wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:20 AM EST

PDB ID	:	4V7B
EMDB ID	:	EMD-5775
Title	:	Visualization of two tRNAs trapped in transit during EF-G-mediated translocation
Authors	:	Ramrath, D.J.F.; Lancaster, L.; Sprink, T.; Mielke, T.; Loerke, J.; Noller, H.F.; Spahn, C.M.T.
Deposited on	:	2013-10-27
Resolution	:	6.80 Å(reported)
Based on initial model	:	4KIY

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

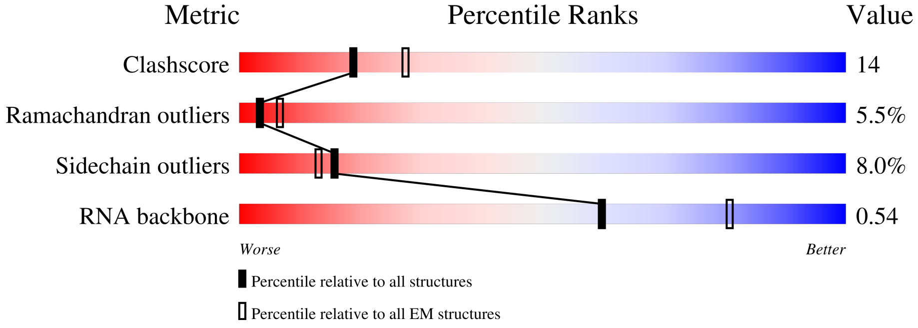
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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

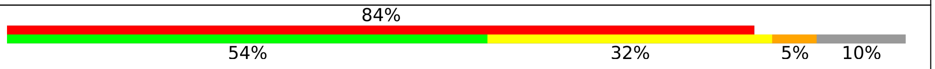
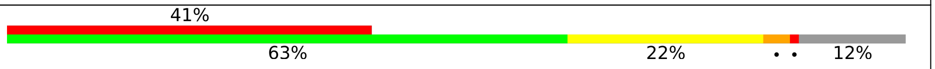
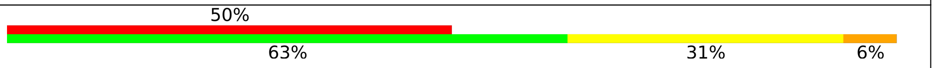
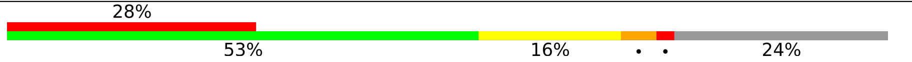
The reported resolution of this entry is 6.80 Å.

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	1542	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	

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Mol	Chain	Length	Quality of chain
8	AH	130	32% 71% 23% 5% •
9	AI	130	38% 44% 45% 8% •
10	AJ	103	48% 60% 30% 5% 5%
11	AK	129	37% 66% 21% • 9%
12	AL	124	50% 66% 27% 6% •
13	AM	118	45% 69% 21% 7% •
14	AN	101	32% 54% 37% • 5%
15	AO	89	16% 78% 20% ••
16	AP	82	29% 72% 26% •
17	AQ	84	25% 65% 27% • 5%
18	AR	75	25% 53% 20% 27%
19	AS	92	26% 58% 23% 5% 14%
20	AT	87	21% 75% 22% • •
21	AU	71	51% 28% 39% • 28%
22	AV	77	13% 19% 64% 14% •
23	AW	77	8% 16% 52% 31% •
24	AX	19	37% 26% 74%
25	AY	704	47% 64% 26% 5% • 5%
26	BB	120	• 66% 25% 8% •
27	BC	273	41% 69% 26% • •
28	BA	2904	• 58% 31% 9% • •
29	BD	209	35% 65% 29% 5% •
30	BE	201	46% 70% 24% 5% •
31	BF	179	42% 65% 30% • ••
32	BG	177	26% 62% 29% 8% ••

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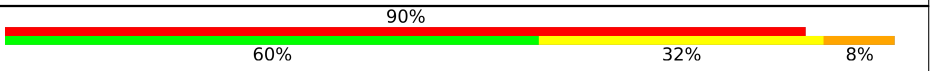
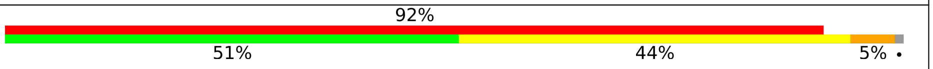
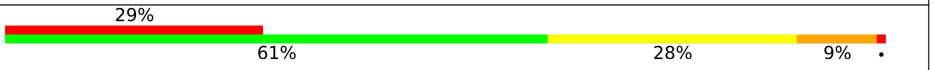
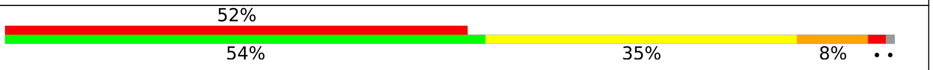
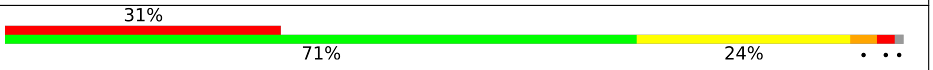
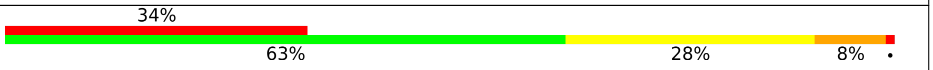
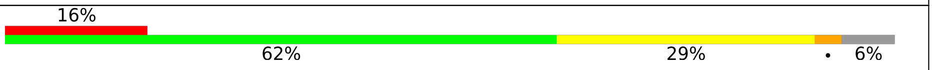
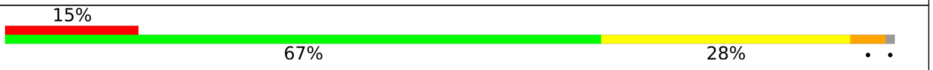
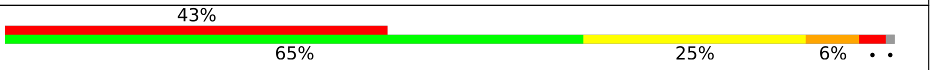
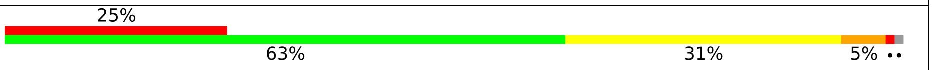
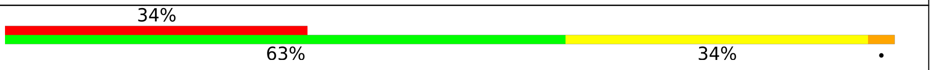
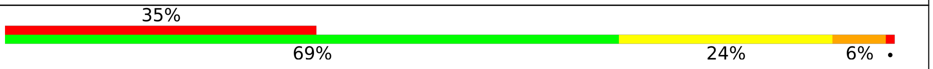
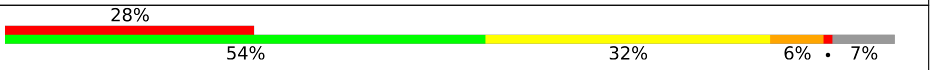
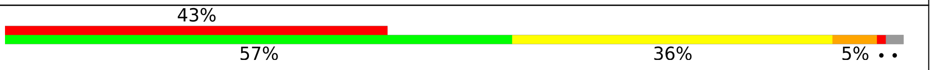
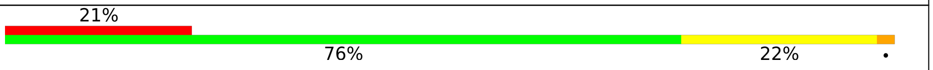
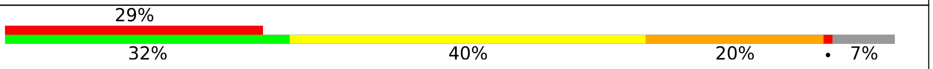
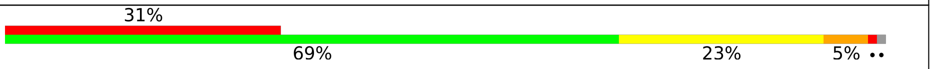
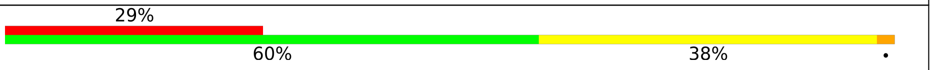
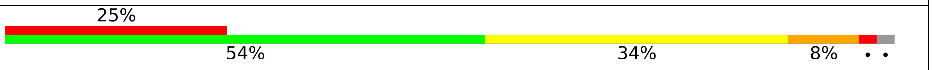
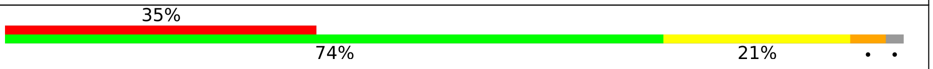
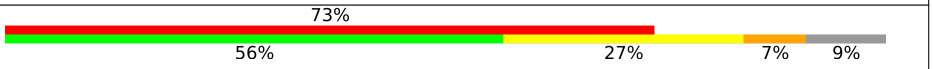
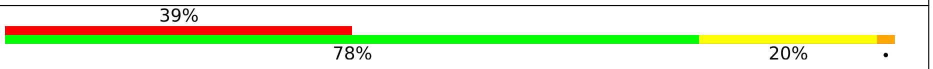
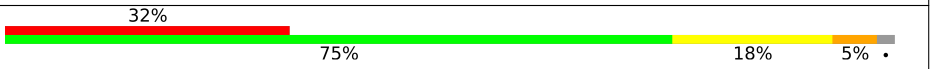
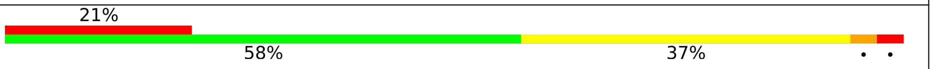
Mol	Chain	Length	Quality of chain
33	BH	50	
34	BI	142	
35	BJ	142	
36	BK	123	
37	BL	144	
38	BM	136	
39	BN	127	
40	BO	117	
41	BP	115	
42	BQ	118	
43	BR	103	
44	BS	110	
45	BT	100	
46	BU	104	
47	BV	94	
48	BW	85	
49	BX	78	
50	BY	63	
51	BZ	59	
52	B0	57	
53	B1	55	
54	B2	46	
55	B3	65	
56	B4	38	
57	B5	165	

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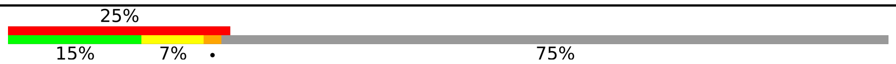
Mol	Chain	Length	Quality of chain
58	B6	121	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	FUA	AY	801	-	-	X	-
60	GDP	AY	802	-	-	X	-

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 150958 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	1533	32895	14671	6036	10655	1533	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	218	1704	1081	305	311	7	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	1624	1028	305	288	3	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	205	1643	1026	315	298	4	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	1105	687	211	201	6	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	102	832	525	150	150	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	151	1181	735	227	215	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AH	129	979	616	173	184	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AI	127	1022	634	206	179	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AJ	98	786	493	150	142	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AK	117	877	540	174	160	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	123	955	590	196	165	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AM	114	883	546	178	156	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total 774	C 483	N 160	O 128	S 3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total 714	C 439	N 144	O 130	S 1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total 649	C 406	N 128	O 114	S 1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total 648	C 411	N 121	O 113	S 3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total 455	C 288	N 86	O 81	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total 637	C 408	N 120	O 107	S 2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total 425	C 265	N 86	O 73	S 1	0	0

- Molecule 22 is a RNA chain called modified formyl-methionine specific initiator transfer RNA.

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

- Molecule 23 is a RNA chain called formyl-methionine specific initiator transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	77	Total 1635	C 732	N 291	O 536	P 76	0	0

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	19	Total 416	C 187	N 86	O 124	P 19	0	0

- Molecule 25 is a protein called Elongation Factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	671	Total 5194	C 3278	N 895	O 998	S 23	0	0

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	118	Total 2529	C 1126	N 464	O 821	P 118	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	271	Total 2082	C 1288	N 423	O 364	S 7	0	0

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	BA	2854	61274	27334	11279	19807	2854	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BE	201	1552	974	283	290	5	0	0

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BF	177	1410	899	249	256	6	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BG	176	1323	832	243	246	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BH	50	384	247	68	68	1	0	0

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	122	Total 938	C 587	N 180	O 165	S 6	0	0

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	143	Total 1045	C 649	N 206	O 189	S 1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	136	Total 1074	C 686	N 205	O 177	S 6	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	120	Total 960	C 593	N 196	O 166	S 5	0	0

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	BQ	117	947	604	192	151	0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BR	103	816	516	153	145	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BS	110	857	532	166	156	3	0	0

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BT	93	738	466	139	131	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	BU	102	779	492	146	141	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BW	79	596	367	120	108	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BX	77	625	388	129	106	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BY	63	509	313	99	95	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BZ	58	449	281	87	79	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	B0	56	444	269	94	80	1	0	0

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	B1	50	409	263	75	71	0	0

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	B2	46	377	228	90	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	B3	64	504	323	105	74	2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

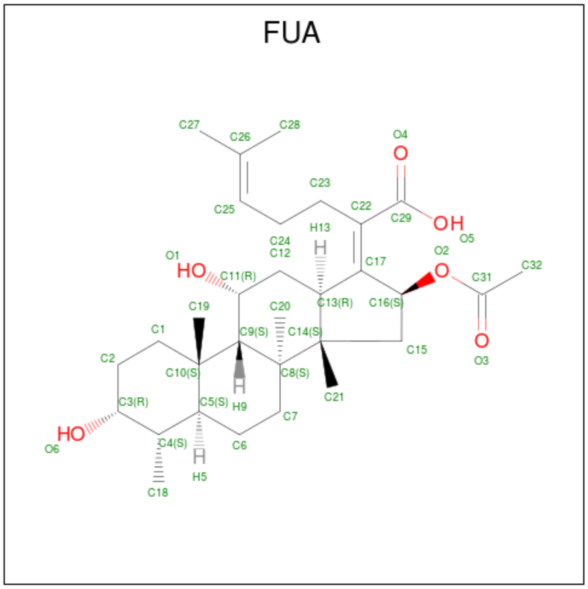
- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

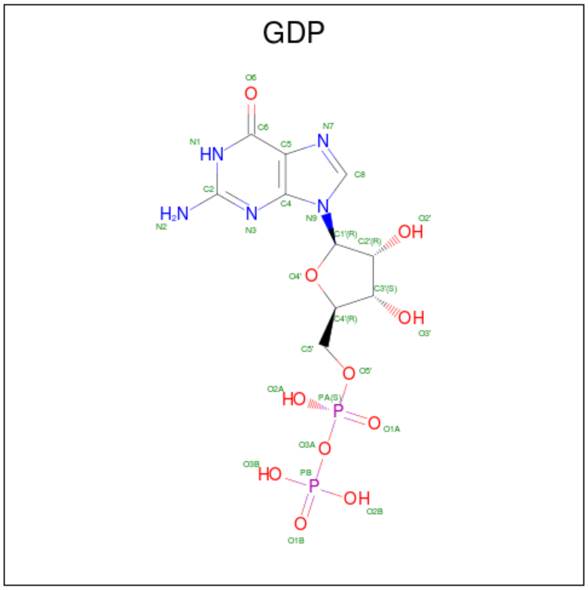
Mol	Chain	Residues	Atoms					AltConf	Trace
58	B6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 59 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



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

- Molecule 60 is GUANOSINE-5’-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

