wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 07:03 am GMT

PDB ID	:	4D61
EMDB ID	:	EMD-2813
Title	:	Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors	:	Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on	:	2014-11-07
Resolution	:	9.00 Å(reported)

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

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

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

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

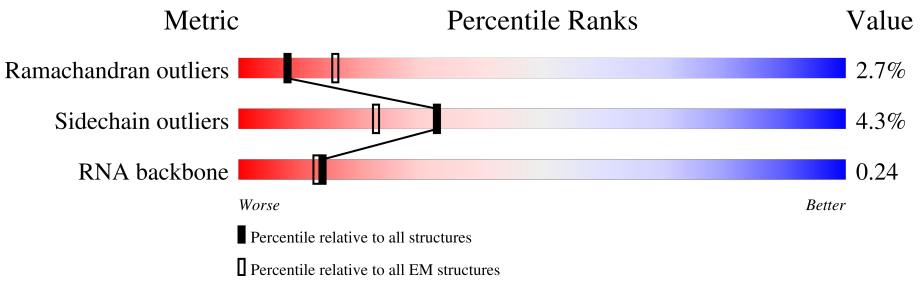
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1	1869	36% 55% • 7%
2	A	295	30% 72% • 26%
3	B	264	12% 71% 8% • 19%
4	C	293	14% 72% • 24%
5	D	243	21% 81% 6% 13%
6	E	263	16% 92% 6% •
7	F	204	20% 84% 8% 8%
8	G	249	16% 87% 6% 7%

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Mol	Chain	Length	Quality of chain
9	H	194	54% 94%
10	I	208	22% 91% 8%
11	J	194	9% 86% 7% 8%
12	K	165	12% 52% 5% 43%
13	L	158	26% 87% 5% 8%
14	M	132	54% 83% 7% 9%
15	N	151	17% 95%
16	O	151	17% 85% 5% 9%
17	P	145	23% 75% 6% 19%
18	Q	146	17% 91% 5%
19	R	135	29% 76% 5% 19%
20	S	152	18% 82% 11% 7%
21	T	145	26% 92% 6%
22	U	119	29% 81% 15%
23	V	83	43% 96%
24	W	130	21% 94% 5%
25	X	143	14% 85% 8% 6%
26	Y	133	17% 84% 8% 8%
27	Z	125	11% 55% 6% 39%
28	a	115	20% 74% 9% 17%
29	b	84	25% 90% 5% 5%
30	c	69	26% 83% 7% 10%
31	d	56	9% 88% 7% 5%
32	e	59	32% 81% 5% 14%
33	f	156	24% 37% 61%

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Mol	Chain	Length	Quality of chain
34	g	317	30% 93% 5%
35	h	436	47% 97%
36	i	426	58% 98%
37	j	201	16% 45% 49% 6%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 86384 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 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1742	37159	16589	6665	12164	1741	0	0

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	218	1719	1091	301	319	8	0	0

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	222	1724	1114	296	304	10	0	0

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	212	1646	1050	299	290	7	0	0

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	257	2031	1298	381	344	8	0	0

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	188	1486	930	283	266	7	0	0

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	232	1884	1176	379	322	7	0	0

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	191	1535	978	282	274	1	0	0

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	207	1695	1064	334	292	5	0	0

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	179	1495	953	299	241	2	0	0

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	94	791	519	138	129	5	0	0

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	146	1199	764	224	205	6	0	0

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	120	931	584	164	174	9	0	0

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	150	1207	773	229	204	1	0	0

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	137	1023	627	200	190	6	0	0

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	118	981	625	183	166	7	0	0

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	139	1108	704	210	191	3	0	0

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	109	893	561	170	159	3	0	0

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	142	1172	736	236	199	1	0	0

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	143	1112	697	214	198	3	0	0

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	101	803	502	153	144	4	0	0

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	83	636	393	117	121	5	0	0

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	129	1033	659	193	175	6	0	0

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	134	1046	663	205	176	2	0	0

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	122	1002	635	196	166	5	0	0

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	76	605	387	112	105	1	0	0

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	96	767	476	159	127	5	0	0

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	80	625	391	116	111	7	0	0

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	62	490	298	99	91	2	0	0

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	53	444	278	90	71	5	0	0

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	51	412	258	90	63	1	0	0

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	61	497	312	94	84	7	0	0

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	g	314	2440	1537	425	466	12	0	0

- Molecule 35 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	h	436	3450	2193	582	663	12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	438	LEU	-	expression tag	UNP P62495
h	439	GLU	-	expression tag	UNP P62495
h	440	HIS	-	expression tag	UNP P62495

- Molecule 36 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR GTP-BINDING SUBUNIT ERF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	i	426	3357	2135	577	624	21	0	0

- Molecule 37 is a RNA chain called CRICKET PARALYSIS VIRUS IRES RNA.

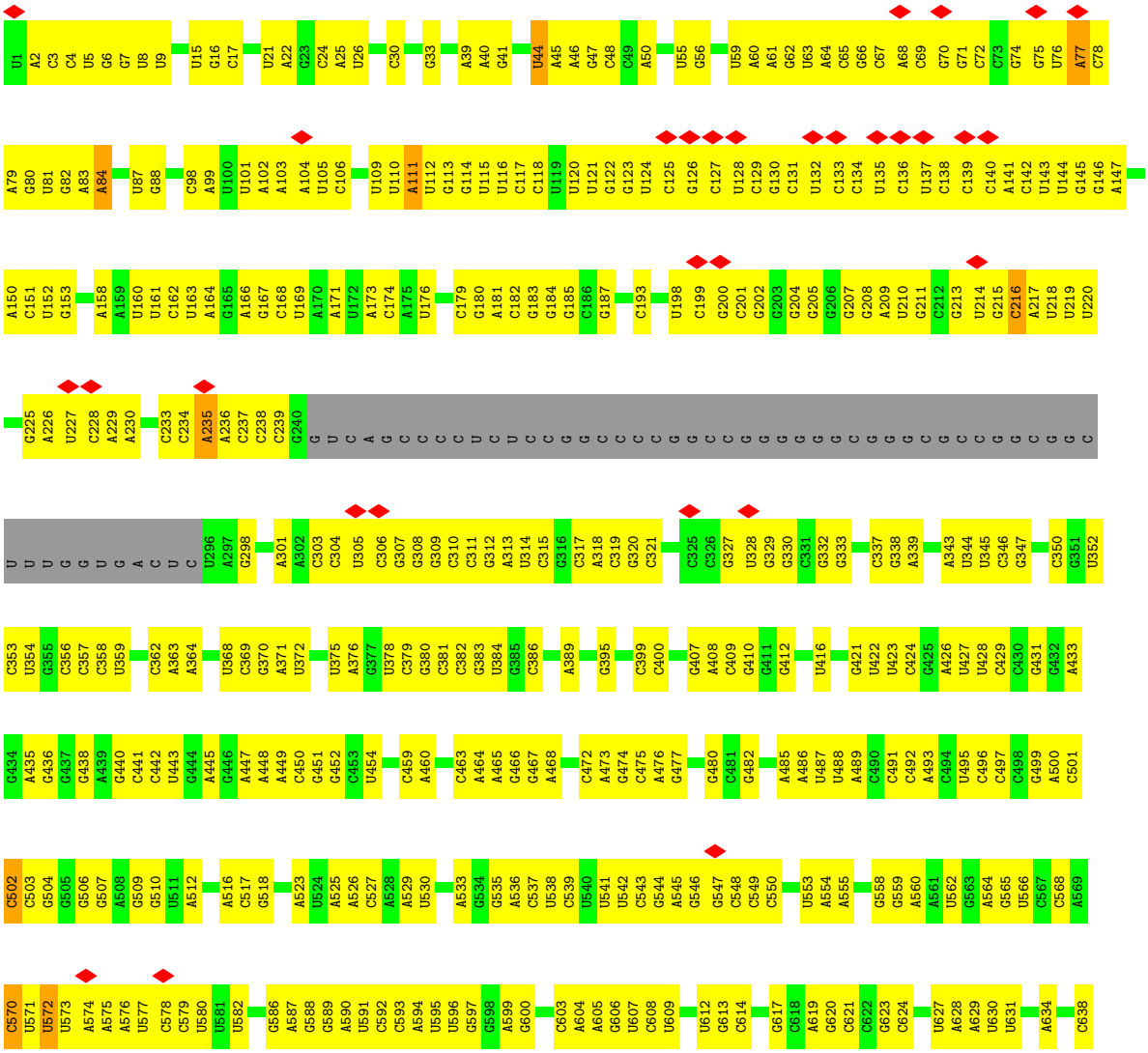
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	j	201	4257	1908	735	1413	201	0	0

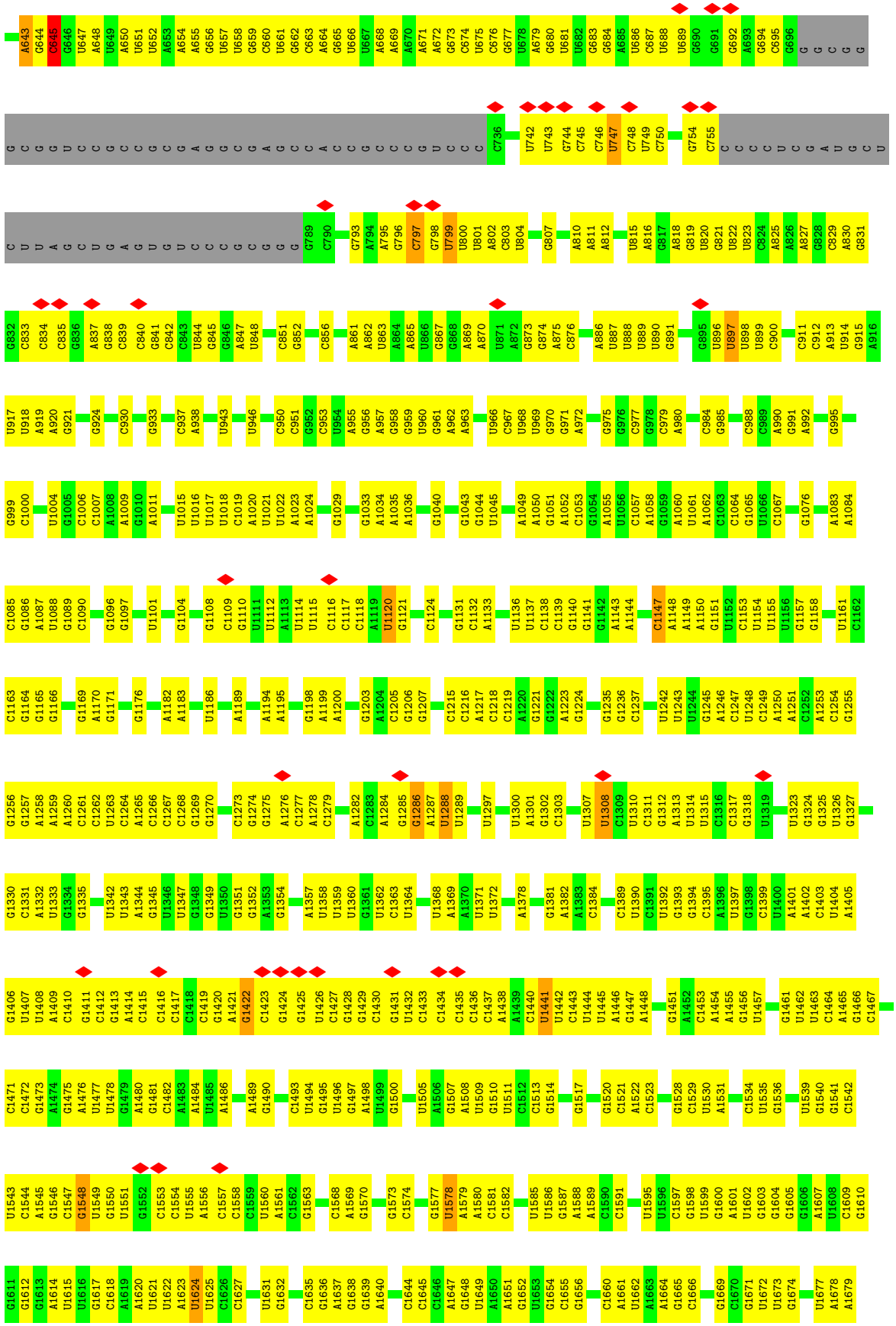
3 Residue-property plots (i)

