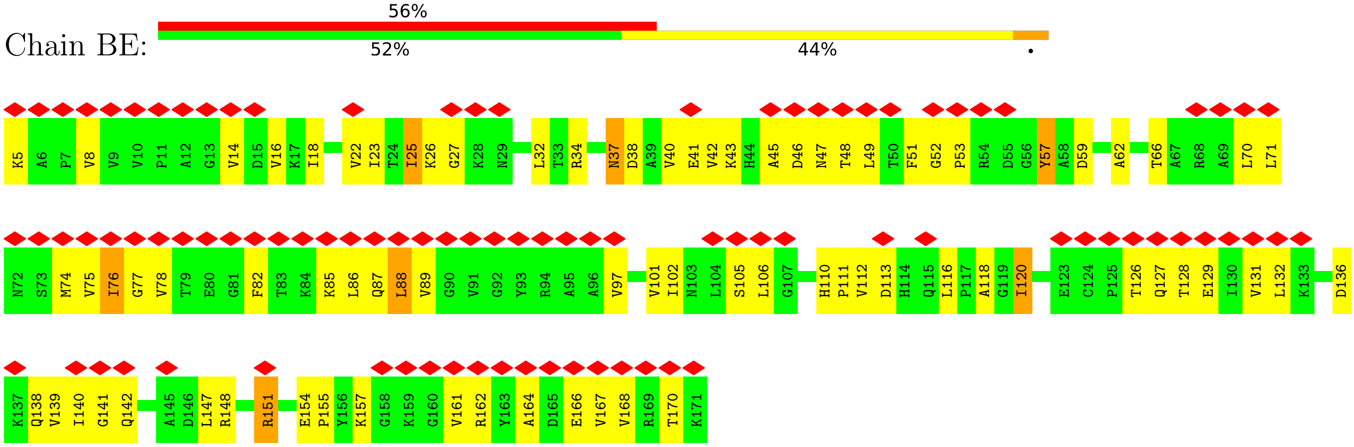




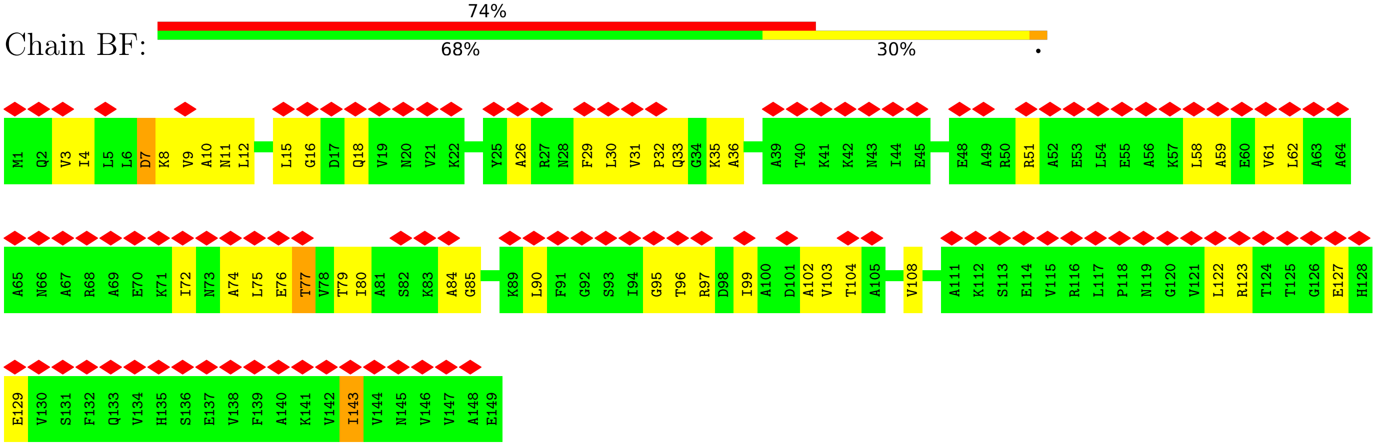
- Molecule 29: 50S ribosomal protein L5



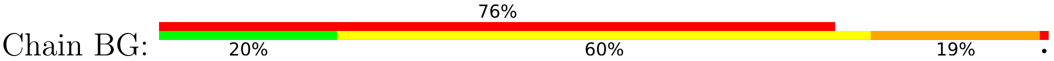
- Molecule 30: 50S ribosomal protein L6

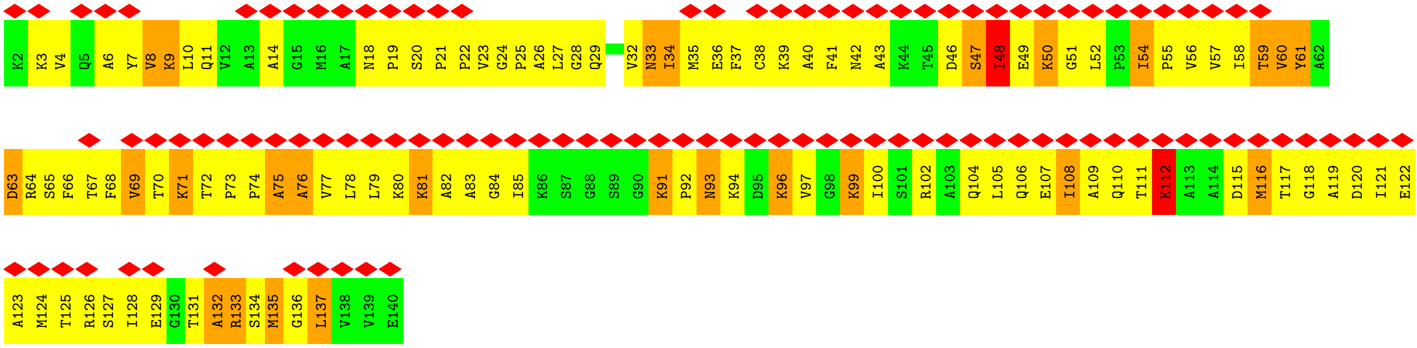


- Molecule 31: 50S ribosomal protein L9



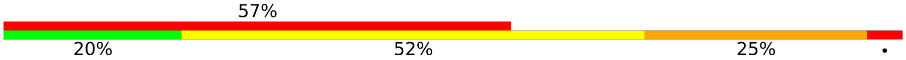
- Molecule 32: 50S ribosomal protein L11

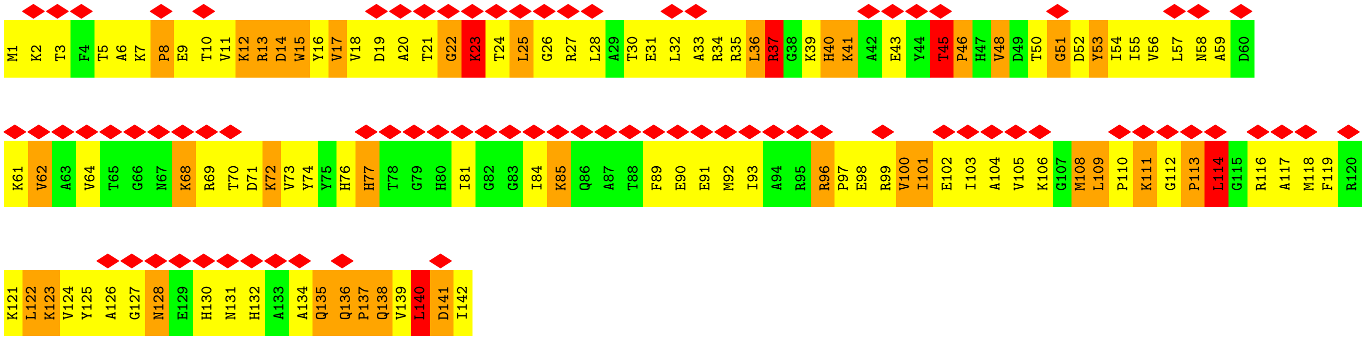




- Molecule 33: 50S ribosomal protein L13

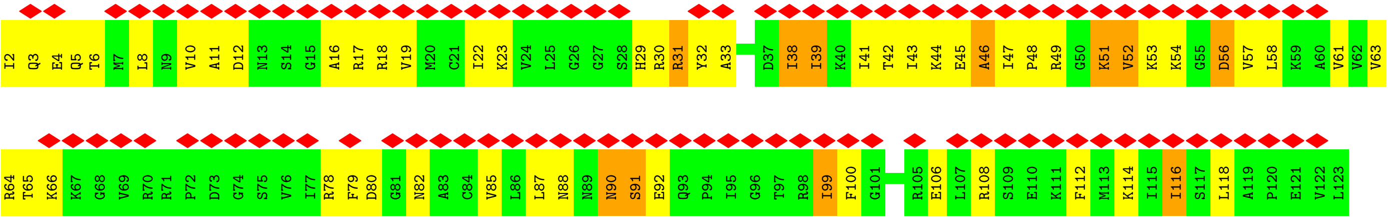
Chain BH:





