wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 02:01 pm GMT

PDB ID	:	4V5M
EMDB ID	:	EMD-1798
Title	:	tRNA tranlocation on the 70S ribosome: the pre-translocational translocation intermediate TI(PRE)
Authors	:	Ratje, A.H.; Loerke, J.; Mikolajka, A.; Bruenner, M.; Hildebrand, P.W.; Starosta, A.L.; Doenhoefer, A.; Connell, S.R.; Fucini, P.; Mielke, T.; Whitford, P.C.; Onuchic, J.N.; Yu, Y.; Sanbonmatsu, K.Y.; Hartmann, R.K.; Penczek, P.A.; Wilson, D.N.; Spahn, C.M.T.
Deposited on	:	2010-10-01
Resolution	:	7.80 Å(reported)
Based on initial models	:	2WRJ, 2WRI

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 (1)) were used in the production of this report:

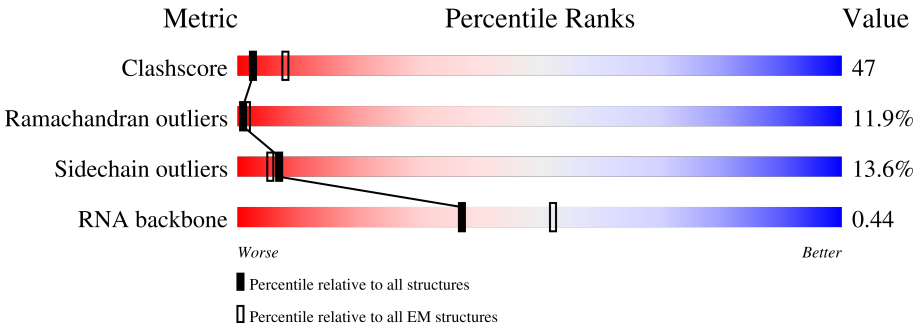
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 7.80 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	1522	24% 57% 17%
2	AB	256	37% 23% 48% 16% 9%
3	AC	239	26% 22% 46% 14% 14%
4	AD	209	26% 29% 49% 17%
5	AE	162	21% 27% 52% 13% 7%

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Mol	Chain	Length	Quality of chain
6	AF	101	25% 24% 52% 16% 8%
7	AG	156	35% 29% 53% 12% 6%
8	AH	138	23% 29% 58% 10%
9	AI	128	30% 23% 53% 19% 5%
10	AJ	105	42% 12% 56% 20% 5% 7%
11	AK	129	32% 37% 43% 12% 8%
12	AL	132	38% 23% 52% 16% 6%
13	AM	126	51% 20% 54% 19% 6%
14	AN	61	21% 23% 49% 23%
15	AO	89	22% 34% 40% 19% 6%
16	AP	88	19% 22% 60% 8% 5% 6%
17	AQ	105	22% 34% 46% 13% 6%
18	AR	88	25% 17% 47% 15% 20%
19	AS	93	31% 12% 45% 23% 16%
20	AT	106	23% 25% 42% 25% 7%
21	AU	27	33% 26% 37% 22% 11%
22	AV	77	10% 14% 64% 22%
23	AX	11	64% 9% 55% 36%
24	AY	691	42% 20% 54% 19%
25	B0	85	32% 33% 51% 12%
26	B1	98	20% 22% 47% 24% 5%
27	B2	72	7% 17% 51% 26%
28	B3	60	15% 22% 62% 13%
29	B4	71	44% 8% 38% 20% 14% 20%
30	B5	60	22% 25% 52% 12% 10%

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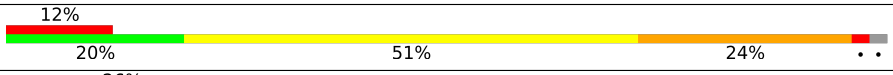
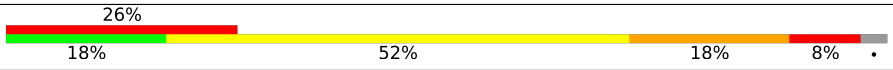
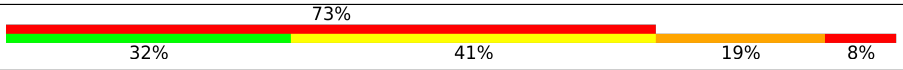
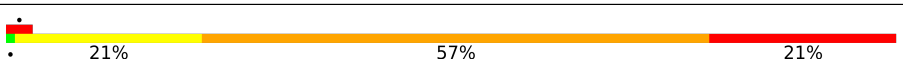
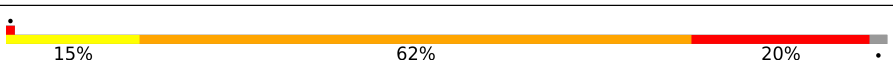
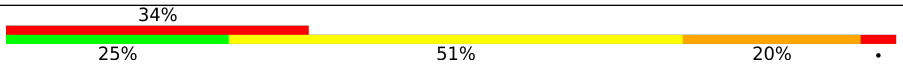
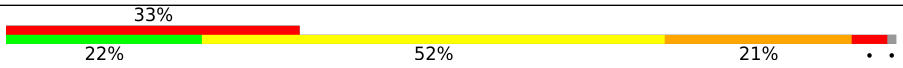
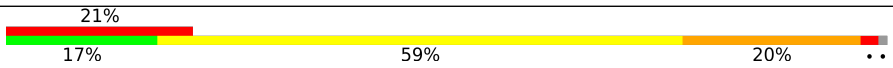
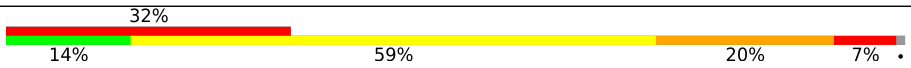
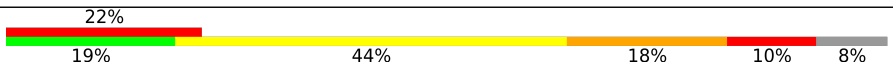
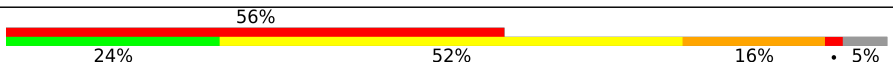
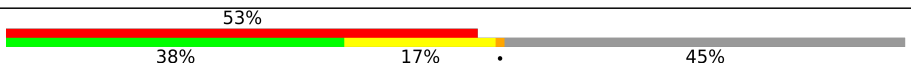
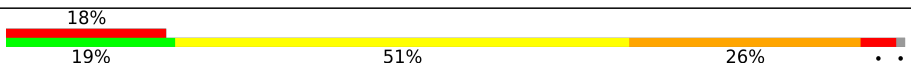
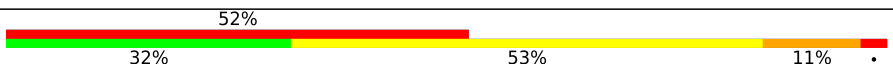
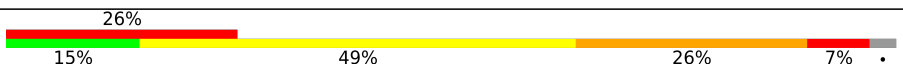
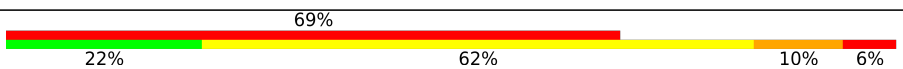
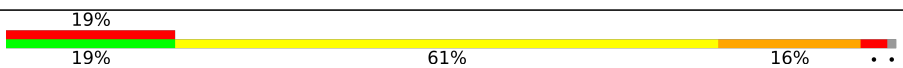
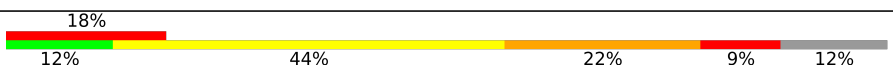
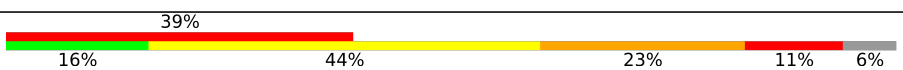
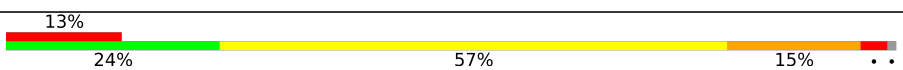
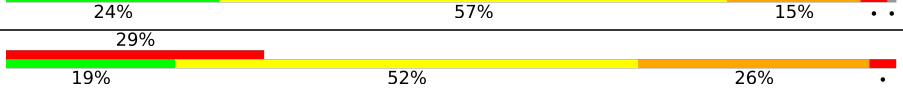
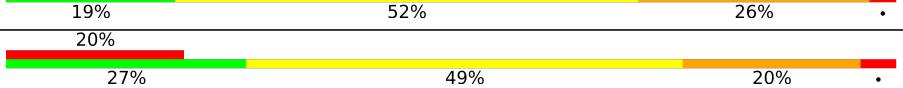
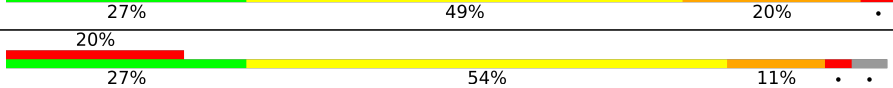
Mol	Chain	Length	Quality of chain
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BK	147	
44	BL	121	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	
55	BX	96	

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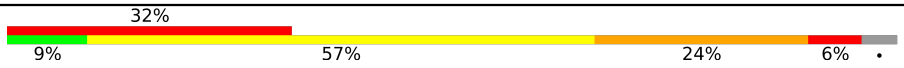
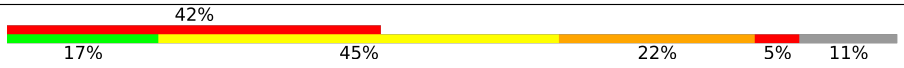
Mol	Chain	Length	Quality of chain
56	BY	110	
57	BZ	206	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 152777 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 RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1504	32329	14390	5992	10444	1503	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	234	1900	1213	341	341	5	0	0

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	206	1612	1016	314	281	1	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	208	1703	1066	339	291	7	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	150	1146	724	217	201	4	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	101	843	531	155	154	3	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AI	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0
			987	611	205	169	2		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	60	Total 492	C 312	N 104	O 72	S 4	0	0

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total 734	C 459	N 147	O 126	S 2	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	83	Total 700	C 443	N 139	O 117	S 1	0	0

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	99	Total 823	C 528	N 151	O 142	S 2	0	0

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	70	Total 574	C 367	N 112	O 95	0	0

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	78	Total 629	C 403	N 114	O 110	S 2	0	0

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	99	Total 763	C 470	N 162	O 129	S 2	0	0

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AU	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a RNA chain called TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0
			230	105	41	74	10		

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AY	666	Total	C	N	O	S	0	0
			5214	3316	892	988	18		

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0
			662	410	140	111	1		

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	93	Total	C	N	O	S	0	0
			731	460	145	125	1		

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0
			598	370	121	106	1		

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B3	59	Total	C	N	O	S	0	0
			467	298	90	78	1		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B4	57	Total	C	N	O	S	0	0
			450	285	77	83	5		

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0
			459	288	90	76	5		

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0
			433	270	88	71	4		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0
			418	257	104	55	2		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B8	63	Total	C	N	O	S	0	0
			507	326	101	78	2		

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0
			62474	27806	11681	20087	2900		

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0
			2551	1136	471	826	118		

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	228	Total	C	N	O	S	0	0
			1742	1101	319	319	3		

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0
			2145	1353	428	361	3		

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	204	Total	C	N	O	S	0	0
			1563	988	299	270	6		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	207	Total	C	N	O	S	0	0
			1623	1035	303	282	3		

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0
			1474	942	268	260	4		

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	166	Total	C	N	O	S	0	0
			1268	803	237	227	1		

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BK	139	Total	C	N	O	S	0	0
			1025	653	181	186	5		

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BL	67	Total	C	N	O	0	0
			477	301	81	95		

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BN	138	Total	C	N	O	S	0	0
			1104	712	206	182	4		

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0
			933	588	171	170	4		

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0
			1114	692	227	193	2		

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0
			1122	715	212	188	7		

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BR	117	Total 960	C 599	N 202	O 159	0	0

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BS	98	Total 770	C 486	N 154	O 130	0	0

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BT	137	Total 1141	C 710	N 234	O 196	S 1	0	0

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BU	117	Total 958	C 604	N 202	O 151	S 1	0	0

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BV	101	Total 779	C 501	N 142	O 135	S 1	0	0

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BW	113	Total 896	C 563	N 176	O 155	S 2	0	0

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	BX	92	Total 725	C 471	N 131	O 123	0	0

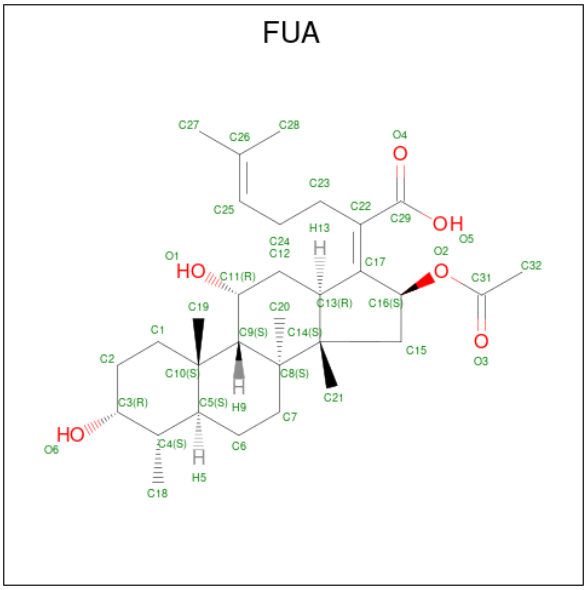
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BY	106	Total	C	N	O	S	0	0
			810	520	154	131	5		

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

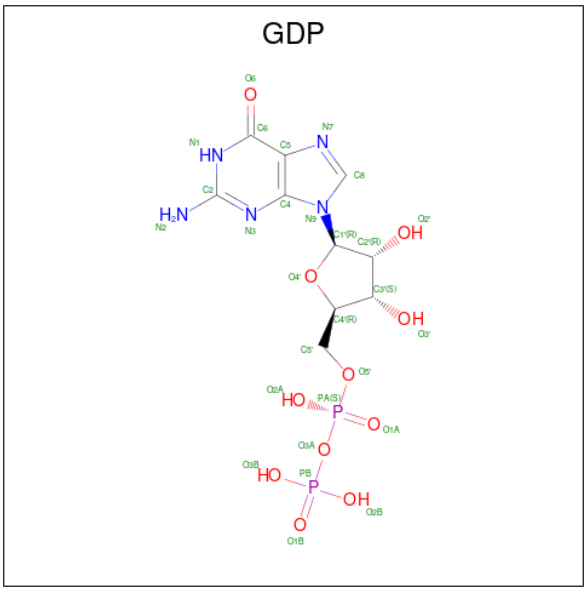
Mol	Chain	Residues	Atoms					AltConf	Trace
57	BZ	184	Total	C	N	O	S	0	0
			1467	936	261	268	2		

- Molecule 58 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			AltConf
58	AY	1	Total	C	O	0
			37	31	6	

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



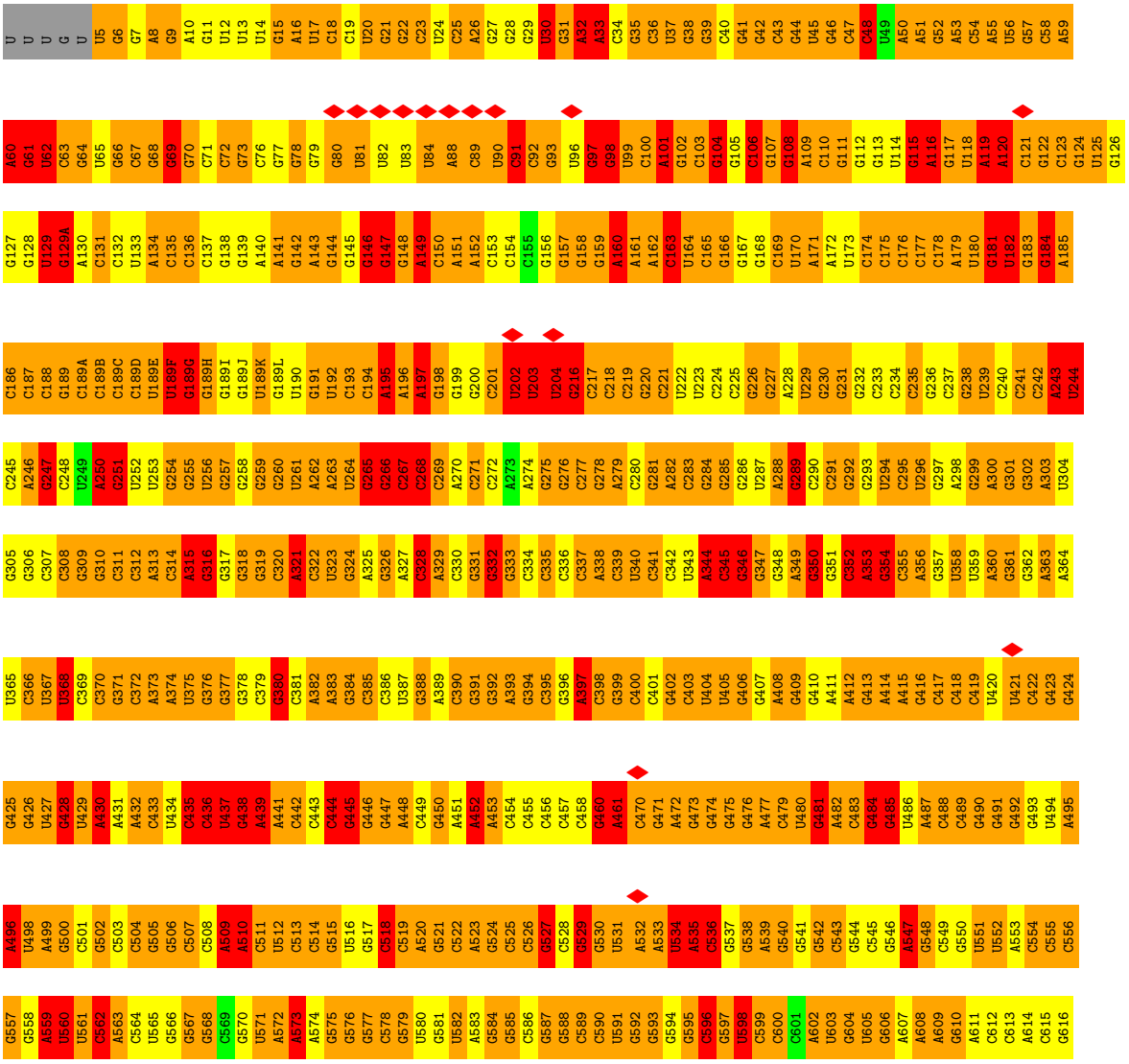
Mol	Chain	Residues	Atoms					AltConf
59	AY	1	Total	C	N	O	P	0
			28	10	5	11	2	

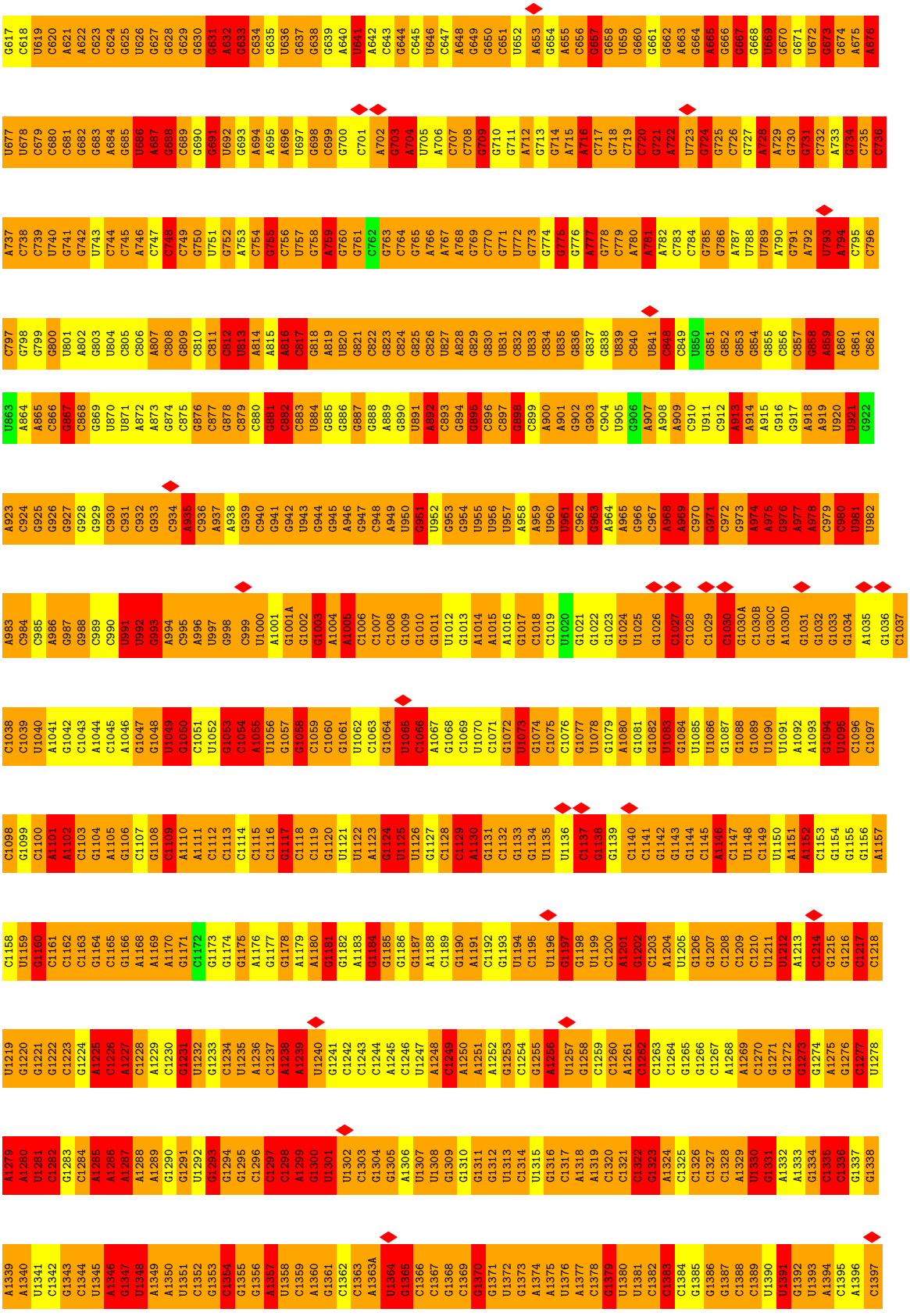
3 Residue-property plots (i)