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: 18S RRNA

Chain 1:

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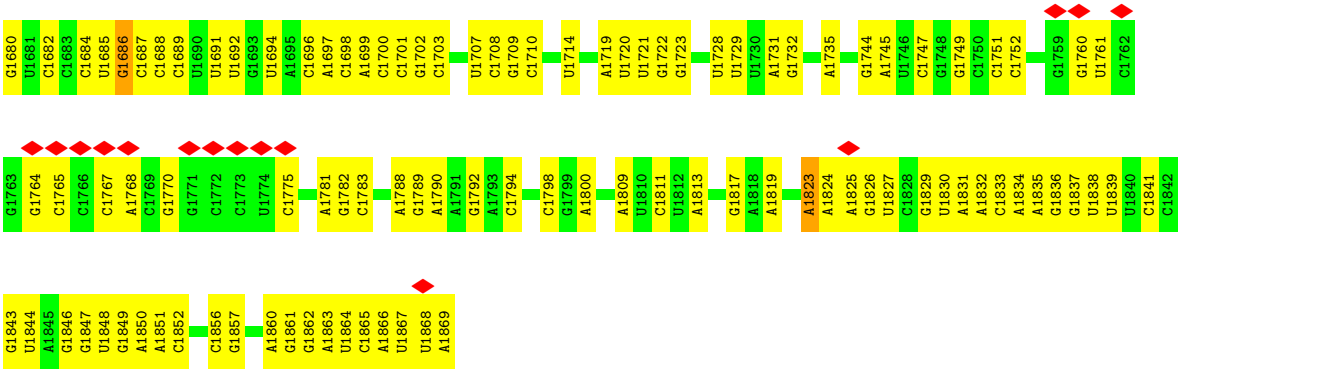
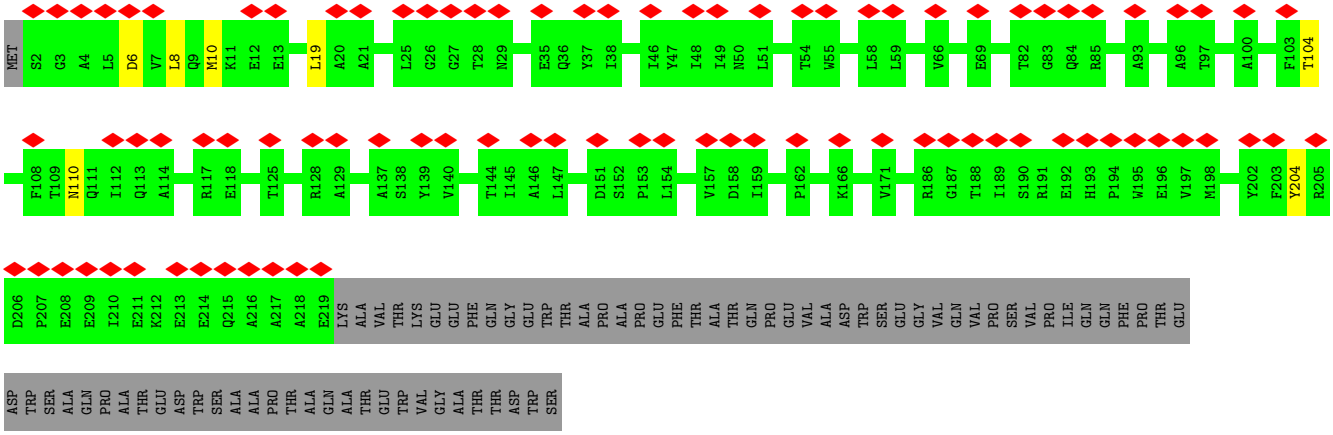
G C G G U C C G C C G C C G U C C C G A G G C C A C C C G U C C C U C G A U G C U
C U U A G C U G A G U G U C C G C G G C C G G C C C C C G U C C C C U C G A U G C U
G832 C833 C834 C835 G836 A837 G838 C839 C840 G841 C842 C843 U844 G845 G846 A847 U848 C851 G852 C856 A861 A862 U863 A864 A865 U866 G867 G868 A869 A870 U871 A872 G873 G874 A875 C876 A886 U887 U888 U889 U890 G891 G895 U896 U897 U898 U899 C900 C911 C912 A913 U914 G915 A916
U917 U918 A919 A920 G921 G924 C930 G933 C937 A938 U943 U946 C950 C951 G952 C953 U954 A955 G956 A957 G958 G959 U960 G961 A962 A963 U966 C967 U968 U969 G970 G971 A972 G975 G976 C977 G978 C979 A980 C984 G985 C988 C989 A990 G991 A992 G995
G999 C1000 U1004 G1005 C1006 C1007 A1008 A1009 G1010 A1011 U1015 U1016 U1017 U1018 C1019 A1020 U1021 U1022 A1023 A1024 G1029 G1033 A1034 A1035 A1036 G1040 G1043 G1044 U1045 A1049 A1050 G1051 A1052 C1053 G1054 A1055 U1056 C1057 A1058 G1059 A1060 U1061 A1062 C1063 C1064 G1065 U1066 C1067 G1076 A1083 A1084
C1085 G1086 A1087 U1088 G1089 C1090 G1096 G1097 U1101 G1104 G1108 C1109 G1110 U1111 U1112 A1113 U1114 U1115 C1116 C1117 C1118 A1119 U1120 G1121 C1124 G1131 C1132 A1133 U1136 U1137 C1138 C1139 G1140 G1141 G1142 A1143 A1144 C1147 A1148 A1149 A1150 G1151 U1152 C1153 U1154 U1155 U1156 G1157 G1158 U1161 C1162
C1163 G1164 G1165 G1166 G1169 A1170 G1171 G1176 A1182 A1183 U1186 A1189 A1194 A1195 G1198 A1199 A1200 G1203 A1204 C1205 G1206 G1207 C1215 C1216 A1217 C1218 C1219 A1220 G1221 G1222 A1223 G1224 G1235 G1236 C1237 U1242 U1243 U1244 G1245 A1246 C1247 U1248 C1249 A1250 A1251 C1252 A1253 C1254 G1255
G1256 G1257 A1258 A1259 A1260 C1261 C1262 U1263 C1264 A1265 C1266 C1267 C1268 G1269 G1270 C1273 G1274 G1275 A1276 C1277 A1278 C1279 A1282 C1283 A1284 C1285 G1286 A1287 U1288 U1289 U1297 U1300 A1301 G1302 C1303 U1307 U1308 C1309 U1310 C1311 G1312 A1313 U1314 U1315 C1316 C1317 G1318 U1319 U1323 G1324 G1325 U1326 G1327
G1330 C1331 A1332 U1333 G1334 G1335 U1342 U1343 A1344 G1345 U1346 U1347 G1348 G1349 U1350 G1351 G1352 A1353 G1354 A1357 U1358 U1359 U1360 G1361 U1362 C1363 U1364 U1368 A1369 A1370 U1371 U1372 A1378 G1381 A1382 A1383 C1384 C1389 U1390 C1391 U1392 G1393 G1394 C1395 A1396 U1397 G1398 C1399 U1400 A1401 A1402 C1403 C1404 A1405
G1406 U1407 U1408 A1409 C1410 G1411 C1412 G1413 A1414 C1415 C1416 C1417 C1418 G1419 G1420 A1421 G1422 C1423 G1424 G1425 U1426 C1427 G1428 G1429 C1430 G1431 U1432 C1433 C1434 C1435 C1436 C1437 A1438 A1439 C1440 U1441 U1442 C1443 U1444 U1445 A1446 G1447 A1448 G1451 A1452 C1453 A1454 A1455 G1456 U1457 G1461 U1462 U1463 C1464 A1465 G1466 C1467
C1471 C1472 G1473 A1474 G1475 A1476 U1477 U1478 G1479 A1480 G1481 C1482 A1483 A1484 U1485 A1486 A1489 G1490 C1493 U1494 G1495 U1496 G1497 A1498 U1499 G1500 U1505 A1506 G1507 A1508 U1509 G1510 U1511 C1512 C1513 G1514 G1517 G1520 C1521 A1522 C1523 G1528 C1529 U1530 A1531 C1534 U1535 G1536 U1539 G1540 G1541 C1542
U1543 C1544 A1545 G1546 C1547 G1548 U1549 G1550 U1551 G1552 C1553 C1554 U1555 A1556 C1557 C1558 C1559 U1560 A1561 C1562 G1563 C1568 A1569 G1570 G1573 C1574 G1577 U1578 A1579 A1580 C1581 C1582 U1585 U1586 G1587 A1588 A1589 C1590 C1591 U1595 U1596 C1597 G1598 U1599 G1600 A1601 U1602 G1603 G1604 G1605 G1606 A1607 U1608 C1609 G1610
G1611 G1612 G1613 A1614 U1615 U1616 G1617 C1618 A1619 A1620 U1621 U1622 A1623 U1624 U1625 C1626 C1627 U1631 G1632 C1635 G1636 A1637 G1638 G1639 A1640 C1644 C1645 C1646 A1647 G1648 U1649 A1650 A1651 G1652 U1653 G1654 C1655 G1656 C1660 A1661 U1662 A1663 A1664 G1665 C1666 G1669 C1670 G1671 U1672 U1673 G1674 U1677 A1678 A1679



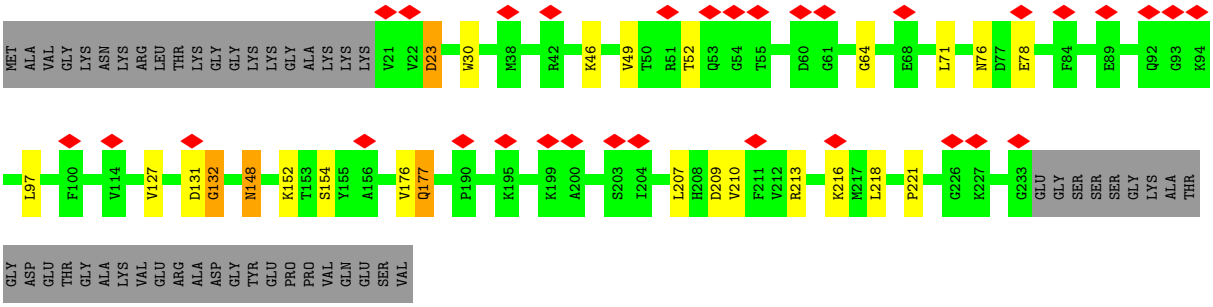
- Molecule 2: 40S RIBOSOMAL PROTEIN SA

Chain A:



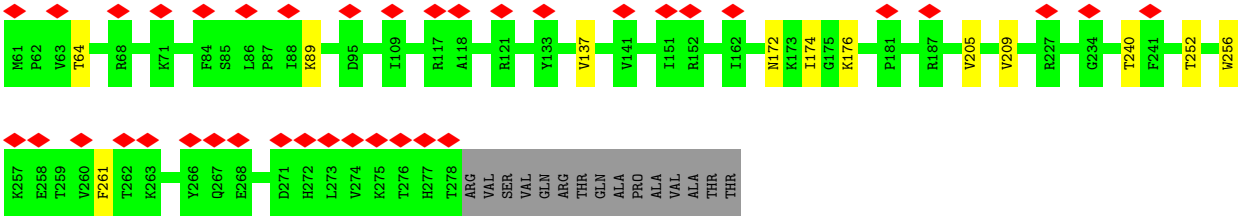
- Molecule 3: 40S RIBOSOMAL PROTEIN S3A

Chain B:



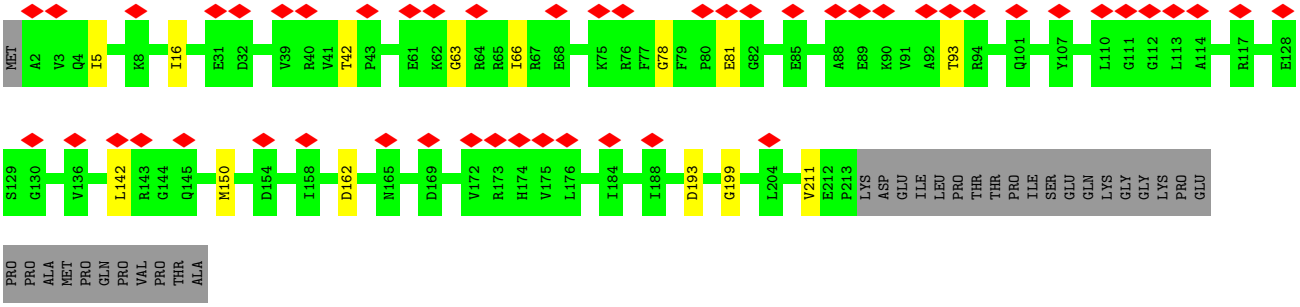
- Molecule 4: 40S RIBOSOMAL PROTEIN S2

Chain C:



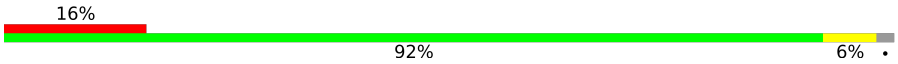
- Molecule 5: 40S RIBOSOMAL PROTEIN S3

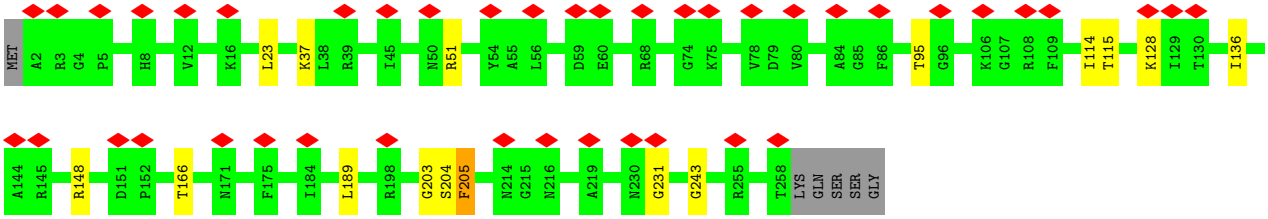
Chain D:



- Molecule 6: 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1

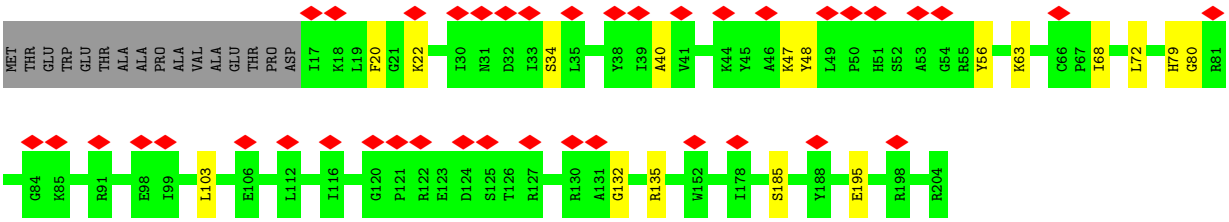
Chain E:





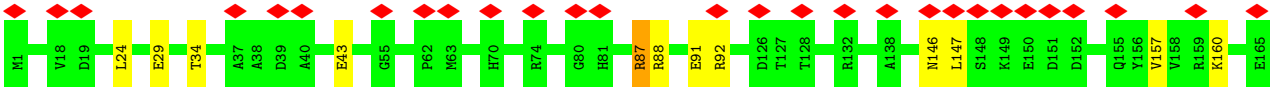
- Molecule 7: 40S RIBOSOMAL PROTEIN S5

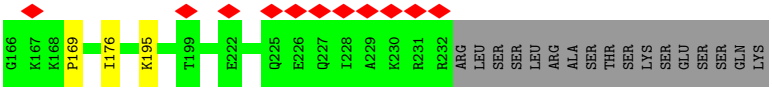
Chain F:



- Molecule 8: 40S RIBOSOMAL PROTEIN S6

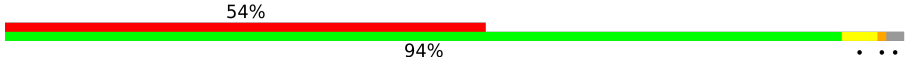
Chain G:

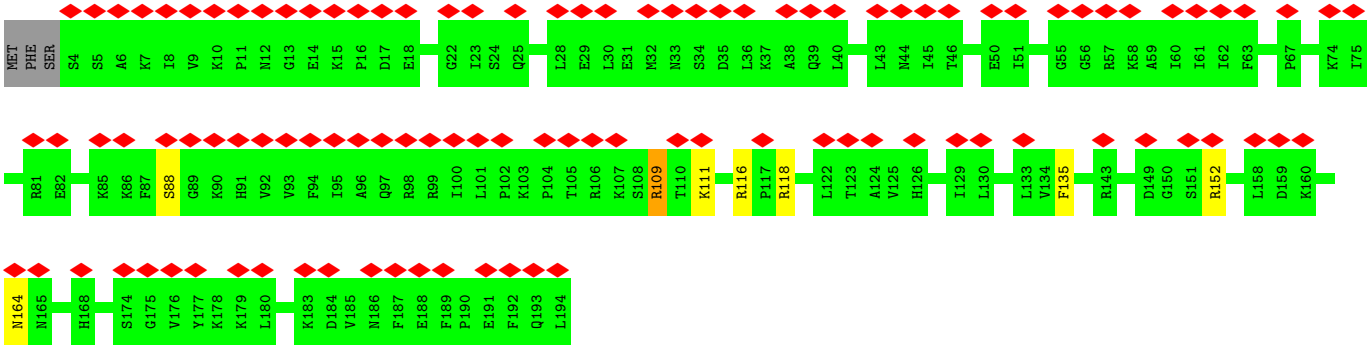




• Molecule 9: 40S RIBOSOMAL PROTEIN S7

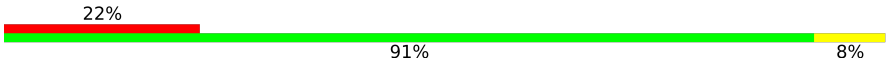
Chain H:

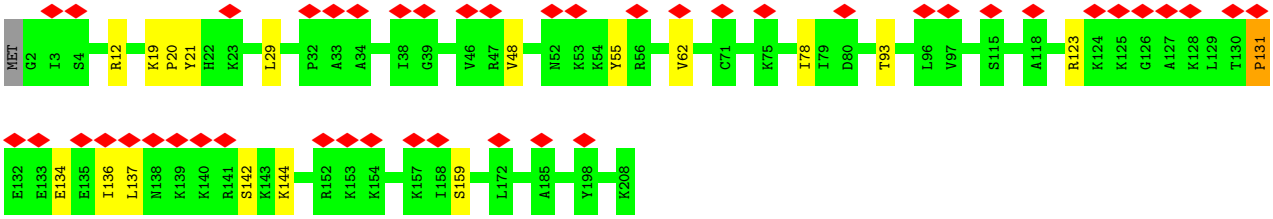




• Molecule 10: 40S RIBOSOMAL PROTEIN S8

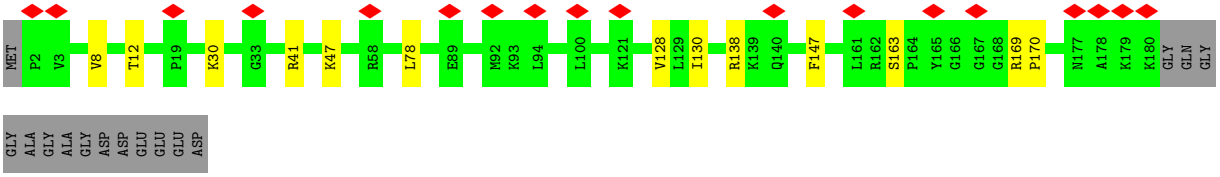
Chain I:





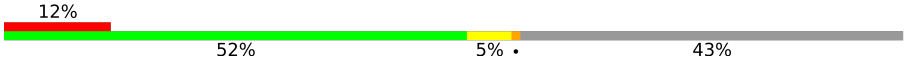
• Molecule 11: 40S RIBOSOMAL PROTEIN S9

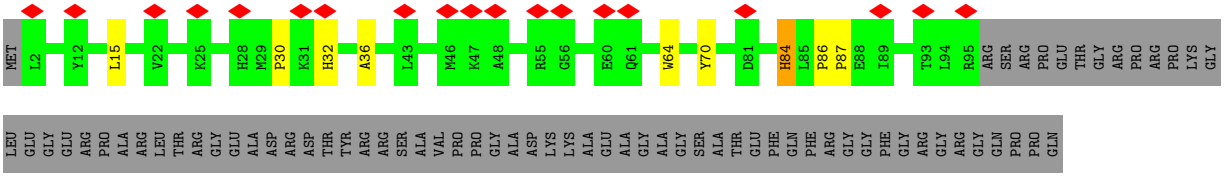
Chain J:



• Molecule 12: 40S RIBOSOMAL PROTEIN S10

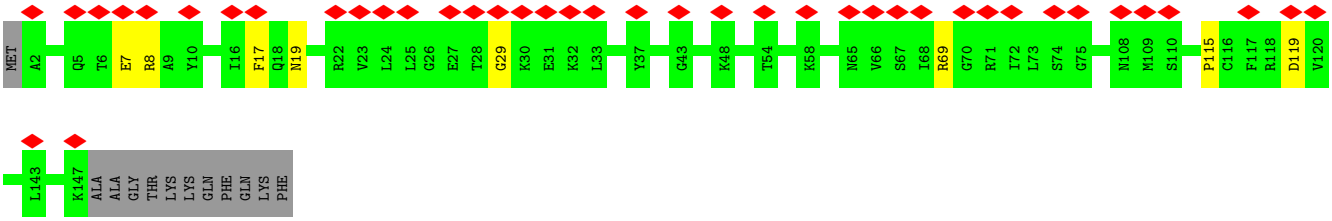
Chain K:





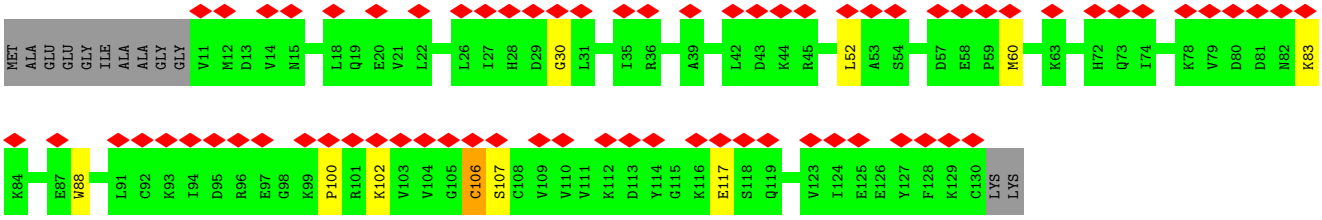
• Molecule 13: 40S RIBOSOMAL PROTEIN S11

Chain L:



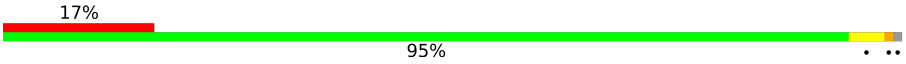
- Molecule 14: 40S RIBOSOMAL PROTEIN S12

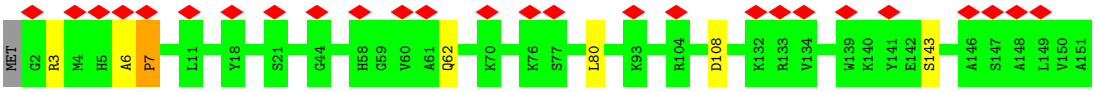
Chain M:



- Molecule 15: 40S RIBOSOMAL PROTEIN S13

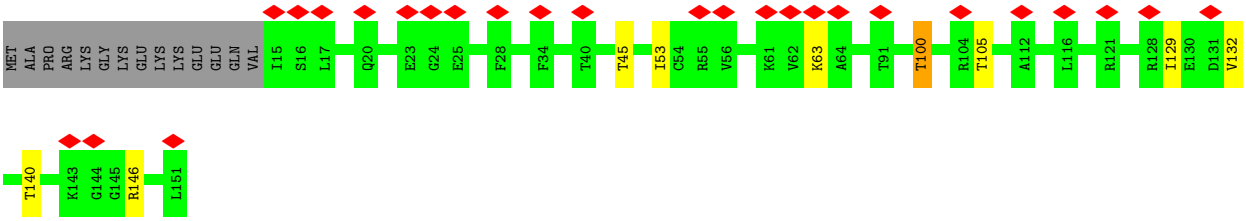
Chain N:





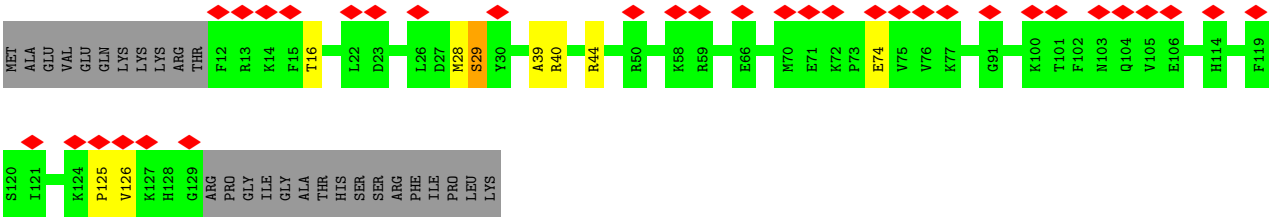
- Molecule 16: 40S RIBOSOMAL PROTEIN S14

Chain O:



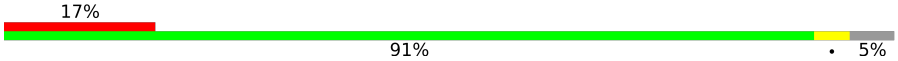
- Molecule 17: 40S RIBOSOMAL PROTEIN S15

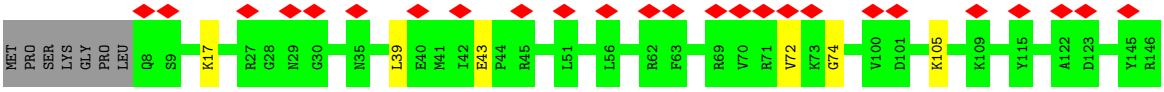
Chain P:



- Molecule 18: 40S RIBOSOMAL PROTEIN S16

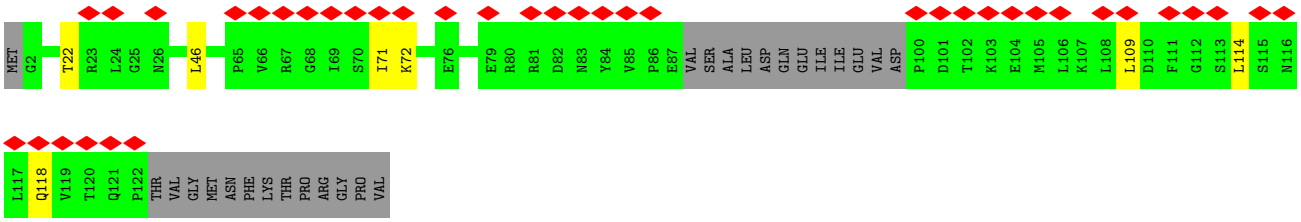
Chain Q:





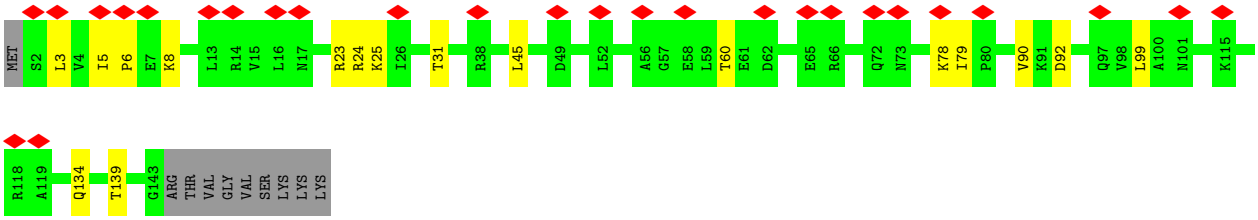
- Molecule 19: 40S RIBOSOMAL PROTEIN S17

Chain R:



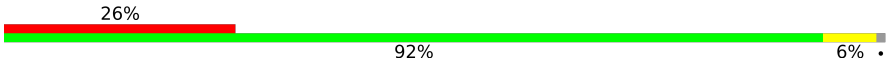
- Molecule 20: 40S RIBOSOMAL PROTEIN S18

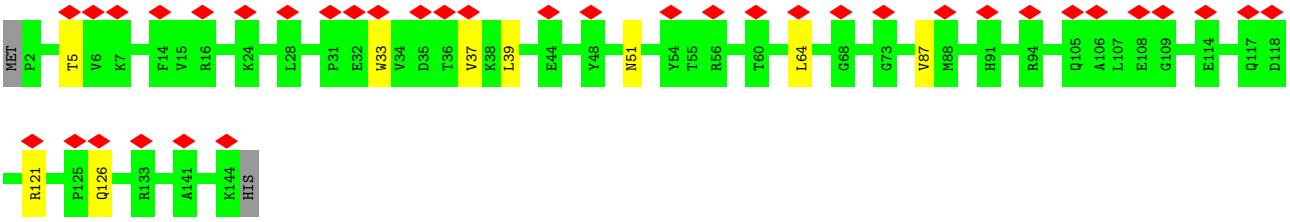
Chain S:



- Molecule 21: 40S RIBOSOMAL PROTEIN S19

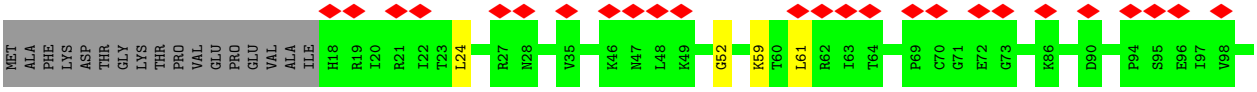
Chain T:

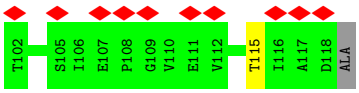




- Molecule 22: 40S RIBOSOMAL PROTEIN S20

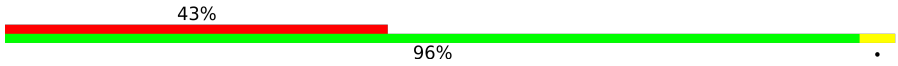
Chain U:

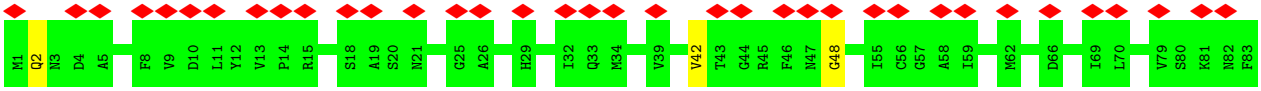




- Molecule 23: 40S RIBOSOMAL PROTEIN S21

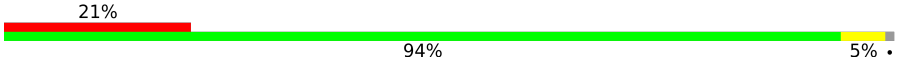
Chain V:

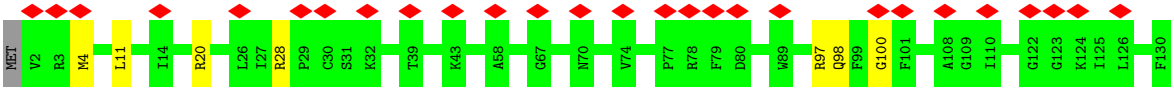




- Molecule 24: 40S RIBOSOMAL PROTEIN S15A

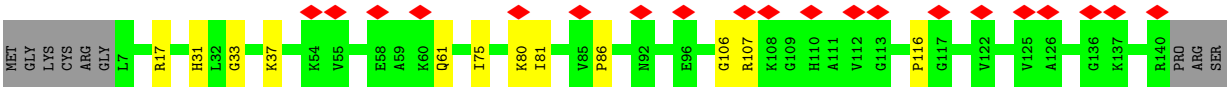
Chain W:





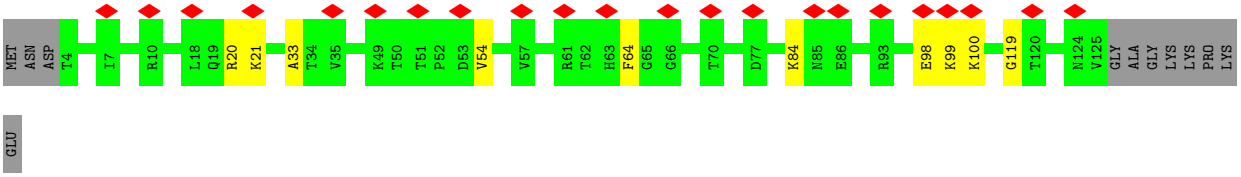
- Molecule 25: 40S RIBOSOMAL PROTEIN S23

Chain X:



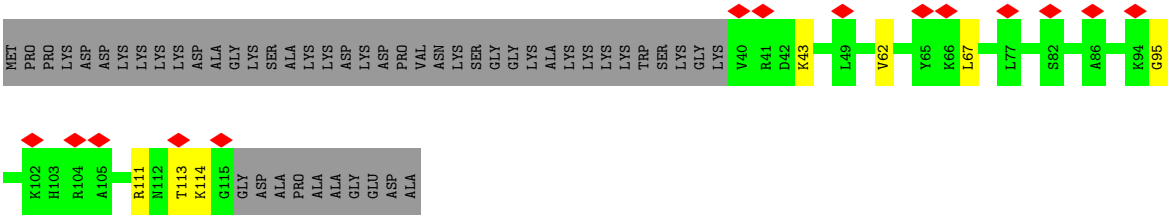
- Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain Y:



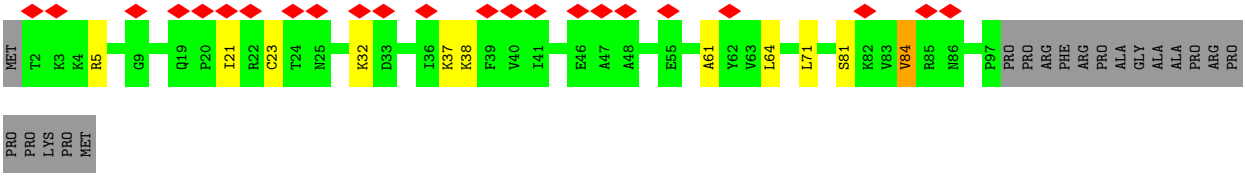
- Molecule 27: 40S RIBOSOMAL PROTEIN S25

Chain Z:



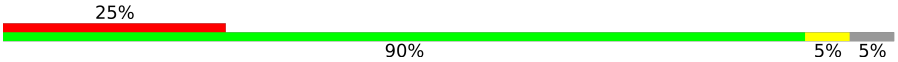
- Molecule 28: 40S RIBOSOMAL PROTEIN S26

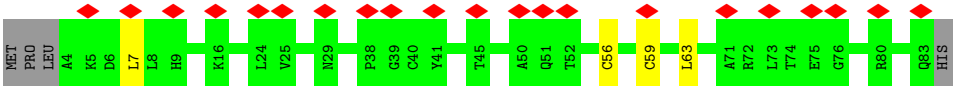
Chain a:



• Molecule 29: 40S RIBOSOMAL PROTEIN S27

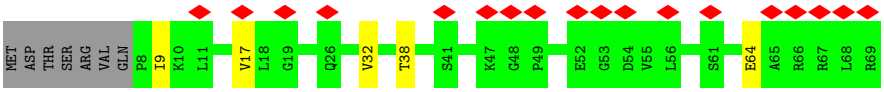
Chain b:





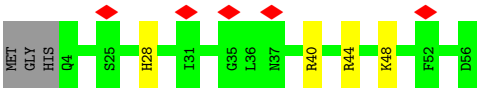
• Molecule 30: 40S RIBOSOMAL PROTEIN S28

Chain c:



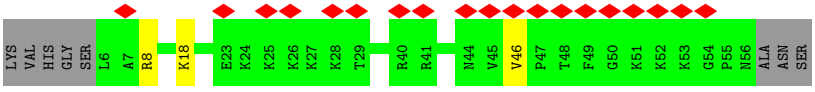
• Molecule 31: 40S RIBOSOMAL PROTEIN S29

Chain d:



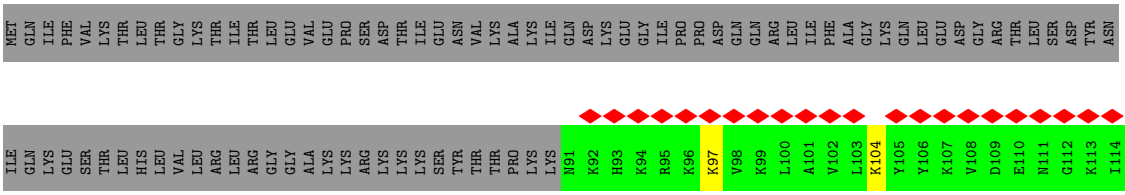
• Molecule 32: 40S RIBOSOMAL PROTEIN S30

Chain e:



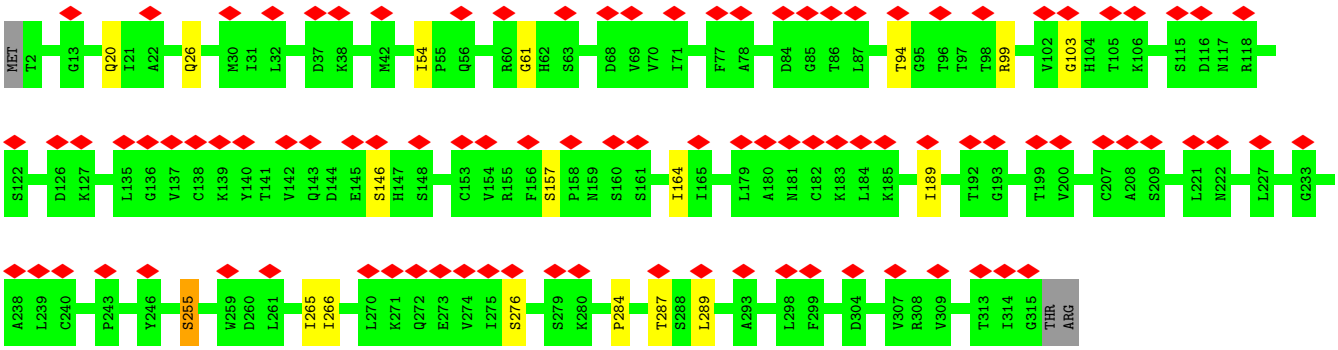
• Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A

Chain f:



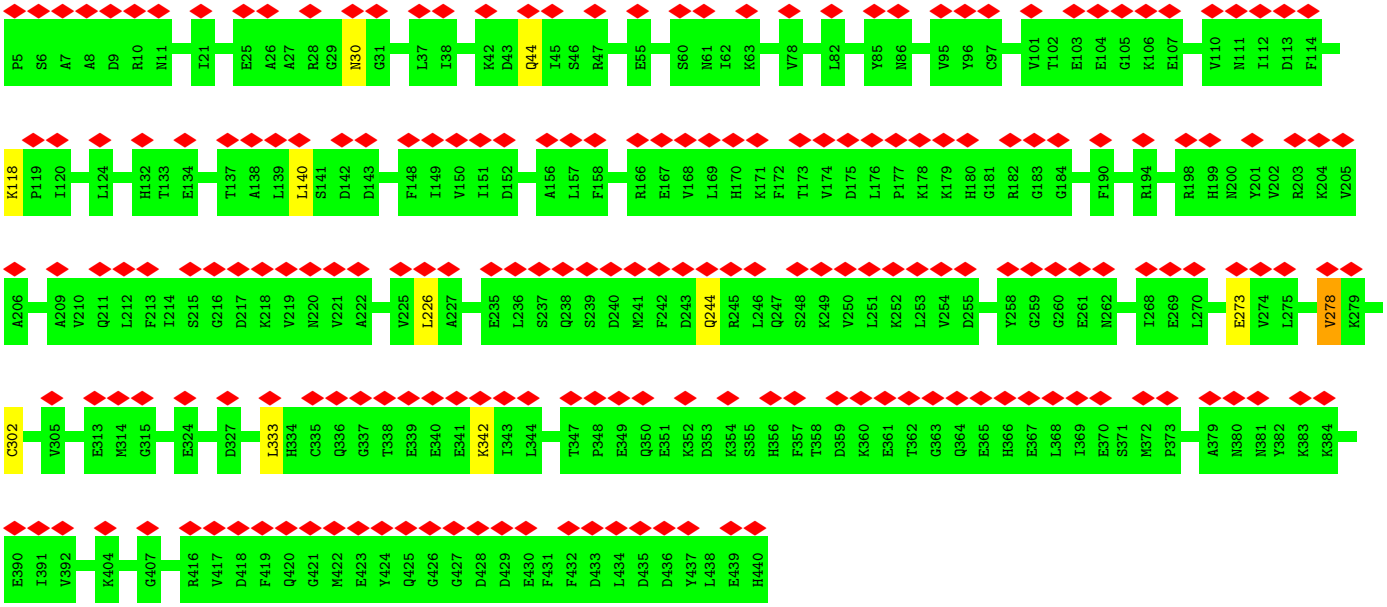
• Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1

Chain g: 30% 93% 5%



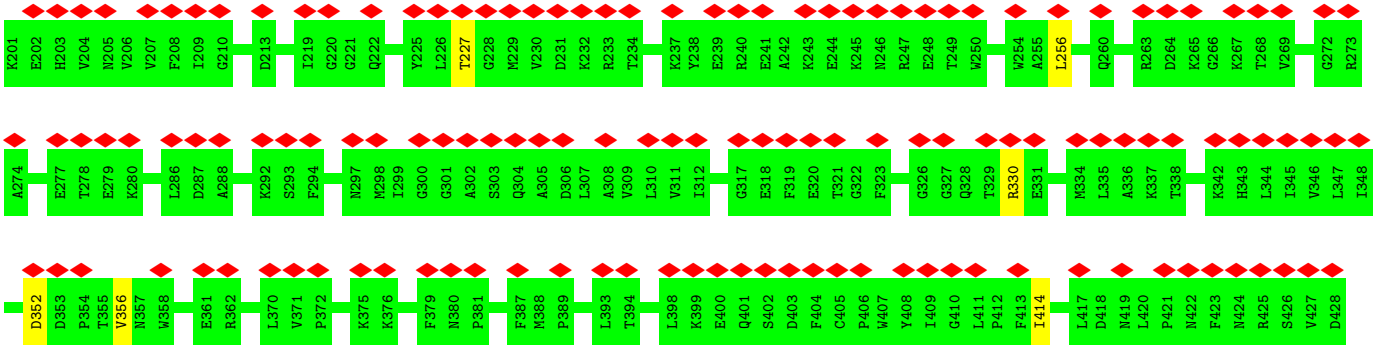
• Molecule 35: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1

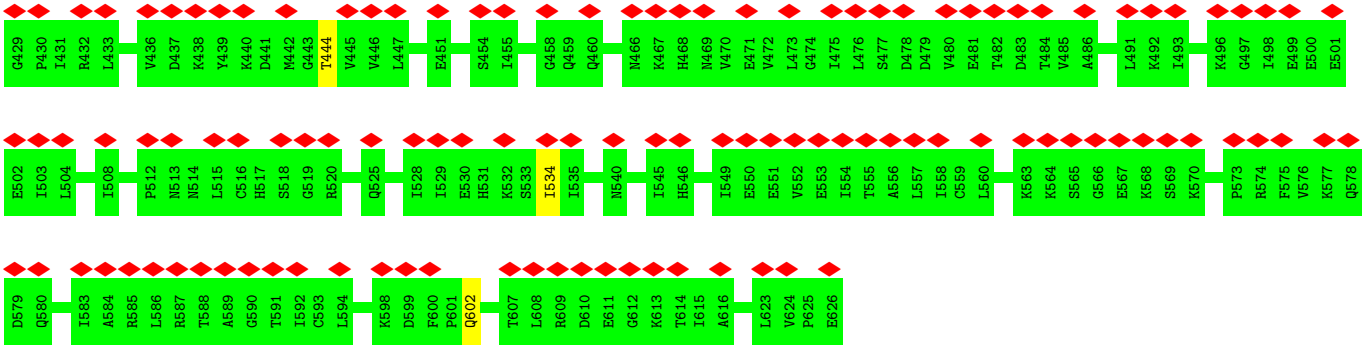
Chain h: 47% 97%



• Molecule 36: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR GTP-BINDING SUBUNIT ERF3A

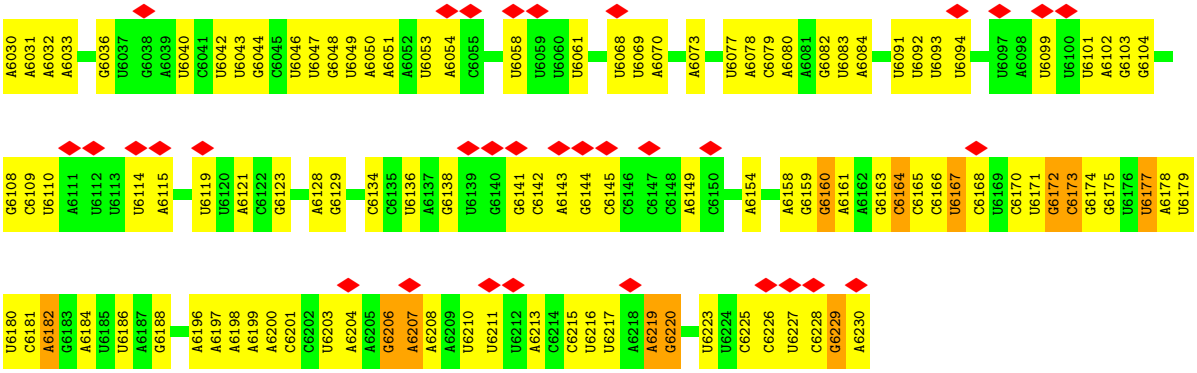
Chain i: 58% 98%





- Molecule 37: CRICKET PARALYSIS VIRUS IRES RNA

Chain j:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64902	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	194805	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	12.165	Depositor
Minimum map value	-4.363	Depositor
Average map value	0.164	Depositor
Map value standard deviation	0.954	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	467.99997, 467.99997, 467.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1	0.37	2/41550 (0.0%)	0.80	6/64763 (0.0%)
2	A	0.51	0/1756	0.68	0/2386
3	B	0.51	0/1756	0.75	1/2350 (0.0%)
4	C	0.42	0/1761	0.65	0/2379
5	D	0.41	0/1672	0.66	0/2250
6	E	0.47	0/2072	0.70	0/2793
7	F	0.43	0/1507	0.74	0/2026
8	G	0.48	0/1907	0.74	0/2538
9	H	0.46	0/1558	0.74	1/2087 (0.0%)
10	I	0.48	0/1724	0.72	0/2298
11	J	0.45	0/1520	0.77	0/2030
12	K	0.48	0/815	0.68	0/1101
13	L	0.45	0/1220	0.72	0/1633
14	M	0.48	0/941	0.72	0/1264
15	N	0.43	0/1231	0.73	1/1656 (0.1%)
16	O	0.46	0/1036	0.71	0/1391
17	P	0.43	0/1000	0.67	0/1335
18	Q	0.43	0/1125	0.66	0/1506
19	R	0.42	0/904	0.67	0/1208
20	S	0.42	0/1190	0.68	0/1594
21	T	0.44	0/1131	0.69	0/1515
22	U	0.50	0/813	0.70	0/1092
23	V	0.47	0/643	0.71	0/860
24	W	0.44	0/1050	0.69	0/1406
25	X	0.46	0/1063	0.70	0/1421
26	Y	0.45	0/1019	0.70	0/1354
27	Z	0.46	0/611	0.71	0/820
28	a	0.48	0/778	0.75	1/1041 (0.1%)
29	b	0.48	0/637	0.68	0/854
30	c	0.46	0/492	0.74	0/657
31	d	0.51	0/454	0.77	0/603
32	e	0.45	0/417	0.69	0/548
33	f	0.53	0/507	0.84	1/673 (0.1%)
34	g	0.45	0/2497	0.67	0/3399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	h	0.35	0/3506	0.56	0/4709
36	i	0.37	0/3418	0.55	0/4600
37	j	1.42	85/4752 (1.8%)	1.74	207/7383 (2.8%)
All	All	0.52	87/92033 (0.1%)	0.83	218/133523 (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
1	1	0	24
37	j	0	1
All	All	0	25

