Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:02 pm GMT

PDB ID	:	5O9Z
EMDB ID	:	EMD-3766
Title	:	Cryo-EM structure of a pre-catalytic human spliceosome primed for activation (B complex)
Authors	:	Bertram, K.; Kastner, B.
Deposited on	:	2017-06-20
Resolution	:	4.50 Å(reported)

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

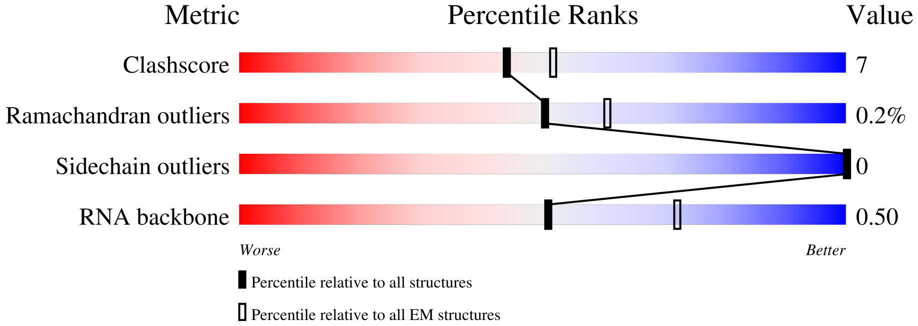
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

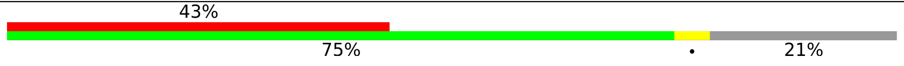
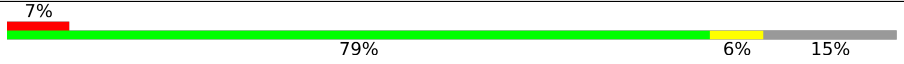
The reported resolution of this entry is 4.50 Å.

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.



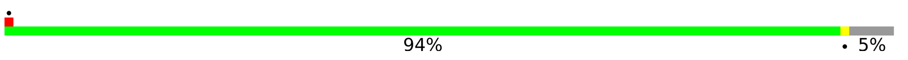
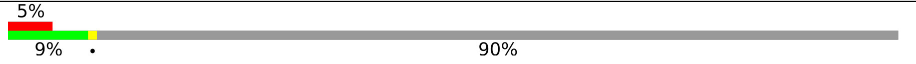
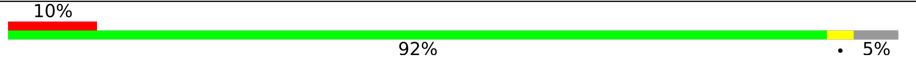
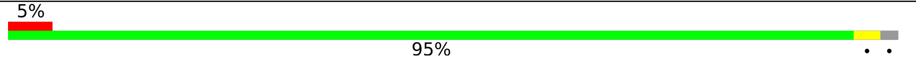
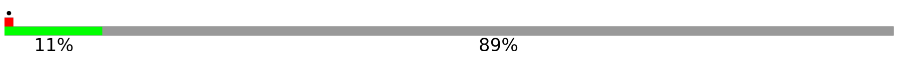
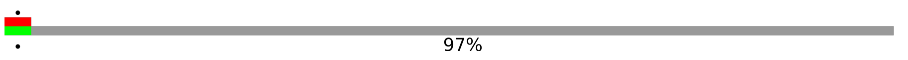
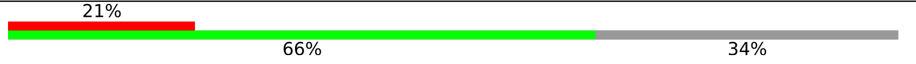
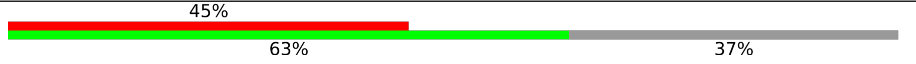
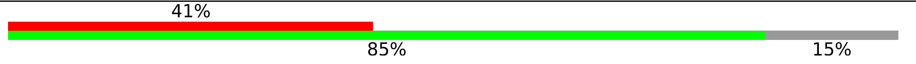
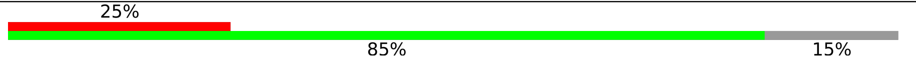
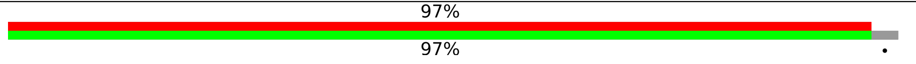
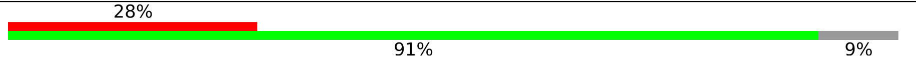
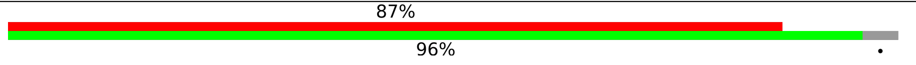
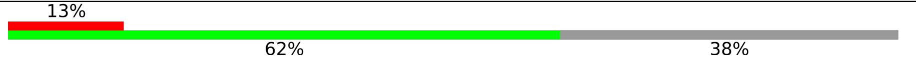
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	2335	
2	B	972	
3	C	2136	
4	D	357	
5	E	683	
6	F	521	
7	G	941	

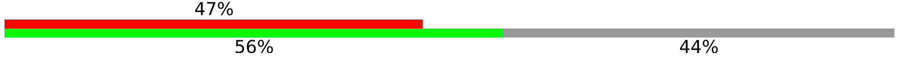
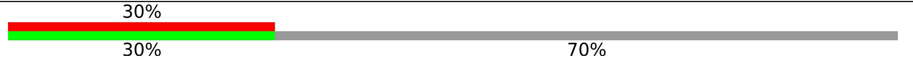
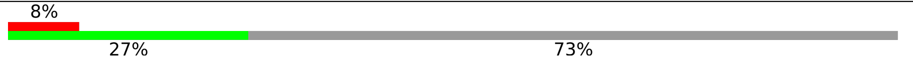
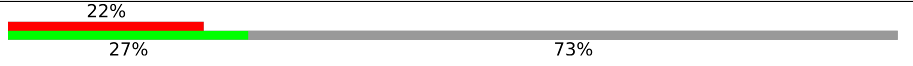
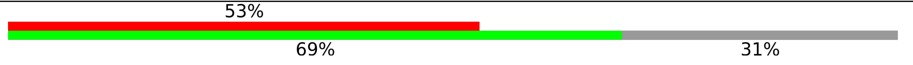
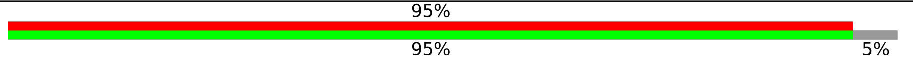
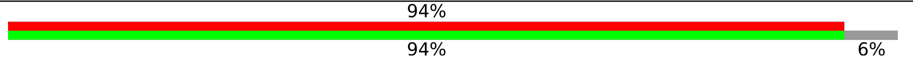
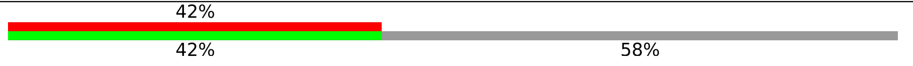
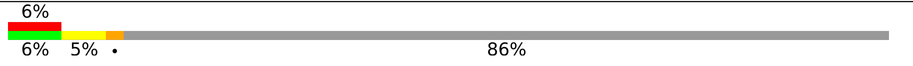
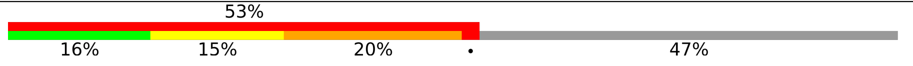
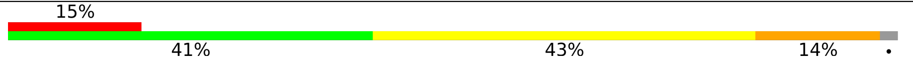
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	499	
9	I	312	
10	J	142	
11	K	439	
12	L	513	
13	M	177	
14	N	199	
15	O	128	
16	P	800	
17	Q	376	
18	R	557	
19	S	118	
19	a	118	
19	h	118	
20	T	86	
20	b	86	
20	i	86	
21	U	92	
21	c	92	
21	j	92	
22	V	76	
22	d	76	
22	k	76	
23	W	126	
23	e	126	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	l	126	
24	X	240	
24	f	240	
24	m	240	
25	Z	119	
25	g	119	
25	n	119	
26	o	95	
27	p	102	
28	q	139	
29	r	91	
30	s	80	
31	t	103	
32	u	96	
33	v	1304	
34	w	1217	
35	x	86	
36	y	110	
37	z	256	
38	1	225	
39	Y	324	
40	2	188	
41	4	145	
42	5	116	
43	6	106	

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 59243 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 protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	2190	Total 11100	C 6725	N 2190	O 2185	0	0

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	844	Total 4264	C 2577	N 844	O 843	0	0

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	1693	Total 8538	C 5154	N 1693	O 1691	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	D	302	Total 302	C 302	0	302

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	219	Total 1101	C 663	N 219	O 219	0	0

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	420	Total 2100	C 1260	N 420	O 420	0	0

- Molecule 7 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	804	4057	2449	804	804	0	0

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	413	2068	1243	413	412	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	176	883	531	176	176	0	0

- Molecule 10 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	J	135	677	408	135	134	0	0

- Molecule 11 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	45	225	135	45	45	0	0

- Molecule 12 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	459	2288	1370	459	459	0	0

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	169	844	506	169	169	0	0

- Molecule 14 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms	AltConf	Trace
14	N	56	Total C N O 277 165 56 56	0	0

- Molecule 15 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
15	O	126	Total C N O 636 385 126 125	0	0

- Molecule 16 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	P	91	Total C N O 458 276 91 91	0	0

- Molecule 17 is a protein called WW domain-binding protein 4.

Mol	Chain	Residues	Atoms	AltConf	Trace
17	Q	75	Total C N O 378 228 75 75	0	0

- Molecule 18 is a protein called Protein Red.

Mol	Chain	Residues	Atoms	AltConf	Trace
18	R	16	Total C N O 79 47 16 16	0	0

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	AltConf	Trace
19	a	78	Total C N O 393 237 78 78	0	0
19	h	74	Total C N O 371 223 74 74	0	0
19	S	87	Total C 87 87	0	87

- Molecule 20 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	AltConf	Trace
20	b	73	Total C N O 364 218 73 73	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
20	i	71	Total C N O 354 212 71 71	0	0
20	T	74	Total C 74 74	0	74

- Molecule 21 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	c	78	Total C N O 388 232 78 78	0	0
21	j	78	Total C N O 388 232 78 78	0	0
21	U	79	Total C 79 79	0	79

- Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	d	69	Total C N O 344 206 69 69	0	0
22	k	73	Total C N O 364 218 73 73	0	0
22	V	74	Total C 74 74	0	74

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	e	78	Total C N O 390 234 78 78	0	0
23	l	71	Total C N O 353 211 71 71	0	0
23	W	80	Total C 80 80	0	80

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	f	64	Total C N O 319 191 64 64	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
24	m	64	Total C N O 316 188 64 64	0	0
24	X	71	Total C 71 71	0	71

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	g	93	Total C N O 469 283 93 93	0	0
25	n	82	Total C N O 412 248 82 82	0	0
25	Z	82	Total C 82 82	0	82

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms	AltConf	Trace
26	o	90	Total C 90 90	0	90

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	p	73	Total C 73 73	0	73

- Molecule 28 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	q	80	Total C 80 80	0	80

- Molecule 29 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	r	76	Total C 76 76	0	76

- Molecule 30 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
30	s	69	69	69	0	69

- Molecule 31 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
31	t	79	79	79	0	79

- Molecule 32 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
32	u	62	62	62	0	62

- Molecule 33 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
33	v	806	806	806	0	806

- Molecule 34 is a protein called Splicing factor 3B subunit 3 (SF3B3).

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
34	w	1140	1140	1140	0	1140

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
35	x	54	54	54	0	54

- Molecule 36 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
36	y	89	89	89	0	89

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
37	z	162	162	162	0	162

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	89	ASP	CYS	conflict	UNP P09661
z	119	CYS	SER	conflict	UNP P09661
z	151A	PHE	-	insertion	UNP P09661

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
38	1	94	94	94	0	94

- Molecule 39 is a RNA chain called MINX pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	Y	46	972	435	167	324	46	0	0

- Molecule 40 is a RNA chain called Human gene for small nuclear RNA U2 (snRNA U2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	2	100	2123	947	367	709	100	0	0

- Molecule 41 is a RNA chain called Homo sapiens U4A snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	4	137	2904	1298	501	968	137	0	0

- Molecule 42 is a RNA chain called Homo sapiens U5 A small nuclear RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	5	114	2397	1074	399	810	114	0	0

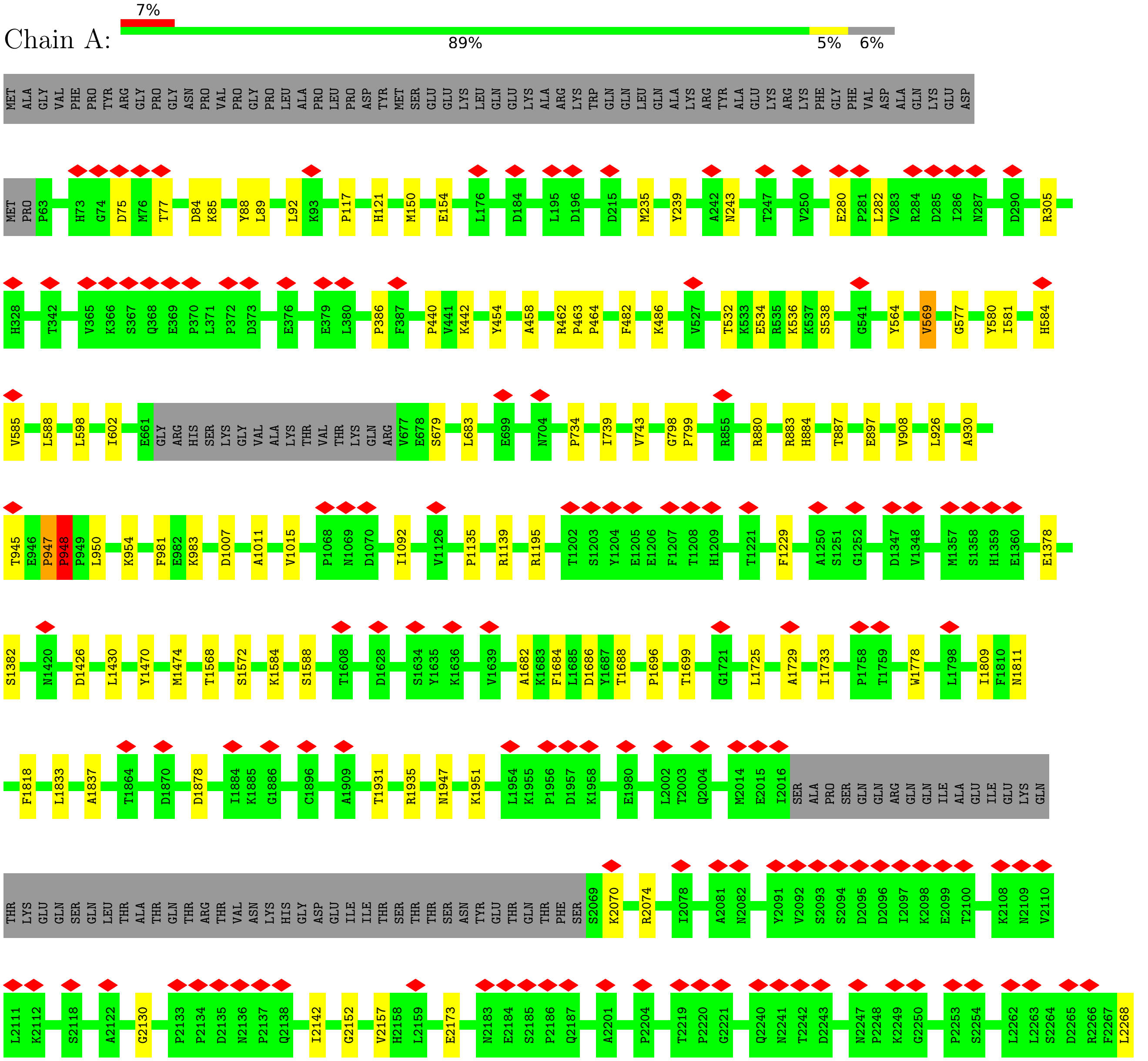
- Molecule 43 is a RNA chain called Homo sapiens RNA, U6 small nuclear 1 (RNU6-1), small nuclear RNA.

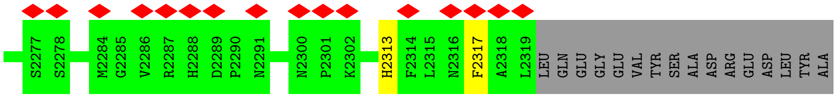
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
43	6	90	1926	861	353	622	90	0	0

3 Residue-property plots

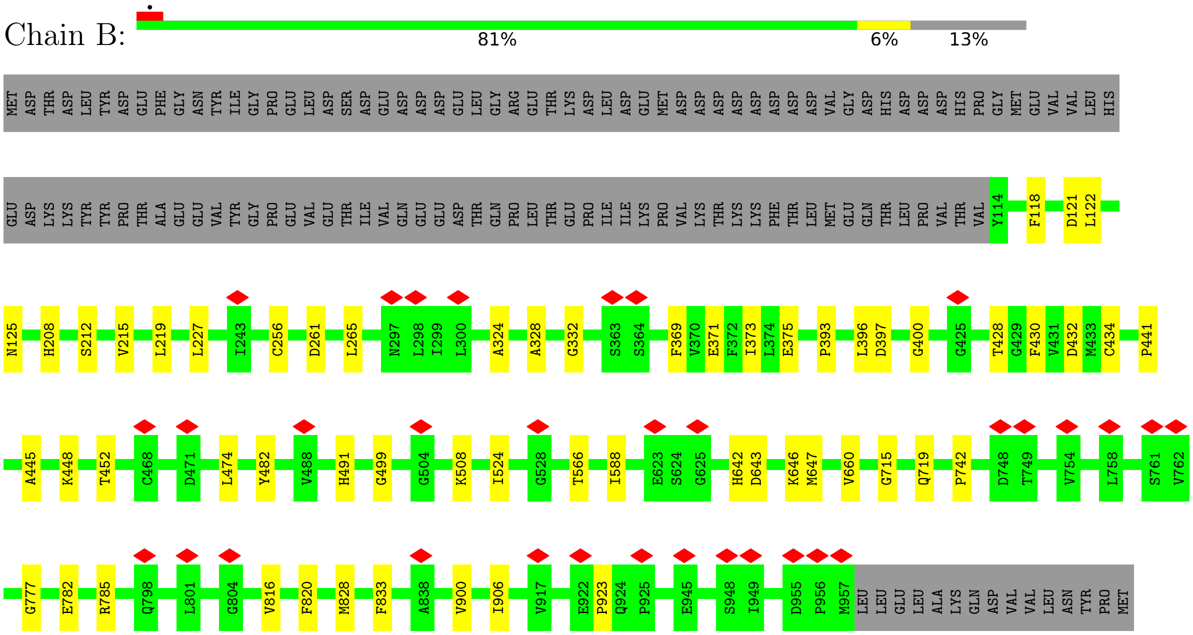
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Pre-mRNA-processing-splicing factor 8