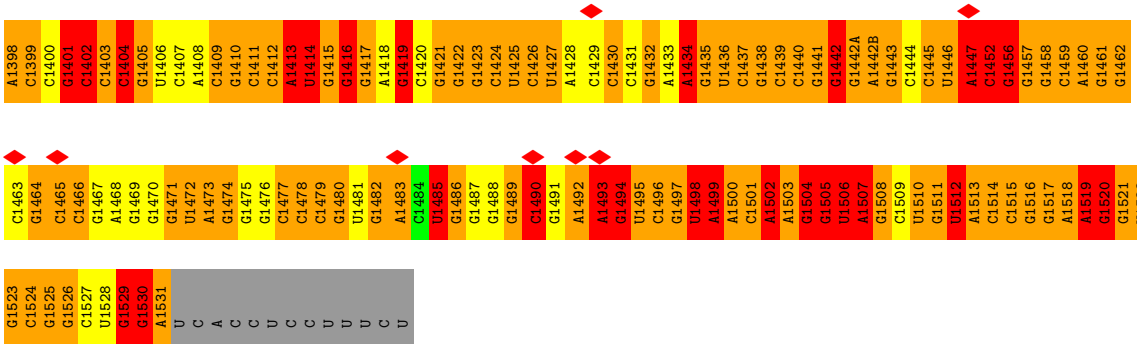
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S RRNA

Chain AA: 24% 57% 17%

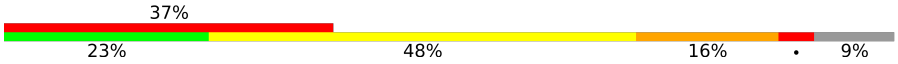


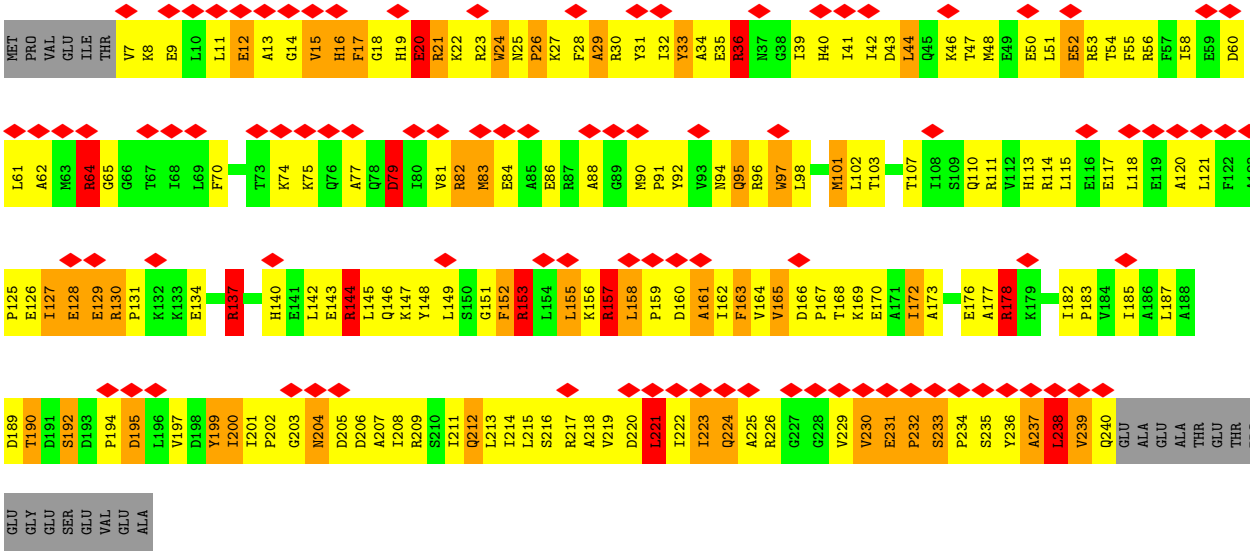

G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 U636 G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 G654 A655 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G668 U669 G670 G671 U672 G673 G674 A675 A676
U677 U678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C699 G700 C701 A702 G703 A704 U705 A706 C707 C708 G709 G710 G711 A712 G713 G714 A715 A716 C717 G718 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736
A737 C738 C739 U740 G741 G742 U743 C744 C745 A746 C747 G748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 G760 G761 C762 G763 C764 G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796
C797 G798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862
U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 G886 G887 G888 A889 G890 U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 C904 U905 G906 A907 A908 A909 C910 U911 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922
A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982
A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037
C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1082 U1083 G1084 U1085 U1086 C1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097
C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 G1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 G1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157
C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 C1166 A1168 A1169 A1170 G1171 C1172 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218
U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 C1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 G1266 C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 G1275 G1276 C1277 U1278
A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 A1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 C1331 A1332 A1333 G1334 C1335 C1336 G1337 G1338
A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1362 C1363 A1363A U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 A1376 A1377 C1378 G1379 U1380 U1381 C1382 C1383 C1384 C1385 G1386 G1387 C1388 C1389 U1390 U1391 G1392 U1393 A1394 C1395 A1396 C1397



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

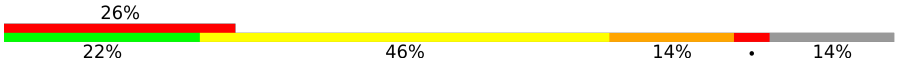
Chain AB:

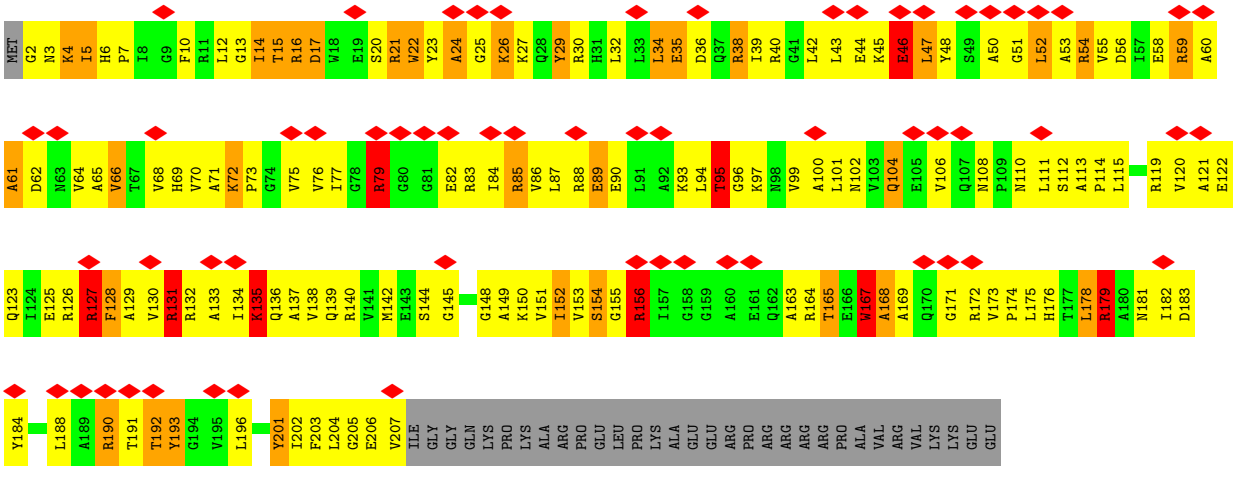




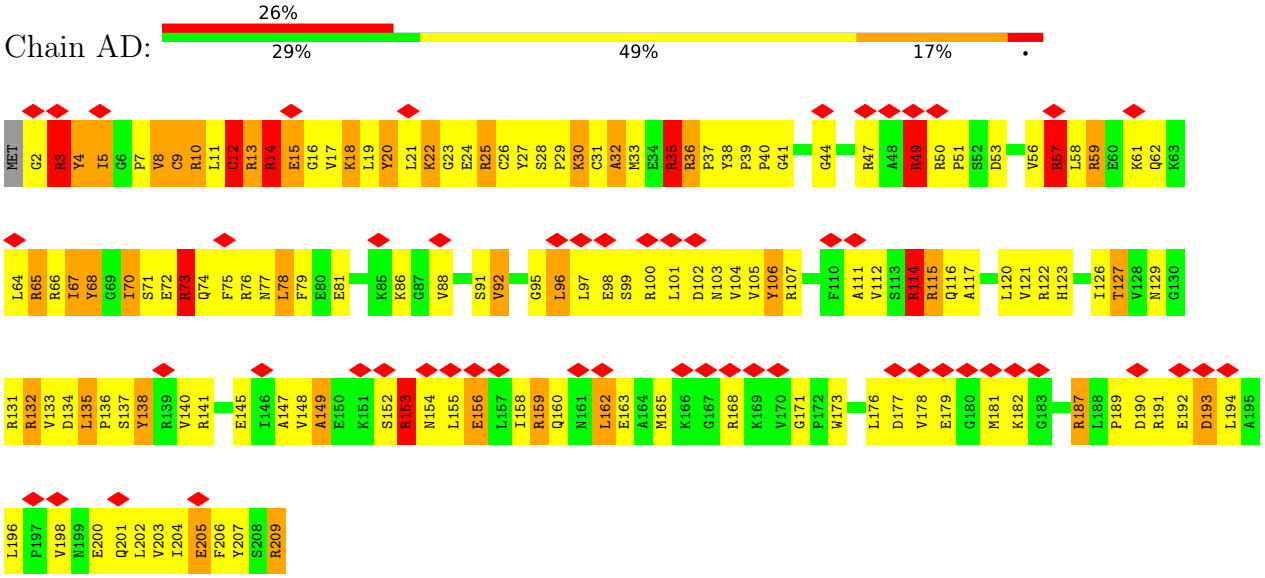
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:

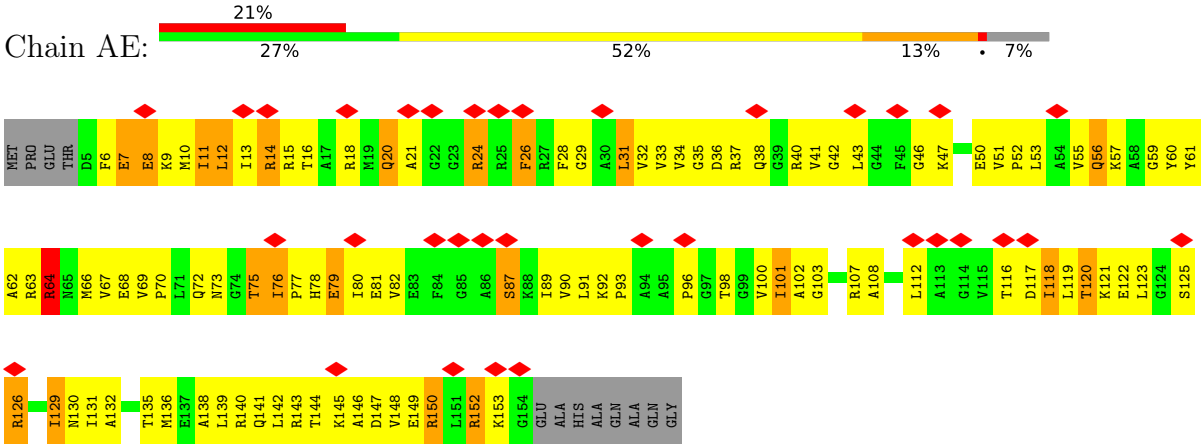




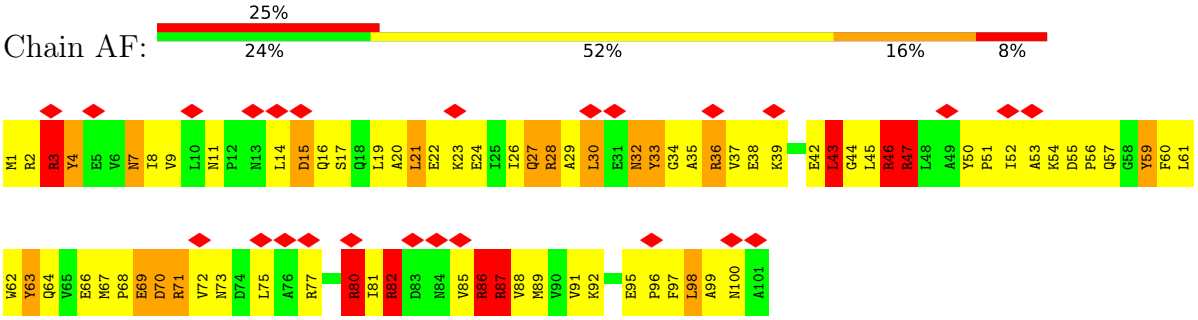
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



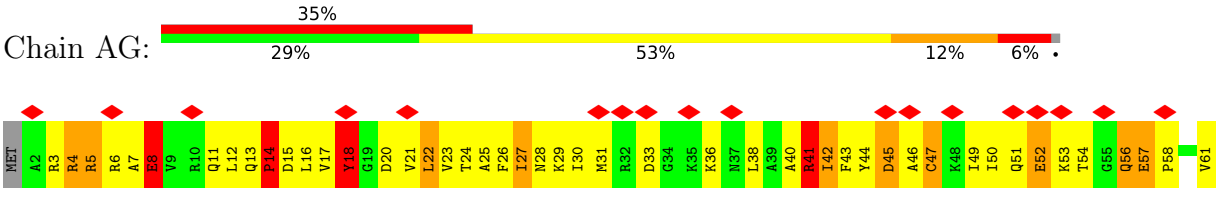
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

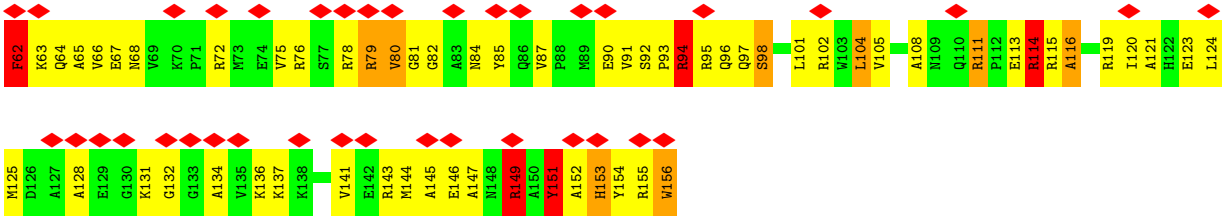


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

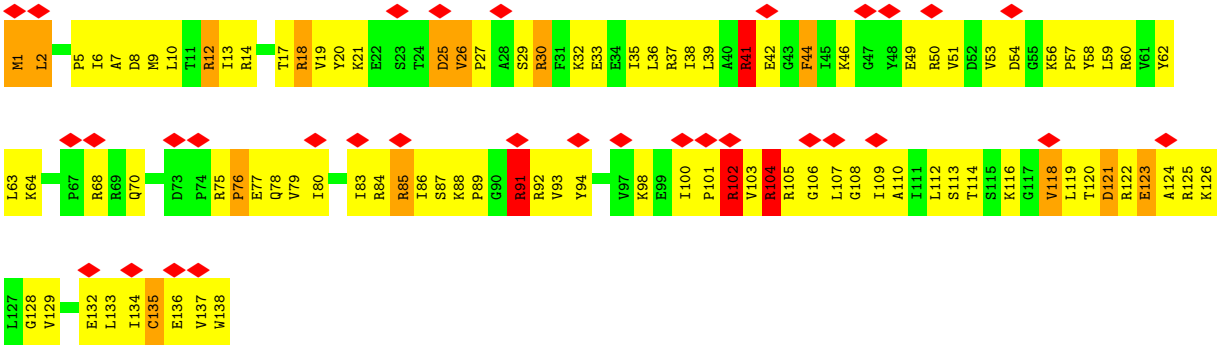


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

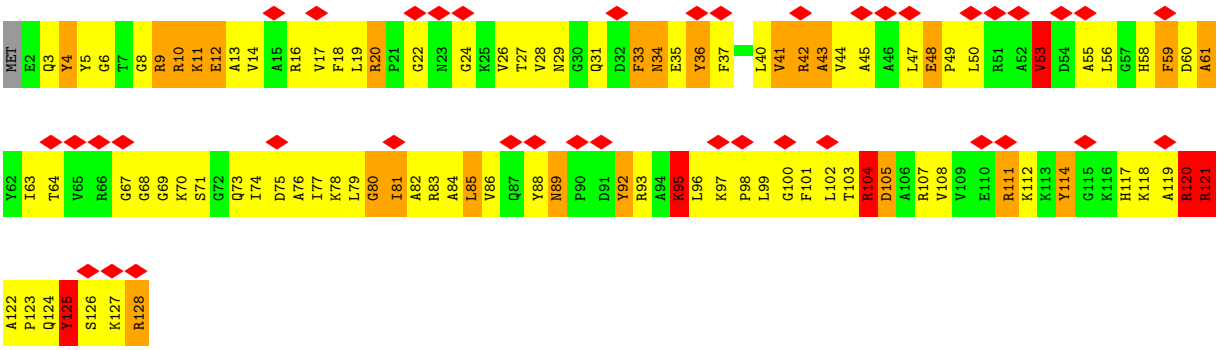




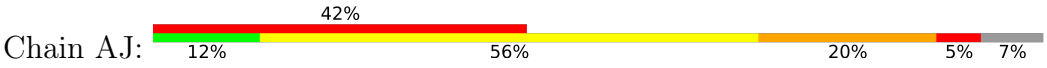
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

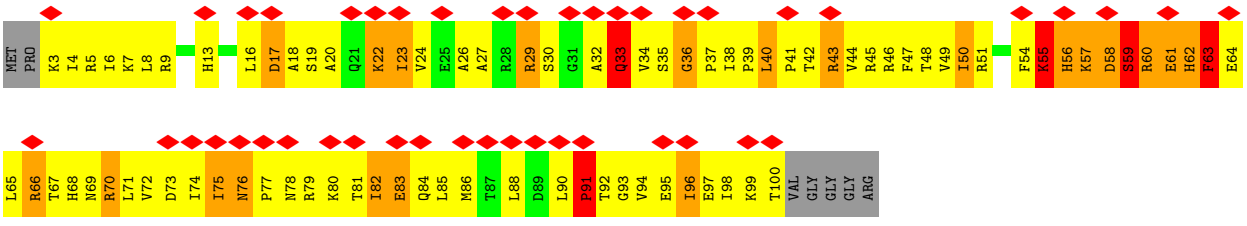


• Molecule 9: 30S RIBOSOMAL PROTEIN S9



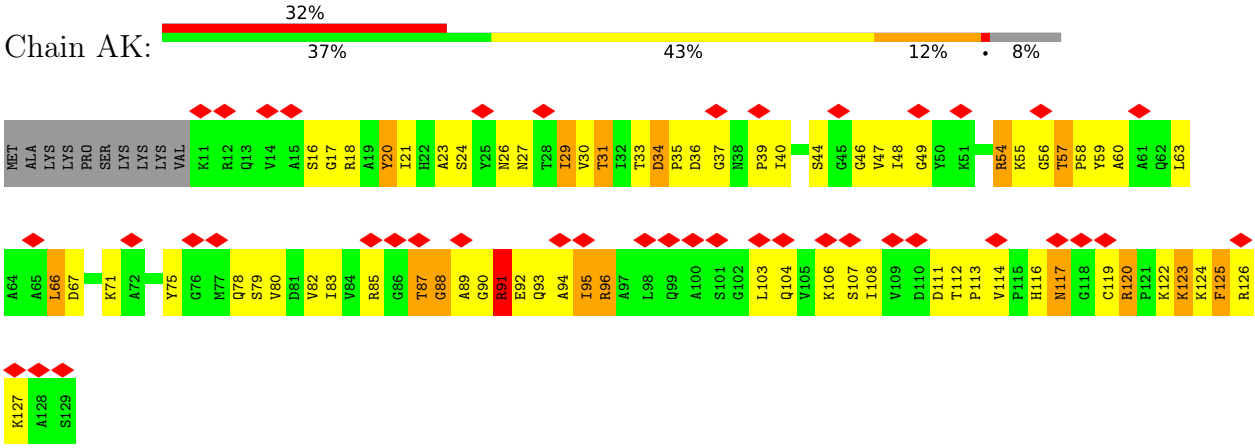
• Molecule 10: 30S RIBOSOMAL PROTEIN S10