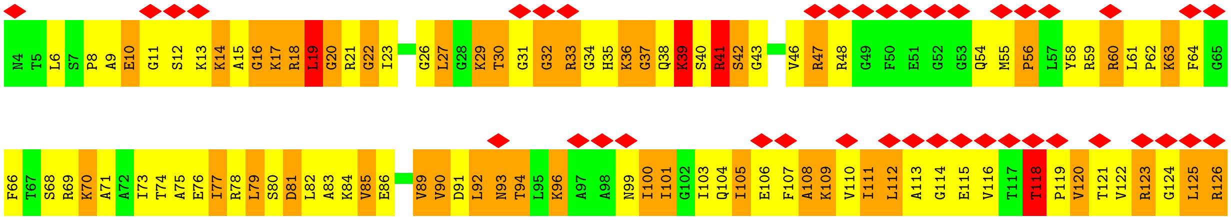
- Molecule 34: 50S ribosomal protein L14

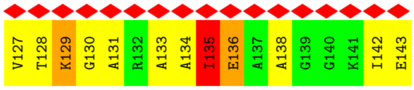
Chain BI:



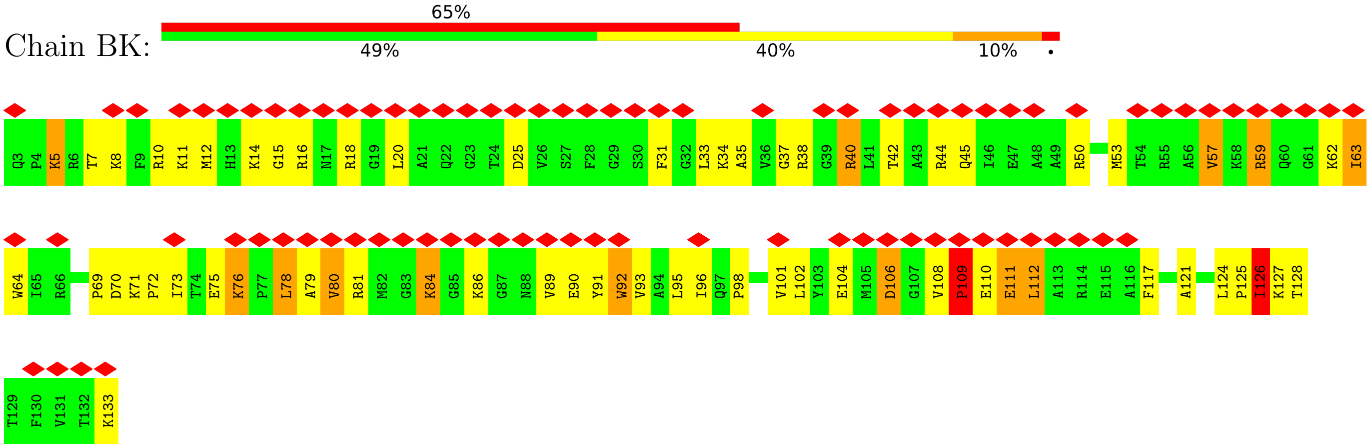
- Molecule 35: 50S ribosomal protein L15

Chain BJ:

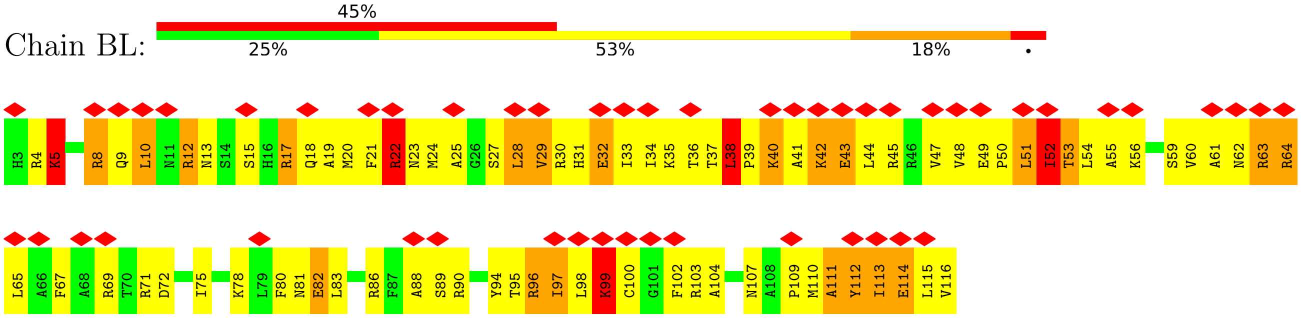




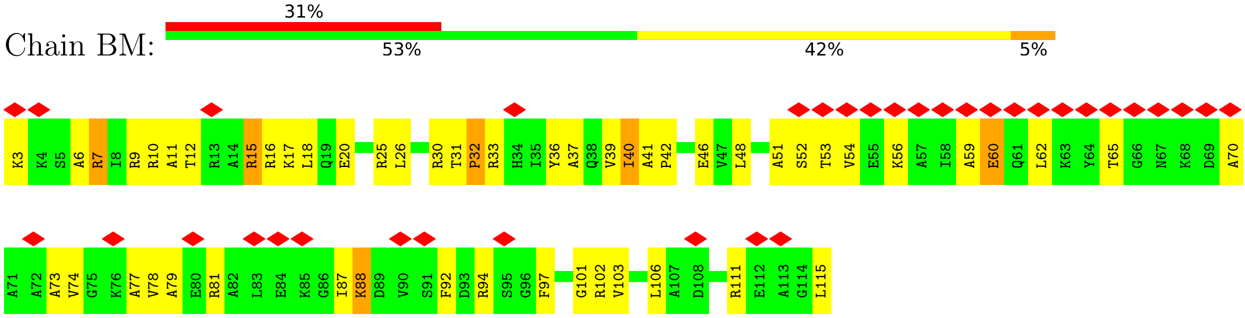
- Molecule 36: 50S ribosomal protein L16



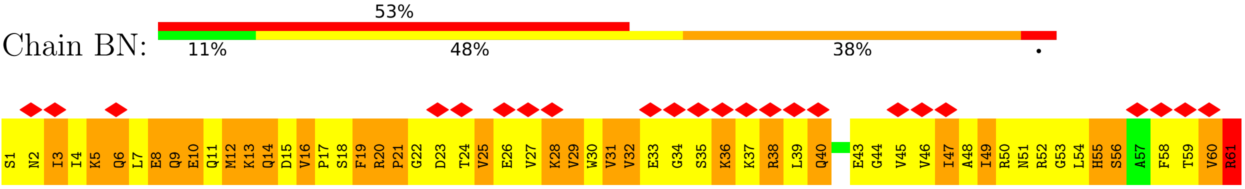
- Molecule 37: 50S ribosomal protein L17