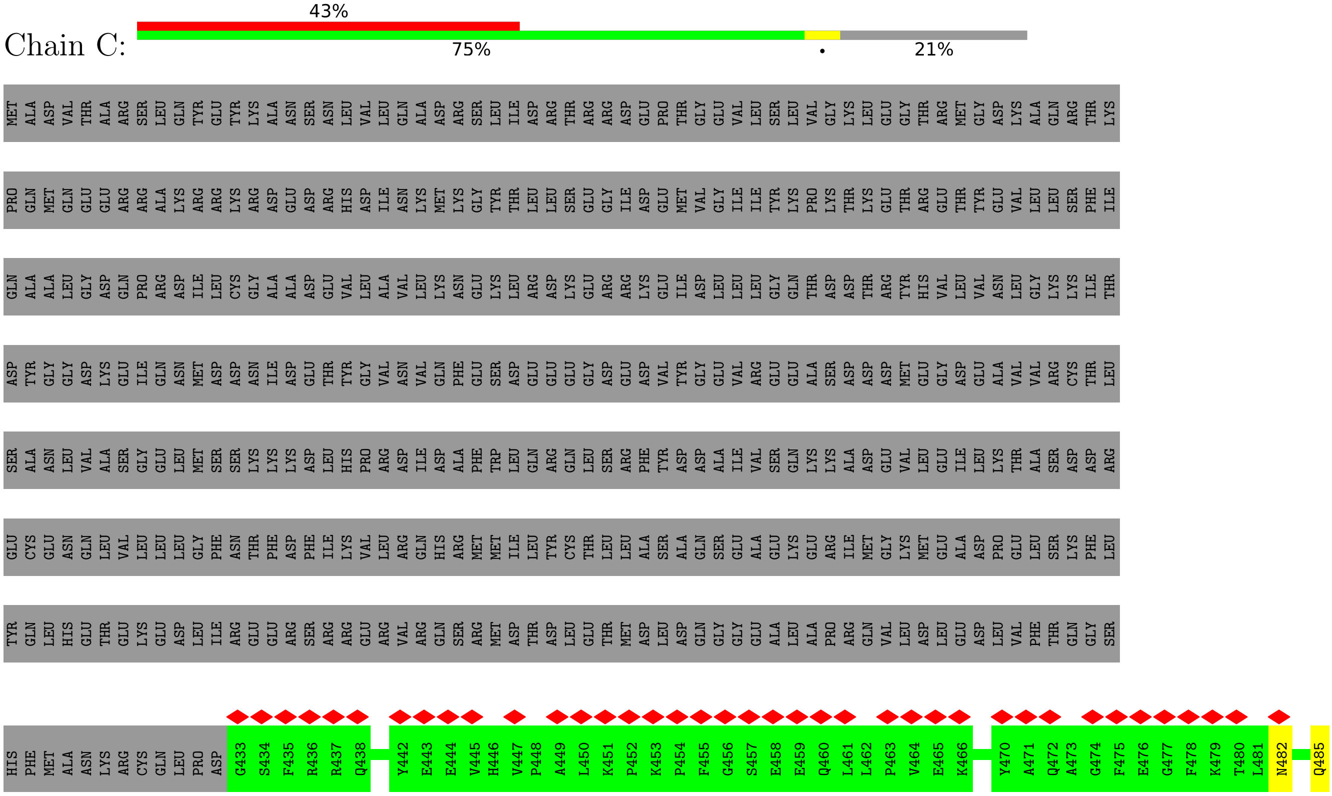


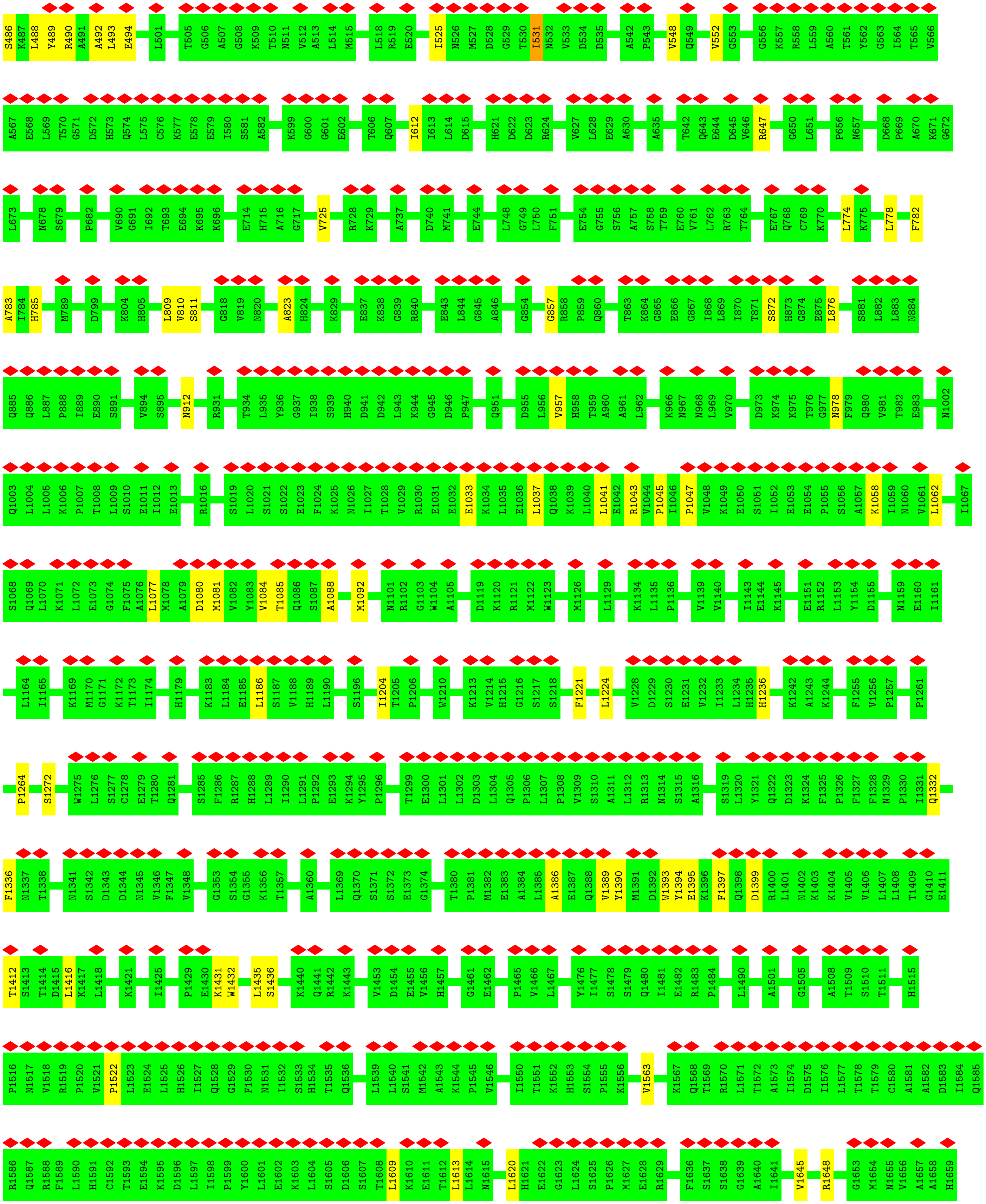


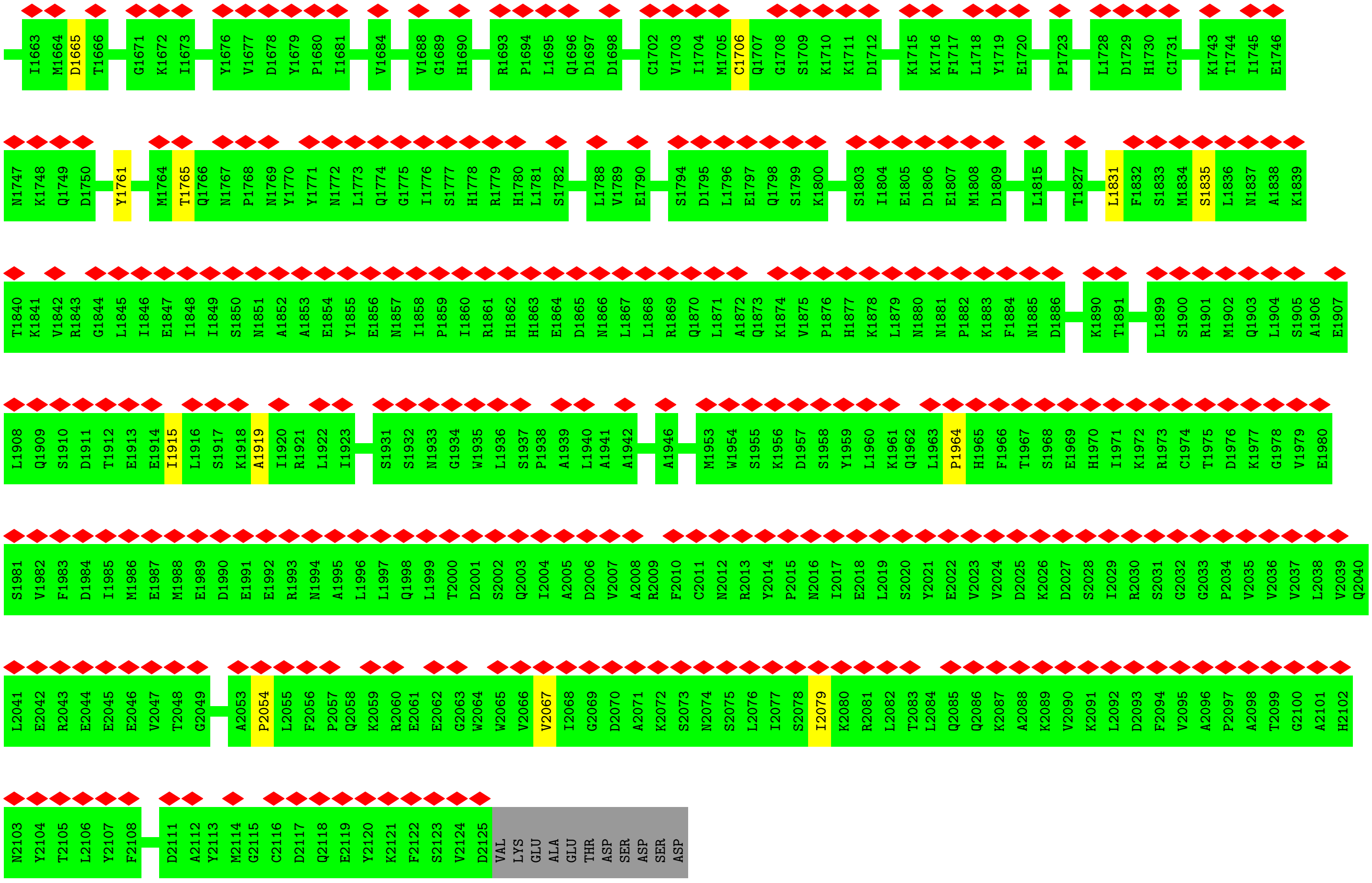
- Molecule 2: 116 kDa U5 small nuclear ribonucleoprotein component



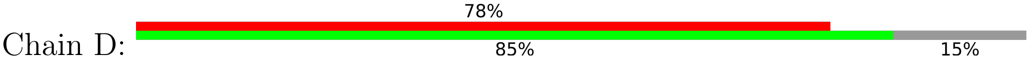
- Molecule 3: U5 small nuclear ribonucleoprotein 200 kDa helicase

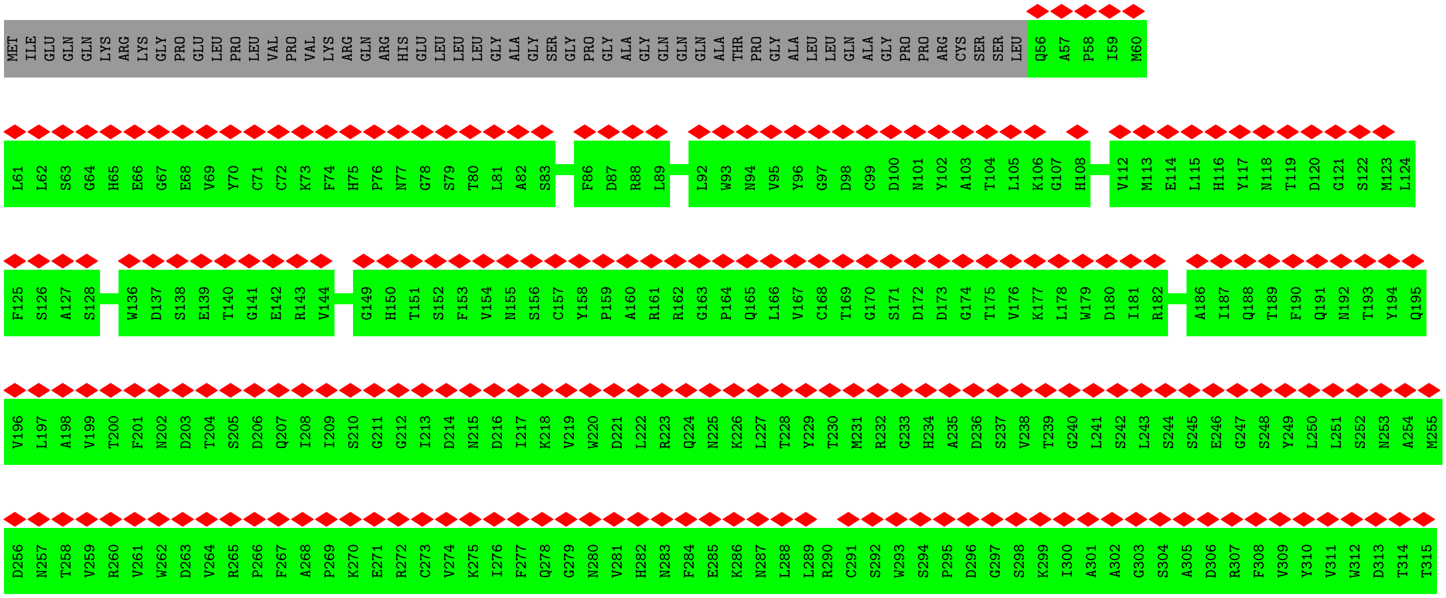


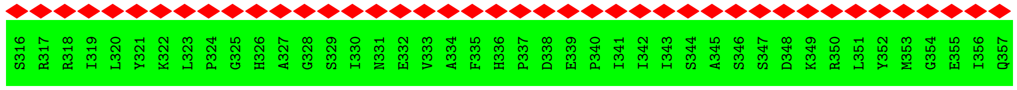

S486 K487 L488 Y489 R490 A491 A492 L493 E494 L501 T505 G506 A507 G508 K509 T510 N511 V512 A513 L514 M515 L518 R519 E520 I525 N526 M527 D528 G529 T530 I531 N532 V533 D534 D535 A542 P543 V548 Q549 V552 G553 G556 K557 R558 L559 A560 T561 Y562 G563 I564 T565 V566
A567 E568 L569 T570 G571 D572 H573 Q574 L575 C576 K577 E578 E579 I580 S581 A582 K599 G600 G601 E602 T606 Q607 I612 I613 L614 D615 H621 D622 D623 R624 V627 L628 E629 A630 A635 T642 Q643 E644 D645 V646 R647 G650 L651 P656 N657 D668 P669 A670 K671 G672
L673 N678 S679 P682 V690 G691 I692 T693 E694 K695 K696 E714 H715 A716 G717 V725 R728 K729 A737 D740 M741 E744 L748 G749 L750 F751 E754 G755 S756 A757 S758 T759 E760 V761 L762 R763 T764 E767 Q768 C769 K770 L774 K775 L778 F782
A783 I784 H785 M789 D799 K804 H805 L809 V810 S811 G818 V819 N820 A823 H824 K829 E837 K838 G839 R840 E843 L844 G845 A846 G854 G857 R858 P859 Q860 T863 K864 G865 E866 G867 I868 L869 I870 T871 S872 H873 G874 E875 L876 S881 L882 L883 N884
Q885 Q886 L887 P888 I889 E890 S891 V894 S895 N912 R931 T934 L935 Y936 G937 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 Q951 D955 L956 V957 H958 T959 A960 A961 L962 K966 N967 N968 L969 V970 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 N1002
Q1003 L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 R1016 S1019 L1020 S1021 S1022 E1023 F1024 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 L1041 E1042 R1043 V1044 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053 E1054 P1055 S1056 A1057 K1058 I1059 N1060 V1061 L1062 I1067
S1068 Q1069 L1070 K1071 L1072 E1073 G1074 F1075 A1076 L1077 M1078 A1079 D1080 M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 A1088 M1092 N1101 R1102 G1103 W1104 A1105 D1119 K1120 R1121 M1122 W1123 M1126 L1129 K1134 L1135 P1136 V1139 V1140 I1143 E1144 K1145 E1151 R1152 L1153 Y1154 D1155 N1159 E1160 I1161
L1164 I1165 K1169 M1170 G1171 K1172 T1173 I1174 H1179 K1183 L1184 E1185 L1186 S1187 V1188 H1189 L1190 S1196 I1204 T1205 P1206 W1210 K1213 V1214 H1215 G1216 S1217 S1218 F1221 L1224 V1228 D1229 S1230 E1231 V1232 I1233 L1234 H1235 H1236 K1242 A1243 K1244 F1255 V1256 P1257 P1261
P1264 S1272 W1275 L1276 S1277 C1278 E1279 T1280 Q1281 S1285 F1286 R1287 H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 T1299 E1300 L1301 L1302 D1303 L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332
F1336 N1337 T1338 N1341 S1342 D1343 D1344 N1345 V1346 F1347 V1348 G1353 S1354 G1355 K1356 T1357 A1360 L1369 Q1370 S1371 S1372 E1373 G1374 T1380 P1381 M1382 E1383 A1384 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 L1407 L1408 T1409 G1410 E1411
T1412 S1413 T1414 D1415 L1416 K1417 L1418 K1421 I1425 P1429 E1430 K1431 W1432 L1435 S1436 K1440 Q1441 R1442 K1443 V1453 D1454 E1455 V1456 H1457 G1461 E1462 P1465 V1466 L1467 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 L1490 A1501 G1505 A1508 T1509 S1510 T1511 H1515
P1516 N1517 V1518 R1519 P1520 V1521 P1522 L1523 E1524 L1525 H1526 I1527 Q1528 G1529 F1530 N1531 I1532 S1533 H1534 T1535 Q1536 L1539 L1540 S1541 M1542 A1543 K1544 P1545 V1546 I1550 T1551 K1552 H1553 S1554 P1555 K1556 V1563 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585
R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615 L1620 H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 F1636 S1637 S1638 G1639 A1640 I1641 V1645 R1648 G1653 M1654 N1655 V1656 A1657 A1658 H1659



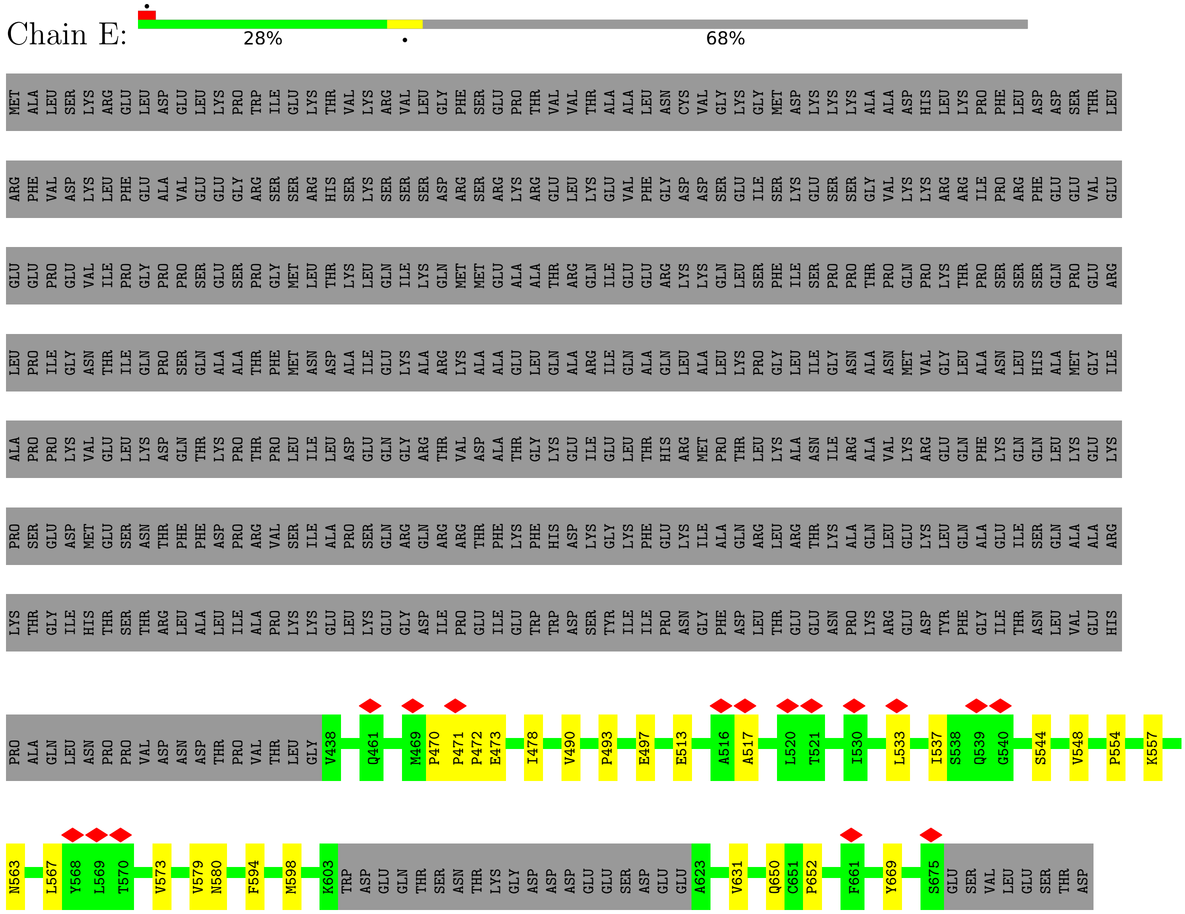
- Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein



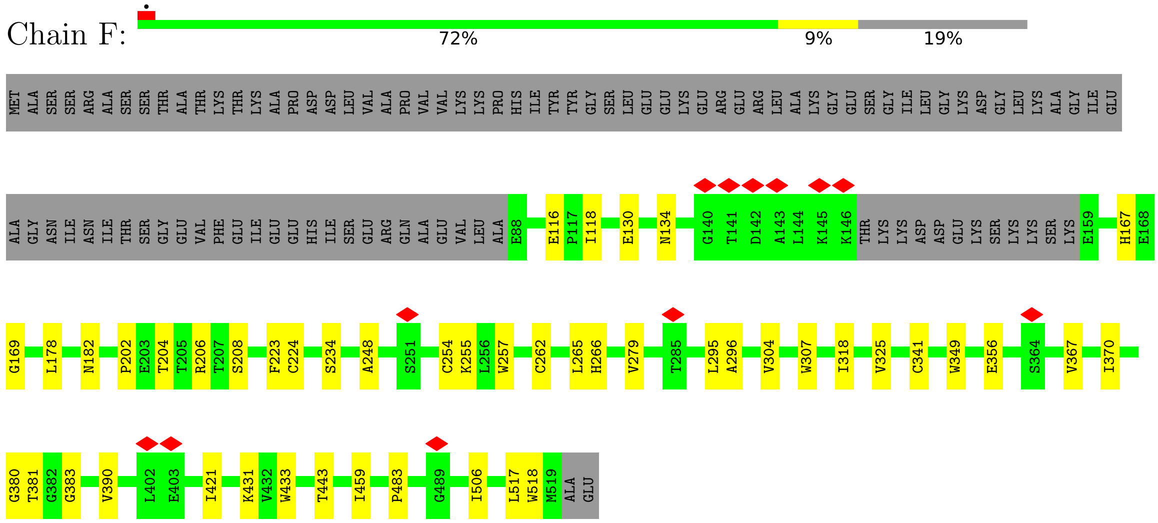




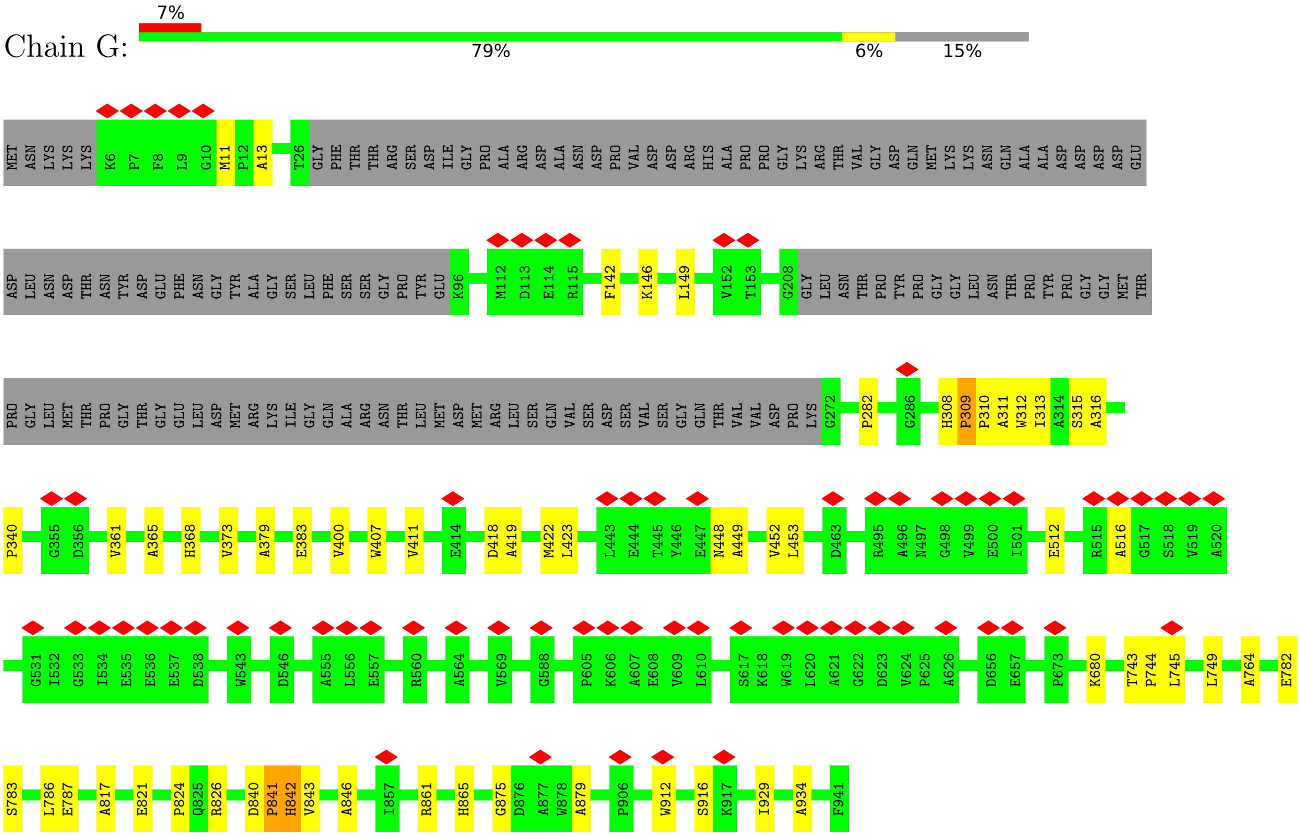
- Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp3



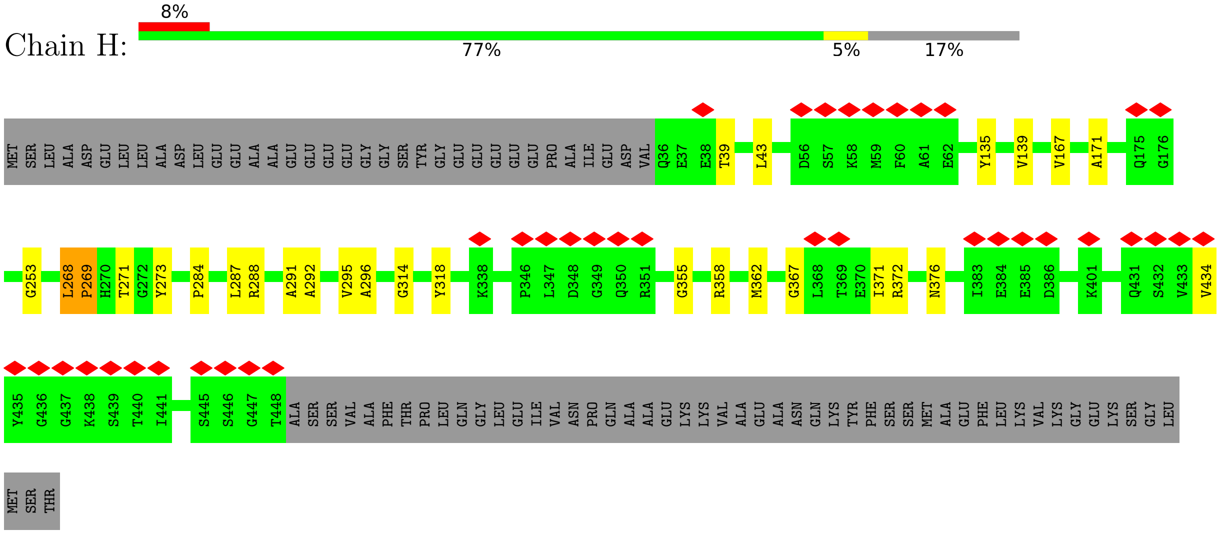
- Molecule 6: U4/U6 small nuclear ribonucleoprotein Prp4



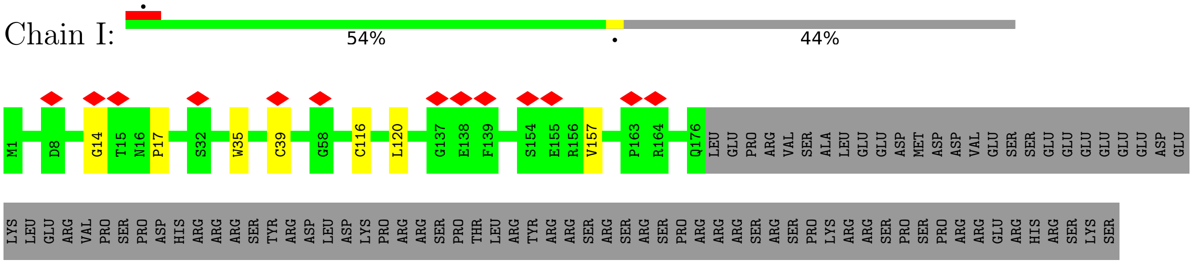
- Molecule 7: Pre-mRNA-processing factor 6



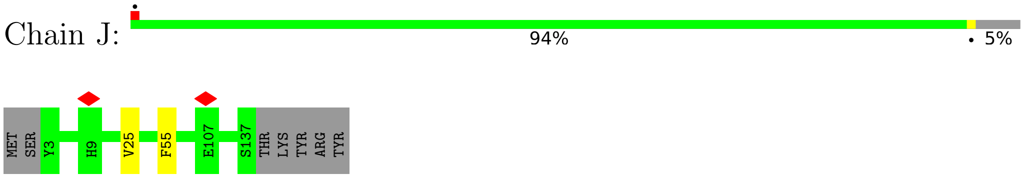
- Molecule 8: U4/U6 small nuclear ribonucleoprotein Prp31



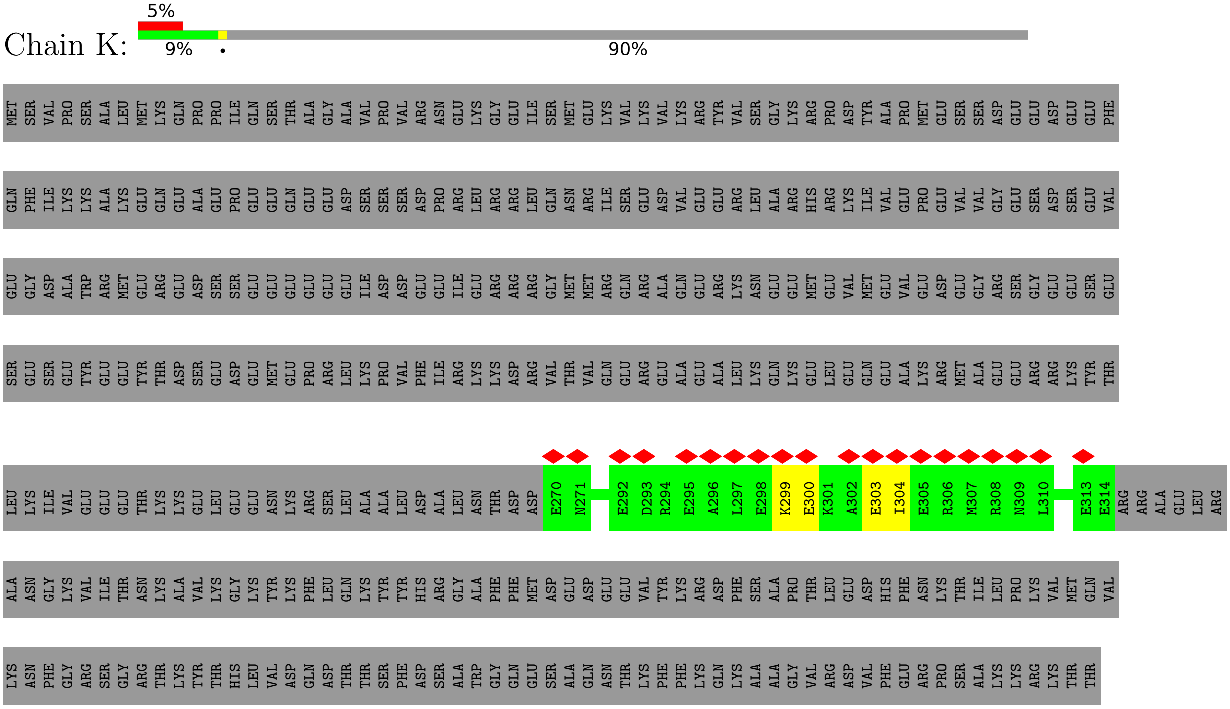
- Molecule 9: Pre-mRNA-splicing factor 38A