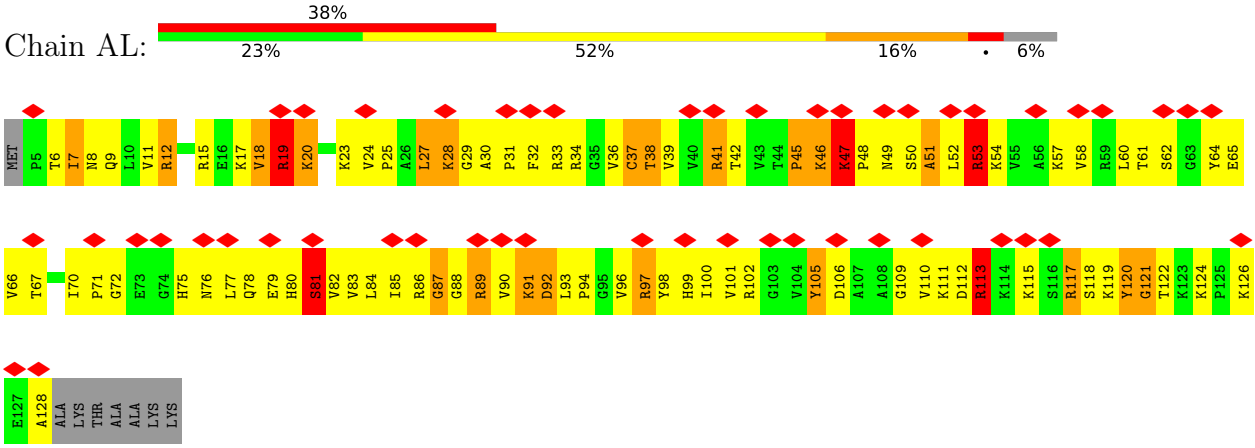
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



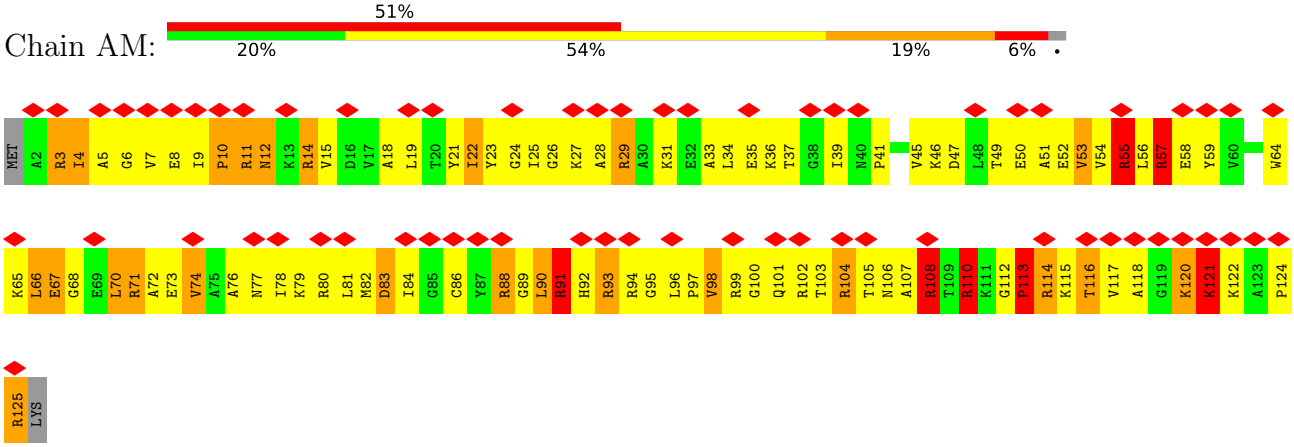
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



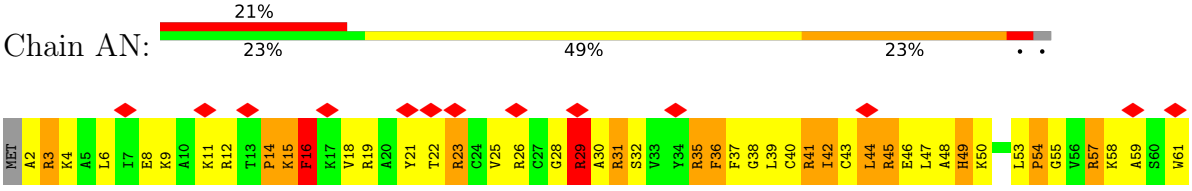
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



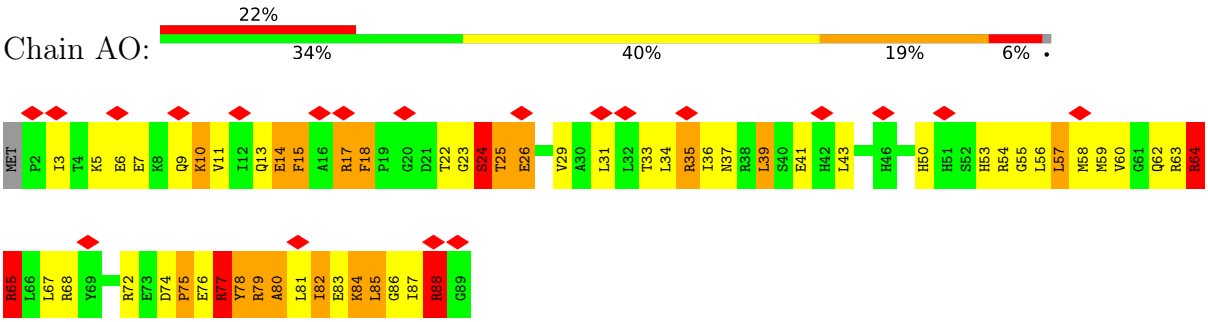
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



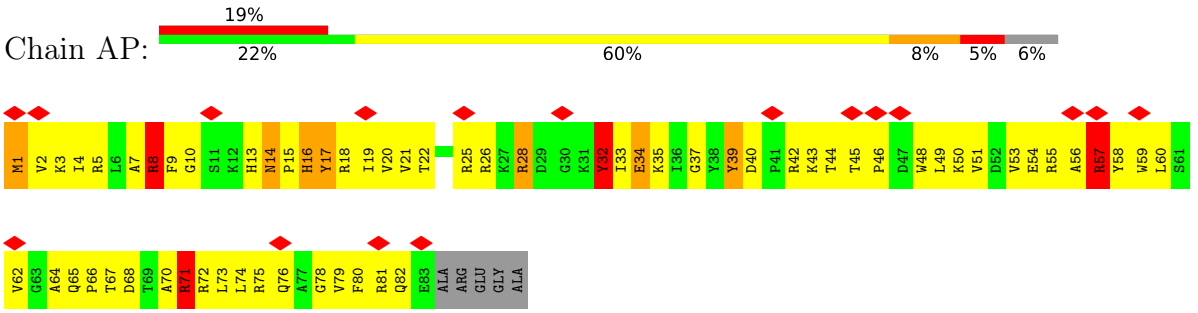
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



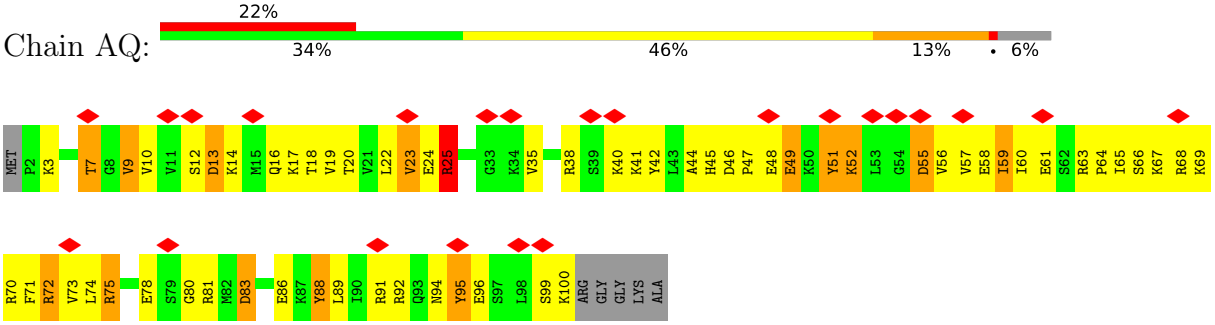
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



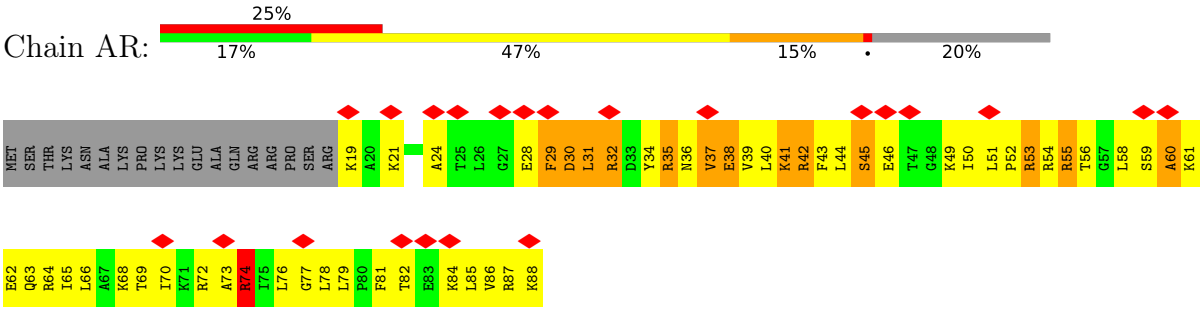
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



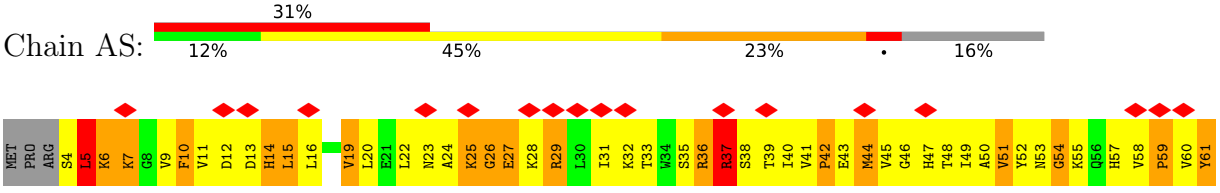
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

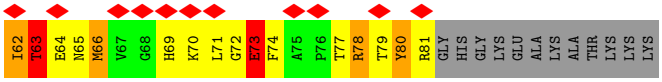
Chain AR:



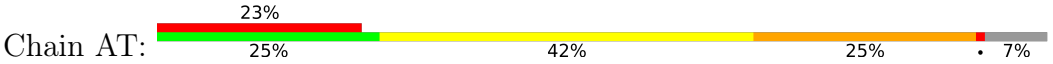
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

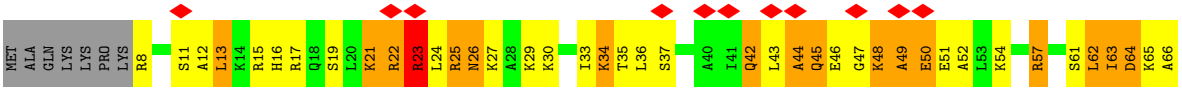
Chain AS:

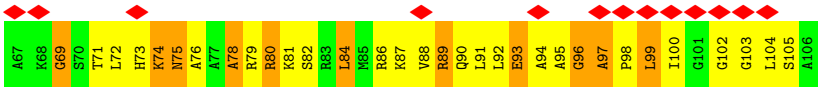




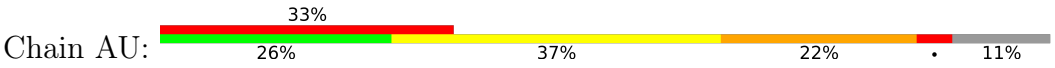
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



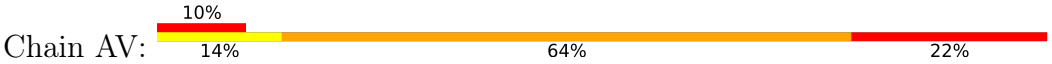


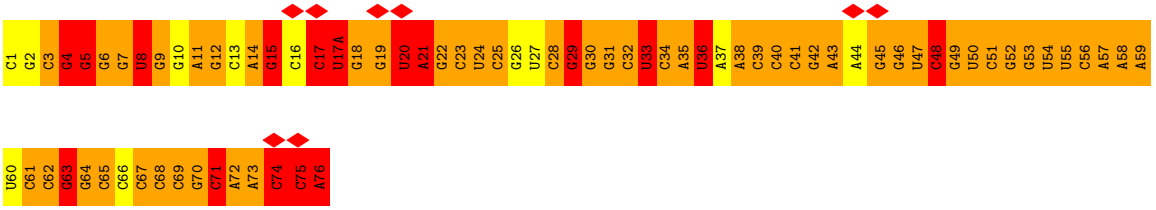


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

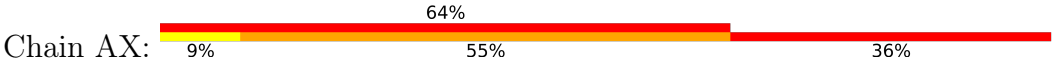


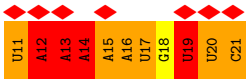
• Molecule 22: TRNA



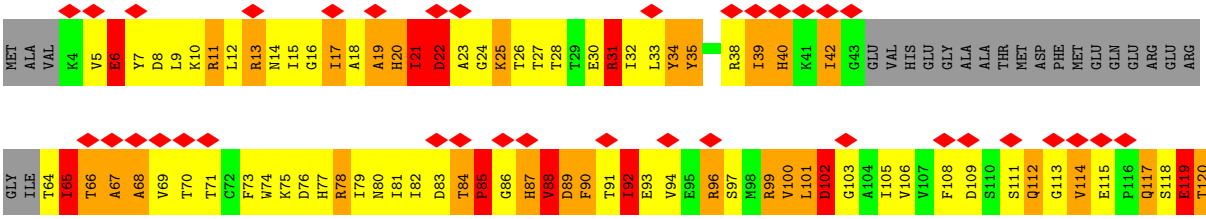


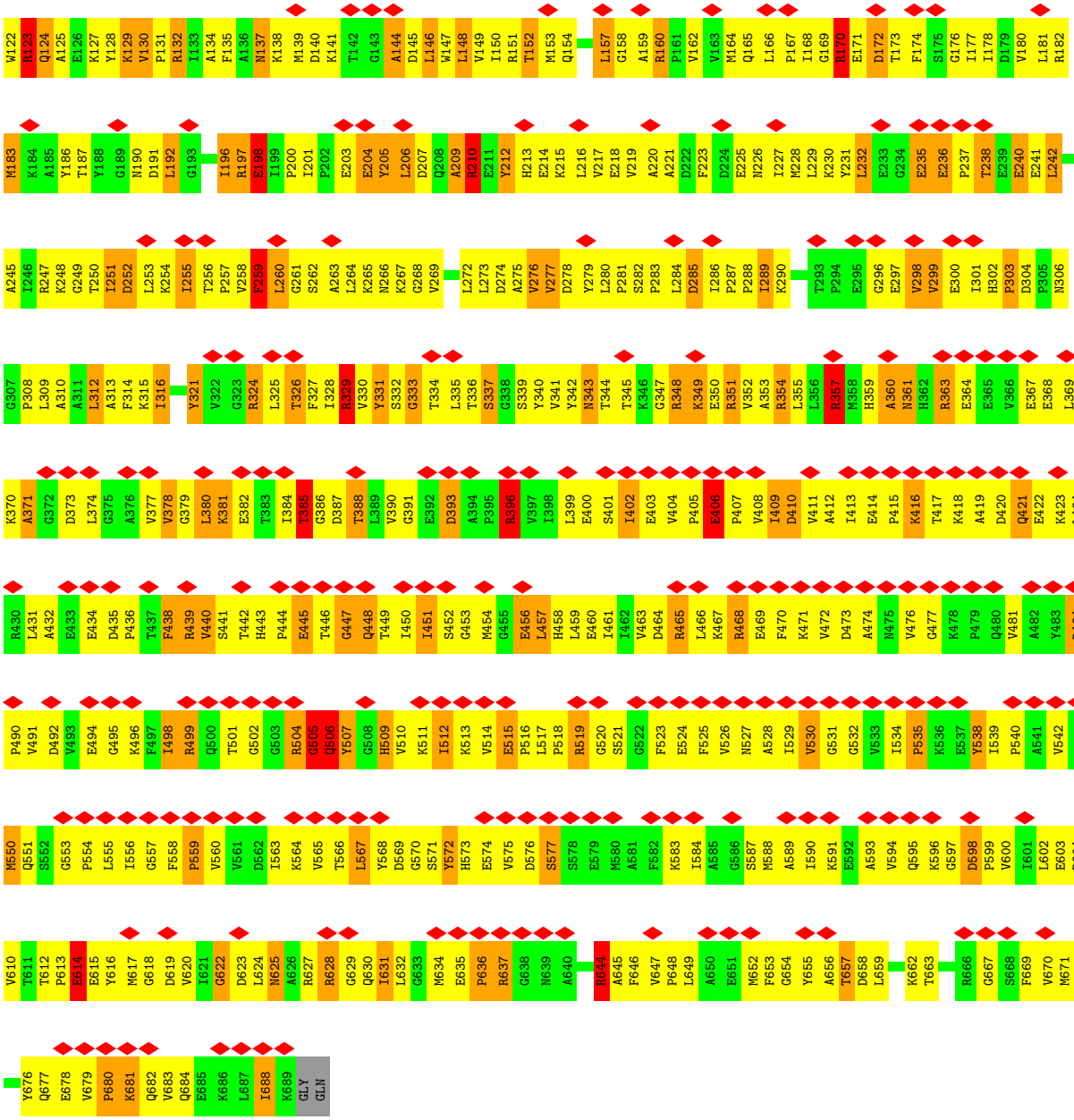
• Molecule 23: MRNA





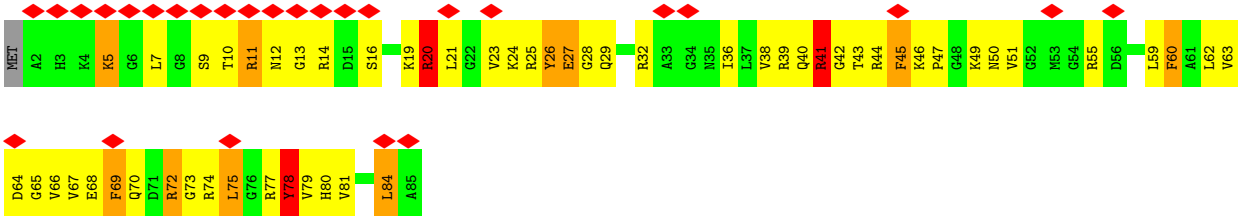
• Molecule 24: ELONGATION FACTOR G





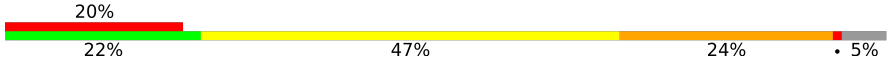
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

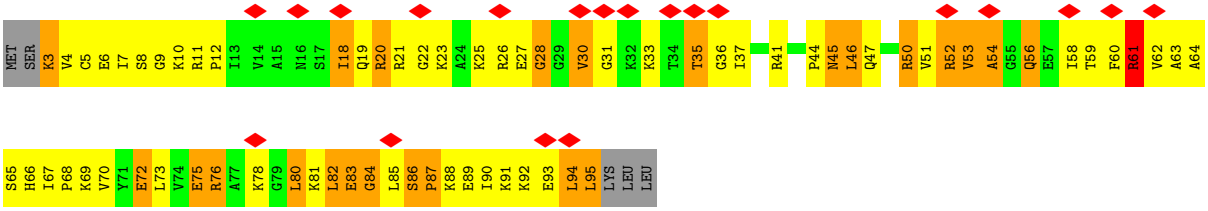
Chain B0:



• Molecule 26: 50S RIBOSOMAL PROTEIN L28

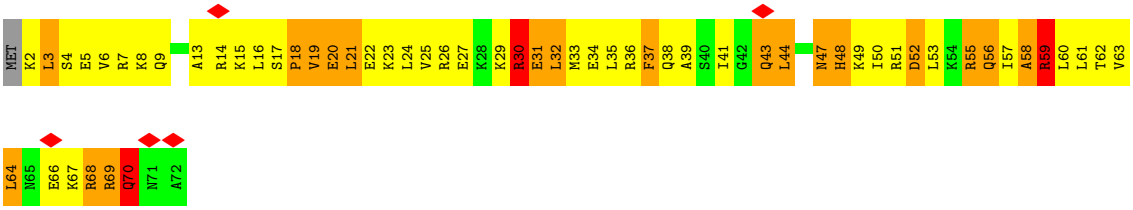
Chain B1:





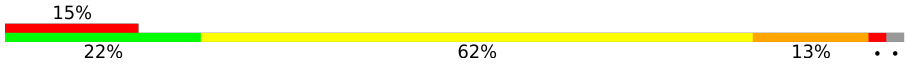
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

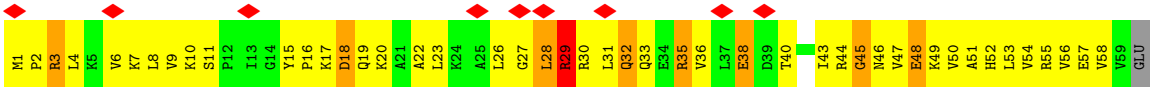
Chain B2:



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

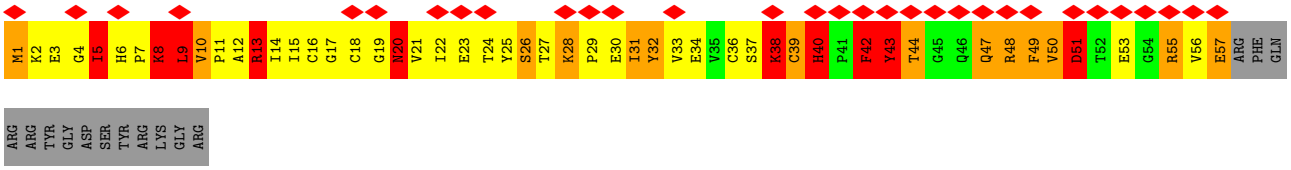
Chain B3:





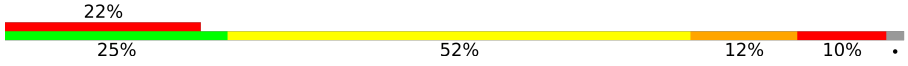
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

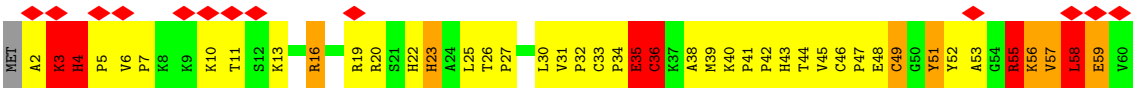
Chain B4:



• Molecule 30: 50S RIBOSOMAL PROTEIN L32

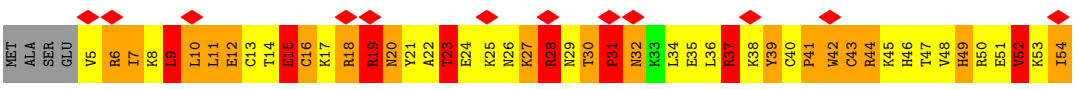
Chain B5:





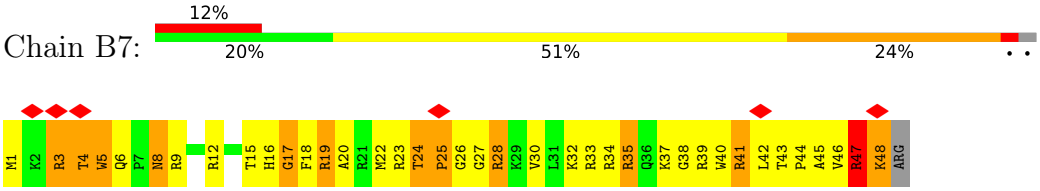
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



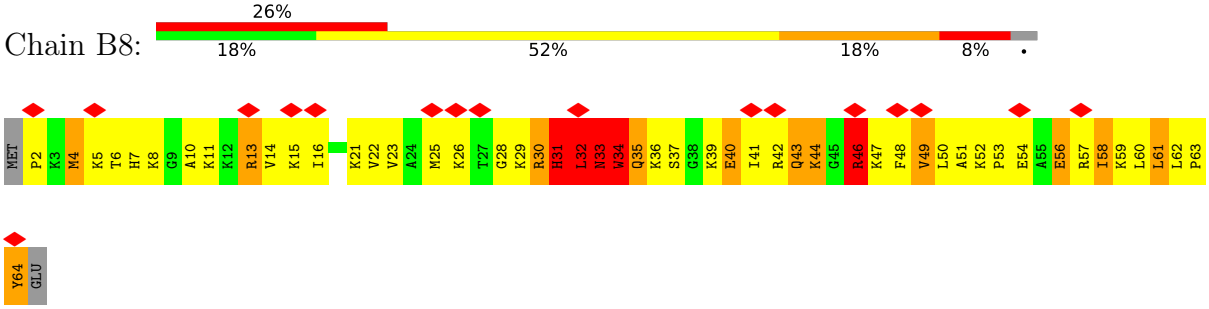
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:



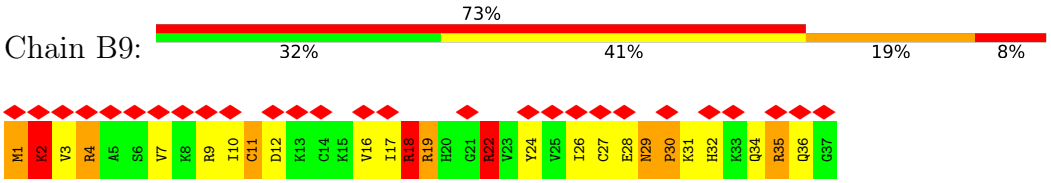
• Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



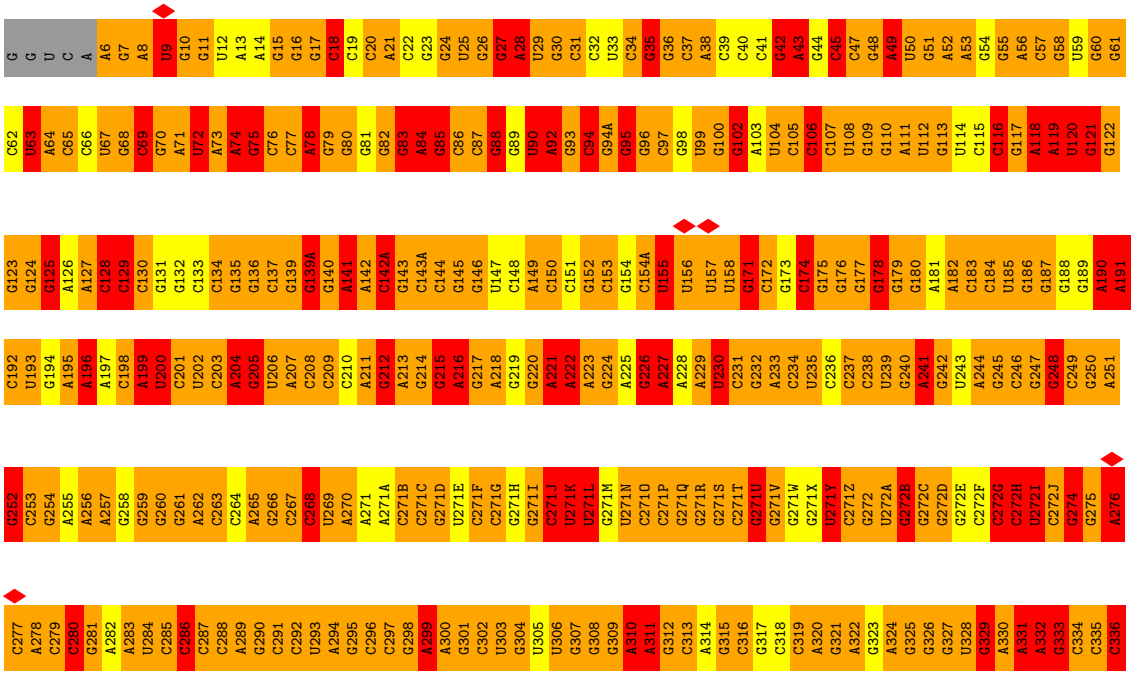
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

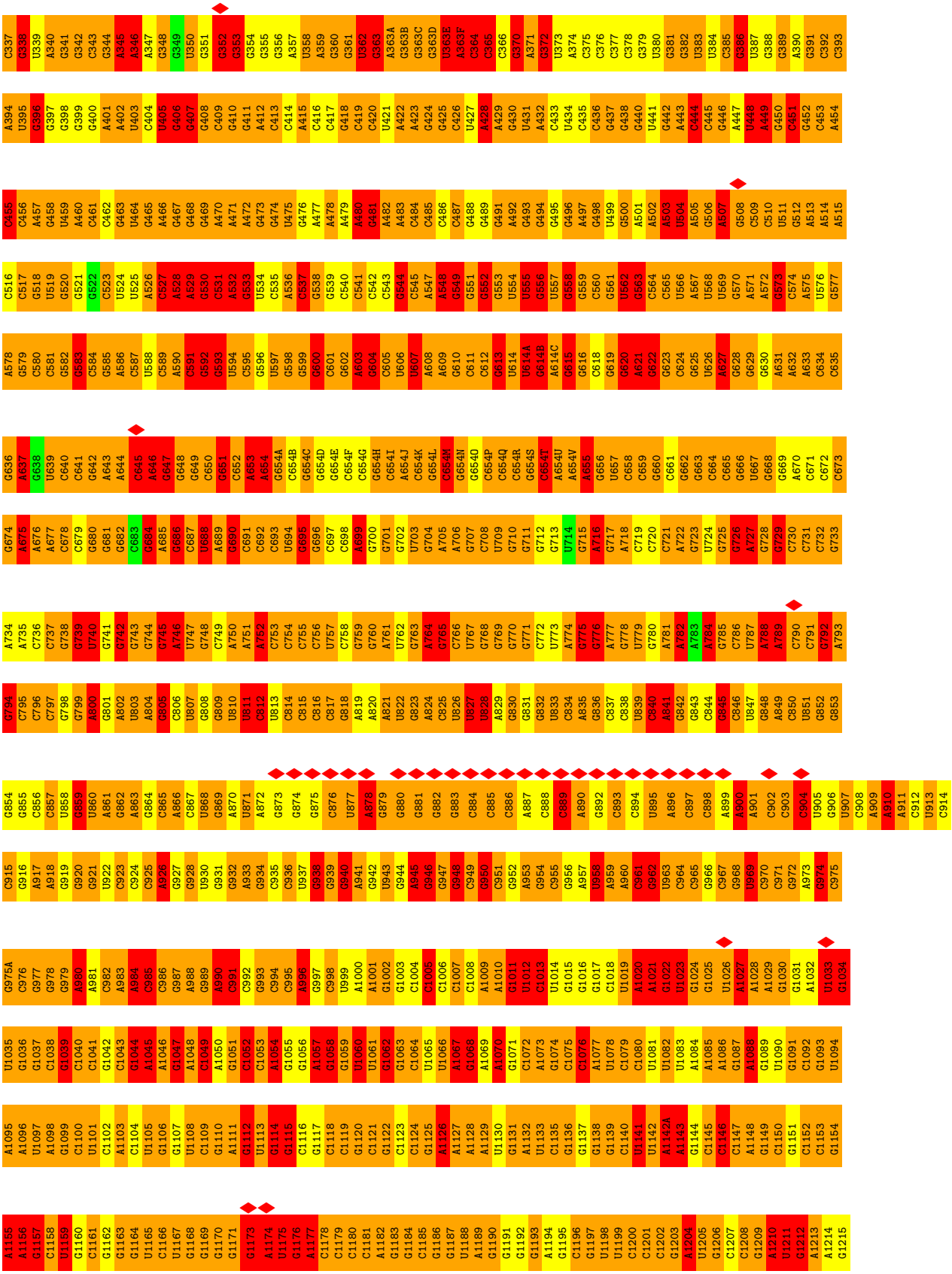
Chain B9:

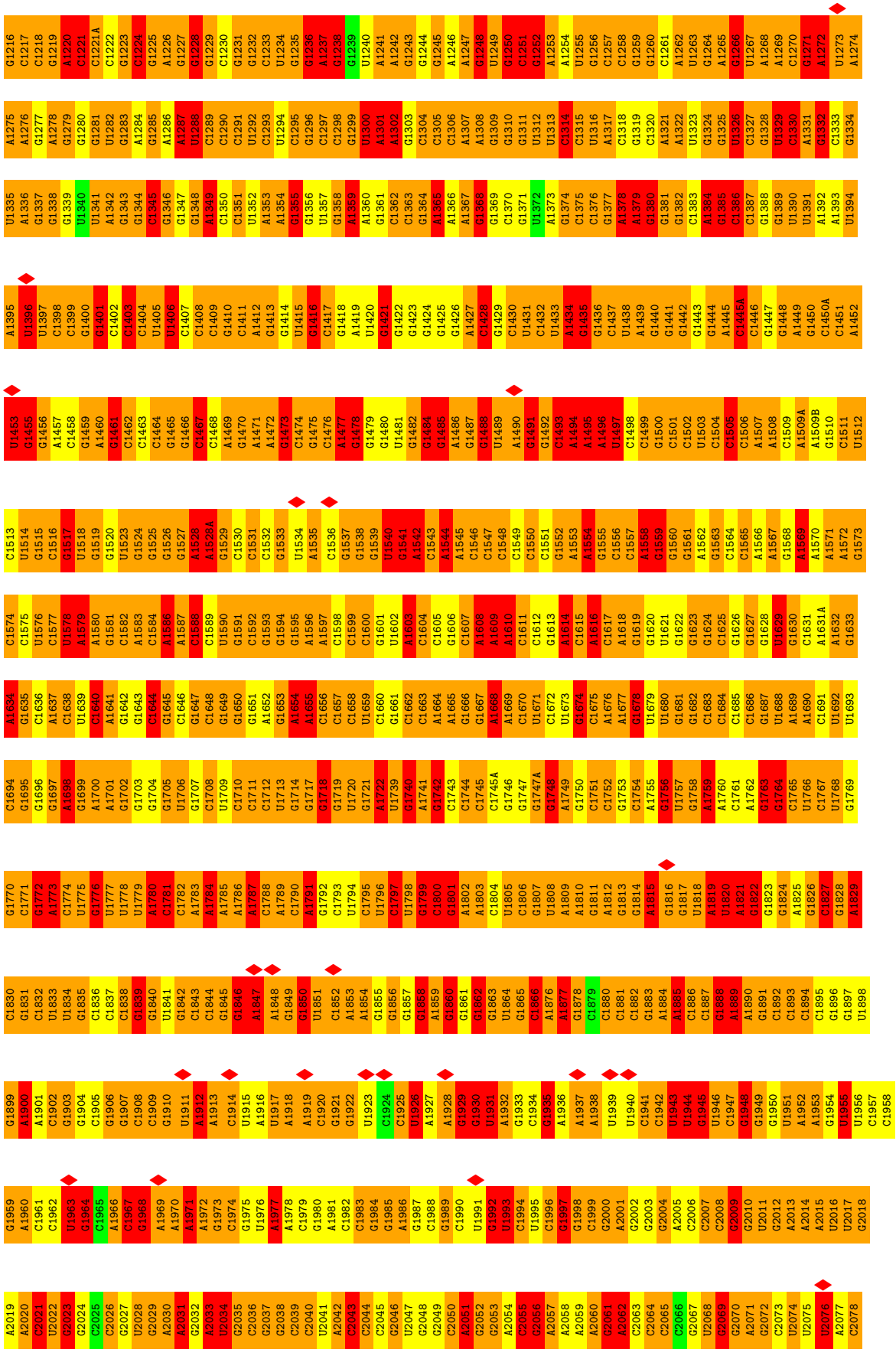


• Molecule 35: 23S RIBOSOMAL RNA

Chain BA:



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C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 U1841 G1842 C1843 C1844 G1845 G1846 A1847 A1848 G1849 G1850 U1851 C1852 A1853 A1854 G1855 G1856 G1857 G1858 A1859 G1860 G1861 G1862 G1863 A1864 U1865 C1866 A1876 A1877 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 G1891 C1892 C1893 C1894 C1895 G1896 G1897 U1898
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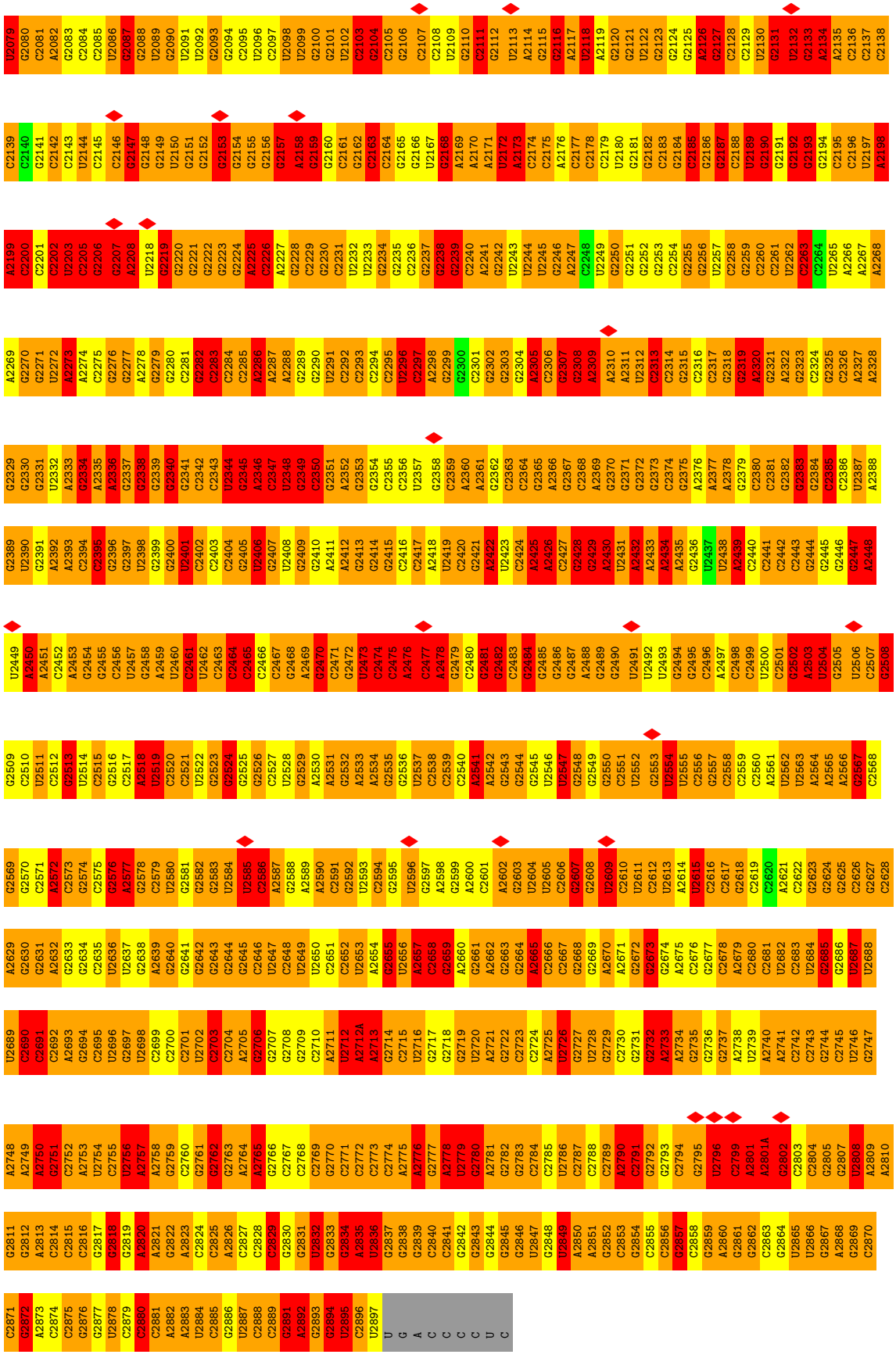
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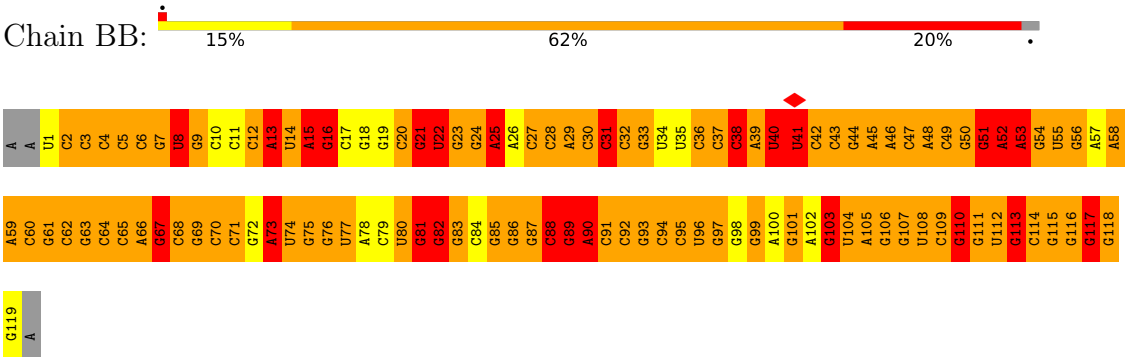
G2569 G2570 C2571 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 G2581 G2582 C2583 U2584 U2585 C2586 A2587 G2588 A2589 A2590 A2591 C2592 U2593 C2594 G2595 U2596 G2597 A2598 G2599 A2600 C2601 A2602 G2603 U2604 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 C2617 G2618 C2619 C2620 A2621 C2622 G2623 G2624 G2625 C2626 U2687 U2688
A2629 G2630 G2631 A2632 G2633 G2634 C2635 U2636 U2637 G2638 A2639 G2640 G2641 G2642 G2643 G2644 G2645 C2646 U2647 G2648 U2649 U2650 C2651 C2652 U2653 A2654 G2655 U2656 A2657 C2658 C2659 A2660 G2661 A2662 G2663 G2664 A2665 C2666 C2667 G2668 C2669 A2670 A2671 G2672 G2673 G2674 A2675 C2676 C2677 C2678 A2679 C2680 C2681 U2682 C2683 U2684 G2685 G2686
U2689 C2690 C2691 C2692 A2693 G2694 C2695 U2696 G2697 U2698 C2699 C2700 C2701 U2702 C2703 C2704 A2705 G2706 G2707 G2708 G2709 C2710 A2711 U2712 A2712A A2713 G2714 C2715 U2716 C2717 G2718 G2719 U2720 A2721 G2722 C2723 C2724 A2725 U2726 G2727 U2728 G2729 C2730 G2731 G2732 A2733 A2734 G2735 G2736 G2737 A2738 U2739 A2740 A2741 C2742 C2743 G2744 C2745 U2746 G2747
A2748 A2749 A2750 G2751 C2752 A2753 U2754 C2755 U2756 A2757 A2758 G2759 C2760 G2761 G2762 G2763 A2764 A2765 G2766 C2767 C2768 C2769 G2770 C2771 C2772 C2773 C2774 A2775 A2776 G2777 A2778 U2779 G2780 A2781 G2782 G2783 C2784 C2785 U2786 C2787 C2788 C2789 A2790 C2791 G2792 G2793 C2794 G2795 U2796 C2799 A2801 A2801A C2802 C2803 C2804 C2805 G2807 U2808 A2809 A2810
G2811 G2812 A2813 C2814 C2815 C2816 G2817 G2818 G2819 A2820 A2821 G2822 A2823 C2824 C2825 A2826 C2827 C2828 C2829 G2830 G2831 U2832 G2833 G2834 A2835 U2836 G2837 G2838 G2839 C2840 C2841 G2842 G2843 G2844 G2845 G2846 U2847 G2848 U2849 A2850 A2851 G2852 C2853 G2854 C2855 C2856 G2857 C2858 G2859 A2860 G2861 G2862 C2863 G2864 U2865 U2866 G2867 A2868 G2869 C2870
C2871 G2872 A2873 C2874 C2875 C2876 G2877 U2878 C2879 C2880 C2881 A2882 A2883 U2884 C2885 G2886 U2887 C2888 C2889 G2891 A2892 G2893 G2894 U2895 C2896 U2897 U G A C C C U C