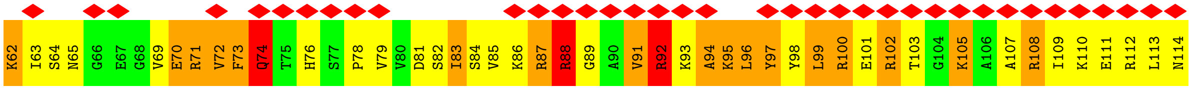


- Molecule 38: 50S ribosomal protein L18

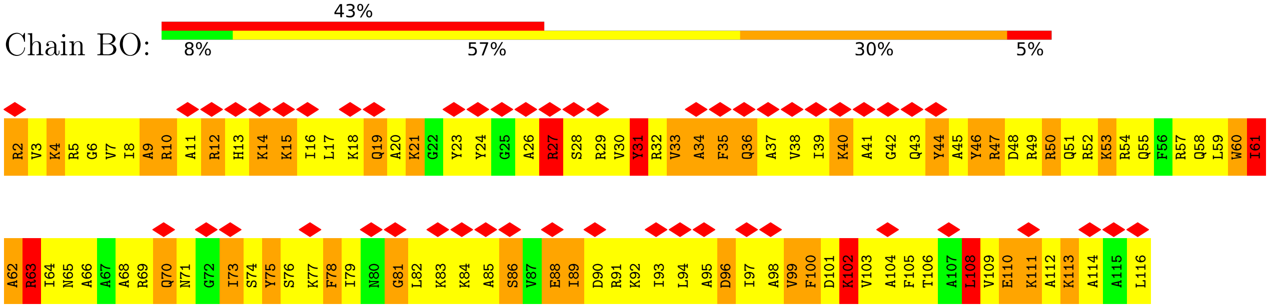


- Molecule 39: 50S ribosomal protein L19

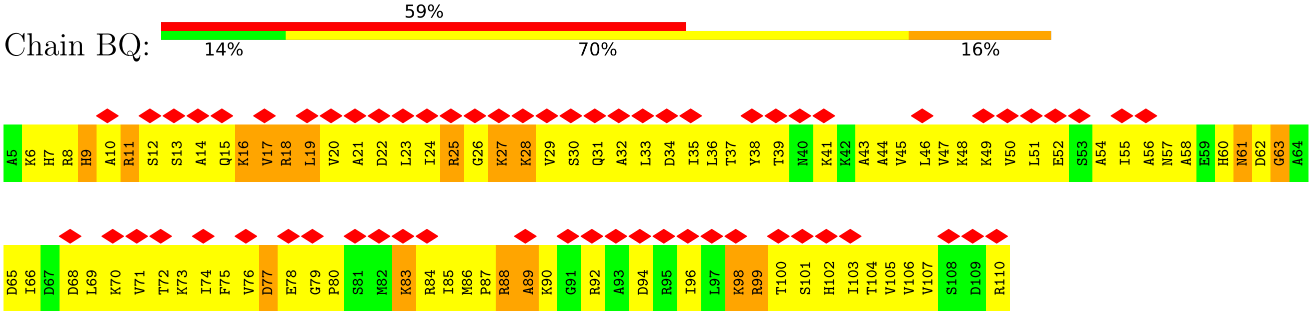




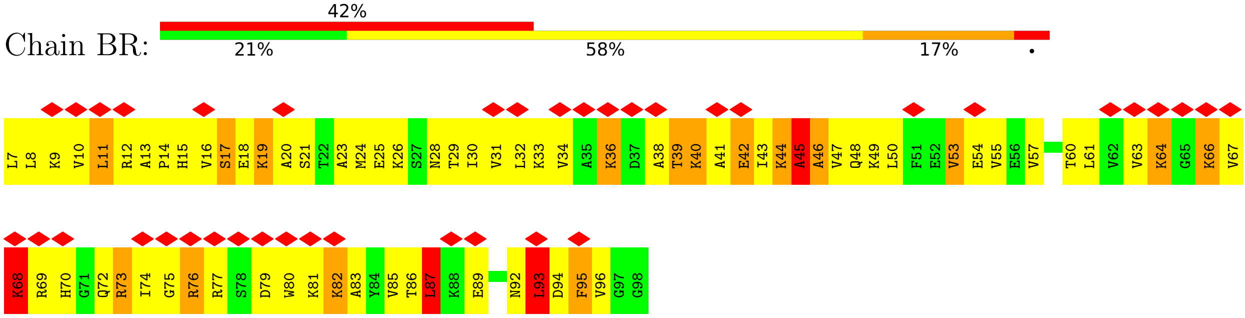
- Molecule 40: 50S RIBOSOMAL PROTEIN L20



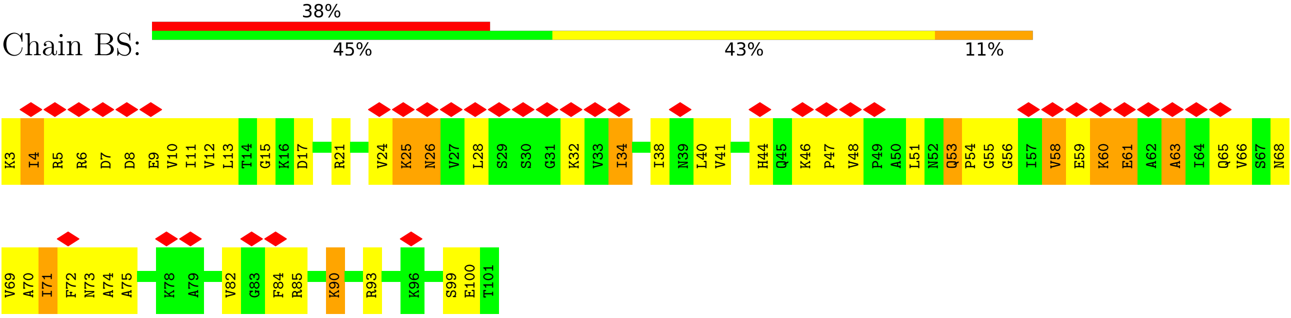
- Molecule 41: 50S ribosomal protein L22



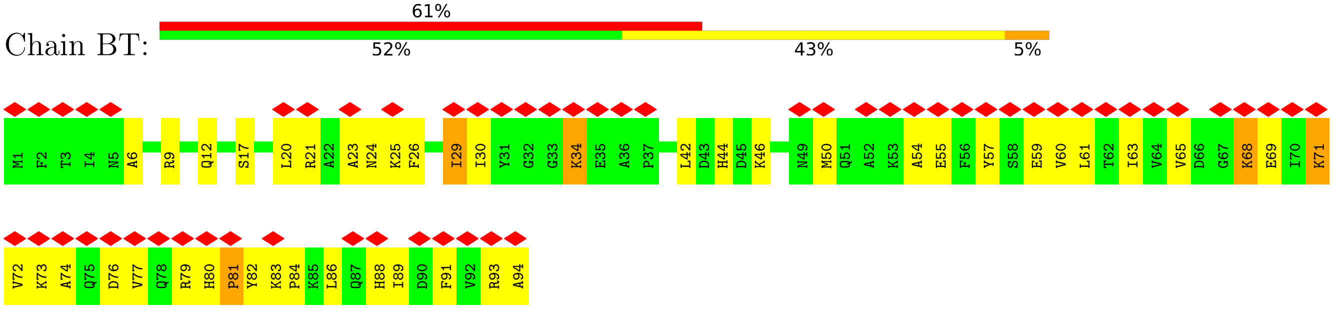
- Molecule 42: 50S ribosomal protein L23



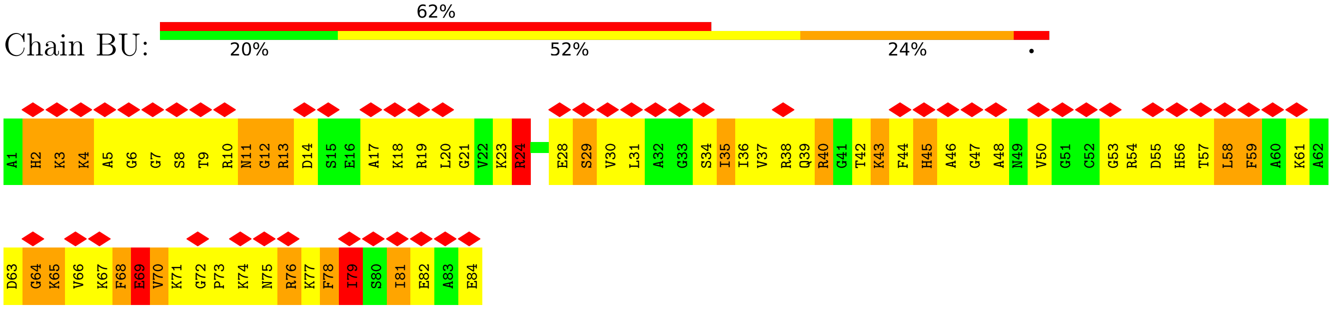
- Molecule 43: 50S ribosomal protein L24



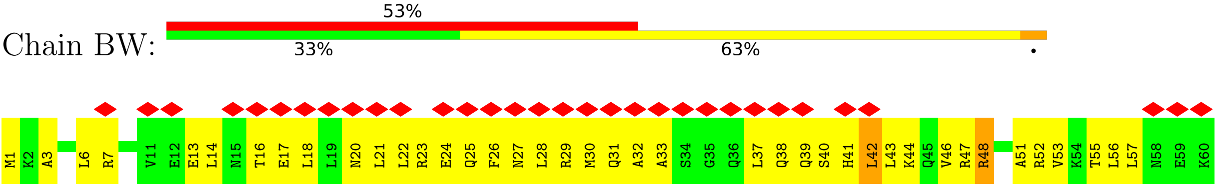
- Molecule 44: 50S ribosomal protein L25



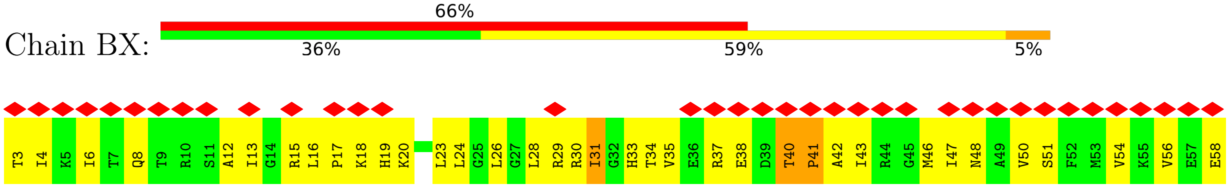
- Molecule 45: 50S ribosomal protein L27



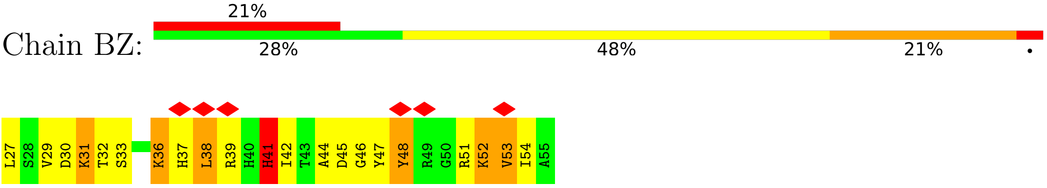
- Molecule 46: 50S ribosomal protein L29