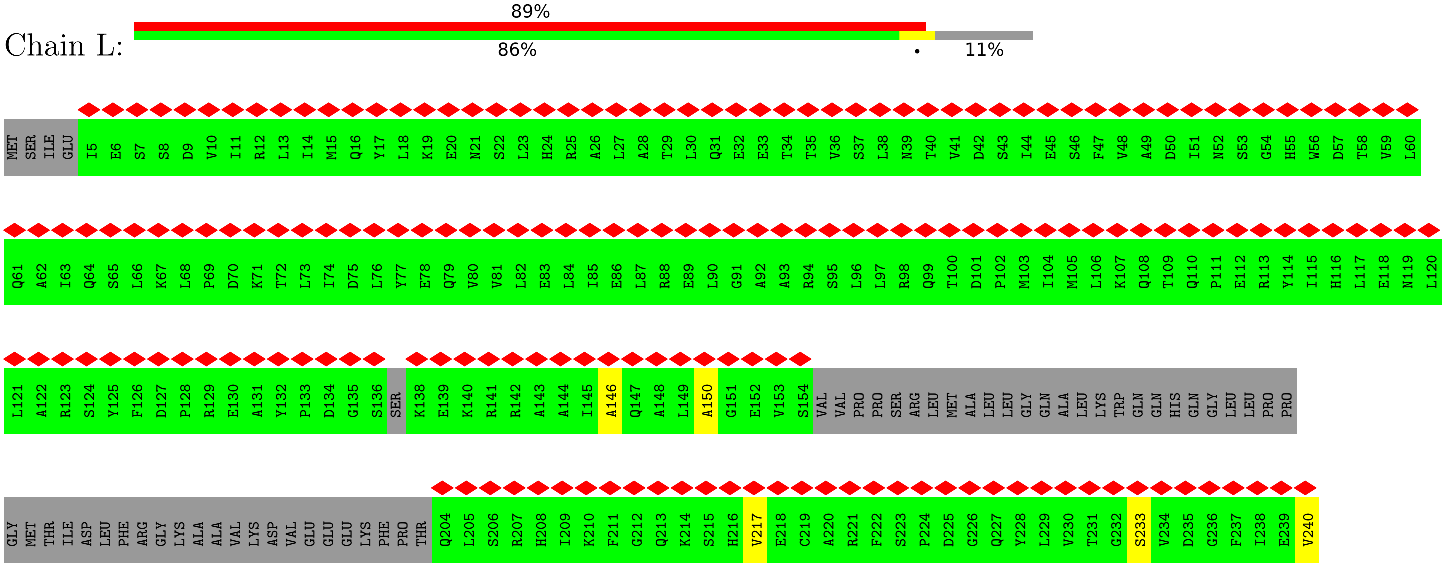
- Molecule 10: Thioredoxin-like protein 4A

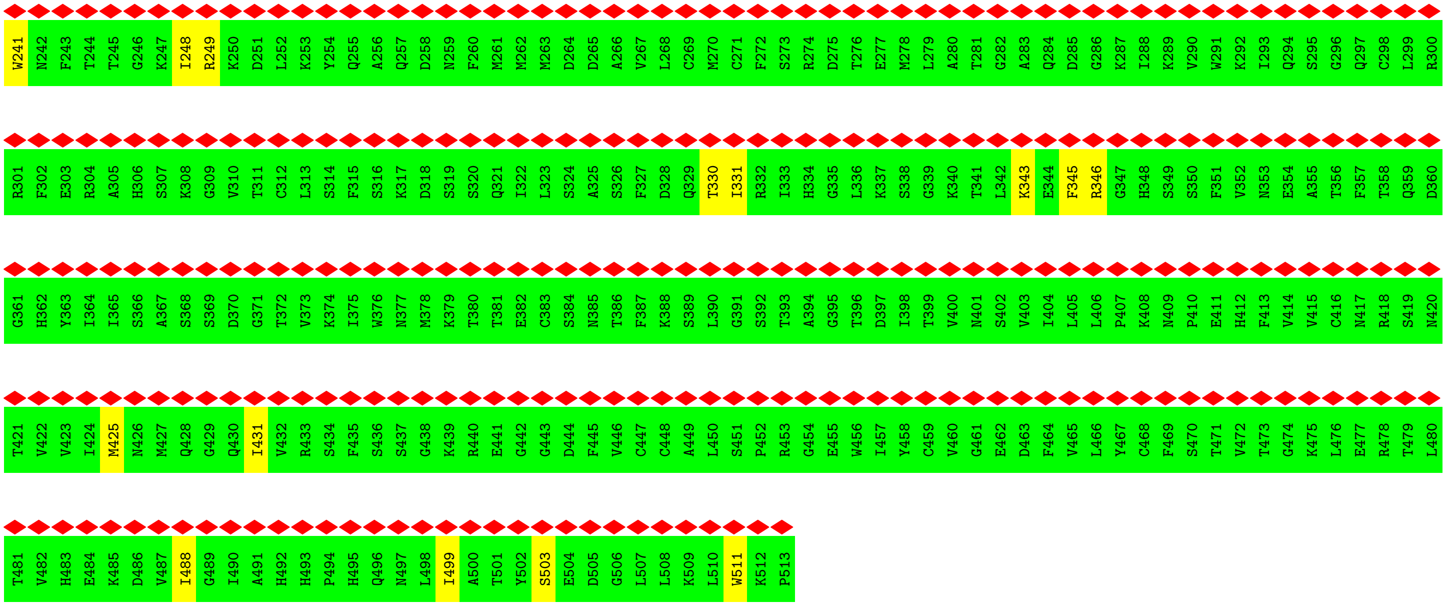


- Molecule 11: Microfibrillar-associated protein 1

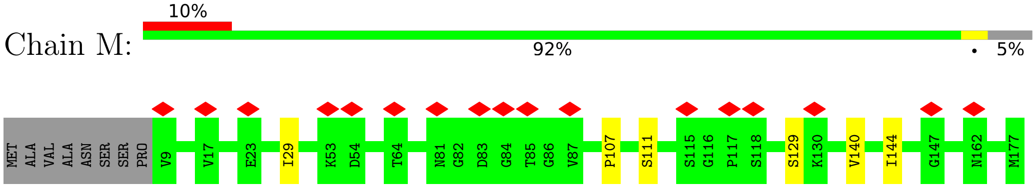


- Molecule 12: WD40 repeat-containing protein SMU1

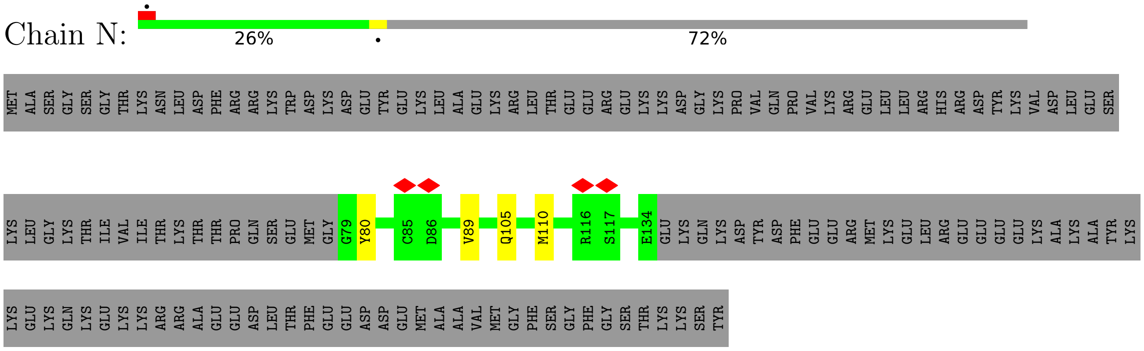




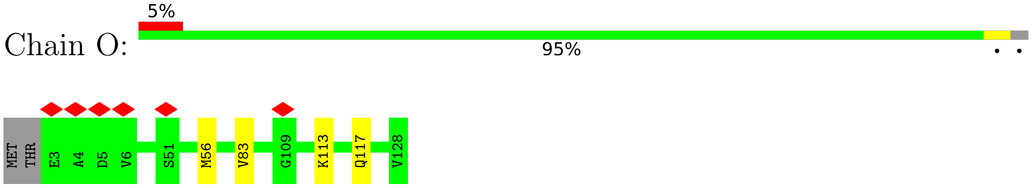
- Molecule 13: Peptidyl-prolyl cis-trans isomerase H



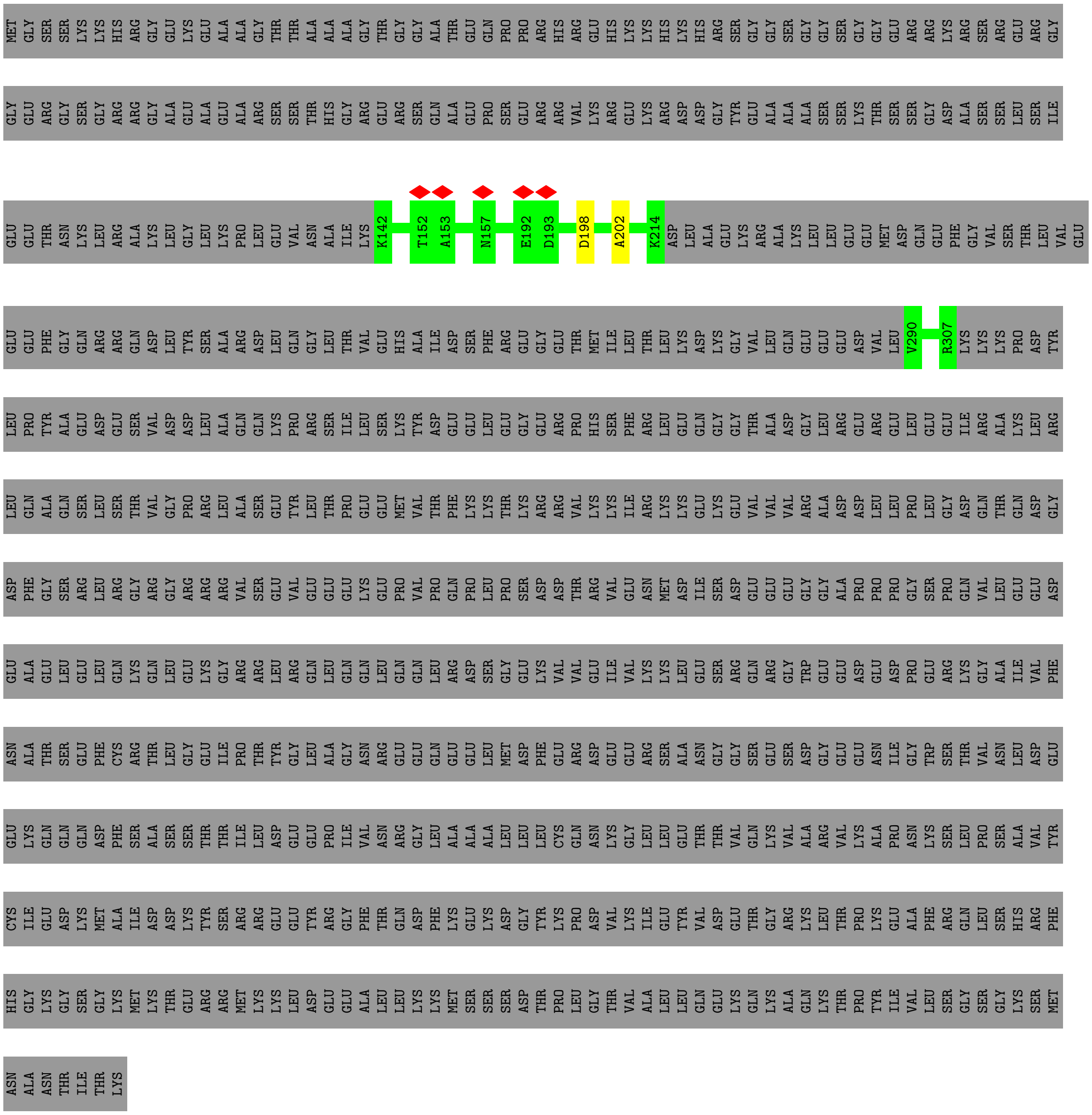
- Molecule 14: Zinc finger matrin-type protein 2



- Molecule 15: NHP2-like protein 1

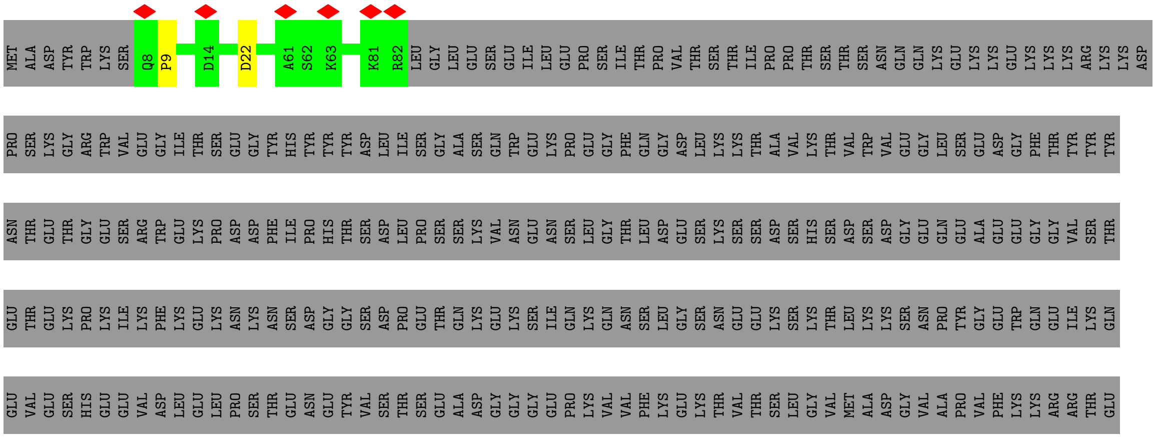


- Molecule 16: U4/U6.U5 tri-snRNP-associated protein 1



- Molecule 17: WW domain-binding protein 4

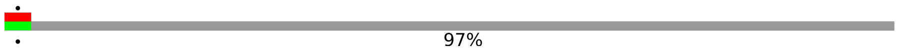
Chain Q:



ASN GLY LYS SER ARG ASN LEU ARG GLN ARG GLY ASP ASP GLN

- Molecule 18: Protein Red

Chain R:



MET PRO GLU ARG ASP SER GLU PRO PHE SER ASN PRO LEU ALA PRO ASP GLY HIS ASP VAL ASP ASP PRO HIS SER PHE HIS GLN SER LYS LEU THR ASN GLU ASP PHE ARG LYS LEU LEU MET THR PRO ARG ALA ALA PRO THR SER ALA PRO PRO SER LYS SER ARG HIS HIS GLU MET

PRO ARG GLU TYR ASN GLU ASP GLU ASP PRO ALA ALA ARG ARG LYS LYS LYS SER TYR TYR ALA LYS LEU ARG GLN GLU ILE GLU ARG GLU ARG GLU LEU ALA GLU LYS TYR ARG ASP ARG ALA LYS GLU ARG ARG ASP GLY VAL ASN LYS ASP TYR GLU GLU THR GLU LEU ILE

SER THR THR ALA ASN TYR ARG ALA VAL GLY PRO THR ALA GLU ALA ASP LYS SER ALA ALA GLU LYS ARG ARG GLN LEU ILE GLN GLU SER LYS PHE LEU GLY GLY ASP MET GLU HIS THR HIS LEU VAL LYS GLY LEU ASP PHE ALA LEU LEU GLN LYS VAL ARG ALA GLU ILE ALA SER

LYS GLU LYS GLU GLU GLU LEU MET GLU LYS PRO GLN LYS GLU THR LYS LYS ASP GLU ASP PRO GLU ASN LYS ILE E207 F208 K209 T210 R211 L212 G213 R214 N215 V216 Y217 R218 M219 L220 F221 K222 SER LYS ALA TYR GLU ARG ASN GLU LEU PHE LEU PRO GLY ARG MET ALA TYR VAL

VAL ASP LEU ASP ASP GLU TYR ALA ASP THR ASP ILE PRO THR THR LEU ILE ARG SER LYS ALA ASP CYS PRO THR MET GLU ALA GLN THR THR LEU THR THR ASN ASP ILE VAL ILE SER LYS LEU THR GLN ILE LEU SER TYR LEU ARG GLN GLY THR ARG ASN LYS LYS LEU LYS LYS

LYS ASP LYS GLY LYS LEU GLU GLU LYS LYS PRO PRO GLU ALA ASP MET ASN ILE PHE GLU ASP ILE GLY ASP TYR VAL PRO SER THR THR LYS THR PRO ARG ASP LYS GLU ARG GLU ARG TYR ARG GLU ARG GLU ARG ASP ARG GLU ARG ASP ARG ASP ARG ASP ARG GLU ARG GLU ARG

GLU ARG ASP ARG GLU ARG GLU ARG GLU ARG ASP ARG GLU ARG GLU GLU GLU LYS LYS ARG HIS SER TYR PHE GLU LYS PRO LYS VAL ASP ASP GLU PRO MET ASP VAL ASP LYS GLY PRO GLY SER THR LYS GLU LEU ILE LYS SER ILE ASN GLU LYS PHE ALA GLY SER ALA GLY TRP

GLU GLY THR GLU SER LEU LYS LYS PRO GLU ASP LYS LYS GLN LEU GLY ASP PHE PHE GLY MET SER ASN SER TYR ALA GLU CYS TYR PRO ALA THR MET ASP ASP MET ALA VAL ASP SER ASP GLU GLU VAL ASP TYR SER LYS MET ASP GLN GLY ASN LYS LYS GLY PRO LEU GLY ARG

TRP ASP PHE ASP THR GLN GLU GLU TYR SER GLU TYR MET ASN ASN LYS GLU ALA LEU PRO LYS ALA ALA PHE GLN TYR GLY ILE LYS MET SER GLU GLY ARG LYS THR ARG ARG PHE LYS GLU THR ASN ASP LYS ALA GLU LEU ASP ARG GLN TRP LYS LYS ILE SER ALA ILE ILE GLU

LYS ARG LYS LYS MET GLU ALA ASP GLY VAL GLU VAL LYS ARG PRO LYS TYR

- Molecule 19: Small nuclear ribonucleoprotein Sm D2

Chain a:

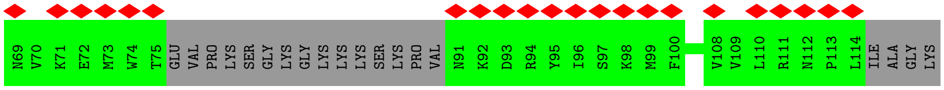
MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG GLU GLU GLU PHE ASN T26 Q34 S35 V36 K37 N38 N39 T40 Q41 R55 V56 K57 A58 E68 T75 E76 V77 PRO LYS SER GLY LYS GLY LYS LYS SER LYS P89 V90 N91

K92 D93 R94 Y95 I96 S97 K98 V108 V109 L110 R111 N112 P113 L114 ILE ALA GLY LYS

- Molecule 19: Small nuclear ribonucleoprotein Sm D2

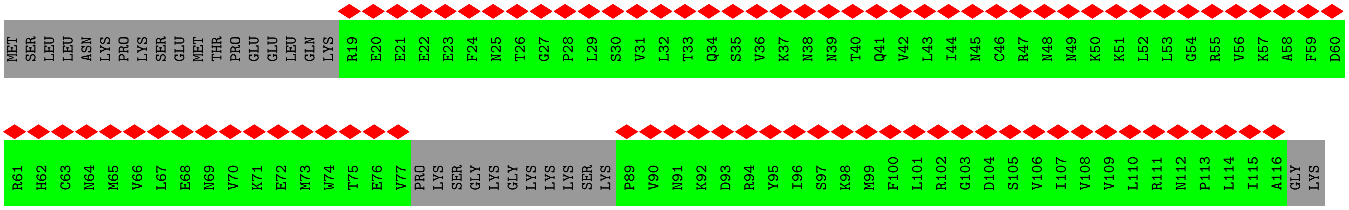
Chain h:

MET SER LEU LEU ASN LYS PRO LYS SER GLU MET THR PRO GLU GLU LEU GLN LYS ARG GLU GLU GLU PHE ASN T26 G27 P28 L29 S30 V31 L32 T33 Q34 S35 V36 K37 N38 N39 T40 Q41 V42 L43 I44 N45 L52 L53 G54 R55 V56 K57 A58 R61 H62 V66 L67 E68



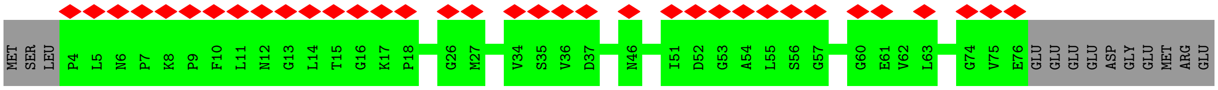
- Molecule 19: Small nuclear ribonucleoprotein Sm D2

Chain S:



- Molecule 20: Small nuclear ribonucleoprotein F

Chain b:



- Molecule 20: Small nuclear ribonucleoprotein F

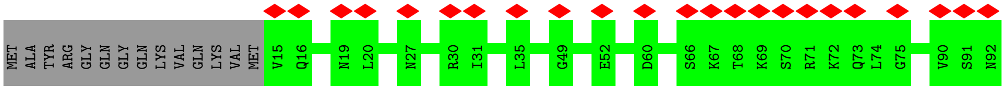
Chain i:

- Molecule 20: Small nuclear ribonucleoprotein F

Chain T:

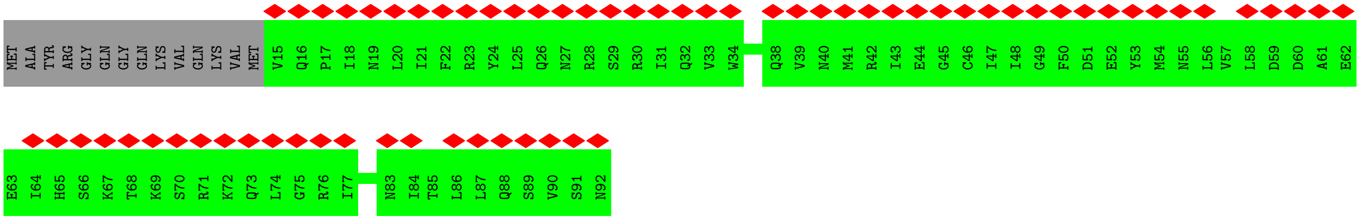
- Molecule 21: Small nuclear ribonucleoprotein E

Chain c:



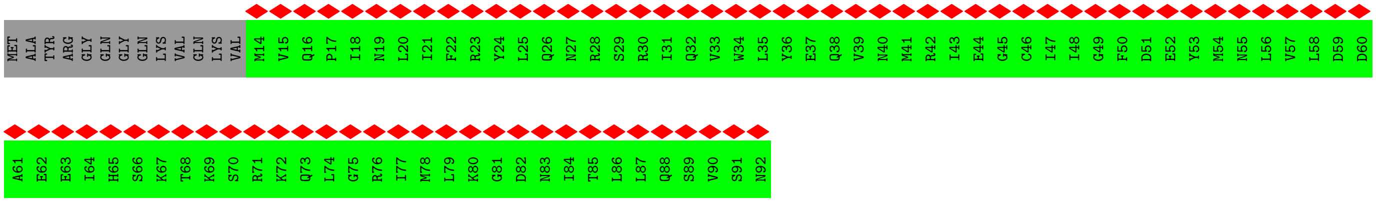
• Molecule 21: Small nuclear ribonucleoprotein E

Chain j:



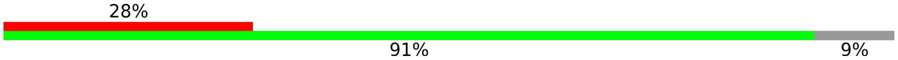
• Molecule 21: Small nuclear ribonucleoprotein E

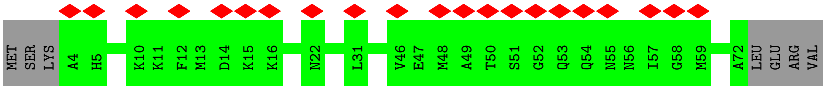
Chain U:



• Molecule 22: Small nuclear ribonucleoprotein G

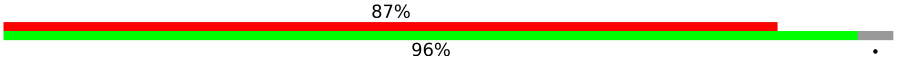
Chain d:

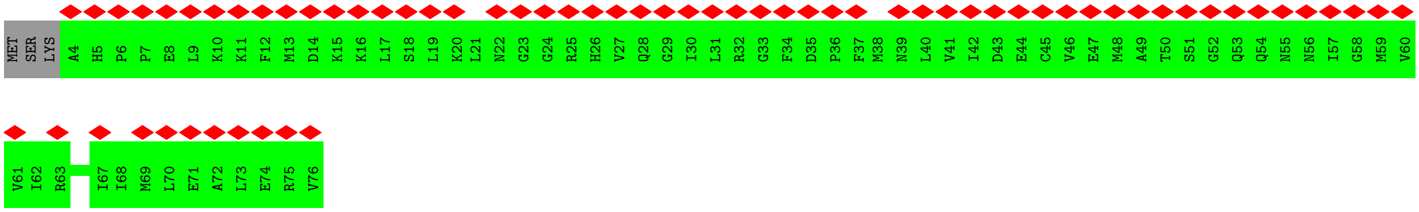




• Molecule 22: Small nuclear ribonucleoprotein G

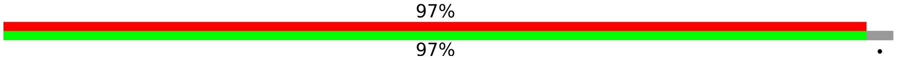
Chain k:





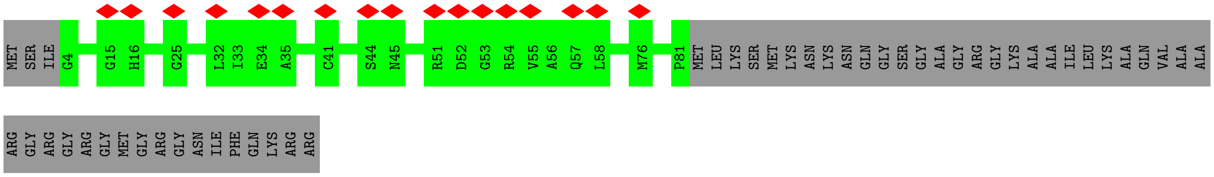
• Molecule 22: Small nuclear ribonucleoprotein G

Chain V:



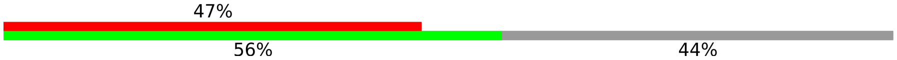
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

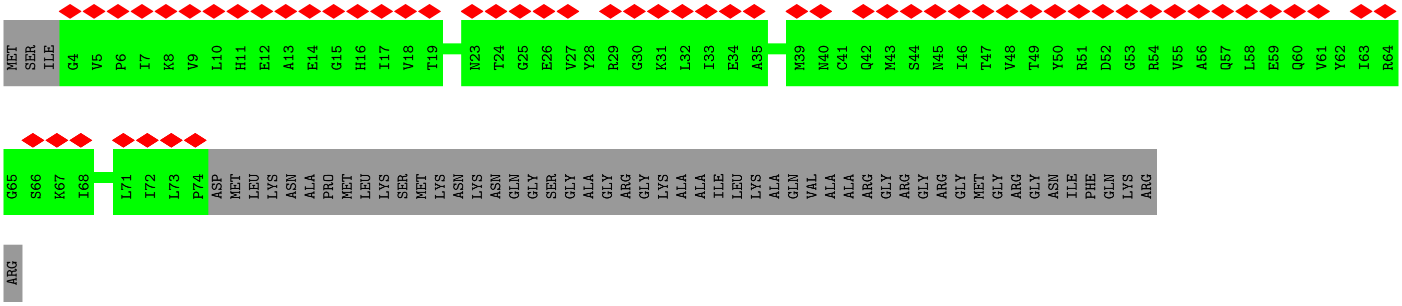
Chain e:



- Molecule 23: Small nuclear ribonucleoprotein Sm D3

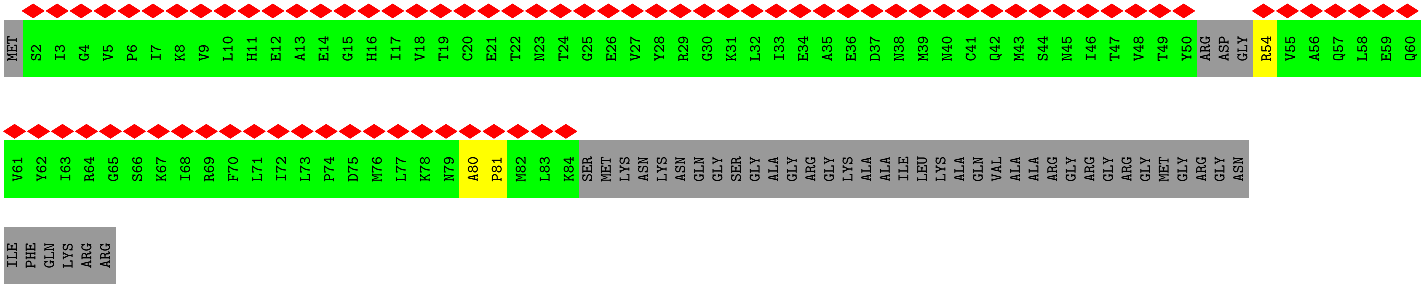
Chain l:





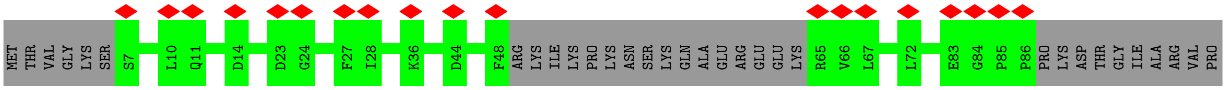
- Molecule 23: Small nuclear ribonucleoprotein Sm D3

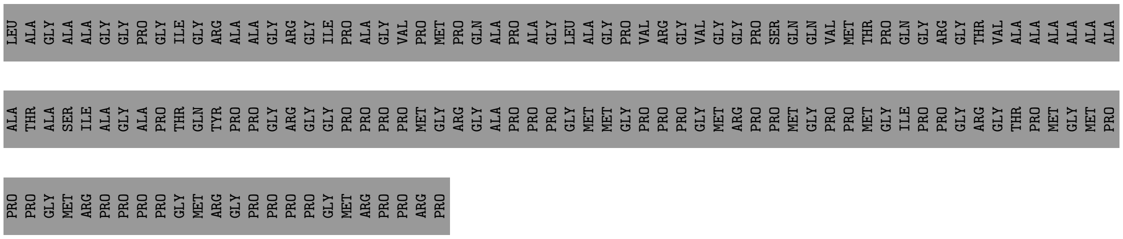
Chain W:



- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B’

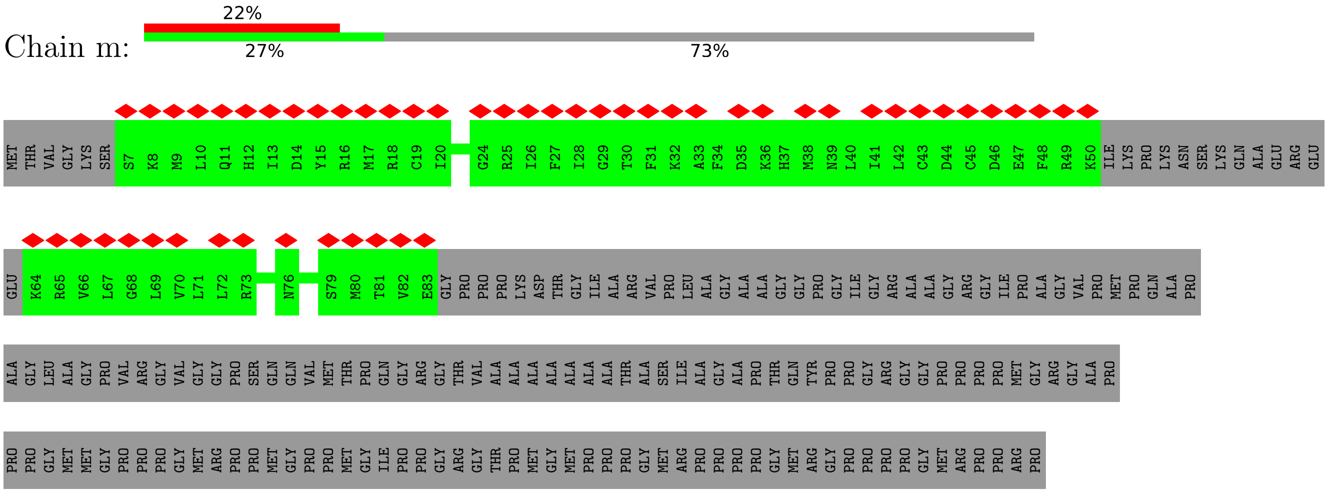
Chain f:





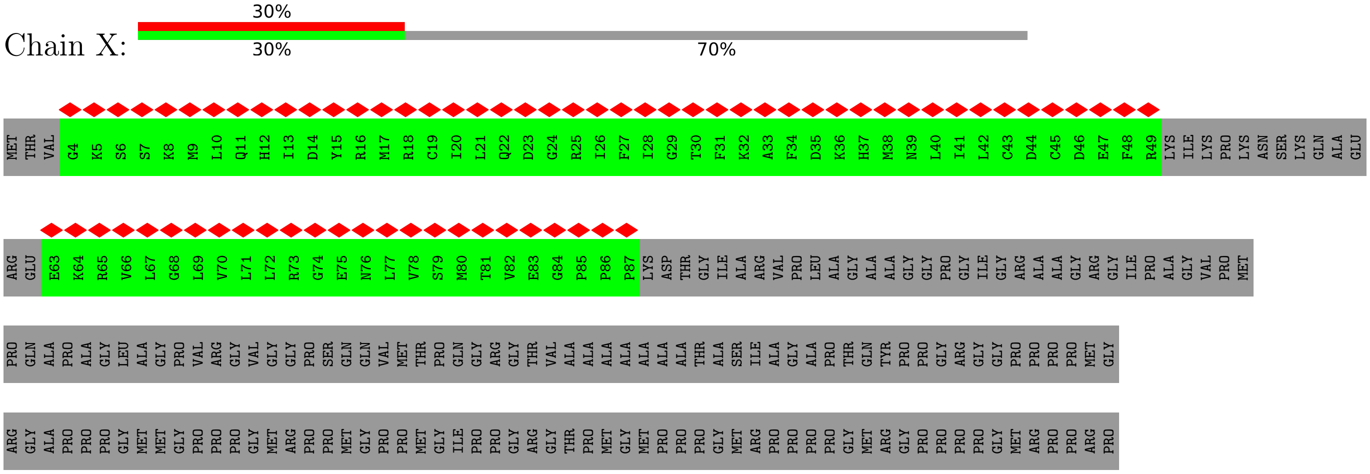
- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B’

Chain m:



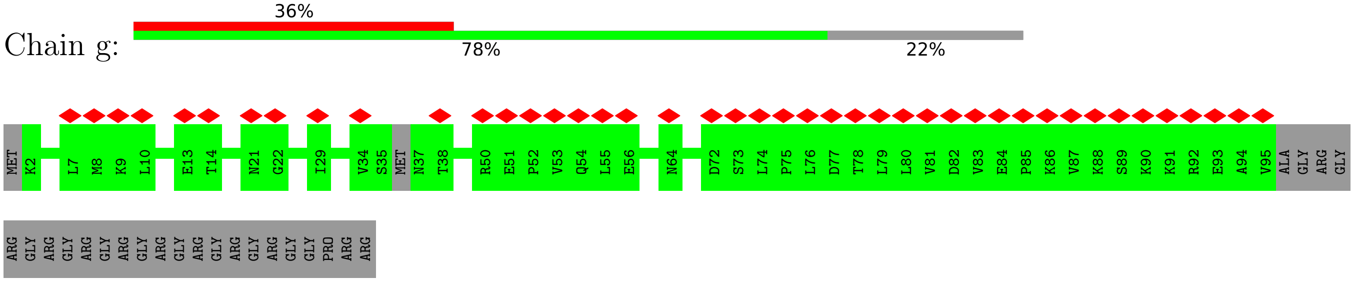
- Molecule 24: Small nuclear ribonucleoprotein-associated proteins B and B’

Chain X:



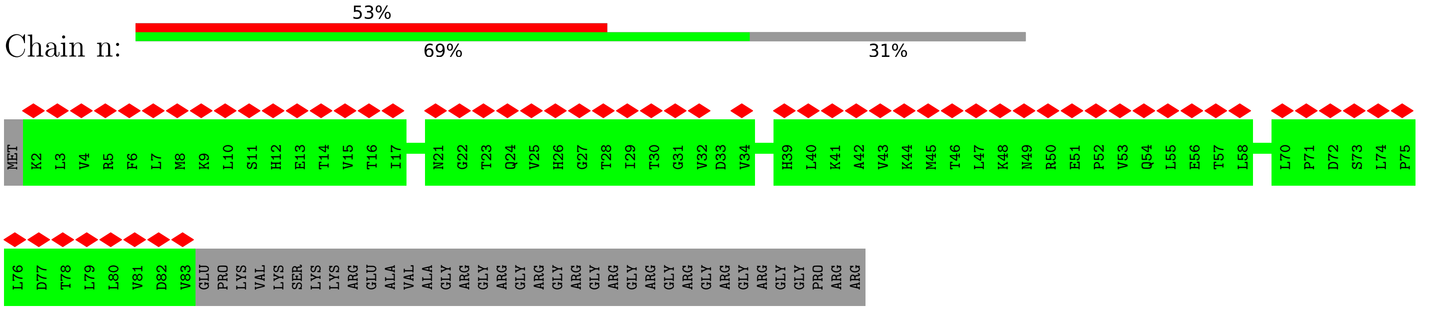
- Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain g:



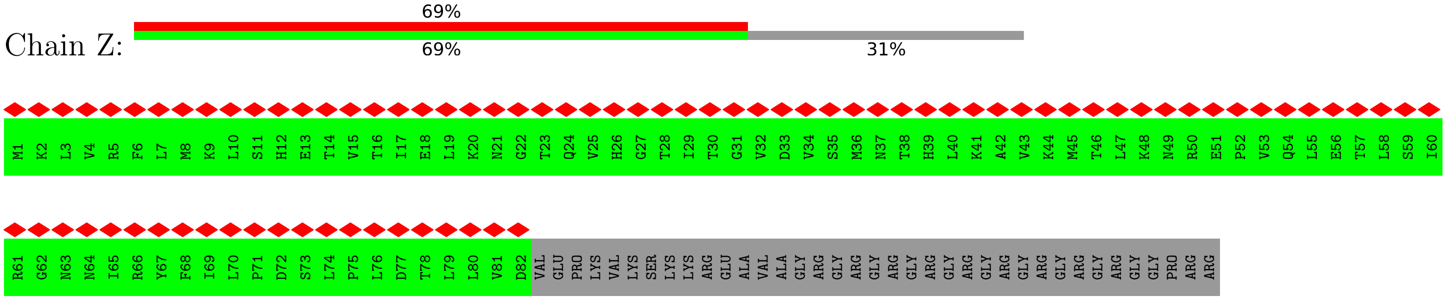
- Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain n:



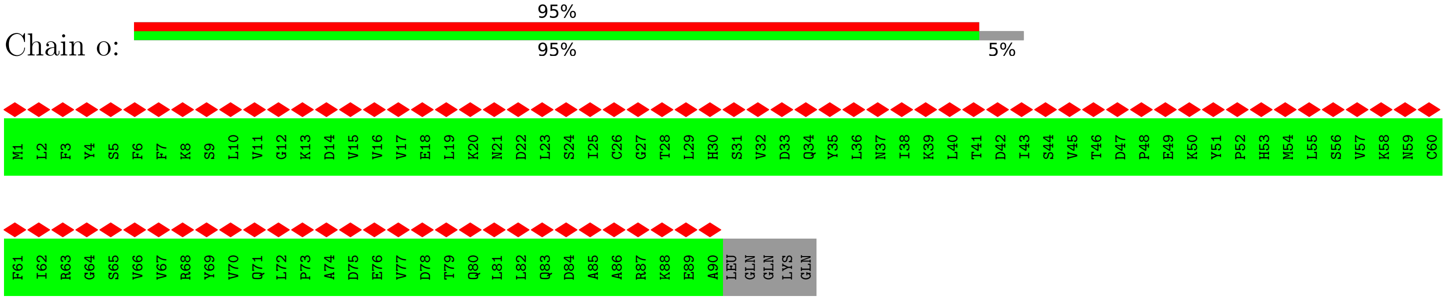
- Molecule 25: Small nuclear ribonucleoprotein Sm D1

Chain Z:



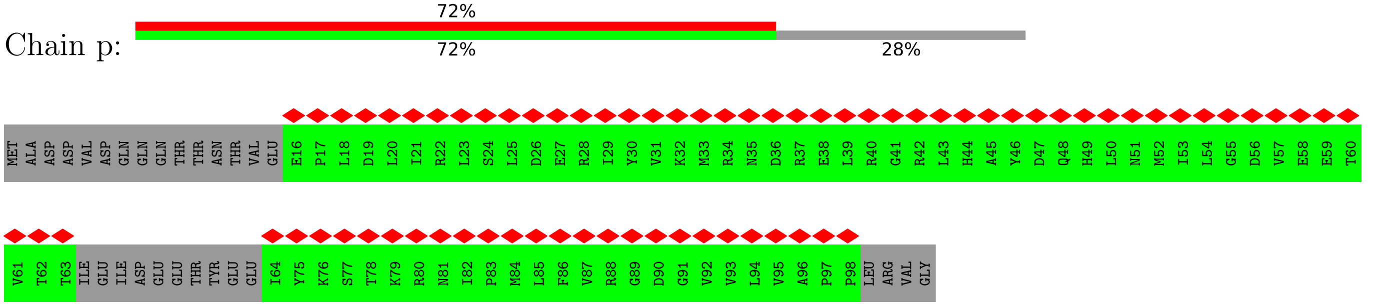
- Molecule 26: U6 snRNA-associated Sm-like protein LSm2

Chain o:



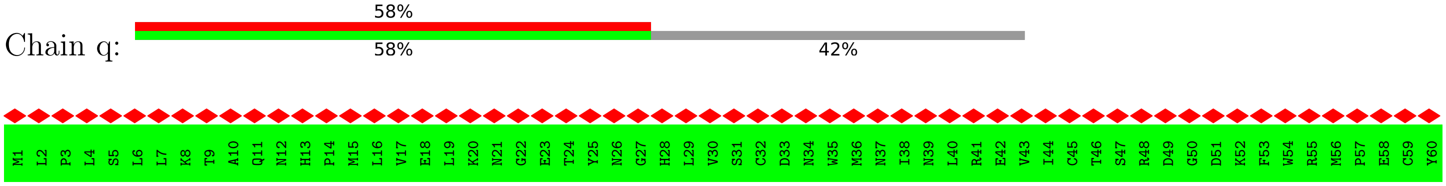
- Molecule 27: U6 snRNA-associated Sm-like protein LSm3

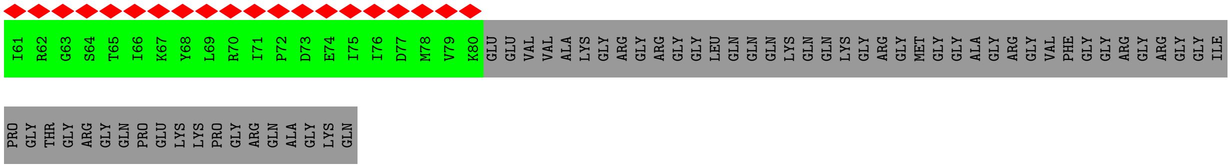
Chain p:



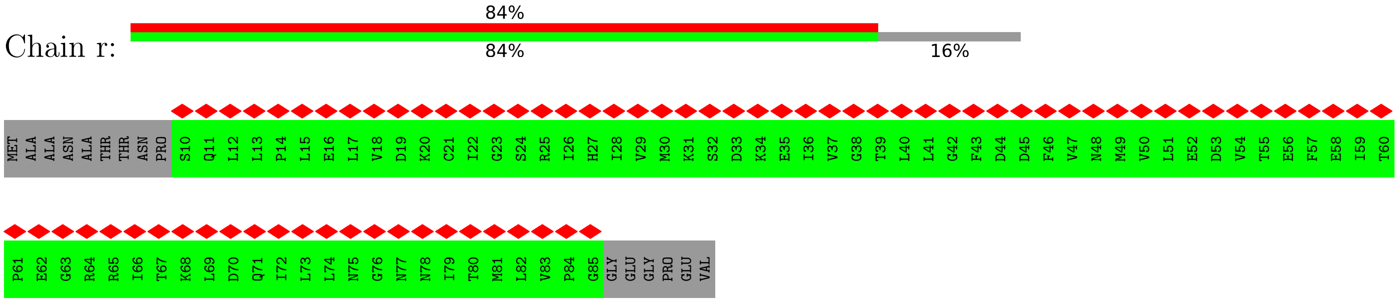
- Molecule 28: U6 snRNA-associated Sm-like protein LSm4

Chain q:

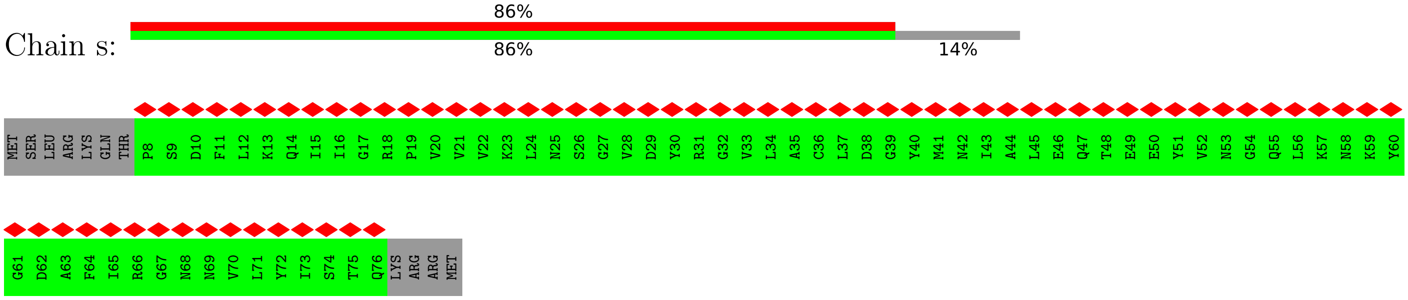




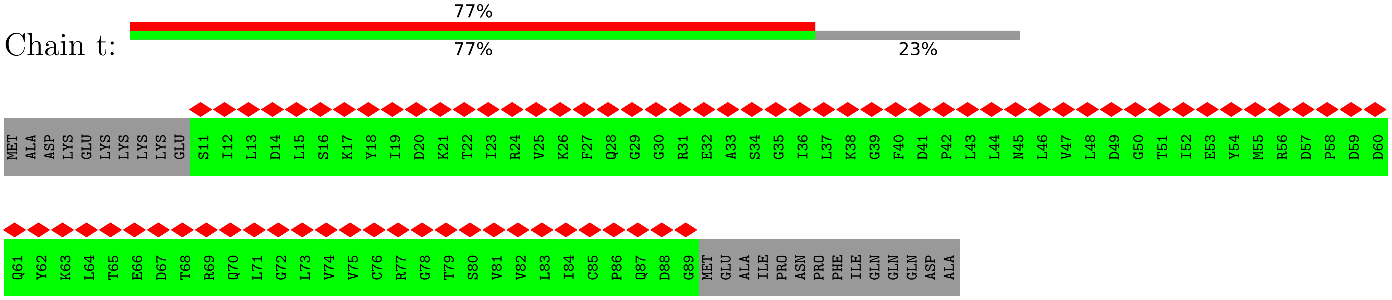
- Molecule 29: U6 snRNA-associated Sm-like protein LSm5



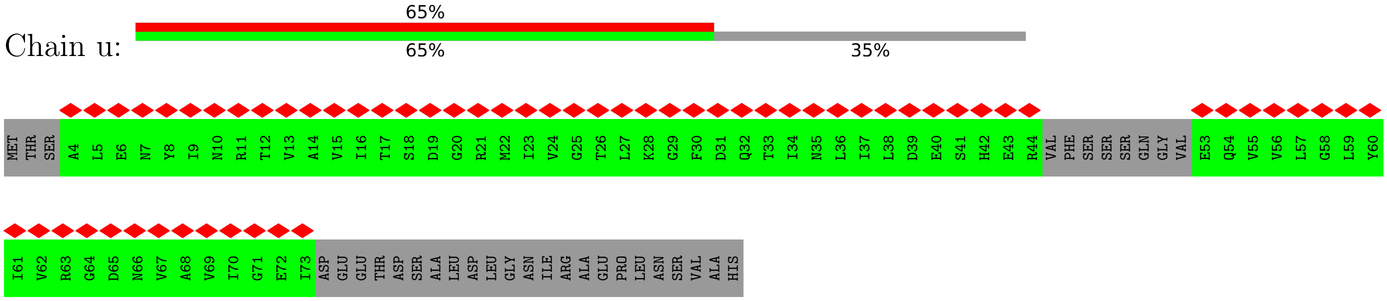
- Molecule 30: U6 snRNA-associated Sm-like protein LSm6



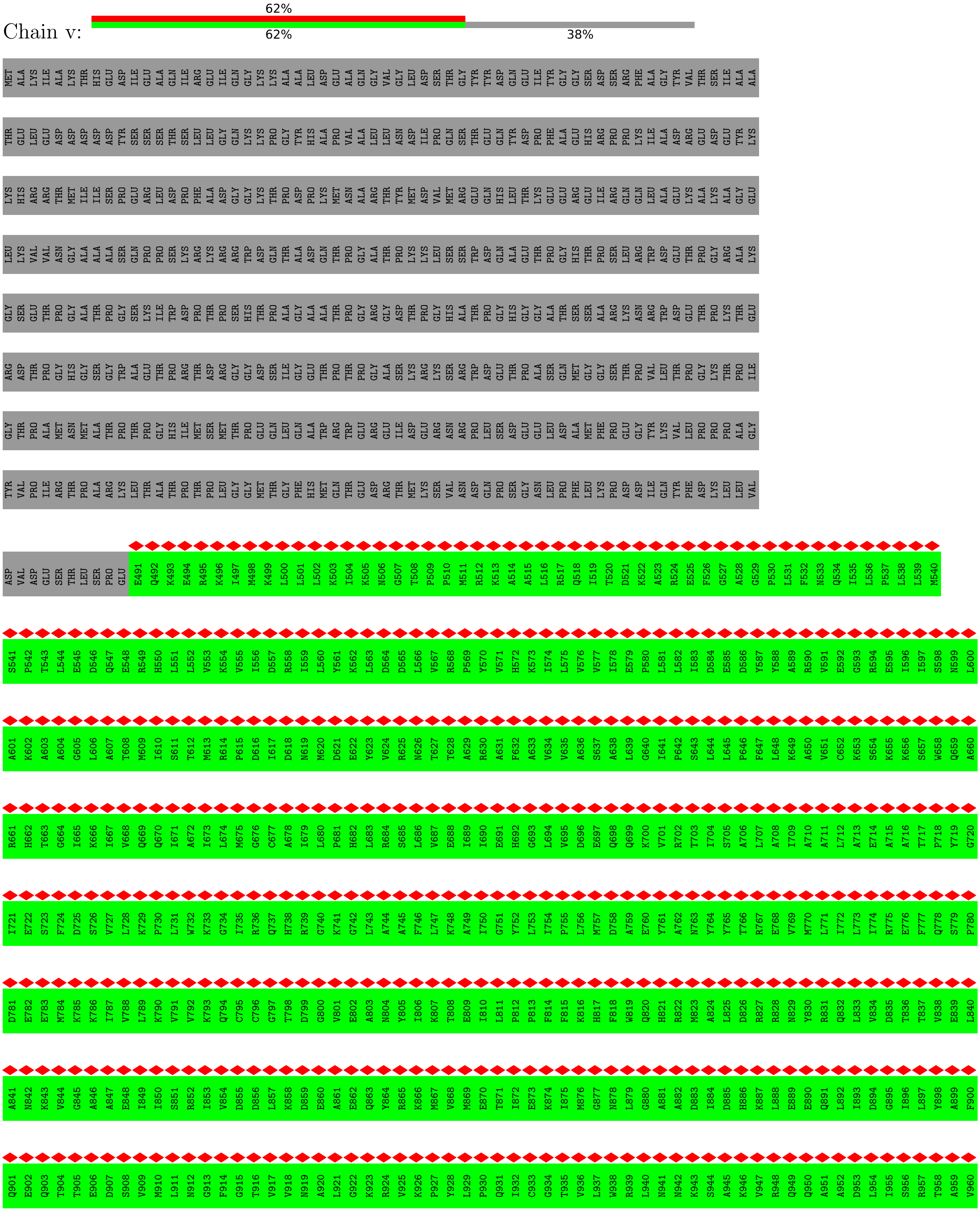
- Molecule 31: U6 snRNA-associated Sm-like protein LSm7