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	j	6173	C	O3'-P	-20.14	1.36	1.61
37	j	6229	G	O3'-P	19.64	1.84	1.61
37	j	6079	C	N3-C4	19.19	1.47	1.33
37	j	6177	U	O3'-P	-18.39	1.39	1.61
37	j	6219	A	O3'-P	-15.97	1.42	1.61

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	6079	C	C5-C6-N1	19.25	130.62	121.00
37	j	6114	U	C4-C5-C6	-18.58	108.55	119.70
37	j	6114	U	N3-C4-C5	17.39	125.03	114.60
37	j	6077	U	C2-N3-C4	-15.00	118.00	127.00
37	j	6161	A	N1-C2-N3	-15.00	121.80	129.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	111	A	Sidechain
1	1	44	U	Sidechain
1	1	77	A	Sidechain
1	1	84	A	Sidechain

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Mol	Chain	Res	Type	Group
1	1	88	G	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	216/295 (73%)	209 (97%)	5 (2%)	2 (1%)	17	57
3	B	211/264 (80%)	176 (83%)	18 (8%)	17 (8%)	1	12
4	C	220/293 (75%)	213 (97%)	2 (1%)	5 (2%)	6	34
5	D	210/243 (86%)	201 (96%)	4 (2%)	5 (2%)	6	33
6	E	255/263 (97%)	237 (93%)	13 (5%)	5 (2%)	7	38
7	F	186/204 (91%)	163 (88%)	13 (7%)	10 (5%)	2	19
8	G	230/249 (92%)	216 (94%)	5 (2%)	9 (4%)	3	23
9	H	189/194 (97%)	178 (94%)	7 (4%)	4 (2%)	7	36
10	I	205/208 (99%)	184 (90%)	14 (7%)	7 (3%)	3	26
11	J	177/194 (91%)	168 (95%)	6 (3%)	3 (2%)	9	42
12	K	92/165 (56%)	84 (91%)	1 (1%)	7 (8%)	1	13
13	L	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	3	22
14	M	118/132 (89%)	111 (94%)	1 (1%)	6 (5%)	2	19
15	N	148/151 (98%)	138 (93%)	5 (3%)	5 (3%)	3	26
16	O	135/151 (89%)	129 (96%)	3 (2%)	3 (2%)	6	35
17	P	116/145 (80%)	106 (91%)	5 (4%)	5 (4%)	2	22
18	Q	137/146 (94%)	129 (94%)	6 (4%)	2 (2%)	10	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	R	105/135 (78%)	99 (94%)	4 (4%)	2 (2%)	8	38
20	S	140/152 (92%)	125 (89%)	7 (5%)	8 (6%)	1	18
21	T	141/145 (97%)	135 (96%)	4 (3%)	2 (1%)	11	46
22	U	99/119 (83%)	95 (96%)	3 (3%)	1 (1%)	15	55
23	V	81/83 (98%)	78 (96%)	1 (1%)	2 (2%)	5	32
24	W	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	9	44
25	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2	19
26	Y	120/133 (90%)	114 (95%)	2 (2%)	4 (3%)	4	26
27	Z	74/125 (59%)	71 (96%)	0	3 (4%)	3	23
28	a	94/115 (82%)	85 (90%)	5 (5%)	4 (4%)	2	22
29	b	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
30	c	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	4	26
31	d	51/56 (91%)	44 (86%)	7 (14%)	0	100	100
32	e	49/59 (83%)	43 (88%)	5 (10%)	1 (2%)	7	38
33	f	59/156 (38%)	53 (90%)	6 (10%)	0	100	100
34	g	312/317 (98%)	291 (93%)	14 (4%)	7 (2%)	6	35
35	h	428/436 (98%)	410 (96%)	14 (3%)	4 (1%)	17	57
36	i	414/426 (97%)	403 (97%)	9 (2%)	2 (0%)	29	69
All	All	5553/6338 (88%)	5186 (93%)	215 (4%)	152 (3%)	8	31

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	76	ASN
3	B	132	GLY
3	B	148	ASN
3	B	154	SER
3	B	176	VAL

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	A	181/243 (74%)	176 (97%)	5 (3%)	43	65
3	B	194/231 (84%)	183 (94%)	11 (6%)	20	45
4	C	188/225 (84%)	181 (96%)	7 (4%)	34	58
5	D	175/202 (87%)	166 (95%)	9 (5%)	24	48
6	E	220/225 (98%)	208 (94%)	12 (6%)	21	47
7	F	158/170 (93%)	151 (96%)	7 (4%)	28	53
8	G	202/218 (93%)	195 (96%)	7 (4%)	36	59
9	H	171/174 (98%)	167 (98%)	4 (2%)	50	70
10	I	179/180 (99%)	167 (93%)	12 (7%)	16	41
11	J	160/168 (95%)	150 (94%)	10 (6%)	18	43
12	K	85/136 (62%)	82 (96%)	3 (4%)	36	59
13	L	133/142 (94%)	131 (98%)	2 (2%)	65	80
14	M	102/108 (94%)	97 (95%)	5 (5%)	25	50
15	N	130/131 (99%)	128 (98%)	2 (2%)	65	80
16	O	107/119 (90%)	100 (94%)	7 (6%)	17	42
17	P	107/130 (82%)	102 (95%)	5 (5%)	26	51
18	Q	115/121 (95%)	111 (96%)	4 (4%)	36	59
19	R	99/122 (81%)	94 (95%)	5 (5%)	24	48
20	S	123/132 (93%)	114 (93%)	9 (7%)	14	39
21	T	113/115 (98%)	106 (94%)	7 (6%)	18	43
22	U	93/107 (87%)	89 (96%)	4 (4%)	29	53
23	V	67/67 (100%)	66 (98%)	1 (2%)	65	80
24	W	112/113 (99%)	107 (96%)	5 (4%)	27	52
25	X	108/115 (94%)	103 (95%)	5 (5%)	27	52
26	Y	107/115 (93%)	101 (94%)	6 (6%)	21	46
27	Z	67/103 (65%)	63 (94%)	4 (6%)	19	44
28	a	83/98 (85%)	76 (92%)	7 (8%)	11	33
29	b	72/76 (95%)	68 (94%)	4 (6%)	21	46
30	c	55/62 (89%)	52 (94%)	3 (6%)	21	47
31	d	47/49 (96%)	43 (92%)	4 (8%)	10	33
32	e	42/48 (88%)	40 (95%)	2 (5%)	25	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	f	54/140 (39%)	51 (94%)	3 (6%)	21	46
34	g	272/275 (99%)	260 (96%)	12 (4%)	28	53
35	h	376/376 (100%)	368 (98%)	8 (2%)	53	72
36	i	371/371 (100%)	364 (98%)	7 (2%)	57	75
All	All	4868/5407 (90%)	4660 (96%)	208 (4%)	33	53

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	109	LEU
25	X	17	ARG
35	h	333	LEU
20	S	8	LYS
21	T	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
21	T	63	HIS
28	a	19	GLN
36	i	578	GLN
22	U	100	GLN
25	X	73	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1738/1869 (92%)	1037 (59%)	152 (8%)
37	j	195/201 (97%)	50 (25%)	0
All	All	1933/2070 (93%)	1087 (56%)	152 (7%)

5 of 1087 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	3	C
1	1	4	C
1	1	5	U
1	1	6	G

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1494	U
1	1	1824	A
1	1	1534	C
1	1	1637	A
1	1	1862	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	j	10
36	i	5
35	h	3

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	j	6150:C	O3'	6151:A	P	11.37
1	j	6065:A	O3'	6066:G	P	10.23
1	j	6106:U	O3'	6107:A	P	9.31
1	j	6136:U	O3'	6137:A	P	8.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	325:LYS	C	326:GLY	N	5.91

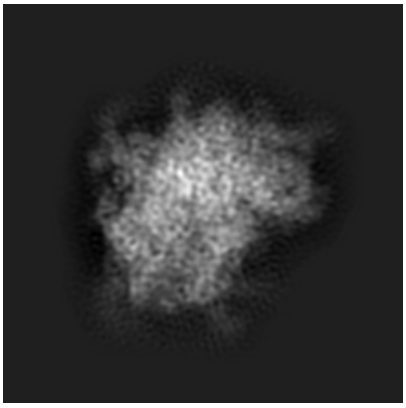
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2813. These allow visual inspection of the internal detail of the map and identification of artifacts.

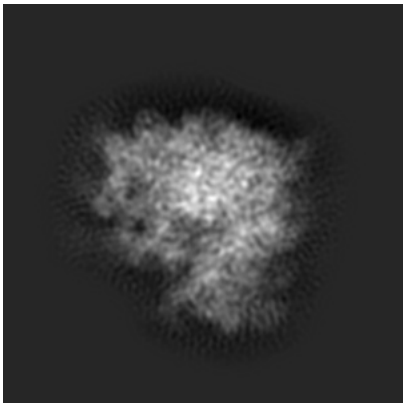
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

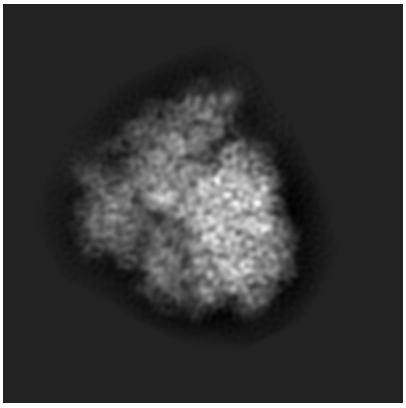
6.1.1 Primary map



X



Y

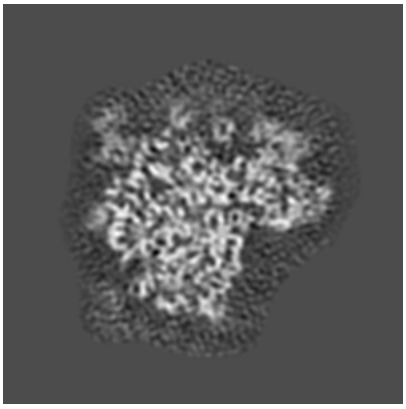


Z

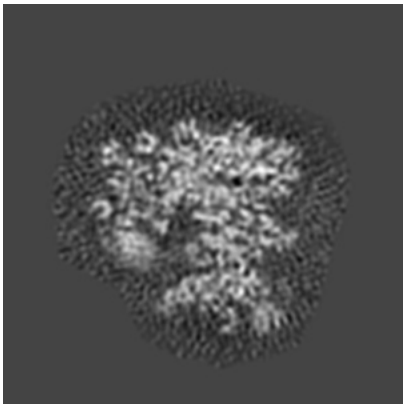
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