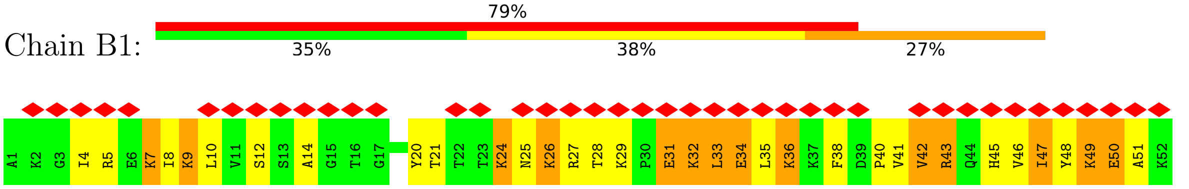
- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52181	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction of 3D-maps by Wiener filtration	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	1.1	Depositor
Maximum defocus (nm)	3.8	Depositor
Magnification	49696	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	250.773	Depositor
Minimum map value	-142.587	Depositor
Average map value	1.513	Depositor
Map value standard deviation	24.331	Depositor
Recommended contour level	43.4	Depositor
Map size (Å)	366.6, 366.6, 366.6	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.82, 2.82, 2.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.31	12/35745 (0.0%)	0.67	10/55764 (0.0%)
2	AU	1.35	6/1814 (0.3%)	2.20	9/2827 (0.3%)
2	AV	0.20	0/1814	0.66	0/2827
2	AW	0.20	0/1814	0.65	0/2827
3	AB	0.25	0/1877	0.42	0/2523
4	AC	0.23	0/1652	0.44	0/2225
5	AD	0.22	0/1660	0.41	0/2220
6	AE	0.24	0/1106	0.44	0/1488
7	AF	0.24	0/802	0.49	0/1081
8	AG	0.23	0/1093	0.42	0/1467
9	AH	0.23	0/978	0.45	0/1311
10	AI	0.24	0/1026	0.49	1/1364 (0.1%)
11	AJ	0.23	0/783	0.52	0/1058
12	AK	0.25	0/886	0.46	0/1195
13	AL	0.22	0/799	0.46	0/1070
14	AM	0.22	0/900	0.48	0/1201
15	AN	0.25	0/510	0.42	0/679
16	AO	0.23	0/705	0.42	0/942
17	AP	0.26	0/632	0.49	0/848
18	AQ	0.24	0/649	0.47	0/870
19	AR	0.25	0/585	0.40	0/782
20	AS	0.25	0/712	0.48	0/955
21	AT	0.26	0/655	0.40	0/866
22	B0	0.41	28/65882 (0.0%)	0.71	50/102783 (0.0%)
23	B9	0.21	0/2583	0.66	0/4028
24	B2	0.46	2/1665 (0.1%)	0.56	1/2240 (0.0%)
25	B3	0.43	0/846	0.67	1/1135 (0.1%)
25	B5	0.23	0/845	0.48	0/1132
26	BA	0.55	2/1759 (0.1%)	0.90	9/2356 (0.4%)
27	BB	0.27	0/1582	0.54	0/2122
28	BC	0.26	0/1549	0.57	0/2082
29	BD	0.26	0/1438	0.54	0/1927
30	BE	0.23	0/1273	0.46	0/1725
31	BF	0.24	0/1120	0.47	0/1509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BG	0.26	0/1032	0.69	1/1388 (0.1%)
33	BH	0.38	0/1152	0.80	5/1551 (0.3%)
34	BI	0.23	0/948	0.50	0/1269
35	BJ	0.27	0/1025	0.69	0/1363
36	BK	0.26	0/1055	0.52	0/1409
37	BL	0.26	0/920	0.72	2/1229 (0.2%)
38	BM	0.22	0/873	0.43	0/1170
39	BN	0.28	0/929	0.60	0/1242
40	BO	1.30	6/949 (0.6%)	3.63	12/1261 (1.0%)
41	BQ	0.24	0/832	0.69	1/1113 (0.1%)
42	BR	0.25	0/723	0.67	1/965 (0.1%)
43	BS	0.26	0/769	0.50	0/1023
44	BT	0.25	0/766	0.44	0/1025
45	BU	0.28	0/642	0.62	0/848
46	BW	0.23	0/496	0.45	0/658
47	BX	0.24	0/439	0.50	0/587
48	BZ	0.25	0/238	0.53	0/316
49	B1	0.27	0/431	0.51	0/572
All	All	0.39	56/153958 (0.0%)	0.75	103/230418 (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
1	AA	3	0
2	AU	0	1
22	B0	5	12
23	B9	0	1
26	BA	0	1
40	BO	0	1
All	All	8	16

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AU	39	U	C5-C6	32.23	1.63	1.34
22	B0	1499	U	N3-C4	30.48	1.65	1.38
22	B0	2131	U	N3-C4	28.17	1.63	1.38
22	B0	2136	G	C2-N3	26.30	1.53	1.32
2	AU	39	U	N1-C6	25.41	1.60	1.38

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	BO	100	PHE	CZ-CE2-CD2	-70.55	35.44	120.10
40	BO	100	PHE	CD1-CE1-CZ	-68.43	37.99	120.10
2	AU	39	U	N3-C4-C5	-67.79	73.93	114.60
40	BO	100	PHE	CE1-CZ-CE2	-53.38	23.91	120.00
2	AU	39	U	N1-C2-N3	-50.81	84.42	114.90

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	190	A	C1’
1	AA	1502	A	C1’
1	AA	1503	A	C1’
22	B0	301	G	C1’
22	B0	1593	G	C1’

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AU	39	U	Sidechain
22	B0	1417	U	Sidechain
22	B0	1418	G	Sidechain
22	B0	611	C	Sidechain
22	B0	884	U	Sidechain

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	AA	31924	0	16068	1365	0
2	AU	1622	0	820	98	0
2	AV	1622	0	821	63	0
2	AW	1622	0	821	61	0
3	AB	1847	0	1855	113	0
4	AC	1625	0	1699	163	0
5	AD	1638	0	1702	148	0
6	AE	1093	0	1132	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AF	784	0	776	98	0
8	AG	1079	0	1108	48	0
9	AH	968	0	1021	101	0
10	AI	1014	0	1064	148	0
11	AJ	773	0	812	137	0
12	AK	870	0	878	118	0
13	AL	787	0	825	86	0
14	AM	892	0	954	68	0
15	AN	500	0	526	54	0
16	AO	697	0	716	52	0
17	AP	622	0	637	75	0
18	AQ	640	0	678	52	0
19	AR	576	0	599	53	0
20	AS	695	0	725	107	0
21	AT	649	0	697	79	0
22	B0	58824	0	29589	4577	0
23	B9	2310	0	1173	65	0
24	B2	1652	0	1729	250	0
25	B3	845	0	880	418	0
25	B5	845	0	879	165	0
26	BA	1733	0	1766	956	0
27	BB	1565	0	1612	294	0
28	BC	1531	0	1593	456	0
29	BD	1415	0	1451	191	0
30	BE	1253	0	1289	79	0
31	BF	1111	0	1146	40	0
32	BG	1019	0	1076	168	0
33	BH	1129	0	1162	326	0
34	BI	939	0	1011	79	0
35	BJ	1017	0	1086	330	0
36	BK	1036	0	1109	91	0
37	BL	908	0	946	216	0
38	BM	864	0	902	61	0
39	BN	917	0	965	265	0
40	BO	937	0	1008	276	0
41	BQ	825	0	886	176	0
42	BR	717	0	773	166	0
43	BS	762	0	809	91	0
44	BT	753	0	780	39	0
45	BU	634	0	656	204	0
46	BW	495	0	530	53	0
47	BX	435	0	470	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BZ	234	0	235	49	0
49	B1	424	0	461	60	0
All	All	141668	0	94906	11577	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 49.

The worst 5 of 11577 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)
26:BA:155:ARG:NE	26:BA:155:ARG:CD	1.68	1.53
22:B0:1499:U:N3	26:BA:155:ARG:CD	1.67	1.52
22:B0:1083:U:C5’	25:B3:85:ASP:H	1.29	1.45
22:B0:2127:G:H3’	22:B0:2166:U:C5’	1.47	1.45
22:B0:2127:G:C8	22:B0:2166:U:H5”	1.52	1.42