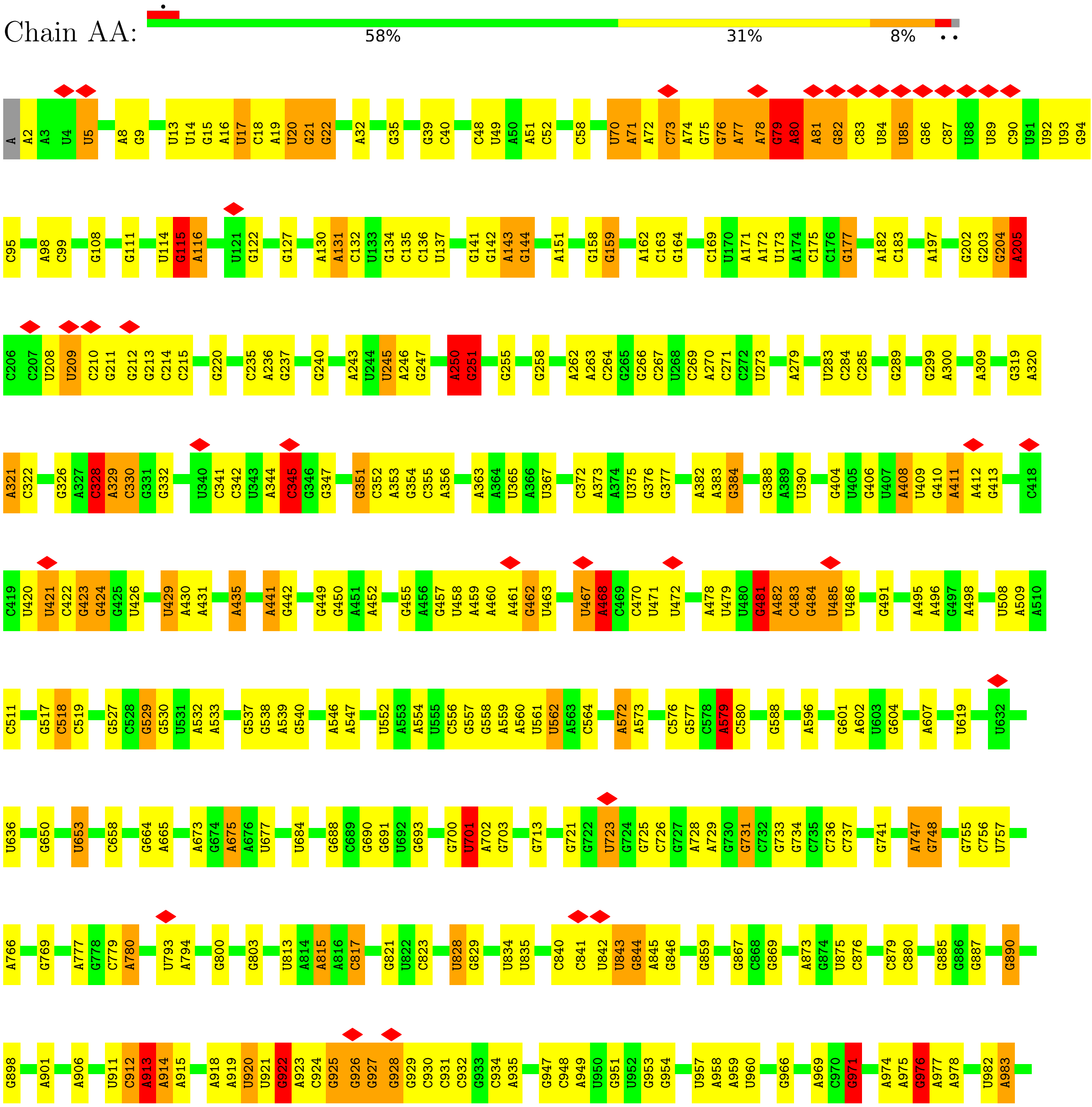


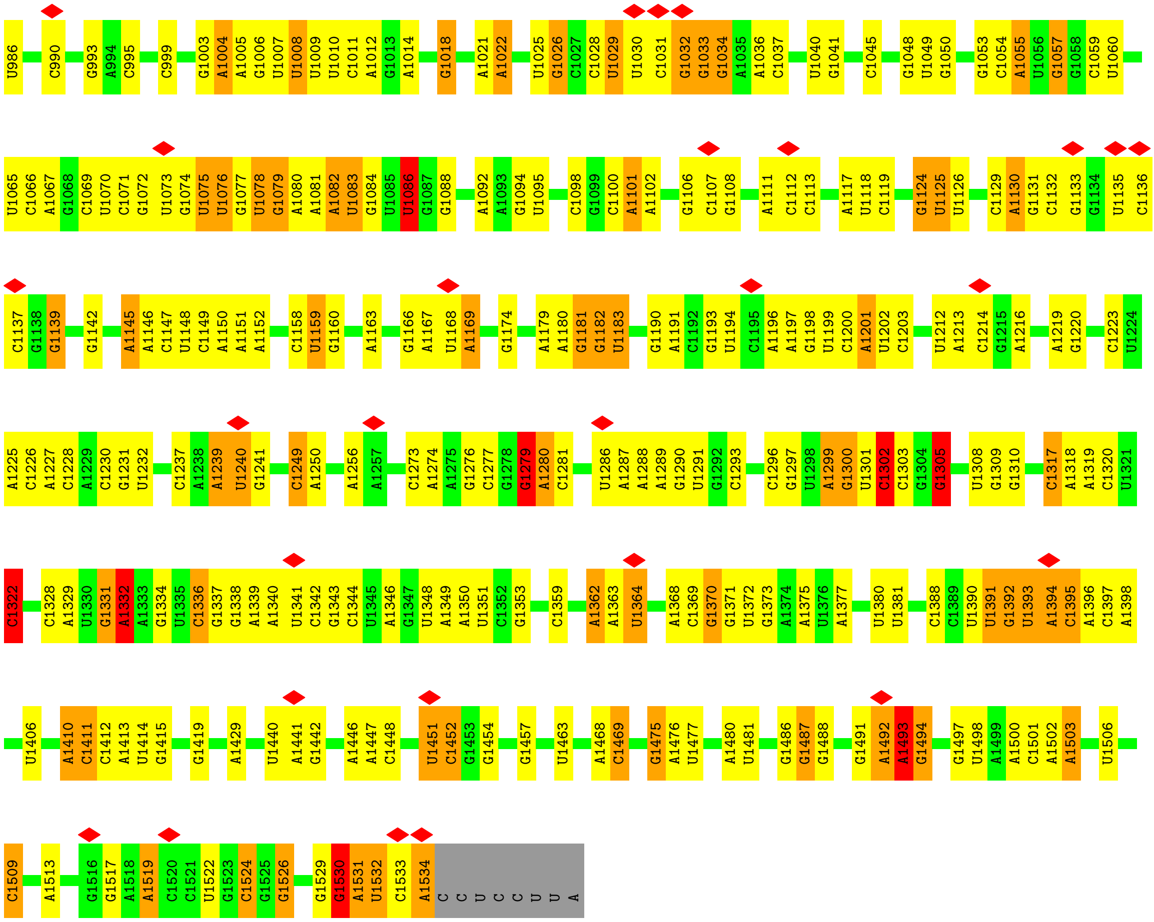
Mol	Chain	Residues	Atoms					AltConf
60	AY	1	Total 28	C 10	N 5	O 11	P 2	0

3 Residue-property plots ⓘ

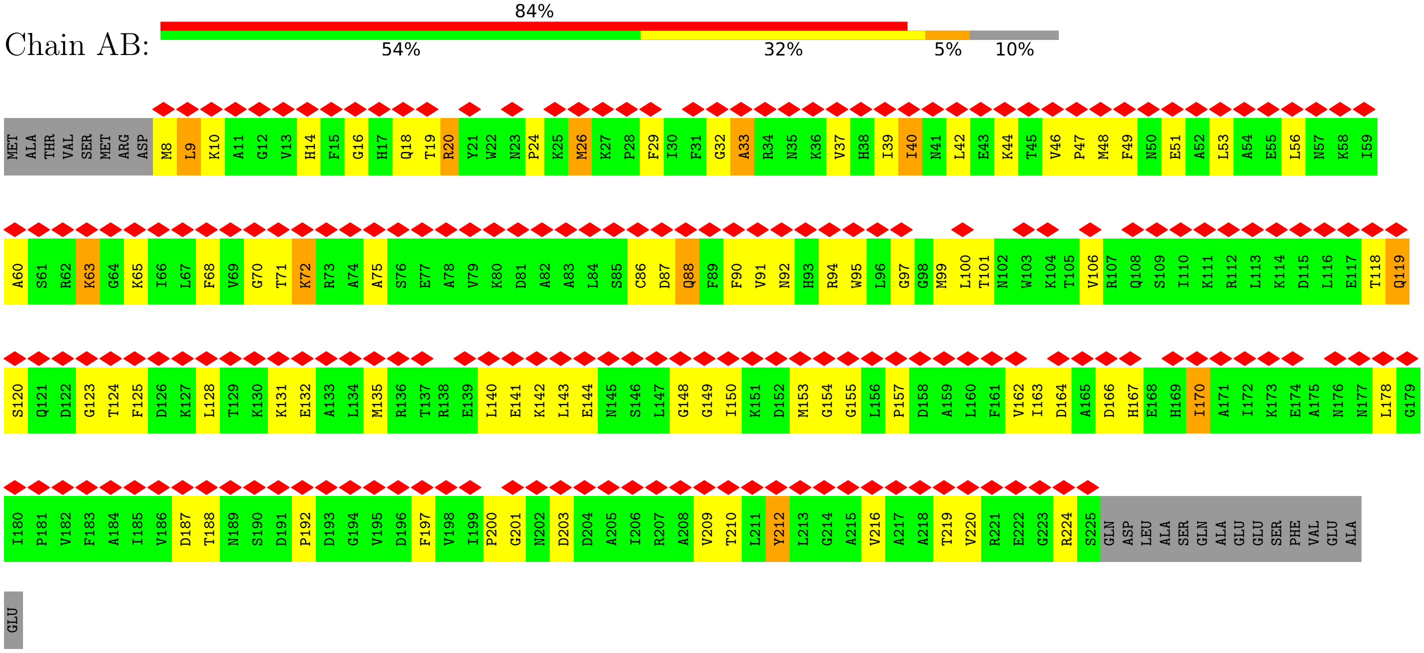
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



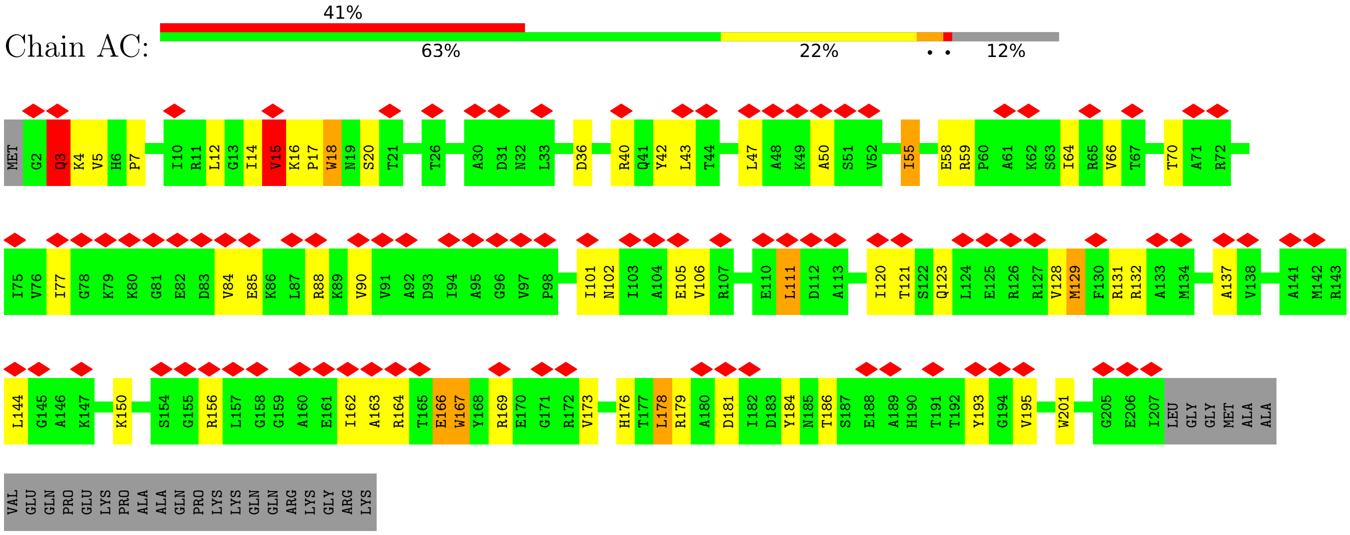


- Molecule 2: 30S ribosomal protein S2



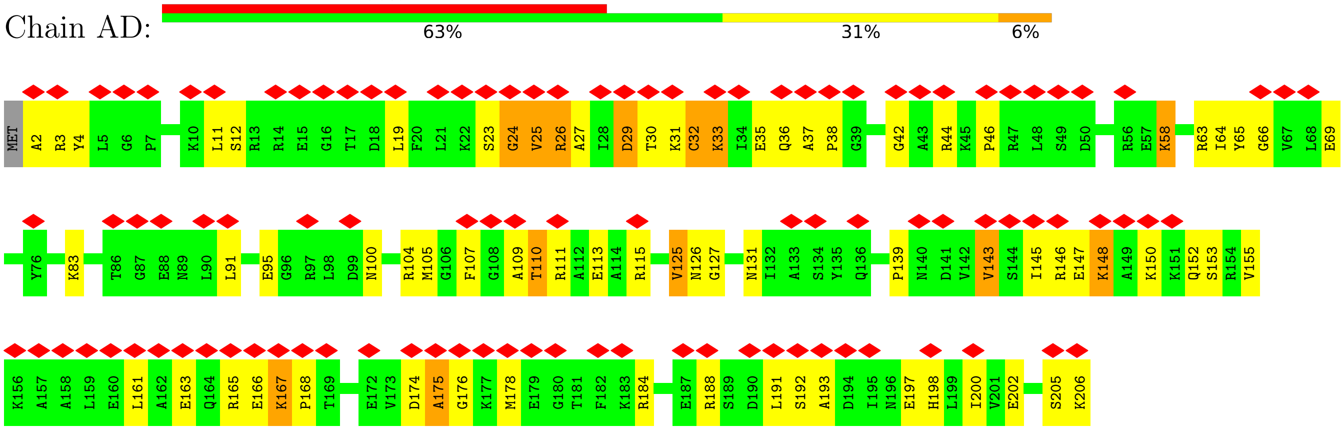
- Molecule 3: 30S ribosomal protein S3

Chain AC:



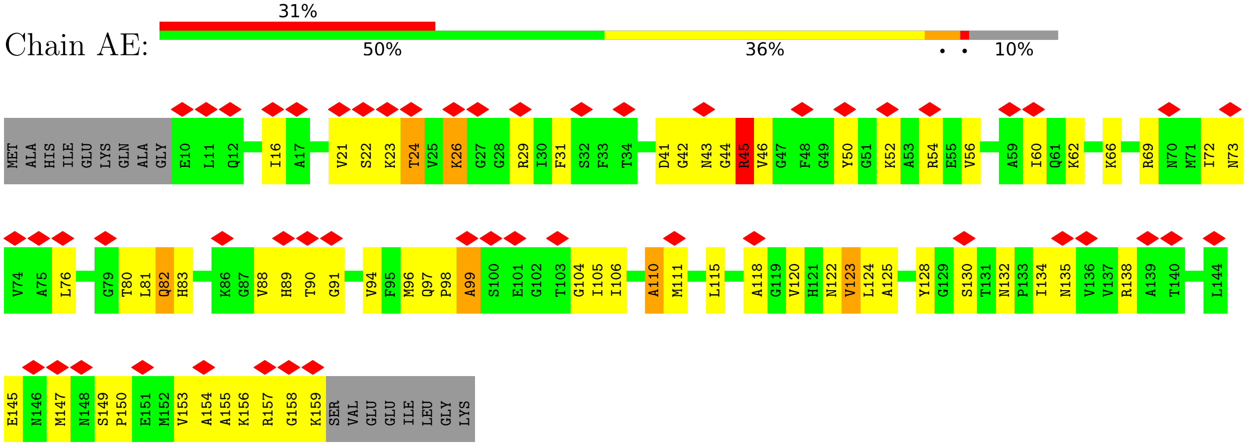
- Molecule 4: 30S ribosomal protein S4

Chain AD:



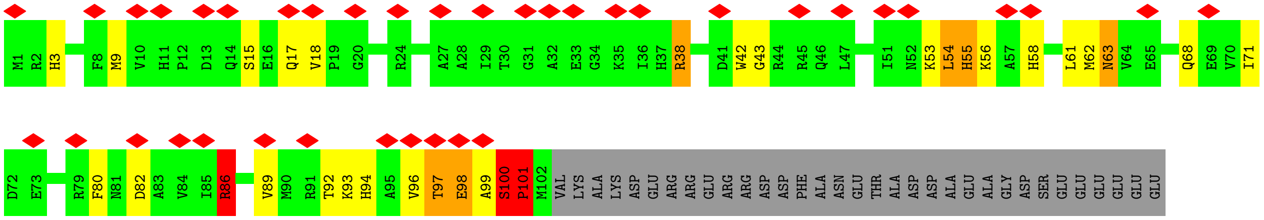
- Molecule 5: 30S ribosomal protein S5

Chain AE:



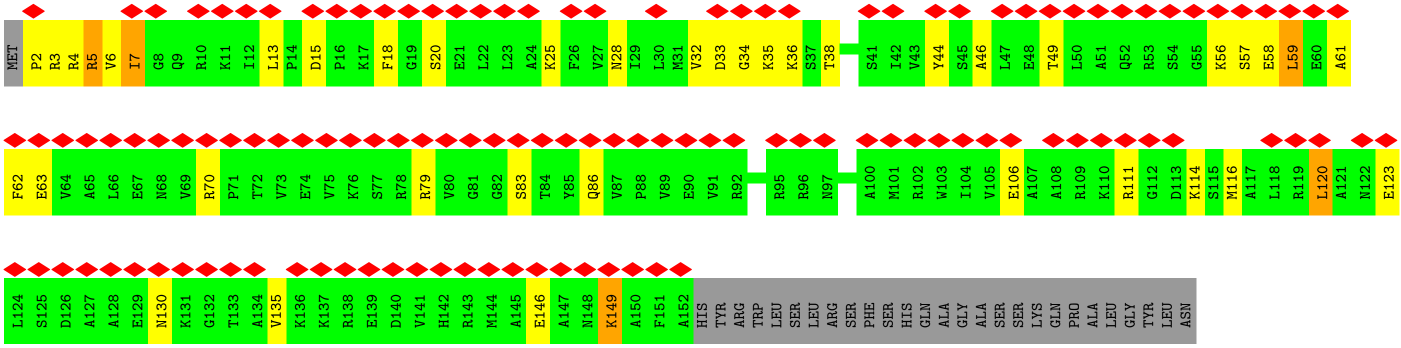
- Molecule 6: 30S ribosomal protein S6

Chain AF:



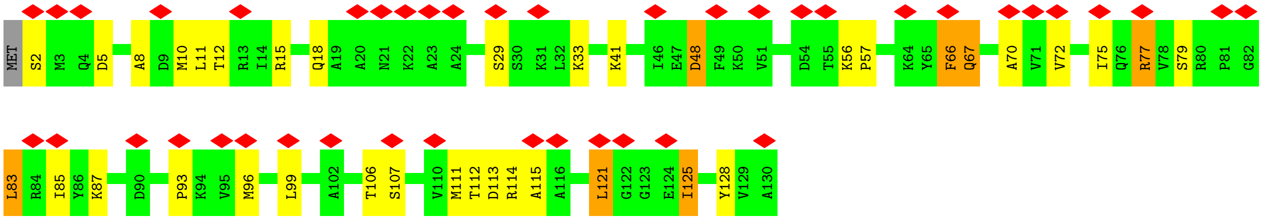
- Molecule 7: 30S ribosomal protein S7

Chain AG:

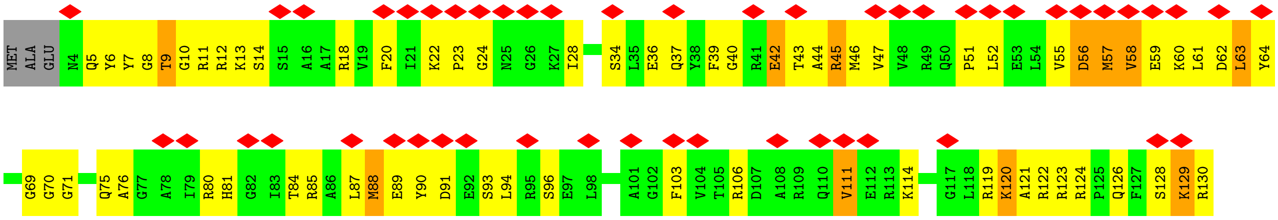
- Molecule 8: 30S ribosomal protein S8

Chain AH:

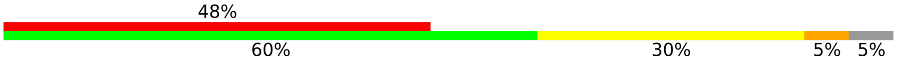



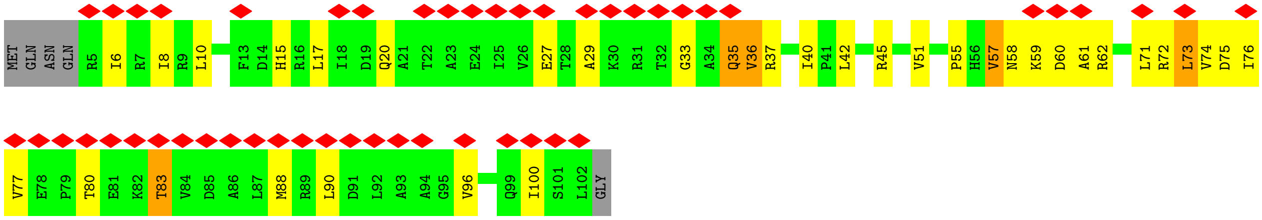
- Molecule 9: 30S ribosomal protein S9

Chain AI:

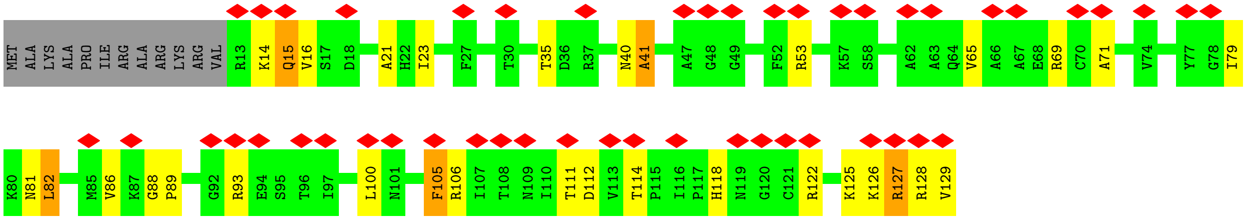
- Molecule 10: 30S ribosomal protein S10

Chain AJ:




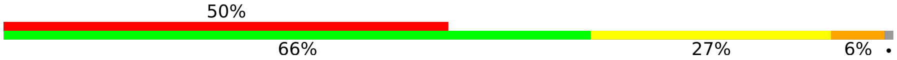
- Molecule 11: 30S ribosomal protein S11