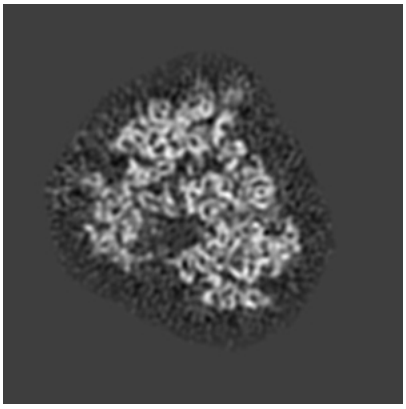
6.2.1 Primary map



X Index: 150



Y Index: 150

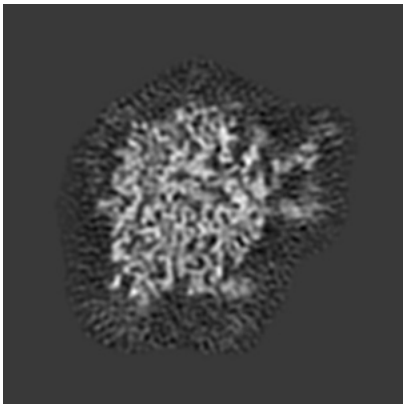


Z Index: 150

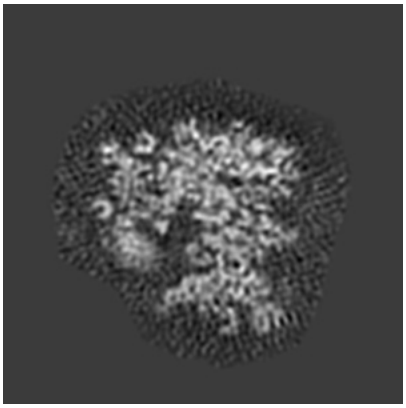
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

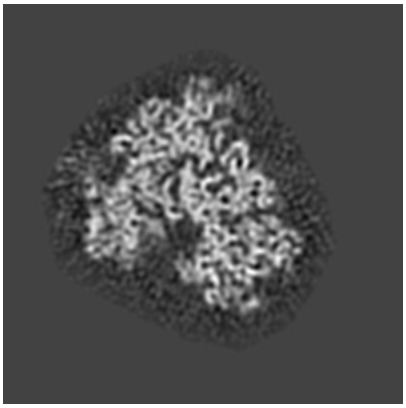
6.3.1 Primary map



X Index: 172



Y Index: 149



Z Index: 154

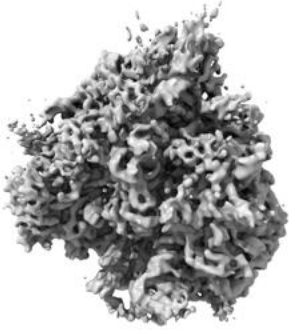
The images above show the largest variance slices of the map in three orthogonal directions.

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

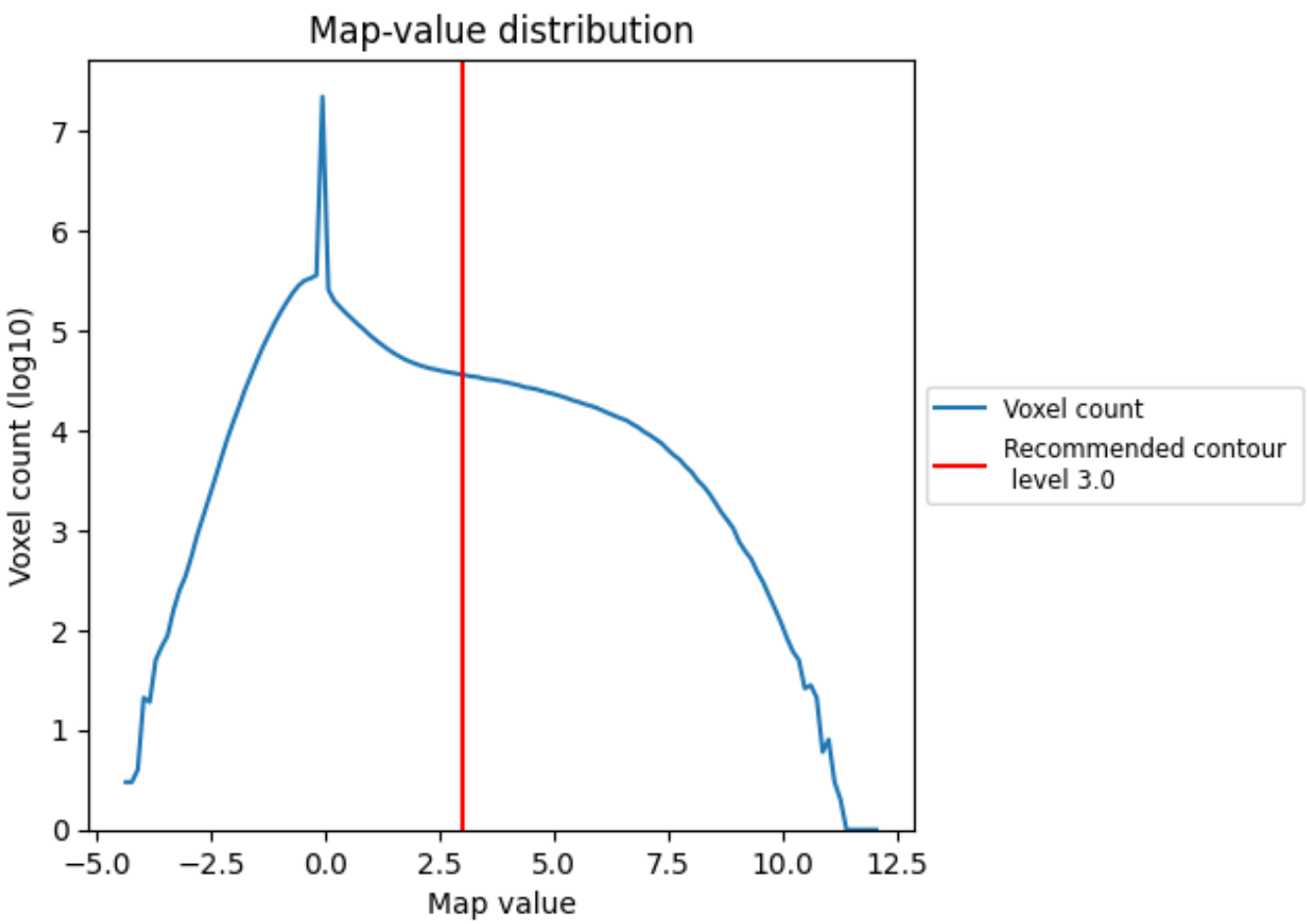
6.5 Mask visualisation (i)

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

7 Map analysis (i)

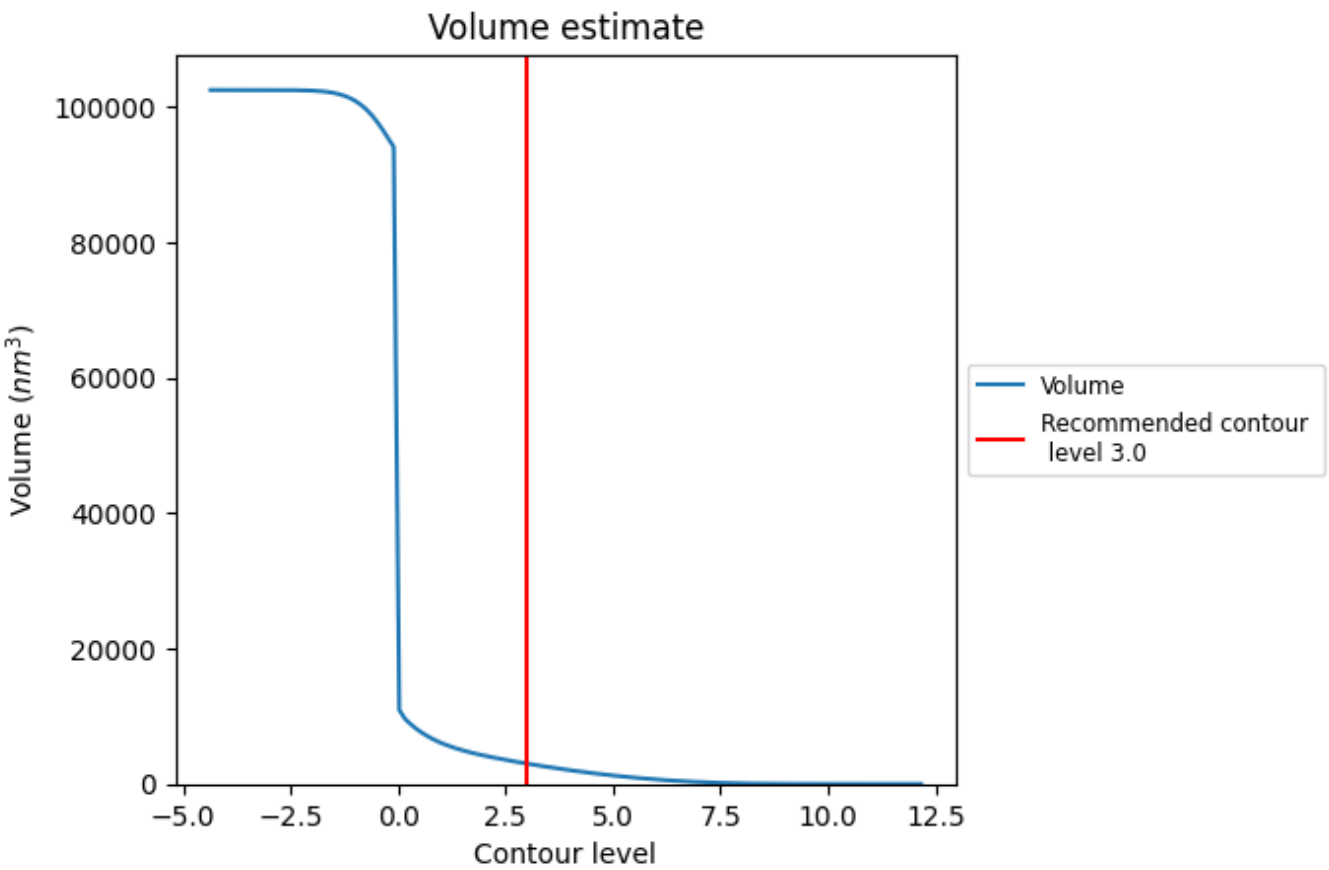
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

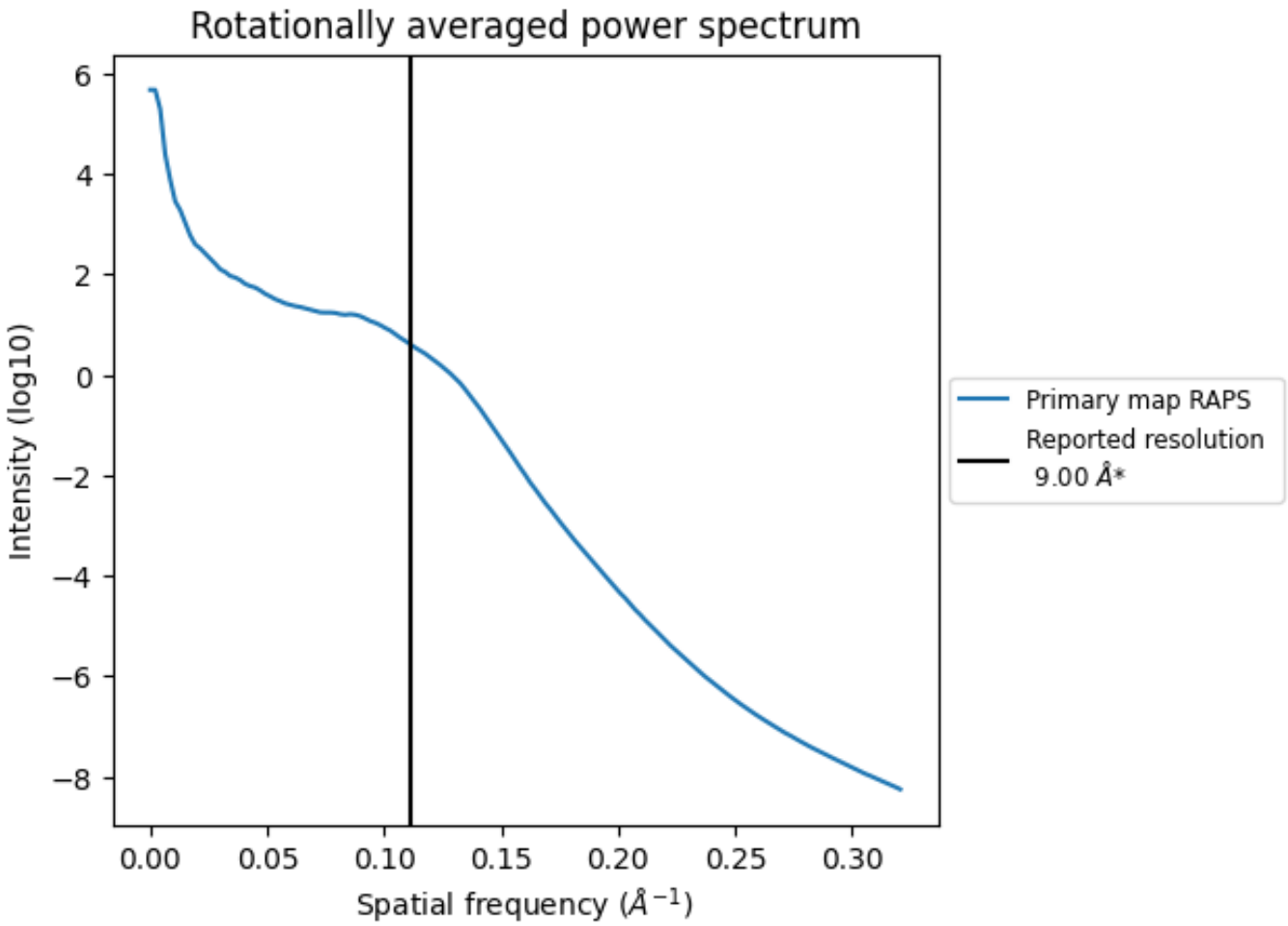
7.2 Volume estimate (i)