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
3	AB	230/236 (98%)	192 (84%)	27 (12%)	11 (5%)	2 21
4	AC	204/206 (99%)	159 (78%)	33 (16%)	12 (6%)	1 17
5	AD	202/204 (99%)	180 (89%)	18 (9%)	4 (2%)	7 38
6	AE	146/148 (99%)	139 (95%)	5 (3%)	2 (1%)	11 46
7	AF	93/95 (98%)	81 (87%)	8 (9%)	4 (4%)	2 22
8	AG	135/137 (98%)	126 (93%)	8 (6%)	1 (1%)	22 63
9	AH	125/127 (98%)	114 (91%)	10 (8%)	1 (1%)	19 60
10	AI	124/126 (98%)	101 (82%)	14 (11%)	9 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AJ	94/96 (98%)	75 (80%)	13 (14%)	6 (6%)	1	16
12	AK	114/116 (98%)	96 (84%)	10 (9%)	8 (7%)	1	14
13	AL	99/101 (98%)	76 (77%)	18 (18%)	5 (5%)	2	19
14	AM	111/115 (96%)	100 (90%)	7 (6%)	4 (4%)	3	25
15	AN	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	1	15
16	AO	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
17	AP	76/78 (97%)	69 (91%)	6 (8%)	1 (1%)	12	48
18	AQ	77/79 (98%)	69 (90%)	6 (8%)	2 (3%)	5	31
19	AR	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
20	AS	85/87 (98%)	67 (79%)	12 (14%)	6 (7%)	1	14
21	AT	81/83 (98%)	68 (84%)	11 (14%)	2 (2%)	5	32
24	B2	216/222 (97%)	174 (81%)	29 (13%)	13 (6%)	1	17
25	B3	114/119 (96%)	90 (79%)	12 (10%)	12 (10%)	0	8
25	B5	113/119 (95%)	87 (77%)	16 (14%)	10 (9%)	1	11
26	BA	217/227 (96%)	121 (56%)	47 (22%)	49 (23%)	0	1
27	BB	199/209 (95%)	157 (79%)	30 (15%)	12 (6%)	1	17
28	BC	194/198 (98%)	127 (66%)	41 (21%)	26 (13%)	0	5
29	BD	173/177 (98%)	94 (54%)	51 (30%)	28 (16%)	0	3
30	BE	165/167 (99%)	147 (89%)	16 (10%)	2 (1%)	13	50
31	BF	143/149 (96%)	121 (85%)	17 (12%)	5 (4%)	3	25
32	BG	135/139 (97%)	80 (59%)	37 (27%)	18 (13%)	0	5
33	BH	140/142 (99%)	78 (56%)	37 (26%)	25 (18%)	0	3
34	BI	120/122 (98%)	96 (80%)	19 (16%)	5 (4%)	3	22
35	BJ	136/140 (97%)	70 (52%)	33 (24%)	33 (24%)	0	1
36	BK	129/131 (98%)	97 (75%)	25 (19%)	7 (5%)	2	19
37	BL	110/114 (96%)	68 (62%)	25 (23%)	17 (16%)	0	3
38	BM	111/113 (98%)	91 (82%)	16 (14%)	4 (4%)	3	25
39	BN	112/114 (98%)	46 (41%)	38 (34%)	28 (25%)	0	1
40	BO	111/115 (96%)	65 (59%)	28 (25%)	18 (16%)	0	3
41	BQ	104/106 (98%)	73 (70%)	25 (24%)	6 (6%)	1	18
42	BR	88/92 (96%)	43 (49%)	31 (35%)	14 (16%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BS	95/99 (96%)	71 (75%)	16 (17%)	8 (8%)	1	12
44	BT	92/94 (98%)	76 (83%)	12 (13%)	4 (4%)	2	22
45	BU	82/84 (98%)	37 (45%)	29 (35%)	16 (20%)	0	2
46	BW	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	9	42
47	BX	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
48	BZ	27/29 (93%)	11 (41%)	10 (37%)	6 (22%)	0	1
49	B1	50/52 (96%)	28 (56%)	13 (26%)	9 (18%)	0	3
All	All	5494/5639 (97%)	4152 (76%)	884 (16%)	458 (8%)	2	12

5 of 458 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	14	HIS
3	AB	225	SER
4	AC	14	VAL
4	AC	126	ARG
9	AH	47	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AB	195/195 (100%)	189 (97%)	6 (3%)	40	62
4	AC	170/170 (100%)	162 (95%)	8 (5%)	26	51
5	AD	172/172 (100%)	170 (99%)	2 (1%)	71	83
6	AE	112/112 (100%)	106 (95%)	6 (5%)	22	47
7	AF	83/83 (100%)	79 (95%)	4 (5%)	25	51
8	AG	112/112 (100%)	107 (96%)	5 (4%)	27	52
9	AH	103/103 (100%)	99 (96%)	4 (4%)	32	56
10	AI	104/104 (100%)	99 (95%)	5 (5%)	25	51
11	AJ	84/84 (100%)	79 (94%)	5 (6%)	19	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AK	89/89 (100%)	87 (98%)	2 (2%)	52	71
13	AL	85/85 (100%)	84 (99%)	1 (1%)	71	83
14	AM	93/93 (100%)	90 (97%)	3 (3%)	39	61
15	AN	52/52 (100%)	50 (96%)	2 (4%)	33	57
16	AO	74/74 (100%)	74 (100%)	0	100	100
17	AP	63/63 (100%)	61 (97%)	2 (3%)	39	61
18	AQ	73/73 (100%)	71 (97%)	2 (3%)	44	65
19	AR	60/60 (100%)	59 (98%)	1 (2%)	60	78
20	AS	75/75 (100%)	73 (97%)	2 (3%)	44	65
21	AT	63/63 (100%)	54 (86%)	9 (14%)	3	16
24	B2	172/172 (100%)	165 (96%)	7 (4%)	30	55
25	B3	83/83 (100%)	76 (92%)	7 (8%)	11	33
25	B5	83/83 (100%)	79 (95%)	4 (5%)	25	51
26	BA	176/176 (100%)	147 (84%)	29 (16%)	2	12
27	BB	164/164 (100%)	160 (98%)	4 (2%)	49	69
28	BC	163/163 (100%)	153 (94%)	10 (6%)	18	44
29	BD	149/149 (100%)	123 (83%)	26 (17%)	2	11
30	BE	130/130 (100%)	123 (95%)	7 (5%)	22	47
31	BF	114/114 (100%)	113 (99%)	1 (1%)	78	87
32	BG	108/108 (100%)	87 (81%)	21 (19%)	1	8
33	BH	116/116 (100%)	96 (83%)	20 (17%)	2	11
34	BI	103/103 (100%)	97 (94%)	6 (6%)	20	45
35	BJ	99/99 (100%)	73 (74%)	26 (26%)	0	3
36	BK	104/104 (100%)	91 (88%)	13 (12%)	4	19
37	BL	94/94 (100%)	76 (81%)	18 (19%)	1	8
38	BM	83/83 (100%)	78 (94%)	5 (6%)	19	44
39	BN	99/99 (100%)	73 (74%)	26 (26%)	0	3
40	BO	89/89 (100%)	64 (72%)	25 (28%)	0	3
41	BQ	89/89 (100%)	77 (86%)	12 (14%)	4	17
42	BR	77/77 (100%)	65 (84%)	12 (16%)	2	14
43	BS	82/82 (100%)	77 (94%)	5 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BT	78/78 (100%)	75 (96%)	3 (4%)	33	57
45	BU	62/62 (100%)	49 (79%)	13 (21%)	1	6
46	BW	55/55 (100%)	53 (96%)	2 (4%)	35	59
47	BX	47/47 (100%)	44 (94%)	3 (6%)	17	42
48	BZ	24/24 (100%)	18 (75%)	6 (25%)	0	3
49	B1	46/46 (100%)	37 (80%)	9 (20%)	1	8
All	All	4551/4551 (100%)	4162 (92%)	389 (8%)	14	33

5 of 389 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	BJ	111	ILE
39	BN	61	ARG
36	BK	18	ARG
37	BL	43	GLU
40	BO	4	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
40	BO	36	GLN
42	BR	48	GLN
46	BW	38	GLN
16	AO	39	GLN
16	AO	36	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1487/1488 (99%)	249 (16%)	95 (6%)
2	AU	75/76 (98%)	16 (21%)	7 (9%)
2	AV	75/76 (98%)	15 (20%)	7 (9%)
2	AW	75/76 (98%)	14 (18%)	7 (9%)
22	B0	2739/2740 (99%)	580 (21%)	182 (6%)
23	B9	107/108 (99%)	23 (21%)	6 (5%)
All	All	4558/4564 (99%)	897 (19%)	304 (6%)

5 of 897 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	31	G
1	AA	32	A

5 of 304 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	B0	1929	G
22	B0	2644	G
22	B0	1996	C
22	B0	2164	C
23	B9	56	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	7
26	BA	4
27	BB	4

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Mol	Chain	Number of breaks
25	B5	3
25	B3	2
3	AB	2
31	BF	2
24	B2	2
29	BD	1
28	BC	1
14	AM	1
43	BS	1
37	BL	1
32	BG	1
40	BO	1
42	BR	1
35	BJ	1

The worst 5 of 35 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	52:THR	C	53:GLU	N	8.77
1	B5	51:LYS	C	52:THR	N	8.07
1	BA	60:ALA	C	61:TYR	N	8.05
1	B3	53:GLU	C	54:PHE	N	7.33
1	BB	167:ASN	C	168:GLU	N	7.32

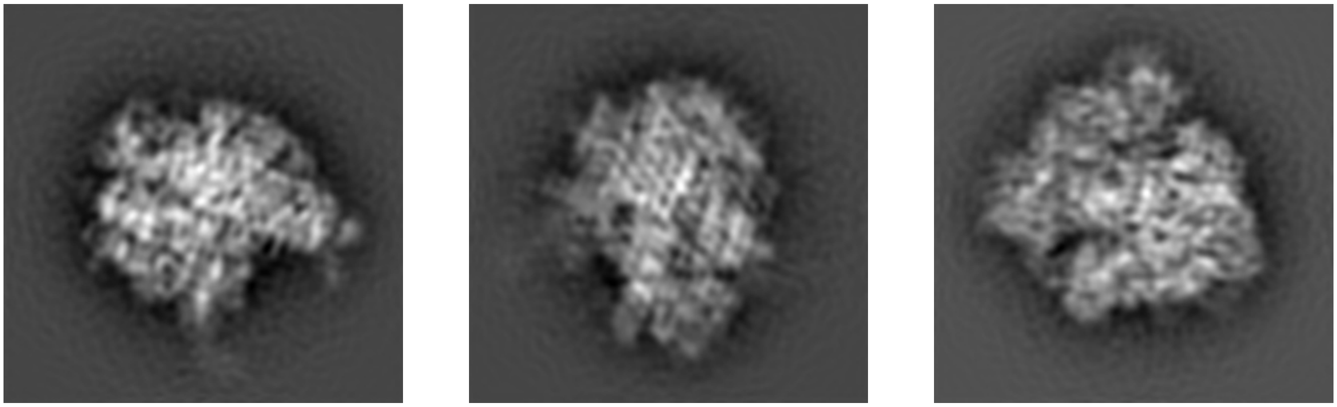
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1056. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map