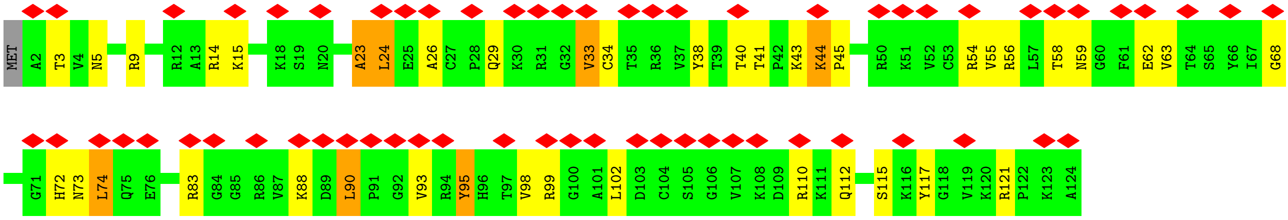
Chain AK:



- Molecule 12: 30S ribosomal protein S12

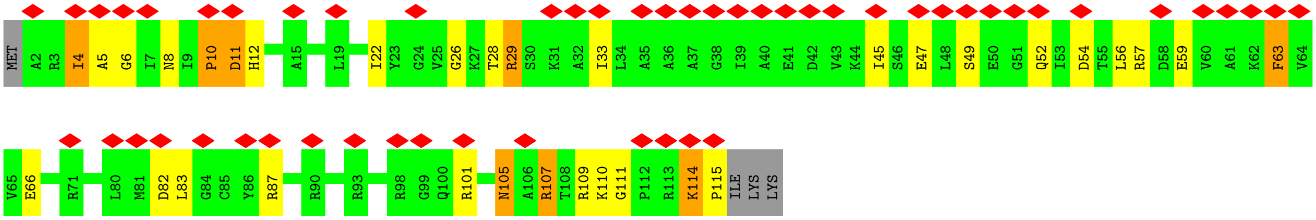
Chain AL:





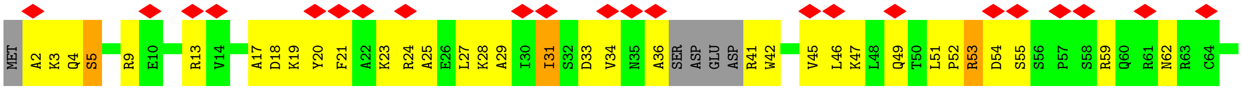
- Molecule 13: 30S ribosomal protein S13

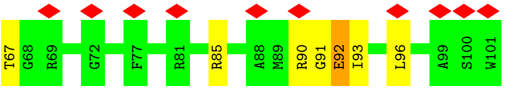
Chain AM:



- Molecule 14: 30S ribosomal protein S14

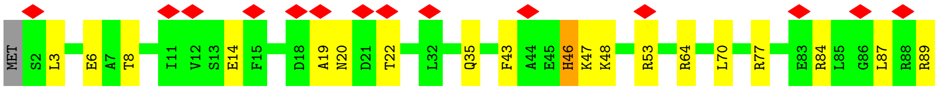
Chain AN:





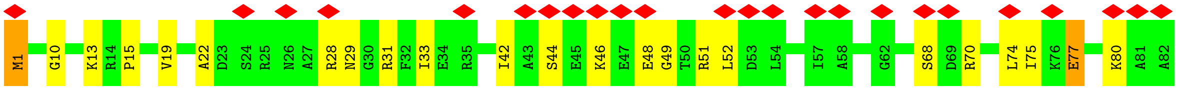
- Molecule 15: 30S ribosomal protein S15

Chain AO:



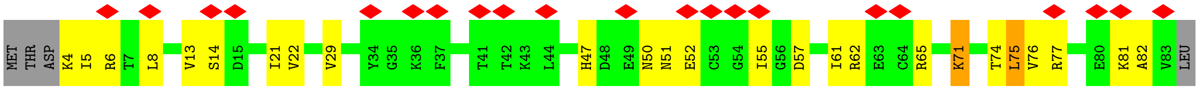
- Molecule 16: 30S ribosomal protein S16

Chain AP:



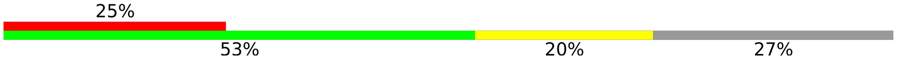
- Molecule 17: 30S ribosomal protein S17

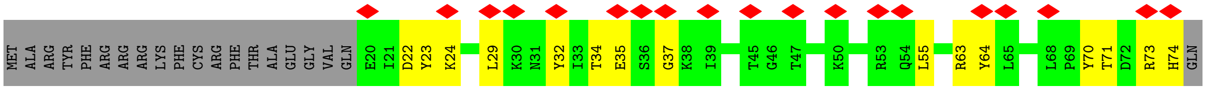
Chain AQ:



- Molecule 18: 30S ribosomal protein S18

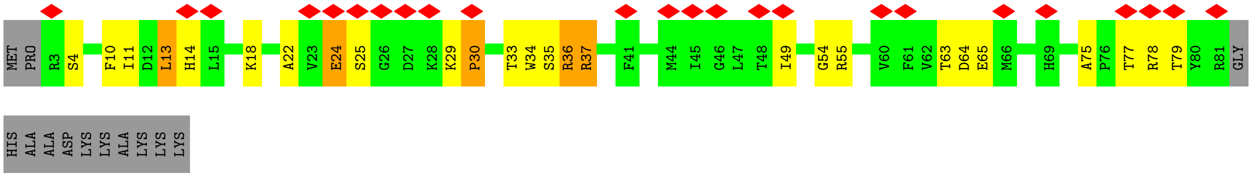
Chain AR:





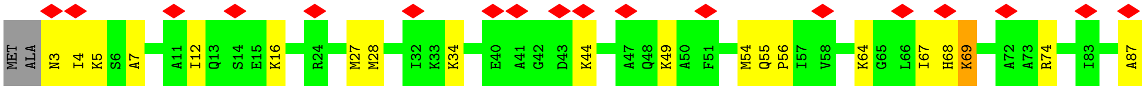
- Molecule 19: 30S ribosomal protein S19

Chain AS:



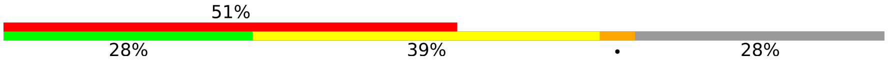
- Molecule 20: 30S ribosomal protein S20

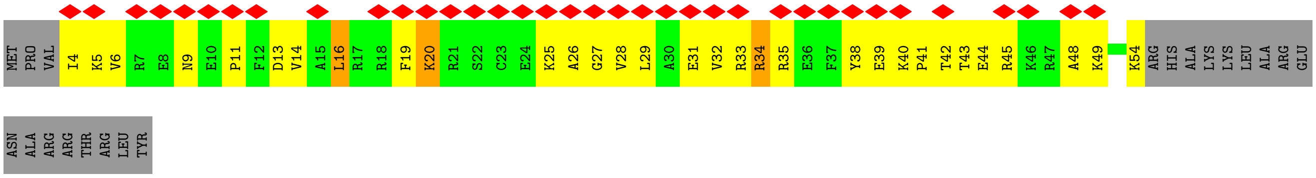
Chain AT:



- Molecule 21: 30S ribosomal protein S21

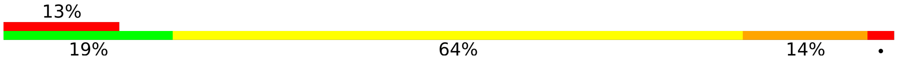
Chain AU:

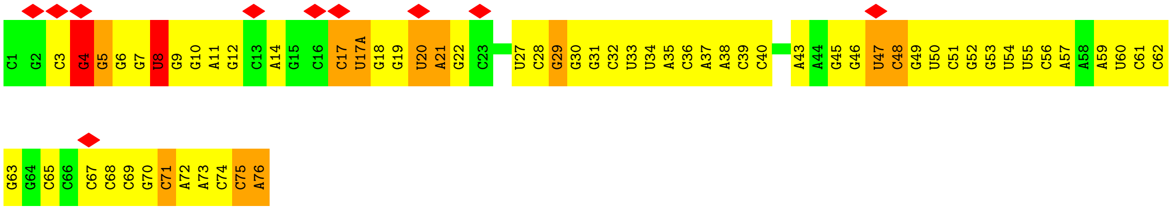




- Molecule 22: modified formyl-methionine specific initiator transfer RNA

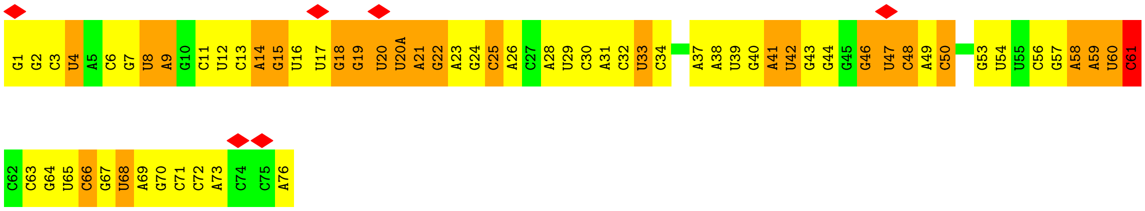
Chain AV:





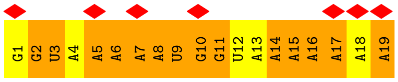
- Molecule 23: formyl-methionine specific initiator transfer RNA

Chain AW:



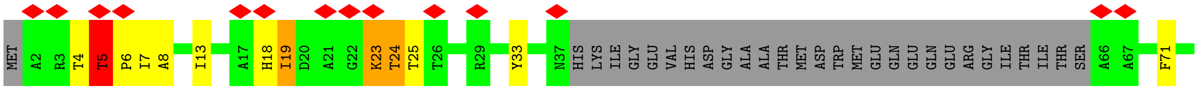
- Molecule 24: messenger RNA

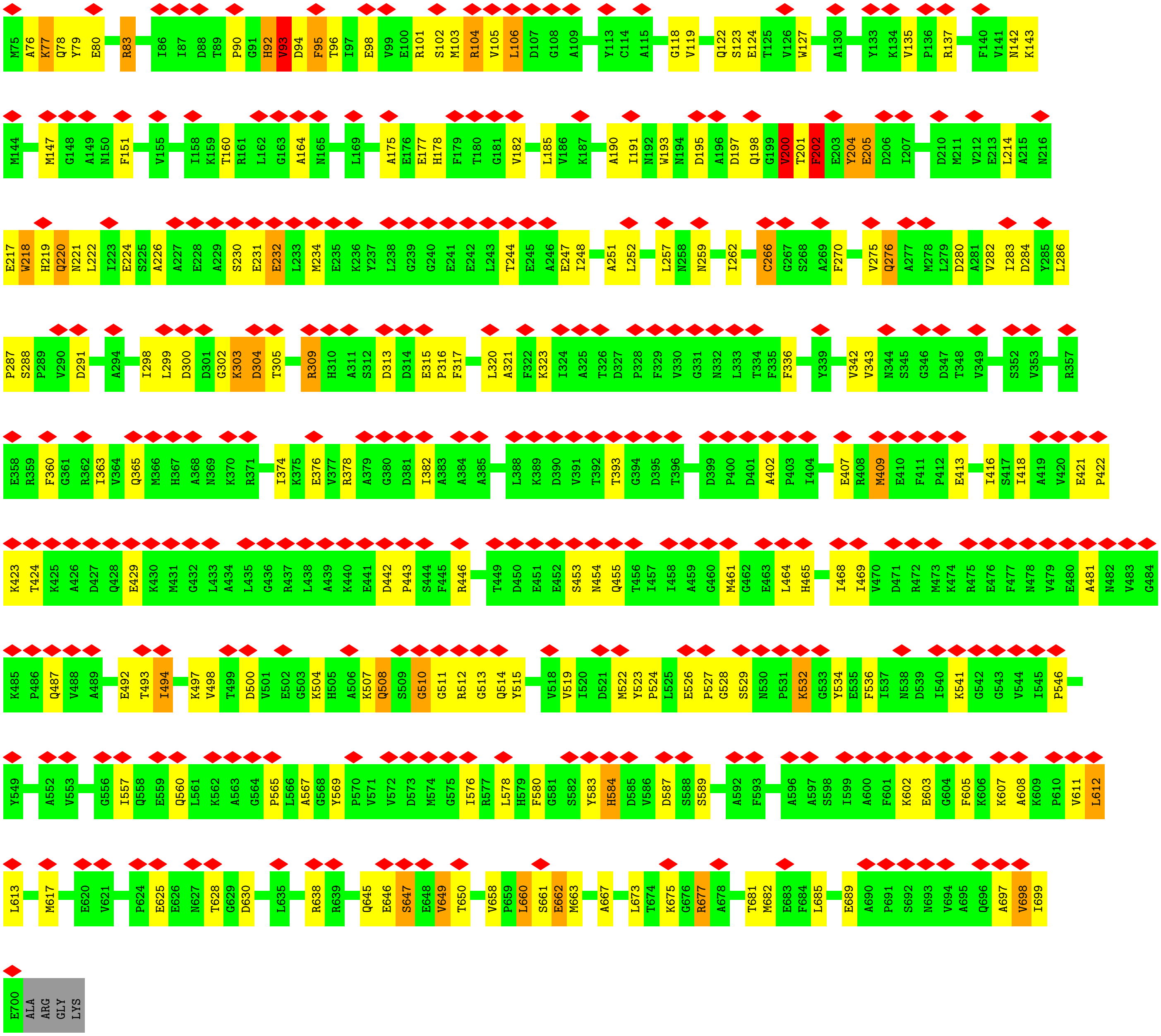
Chain AX:



- Molecule 25: Elongation Factor G

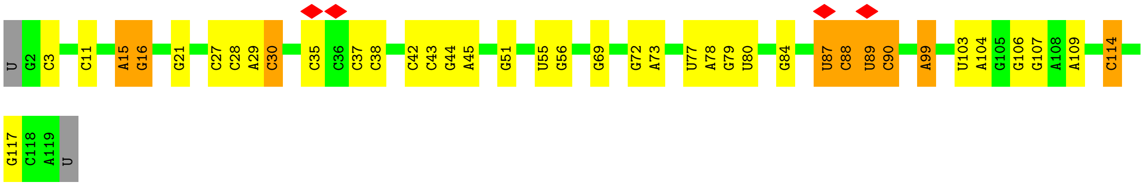
Chain AY:





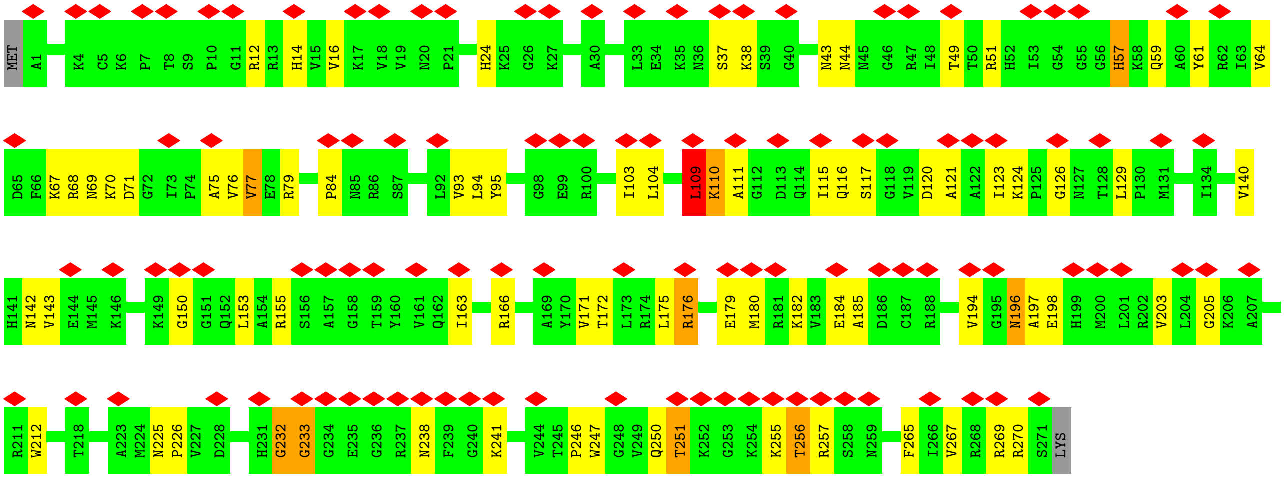
- Molecule 26: 5S ribosomal RNA

Chain BB:



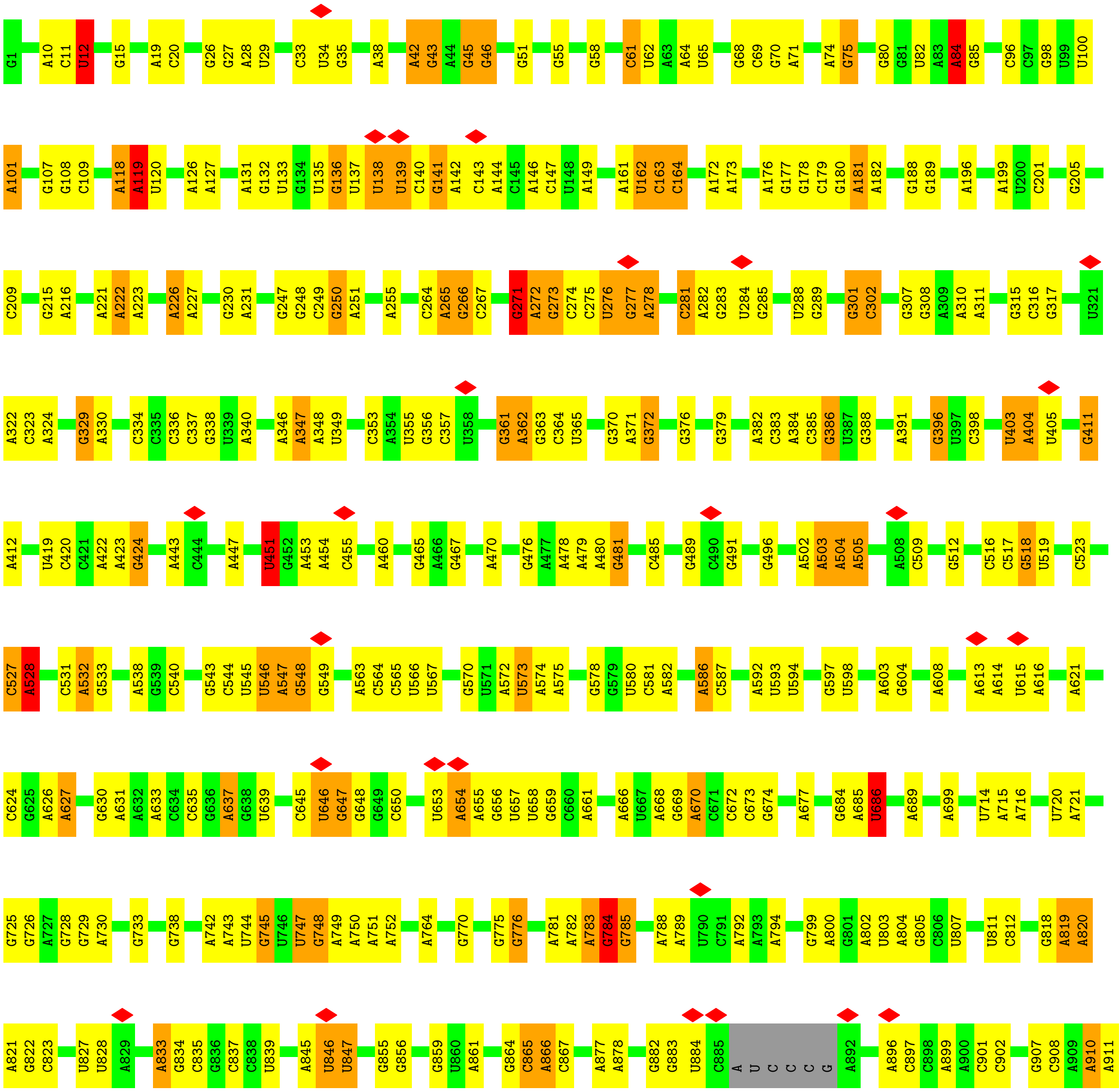
- Molecule 27: 50S ribosomal protein L2

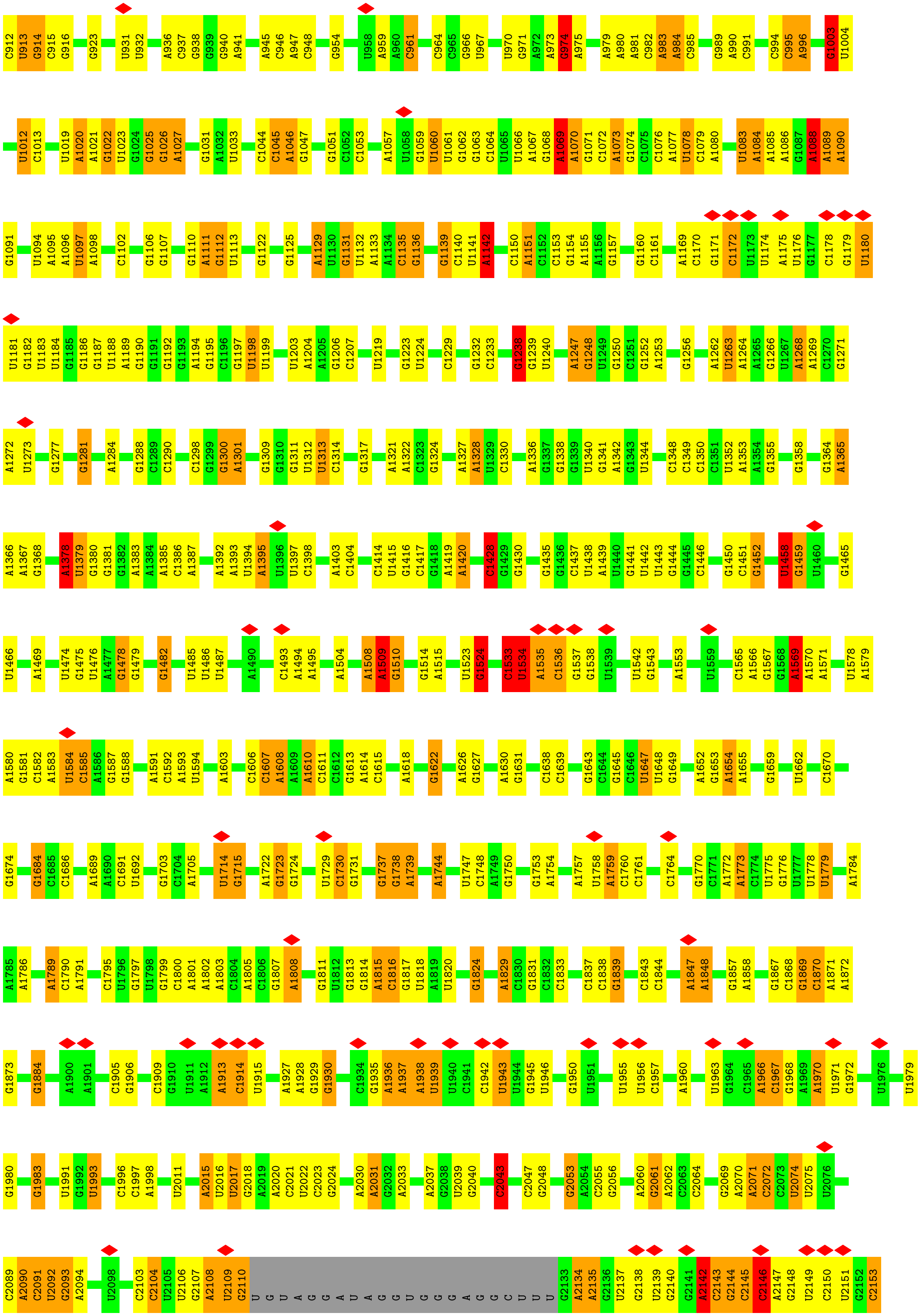
Chain BC:



- Molecule 28: 23S ribosomal RNA

Chain BA:

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U1012 C1013 U1019 A1020 A1021 G1022 U1023 G1024 G1025 G1026 A1027 G1031 A1032 U1033 C1044 C1045 A1046 G1047 G1051 C1052 C1053 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 U1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090
G1091 U1094 A1095 A1096 U1097 A1098 C1102 G1106 G1107 G1110 A1111 G1112 U1113 G1122 G1125 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141 A1142 C1150 A1151 C1152 C1153 G1154 A1155 A1156 G1157 G1160 C1161 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180
U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 U1203 A1204 A1205 G1206 C1207 U1219 G1223 U1224 C1229 G1232 C1233 G1238 G1239 U1240 A1247 G1248 U1249 G1250 C1251 G1252 A1253 G1256 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271
A1272 U1273 G1277 G1281 A1284 G1288 C1289 C1290 C1298 G1299 G1300 A1301 G1309 C1310 G1311 U1312 U1313 C1314 G1317 A1321 A1322 C1323 G1324 A1327 A1328 U1329 C1330 A1336 G1337 G1338 G1339 U1340 G1341 A1342 G1343 U1344 C1348 C1349 C1350 C1351 U1352 A1353 A1354 G1355 G1358 G1364 A1365
A1366 A1367 G1368 A1378 U1379 G1380 G1381 G1382 A1383 A1384 A1385 C1386 A1387 A1392 A1393 U1394 A1395 U1396 U1397 C1398 A1403 C1404 C1414 U1415 G1416 C1417 G1418 A1419 A1420 C1428 G1429 G1430 G1435 G1436 C1437 A1438 A1439 U1440 G1441 U1442 U1443 G1444 G1445 C1446 G1450 C1451 G1452 U1458 G1459 U1460 G1465
U1466 A1469 U1474 G1475 U1476 A1477 G1478 G1479 G1482 U1485 U1486 U1487 A1490 C1493 A1494 A1495 A1504 A1508 A1509 G1510 G1514 A1515 U1523 G1524 C1533 U1534 A1535 C1536 G1537 G1538 U1539 U1542 G1543 A1553 U1559 C1565 A1566 G1567 G1568 A1569 A1570 A1571 U1578 A1579
A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 A1591 C1592 A1593 U1594 A1603 C1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1618 G1622 A1626 G1627 A1630 G1631 C1638 C1639 G1643 C1644 G1645 C1646 U1647 U1648 G1649 A1652 G1653 A1654 A1655 G1659 U1662 C1670
G1674 G1684 C1685 C1686 A1689 A1690 C1691 U1692 G1703 C1704 A1705 U1714 G1715 A1722 G1723 G1724 U1729 C1730 G1731 G1737 G1738 A1739 A1744 U1747 C1748 A1749 G1750 G1753 A1754 A1757 U1758 A1759 C1760 C1761 C1764 G1770 C1771 A1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1784
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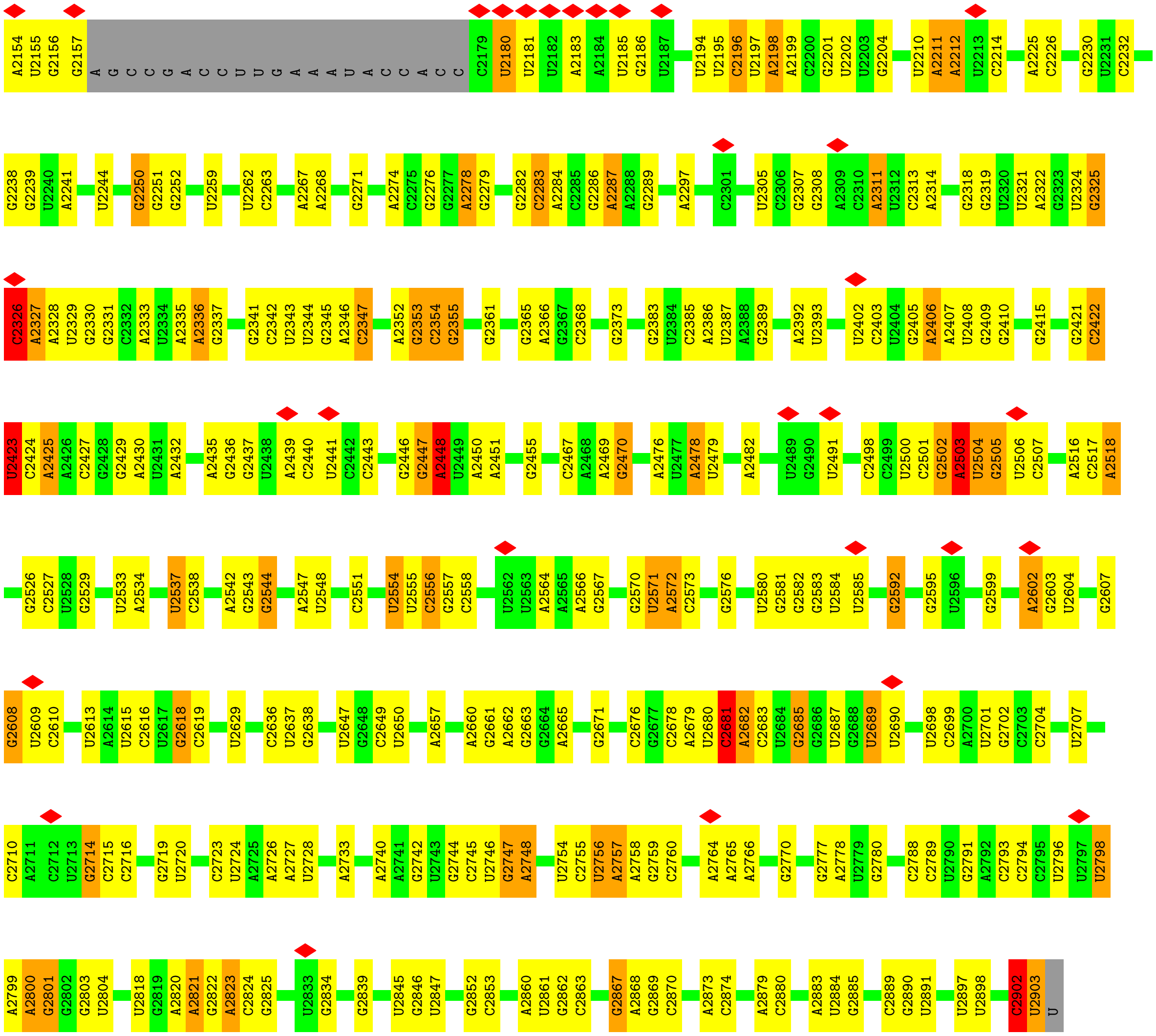
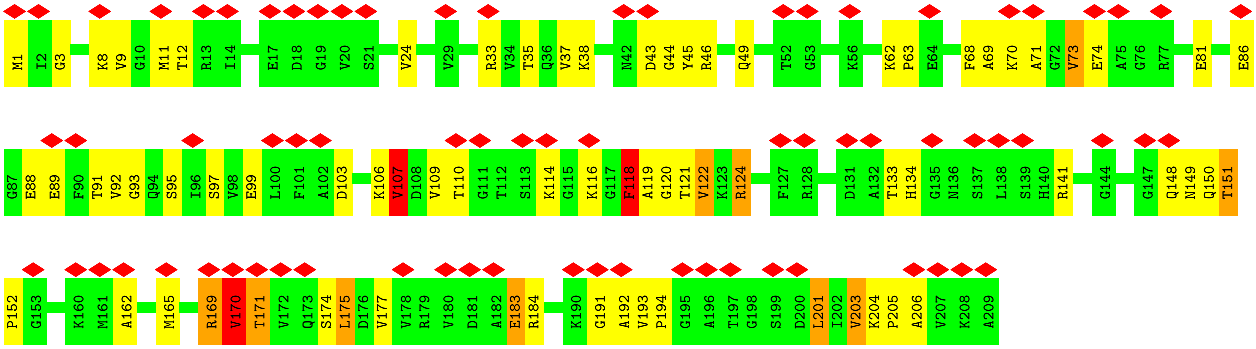
G1873 G1884 A1900 A1901 C1905 G1906 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1927 A1928 G1929 G1930 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 U1946 G1950 U1951 U1955 U1956 C1957 A1960 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 U1976 U1979
G1980 G1983 U1991 G1992 U1993 C1996 C1997 A1998 U2011 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 C2023 G2024 A2030 A2031 G2032 A2033 A2037 G2038 U2039 G2040 C2043 C2047 G2048 G2053 A2054 C2055 G2056 A2060 G2061 A2062 C2063 C2064 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2076
C2089 A2090 C2091 U2092 G2093 A2094 U2098 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U G U A G G A U A G G U G G G A G G C U U U G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153



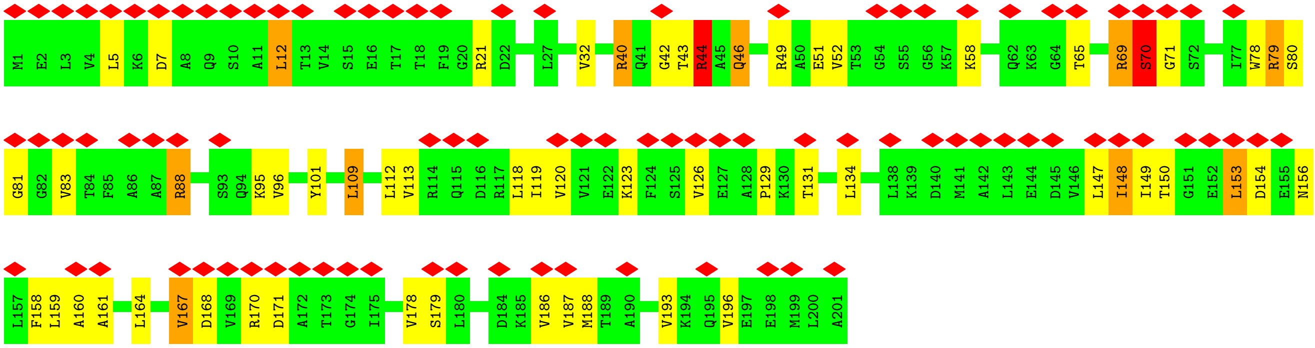
- Molecule 29: 50S ribosomal protein L3

Chain BD:



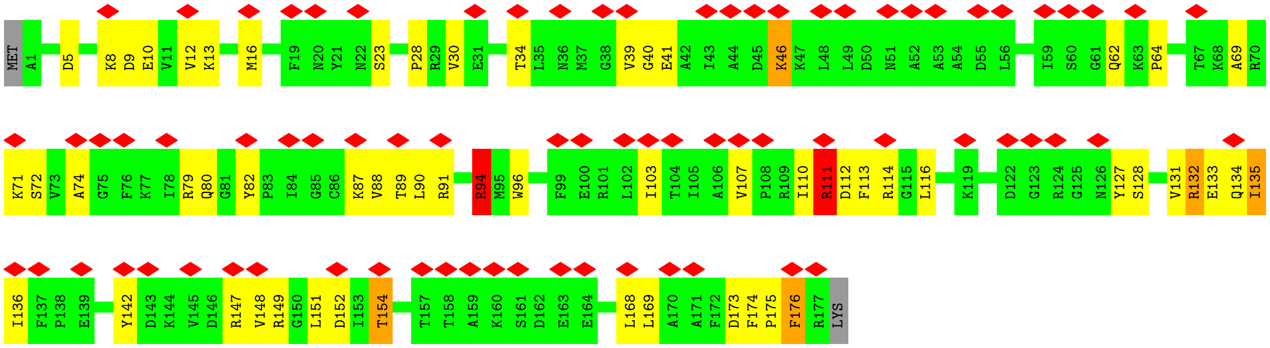
- Molecule 30: 50S ribosomal protein L4

Chain BE:



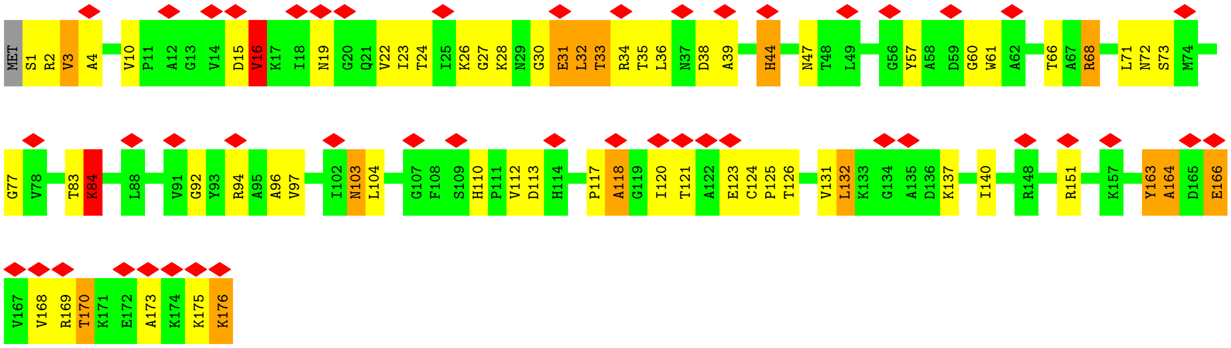
- Molecule 31: 50S ribosomal protein L5

Chain BF:



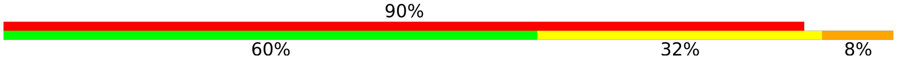
- Molecule 32: 50S ribosomal protein L6

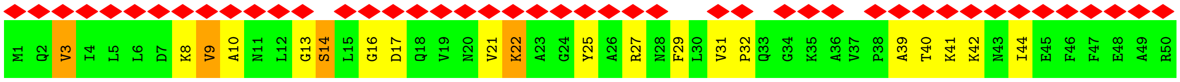
Chain BG:



- Molecule 33: 50S ribosomal protein L9

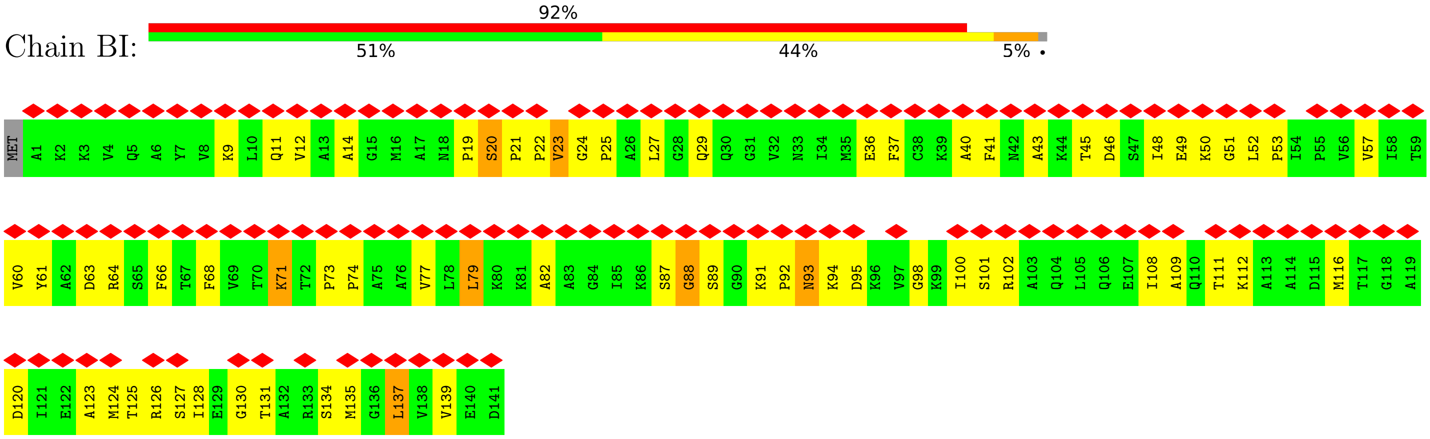
Chain BH:





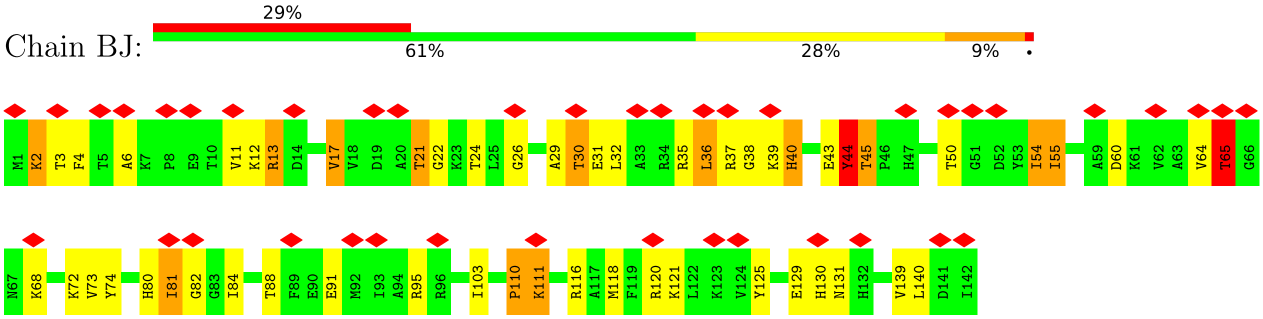
- Molecule 34: 50S ribosomal protein L11

Chain BI:



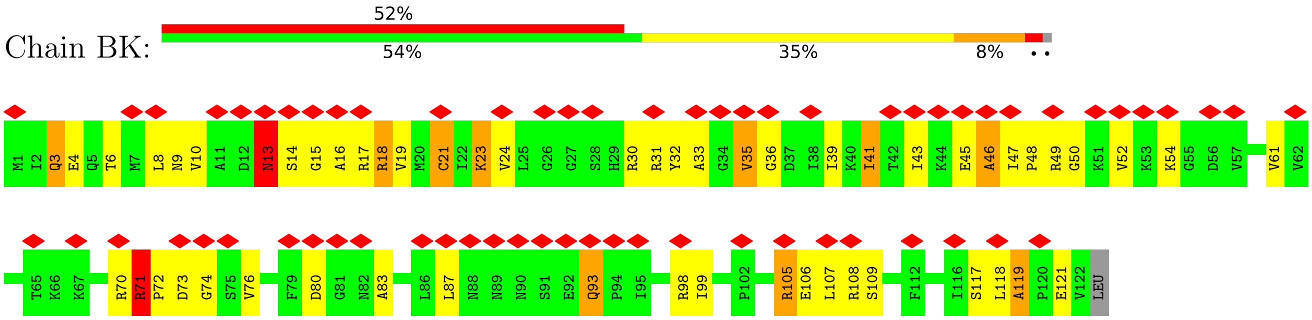
- Molecule 35: 50S ribosomal protein L13

Chain BJ:



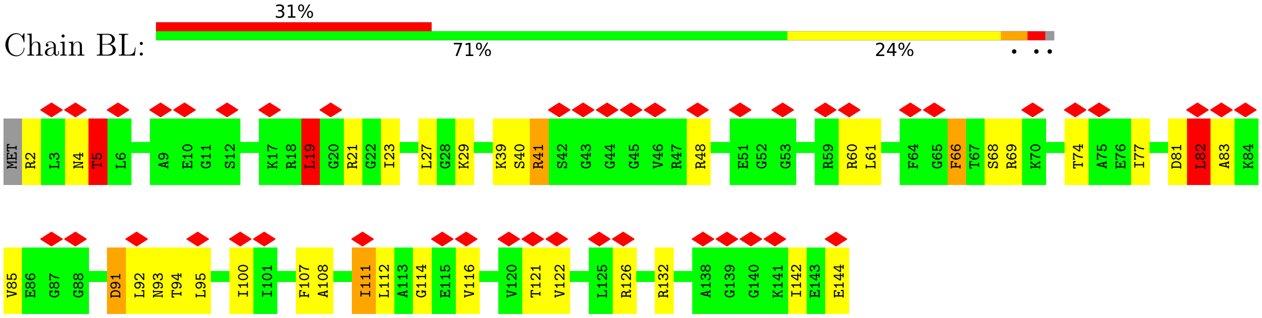
- Molecule 36: 50S ribosomal protein L14

Chain BK:



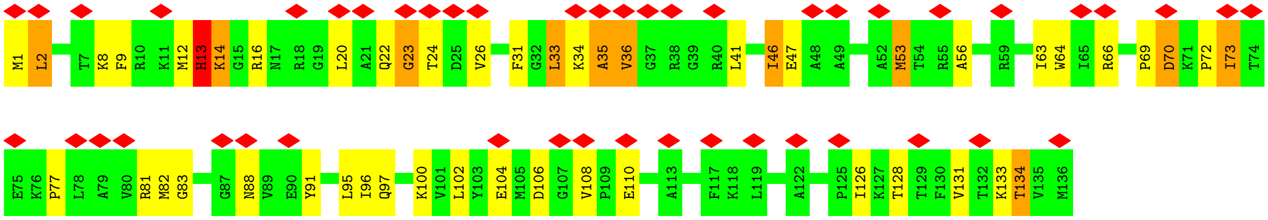
- Molecule 37: 50S ribosomal protein L15

Chain BL:

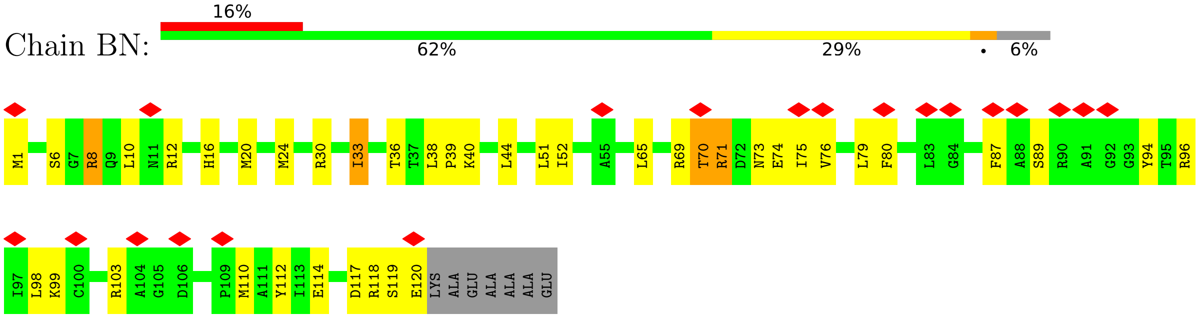


- Molecule 38: 50S ribosomal protein L16

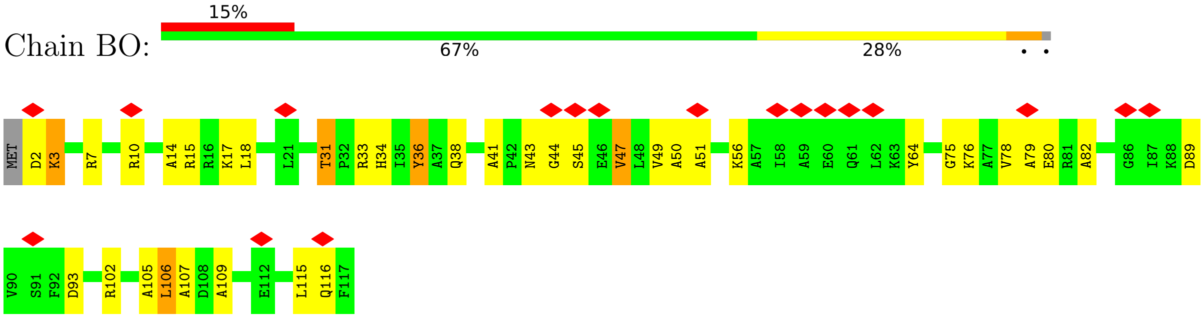
Chain BM:



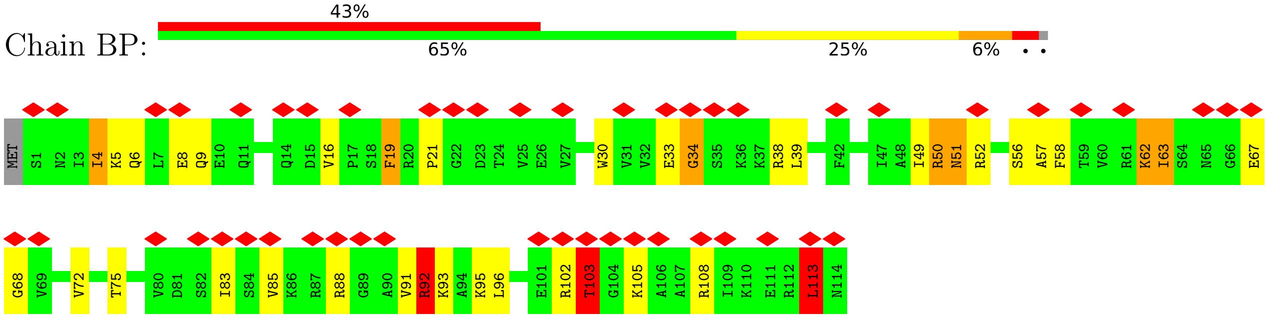
- Molecule 39: 50S ribosomal protein L17



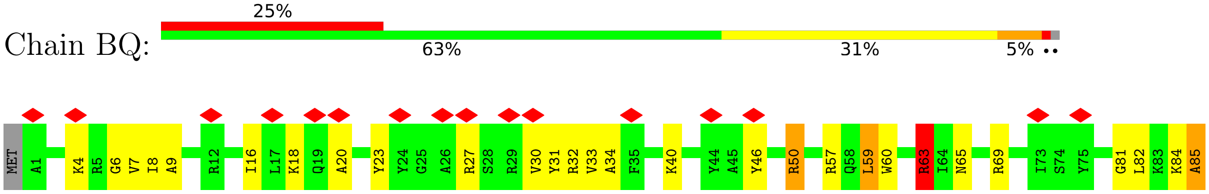
- Molecule 40: 50S ribosomal protein L18

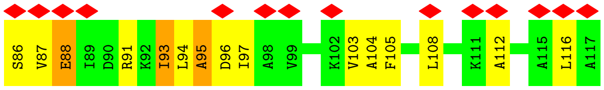


- Molecule 41: 50S ribosomal protein L19



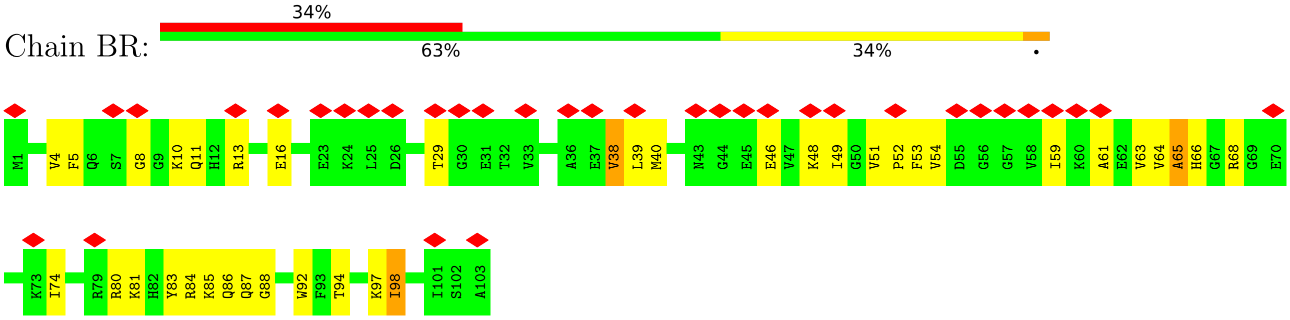
- Molecule 42: 50S ribosomal protein L20





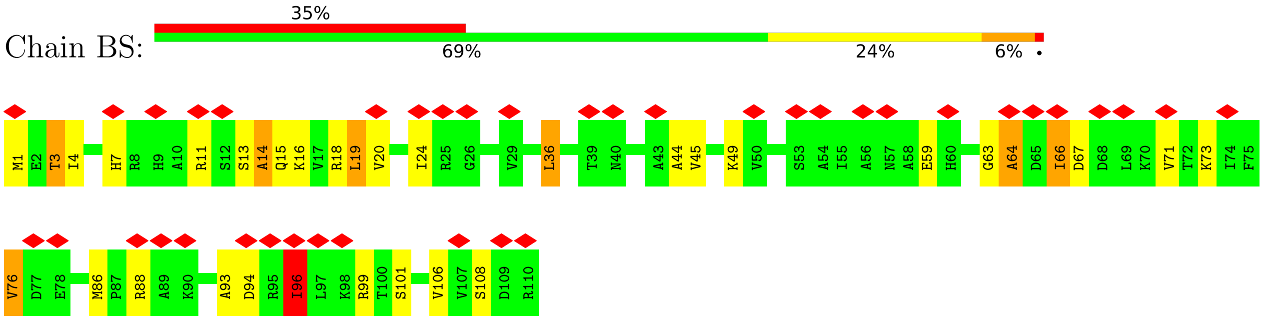
- Molecule 43: 50S ribosomal protein L21

Chain BR:



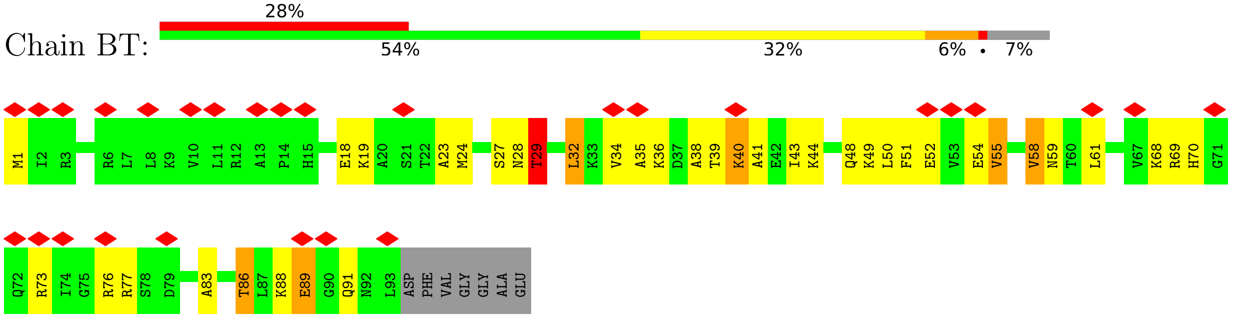
- Molecule 44: 50S ribosomal protein L22

Chain BS:



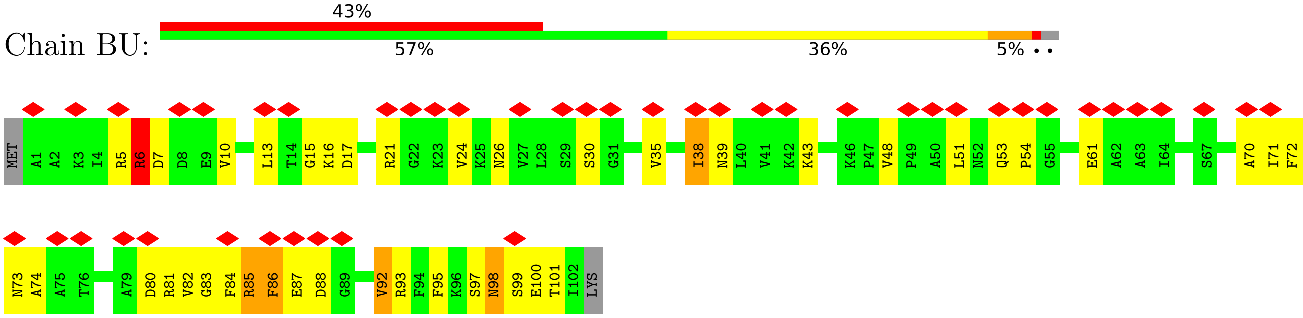
- Molecule 45: 50S ribosomal protein L23

Chain BT:



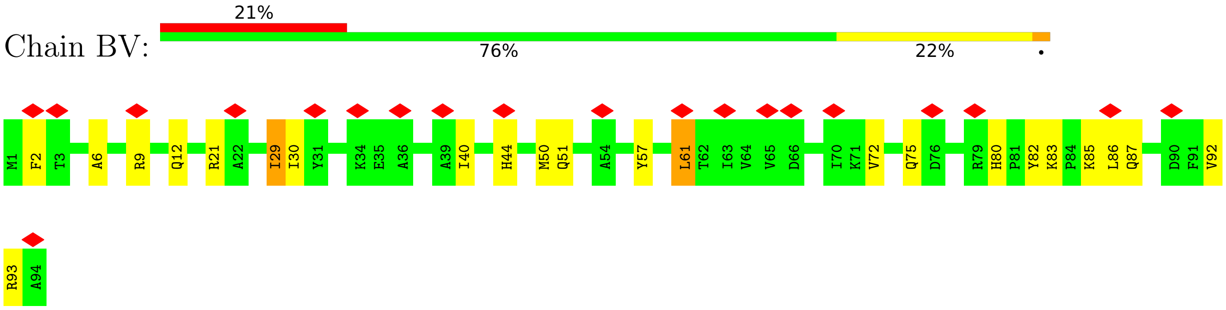
- Molecule 46: 50S ribosomal protein L24

Chain BU:



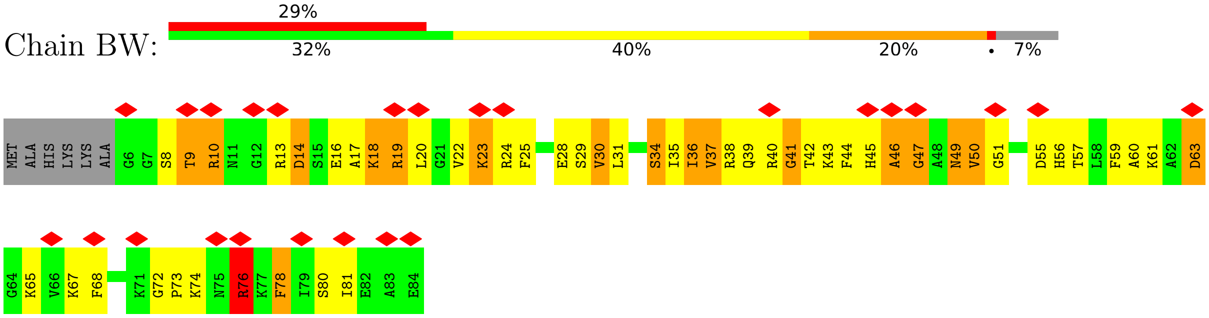
- Molecule 47: 50S ribosomal protein L25

Chain BV:



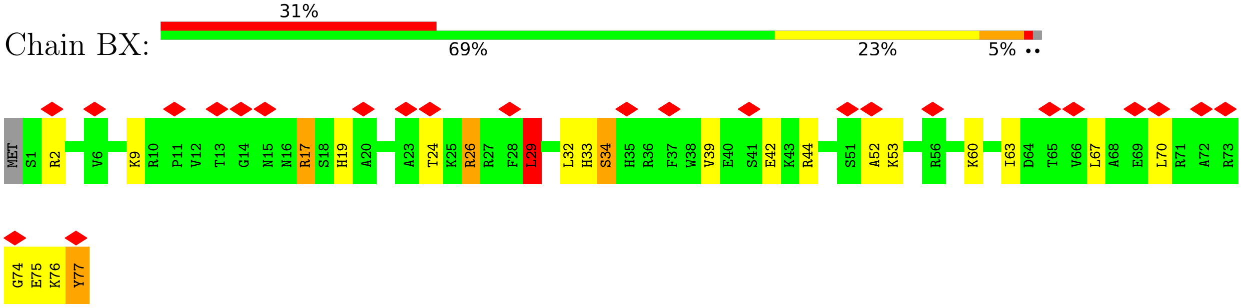
- Molecule 48: 50S ribosomal protein L27

Chain BW:



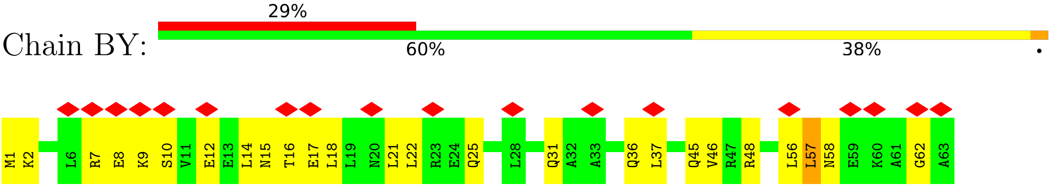
- Molecule 49: 50S ribosomal protein L28

Chain BX:



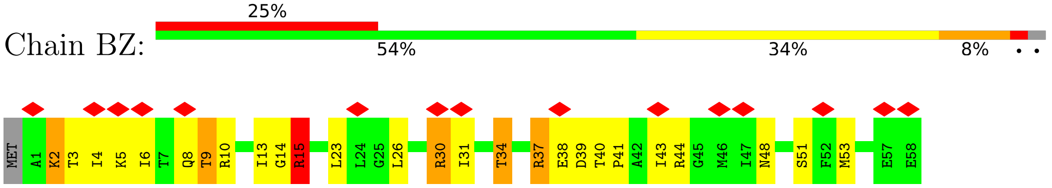
- Molecule 50: 50S ribosomal protein L29

Chain BY:



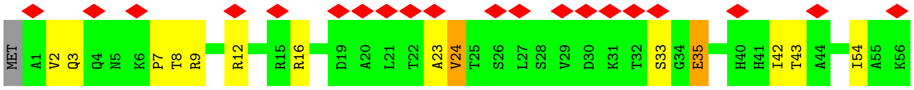
- Molecule 51: 50S ribosomal protein L30

Chain BZ:

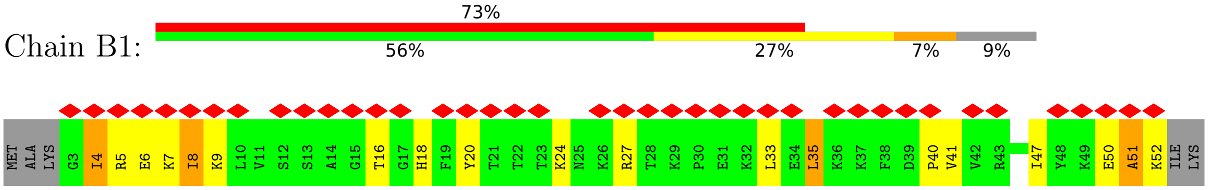


- Molecule 52: 50S ribosomal protein L32

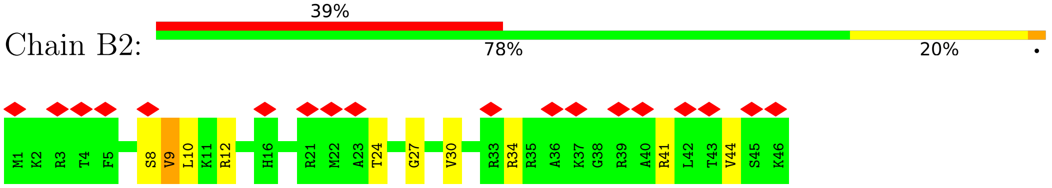
Chain B0:



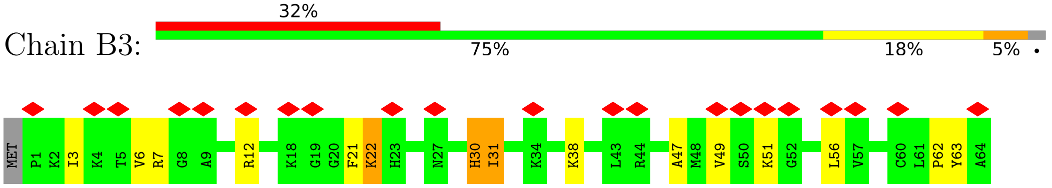
- Molecule 53: 50S ribosomal protein L33



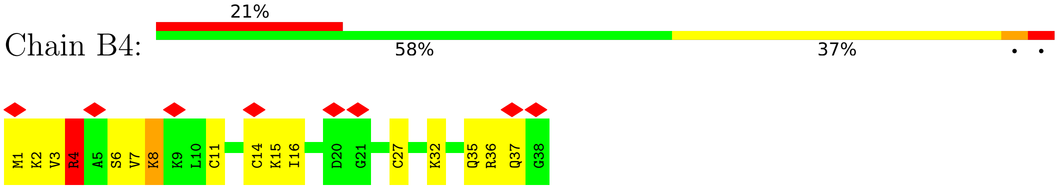
- Molecule 54: 50S ribosomal protein L34



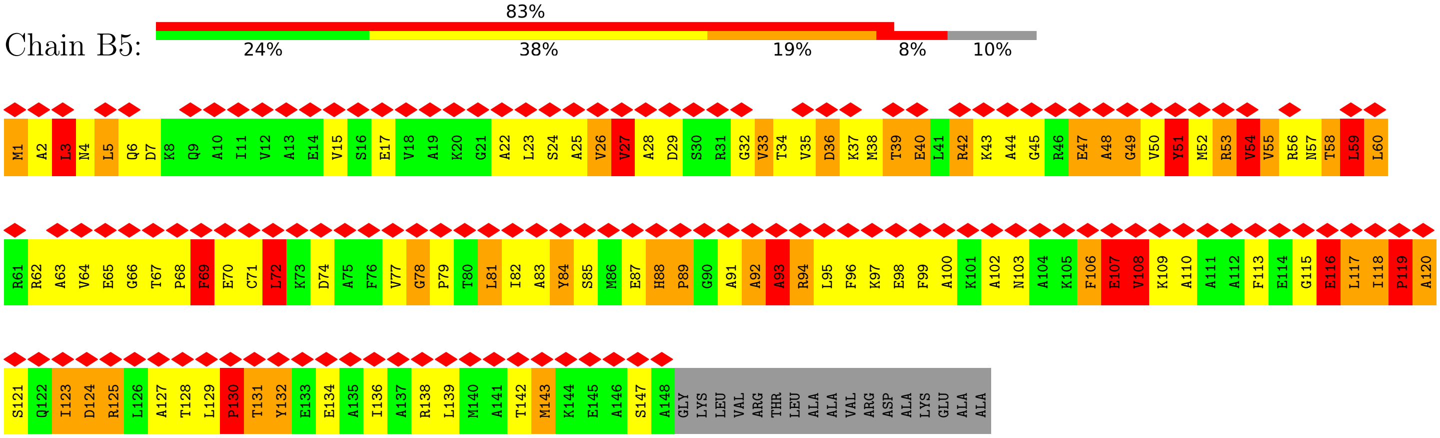
- Molecule 55: 50S ribosomal protein L35



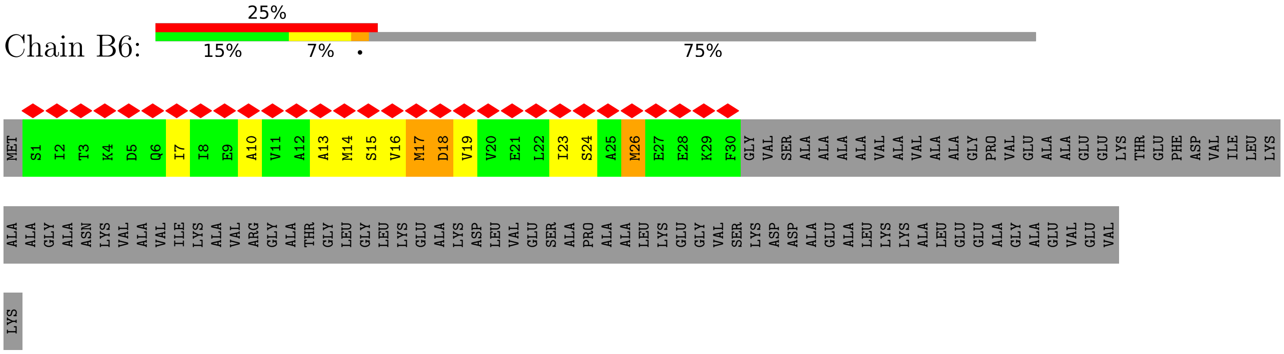
- Molecule 56: 50S ribosomal protein L36



- Molecule 57: 50S ribosomal protein L10



- Molecule 58: 50S ribosomal protein L7/L12


Chain B6:
25%
15%
7%
•
75%
MET S1 I2 T3 K4 D5 Q6 I7 I8 E9 A10 V11 A12 A13 M14 S15 V16 M17 D18 V19 V20 E21 L22 I23 S24 A25 M26 E27 E28 K29 F30 GLY VAL SER ALA ALA ALA ALA VAL ALA VAL ALA ALA GLY PRO VAL GLU ALA ALA GLU GLU LYS THR GLU PHE ASP VAL ILE LEU LYS
ALA ALA GLY ALA ASN LYS VAL ALA VAL ILE LYS ALA VAL ARG GLY ALA THR GLY LEU GLY LEU LYS GLU ALA LYS ASP LEU VAL GLU SER ALA PRO ALA ALA LEU LYS GLU GLY VAL SER LYS ASP ASP ALA GLU ALA LEU LYS LYS ALA LEU GLU GLU ALA GLY ALA GLU VAL GLU VAL
LYS

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	279309	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	The volumes were CTF-corrected in defocus groups with an average of approximately 906 individual images per group.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	20.00	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	12.702	Depositor
Minimum map value	-5.078	Depositor
Average map value	0.197	Depositor
Map value standard deviation	0.875	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, FUA, 5MU

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	0.65	4/36834 (0.0%)	1.13	100/57462 (0.2%)
2	AB	0.49	0/1735	0.72	0/2338
3	AC	0.45	0/1651	0.69	0/2225
4	AD	0.53	0/1665	0.79	0/2227
5	AE	0.49	0/1118	0.76	0/1504
6	AF	0.50	0/851	0.70	0/1150
7	AG	0.49	0/1195	0.67	0/1602
8	AH	0.48	0/989	0.65	0/1326
9	AI	0.54	0/1034	0.81	0/1375
10	AJ	0.54	0/796	0.80	0/1077
11	AK	0.50	0/893	0.74	0/1205
12	AL	0.54	0/969	0.82	0/1300
13	AM	0.48	0/892	0.70	0/1193
14	AN	0.48	0/785	0.78	0/1043
15	AO	0.44	0/722	0.66	0/964
16	AP	0.48	0/659	0.74	0/884
17	AQ	0.46	0/657	0.73	0/881
18	AR	0.45	0/462	0.62	0/621
19	AS	0.47	0/652	0.81	0/877
20	AT	0.47	0/671	0.61	0/888
21	AU	0.66	0/430	0.84	0/570
22	AV	0.57	0/1810	0.74	0/2821
23	AW	0.43	0/1827	1.14	6/2845 (0.2%)
24	AX	0.30	0/469	0.70	0/730
25	AY	0.46	0/5291	0.67	2/7160 (0.0%)
26	BB	0.66	0/2828	1.10	2/4410 (0.0%)
27	BC	0.54	0/2121	0.79	2/2852 (0.1%)
28	BA	0.81	17/68626 (0.0%)	1.22	303/107056 (0.3%)
29	BD	0.57	0/1586	0.77	1/2134 (0.0%)
30	BE	0.53	0/1571	0.76	2/2113 (0.1%)
31	BF	0.49	0/1434	0.71	1/1926 (0.1%)
32	BG	0.55	0/1343	0.73	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BH	0.53	0/389	0.73	0/523
34	BI	0.62	0/1046	0.84	1/1410 (0.1%)
35	BJ	0.63	1/1152 (0.1%)	0.78	0/1551
36	BK	0.65	1/947 (0.1%)	0.77	0/1268
37	BL	0.56	0/1054	0.79	2/1403 (0.1%)
38	BM	0.61	0/1093	0.77	0/1460
39	BN	0.51	0/973	0.68	0/1301
40	BO	0.46	0/902	0.70	0/1209
41	BP	0.52	0/929	0.78	1/1242 (0.1%)
42	BQ	0.62	0/960	0.71	1/1278 (0.1%)
43	BR	0.61	1/829 (0.1%)	0.76	0/1107
44	BS	0.54	0/864	0.73	0/1156
45	BT	0.55	0/744	0.85	1/994 (0.1%)
46	BU	0.56	0/787	0.78	0/1051
47	BV	0.48	0/766	0.67	1/1025 (0.1%)
48	BW	0.69	0/603	1.00	1/797 (0.1%)
49	BX	0.50	0/635	0.79	1/848 (0.1%)
50	BY	0.46	0/510	0.75	0/677
51	BZ	0.54	0/453	0.84	1/605 (0.2%)
52	B0	0.54	0/450	0.69	0/599
53	B1	0.53	0/416	0.74	0/554
54	B2	0.53	0/380	0.70	0/498
55	B3	0.53	0/513	0.75	0/676
56	B4	0.58	0/303	0.84	0/397
57	B5	0.74	0/1131	1.32	26/1524 (1.7%)
58	B6	0.59	0/227	0.65	0/304
All	All	0.69	24/163622 (0.0%)	1.08	455/244032 (0.2%)

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
6	AF	0	1
12	AL	0	1
22	AV	0	3
25	AY	0	1
27	BC	0	1
29	BD	0	1
35	BJ	0	1
36	BK	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	B5	0	1
All	All	0	11

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	922	G	O3'-P	9.48	1.72	1.61
28	BA	984	A	N9-C4	-8.58	1.32	1.37
1	AA	1362	A	N7-C5	7.93	1.44	1.39
28	BA	528	A	N9-C4	-6.68	1.33	1.37
28	BA	1142	A	N9-C4	-6.58	1.33	1.37

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BA	1073	A	N1-C6-N6	-20.01	106.59	118.60
28	BA	1073	A	C5-C6-N6	14.04	134.94	123.70
28	BA	2053	G	N1-C6-O6	13.92	128.25	119.90
1	AA	922	G	P-O3'-C3'	13.08	135.40	119.70
28	BA	2504	U	N3-C4-O4	13.06	128.54	119.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AF	101	PRO	Peptide
12	AL	23	ALA	Peptide
22	AV	29	G	Sidechain
22	AV	4	G	Sidechain
22	AV	8	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	32895	0	16542	956	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1704	0	1732	90	0
3	AC	1624	0	1696	41	0
4	AD	1643	0	1707	68	0
5	AE	1105	0	1147	147	0
6	AF	832	0	824	26	0
7	AG	1181	0	1236	53	0
8	AH	979	0	1031	28	0
9	AI	1022	0	1067	121	0
10	AJ	786	0	828	23	0
11	AK	877	0	887	32	0
12	AL	955	0	1016	36	0
13	AM	883	0	941	31	0
14	AN	774	0	824	35	0
15	AO	714	0	733	11	0
16	AP	649	0	666	14	0
17	AQ	648	0	691	11	0
18	AR	455	0	478	10	0
19	AS	637	0	665	39	0
20	AT	665	0	714	11	0
21	AU	425	0	449	43	0
22	AV	1640	0	832	136	0
23	AW	1635	0	829	97	0
24	AX	416	0	207	169	0
25	AY	5194	0	5170	222	0
26	BB	2529	0	1281	21	0
27	BC	2082	0	2157	50	0
28	BA	61274	0	30812	852	0
29	BD	1565	0	1616	52	0
30	BE	1552	0	1619	37	0
31	BF	1410	0	1442	59	0
32	BG	1323	0	1374	45	0
33	BH	384	0	405	35	0
34	BI	1032	0	1088	57	0
35	BJ	1129	0	1162	52	0
36	BK	938	0	1012	40	0
37	BL	1045	0	1117	34	0
38	BM	1074	0	1156	48	0
39	BN	960	0	1000	30	0
40	BO	892	0	923	22	0
41	BP	917	0	965	51	0
42	BQ	947	0	1022	50	0
43	BR	816	0	839	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BS	857	0	922	28	0
45	BT	738	0	807	35	0
46	BU	779	0	834	29	0
47	BV	753	0	780	14	0
48	BW	596	0	610	82	0
49	BX	625	0	655	16	0
50	BY	509	0	543	12	0
51	BZ	449	0	491	17	0
52	B0	444	0	461	17	0
53	B1	409	0	440	16	0
54	B2	377	0	418	5	0
55	B3	504	0	574	10	0
56	B4	302	0	340	15	0
57	B5	1117	0	1155	120	0
58	B6	227	0	237	7	0
59	AY	37	0	44	59	0
60	AY	28	0	12	26	0
All	All	150958	0	103225	3593	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 14.