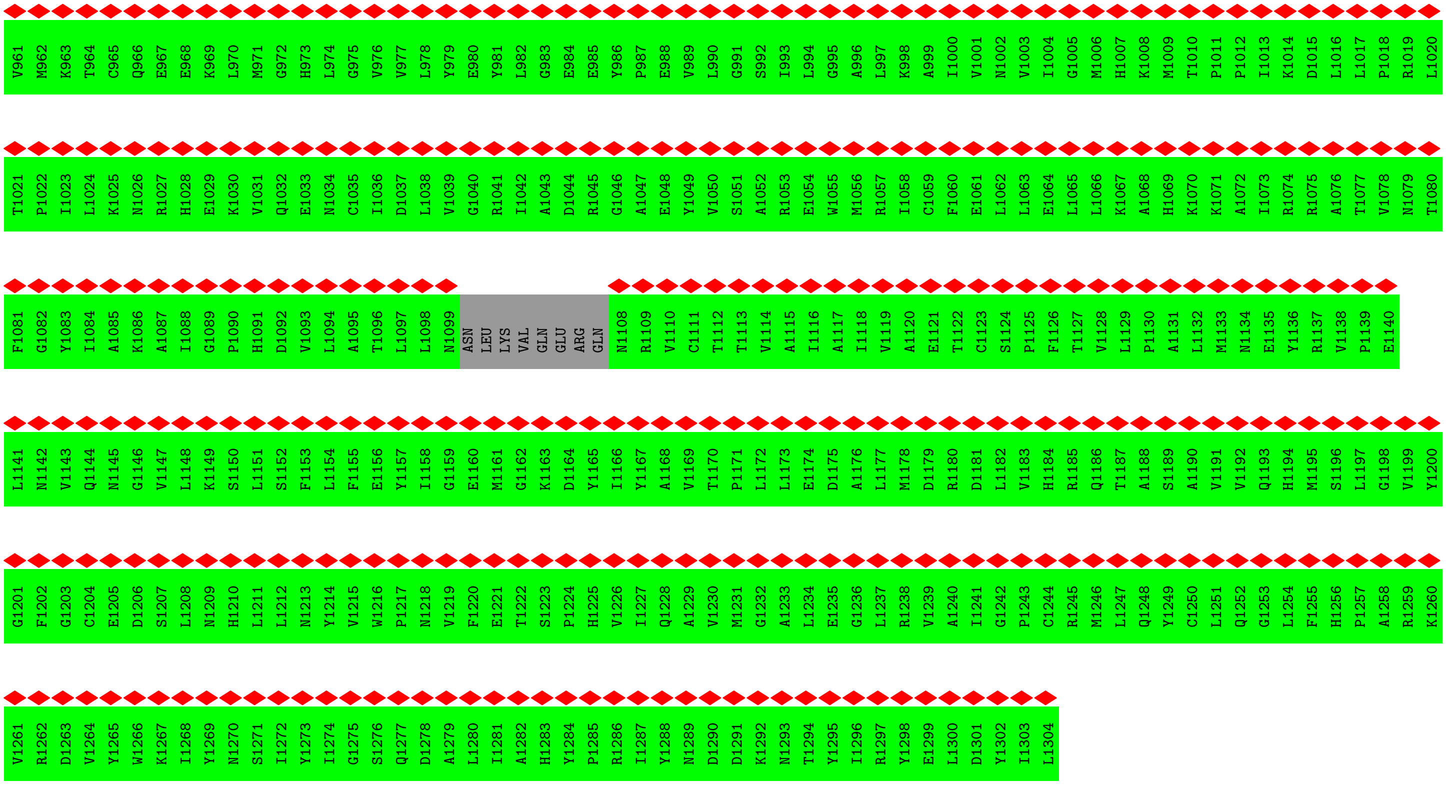


- Molecule 32: U6 snRNA-associated Sm-like protein LSm8

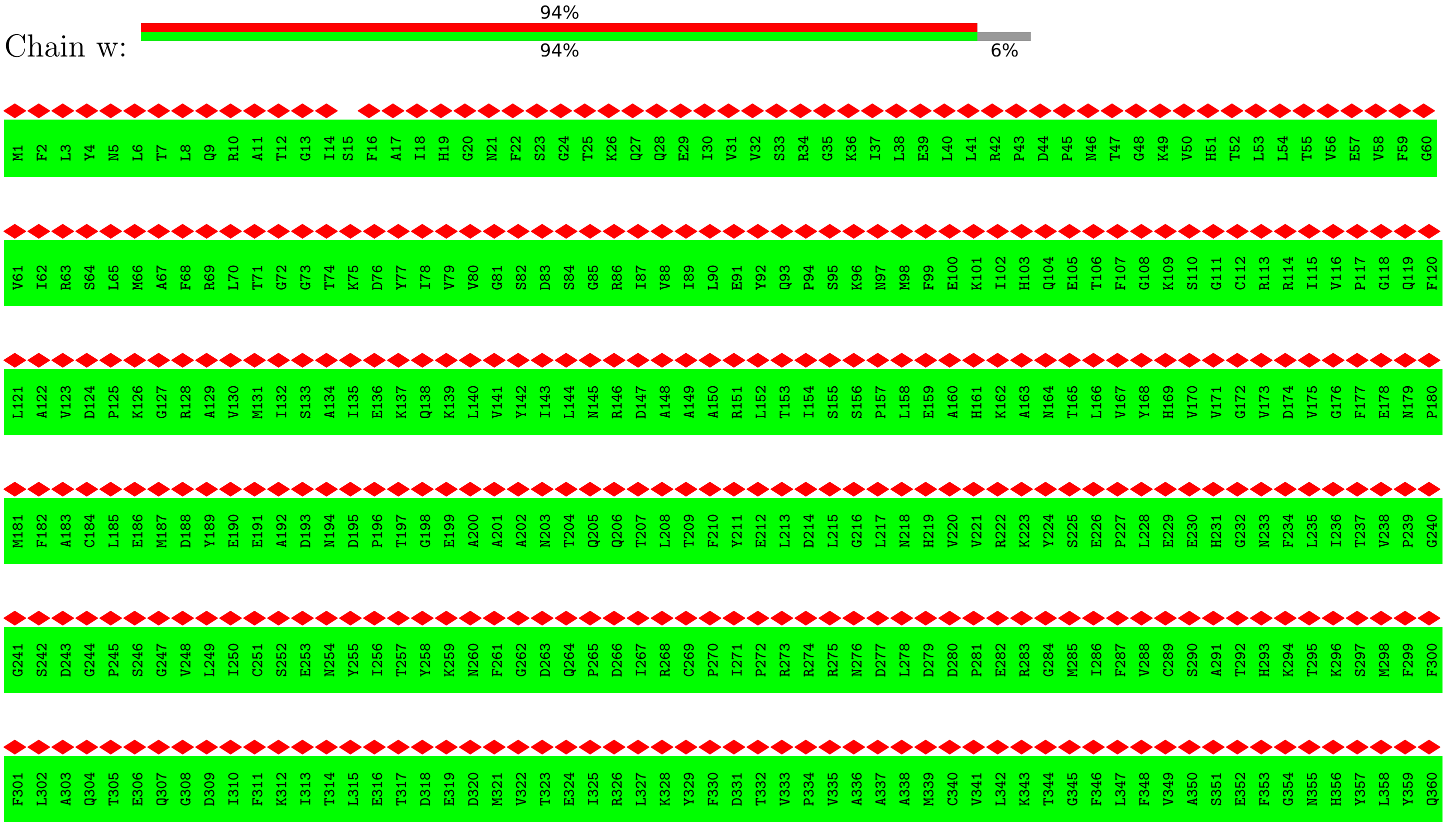


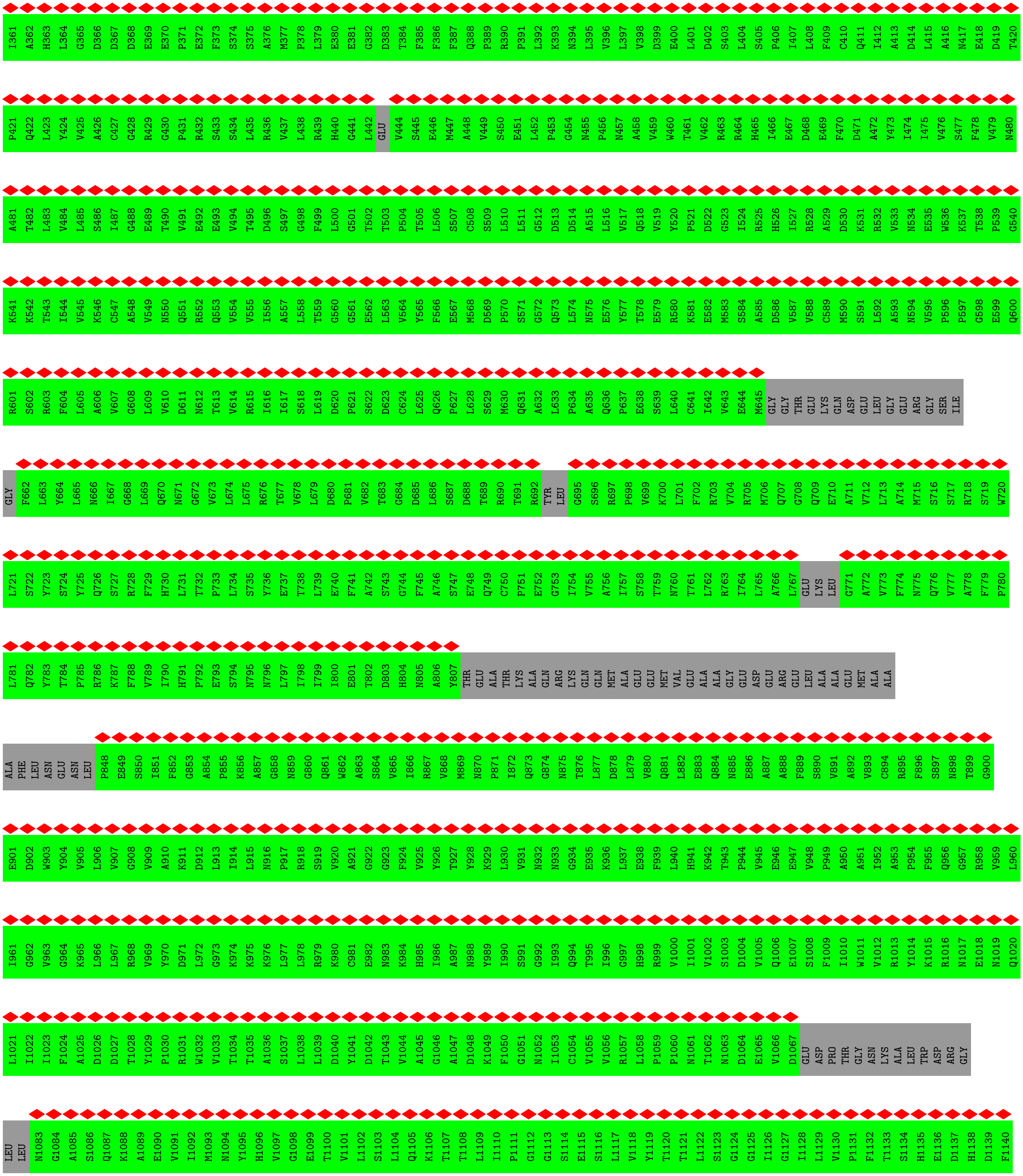
- Molecule 33: Splicing factor 3B subunit 1


62%
Chain v:
62%
38%
MET ALA LYS ILE ALA LYS THR HIS GLU ASP ILE GLU ALA GLN ILE ARG GLU ILE GLN GLY LYS LYS ALA ALA LEU ASP GLU ALA GLN GLY VAL GLY LEU ASP SER THR GLY TYR TYR ASP GLN GLU ILE TYR GLY GLY SER ASP SER ARG PHE ALA GLY TYR VAL THR SER ILE ALA ALA
THR GLU LEU GLU ASP ASP ASP ASP ASP TYR SER SER SER THR SER LEU LEU GLY GLN LYS LYS PRO GLY TYR HIS ALA PRO VAL ALA LEU LEU ASN ASP ILE PRO GLN SER THR GLU GLN TYR ASP PRO PHE ALA GLU HIS ARG PRO PRO LYS ILE ALA ASP ARG GLU ASP GLU TYR LYS
LYS HIS ARG ARG THR MET ILE ILE SER PRO GLU ARG LEU ASP PRO PHE ALA ASP GLY GLY LYS THR PRO ASP PRO LYS MET ASN ALA ARG THR TYR MET ASP VAL MET ARG GLU GLN HIS LEU THR LYS GLU GLU ARG GLU ILE ARG GLN GLN LEU ALA GLU LYS ALA LYS ALA GLY GLU
LEU LYS VAL VAL ASN GLY ALA ALA ALA SER GLN PRO PRO SER LYS ARG LYS ARG ARG TRP ASP GLN THR ALA ASP GLN THR PRO GLY ALA THR PRO LYS LYS LEU SER SER TRP ASP GLN ALA GLU THR PRO GLY HIS THR PRO SER LEU ARG TRP ASP GLU THR PRO GLY ARG ALA LYS
GLY SER GLU THR PRO GLY ALA THR PRO GLY SER LYS ILE TRP ASP PRO THR PRO SER HIS THR PRO ALA GLY ALA ALA THR PRO GLY ARG GLY ASP THR PRO GLY HIS ALA THR PRO GLY HIS GLY GLY ALA THR SER SER ALA ARG LYS ASN ARG TRP ASP GLU THR PRO LYS THR GLU
ARG ASP THR PRO GLY HIS GLY SER GLY TRP ALA GLU THR PRO ARG THR ASP ARG GLY GLY ASP SER ILE GLY GLU THR PRO THR PRO GLY ALA SER LYS ARG LYS SER ARG TRP ASP GLU THR PRO ALA SER GLN MET GLY GLY SER THR PRO VAL LEU THR PRO GLY LYS THR PRO ILE
GLY THR PRO ALA MET ASN MET ALA THR PRO THR PRO GLY HIS ILE MET SER MET THR PRO GLU GLN LEU GLN ALA TRP ARG TRP GLU ARG GLU ILE ASP GLU ARG ASN ARG PRO LEU SER ASP GLU GLU LEU ASP ALA MET PHE PRO GLU GLY TYR LYS VAL LEU PRO PRO PRO ALA GLY
TYR VAL PRO ILE ARG THR PRO ALA ARG LYS LEU THR ALA THR PRO THR PRO LEU GLY GLY MET THR GLY PHE HIS MET GLN THR GLU ASP ARG THR MET LYS SER VAL ASN ASP GLN PRO SER GLY ASN LEU PRO PHE LEU LYS PRO ASP ASP ILE GLN TYR PHE ASP LYS LEU LEU VAL
ASP VAL ASP GLU SER THR LEU SER PRO GLU E491 Q492 K493 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 N506 G507 T508 P509 P510 M511 R512 K513 A514 A515 L516 R517 Q518 I519 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 F532 N533 Q534 I535 L536 P537 L538 L539 M540
S541 P542 T543 L544 E545 D546 Q547 E548 R549 H550 L551 L552 V553 K554 V555 I556 D557 R558 I559 L560 Y561 K562 L563 D564 D565 L566 V567 R568 P569 Y570 V571 H572 K573 I574 L575 V576 V577 I578 E579 P580 L581 L582 I583 D584 E585 D586 Y587 Y588 A589 R590 V591 E592 G593 R594 E595 I596 I597 S598 N599 L600
A601 K602 A603 A604 G605 L606 A607 T608 M609 I610 S611 T612 M613 R614 P615 D616 I617 D618 N619 M620 D621 E622 Y623 V624 R625 N626 T627 T628 A629 R630 A631 F632 A633 V634 V635 A636 S637 A638 L639 G640 I641 P642 S643 L644 L645 P646 F647 L648 K649 A650 V651 C652 K653 S654 K655 K656 S657 W658 Q659 A660
R661 H662 T663 G664 I665 K666 I667 V668 Q669 Q670 I671 A672 I673 L674 M675 G676 C677 A678 I679 L680 P681 H682 L683 R684 S685 L686 V687 E688 I689 I690 E691 H692 G693 L694 V695 D696 E697 Q698 Q699 K700 V701 R702 T703 I704 S705 A706 L707 A708 I709 A710 A711 L712 A713 E714 A715 A716 T717 P718 Y719 G720
I721 E722 S723 F724 D725 S726 V727 L728 K729 P730 L731 W732 K733 G734 I735 R736 Q737 H738 R739 G740 K741 G742 L743 A744 A745 F746 L747 K748 A749 I750 G751 Y752 L753 I754 P755 L756 M757 D758 A759 E760 Y761 A762 N763 Y764 Y765 T766 R767 E768 V769 M770 L771 I772 L773 I774 R775 E776 F777 Q778 S779 P780
D781 E782 E783 M784 K785 K786 I787 V788 L789 K790 V791 V792 K793 Q794 C795 C796 G797 T798 D799 G800 V801 E802 A803 N804 Y805 I806 K807 T808 E809 I810 L811 P812 P813 F814 F815 K816 H817 F818 W819 Q820 H821 R822 M823 A824 L825 D826 R827 R828 N829 Y830 R831 Q832 L833 V834 D835 T836 T837 V838 E839 L840
A841 N842 K843 V844 G845 A846 A847 E848 I849 I850 S851 R852 I853 V854 D855 D856 L857 K858 D859 E860 A861 E862 Q863 Y864 R865 K866 M867 V868 M869 E870 T871 I872 E873 K874 I875 M876 G877 N878 L879 G880 A881 A882 D883 I884 D885 H886 K887 L888 E889 E890 Q891 L892 I893 D894 G895 I896 L897 Y898 A899 F900
Q901 E902 Q903 T904 T905 E906 D907 S908 V909 M910 L911 N912 G913 F914 G915 T916 V917 V918 N919 A920 L921 G922 K923 R924 V925 K926 P927 Y928 L929 P930 Q931 I932 C933 G934 T935 V936 L937 W938 R939 L940 N941 N942 K943 S944 A945 K946 V947 R948 Q949 Q950 A951 A952 D953 L954 I955 S956 R957 T958 A959 V960



- Molecule 34: Splicing factor 3B subunit 3 (SF3B3)





I361 A362 H363 L364 G365 D366 D367 D368 E369 E370 P371 E372 F373 S374 S375 A376 M377 P378 L379 E380 E381 G382 D383 T384 F385 F386 F387 Q388 P389 R390 P391 L392 K393 N394 L395 V396 L397 V398 D399 E400 L401 D402 S403 L404 S405 P406 I407 L408 F409 C410 Q411 I412 A413 D414 L415 A416 N417 E418 D419 T420

P421 Q422 L423 Y424 V425 A426 C427 G428 R429 G430 P431 R432 S433 S434 L435 R436 V437 L438 R439 H440 G441 L442 GLU V444 S445 E446 M447 A448 V449 S450 E451 L452 P453 G454 N455 P456 N457 A458 V459 W460 T461 V462 R463 R464 H465 I466 E467 D468 E469 F470 D471 A472 Y473 I474 I475 V476 S477 F478 V479 N480

A481 T482 L483 V484 L485 S486 I487 G488 E489 T490 V491 E492 E493 V494 T495 D496 S497 G498 F499 L500 G501 T502 T503 P504 T505 L506 S507 C508 S509 L510 L511 G512 D513 D514 A515 L516 V517 Q518 V519 Y520 P521 D522 G523 I524 R525 H526 I527 R528 A529 D530 K531 R532 V533 N534 E535 W536 K537 T538 P539 G540

K541 K542 T543 I544 V545 K546 C547 A548 V549 N550 Q551 R552 Q553 V554 V555 I556 A557 L558 T559 G560 G561 E562 L563 V564 Y565 F566 E567 M568 D569 P570 S571 G572 Q573 L574 N575 E576 Y577 T578 E579 R580 K581 E582 M583 S584 A585 D586 V587 V588 C589 M590 S591 L592 A593 N594 V595 P596 P597 G598 E599 Q600

R601 S602 R603 F604 L605 A606 V607 G608 L609 V610 D611 N612 T613 V614 R615 I616 I617 S618 L619 D620 P621 S622 D623 C624 L625 Q626 P627 L628 S629 M630 Q631 A632 L633 P634 A635 Q636 P637 E638 S639 L640 C641 I642 V643 E644 M645 GLY GLY THR GLU LYS GLN ASP GLU LEU GLY GLU ARG GLY SER ILE

GLY F662 L663 Y664 L665 N666 I667 G668 L669 Q670 N671 G672 V673 L674 L675 R676 T677 V678 L679 D680 P681 V682 T683 G684 D685 L686 S687 D688 T689 R690 T691 R692 TYR LEU G695 S696 R697 P698 V699 K700 L701 F702 R703 V704 R705 M706 Q707 G708 Q709 E710 A711 V712 L713 A714 M715 S716 S717 R718 S719 W720

L721 S722 Y723 S724 Y725 Q726 S727 R728 F729 H730 L731 T732 P733 L734 S735 Y736 E737 T738 L739 E740 F741 A742 S743 G744 F745 A746 S747 E748 Q749 C750 P751 E752 G753 I754 V755 A756 I757 S758 T759 N760 T761 L762 R763 I764 L765 A766 L767 GLU LYS LEU G771 A772 V773 F774 N775 Q776 V777 A778 F779 P780

L781 Q782 Y783 T784 P785 R786 K787 F788 V789 I790 H791 P792 E793 S794 N795 N796 L797 I798 I799 I800 E801 T802 D803 H804 N805 A806 Y807 THR GLU ALA THR LYS ALA GLN ARG LYS GLN GLN MET ALA GLU GLU MET VAL GLU ALA ALA GLY GLU ASP GLU ARG GLU LEU ALA ALA GLU MET ALA ALA

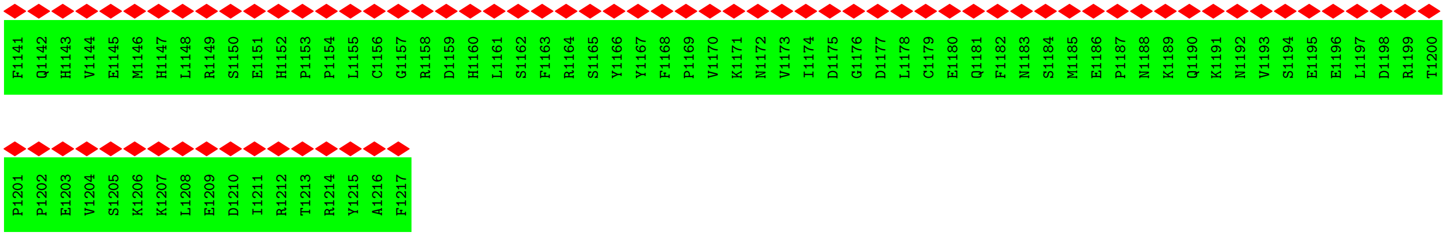
ALA PHE LEU ASN GLU ASN LEU P848 E849 S850 I851 F852 G853 A854 P855 K856 A857 G858 N859 G860 Q861 W862 A863 S864 V865 I866 R867 V868 M869 N870 P871 I872 Q873 G874 N875 T876 L877 D878 L879 V880 Q881 L882 E883 Q884 N885 E886 A887 A888 F889 S890 V891 A892 V893 C894 R895 F896 S897 N898 T899 G900

E901 D902 W903 Y904 V905 L906 V907 G908 V909 A910 K911 D912 L913 I914 L915 N916 P917 R918 S919 V920 A921 G922 G923 F924 V925 Y926 T927 Y928 K929 L930 V931 N932 E933 G934 E935 K936 L937 E938 F939 L940 H941 K942 T943 P944 V945 E946 E947 V948 P949 A950 A951 I952 A953 P954 F955 Q956 G957 R958 V959 L960

I961 G962 V963 G964 K965 L966 L967 R968 V969 Y970 D971 L972 G973 K974 K975 K976 L977 L978 R979 K980 C981 E982 N983 K984 H985 I986 A987 N988 Y989 I990 S991 G992 I993 Q994 T995 I996 G997 H998 R999 V1000 I1001 V1002 S1003 D1004 V1005 Q1006 E1007 S1008 F1009 I1010 W1011 V1012 R1013 Y1014 K1015 R1016 N1017 E1018 N1019 Q1020

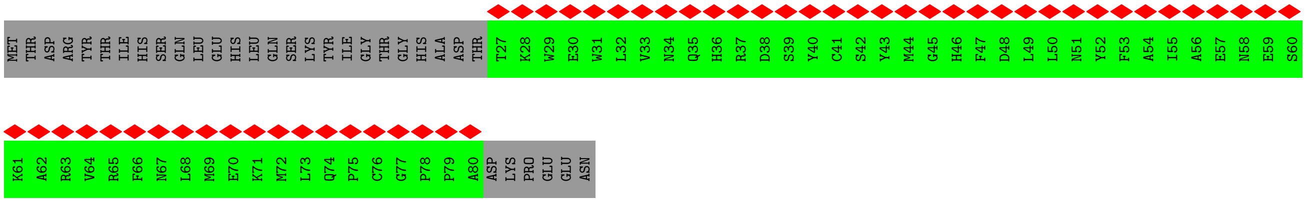
L1021 I1022 I1023 F1024 A1025 D1026 D1027 T1028 Y1029 P1030 R1031 W1032 V1033 T1034 T1035 A1036 S1037 L1038 L1039 D1040 Y1041 D1042 T1043 V1044 A1045 G1046 A1047 D1048 K1049 F1050 G1051 N1052 I1053 C1054 V1055 V1056 R1057 L1058 P1059 P1060 N1061 T1062 N1063 D1064 E1065 V1066 D1067 GLU ASP PRO THR GLY ASN LYS ALA LEU TRP ASP ARG GLY