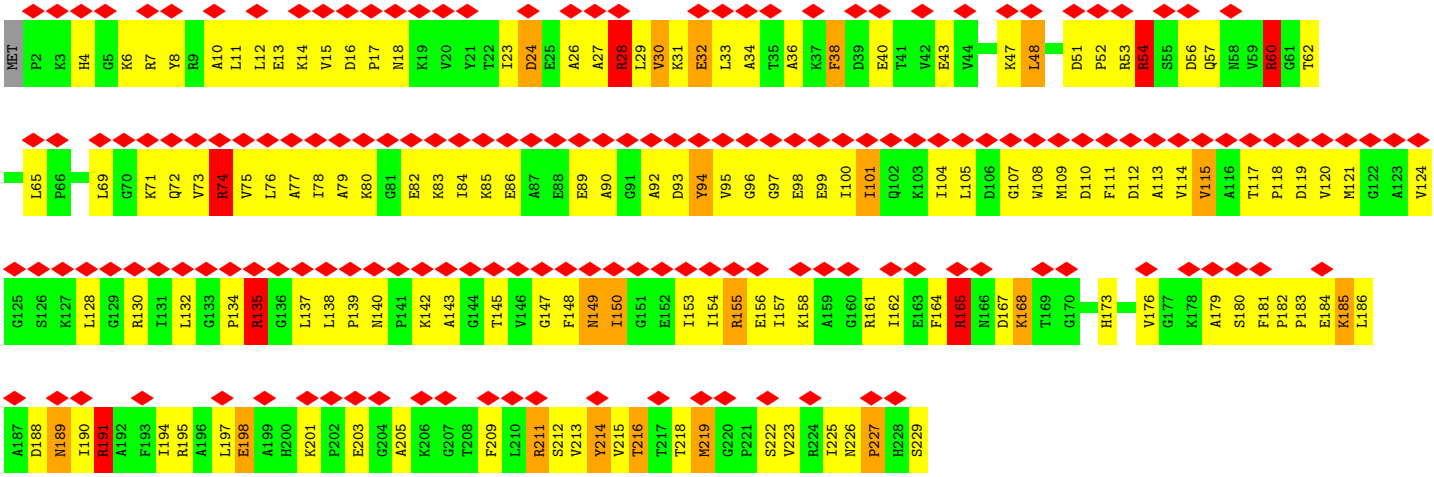
• Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



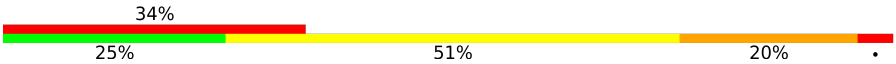
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

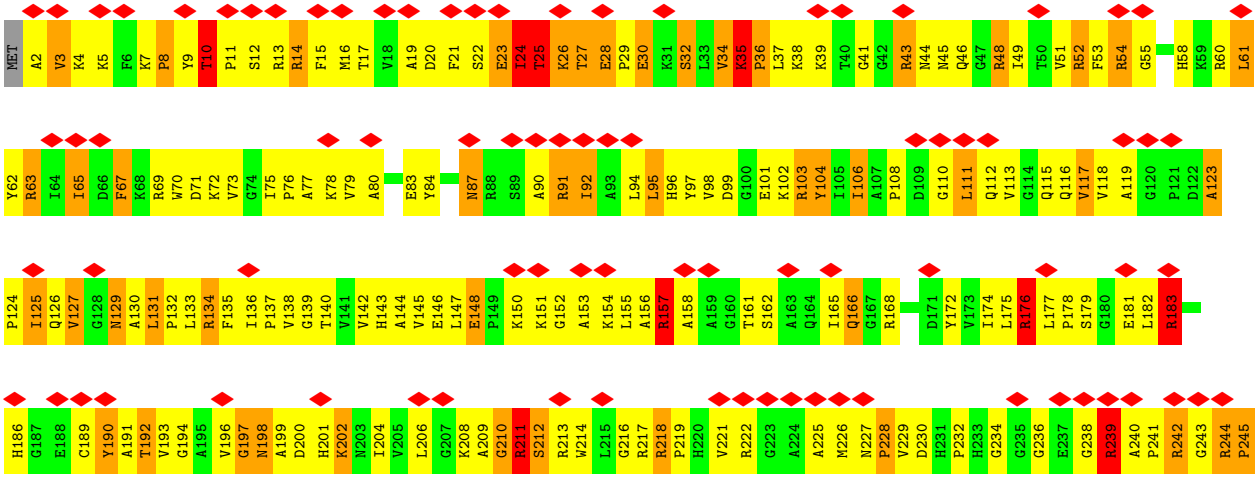
Chain BC:

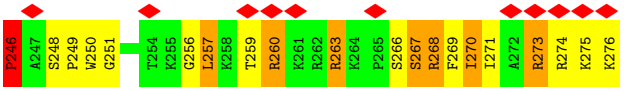


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:

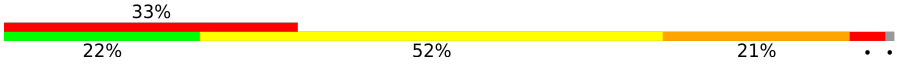


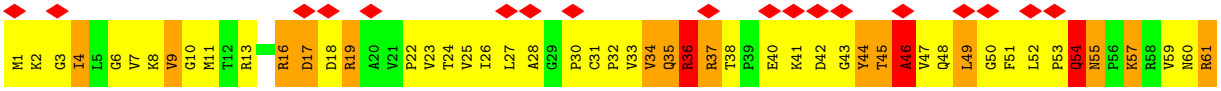


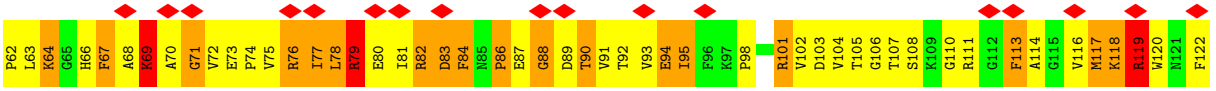


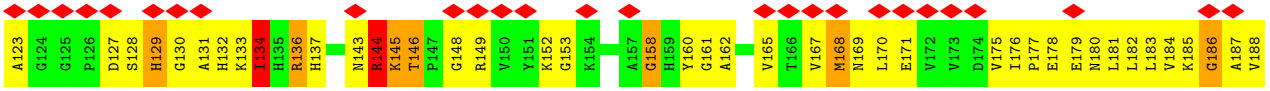
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

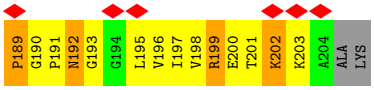
Chain BE:





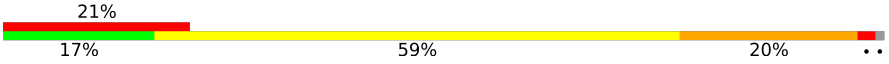


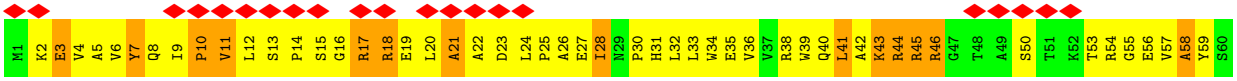


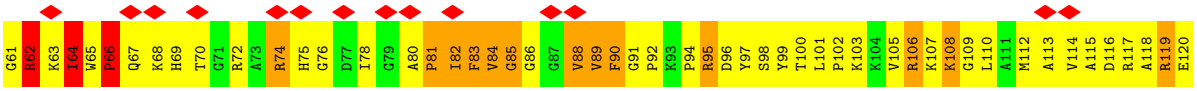


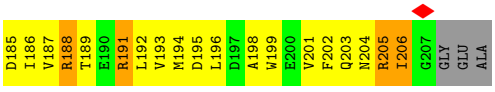
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



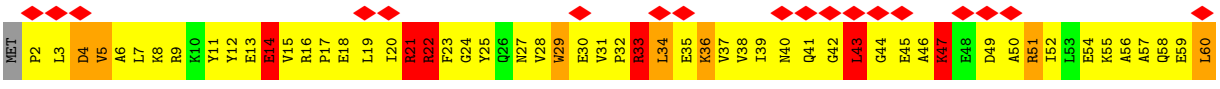


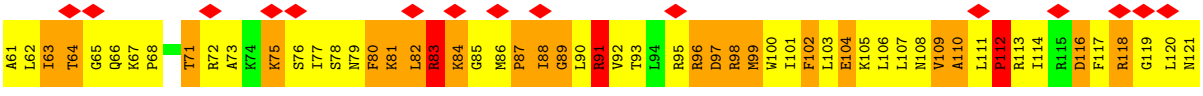


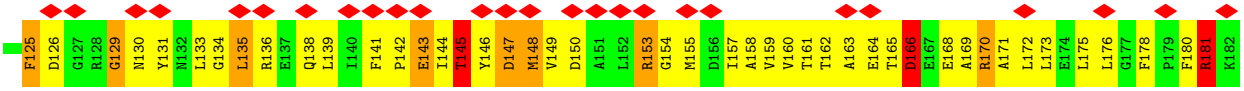


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:

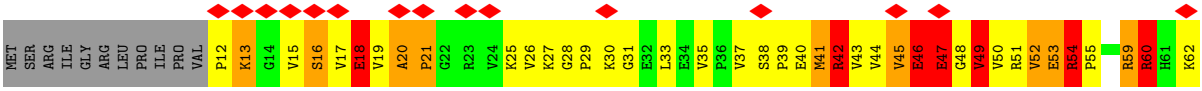


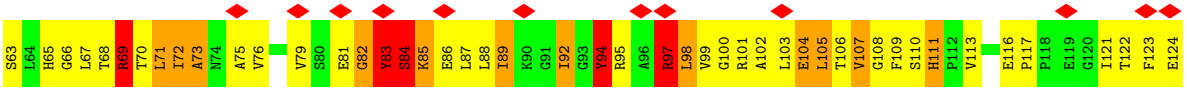




• Molecule 42: 50S RIBOSOMAL PROTEIN L6

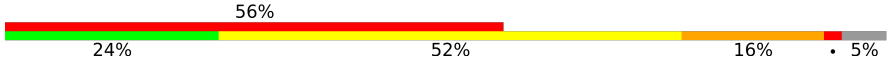
Chain BH:

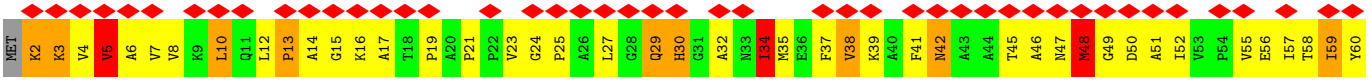


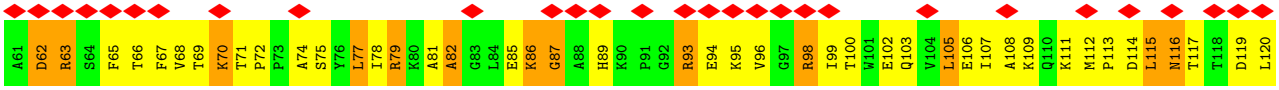


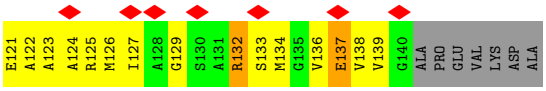
• Molecule 43: 50S RIBOSOMAL PROTEIN L11

Chain BK:



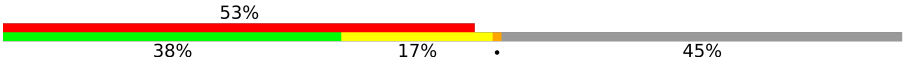


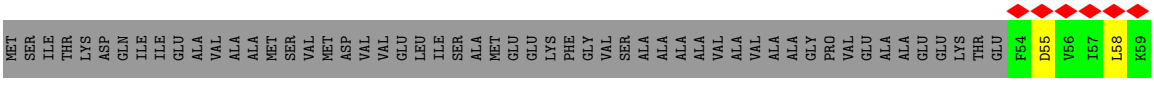


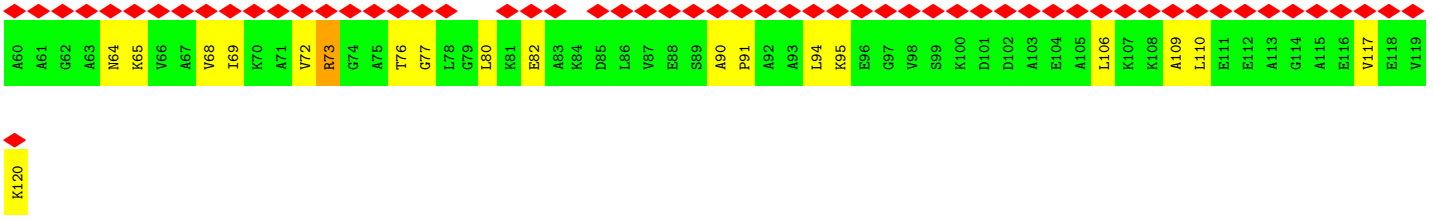


• Molecule 44: 50S RIBOSOMAL PROTEIN L7/L12

Chain BL:

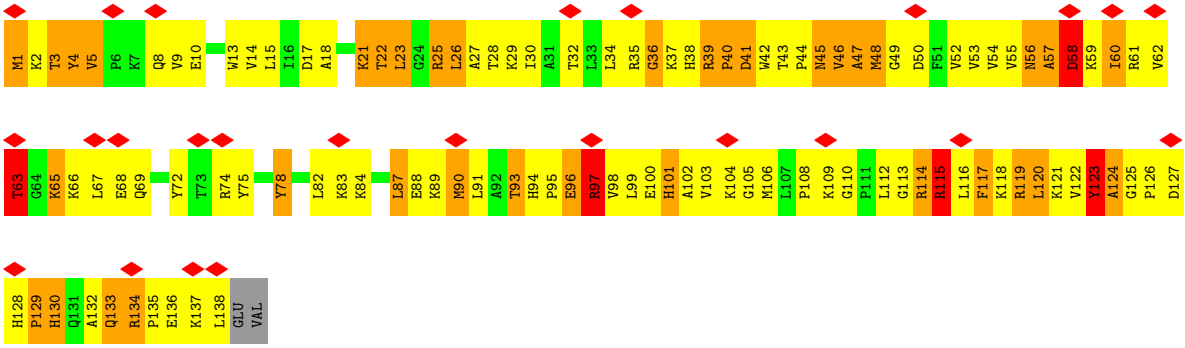






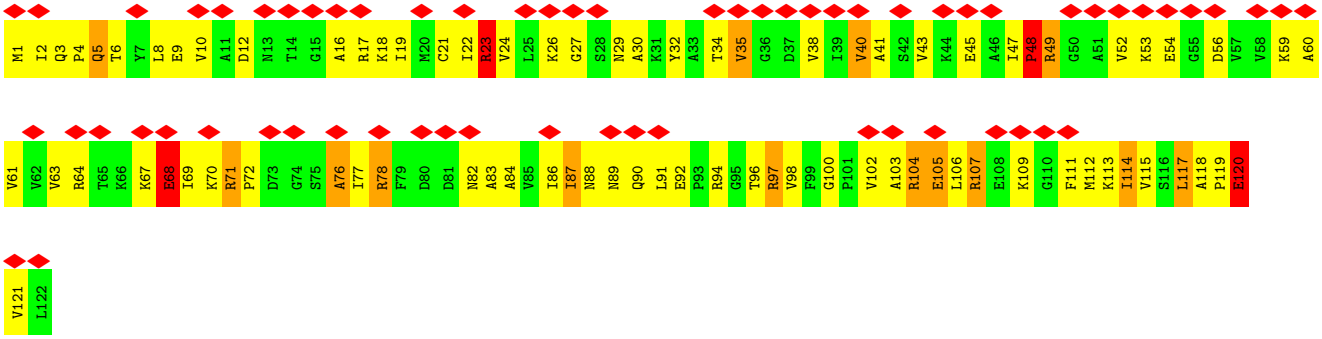
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN:



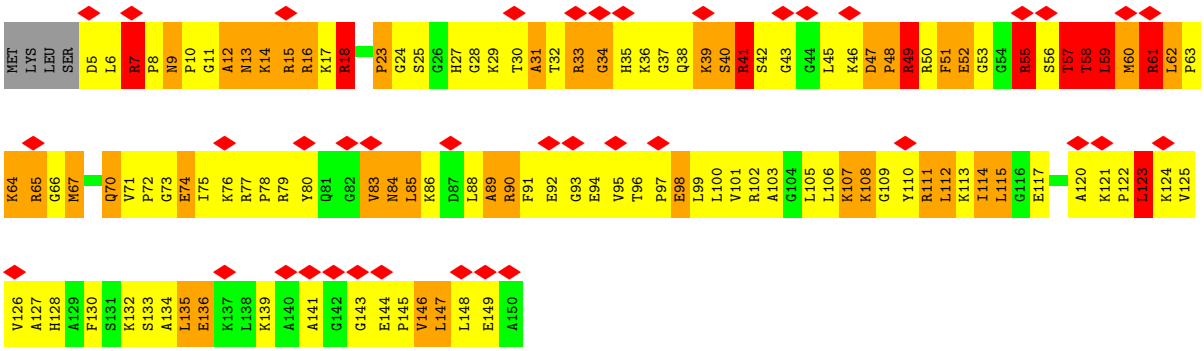
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:



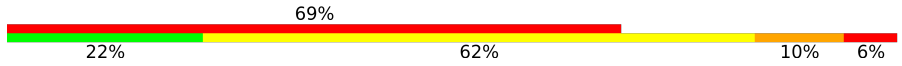
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

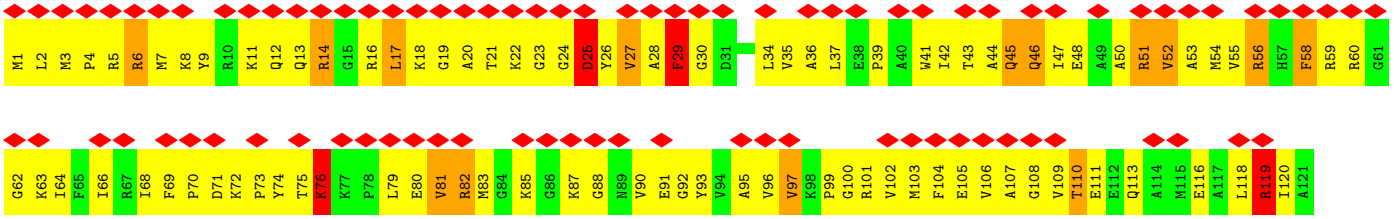
Chain BP:

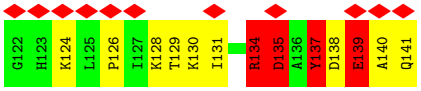


• Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:

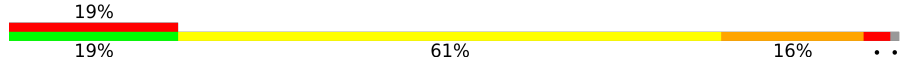


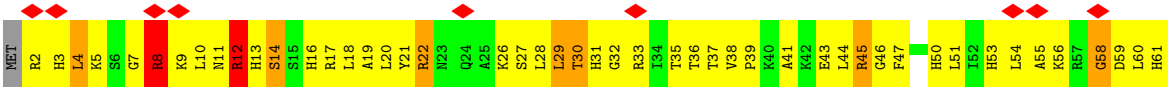


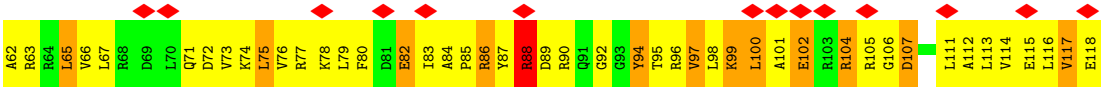


• Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR:

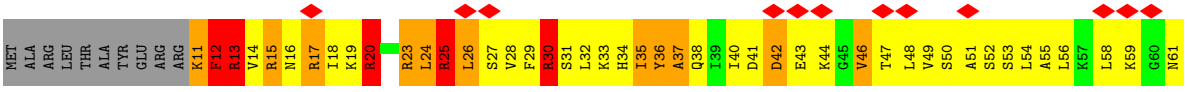


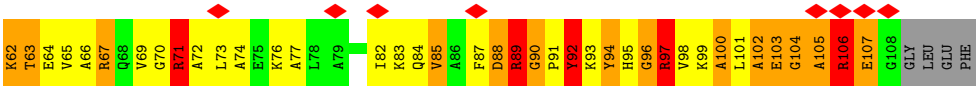




• Molecule 50: 50S RIBOSOMAL PROTEIN L18

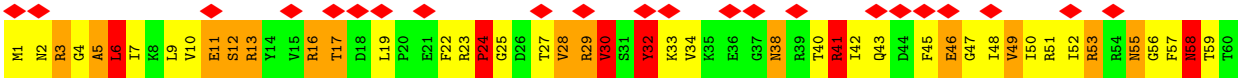
Chain BS:

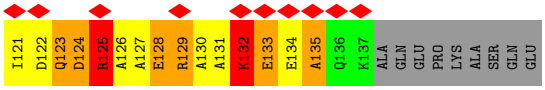




• Molecule 51: 50S RIBOSOMAL PROTEIN L19

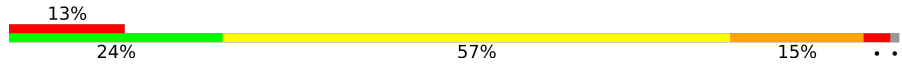
Chain BT:

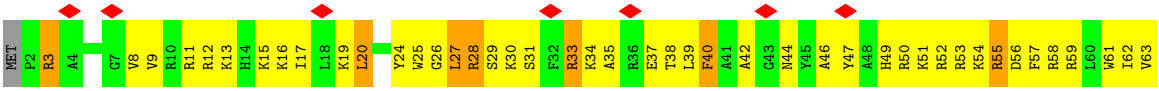


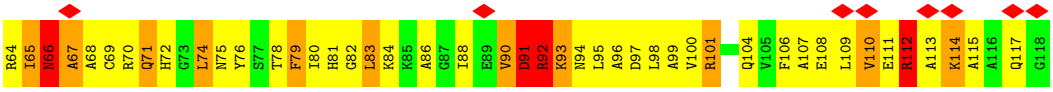


• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:

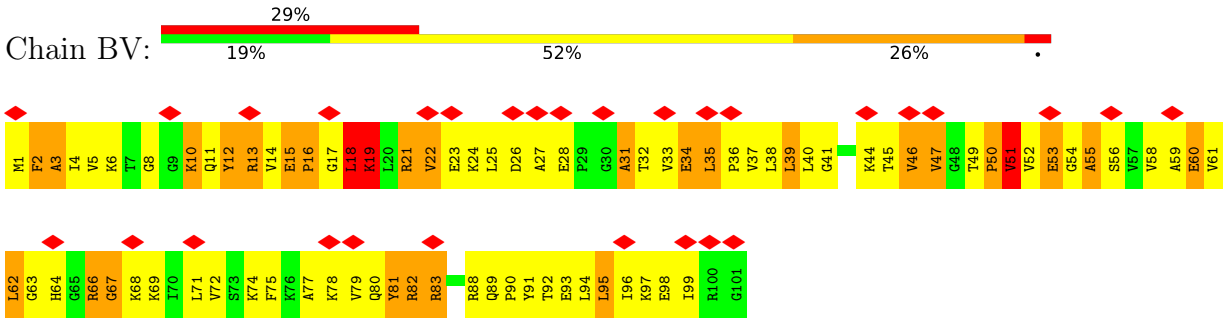






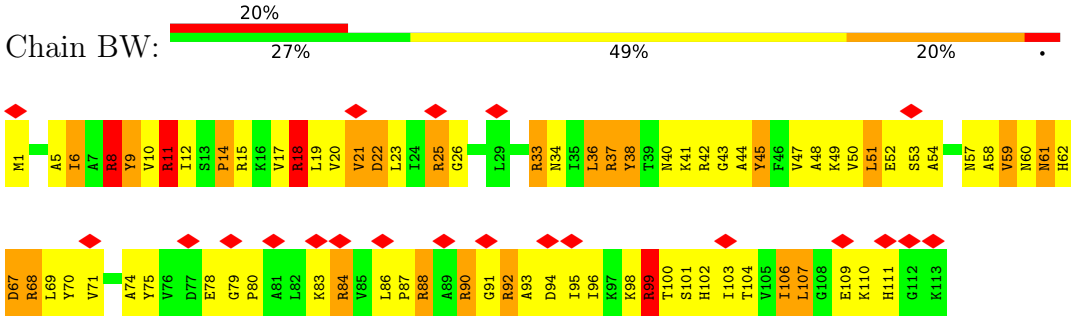
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain BV:



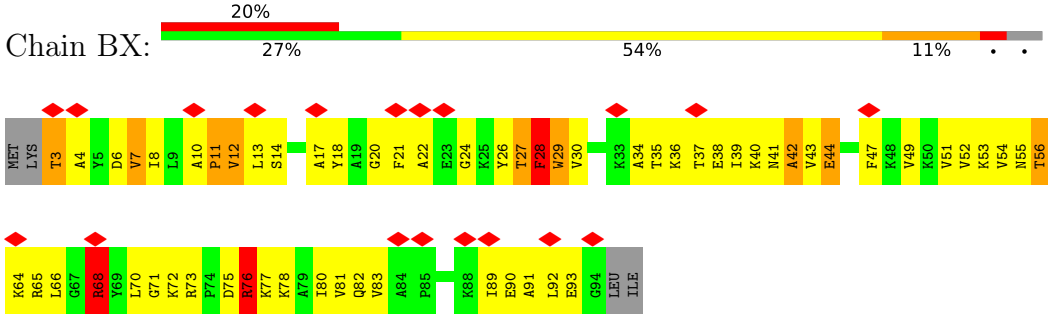
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain BW:



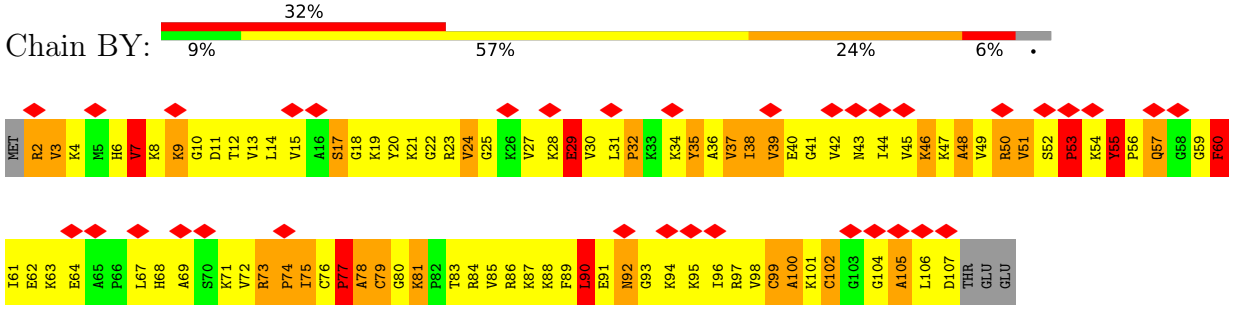
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain BX:



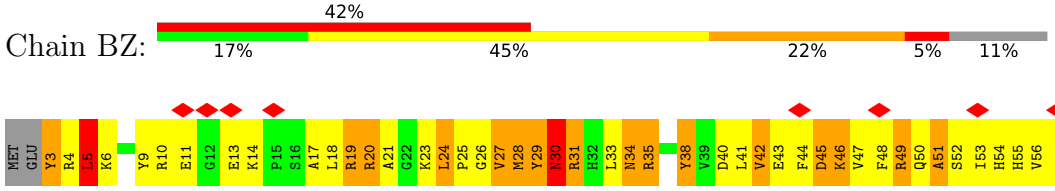
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

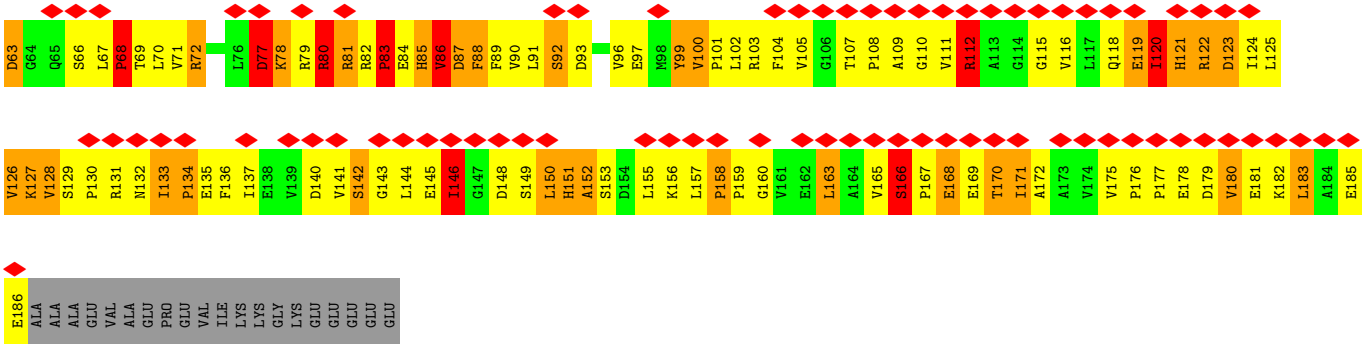
Chain BY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ:




D63 G64 Q65 S66 L67 P68 T69 L70 V71 R72 L76 D77 K78 R79 R80 R81 R82 P83 E84 H85 V86 D87 F88 F89 V90 L91 S92 D93 V96 E97 M98 Y99 V100 P101 L102 R103 F104 V105 G106 T107 P108 A109 G110 V111 R112 A113 G114 G115 V116 L117 Q118 E119 I120 H121 R122 D123 I124 L125
V126 K127 V128 S129 P130 R131 N132 I133 P134 E135 F136 I137 E138 V139 D140 V141 S142 G143 L144 E145 I146 G147 D148 S149 L150 H151 A152 S153 D154 L155 K156 L157 P158 P159 G160 V161 E162 L163 A164 V165 S166 P167 E168 E169 T170 I171 A172 A173 V174 V175 P176 P177 E178 D179 V180 E181 K182 L183 A184 E185
E186 ALA ALA ALA GLU VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	13410.900	Depositor
Minimum map value	-6356.590	Depositor
Average map value	213.063	Depositor
Map value standard deviation	916.721	Depositor
Recommended contour level	3000.0	Depositor
Map size (Å)	378, 378, 378	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	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: GDP, FUA

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	2.74	2653/36190 (7.3%)	2.42	3123/56486 (5.5%)
2	AB	1.43	2/1935 (0.1%)	1.55	20/2609 (0.8%)
3	AC	1.49	3/1636 (0.2%)	1.59	25/2205 (1.1%)
4	AD	1.40	1/1733 (0.1%)	1.59	25/2318 (1.1%)
5	AE	1.48	1/1162 (0.1%)	1.54	9/1564 (0.6%)
6	AF	1.39	3/856 (0.4%)	1.69	15/1154 (1.3%)
7	AG	1.39	1/1276 (0.1%)	1.51	15/1709 (0.9%)
8	AH	1.48	2/1136 (0.2%)	1.67	20/1527 (1.3%)
9	AI	1.47	2/1029 (0.2%)	2.08	19/1379 (1.4%)
10	AJ	1.35	0/807	1.50	6/1085 (0.6%)
11	AK	1.40	1/900 (0.1%)	1.48	9/1213 (0.7%)
12	AL	1.45	0/986	1.56	9/1320 (0.7%)
13	AM	1.39	1/998 (0.1%)	1.64	17/1336 (1.3%)
14	AN	1.49	2/501 (0.4%)	1.71	9/664 (1.4%)
15	AO	1.35	0/745	1.59	13/992 (1.3%)
16	AP	1.34	1/716 (0.1%)	1.62	11/963 (1.1%)
17	AQ	1.45	2/836 (0.2%)	1.57	11/1117 (1.0%)
18	AR	1.40	0/579	1.59	7/768 (0.9%)
19	AS	1.28	0/642	1.48	5/865 (0.6%)
20	AT	1.31	0/765	1.52	12/1007 (1.2%)
21	AU	1.33	0/212	1.76	6/277 (2.2%)
22	AV	2.74	134/1832 (7.3%)	2.54	182/2855 (6.4%)
23	AX	2.60	15/257 (5.8%)	2.50	24/398 (6.0%)
24	AY	1.31	7/5312 (0.1%)	1.51	49/7193 (0.7%)
25	B0	1.27	0/671	1.52	11/892 (1.2%)
26	B1	1.37	2/738 (0.3%)	1.59	6/981 (0.6%)
27	B2	1.25	0/600	1.51	4/793 (0.5%)
28	B3	1.35	0/472	1.46	4/634 (0.6%)
29	B4	1.32	0/460	1.78	10/621 (1.6%)
30	B5	1.35	1/473 (0.2%)	1.48	3/639 (0.5%)
31	B6	1.49	3/440 (0.7%)	1.68	7/586 (1.2%)
32	B7	1.38	0/426	1.66	9/561 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	B8	1.33	1/515 (0.2%)	1.56	6/679 (0.9%)
34	B9	1.37	0/310	1.59	6/407 (1.5%)
35	BA	2.69	4866/69972 (7.0%)	2.42	6058/109237 (5.5%)
36	BB	2.71	196/2853 (6.9%)	2.45	289/4451 (6.5%)
37	BC	1.35	0/1774	1.44	16/2391 (0.7%)
38	BD	1.38	3/2195 (0.1%)	1.59	25/2955 (0.8%)
39	BE	1.37	1/1596 (0.1%)	1.58	19/2153 (0.9%)
40	BF	1.40	2/1658 (0.1%)	1.63	27/2244 (1.2%)
41	BG	1.35	1/1499 (0.1%)	1.93	24/2016 (1.2%)
42	BH	1.35	4/1292 (0.3%)	1.51	12/1744 (0.7%)
43	BK	1.29	2/1044 (0.2%)	1.38	4/1416 (0.3%)
44	BL	1.10	0/478	1.50	2/640 (0.3%)
45	BN	1.33	2/1131 (0.2%)	1.57	13/1525 (0.9%)
46	BO	1.43	1/943 (0.1%)	1.50	11/1269 (0.9%)
47	BP	1.34	0/1131	1.64	13/1504 (0.9%)
48	BQ	1.38	2/1143 (0.2%)	1.52	11/1527 (0.7%)
49	BR	1.28	0/974	1.52	12/1302 (0.9%)
50	BS	1.31	1/778 (0.1%)	1.74	23/1036 (2.2%)
51	BT	1.37	1/1155 (0.1%)	1.78	25/1542 (1.6%)
52	BU	1.38	0/975	1.51	8/1297 (0.6%)
53	BV	1.34	2/790 (0.3%)	1.49	7/1057 (0.7%)
54	BW	1.31	1/907 (0.1%)	1.59	14/1216 (1.2%)
55	BX	1.39	0/739	1.46	5/993 (0.5%)
56	BY	1.24	1/823 (0.1%)	1.55	9/1098 (0.8%)
57	BZ	1.34	0/1499	1.53	18/2035 (0.9%)
All	All	2.36	7924/165495 (4.8%)	2.21	10352/246445 (4.2%)

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	0	107
2	AB	0	5
3	AC	0	3
4	AD	0	3
5	AE	0	4
6	AF	0	6
7	AG	0	6
8	AH	0	4
9	AI	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	AJ	0	2
11	AK	0	2
12	AL	0	3
13	AM	0	3
14	AN	0	2
15	AO	0	3
16	AP	0	6
17	AQ	0	3
18	AR	0	3
19	AS	0	3
20	AT	0	2
21	AU	0	3
22	AV	0	5
23	AX	0	1
24	AY	0	13
25	B0	0	1
26	B1	0	3
27	B2	0	6
28	B3	0	2
29	B4	0	3
30	B5	0	2
31	B6	0	3
32	B7	0	1
33	B8	0	2
34	B9	0	2
35	BA	1	152
36	BB	0	6
37	BC	0	6
38	BD	0	2
39	BE	0	3
40	BF	0	3
41	BG	0	5
42	BH	0	8
43	BK	0	3
45	BN	0	3
46	BO	0	3
47	BP	0	5
48	BQ	0	3
49	BR	0	2
50	BS	0	6
51	BT	0	6
52	BU	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	BV	0	2
54	BW	0	4
55	BX	0	2
56	BY	0	3
57	BZ	0	4
All	All	1	457

The worst 5 of 7924 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	473	G	N7-C5	-17.52	1.28	1.39
1	AA	710	G	C8-N7	-15.43	1.21	1.30
1	AA	809	G	C8-N7	-15.17	1.21	1.30
1	AA	188	C	N1-C6	-15.00	1.28	1.37
1	AA	1311	G	C8-N7	-14.67	1.22	1.30

The worst 5 of 10352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BG	112	PRO	O-C-N	-40.65	57.66	122.70
9	AI	53	VAL	O-C-N	-36.52	64.27	122.70
9	AI	104	ARG	O-C-N	-30.37	74.11	122.70
41	BG	112	PRO	CA-C-N	21.56	164.63	117.20
26	B1	20	ARG	NE-CZ-NH2	-18.37	111.11	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	1992	G	C3'

5 of 457 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	106	C	Sidechain
1	AA	108	G	Sidechain
1	AA	30	U	Sidechain
1	AA	5	U	Sidechain
1	AA	69	G	Sidechain

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	AA	32329	0	16041	1543	0
2	AB	1900	0	1951	244	0
3	AC	1612	0	1677	208	0
4	AD	1703	0	1767	205	0
5	AE	1146	0	1207	140	0
6	AF	843	0	857	95	0
7	AG	1257	0	1296	119	0
8	AH	1116	0	1177	110	0
9	AI	1010	0	1037	142	0
10	AJ	794	0	840	185	0
11	AK	885	0	904	92	0
12	AL	970	0	1057	144	0
13	AM	987	0	1059	139	0
14	AN	492	0	533	78	0
15	AO	734	0	771	74	0
16	AP	700	0	720	83	0
17	AQ	823	0	891	68	0
18	AR	574	0	644	77	0
19	AS	629	0	652	116	0
20	AT	763	0	861	112	0
21	AU	208	0	221	28	0
22	AV	1640	0	831	100	0
23	AX	230	0	114	17	0
24	AY	5214	0	5288	791	0
25	B0	662	0	688	91	0
26	B1	731	0	808	116	0
27	B2	598	0	653	94	0
28	B3	467	0	523	53	0
29	B4	450	0	449	93	0
30	B5	459	0	480	98	0
31	B6	433	0	461	148	0
32	B7	418	0	467	58	0
33	B8	507	0	576	103	0
34	B9	307	0	338	35	0
35	BA	62474	0	31032	3276	0
36	BB	2551	0	1281	164	0
37	BC	1742	0	1798	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	305	0
39	BE	1563	0	1629	246	0
40	BF	1623	0	1677	283	0
41	BG	1474	0	1535	287	0
42	BH	1268	0	1337	232	0
43	BK	1025	0	1066	177	0
44	BL	477	0	509	14	0
45	BN	1104	0	1180	202	0
46	BO	933	0	996	124	0
47	BP	1114	0	1187	295	0
48	BQ	1122	0	1179	166	0
49	BR	960	0	1021	158	0
50	BS	770	0	832	168	0
51	BT	1141	0	1202	228	0
52	BU	958	0	1015	170	0
53	BV	779	0	852	148	0
54	BW	896	0	953	103	0
55	BX	725	0	778	93	0
56	BY	810	0	901	186	0
57	BZ	1467	0	1492	230	0
58	AY	37	0	47	12	0
59	AY	28	0	12	7	0
All	All	152777	0	105584	12183	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 47.