The volume at the recommended contour level is 3001 nm^3; this corresponds to an approximate mass of 2711 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 0.111 Å^{-1}

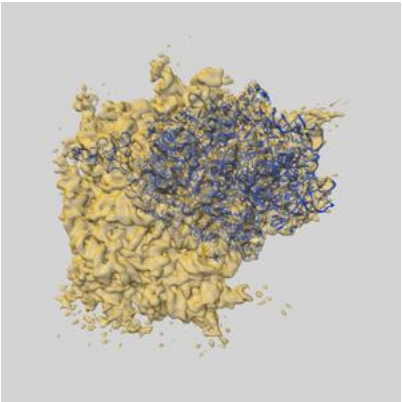
8 Fourier-Shell correlation (i)

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

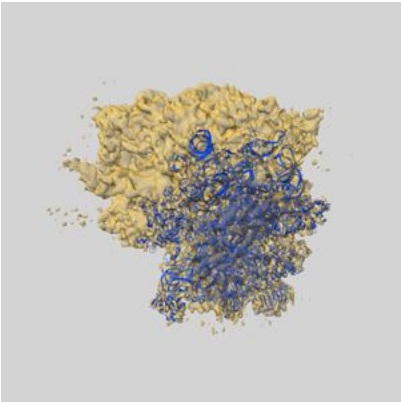
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2813 and PDB model 4D61. Per-residue inclusion information can be found in section 3 on page 11.

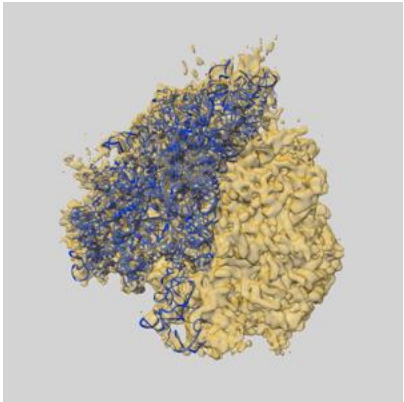
9.1 Map-model overlay (i)



X



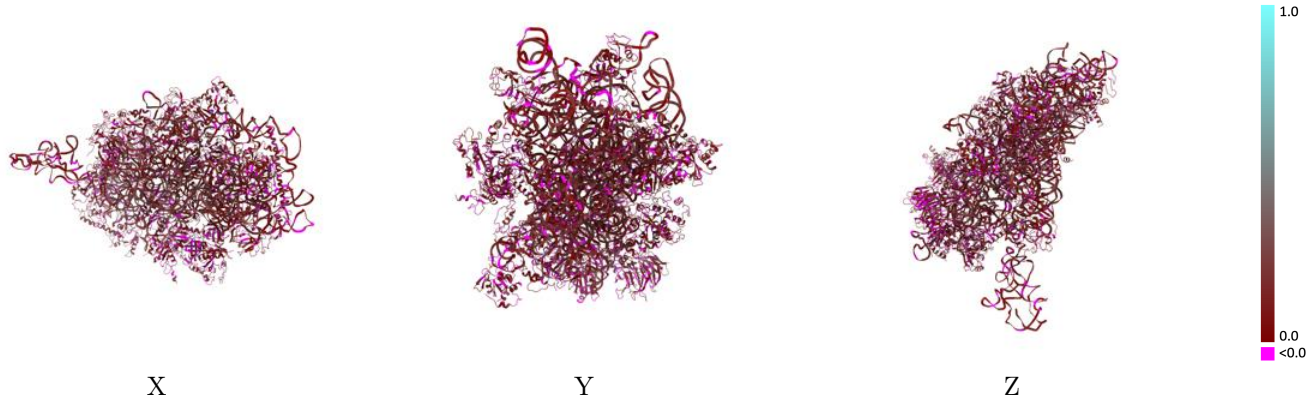
Y



Z

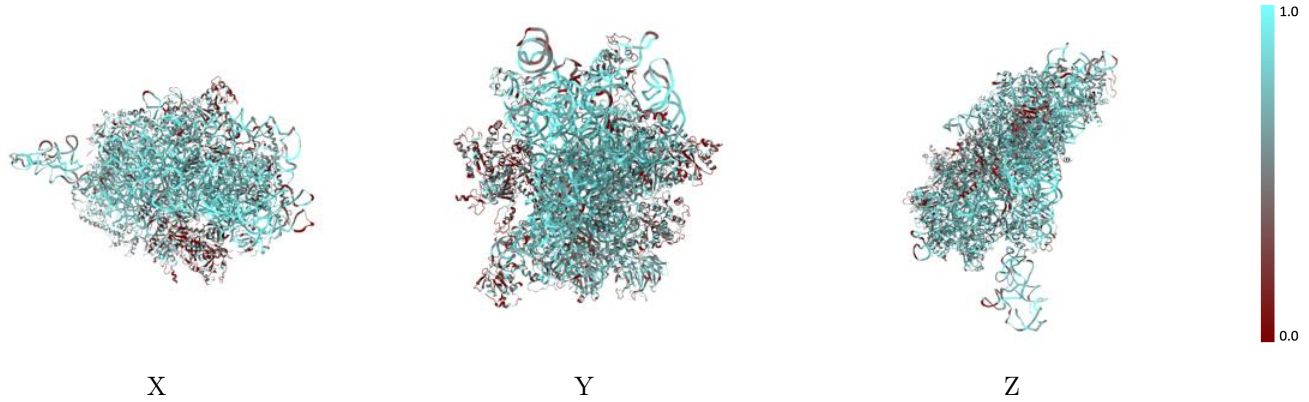
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



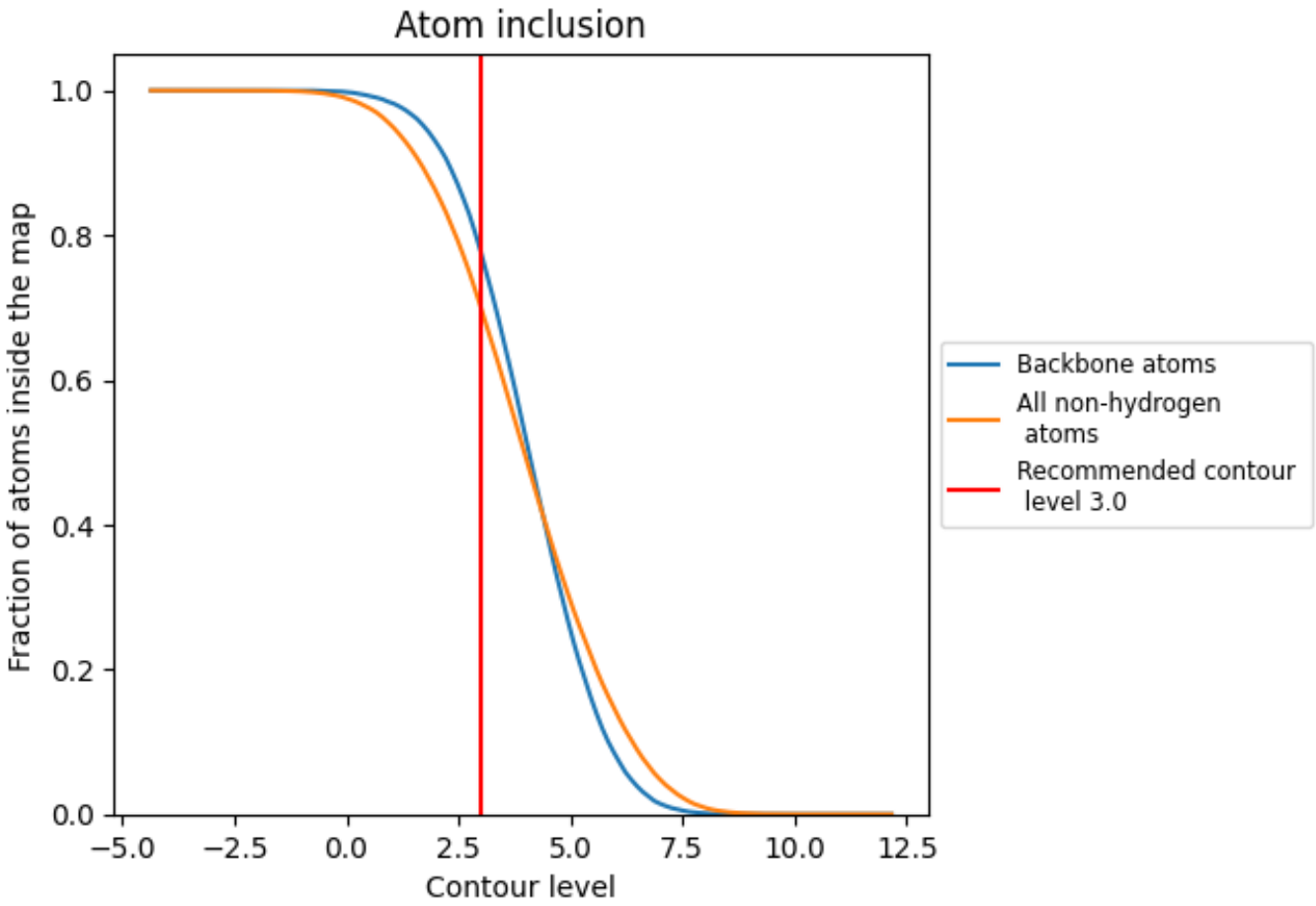
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (i)



At the recommended contour level, 78% of all backbone atoms, 70% 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	0.7002	0.1270
1	0.8652	0.1580
A	0.4654	0.1120
B	0.6698	0.1340
C	0.6099	0.1280
D	0.5852	0.1170
E	0.6687	0.1090
F	0.6284	0.0970
G	0.6601	0.0980
H	0.3619	0.1000
I	0.6253	0.0930
J	0.6794	0.1080
K	0.6365	0.0860
L	0.6040	0.1150
M	0.3293	0.0670
N	0.6080	0.1130
O	0.6439	0.1060
P	0.5920	0.0850
Q	0.6791	0.0870
R	0.4925	0.0900
S	0.6546	0.1070
T	0.6322	0.0850
U	0.5371	0.0690
V	0.4855	0.1050
W	0.6244	0.1050
X	0.6256	0.1140
Y	0.6204	0.1000
Z	0.6559	0.1180
a	0.6206	0.0910
b	0.6020	0.1140
c	0.5681	0.1030
d	0.7160	0.0630
e	0.5214	0.1160
f	0.3706	0.0750
g	0.5858	0.0860

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Chain	Atom inclusion	Q-score
h	0.4202	0.0970
i	0.3540	0.0920
j	0.6869	0.1270