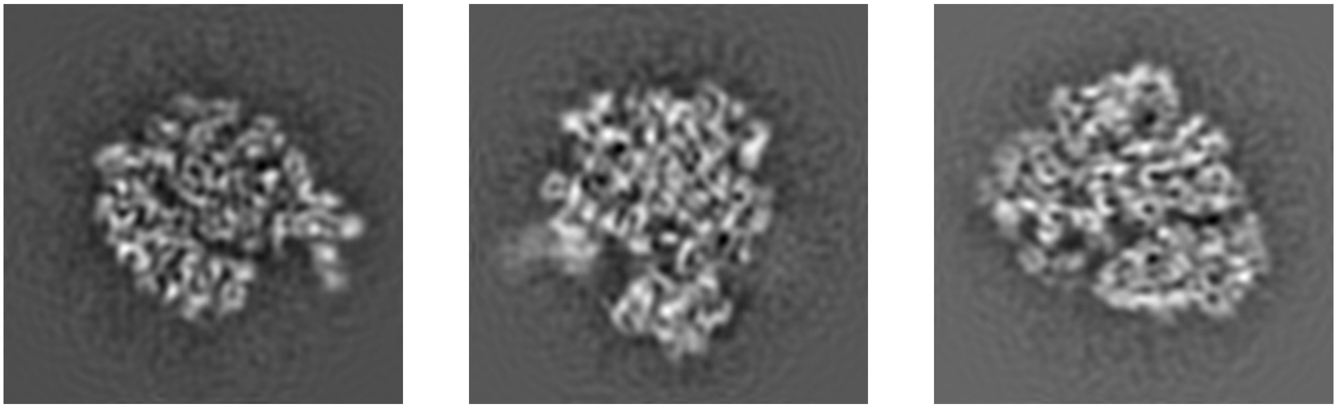


X Y Z

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

6.2 Central slices (i)

6.2.1 Primary map

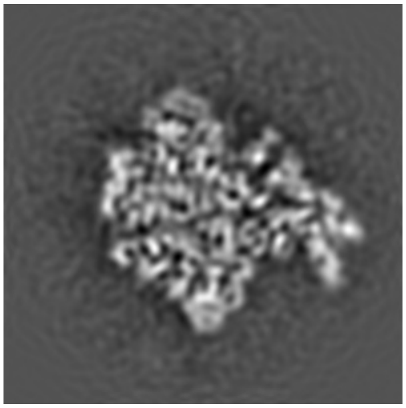


X Index: 65 Y Index: 65 Z Index: 65

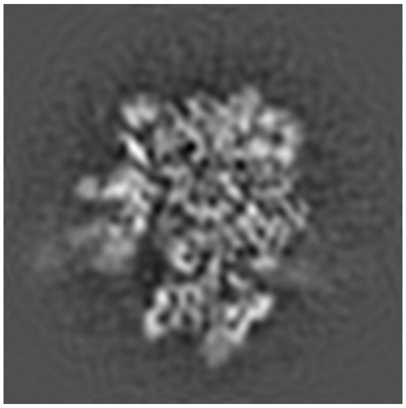
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

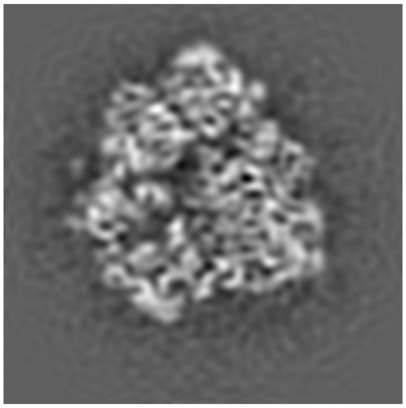
6.3.1 Primary map



X Index: 68



Y Index: 68

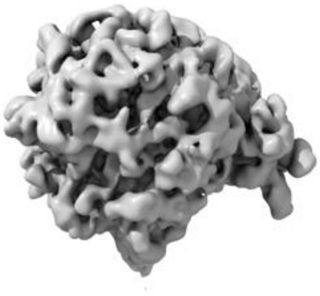


Z Index: 58

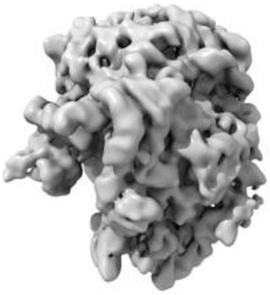
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

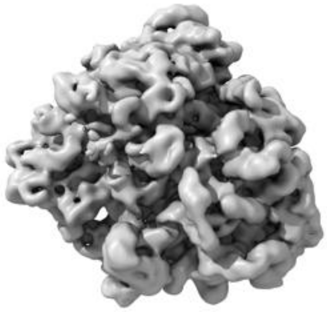
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 43.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

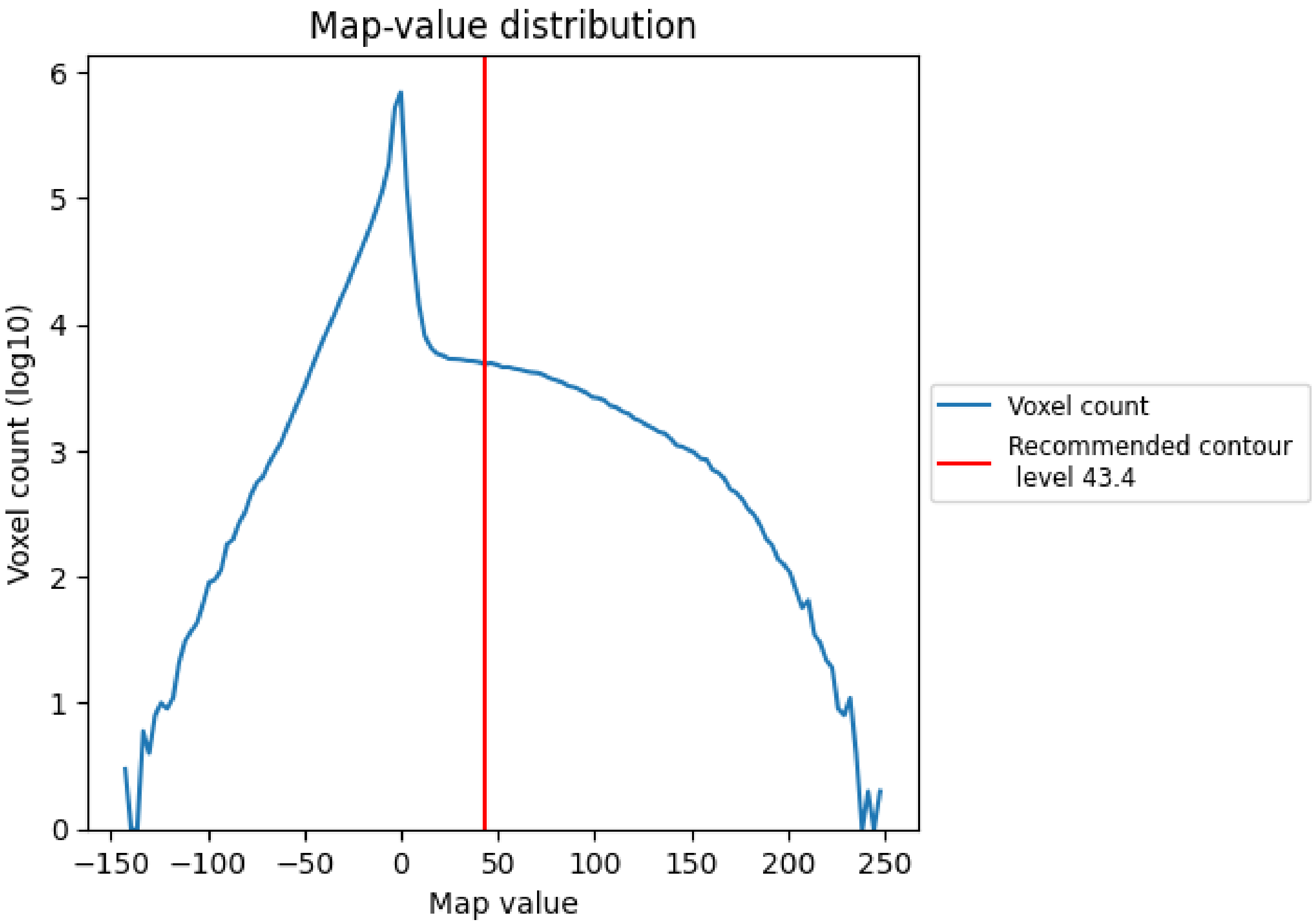
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