The worst 5 of 12183 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)
1:AA:509:A:H5'	1:AA:510:A:OP2	1.26	1.30
24:AY:496:LYS:HE2	24:AY:498:ILE:CD1	1.66	1.25
53:BV:15:GLU:HB3	53:BV:16:PRO:HD2	1.23	1.20
41:BG:63:ILE:HA	41:BG:143:GLU:HG3	1.22	1.19
35:BA:925:C:H2'	35:BA:926:A:H5"	1.24	1.18

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
2	AB	232/256 (91%)	146 (63%)	55 (24%)	31 (13%)	0 5
3	AC	204/239 (85%)	129 (63%)	58 (28%)	17 (8%)	1 12
4	AD	206/209 (99%)	133 (65%)	52 (25%)	21 (10%)	0 9
5	AE	148/162 (91%)	116 (78%)	27 (18%)	5 (3%)	3 26
6	AF	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	1 17
7	AG	153/156 (98%)	107 (70%)	34 (22%)	12 (8%)	1 13
8	AH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	2 19
9	AI	125/128 (98%)	84 (67%)	26 (21%)	15 (12%)	0 6
10	AJ	96/105 (91%)	64 (67%)	19 (20%)	13 (14%)	0 4
11	AK	117/129 (91%)	93 (80%)	18 (15%)	6 (5%)	2 19
12	AL	122/132 (92%)	81 (66%)	26 (21%)	15 (12%)	0 5
13	AM	122/126 (97%)	77 (63%)	25 (20%)	20 (16%)	0 3
14	AN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1 15
15	AO	86/89 (97%)	53 (62%)	25 (29%)	8 (9%)	0 11
16	AP	81/88 (92%)	58 (72%)	19 (24%)	4 (5%)	2 20
17	AQ	97/105 (92%)	76 (78%)	16 (16%)	5 (5%)	2 19
18	AR	68/88 (77%)	51 (75%)	11 (16%)	6 (9%)	1 11
19	AS	76/93 (82%)	39 (51%)	20 (26%)	17 (22%)	0 1
20	AT	97/106 (92%)	52 (54%)	30 (31%)	15 (16%)	0 3
21	AU	22/27 (82%)	14 (64%)	6 (27%)	2 (9%)	1 11
24	AY	662/691 (96%)	442 (67%)	135 (20%)	85 (13%)	0 5
25	B0	82/85 (96%)	64 (78%)	16 (20%)	2 (2%)	6 33
26	B1	91/98 (93%)	60 (66%)	20 (22%)	11 (12%)	0 6
27	B2	69/72 (96%)	34 (49%)	22 (32%)	13 (19%)	0 2
28	B3	57/60 (95%)	41 (72%)	12 (21%)	4 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	B4	55/71 (78%)	25 (46%)	16 (29%)	14 (26%)	0 1
30	B5	57/60 (95%)	40 (70%)	6 (10%)	11 (19%)	0 2
31	B6	48/54 (89%)	22 (46%)	10 (21%)	16 (33%)	0 0
32	B7	46/49 (94%)	35 (76%)	9 (20%)	2 (4%)	2 22
33	B8	61/65 (94%)	35 (57%)	17 (28%)	9 (15%)	0 3
34	B9	35/37 (95%)	23 (66%)	8 (23%)	4 (11%)	0 7
37	BC	226/229 (99%)	173 (76%)	42 (19%)	11 (5%)	2 20
38	BD	273/276 (99%)	185 (68%)	55 (20%)	33 (12%)	0 6
39	BE	202/206 (98%)	121 (60%)	49 (24%)	32 (16%)	0 3
40	BF	205/210 (98%)	134 (65%)	44 (22%)	27 (13%)	0 5
41	BG	179/182 (98%)	113 (63%)	44 (25%)	22 (12%)	0 5
42	BH	164/180 (91%)	89 (54%)	37 (23%)	38 (23%)	0 1
43	BK	137/147 (93%)	89 (65%)	36 (26%)	12 (9%)	1 11
44	BL	65/121 (54%)	56 (86%)	9 (14%)	0	100 100
45	BN	136/140 (97%)	89 (65%)	31 (23%)	16 (12%)	0 6
46	BO	120/122 (98%)	94 (78%)	17 (14%)	9 (8%)	1 13
47	BP	144/150 (96%)	75 (52%)	44 (31%)	25 (17%)	0 3
48	BQ	139/141 (99%)	104 (75%)	28 (20%)	7 (5%)	2 20
49	BR	115/118 (98%)	79 (69%)	24 (21%)	12 (10%)	0 8
50	BS	96/112 (86%)	43 (45%)	34 (35%)	19 (20%)	0 2
51	BT	135/146 (92%)	76 (56%)	34 (25%)	25 (18%)	0 2
52	BU	115/118 (98%)	70 (61%)	33 (29%)	12 (10%)	0 8
53	BV	99/101 (98%)	67 (68%)	15 (15%)	17 (17%)	0 3
54	BW	111/113 (98%)	80 (72%)	18 (16%)	13 (12%)	0 6
55	BX	90/96 (94%)	62 (69%)	23 (26%)	5 (6%)	2 19
56	BY	104/110 (94%)	45 (43%)	35 (34%)	24 (23%)	0 1
57	BZ	182/206 (88%)	108 (59%)	41 (22%)	33 (18%)	0 3
All	All	6645/7104 (94%)	4378 (66%)	1475 (22%)	792 (12%)	1 6

5 of 792 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	13	ALA

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Mol	Chain	Res	Type
2	AB	20	GLU
2	AB	95	GLN
2	AB	190	THR
2	AB	195	ASP

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
2	AB	202/220 (92%)	178 (88%)	24 (12%)	5 20
3	AC	160/188 (85%)	133 (83%)	27 (17%)	2 12
4	AD	180/181 (99%)	158 (88%)	22 (12%)	5 20
5	AE	115/123 (94%)	101 (88%)	14 (12%)	5 20
6	AF	90/90 (100%)	80 (89%)	10 (11%)	6 22
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7 25
8	AH	119/119 (100%)	106 (89%)	13 (11%)	6 23
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7 25
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	3 15
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9 30
12	AL	104/109 (95%)	93 (89%)	11 (11%)	6 24
13	AM	99/101 (98%)	86 (87%)	13 (13%)	4 18
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3 16
15	AO	79/80 (99%)	70 (89%)	9 (11%)	5 21
16	AP	72/74 (97%)	69 (96%)	3 (4%)	30 54
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10 33
18	AR	61/77 (79%)	58 (95%)	3 (5%)	25 50
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3 15
20	AT	76/82 (93%)	66 (87%)	10 (13%)	4 18
21	AU	19/22 (86%)	19 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	AY	563/582 (97%)	481 (85%)	82 (15%)	3 15
25	B0	66/67 (98%)	56 (85%)	10 (15%)	3 14
26	B1	78/83 (94%)	64 (82%)	14 (18%)	2 10
27	B2	66/67 (98%)	58 (88%)	8 (12%)	5 20
28	B3	51/52 (98%)	47 (92%)	4 (8%)	12 36
29	B4	51/63 (81%)	36 (71%)	15 (29%)	0 2
30	B5	51/52 (98%)	45 (88%)	6 (12%)	5 20
31	B6	49/52 (94%)	37 (76%)	12 (24%)	0 3
32	B7	41/42 (98%)	34 (83%)	7 (17%)	2 11
33	B8	53/55 (96%)	46 (87%)	7 (13%)	4 18
34	B9	34/34 (100%)	28 (82%)	6 (18%)	2 11
37	BC	180/181 (99%)	162 (90%)	18 (10%)	7 26
38	BD	217/218 (100%)	178 (82%)	39 (18%)	1 10
39	BE	165/166 (99%)	141 (86%)	24 (14%)	3 15
40	BF	165/166 (99%)	154 (93%)	11 (7%)	16 41
41	BG	155/156 (99%)	129 (83%)	26 (17%)	2 12
42	BH	136/148 (92%)	118 (87%)	18 (13%)	4 18
43	BK	104/111 (94%)	88 (85%)	16 (15%)	2 14
44	BL	46/85 (54%)	41 (89%)	5 (11%)	6 23
45	BN	117/119 (98%)	95 (81%)	22 (19%)	1 9
46	BO	100/100 (100%)	92 (92%)	8 (8%)	12 35
47	BP	112/116 (97%)	86 (77%)	26 (23%)	1 4
48	BQ	111/111 (100%)	94 (85%)	17 (15%)	2 14
49	BR	100/101 (99%)	89 (89%)	11 (11%)	6 22
50	BS	77/88 (88%)	66 (86%)	11 (14%)	3 16
51	BT	120/127 (94%)	95 (79%)	25 (21%)	1 6
52	BU	92/94 (98%)	82 (89%)	10 (11%)	6 23
53	BV	82/82 (100%)	70 (85%)	12 (15%)	3 15
54	BW	91/92 (99%)	78 (86%)	13 (14%)	3 16
55	BX	74/78 (95%)	63 (85%)	11 (15%)	3 15
56	BY	87/91 (96%)	75 (86%)	12 (14%)	3 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	BZ	162/179 (90%)	134 (83%)	28 (17%)	2 11
All	All	5586/5868 (95%)	4824 (86%)	762 (14%)	7 17

5 of 762 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BE	61	ARG
45	BN	96	GLU
39	BE	192	ASN
39	BE	54	GLN
42	BH	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
39	BE	129	HIS
48	BQ	12	GLN
39	BE	192	ASN
43	BK	30	HIS
50	BS	38	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	277 (18%)	47 (3%)
22	AV	76/77 (98%)	17 (22%)	0
23	AX	10/11 (90%)	5 (50%)	0
35	BA	2900/2915 (99%)	633 (21%)	77 (2%)
36	BB	118/122 (96%)	27 (22%)	2 (1%)
All	All	4607/4647 (99%)	959 (20%)	126 (2%)

5 of 959 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	332	A
35	BA	2425	A
35	BA	1020	A
35	BA	2422	A
35	BA	2779	U

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	GDP	AY	702	-	24,30,30	1.57	6 (25%)	30,47,47	1.71	7 (23%)
58	FUA	AY	701	-	39,40,40	2.10	12 (30%)	49,64,64	1.79	11 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	AY	702	-	-	2/12/32/32	0/3/3/3
58	FUA	AY	701	-	-	5/15/92/92	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	701	FUA	C23-C22	-5.40	1.37	1.51
58	AY	701	FUA	C23-C24	-4.19	1.39	1.53
59	AY	702	GDP	C5-C6	-4.16	1.39	1.47
58	AY	701	FUA	C15-C14	-3.97	1.46	1.54
58	AY	701	FUA	C29-C22	3.88	1.53	1.47

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	AY	701	FUA	C8-C9-C10	-6.55	109.63	116.34
58	AY	701	FUA	C6-C5-C10	-4.41	106.16	111.65
59	AY	702	GDP	PA-O3A-PB	-4.24	118.26	132.83
59	AY	702	GDP	C2-N1-C6	-3.60	118.46	125.10
58	AY	701	FUA	O6-C3-C2	-3.46	101.66	109.96

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AY	701	FUA	C13-C17-C22-C29
58	AY	701	FUA	C17-C22-C23-C24
58	AY	701	FUA	C29-C22-C23-C24
59	AY	702	GDP	C5'-O5'-PA-O3A
59	AY	702	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

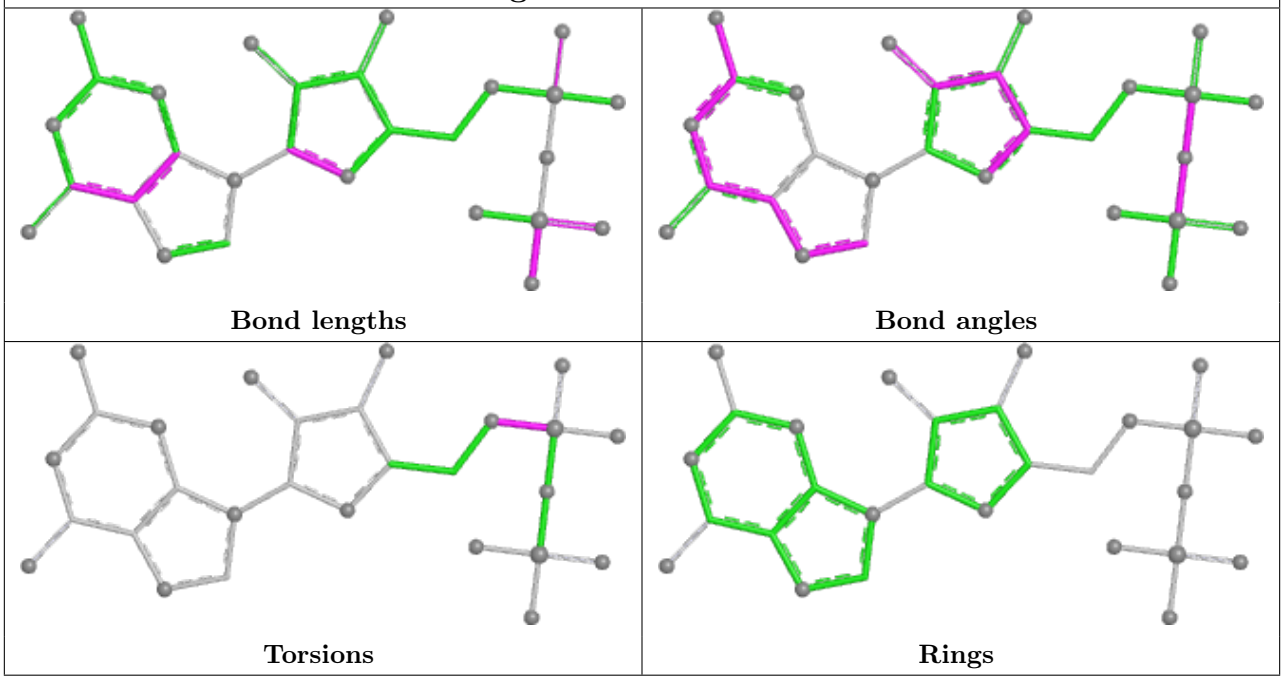
2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AY	702	GDP	7	0
58	AY	701	FUA	12	0

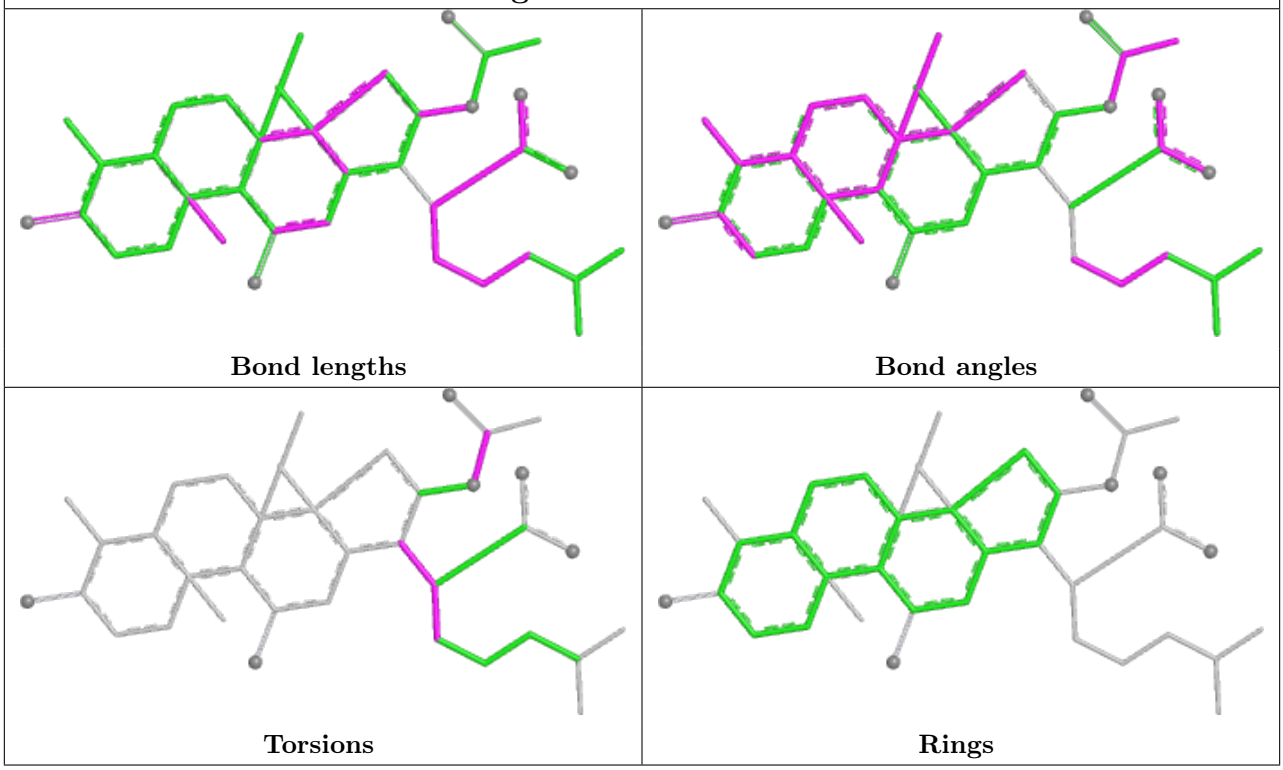
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP AY 702



Ligand FUA AY 701



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.

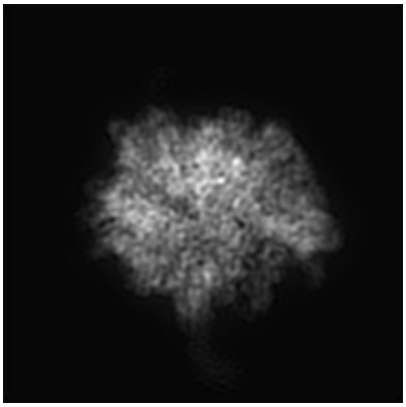
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1798. These allow visual inspection of the internal detail of the map and identification of artifacts.

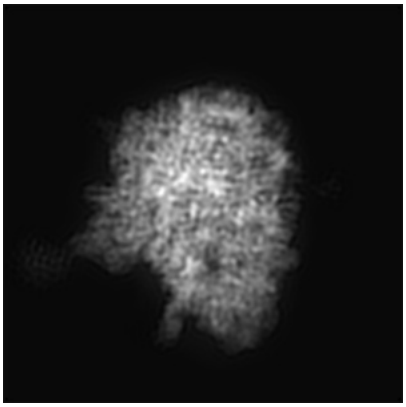
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

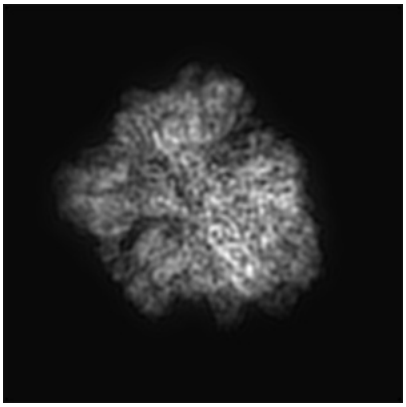
6.1.1 Primary map



X



Y

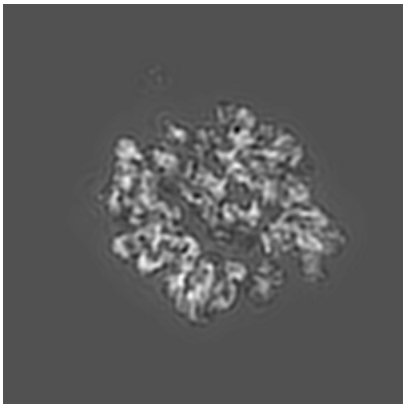


Z

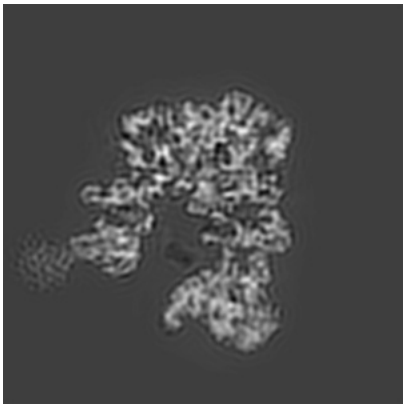
The images above show the map projected in three orthogonal directions.