The worst 5 of 3593 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)
25:AY:92:HIS:CE1	59:AY:801:FUA:H283	1.23	1.69
1:AA:1498:U:C5	24:AX:12:U:H5”	1.26	1.64
1:AA:1498:U:C4	24:AX:12:U:H5”	1.32	1.61
24:AX:14:A:H2’	24:AX:15:A:C5’	1.24	1.58
24:AX:14:A:C2’	24:AX:15:A:H5”	1.16	1.57

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	16
3	AC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	5	32
4	AD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	2	19
5	AE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	2	21
6	AF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	1	17
7	AG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	22	63
8	AH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	19	60
9	AI	125/130 (96%)	104 (83%)	15 (12%)	6 (5%)	2	21
10	AJ	96/103 (93%)	69 (72%)	20 (21%)	7 (7%)	1	14
11	AK	115/129 (89%)	97 (84%)	12 (10%)	6 (5%)	2	19
12	AL	121/124 (98%)	101 (84%)	16 (13%)	4 (3%)	4	26
13	AM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2	19
14	AN	92/101 (91%)	73 (79%)	13 (14%)	6 (6%)	1	16
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	34
16	AP	80/82 (98%)	60 (75%)	17 (21%)	3 (4%)	3	24
17	AQ	78/84 (93%)	59 (76%)	15 (19%)	4 (5%)	2	19
18	AR	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
19	AS	77/92 (84%)	65 (84%)	11 (14%)	1 (1%)	12	48
20	AT	83/87 (95%)	74 (89%)	7 (8%)	2 (2%)	6	33
21	AU	49/71 (69%)	26 (53%)	20 (41%)	3 (6%)	1	17
25	AY	667/704 (95%)	541 (81%)	92 (14%)	34 (5%)	2	19
27	BC	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	18
29	BD	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	15
30	BE	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	2	20
31	BF	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	6	34
32	BG	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	0	9
33	BH	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	0	8
34	BI	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	16
35	BJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	16
36	BK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	3	25
38	BM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	12
39	BN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	19	60
40	BO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	17	57
41	BP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	12
42	BQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	25
43	BR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	4	28
44	BS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	21
45	BT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	7
46	BU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0	9
47	BV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
48	BW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	2
49	BX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	3	23
50	BY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	15
51	BZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	3	25
52	B0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	13
53	B1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	17
54	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
55	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4	26
56	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	12
57	B5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	2
58	B6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	3	25
All	All	6365/6876 (93%)	5040 (79%)	977 (15%)	348 (6%)	3	19

5 of 348 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	33	ALA
2	AB	40	ILE
2	AB	119	GLN
3	AC	101	ILE
4	AD	24	GLY

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	
2	AB	180/199 (90%)	170 (94%)	10 (6%)	21	46
3	AC	170/190 (90%)	156 (92%)	14 (8%)	11	34
4	AD	172/173 (99%)	165 (96%)	7 (4%)	30	55
5	AE	113/126 (90%)	108 (96%)	5 (4%)	28	53
6	AF	89/116 (77%)	82 (92%)	7 (8%)	12	35
7	AG	124/147 (84%)	115 (93%)	9 (7%)	14	39
8	AH	104/105 (99%)	96 (92%)	8 (8%)	13	37
9	AI	105/107 (98%)	96 (91%)	9 (9%)	10	32
10	AJ	86/90 (96%)	83 (96%)	3 (4%)	36	59
11	AK	90/99 (91%)	85 (94%)	5 (6%)	21	46
12	AL	103/104 (99%)	96 (93%)	7 (7%)	16	41
13	AM	92/96 (96%)	88 (96%)	4 (4%)	29	53
14	AN	79/84 (94%)	75 (95%)	4 (5%)	24	48
15	AO	76/77 (99%)	72 (95%)	4 (5%)	22	47
16	AP	65/65 (100%)	61 (94%)	4 (6%)	18	43
17	AQ	74/78 (95%)	66 (89%)	8 (11%)	6	23
18	AR	48/65 (74%)	47 (98%)	1 (2%)	53	72
19	AS	70/79 (89%)	64 (91%)	6 (9%)	10	32
20	AT	65/66 (98%)	60 (92%)	5 (8%)	13	37
21	AU	44/61 (72%)	36 (82%)	8 (18%)	1	10
25	AY	552/578 (96%)	505 (92%)	47 (8%)	10	33
27	BC	216/218 (99%)	202 (94%)	14 (6%)	17	42
29	BD	164/164 (100%)	151 (92%)	13 (8%)	12	35
30	BE	165/165 (100%)	146 (88%)	19 (12%)	5	21
31	BF	148/150 (99%)	138 (93%)	10 (7%)	16	41
32	BG	137/138 (99%)	122 (89%)	15 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BH	40/40 (100%)	38 (95%)	2 (5%)	24	49
34	BI	109/110 (99%)	105 (96%)	4 (4%)	34	58
35	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	17
36	BK	103/104 (99%)	92 (89%)	11 (11%)	6	23
37	BL	102/103 (99%)	95 (93%)	7 (7%)	15	40
38	BM	109/109 (100%)	93 (85%)	16 (15%)	3	15
39	BN	100/103 (97%)	93 (93%)	7 (7%)	15	40
40	BO	86/87 (99%)	78 (91%)	8 (9%)	9	28
41	BP	99/100 (99%)	91 (92%)	8 (8%)	11	35
42	BQ	89/90 (99%)	81 (91%)	8 (9%)	9	30
43	BR	84/84 (100%)	78 (93%)	6 (7%)	14	39
44	BS	93/93 (100%)	84 (90%)	9 (10%)	8	27
45	BT	80/84 (95%)	77 (96%)	3 (4%)	33	57
46	BU	83/85 (98%)	76 (92%)	7 (8%)	11	33
47	BV	78/78 (100%)	75 (96%)	3 (4%)	33	57
48	BW	59/63 (94%)	53 (90%)	6 (10%)	7	25
49	BX	67/68 (98%)	61 (91%)	6 (9%)	9	30
50	BY	55/55 (100%)	52 (94%)	3 (6%)	21	47
51	BZ	48/49 (98%)	40 (83%)	8 (17%)	2	12
52	B0	47/48 (98%)	46 (98%)	1 (2%)	53	72
53	B1	45/49 (92%)	42 (93%)	3 (7%)	16	41
54	B2	38/38 (100%)	35 (92%)	3 (8%)	12	35
55	B3	51/52 (98%)	46 (90%)	5 (10%)	8	26
56	B4	34/34 (100%)	31 (91%)	3 (9%)	10	31
57	B5	112/123 (91%)	93 (83%)	19 (17%)	2	12
58	B6	26/85 (31%)	22 (85%)	4 (15%)	2	14
All	All	5284/5590 (94%)	4862 (92%)	422 (8%)	16	35

5 of 422 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	BG	3	VAL
38	BM	12	MET

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Mol	Chain	Res	Type
57	B5	1	MET
32	BG	110	HIS
35	BJ	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
25	AY	465	HIS
31	BF	26	GLN
55	B3	30	HIS
25	AY	645	GLN
34	BI	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1542 (99%)	282 (18%)	18 (1%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	27 (35%)	2 (2%)
24	AX	18/19 (94%)	14 (77%)	1 (5%)
26	BB	117/120 (97%)	17 (14%)	0
28	BA	2850/2904 (98%)	462 (16%)	41 (1%)
All	All	4669/4739 (98%)	817 (17%)	62 (1%)

5 of 817 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	17	U
1	AA	20	U
1	AA	21	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	BA	527	C
28	BA	2211	A
28	BA	931	U
28	BA	2142	A

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Mol	Chain	Res	Type
28	BA	2756	U

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
22	5MU	AV	54	22	18,21,23	0.40	0	26,30,35	0.48	0

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
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	FUA	AY	801	-	39,40,40	1.68	7 (17%)	49,64,64	1.51	5 (10%)
60	GDP	AY	802	-	24,30,30	1.27	2 (8%)	30,47,47	1.57	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FUA	AY	801	-	-	6/15/92/92	0/4/4/4
60	GDP	AY	802	-	-	3/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AY	801	FUA	C23-C22	-4.38	1.39	1.51
59	AY	801	FUA	C23-C24	-4.29	1.39	1.53
59	AY	801	FUA	C29-C22	4.17	1.53	1.47
60	AY	802	GDP	C5-C6	-3.91	1.39	1.47
59	AY	801	FUA	C24-C25	-3.27	1.39	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	AY	801	FUA	C13-C12-C11	-4.35	105.81	111.90
60	AY	802	GDP	PA-O3A-PB	-3.92	119.36	132.83
59	AY	801	FUA	C16-O2-C31	-3.91	111.11	117.06
59	AY	801	FUA	C8-C9-C10	-3.43	112.82	116.34
60	AY	802	GDP	C2-N1-C6	-3.16	119.27	125.10

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AY	801	FUA	C13-C17-C22-C29
59	AY	801	FUA	C17-C22-C23-C24
59	AY	801	FUA	C29-C22-C23-C24
60	AY	802	GDP	C5'-O5'-PA-O3A
60	AY	802	GDP	C5'-O5'-PA-O1A

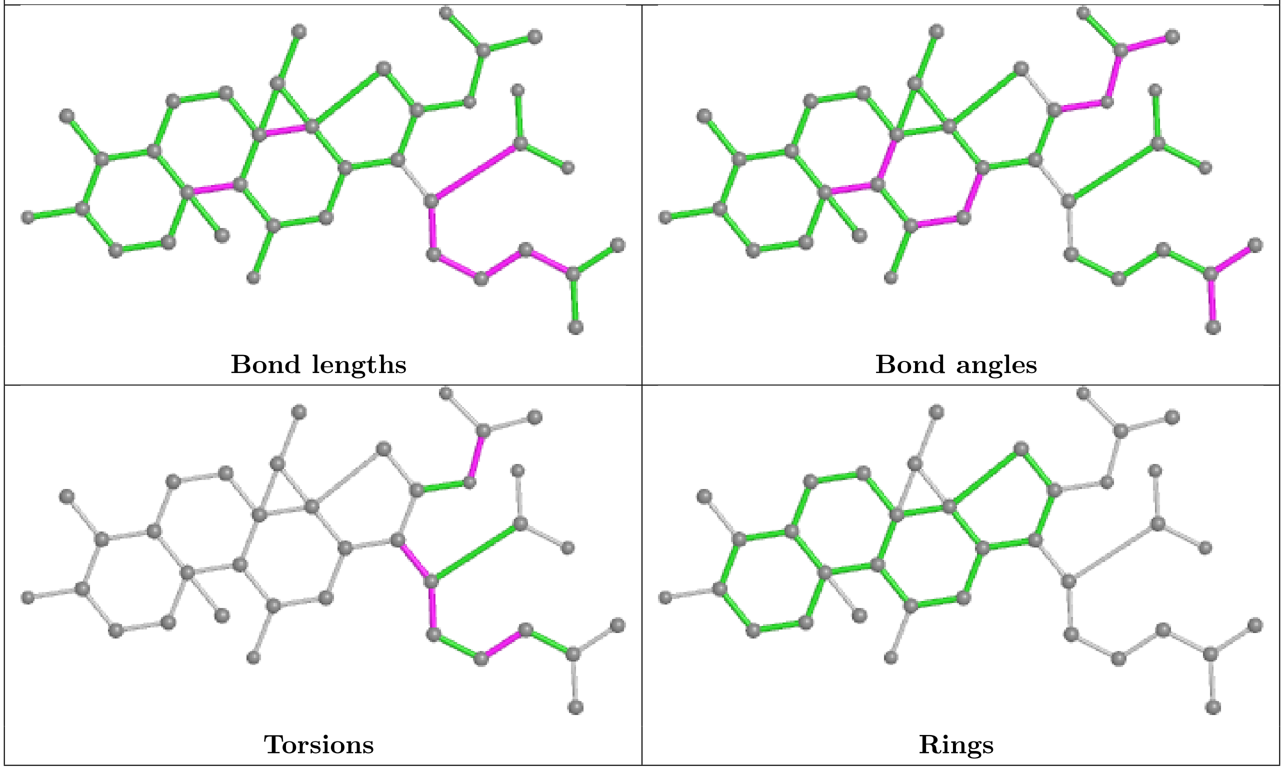
There are no ring outliers.

2 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AY	801	FUA	59	0
60	AY	802	GDP	26	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 FUA AY 801



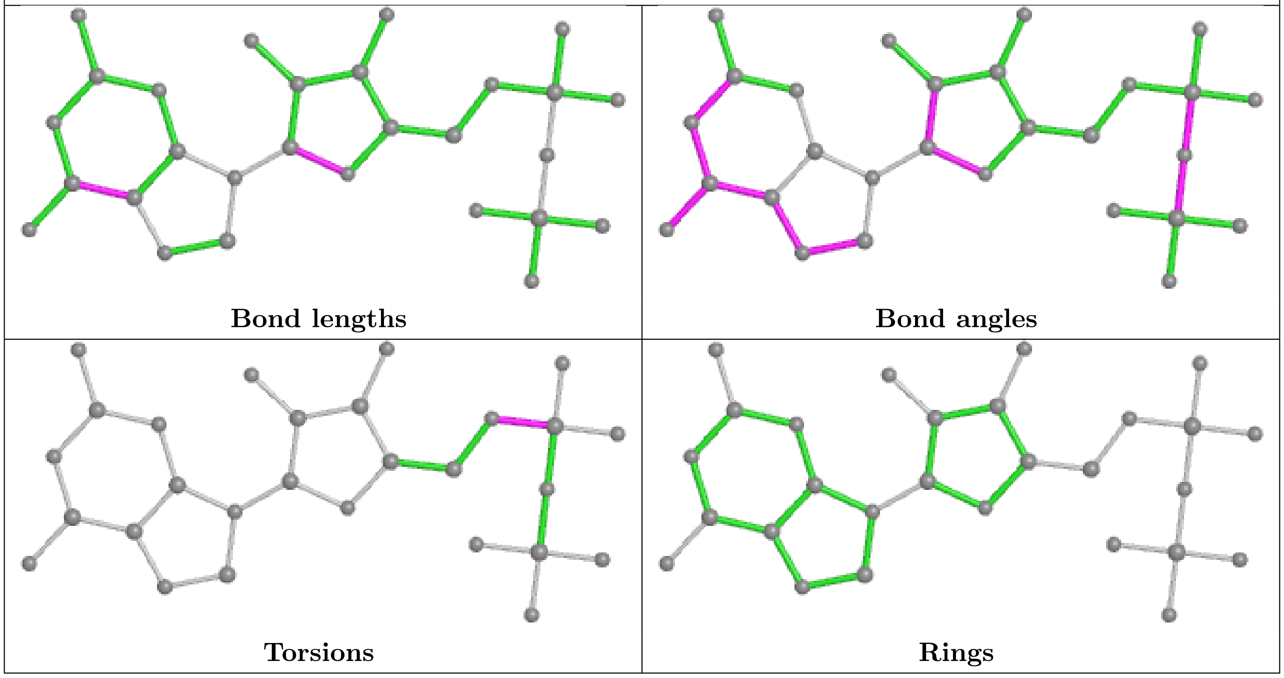
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP AY 802



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

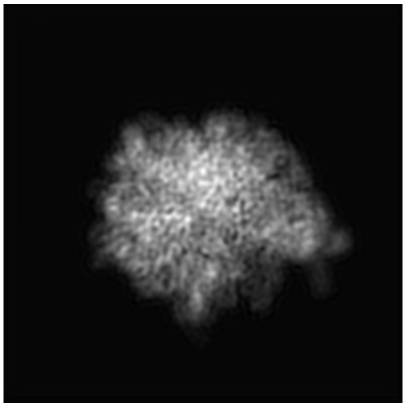
6 Map visualisation

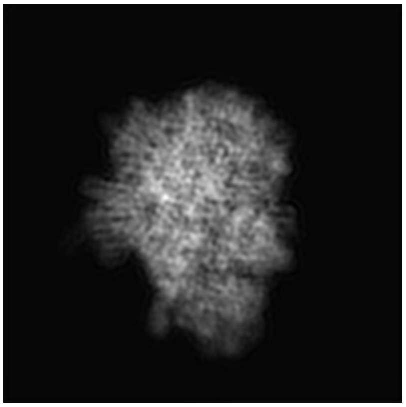
This section contains visualisations of the EMDB entry EMD-5775. These allow visual inspection of the internal detail of the map and identification of artifacts.

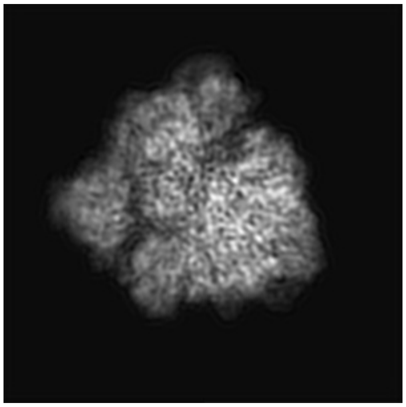
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

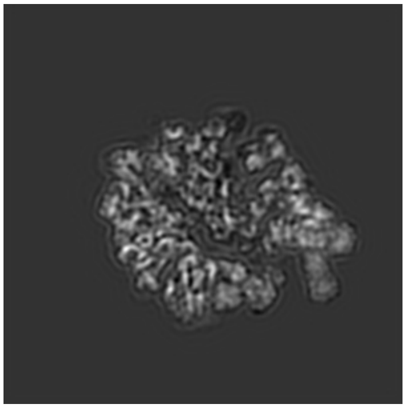

Y

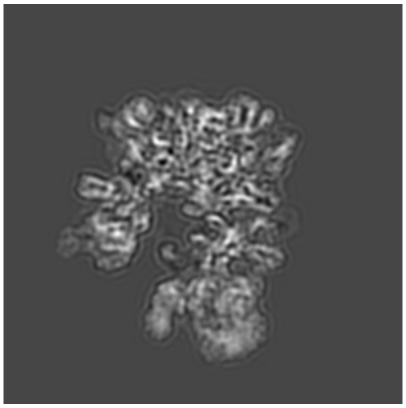

Z

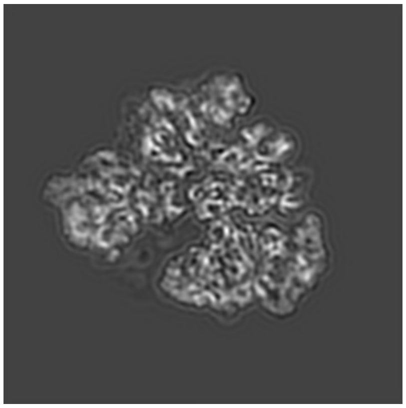
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 150


Y Index: 150


Z Index: 150

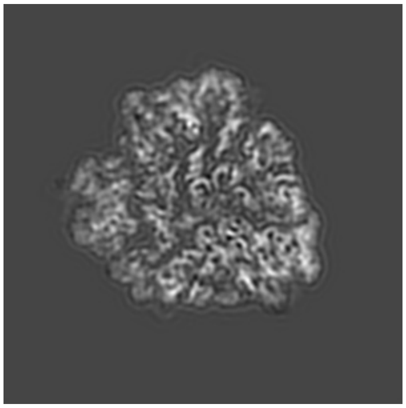
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map

X Index: 141

Y Index: 154



Z Index: 141

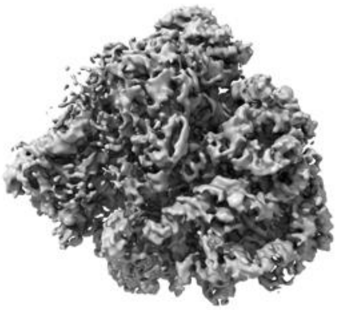
The images above show the largest variance slices of the map in three orthogonal directions.