LEU LEU N1083 G1084 A1085 S1086 Q1087 K1088 A1089 E1090 V1091 I1092 M1093 N1094 Y1095 H1096 V1097 G1098 E1099 T1100 V1101 L1102 S1103 L1104 Q1105 K1106 T1107 T1108 L1109 I1110 P1111 G1112 G1113 S1114 E1115 S1116 L1117 V1118 Y1119 T1120 T1121 L1122 S1123 G1124 G1125 I1126 G1127 I1128 L1129 V1130 P1131 F1132 T1133 S1134 H1135 E1136 D1137 H1138 D1139 F1140



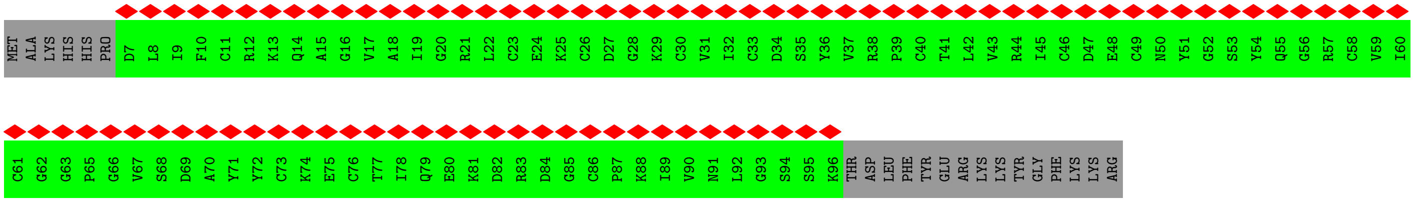
- Molecule 35: Splicing factor 3B subunit 5

Chain x:



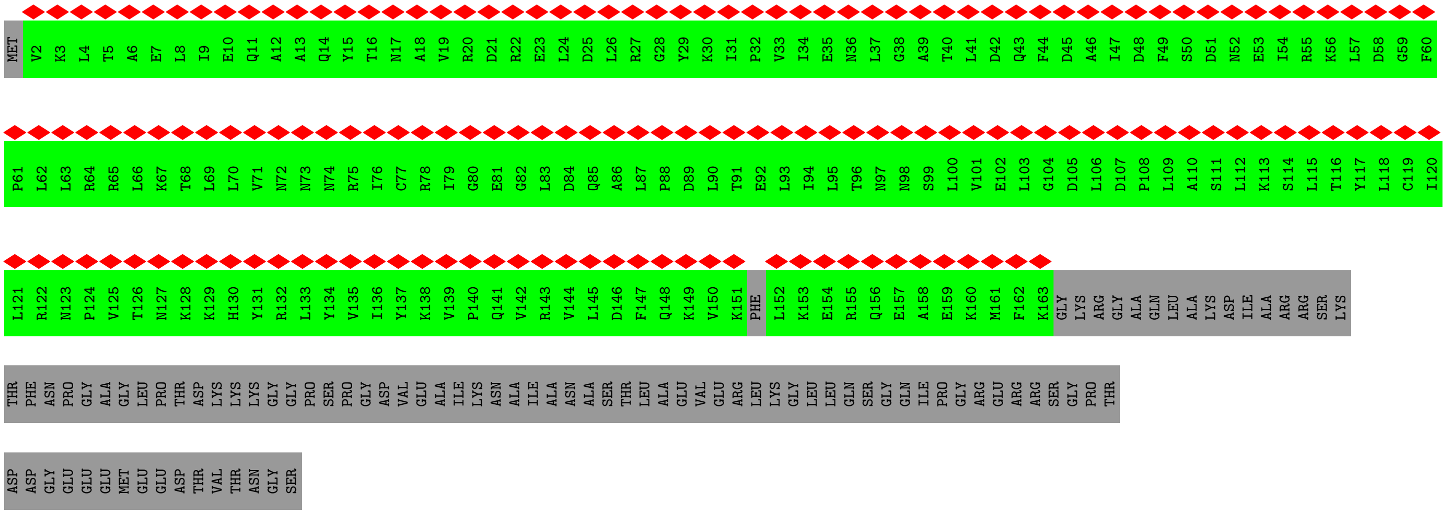
- Molecule 36: PHD finger-like domain-containing protein 5A

Chain y:

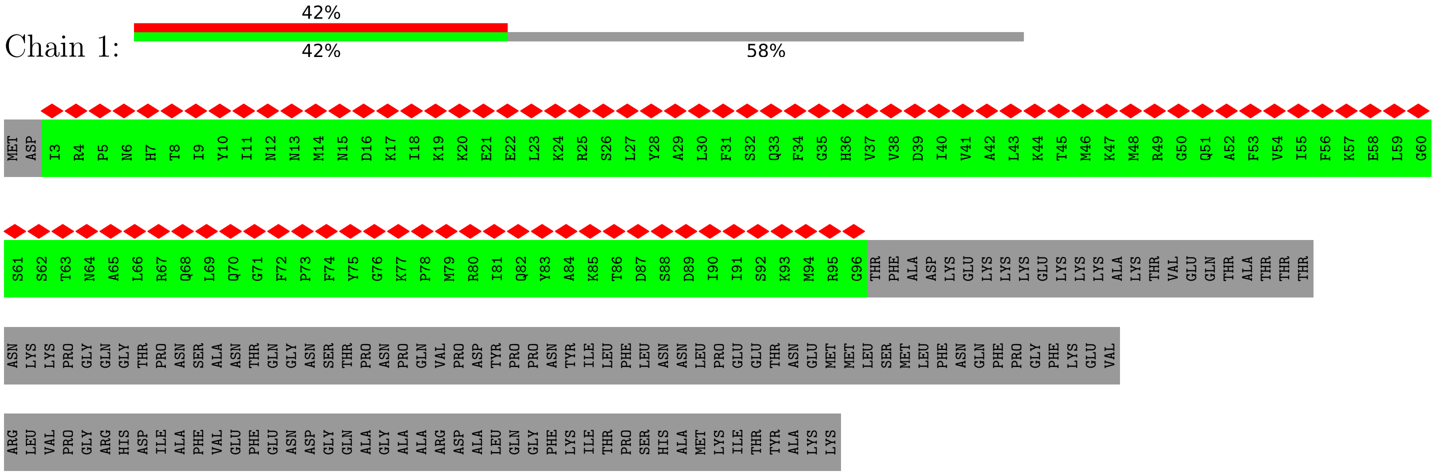


- Molecule 37: U2 small nuclear ribonucleoprotein A'

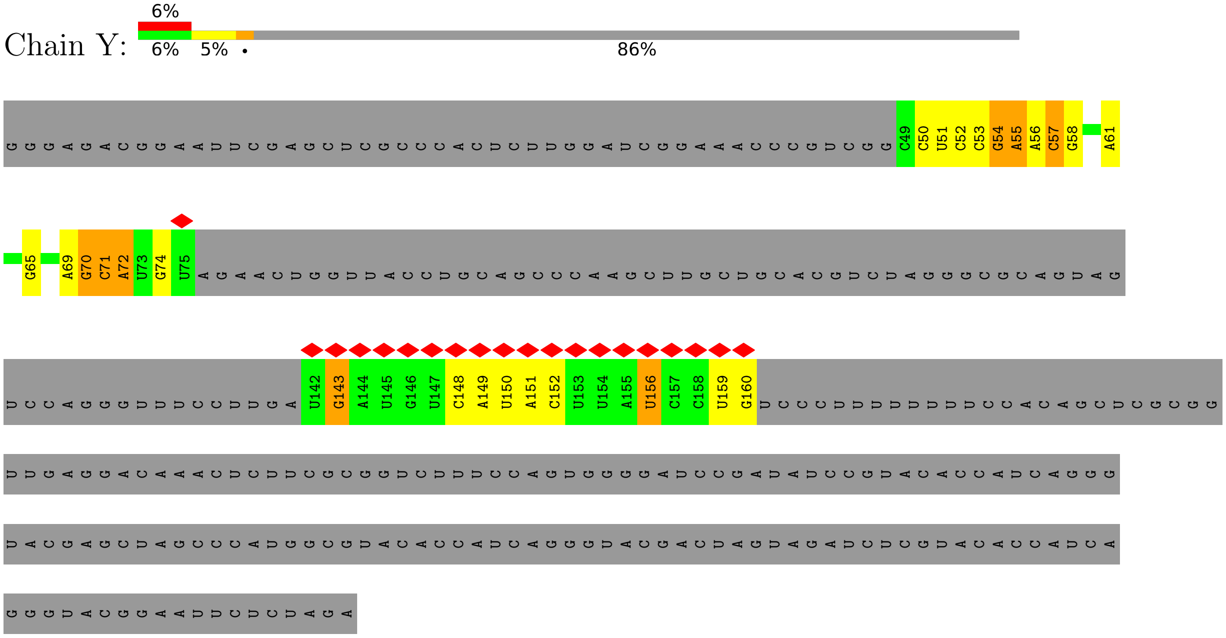
Chain z:



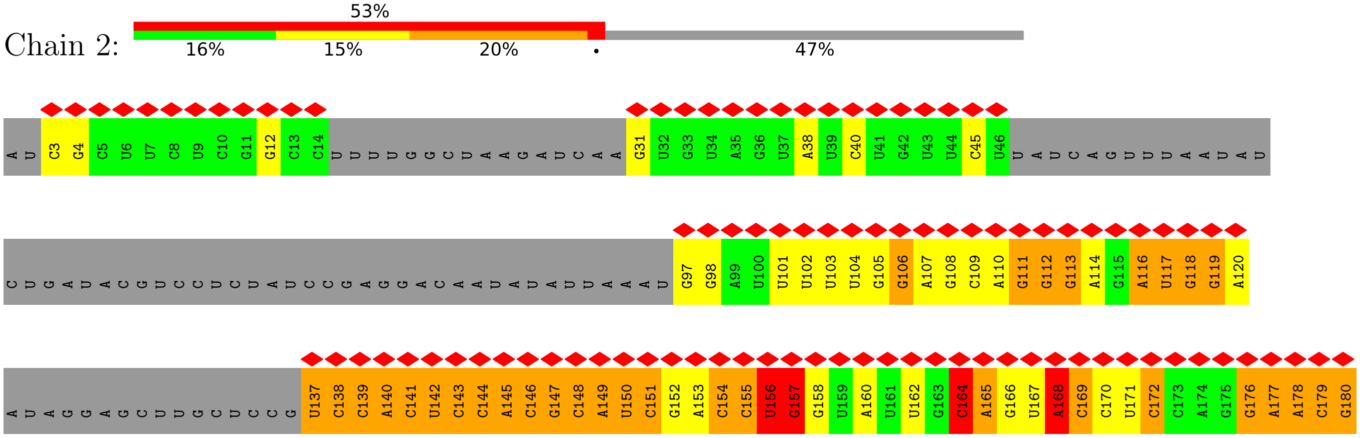
- Molecule 38: U2 small nuclear ribonucleoprotein B"

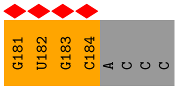


- Molecule 39: MINX pre-mRNA



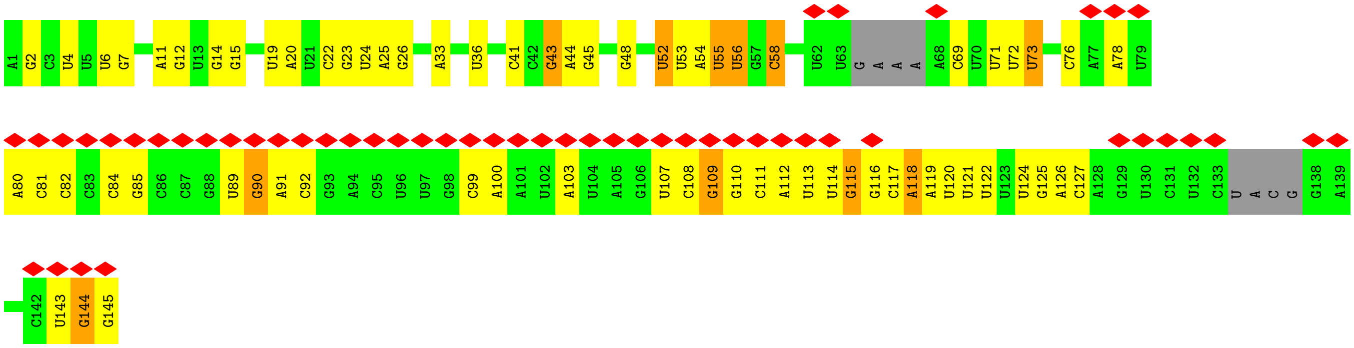
- Molecule 40: Human gene for small nuclear RNA U2 (snRNA U2)





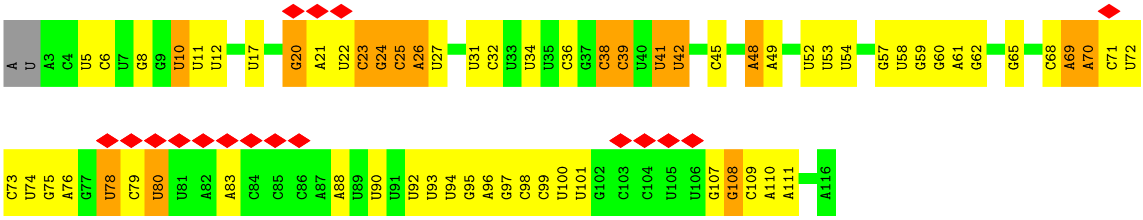
- Molecule 41: Homo sapiens U4A snRNA

Chain 4:



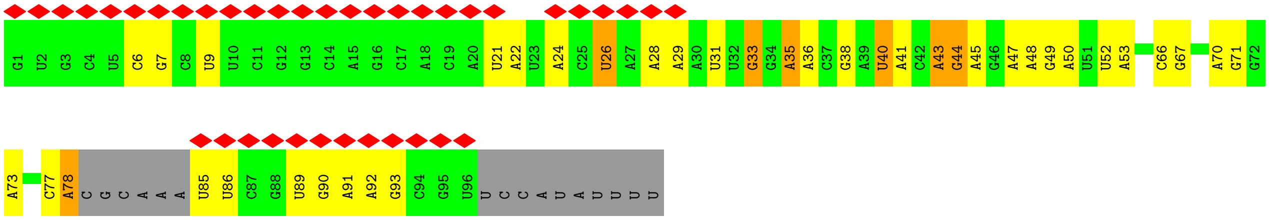
- Molecule 42: Homo sapiens U5 A small nuclear RNA

Chain 5:



- Molecule 43: Homo sapiens RNA, U6 small nuclear 1 (RNU6-1), small nuclear RNA

Chain 6:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	501.12, 501.12, 501.12	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/11222	0.41	0/15747
2	B	0.24	0/4312	0.43	0/6043
3	C	0.23	0/8613	0.41	0/12069
5	E	0.23	0/1107	0.42	0/1547
6	F	0.24	0/2115	0.45	0/2951
7	G	0.26	1/4089 (0.0%)	0.40	0/5728
8	H	0.49	1/2082 (0.0%)	0.40	0/2910
9	I	0.23	0/888	0.40	0/1241
10	J	0.23	0/681	0.38	0/952
11	K	0.22	0/224	0.29	0/312
12	L	0.24	0/2295	0.44	0/3198
13	M	0.24	0/853	0.47	0/1188
14	N	0.22	0/276	0.43	0/383
15	O	0.22	0/641	0.39	0/898
16	P	0.22	0/459	0.36	0/640
17	Q	0.24	0/379	0.35	0/530
18	R	0.21	0/78	0.35	0/107
19	a	0.22	0/394	0.44	0/548
19	h	0.22	0/371	0.44	0/516
20	b	0.24	0/367	0.45	0/509
20	i	0.24	0/357	0.46	0/495
21	c	0.22	0/388	0.46	0/540
21	j	0.22	0/388	0.45	0/540
22	d	0.23	0/346	0.48	0/481
22	k	0.23	0/366	0.47	0/509
23	e	0.23	0/392	0.47	0/546
23	l	0.23	0/354	0.45	0/492
24	f	0.23	0/319	0.43	0/442
24	m	0.22	0/314	0.44	0/434
25	g	0.23	0/471	0.42	0/657
25	n	0.22	0/414	0.45	0/578
39	Y	0.44	4/1083 (0.4%)	0.75	0/1681
40	2	0.88	16/2366 (0.7%)	1.55	70/3677 (1.9%)
41	4	0.16	0/3240	0.71	0/5039

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
42	5	0.16	0/2672	0.76	0/4154
43	6	0.14	0/2155	0.70	0/3355
All	All	0.30	22/57071 (0.0%)	0.58	70/81637 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
7	G	0	3
All	All	0	5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	268	LEU	C-N	19.79	1.71	1.34
40	2	150	U	C1'-N1	6.93	1.59	1.48
40	2	111	G	C1'-N9	-6.89	1.37	1.46
40	2	182	U	C1'-N1	6.86	1.59	1.48
40	2	142	U	C1'-N1	6.77	1.58	1.48
40	2	137	U	C1'-N1	6.76	1.58	1.48
40	2	148	C	C1'-N1	6.49	1.58	1.48
40	2	143	C	C1'-N1	6.35	1.58	1.48
7	G	400	VAL	C-N	6.35	1.46	1.34
40	2	141	C	C1'-N1	6.31	1.58	1.48
40	2	139	C	C1'-N1	6.31	1.58	1.48
40	2	97	G	C1'-N9	-6.30	1.38	1.46
39	Y	143	G	C1'-N9	-6.30	1.38	1.46
40	2	179	C	C1'-N1	6.29	1.58	1.48
40	2	151	C	C1'-N1	6.23	1.58	1.48
40	2	144	C	C1'-N1	6.23	1.58	1.48
40	2	138	C	C1'-N1	6.21	1.58	1.48
40	2	184	C	C1'-N1	6.21	1.58	1.48
40	2	110	A	C1'-N9	-5.70	1.38	1.46
39	Y	148	C	C1'-N1	5.48	1.56	1.48
39	Y	152	C	C1'-N1	5.38	1.56	1.48
39	Y	156	U	C1'-N1	5.25	1.56	1.48

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	2	167	U	C5-C4-O4	11.77	132.96	125.90
40	2	164	C	N1-C2-O2	-10.19	112.78	118.90
40	2	162	U	N3-C2-O2	-9.05	115.87	122.20
40	2	164	C	C5'-C4'-O4'	-8.38	99.04	109.10
40	2	169	C	P-O3'-C3'	8.20	129.53	119.70
40	2	167	U	N3-C4-O4	-8.02	113.78	119.40
40	2	166	G	O4'-C1'-N9	7.91	114.53	108.20
40	2	164	C	P-O3'-C3'	7.55	128.76	119.70
40	2	164	C	N3-C2-O2	7.50	127.15	121.90
40	2	167	U	N1-C2-O2	7.27	127.89	122.80
40	2	179	C	OP2-P-O3'	7.27	121.19	105.20
40	2	141	C	OP2-P-O3'	7.25	121.15	105.20
40	2	151	C	OP2-P-O3'	7.25	121.15	105.20
40	2	143	C	OP2-P-O3'	7.24	121.12	105.20
40	2	139	C	OP2-P-O3'	7.24	121.12	105.20
40	2	149	A	OP2-P-O3'	7.22	121.09	105.20
40	2	150	U	OP2-P-O3'	7.22	121.08	105.20
40	2	140	A	OP2-P-O3'	7.21	121.06	105.20
40	2	180	G	OP2-P-O3'	7.21	121.06	105.20
40	2	119	G	OP2-P-O3'	7.20	121.04	105.20
40	2	181	G	OP2-P-O3'	7.19	121.02	105.20
40	2	182	U	OP2-P-O3'	7.19	121.02	105.20
40	2	138	C	OP2-P-O3'	7.19	121.01	105.20
40	2	142	U	OP2-P-O3'	7.18	121.00	105.20
40	2	148	C	OP2-P-O3'	7.16	120.94	105.20
40	2	183	G	OP2-P-O3'	7.14	120.92	105.20
40	2	137	U	OP2-P-O3'	7.14	120.92	105.20
40	2	168	A	P-O5'-C5'	-7.14	109.48	120.90
40	2	167	U	N3-C2-O2	-7.04	117.27	122.20
40	2	106	G	O5'-P-OP1	6.92	119.00	110.70
40	2	119	G	O3'-P-O5'	-6.80	91.08	104.00
40	2	151	C	O3'-P-O5'	-6.80	91.08	104.00
40	2	181	G	O3'-P-O5'	-6.80	91.09	104.00
40	2	183	G	O3'-P-O5'	-6.79	91.10	104.00
40	2	142	U	O3'-P-O5'	-6.79	91.10	104.00
40	2	141	C	O3'-P-O5'	-6.78	91.11	104.00
40	2	150	U	O3'-P-O5'	-6.78	91.11	104.00
40	2	166	G	C8-N9-C4	-6.78	103.69	106.40
40	2	182	U	O3'-P-O5'	-6.78	91.12	104.00
40	2	180	G	O3'-P-O5'	-6.77	91.14	104.00
40	2	137	U	O3'-P-O5'	-6.77	91.14	104.00
40	2	139	C	O3'-P-O5'	-6.76	91.15	104.00
40	2	140	A	O3'-P-O5'	-6.76	91.16	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	2	179	C	O3'-P-O5'	-6.76	91.16	104.00
40	2	149	A	O3'-P-O5'	-6.75	91.17	104.00
40	2	138	C	O3'-P-O5'	-6.73	91.22	104.00
40	2	143	C	O3'-P-O5'	-6.72	91.22	104.00
40	2	148	C	O3'-P-O5'	-6.72	91.24	104.00
40	2	155	C	P-O3'-C3'	6.69	127.72	119.70
40	2	157	G	C5-C6-O6	-6.29	124.83	128.60
40	2	162	U	N1-C2-O2	6.28	127.20	122.80
40	2	157	G	N1-C6-O6	6.26	123.66	119.90
40	2	166	G	N9-C4-C5	6.24	107.90	105.40
40	2	165	A	O4'-C1'-N9	-6.16	103.27	108.20
40	2	166	G	N3-C4-C5	-5.95	125.63	128.60
40	2	172	C	P-O3'-C3'	5.87	126.75	119.70
40	2	167	U	O3'-P-O5'	-5.79	93.01	104.00
40	2	168	A	C5'-C4'-C3'	-5.79	106.75	116.00
40	2	164	C	C5-C4-N4	-5.72	116.19	120.20
40	2	156	U	P-O3'-C3'	-5.72	112.84	119.70
40	2	166	G	C6-N1-C2	-5.40	121.86	125.10
40	2	156	U	OP2-P-O3'	5.39	117.06	105.20
40	2	157	G	P-O5'-C5'	-5.22	112.55	120.90
40	2	160	A	C4'-C3'-C2'	-5.21	97.39	102.60
40	2	162	U	C2-N3-C4	-5.20	123.88	127.00
40	2	160	A	P-O5'-C5'	-5.15	112.66	120.90
40	2	170	C	N3-C4-C5	-5.14	119.84	121.90
40	2	156	U	C4'-C3'-C2'	5.12	107.72	102.60
40	2	170	C	O4'-C1'-C2'	-5.12	100.68	105.80
40	2	176	G	OP1-P-OP2	-5.11	111.93	119.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	ARG	Peptide
1	A	948	PRO	Peptide
7	G	308	HIS	Peptide
7	G	840	ASP	Peptide
7	G	841	PRO	Peptide

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	A	11100	0	5431	72	0
2	B	4264	0	2120	32	0
3	C	8538	0	4146	60	0
4	D	302	0	0	0	0
5	E	1101	0	543	15	0
6	F	2100	0	1038	24	0
7	G	4057	0	2089	37	0
8	H	2068	0	1019	20	0
9	I	883	0	414	4	0
10	J	677	0	316	1	0
11	K	225	0	98	2	0
12	L	2288	0	1076	10	0
13	M	844	0	426	3	0
14	N	277	0	114	2	0
15	O	636	0	322	2	0
16	P	458	0	225	1	0
17	Q	378	0	190	1	0
18	R	79	0	32	0	0
19	S	87	0	0	0	0
19	a	393	0	176	0	0
19	h	371	0	162	0	0
20	T	74	0	0	0	0
20	b	364	0	181	0	0
20	i	354	0	177	0	0
21	U	79	0	0	0	0
21	c	388	0	167	0	0
21	j	388	0	167	0	0
22	V	74	0	0	0	0
22	d	344	0	168	0	0
22	k	364	0	176	0	0
23	W	80	0	0	2	0
23	e	390	0	188	0	0
23	l	353	0	166	0	0
24	X	71	0	0	0	0
24	f	319	0	144	0	0
24	m	316	0	133	0	0
25	Z	82	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	g	469	0	214	0	0
25	n	412	0	185	0	0
26	o	90	0	0	0	0
27	p	73	0	0	0	0
28	q	80	0	0	0	0
29	r	76	0	0	0	0
30	s	69	0	0	0	0
31	t	79	0	0	0	0
32	u	62	0	0	0	0
33	v	806	0	0	0	0
34	w	1140	0	0	0	0
35	x	54	0	0	0	0
36	y	89	0	0	0	0
37	z	162	0	0	0	0
38	1	94	0	0	0	0
39	Y	972	0	495	31	0
40	2	2123	0	1076	178	0
41	4	2904	0	1470	44	0
42	5	2397	0	1216	40	0
43	6	1926	0	973	33	0
All	All	59243	0	27233	553	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 7.