6.2 Central slices

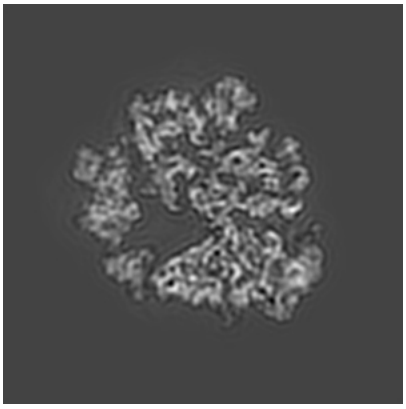
6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

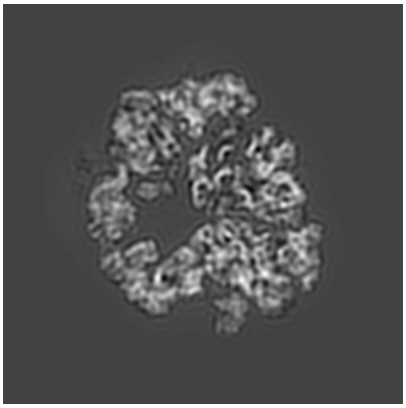
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 162

Y Index: 152

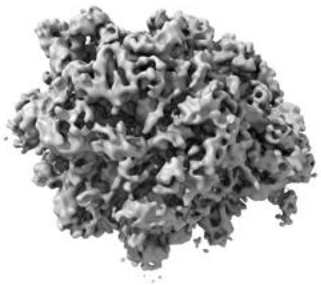


Z Index: 142

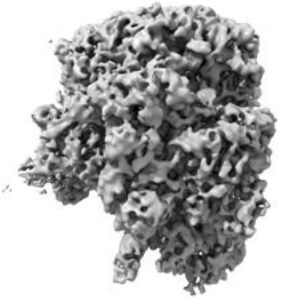
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 3000.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

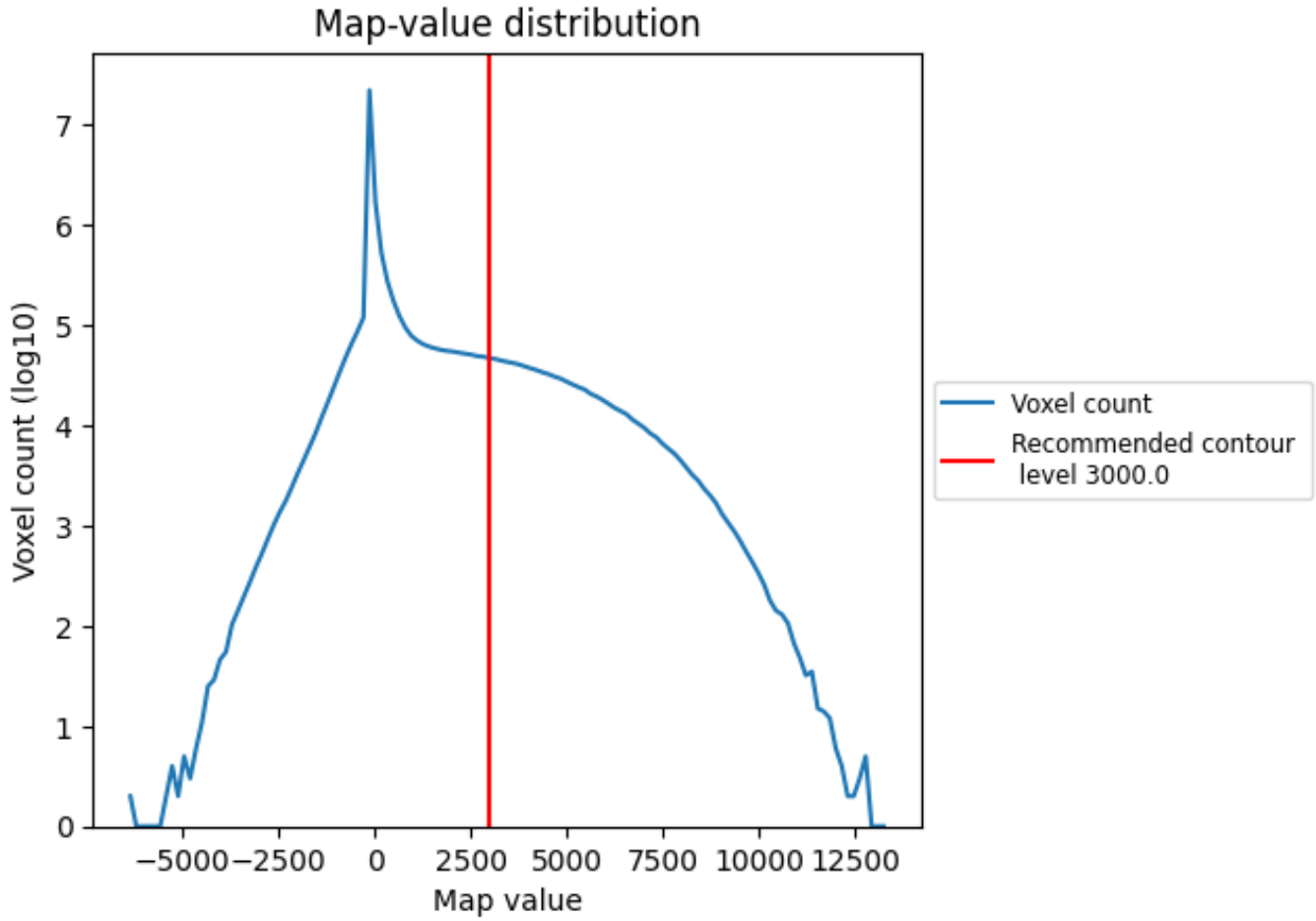
6.5 Mask visualisation (i)

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

7 Map analysis

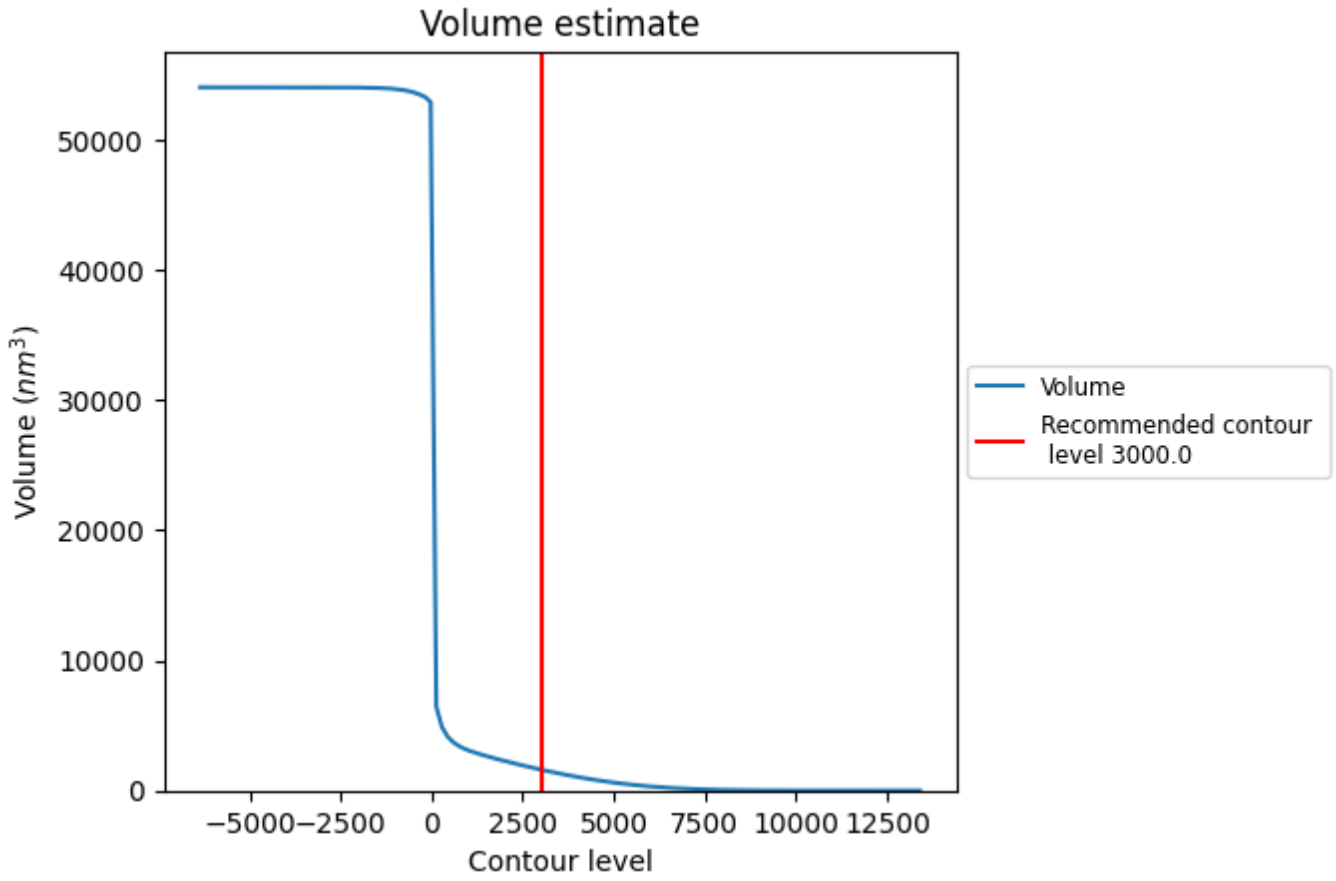
This section contains the results of statistical analysis of the map.

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.

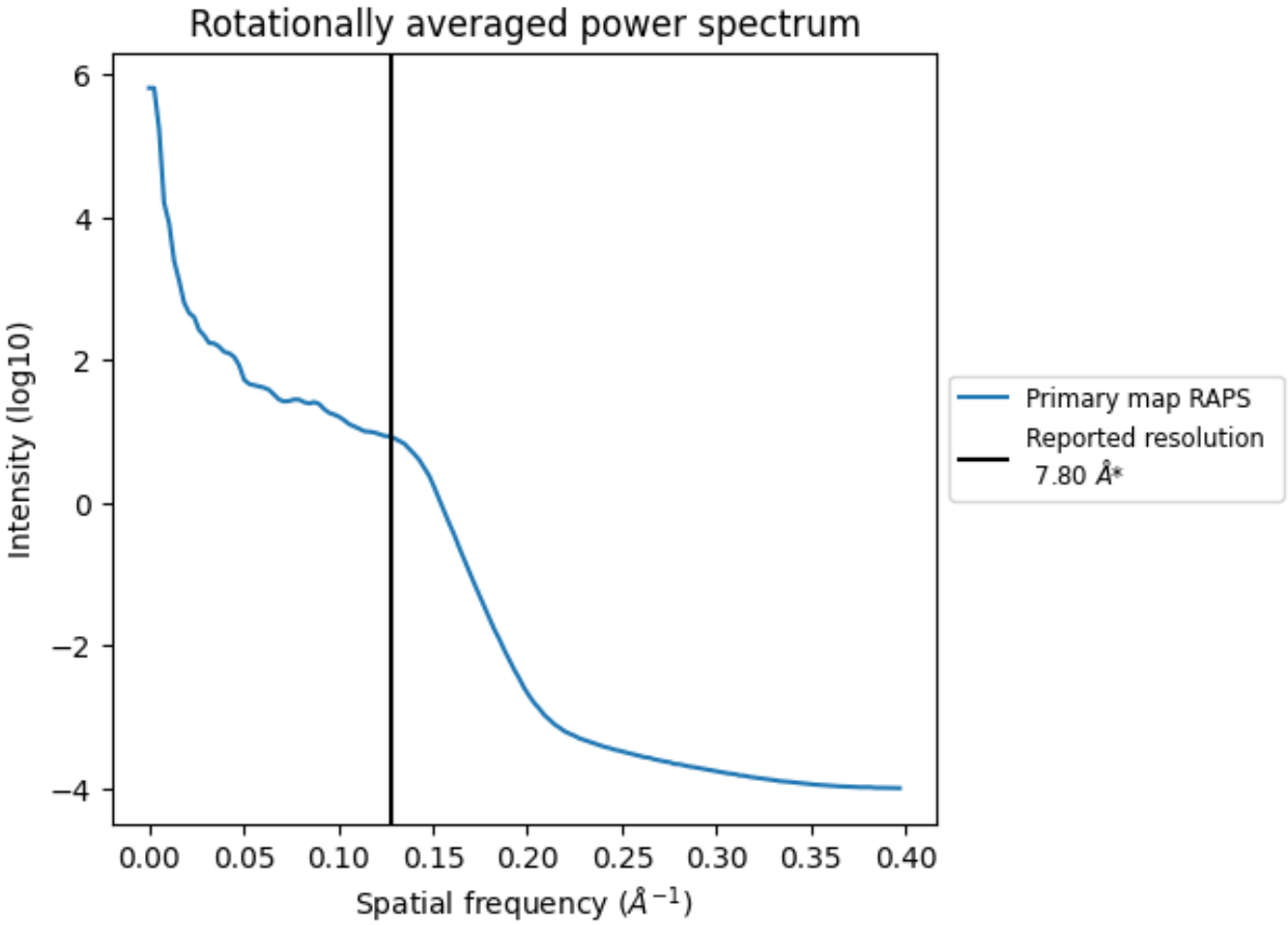
7.2 Volume estimate (i)



The volume at the recommended contour level is 1609 nm^3; this corresponds to an approximate mass of 1453 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 0.128 Å^{-1}

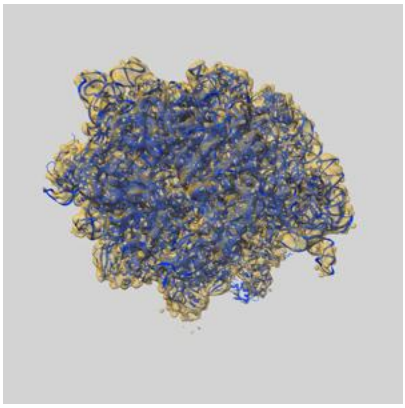
8 Fourier-Shell correlation (i)

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

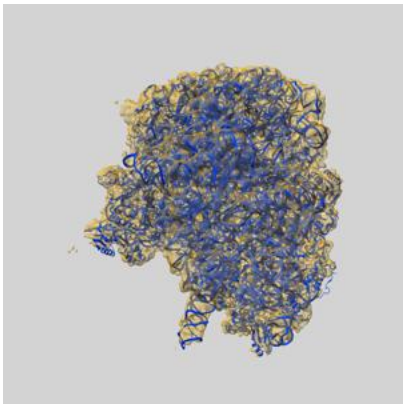
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1798 and PDB model 4V5M. Per-residue inclusion information can be found in section 3 on page 16.

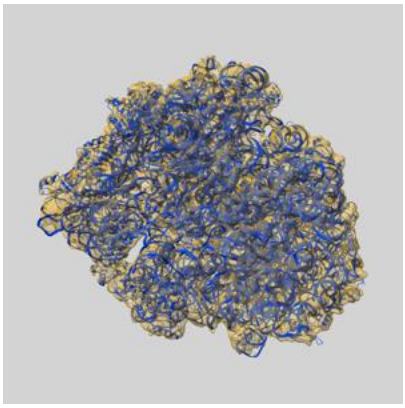
9.1 Map-model overlay



X



Y



Z

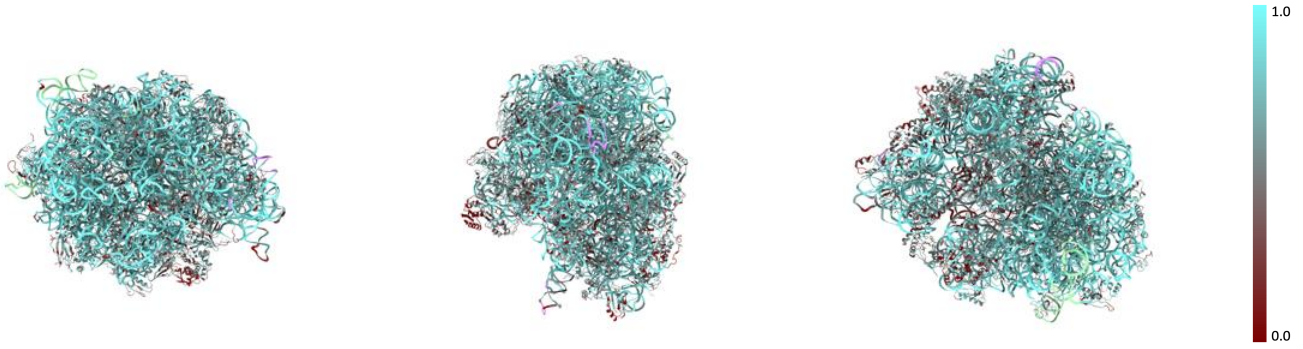
The images above show the 3D surface view of the map at the recommended contour level 3000.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

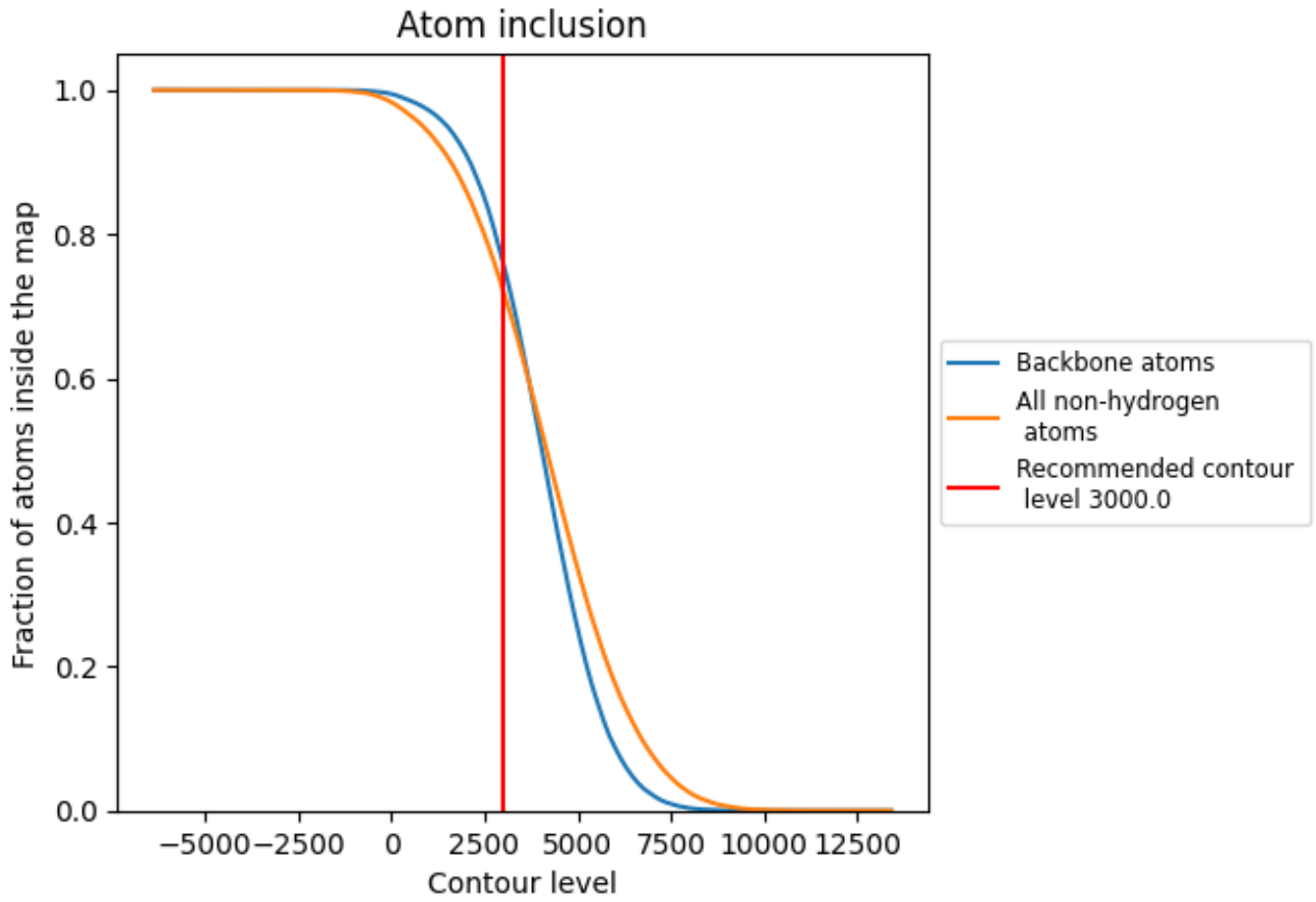
9.3 Atom inclusion mapped to coordinate model (i)



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 (3000.0).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (3000.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.1590
AA	0.8289	0.1700
AB	0.4670	0.1320
AC	0.5498	0.1360
AD	0.5930	0.1270
AE	0.5824	0.1350
AF	0.5400	0.1510
AG	0.4983	0.1130
AH	0.5837	0.1400
AI	0.5864	0.0960
AJ	0.4571	0.0840
AK	0.5295	0.1310
AL	0.4578	0.1200
AM	0.4246	0.0790
AN	0.5974	0.1230
AO	0.5989	0.1410
AP	0.6297	0.1120
AQ	0.5514	0.1200
AR	0.5226	0.1210
AS	0.5220	0.0840
AT	0.5602	0.1220
AU	0.4764	0.0650
AV	0.6488	0.1350
AX	0.2696	0.0910
AY	0.4490	0.1190
B0	0.5205	0.0990
B1	0.5769	0.1340
B2	0.6332	0.1500
B3	0.6035	0.1520
B4	0.3878	0.1080
B5	0.5996	0.1540
B6	0.5938	0.0930
B7	0.6160	0.1230
B8	0.5535	0.1240
B9	0.2823	0.0620

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Chain	Atom inclusion	Q-score
BA	0.8406	0.1880
BB	0.8675	0.1790
BC	0.2516	0.0480
BD	0.5135	0.1240
BE	0.5332	0.1270
BF	0.6151	0.1380
BG	0.5165	0.0980
BH	0.5734	0.1330
BK	0.3594	0.0890
BL	0.0589	0.0440
BN	0.5870	0.1450
BO	0.3677	0.1210
BP	0.5853	0.1430
BQ	0.2793	0.0930
BR	0.5996	0.1370
BS	0.6622	0.1480
BT	0.4784	0.1260
BU	0.6310	0.1220
BV	0.5538	0.1420
BW	0.6049	0.1280
BX	0.6141	0.1420
BY	0.4968	0.1340
BZ	0.4570	0.0750