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

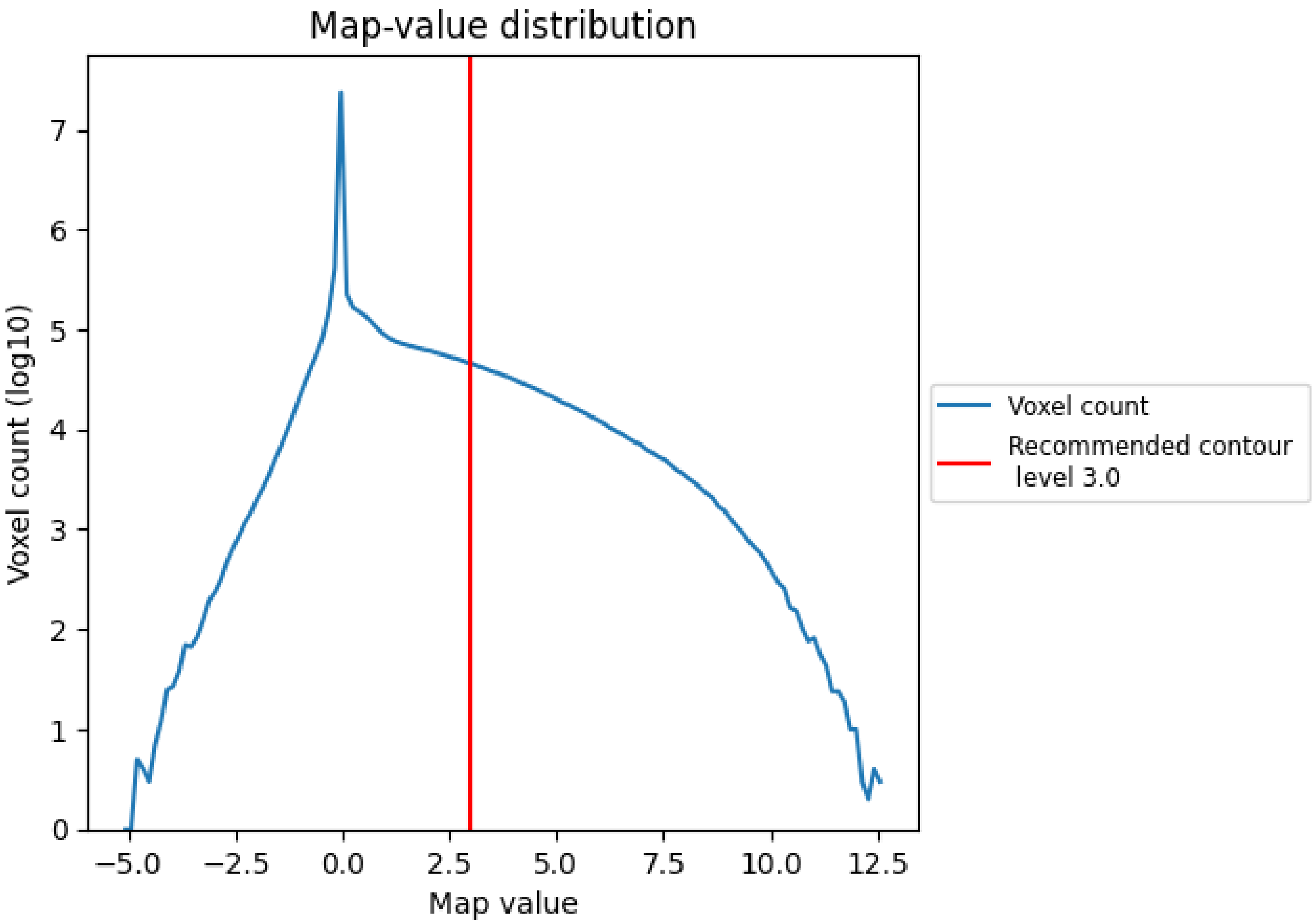
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

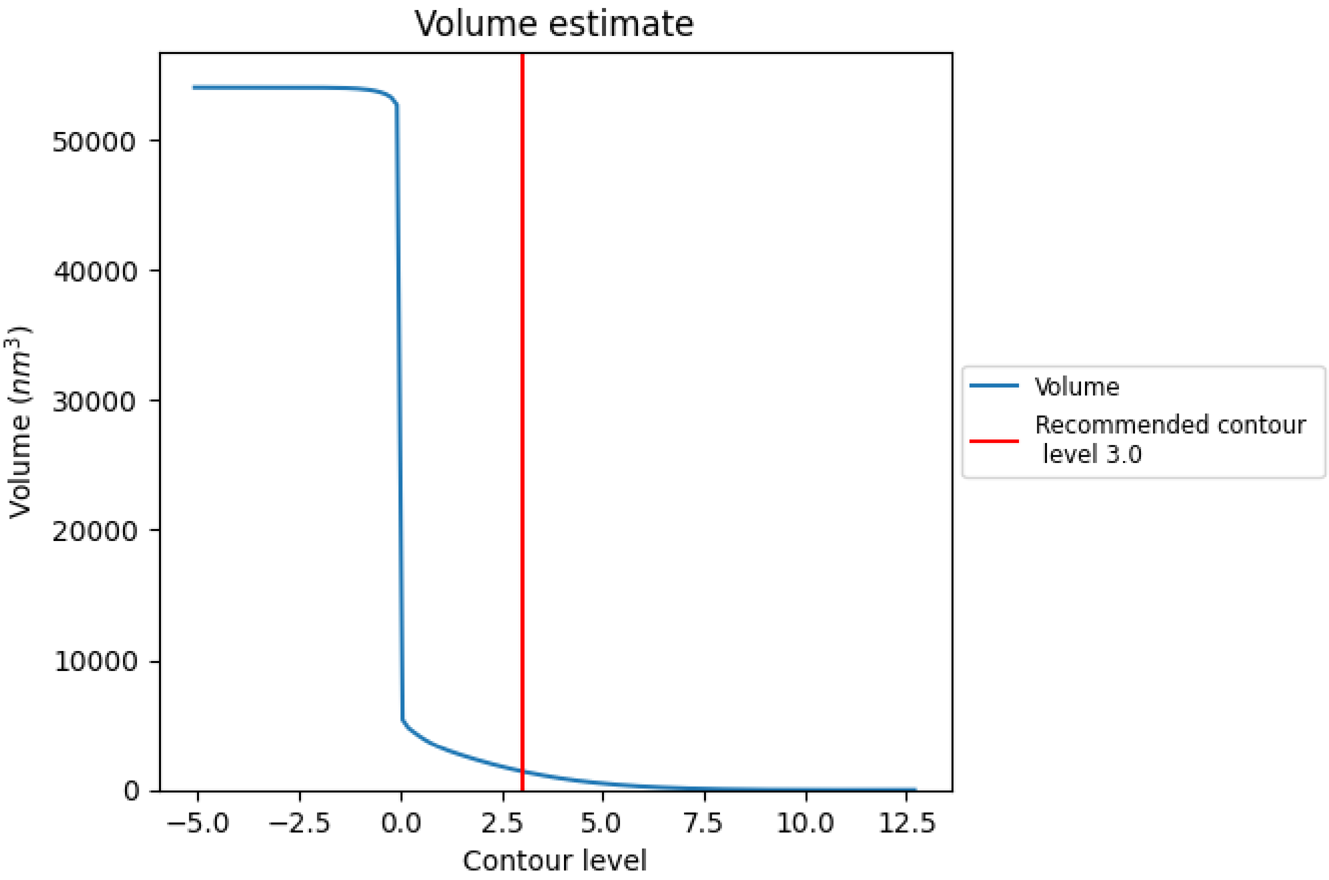
This section contains the results of statistical analysis of the map.

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.

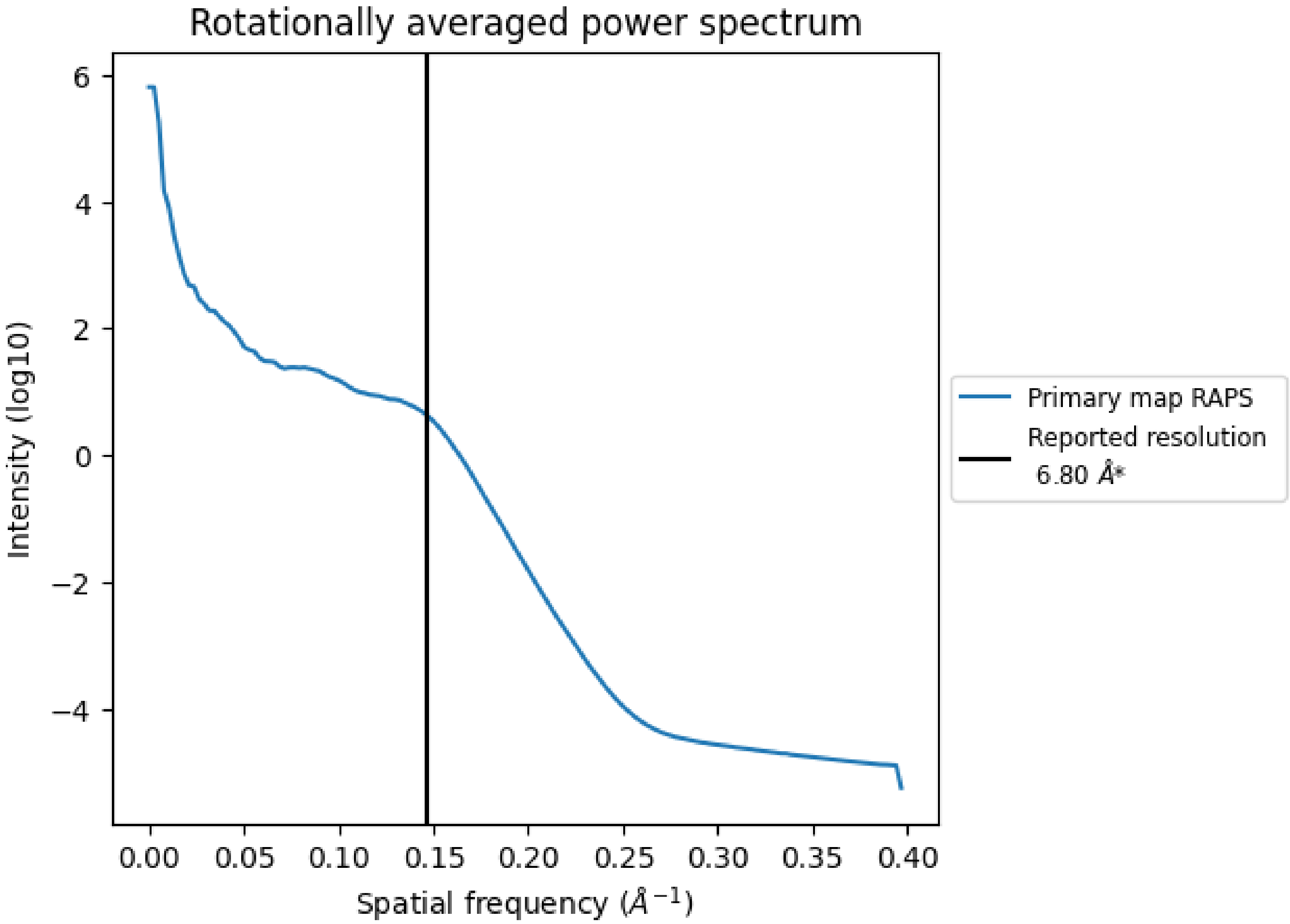
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1436 nm^3; this corresponds to an approximate mass of 1297 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 0.147 Å^{-1}

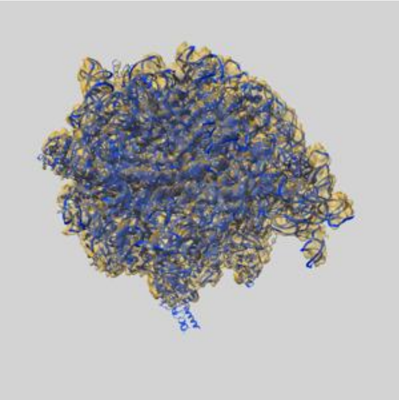
8 Fourier-Shell correlation ⓘ

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

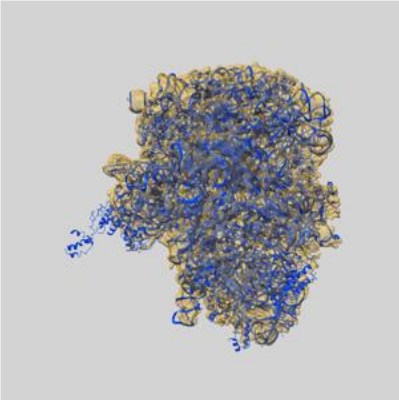
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5775 and PDB model 4V7B. Per-residue inclusion information can be found in section 3 on page 16.

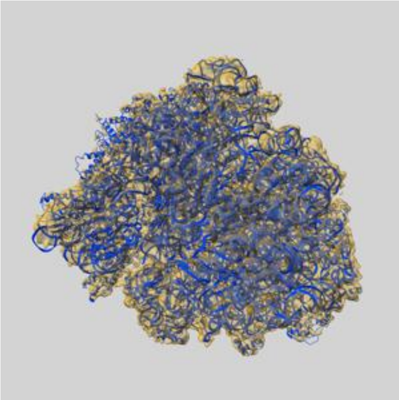
9.1 Map-model overlay (i)



X



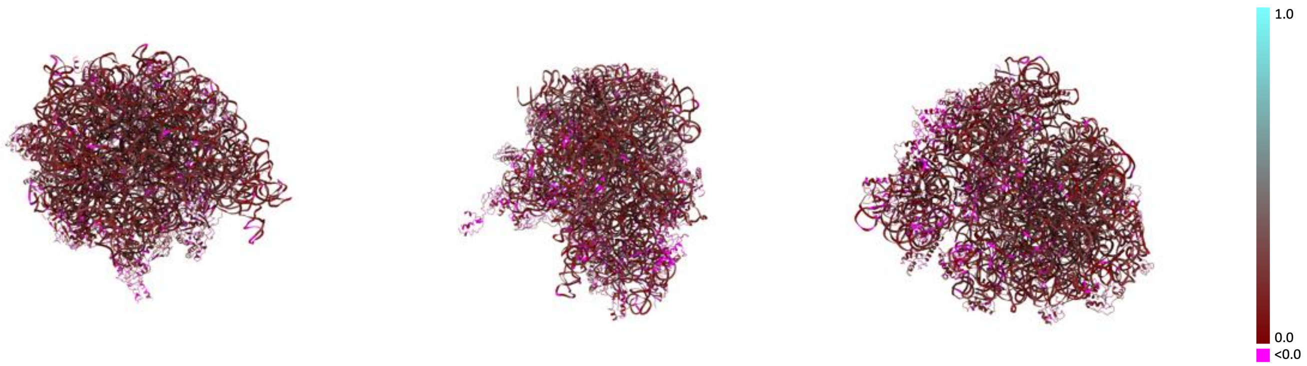
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

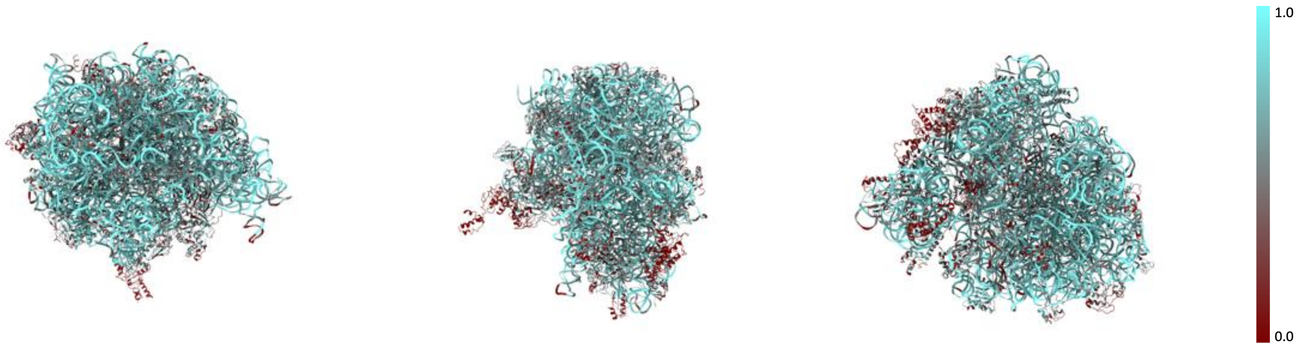
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

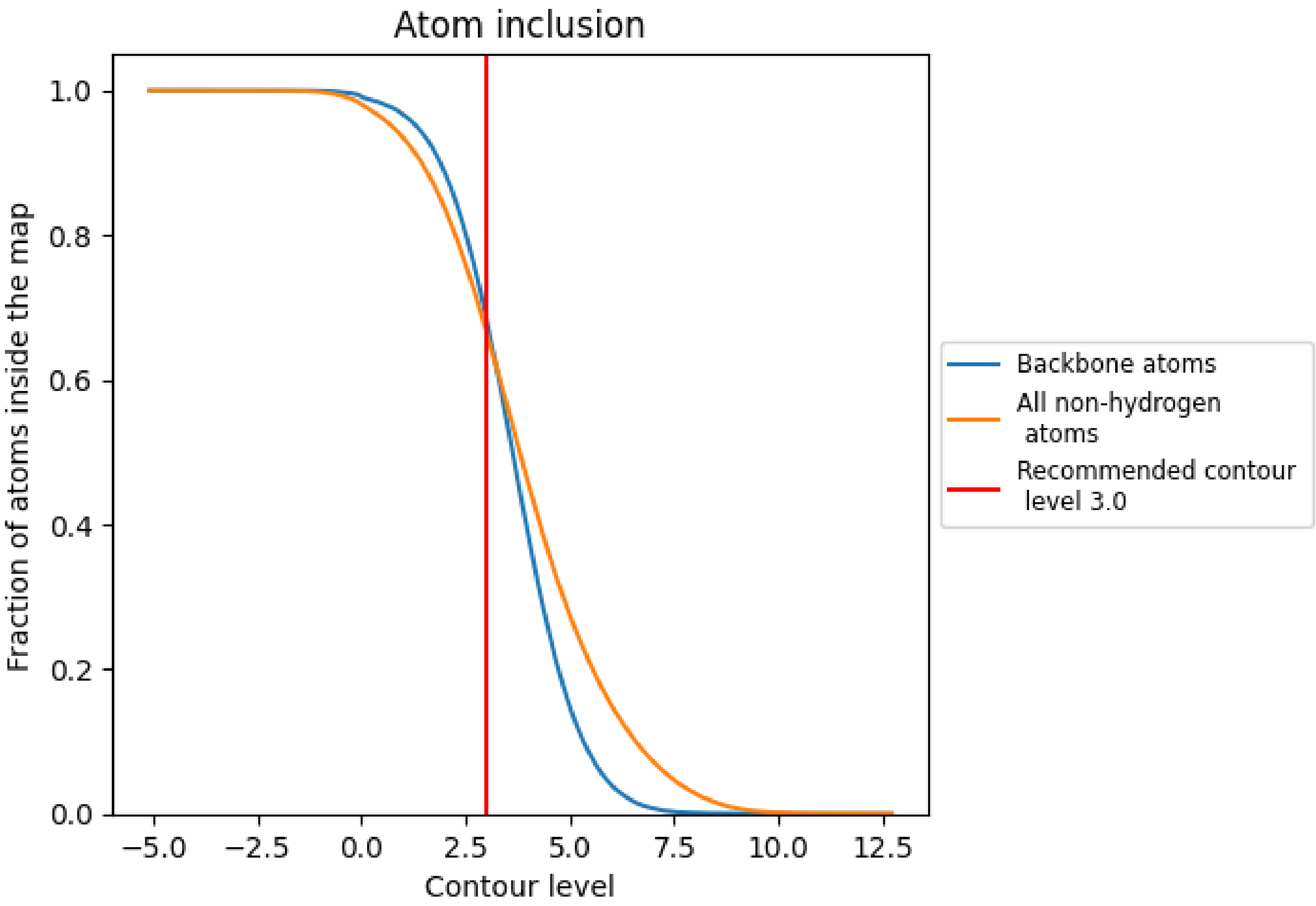
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6656	0.1610
AA	0.7855	0.1720
AB	0.0884	0.0200
AC	0.4423	0.1190
AD	0.4239	0.1010
AE	0.5125	0.1290
AF	0.4908	0.0840
AG	0.1705	0.0750
AH	0.5094	0.1360
AI	0.5087	0.1040
AJ	0.3706	0.1080
AK	0.4842	0.1240
AL	0.3909	0.1350
AM	0.4442	0.1130
AN	0.5168	0.1330
AO	0.5580	0.1320
AP	0.5678	0.1500
AQ	0.5253	0.1240
AR	0.5298	0.1380
AS	0.5201	0.1130
AT	0.5800	0.1490
AU	0.2635	0.0750
AV	0.5902	0.1730
AW	0.6869	0.1750
AX	0.4663	0.1420
AY	0.4012	0.1200
B0	0.4883	0.1490
B1	0.2170	0.0820
B2	0.4535	0.1290
B3	0.4847	0.1390
B4	0.5651	0.1340
B5	0.0612	0.0430
B6	0.0000	-0.0070
BA	0.7821	0.1890
BB	0.8296	0.1790

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Chain	Atom inclusion	Q-score
BC	0.4658	0.1220
BD	0.4863	0.1390
BE	0.4072	0.1510
BF	0.4618	0.0710
BG	0.5775	0.1650
BH	0.1029	0.0470
BI	0.1086	0.0710
BJ	0.5336	0.1320
BK	0.3746	0.1530
BL	0.5315	0.1540
BM	0.5038	0.1650
BN	0.5738	0.1350
BO	0.6292	0.1580
BP	0.4369	0.1500
BQ	0.5606	0.1150
BR	0.4969	0.1460
BS	0.4904	0.1310
BT	0.5000	0.1400
BU	0.4472	0.1040
BV	0.5813	0.1310
BW	0.5241	0.1290
BX	0.5058	0.1570
BY	0.5392	0.1350
BZ	0.5538	0.1400