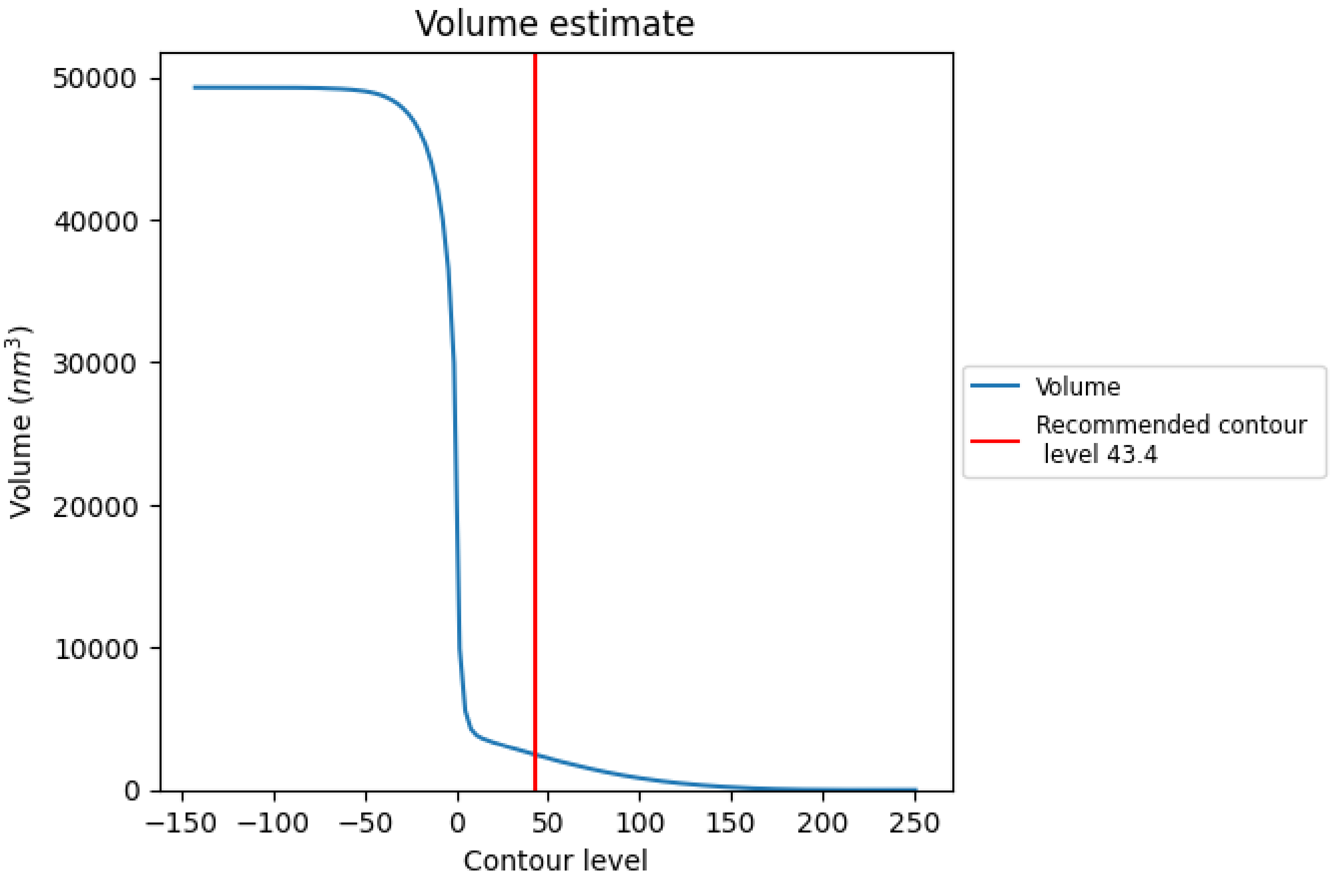
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

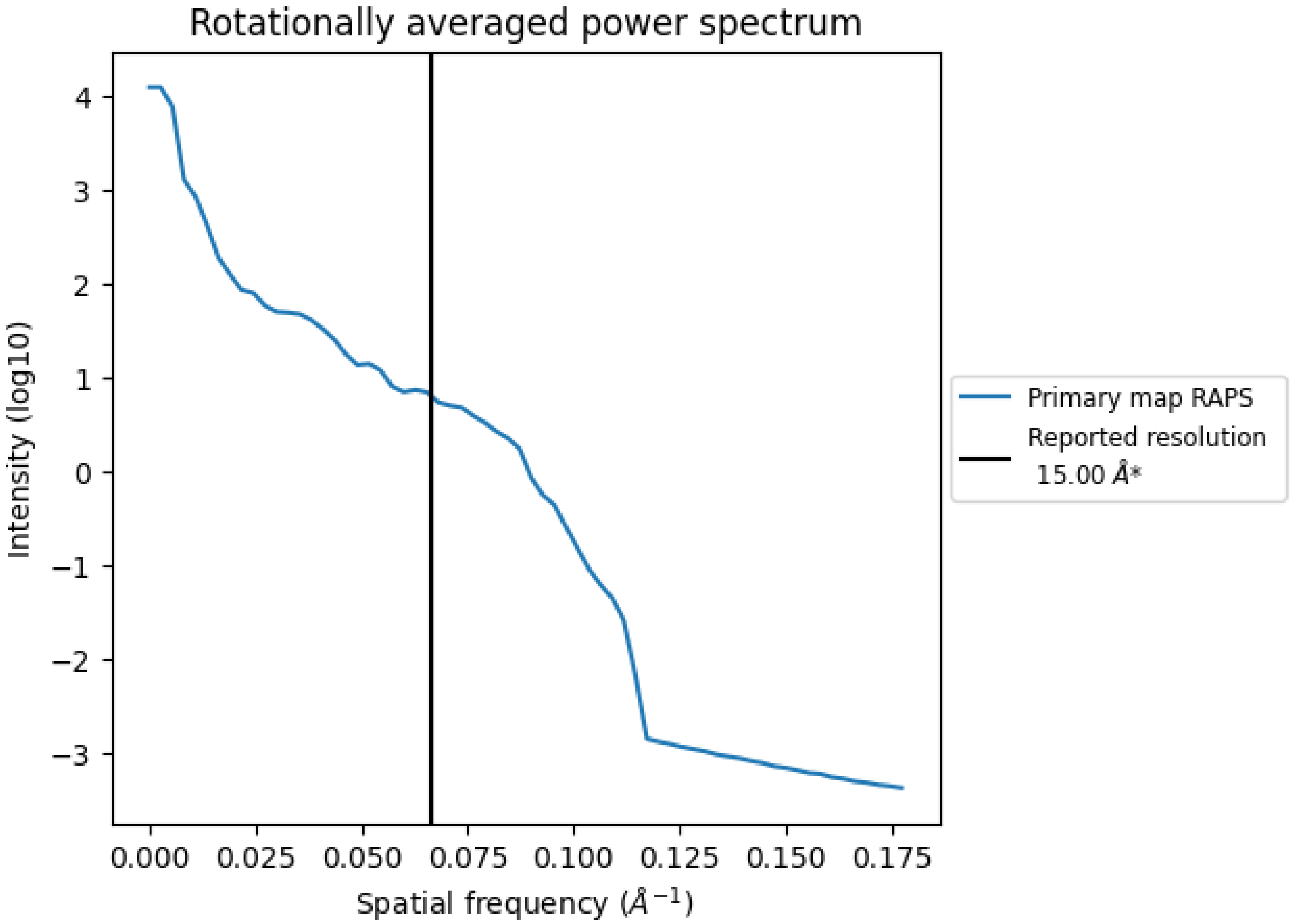
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2462 nm^3; this corresponds to an approximate mass of 2224 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 0.067 $Å^{-1}$

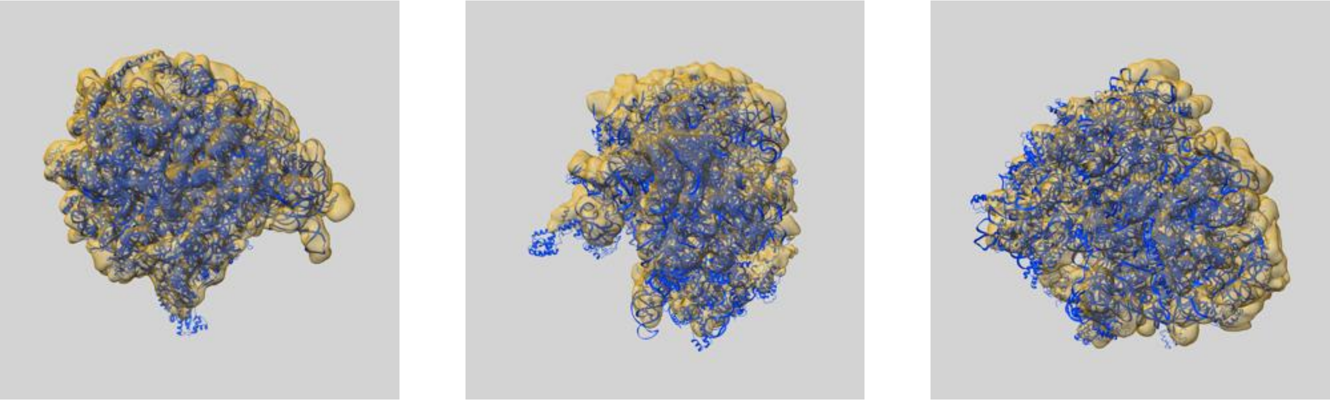
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-1056 and PDB model 4V4V. Per-residue inclusion information can be found in section 3 on page 13.