All (553) 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)
40:2:153:A:H2	40:2:178:A:N1	1.00	1.46
1:A:2313:HIS:CB	3:C:1045:PRO:HB3	1.47	1.44
40:2:153:A:C2'	40:2:154:C:H5'	1.46	1.42
8:H:268:LEU:C	8:H:269:PRO:N	1.71	1.39
40:2:153:A:N1	40:2:178:A:N6	1.73	1.37
40:2:153:A:C2	40:2:178:A:N1	1.91	1.36
40:2:106:G:H21	40:2:107:A:N6	1.23	1.35
40:2:106:G:N2	40:2:107:A:C6	1.97	1.29
39:Y:149:A:N1	40:2:40:C:N4	1.78	1.29
40:2:153:A:O2'	40:2:154:C:C5'	1.79	1.29
40:2:108:G:H2'	40:2:109:C:C6	1.68	1.27
39:Y:143:G:O6	40:2:45:C:N4	1.71	1.21
40:2:153:A:C2	40:2:178:A:C6	2.31	1.18

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
40:2:153:A:O2'	40:2:154:C:H5'	1.01	1.17
40:2:153:A:C2'	40:2:154:C:C5'	2.22	1.16
40:2:106:G:N2	40:2:107:A:N6	1.94	1.13
40:2:156:U:H6	40:2:156:U:H5"	1.10	1.10
40:2:154:C:O2	40:2:178:A:N6	1.85	1.09
1:A:2268:LEU:O	3:C:1264:PRO:HG2	1.53	1.08
39:Y:149:A:H61	40:2:40:C:N4	1.50	1.07
39:Y:149:A:N6	40:2:40:C:N4	2.03	1.07
1:A:2268:LEU:O	3:C:1264:PRO:CG	2.04	1.06
39:Y:149:A:C6	40:2:40:C:N4	2.19	1.06
40:2:105:G:H2'	40:2:106:G:H5"	1.37	1.05
40:2:153:A:H2'	40:2:154:C:C5'	1.81	1.05
1:A:2074:ARG:CB	3:C:1047:PRO:HG2	1.86	1.03
39:Y:72:A:N6	43:6:33:G:H1	1.53	1.03
1:A:2313:HIS:CB	3:C:1045:PRO:CB	2.37	1.01
40:2:153:A:H2	40:2:178:A:C6	1.74	1.01
40:2:153:A:C2	40:2:178:A:N6	2.28	1.00
40:2:168:A:C8	40:2:168:A:H5"	1.99	0.98
40:2:112:G:C2	40:2:113:G:C5	2.51	0.97
42:5:12:U:H3	42:5:65:G:H1	1.12	0.97
41:4:91:A:H2	41:4:110:G:N2	1.61	0.97
40:2:153:A:H2'	40:2:154:C:H5'	1.34	0.96
40:2:112:G:H2'	40:2:113:G:H8	1.29	0.96
41:4:4:U:H3	43:6:71:G:H1	0.98	0.94
40:2:156:U:H5"	40:2:156:U:C6	2.02	0.93
39:Y:149:A:N1	40:2:40:C:C4	2.37	0.93
39:Y:149:A:N6	40:2:40:C:H42	1.62	0.93
39:Y:65:G:H1	43:6:40:U:H3	0.99	0.92
40:2:118:G:H2'	40:2:119:G:H8	1.33	0.92
40:2:153:A:N1	40:2:178:A:C6	2.34	0.91
40:2:112:G:O2'	40:2:113:G:H5'	1.69	0.91
40:2:168:A:H5"	40:2:168:A:H8	1.37	0.90
39:Y:149:A:H61	40:2:40:C:H41	1.14	0.90
40:2:112:G:N3	40:2:113:G:C8	2.40	0.89
40:2:144:C:H2'	40:2:145:A:H5"	1.54	0.89
39:Y:58:G:H1	42:5:41:U:H3	0.92	0.89
40:2:112:G:C2	40:2:113:G:N7	2.42	0.87
40:2:144:C:H3'	40:2:145:A:H5'	1.56	0.86
7:G:312:TRP:O	7:G:316:ALA:HB3	1.75	0.86
39:Y:143:G:O6	40:2:45:C:C4	2.29	0.86
40:2:108:G:H2'	40:2:109:C:H6	1.35	0.86

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
40:2:106:G:N2	40:2:107:A:N1	2.22	0.86
40:2:156:U:H6	40:2:156:U:C5’	1.89	0.86
39:Y:74:G:H1	43:6:31:U:H3	0.86	0.85
40:2:105:G:C2’	40:2:106:G:H5”	2.09	0.81
40:2:108:G:H2’	40:2:109:C:C5	2.14	0.81
41:4:91:A:H2	41:4:110:G:H22	0.83	0.81
41:4:108:C:O2’	41:4:109:G:H5’	1.81	0.81
40:2:112:G:C4	40:2:113:G:N7	2.49	0.80
40:2:112:G:N3	40:2:113:G:N7	2.30	0.80
42:5:17:U:H3	42:5:60:G:H1	0.83	0.80
7:G:842:HIS:O	7:G:846:ALA:HB2	1.83	0.80
40:2:101:U:H5”	40:2:102:U:H5’	1.64	0.80
40:2:154:C:C2	40:2:178:A:N6	2.47	0.79
40:2:178:A:O2’	40:2:179:C:H5’	1.85	0.77
39:Y:72:A:H61	43:6:33:G:H1	0.78	0.77
1:A:2070:LYS:O	3:C:1047:PRO:HG3	1.84	0.76
40:2:112:G:H2’	40:2:113:G:C8	2.18	0.76
39:Y:149:A:N1	40:2:40:C:N3	2.33	0.76
40:2:106:G:H4’	40:2:107:A:O4’	1.85	0.76
40:2:178:A:H2’	40:2:179:C:H6	1.49	0.75
1:A:464:PRO:HG2	42:5:20:G:H4’	1.69	0.75
40:2:144:C:H3’	40:2:145:A:C5’	2.17	0.75
1:A:75:ASP:HA	9:I:14:GLY:HA2	1.70	0.73
40:2:118:G:H2’	40:2:119:G:C8	2.23	0.72
2:B:441:PRO:O	2:B:445:ALA:HB2	1.88	0.72
7:G:361:VAL:O	7:G:365:ALA:HB2	1.89	0.72
40:2:153:A:HO2’	40:2:154:C:C5’	2.02	0.72
40:2:109:C:H6	40:2:109:C:O5’	1.73	0.71
39:Y:143:G:O6	40:2:45:C:N3	2.23	0.71
8:H:288:ARG:O	8:H:292:ALA:HB2	1.91	0.70
40:2:153:A:H2’	40:2:154:C:O5’	1.91	0.70
40:2:154:C:H1’	40:2:178:A:N1	2.05	0.70
7:G:842:HIS:O	7:G:846:ALA:CB	2.39	0.70
1:A:2313:HIS:CA	3:C:1045:PRO:HB3	2.19	0.70
40:2:12:G:H1	43:6:86:U:H3	1.39	0.69
40:2:177:A:H2	40:2:178:A:H62	1.39	0.68
40:2:150:U:H3	40:2:181:G:H1	1.41	0.68
7:G:312:TRP:O	7:G:316:ALA:CB	2.42	0.68
8:H:292:ALA:O	8:H:296:ALA:HB2	1.93	0.68
15:O:113:LYS:O	15:O:117:GLN:CB	2.41	0.67
40:2:112:G:N1	40:2:113:G:C6	2.62	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:111:SER:HA	13:M:140:VAL:HA	1.76	0.67
7:G:841:PRO:O	7:G:843:VAL:N	2.27	0.67
41:4:24:U:H3	41:4:48:G:H1	1.42	0.67
41:4:2:G:O6	43:6:73:A:N1	2.27	0.67
11:K:299:LYS:O	11:K:303:GLU:CB	2.43	0.67
39:Y:150:U:H6	39:Y:150:U:O5'	1.77	0.67
41:4:111:C:O5'	41:4:111:C:H6	1.78	0.67
40:2:168:A:C8	40:2:168:A:C5'	2.75	0.66
42:5:78:U:O2'	42:5:80:U:OP1	2.14	0.66
40:2:154:C:O2	40:2:178:A:C6	2.49	0.66
41:4:6:U:H2'	41:4:7:G:H8	1.61	0.65
42:5:58:U:H2'	42:5:59:G:H8	1.62	0.65
1:A:2152:GLY:HA3	1:A:2157:VAL:HA	1.79	0.65
41:4:117:C:O5'	41:4:117:C:H6	1.80	0.65
9:I:35:TRP:O	9:I:39:CYS:CB	2.45	0.65
6:F:349:TRP:HA	6:F:356:GLU:HA	1.78	0.65
40:2:144:C:C3'	40:2:145:A:C5'	2.75	0.65
40:2:153:A:C2'	40:2:154:C:O5'	2.43	0.65
40:2:156:U:C6	40:2:156:U:C5'	2.72	0.64
3:C:1084:VAL:O	3:C:1088:ALA:HB2	1.97	0.64
39:Y:149:A:C2	40:2:40:C:N3	2.65	0.64
3:C:1077:LEU:O	3:C:1081:MET:N	2.27	0.63
40:2:112:G:N1	40:2:113:G:C5	2.66	0.63
40:2:164:C:H6	40:2:164:C:H5'	1.63	0.63
2:B:371:GLU:O	2:B:375:GLU:CB	2.46	0.63
41:4:89:U:C2'	41:4:90:G:H5'	2.29	0.63
40:2:112:G:C2	40:2:113:G:C8	2.85	0.63
41:4:108:C:H2'	41:4:109:G:H8	1.63	0.62
1:A:2074:ARG:CB	3:C:1047:PRO:CG	2.73	0.62
7:G:311:ALA:O	7:G:315:SER:CB	2.47	0.62
41:4:89:U:O2'	41:4:90:G:H5'	1.99	0.62
3:C:1081:MET:O	3:C:1085:THR:CB	2.48	0.62
7:G:407:TRP:O	7:G:411:VAL:CB	2.48	0.62
41:4:91:A:O5'	41:4:91:A:H8	1.82	0.62
1:A:534:GLU:O	1:A:538:SER:CB	2.48	0.62
1:A:2317:PHE:CB	3:C:1043:ARG:CB	2.78	0.62
5:E:513:GLU:O	5:E:517:ALA:HB2	2.00	0.62
7:G:875:GLY:O	7:G:879:ALA:HB2	2.00	0.61
3:C:488:LEU:O	3:C:492:ALA:HB3	2.01	0.61
13:M:107:PRO:HG3	13:M:129:SER:HA	1.81	0.61
2:B:328:ALA:HA	2:B:332:GLY:HA3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:745:LEU:O	7:G:749:LEU:CB	2.47	0.61
1:A:239:TYR:O	1:A:243:ASN:CB	2.49	0.61
40:2:147:G:H2'	40:2:148:C:H6	1.66	0.61
42:5:12:U:O4	42:5:65:G:O6	2.19	0.61
40:2:146:C:O5'	40:2:147:G:H4'	2.01	0.61
23:W:54:ARG:CA	40:2:151:C:O2	2.50	0.60
39:Y:151:A:O5'	39:Y:151:A:H8	1.84	0.60
40:2:146:C:OP2	40:2:147:G:H4'	2.01	0.60
40:2:157:G:H8	40:2:157:G:H5"	1.65	0.60
3:C:1393:TRP:O	3:C:1397:PHE:CB	2.49	0.60
3:C:1080:ASP:O	3:C:1084:VAL:CB	2.50	0.60
7:G:861:ARG:O	7:G:865:HIS:CB	2.50	0.59
3:C:774:LEU:O	3:C:778:LEU:N	2.31	0.59
1:A:1007:ASP:O	1:A:1011:ALA:HB2	2.02	0.59
7:G:379:ALA:O	7:G:383:GLU:CB	2.50	0.59
40:2:176:G:H2'	40:2:177:A:O4'	2.02	0.59
13:M:29:ILE:HA	13:M:144:ILE:HA	1.83	0.59
16:P:198:ASP:HA	16:P:202:ALA:HB3	1.84	0.59
3:C:482:ASN:O	3:C:486:SER:N	2.36	0.58
3:C:1084:VAL:O	3:C:1088:ALA:CB	2.52	0.58
41:4:110:G:O5'	41:4:110:G:H8	1.86	0.58
40:2:118:G:O2'	40:2:119:G:H5'	2.04	0.58
39:Y:143:G:C6	40:2:45:C:N3	2.71	0.58
40:2:114:A:O5'	40:2:114:A:H8	1.86	0.58
41:4:33:A:H62	41:4:43:G:H21	1.49	0.58
1:A:77:THR:HA	9:I:17:PRO:HD3	1.84	0.58
2:B:441:PRO:O	2:B:445:ALA:CB	2.51	0.58
6:F:130:GLU:O	6:F:134:ASN:CB	2.52	0.58
7:G:783:SER:O	7:G:787:GLU:CB	2.52	0.58
40:2:146:C:H2'	40:2:148:C:OP1	2.03	0.58
2:B:208:HIS:O	2:B:212:SER:N	2.37	0.57
2:B:474:LEU:HA	2:B:499:GLY:HA3	1.85	0.57
40:2:112:G:C2'	40:2:113:G:H5'	2.33	0.57
40:2:108:G:C5	40:2:109:C:C4	2.91	0.57
40:2:152:G:H2'	40:2:153:A:H8	1.68	0.57
40:2:144:C:C2'	40:2:145:A:H5"	2.30	0.57
8:H:372:ARG:O	8:H:376:ASN:CB	2.52	0.57
1:A:85:LYS:O	1:A:89:LEU:CB	2.53	0.57
1:A:305:ARG:HA	2:B:923:PRO:HG3	1.85	0.57
39:Y:74:G:O6	43:6:31:U:O4	2.22	0.57
41:4:108:C:C2'	41:4:109:G:H5'	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:THR:O	2:B:432:ASP:CB	2.53	0.56
42:5:61:A:H2'	42:5:62:G:H8	1.69	0.56
1:A:1682:ALA:O	1:A:1686:ASP:CB	2.53	0.56
39:Y:57:C:N4	42:5:42:U:O4	2.36	0.56
40:2:146:C:P	40:2:147:G:H4'	2.45	0.56
40:2:183:G:H2'	40:2:184:C:H6	1.70	0.56
5:E:548:VAL:O	5:E:579:VAL:N	2.26	0.56
6:F:295:LEU:O	6:F:307:TRP:N	2.33	0.56
9:I:116:CYS:O	9:I:120:LEU:CB	2.53	0.56
11:K:300:GLU:O	11:K:304:ILE:CB	2.54	0.56
40:2:143:C:C2	40:2:144:C:C5	2.93	0.56
40:2:109:C:C6	40:2:109:C:O5'	2.57	0.56
40:2:137:U:H2'	40:2:138:C:H6	1.71	0.56
40:2:138:C:C2	40:2:139:C:C5	2.93	0.56
1:A:950:LEU:O	1:A:954:LYS:CB	2.52	0.56
40:2:106:G:C2	40:2:107:A:C6	2.89	0.56
42:5:69:A:O2'	42:5:70:A:N3	2.39	0.56
42:5:109:C:H2'	42:5:110:A:H8	1.70	0.56
40:2:105:G:N2	40:2:107:A:H5'	2.20	0.56
40:2:141:C:H2'	40:2:142:U:H6	1.71	0.56
40:2:141:C:C2	40:2:142:U:C5	2.94	0.56
41:4:111:C:H2'	41:4:112:A:H8	1.69	0.56
3:C:485:GLN:O	3:C:489:TYR:CB	2.53	0.56
40:2:137:U:C2	40:2:138:C:C5	2.94	0.56
40:2:149:A:H2'	40:2:150:U:H6	1.70	0.56
3:C:1395:GLU:O	3:C:1399:ASP:CB	2.54	0.56
39:Y:65:G:O6	43:6:40:U:O4	2.24	0.56
40:2:142:U:C2	40:2:143:C:C5	2.94	0.56
41:4:108:C:H2'	41:4:109:G:C8	2.41	0.56
6:F:202:PRO:O	6:F:206:ARG:CB	2.55	0.55
7:G:11:MET:O	7:G:13:ALA:N	2.38	0.55
40:2:140:A:C4	40:2:141:C:C5	2.95	0.55
40:2:150:U:C2	40:2:151:C:C5	2.94	0.55
1:A:532:THR:O	1:A:536:LYS:CB	2.54	0.55
5:E:544:SER:HA	5:E:631:VAL:HA	1.87	0.55
40:2:147:G:H2'	40:2:148:C:C6	2.40	0.55
3:C:1332:GLN:O	3:C:1336:PHE:CB	2.54	0.55
40:2:143:C:H2'	40:2:144:C:H6	1.71	0.55
42:5:109:C:H2'	42:5:110:A:C8	2.41	0.55
7:G:419:ALA:O	7:G:423:LEU:CB	2.54	0.55
40:2:106:G:N2	40:2:107:A:H61	1.98	0.55