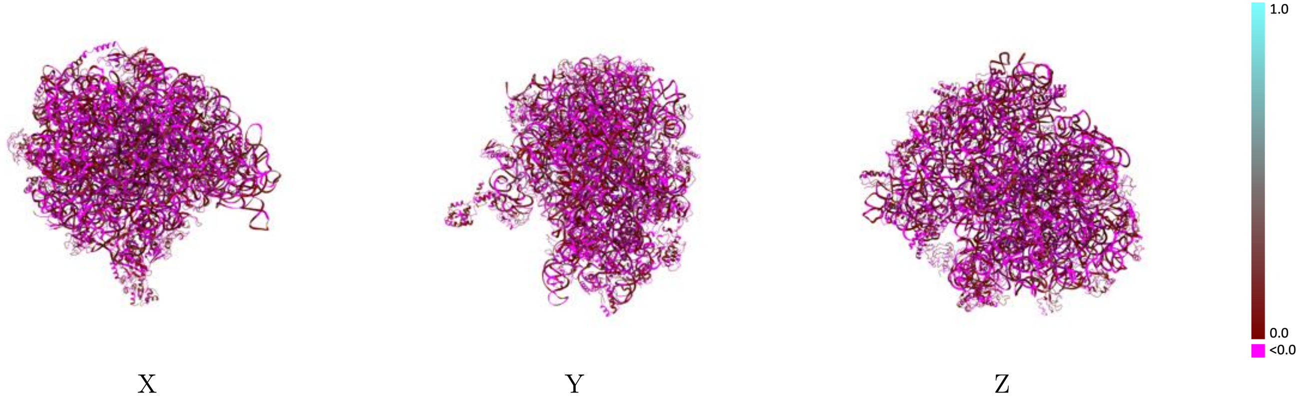
9.1 Map-model overlay ⓘ



X Y Z

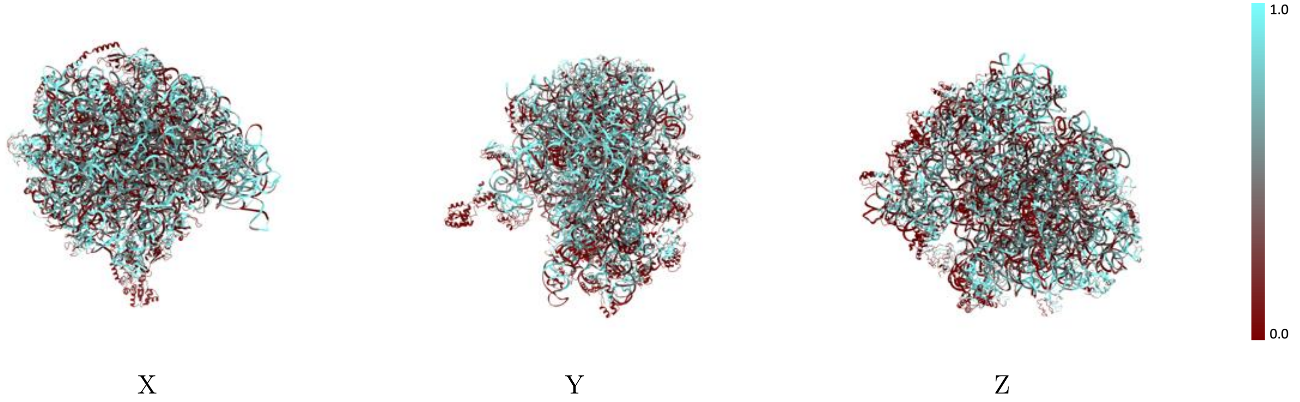
The images above show the 3D surface view of the map at the recommended contour level 43.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



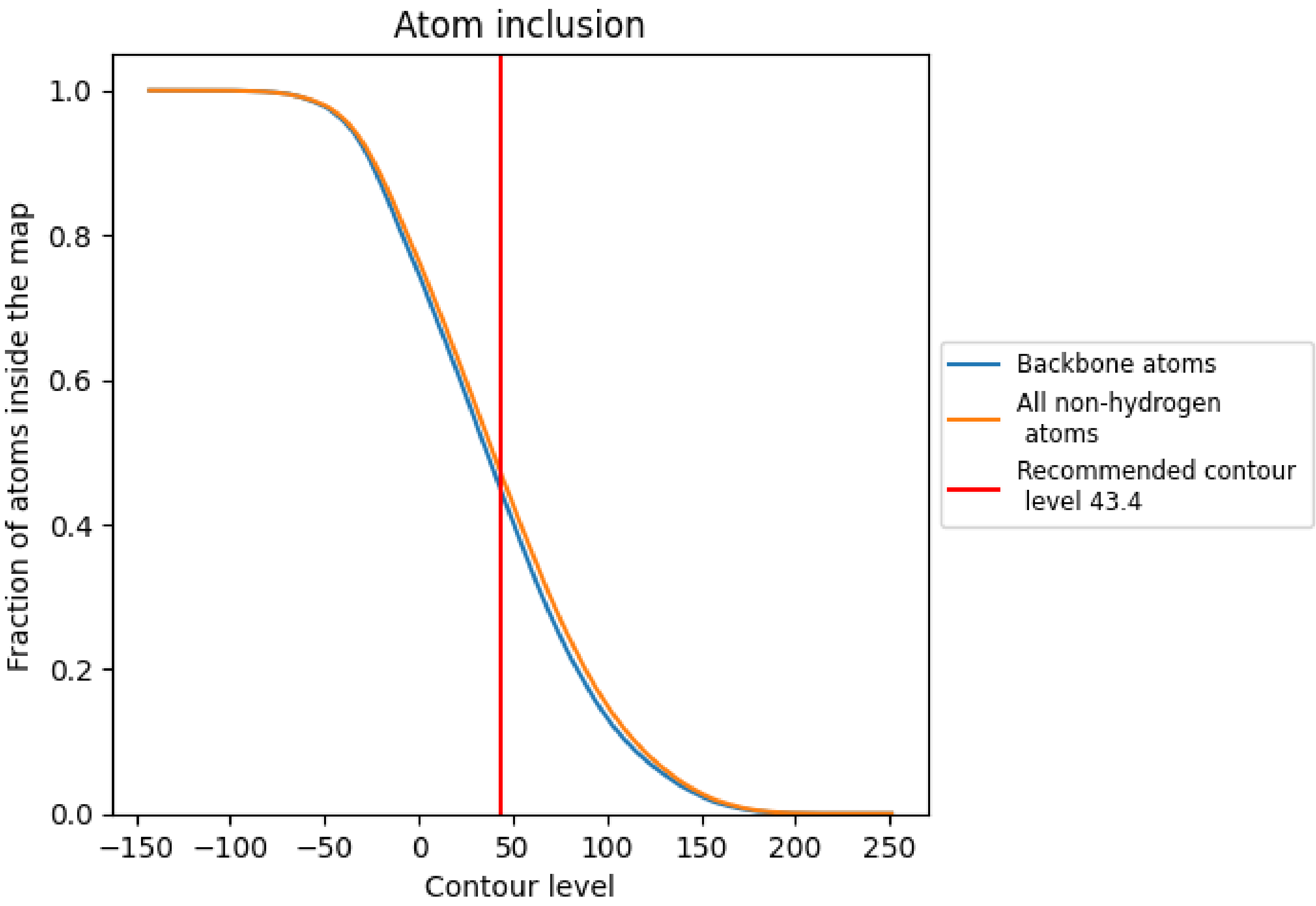
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (43.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 45% of all backbone atoms, 47% 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 (43.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4728	0.0020
AA	0.5227	0.0010
AB	0.3563	-0.0010
AC	0.3205	0.0010
AD	0.2795	-0.0070
AE	0.3277	0.0090
AF	0.4417	0.0080
AG	0.4809	0.0140
AH	0.4341	0.0050
AI	0.4882	0.0030
AJ	0.3503	0.0100
AK	0.2896	0.0060
AL	0.5455	0.0280
AM	0.3209	-0.0080
AN	0.0819	-0.0290
AO	0.6281	0.0110
AP	0.5817	-0.0090
AQ	0.4936	-0.0010
AR	0.2595	0.0140
AS	0.3888	0.0050
AT	0.6546	0.0170
AU	0.4131	0.0110
AV	0.3656	-0.0210
AW	0.3366	-0.0200
B0	0.5043	0.0010
B1	0.2163	0.0070
B2	0.4456	0.0200
B3	0.1898	0.0230
B5	0.0427	0.0170
B9	0.5143	0.0000
BA	0.4502	0.0130
BB	0.4350	0.0080
BC	0.5871	0.0170
BD	0.4224	0.0170
BE	0.4231	-0.0310

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Chain	Atom inclusion	Q-score
BF	0.2400	-0.0250
BG	0.2091	0.0150
BH	0.3882	-0.0020
BI	0.1718	-0.0150
BJ	0.5545	0.0200
BK	0.3237	-0.0140
BL	0.4828	-0.0050
BM	0.6156	0.0330
BN	0.4459	0.0070
BO	0.5367	-0.0010
BQ	0.3794	-0.0280
BR	0.5248	-0.0030
BS	0.5720	0.0030
BT	0.3631	-0.0090
BU	0.3786	0.0060
BW	0.4803	-0.0360
BX	0.2979	-0.0380
BZ	0.7434	0.0410