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
40:2:142:U:H2’	40:2:143:C:H6	1.71	0.55
40:2:178:A:O2’	40:2:179:C:C5’	2.53	0.55
43:6:78:A:N1	43:6:85:U:OP1	2.39	0.55
1:A:584:HIS:O	1:A:588:LEU:CB	2.55	0.55
40:2:118:G:O2’	40:2:119:G:C5’	2.55	0.55
40:2:140:A:H2’	40:2:141:C:H6	1.71	0.55
40:2:181:G:C4	40:2:182:U:C5	2.95	0.55
41:4:113:U:H6	41:4:113:U:O5’	1.90	0.55
1:A:1725:LEU:O	1:A:1729:ALA:CB	2.55	0.55
2:B:588:ILE:HA	2:B:660:VAL:HA	1.89	0.55
40:2:138:C:H2’	40:2:139:C:H6	1.71	0.55
40:2:183:G:C4	40:2:184:C:C5	2.94	0.55
1:A:2268:LEU:O	3:C:1264:PRO:HG3	2.04	0.54
1:A:947:PRO:HG2	1:A:948:PRO:HD2	1.90	0.54
12:L:330:THR:HA	12:L:346:ARG:HA	1.88	0.54
42:5:17:U:O2	42:5:60:G:N2	2.28	0.54
2:B:448:LYS:O	2:B:452:THR:CB	2.55	0.54
5:E:650:GLN:H	5:E:652:PRO:HD2	1.72	0.54
39:Y:159:U:H3	40:2:31:G:H22	1.55	0.54
40:2:150:U:H2’	40:2:151:C:H6	1.71	0.54
40:2:153:A:O2’	40:2:154:C:H5”	1.95	0.54
41:4:2:G:N1	43:6:73:A:C2	2.75	0.54
42:5:107:G:H3’	42:5:108:G:H8	1.73	0.54
1:A:1729:ALA:O	1:A:1733:ILE:CB	2.56	0.54
3:C:489:TYR:O	3:C:493:LEU:CB	2.55	0.54
6:F:223:PHE:N	6:F:517:LEU:O	2.40	0.54
40:2:181:G:H2’	40:2:182:U:H6	1.70	0.54
2:B:324:ALA:O	2:B:328:ALA:CB	2.56	0.54
40:2:146:C:OP2	40:2:147:G:C4’	2.56	0.54
40:2:149:A:C4	40:2:150:U:C5	2.95	0.54
39:Y:58:G:N2	42:5:41:U:O2	2.28	0.53
40:2:164:C:H5’	40:2:164:C:C6	2.44	0.53
1:A:734:PRO:HB3	7:G:149:LEU:HA	1.89	0.53
40:2:178:A:H2’	40:2:179:C:C6	2.37	0.53
2:B:482:TYR:O	2:B:491:HIS:N	2.40	0.53
1:A:235:MET:O	1:A:239:TYR:CB	2.56	0.53
1:A:1426:ASP:O	1:A:1430:LEU:CB	2.57	0.53
3:C:1563:VAL:O	3:C:1648:ARG:N	2.41	0.53
40:2:112:G:N2	40:2:113:G:C4	2.77	0.53
41:4:4:U:O2	43:6:71:G:N2	2.33	0.53
2:B:118:PHE:O	2:B:122:LEU:CB	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:490:ARG:O	3:C:494:GLU:CB	2.57	0.53
42:5:98:C:H2'	42:5:99:C:C6	2.43	0.53
1:A:84:ASP:O	1:A:88:TYR:CB	2.57	0.53
2:B:643:ASP:O	2:B:647:MET:CB	2.57	0.53
8:H:287:LEU:O	8:H:291:ALA:HB3	2.09	0.53
41:4:118:A:OP2	41:4:118:A:H8	1.92	0.53
3:C:1412:THR:O	3:C:1416:LEU:CB	2.57	0.53
1:A:1135:PRO:O	1:A:1139:ARG:N	2.41	0.52
2:B:742:PRO:HG2	2:B:785:ARG:HA	1.90	0.52
8:H:288:ARG:O	8:H:292:ALA:CB	2.56	0.52
7:G:361:VAL:O	7:G:365:ALA:CB	2.55	0.52
1:A:1725:LEU:O	1:A:1729:ALA:HB3	2.09	0.52
5:E:554:PRO:O	5:E:557:LYS:N	2.42	0.52
12:L:425:MET:HA	12:L:431:ILE:HA	1.92	0.52
41:4:2:G:H1	43:6:73:A:H2	1.56	0.52
43:6:52:U:O4	43:6:53:A:N6	2.42	0.52
7:G:875:GLY:O	7:G:879:ALA:CB	2.58	0.52
3:C:1224:LEU:HA	3:C:1236:HIS:HA	1.92	0.52
3:C:1033:GLU:O	3:C:1037:LEU:CB	2.58	0.51
8:H:167:VAL:O	8:H:171:ALA:CB	2.58	0.51
3:C:1389:VAL:O	3:C:1393:TRP:CB	2.57	0.51
39:Y:69:A:O2'	43:6:35:A:N6	2.42	0.51
41:4:143:U:H2'	41:4:144:G:H5"	1.92	0.51
40:2:152:G:H2'	40:2:153:A:C8	2.45	0.51
1:A:1931:THR:O	1:A:1935:ARG:CB	2.59	0.51
5:E:493:PRO:O	5:E:497:GLU:CB	2.59	0.51
7:G:418:ASP:O	7:G:422:MET:CB	2.58	0.51
8:H:355:GLY:H	41:4:58:C:H41	1.56	0.51
1:A:1684:PHE:O	1:A:1688:THR:CB	2.59	0.51
2:B:430:PHE:O	2:B:434:CYS:CB	2.59	0.51
6:F:204:THR:O	6:F:208:SER:CB	2.59	0.51
8:H:292:ALA:O	8:H:296:ALA:CB	2.59	0.51
42:5:99:C:H2'	42:5:100:U:C6	2.46	0.51
40:2:108:G:C2'	40:2:109:C:C6	2.65	0.51
42:5:48:A:H2'	42:5:49:A:H8	1.76	0.51
3:C:1221:PHE:HA	3:C:1272:SER:HA	1.93	0.51
3:C:1432:TRP:O	3:C:1436:SER:CB	2.59	0.51
6:F:224:CYS:HA	7:G:764:ALA:HB2	1.91	0.50
6:F:304:VAL:N	6:F:318:ILE:O	2.39	0.50
2:B:393:PRO:O	2:B:397:ASP:CB	2.58	0.50
3:C:1665:ASP:HA	3:C:1706:CYS:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:573:VAL:N	5:E:580:ASN:O	2.41	0.50
15:O:56:MET:O	15:O:83:VAL:N	2.43	0.50
42:5:97:G:H2'	42:5:98:C:H6	1.77	0.50
6:F:370:ILE:HA	6:F:381:THR:HA	1.92	0.50
40:2:112:G:C4	40:2:113:G:C8	2.96	0.50
40:2:177:A:N3	40:2:178:A:N7	2.58	0.50
1:A:564:TYR:O	1:A:569:VAL:N	2.45	0.50
1:A:1584:LYS:O	1:A:1588:SER:CB	2.59	0.50
7:G:142:PHE:O	7:G:146:LYS:CB	2.59	0.50
8:H:367:GLY:O	8:H:371:ILE:N	2.41	0.50
41:4:52:U:O2'	41:4:56:U:OP2	2.22	0.50
1:A:1378:GLU:O	1:A:1382:SER:CB	2.60	0.50
1:A:1833:LEU:O	1:A:1837:ALA:CB	2.60	0.50
10:J:25:VAL:N	10:J:55:PHE:O	2.40	0.50
1:A:880:ARG:O	1:A:884:HIS:CB	2.60	0.50
1:A:150:MET:O	1:A:154:GLU:CB	2.60	0.49
7:G:782:GLU:O	7:G:786:LEU:CB	2.59	0.49
40:2:117:U:H2'	40:2:118:G:C8	2.47	0.49
40:2:113:G:H2'	40:2:114:A:C8	2.47	0.49
41:4:111:C:H2'	41:4:112:A:C8	2.46	0.49
42:5:97:G:H2'	42:5:98:C:C6	2.47	0.49
42:5:17:U:O4	42:5:60:G:O6	2.31	0.49
42:5:25:C:H2'	42:5:26:A:C8	2.47	0.49
2:B:369:PHE:O	2:B:373:ILE:CB	2.60	0.49
2:B:777:GLY:N	2:B:782:GLU:O	2.46	0.49
5:E:554:PRO:HG3	43:6:78:A:H8	1.78	0.49
6:F:254:CYS:HA	6:F:266:HIS:HA	1.95	0.49
6:F:506:ILE:N	6:F:518:TRP:O	2.41	0.49
3:C:778:LEU:HA	3:C:782:PHE:O	2.13	0.49
3:C:872:SER:O	3:C:876:LEU:N	2.45	0.49
1:A:581:ILE:O	1:A:585:VAL:CB	2.61	0.49
43:6:24:A:H4'	43:6:26:U:H1'	1.94	0.49
1:A:2268:LEU:O	3:C:1264:PRO:CD	2.59	0.49
39:Y:69:A:H62	43:6:35:A:H2'	1.77	0.48
42:5:58:U:H2'	42:5:59:G:C8	2.46	0.48
1:A:280:GLU:O	1:A:282:LEU:N	2.46	0.48
40:2:116:A:O5'	40:2:116:A:H8	1.95	0.48
1:A:1007:ASP:O	1:A:1011:ALA:CB	2.60	0.48
7:G:841:PRO:C	7:G:843:VAL:H	2.17	0.48
2:B:508:LYS:N	2:B:566:THR:O	2.39	0.48
7:G:512:GLU:O	7:G:516:ALA:HB3	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:431:LYS:HA	6:F:443:THR:HA	1.94	0.48
7:G:449:ALA:O	7:G:453:LEU:CB	2.61	0.48
1:A:2070:LYS:O	3:C:1047:PRO:CG	2.59	0.48
7:G:817:ALA:O	7:G:821:GLU:CB	2.61	0.48
42:5:72:U:H2’	42:5:73:C:H6	1.78	0.48
1:A:883:ARG:O	1:A:887:THR:CB	2.62	0.48
41:4:110:G:H2’	41:4:111:C:C6	2.49	0.48
1:A:121:HIS:HA	1:A:482:PHE:HA	1.96	0.48
6:F:178:LEU:O	6:F:182:ASN:CB	2.62	0.48
8:H:268:LEU:C	8:H:269:PRO:CA	2.75	0.48
40:2:108:G:C2’	40:2:109:C:C5	2.92	0.48
41:4:2:G:C6	43:6:73:A:N1	2.82	0.48
1:A:1947:ASN:O	1:A:1951:LYS:CB	2.62	0.47
3:C:612:ILE:N	3:C:647:ARG:O	2.47	0.47
3:C:1037:LEU:O	3:C:1041:LEU:CB	2.62	0.47
39:Y:151:A:H2	40:2:38:A:N1	2.12	0.47
40:2:143:C:H2’	40:2:144:C:C6	2.49	0.47
42:5:23:C:H3’	42:5:24:G:H4’	1.96	0.47
3:C:725:VAL:N	3:C:811:SER:O	2.46	0.47
3:C:1761:TYR:O	3:C:1765:THR:CB	2.62	0.47
1:A:1778:TRP:HA	1:A:1811:ASN:HA	1.96	0.47
2:B:816:VAL:O	2:B:820:PHE:CB	2.63	0.47
3:C:1088:ALA:O	3:C:1092:MET:CB	2.63	0.47
40:2:142:U:H2’	40:2:143:C:C6	2.49	0.47
42:5:98:C:H2’	42:5:99:C:H6	1.80	0.47
42:5:110:A:H2’	42:5:111:A:C8	2.49	0.47
1:A:1568:THR:O	1:A:1572:SER:CB	2.62	0.47
3:C:1964:PRO:HA	3:C:2054:PRO:HG3	1.96	0.47
8:H:135:TYR:O	8:H:139:VAL:CB	2.62	0.47
3:C:1831:LEU:O	3:C:1835:SER:CB	2.62	0.47
7:G:680:LYS:HA	7:G:934:ALA:HB1	1.97	0.47
41:4:109:G:H2’	41:4:110:G:C8	2.50	0.47
1:A:117:PRO:HA	1:A:486:LYS:HA	1.96	0.47
2:B:261:ASP:O	2:B:265:LEU:CB	2.63	0.47
8:H:291:ALA:O	8:H:295:VAL:CB	2.63	0.47
40:2:117:U:H2’	40:2:118:G:H8	1.79	0.47
1:A:1470:TYR:O	1:A:1474:MET:CB	2.63	0.46
3:C:525:ILE:HA	3:C:531:ILE:HA	1.98	0.46
5:E:554:PRO:HG3	43:6:78:A:C8	2.50	0.46
40:2:138:C:H2’	40:2:139:C:C6	2.50	0.46
41:4:11:A:H2’	41:4:12:G:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:C:1620:LEU:N	3:C:1645:VAL:O	2.48	0.46
7:G:309:PRO:HB2	7:G:310:PRO:HD3	1.97	0.46
40:2:154:C:O5'	40:2:154:C:H6	1.97	0.46
41:4:89:U:HO2'	41:4:90:G:H5'	1.81	0.46
6:F:325:VAL:HA	6:F:341:CYS:HA	1.97	0.46
7:G:309:PRO:O	7:G:313:ILE:CB	2.63	0.46
40:2:137:U:H2'	40:2:138:C:C6	2.50	0.46
40:2:149:A:H2'	40:2:150:U:C6	2.50	0.46
1:A:1833:LEU:O	1:A:1837:ALA:HB3	2.14	0.46
8:H:253:GLY:HA3	8:H:273:TYR:H	1.81	0.46
40:2:140:A:H2'	40:2:141:C:C6	2.50	0.46
40:2:150:U:H2'	40:2:151:C:C6	2.50	0.46
40:2:181:G:H2'	40:2:182:U:C6	2.50	0.46
1:A:88:TYR:O	1:A:92:LEU:CB	2.64	0.46
2:B:833:PHE:N	2:B:900:VAL:O	2.41	0.46
6:F:167:HIS:C	6:F:169:GLY:H	2.19	0.46
40:2:180:G:H2'	40:2:181:G:H8	1.81	0.46
1:A:2130:GLY:HA3	1:A:2142:ILE:HA	1.98	0.46
14:N:105:GLN:O	14:N:110:MET:N	2.34	0.46
43:6:40:U:H2'	43:6:41:A:C8	2.51	0.46
2:B:508:LYS:HA	2:B:524:ILE:HA	1.98	0.46
5:E:563:ASN:O	5:E:567:LEU:N	2.48	0.46
8:H:167:VAL:O	8:H:171:ALA:HB3	2.16	0.46
43:6:66:C:H2'	43:6:67:G:C8	2.50	0.46
7:G:512:GLU:O	7:G:516:ALA:CB	2.63	0.46
40:2:112:G:N2	40:2:113:G:C5	2.82	0.46
40:2:112:G:C6	40:2:113:G:O6	2.69	0.46
6:F:421:ILE:N	6:F:433:TRP:O	2.49	0.45
8:H:39:THR:O	8:H:43:LEU:CB	2.64	0.45
40:2:183:G:H2'	40:2:184:C:C6	2.50	0.45
42:5:61:A:H2'	42:5:62:G:C8	2.50	0.45
6:F:255:LYS:N	6:F:265:LEU:O	2.49	0.45
40:2:178:A:C2'	40:2:179:C:O5'	2.64	0.45
1:A:463:PRO:O	42:5:24:G:N2	2.47	0.45
1:A:798:GLY:N	1:A:799:PRO:HD3	2.32	0.45
40:2:3:C:H2'	40:2:4:G:C8	2.51	0.45
40:2:177:A:H2	40:2:178:A:N6	2.09	0.45
7:G:912:TRP:O	7:G:916:SER:CB	2.64	0.45
40:2:148:C:H2'	40:2:149:A:H8	1.82	0.45
40:2:151:C:H2'	40:2:152:G:H8	1.81	0.45
3:C:912:ASN:HA	3:C:978:ASN:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2:179:C:H2'	40:2:180:G:H8	1.81	0.45
1:A:598:LEU:O	1:A:602:ILE:CB	2.64	0.45
17:Q:9:PRO:HB2	17:Q:22:ASP:HA	1.98	0.45
2:B:324:ALA:O	2:B:328:ALA:HB2	2.17	0.45
40:2:112:G:C2	40:2:113:G:C4	3.04	0.45
40:2:182:U:H2'	40:2:183:G:H8	1.81	0.45
42:5:10:U:H2'	42:5:11:U:C6	2.52	0.45
6:F:234:SER:N	6:F:248:ALA:O	2.49	0.45
40:2:119:G:H2'	40:2:120:A:H8	1.82	0.45
2:B:715:GLY:O	2:B:719:GLN:CB	2.64	0.44
40:2:116:A:O5'	40:2:116:A:C8	2.70	0.44
43:6:91:A:H2'	43:6:92:A:H8	1.82	0.44
3:C:2067:VAL:HA	3:C:2079:ILE:HA	2.00	0.44
40:2:141:C:H2'	40:2:142:U:C6	2.50	0.44
1:A:1809:ILE:O	1:A:1818:PHE:N	2.49	0.44
3:C:1522:PRO:HG2	12:L:343:LYS:HA	1.99	0.44
6:F:367:VAL:HA	6:F:383:GLY:HA2	2.00	0.44
7:G:340:PRO:HB2	7:G:368:HIS:O	2.18	0.44
1:A:897:GLU:O	1:A:908:VAL:N	2.48	0.44
3:C:785:HIS:N	3:C:810:VAL:O	2.51	0.44
41:4:115:G:H2'	41:4:116:G:C8	2.52	0.44
40:2:139:C:H2'	40:2:140:A:H8	1.81	0.44
43:6:89:U:H2'	43:6:90:G:C8	2.53	0.44
43:6:90:G:H2'	43:6:91:A:H8	1.82	0.44
5:E:594:PHE:O	5:E:598:MET:CB	2.66	0.44
43:6:91:A:H2'	43:6:92:A:C8	2.53	0.44
40:2:118:G:O6	40:2:140:A:N6	2.51	0.44
41:4:91:A:H2'	41:4:92:C:C6	2.53	0.44
1:A:1878:ASP:HA	7:G:282:PRO:HA	1.99	0.43
41:4:118:A:OP2	41:4:118:A:C8	2.70	0.43
2:B:215:VAL:O	2:B:219:LEU:CB	2.66	0.43
8:H:284:PRO:O	8:H:288:ARG:N	2.48	0.43
40:2:117:U:C2'	40:2:118:G:H5'	2.48	0.43
42:5:72:U:H2'	42:5:73:C:C6	2.53	0.43
8:H:355:GLY:N	41:4:58:C:H41	2.16	0.43
39:Y:71:C:H2'	39:Y:72:A:H8	1.83	0.43
43:6:40:U:H2'	43:6:41:A:H8	1.83	0.43
3:C:1186:LEU:HA	3:C:1204:ILE:HA	2.00	0.43
40:2:108:G:C4	40:2:109:C:C4	3.07	0.43
42:5:74:U:H2'	42:5:75:G:C8	2.52	0.43
5:E:513:GLU:O	5:E:517:ALA:CB	2.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:358:ARG:O	8:H:362:MET:CB	2.66	0.43
12:L:499:ILE:N	12:L:511:TRP:O	2.43	0.43
39:Y:70:G:H22	43:6:36:A:H2	1.66	0.43
6:F:279:VAL:N	6:F:296:ALA:O	2.51	0.43
8:H:314:GLY:O	8:H:318:TYR:CB	2.67	0.43
42:5:31:U:H2'	42:5:32:C:C6	2.54	0.43
1:A:440:PRO:HB2	1:A:442:LYS:H	1.83	0.43
1:A:1195:ARG:O	1:A:1229:PHE:N	2.46	0.43
2:B:642:HIS:O	2:B:646:LYS:CB	2.67	0.43
40:2:144:C:C4	40:2:146:C:OP1	2.72	0.43
40:2:153:A:H2'	40:2:154:C:H6	1.84	0.43
40:2:157:G:H5"	40:2:157:G:C8	2.50	0.43
1:A:679:SER:O	1:A:683:LEU:CB	2.67	0.43
3:C:548:VAL:O	3:C:552:VAL:CB	2.67	0.43
40:2:178:A:H2'	40:2:179:C:O5'	2.18	0.43
43:6:89:U:H2'	43:6:90:G:H8	1.84	0.43
3:C:783:ALA:HB3	3:C:809:LEU:HA	2.01	0.42
6:F:380:GLY:HA2	6:F:390:VAL:HA	2.00	0.42
12:L:488:ILE:H	12:L:503:SER:HA	1.84	0.42
2:B:396:LEU:O	2:B:400:GLY:N	2.51	0.42
40:2:108:G:C5	40:2:109:C:N4	2.87	0.42
40:2:112:G:HO2'	40:2:113:G:H5'	1.79	0.42
40:2:114:A:O5'	40:2:114:A:C8	2.70	0.42
40:2:118:G:C2'	40:2:119:G:O5'	2.67	0.42
12:L:146:ALA:O	12:L:150:ALA:CB	2.68	0.42
1:A:580:TYR:O	1:A:584:HIS:CB	2.67	0.42
3:C:488:LEU:O	3:C:492:ALA:CB	2.66	0.42
3:C:1390:TYR:O	3:C:1394:TYR:CB	2.67	0.42
43:6:92:A:H2'	43:6:93:G:H8	1.83	0.42
7:G:448:ASN:O	7:G:452:VAL:CB	2.68	0.42
12:L:331:ILE:N	12:L:345:PHE:O	2.44	0.42
23:W:80:ALA:CA	23:W:81:PRO:CA	2.98	0.42
40:2:98:G:H5'	40:2:104:U:OP2	2.19	0.42
1:A:926:LEU:O	1:A:930:ALA:CB	2.67	0.42
40:2:155:C:H2'	40:2:156:U:H5"	2.02	0.42
3:C:1386:ALA:O	3:C:1390:TYR:CB	2.68	0.42
7:G:841:PRO:C	7:G:843:VAL:N	2.73	0.42
41:4:90:G:H2'	41:4:91:A:C8	2.55	0.42
2:B:227:LEU:O	2:B:256:CYS:N	2.46	0.42
40:2:157:G:H2'	40:2:158:G:O4'	2.19	0.42
41:4:107:U:H2'	41:4:108:C:H6	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:241:TRP:HA	12:L:248:ILE:HA	2.01	0.42
40:2:3:C:H2'	40:2:4:G:H8	1.84	0.42
2:B:828:MET:HA	2:B:906:ILE:HA	2.01	0.42
41:4:14:G:H2'	41:4:15:G:C8	2.55	0.42
43:6:92:A:H2'	43:6:93:G:C8	2.54	0.42
1:A:2130:GLY:O	1:A:2173:GLU:N	2.53	0.41
1:A:981:PHE:C	1:A:983:LYS:H	2.23	0.41
42:5:75:G:H2'	42:5:76:A:C8	2.55	0.41
1:A:577:GLY:O	1:A:581:ILE:CB	2.68	0.41
3:C:1609:LEU:O	3:C:1613:LEU:CB	2.68	0.41
42:5:31:U:H2'	42:5:32:C:H6	1.85	0.41
42:5:59:G:C2	42:5:60:G:C8	3.08	0.41
3:C:823:ALA:O	3:C:857:GLY:N	2.50	0.41
6:F:257:TRP:N	6:F:262:CYS:O	2.43	0.41
7:G:824:PRO:C	7:G:826:ARG:H	2.24	0.41
40:2:171:U:H2'	40:2:172:C:O4'	2.21	0.41
1:A:1696:PRO:HB2	1:A:1699:THR:O	2.21	0.41
3:C:1915:ILE:O	3:C:1919:ALA:CB	2.69	0.41
41:4:22:C:H2'	41:4:23:G:C8	2.56	0.41
42:5:71:C:H2'	42:5:72:U:C6	2.56	0.41
14:N:80:TYR:O	14:N:89:VAL:N	2.47	0.41
41:4:55:U:H2'	41:4:56:U:C6	2.56	0.41
3:C:1058:LYS:O	3:C:1062:LEU:CB	2.69	0.41
39:Y:54:G:O2'	39:Y:55:A:H5"	2.21	0.41
40:2:117:U:H6	40:2:117:U:H5'	1.85	0.41
42:5:5:U:H2'	42:5:6:C:C6	2.56	0.41
42:5:38:C:N4	42:5:39:C:N3	2.68	0.41
2:B:121:ASP:O	2:B:125:ASN:CB	2.69	0.41
3:C:1431:LYS:O	3:C:1435:LEU:CB	2.69	0.41
40:2:103:U:C3'	40:2:104:U:H5'	2.51	0.41
40:2:107:A:H2'	40:2:108:G:C8	2.56	0.41
41:4:72:U:O2'	41:4:73:U:H5"	2.21	0.41
42:5:100:U:H2'	42:5:101:U:C6	2.57	0.41
43:6:43:A:H3'	43:6:44:G:H8	1.86	0.41
6:F:116:GLU:O	6:F:118:ILE:N	2.52	0.40
7:G:743:THR:N	7:G:744:PRO:HD3	2.36	0.40
12:L:240:VAL:O	12:L:249:ARG:N	2.52	0.40
5:E:470:PRO:O	5:E:472:PRO:HD3	2.21	0.40
12:L:217:VAL:HA	12:L:233:SER:HA	2.04	0.40
40:2:149:A:C6	40:2:150:U:C4	3.09	0.40
43:6:66:C:H2'	43:6:67:G:H8	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:TYR:O	1:A:458:ALA:HB2	2.22	0.40
1:A:739:ILE:O	1:A:743:VAL:CB	2.69	0.40
5:E:471:PRO:O	5:E:473:GLU:N	2.54	0.40
40:2:183:G:C6	40:2:184:C:N4	2.89	0.40
41:4:14:G:H2'	41:4:15:G:H8	1.87	0.40
5:E:669:TYR:HA	6:F:483:PRO:HG3	2.04	0.40
41:4:110:G:O5'	41:4:110:G:C8	2.70	0.40

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	
1	A	2184/2335 (94%)	1969 (90%)	208 (10%)	7 (0%)	41	76
2	B	842/972 (87%)	772 (92%)	70 (8%)	0	100	100
3	C	1689/2136 (79%)	1624 (96%)	63 (4%)	2 (0%)	51	85
5	E	215/683 (32%)	174 (81%)	37 (17%)	4 (2%)	8	41
6	F	416/521 (80%)	376 (90%)	39 (9%)	1 (0%)	47	81
7	G	798/941 (85%)	700 (88%)	94 (12%)	4 (0%)	29	68
8	H	411/499 (82%)	359 (87%)	49 (12%)	3 (1%)	22	62
9	I	174/312 (56%)	158 (91%)	15 (9%)	1 (1%)	25	65
10	J	133/142 (94%)	126 (95%)	7 (5%)	0	100	100
11	K	43/439 (10%)	42 (98%)	1 (2%)	0	100	100
12	L	451/513 (88%)	437 (97%)	14 (3%)	0	100	100
13	M	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
14	N	54/199 (27%)	47 (87%)	7 (13%)	0	100	100
15	O	124/128 (97%)	119 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	87/800 (11%)	79 (91%)	8 (9%)	0	100	100
17	Q	73/376 (19%)	70 (96%)	3 (4%)	0	100	100
18	R	14/557 (2%)	13 (93%)	1 (7%)	0	100	100
19	a	74/118 (63%)	71 (96%)	3 (4%)	0	100	100
19	h	70/118 (59%)	68 (97%)	2 (3%)	0	100	100
20	b	71/86 (83%)	70 (99%)	1 (1%)	0	100	100
20	i	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
21	c	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
21	j	76/92 (83%)	70 (92%)	6 (8%)	0	100	100
22	d	67/76 (88%)	63 (94%)	4 (6%)	0	100	100
22	k	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
23	e	76/126 (60%)	73 (96%)	3 (4%)	0	100	100
23	l	69/126 (55%)	69 (100%)	0	0	100	100
24	f	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
24	m	60/240 (25%)	57 (95%)	3 (5%)	0	100	100
25	g	89/119 (75%)	84 (94%)	5 (6%)	0	100	100
25	n	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
All	All	8883/13444 (66%)	8186 (92%)	675 (8%)	22 (0%)	50	81

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	957	VAL
7	G	842	HIS
7	G	373	VAL
8	H	434	VAL
1	A	1015	VAL
3	C	531	ILE
9	I	157	VAL
1	A	1092	ILE
5	E	478	ILE
5	E	490	VAL
1	A	569	VAL
1	A	945	THR
5	E	533	LEU
7	G	309	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	929	ILE
1	A	948	PRO
8	H	271	THR
1	A	947	PRO
5	E	537	ILE
1	A	386	PRO
8	H	269	PRO
6	F	459	ILE

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	
1	A	125/2108 (6%)	125 (100%)	0	100	100
2	B	49/866 (6%)	49 (100%)	0	100	100
3	C	77/1908 (4%)	77 (100%)	0	100	100
5	E	8/599 (1%)	8 (100%)	0	100	100
6	F	17/441 (4%)	17 (100%)	0	100	100
7	G	35/792 (4%)	35 (100%)	0	100	100
8	H	15/424 (4%)	15 (100%)	0	100	100
9	I	6/293 (2%)	6 (100%)	0	100	100
10	J	5/130 (4%)	5 (100%)	0	100	100
12	L	11/450 (2%)	11 (100%)	0	100	100
13	M	10/148 (7%)	10 (100%)	0	100	100
15	O	6/111 (5%)	6 (100%)	0	100	100
16	P	3/681 (0%)	3 (100%)	0	100	100
17	Q	2/333 (1%)	2 (100%)	0	100	100
19	a	3/110 (3%)	3 (100%)	0	100	100
19	h	2/110 (2%)	2 (100%)	0	100	100
20	b	4/74 (5%)	4 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	i	4/74 (5%)	4 (100%)	0	100	100
21	c	1/84 (1%)	1 (100%)	0	100	100
21	j	1/84 (1%)	1 (100%)	0	100	100
22	d	3/66 (4%)	3 (100%)	0	100	100
22	k	3/66 (4%)	3 (100%)	0	100	100
23	e	3/101 (3%)	3 (100%)	0	100	100
23	l	2/101 (2%)	2 (100%)	0	100	100
24	f	2/177 (1%)	2 (100%)	0	100	100
25	g	4/101 (4%)	4 (100%)	0	100	100
25	n	3/101 (3%)	3 (100%)	0	100	100
All	All	404/10533 (4%)	404 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	Y	44/324 (13%)	14 (31%)	0
40	2	96/188 (51%)	18 (18%)	3 (3%)
41	4	134/145 (92%)	41 (30%)	4 (2%)
42	5	113/116 (97%)	36 (31%)	2 (1%)
43	6	88/106 (83%)	22 (25%)	3 (3%)
All	All	475/879 (54%)	131 (27%)	12 (2%)

All (131) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
39	Y	50	C
39	Y	51	U
39	Y	52	C
39	Y	53	C
39	Y	54	G
39	Y	55	A
39	Y	56	A
39	Y	57	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	Y	61	A
39	Y	70	G
39	Y	71	C
39	Y	72	A
39	Y	156	U
39	Y	160	G
40	2	111	G
40	2	112	G
40	2	113	G
40	2	116	A
40	2	117	U
40	2	118	G
40	2	145	A
40	2	146	C
40	2	147	G
40	2	154	C
40	2	156	U
40	2	157	G
40	2	164	C
40	2	165	A
40	2	168	A
40	2	169	C
40	2	177	A
40	2	178	A
41	4	19	U
41	4	20	A
41	4	25	A
41	4	26	G
41	4	36	U
41	4	41	C
41	4	44	A
41	4	45	G
41	4	52	U
41	4	53	U
41	4	54	A
41	4	55	U
41	4	56	U
41	4	58	C
41	4	69	C
41	4	71	U
41	4	73	U
41	4	76	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	4	78	A
41	4	80	A
41	4	81	C
41	4	82	C
41	4	84	C
41	4	85	G
41	4	90	G
41	4	100	A
41	4	103	A
41	4	109	G
41	4	114	U
41	4	115	G
41	4	118	A
41	4	119	A
41	4	120	U
41	4	121	U
41	4	122	U
41	4	124	U
41	4	125	G
41	4	126	A
41	4	127	C
41	4	144	G
41	4	145	G
42	5	8	G
42	5	10	U
42	5	20	G
42	5	21	A
42	5	22	U
42	5	23	C
42	5	24	G
42	5	25	C
42	5	26	A
42	5	27	U
42	5	34	U
42	5	36	C
42	5	38	C
42	5	39	C
42	5	41	U
42	5	42	U
42	5	45	C
42	5	48	A
42	5	52	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	5	53	U
42	5	54	U
42	5	57	G
42	5	68	C
42	5	69	A
42	5	70	A
42	5	79	C
42	5	80	U
42	5	83	A
42	5	88	A
42	5	90	U
42	5	92	U
42	5	93	U
42	5	94	U
42	5	95	G
42	5	96	A
42	5	108	G
43	6	6	C
43	6	7	G
43	6	9	U
43	6	21	U
43	6	22	A
43	6	26	U
43	6	28	A
43	6	29	A
43	6	33	G
43	6	35	A
43	6	38	G
43	6	40	U
43	6	43	A
43	6	44	G
43	6	45	A
43	6	47	A
43	6	48	A
43	6	49	G
43	6	50	A
43	6	70	A
43	6	77	C
43	6	78	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	2	156	U
40	2	164	C
40	2	168	A
41	4	43	G
41	4	55	U
41	4	99	C
41	4	114	U
42	5	78	U
42	5	94	U
43	6	28	A
43	6	49	G
43	6	77	C

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	L	1
3	C	1
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	39:ASN	C	40:THR	N	8.39
1	C	1296:PRO	C	1297:PRO	N	3.45
1	H	268:LEU	C	269:PRO	N	1.71

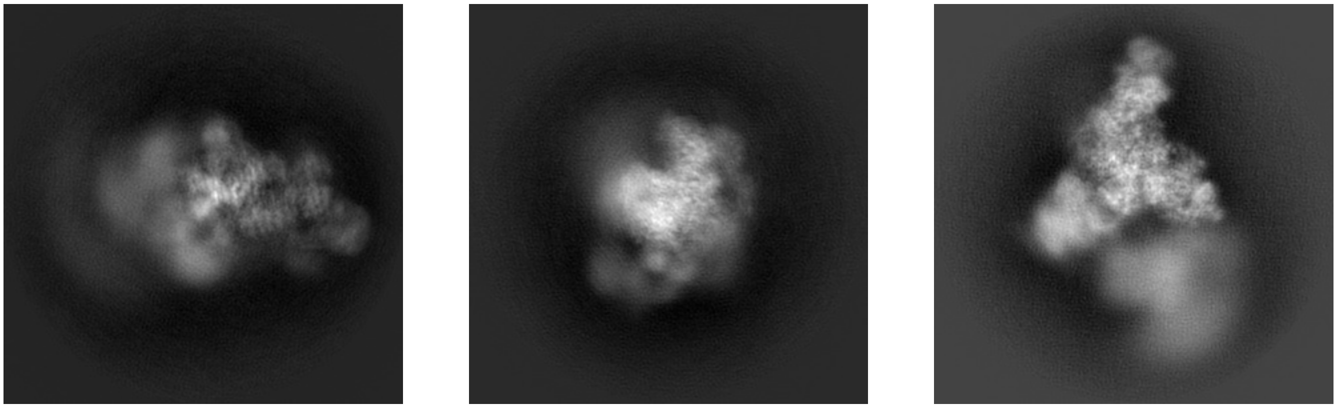
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3766. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

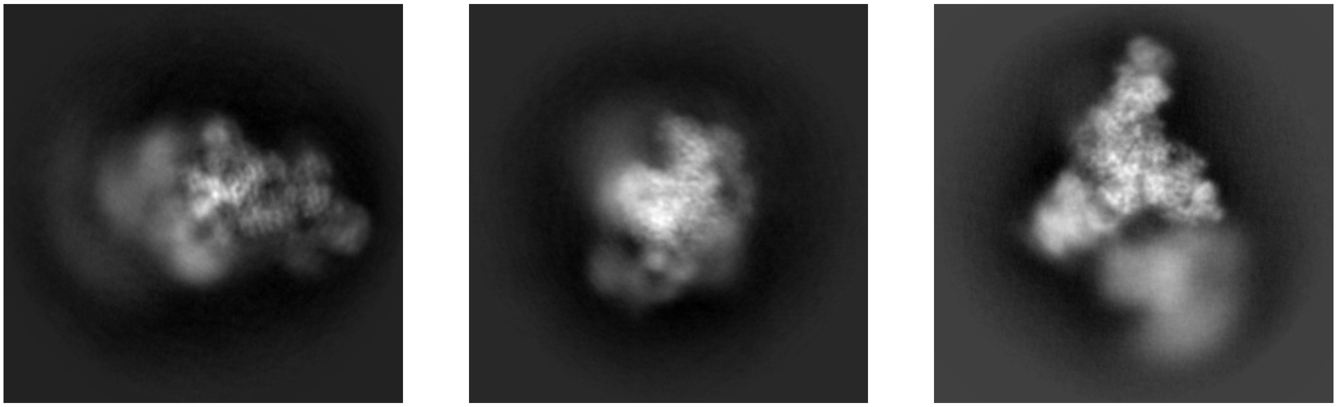
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

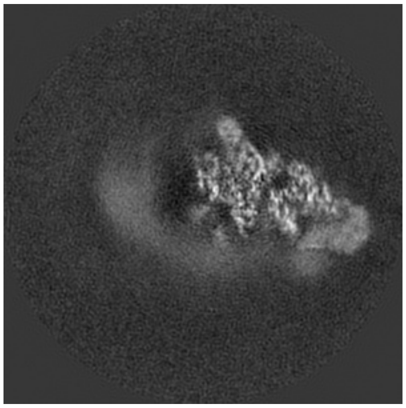


X Y Z

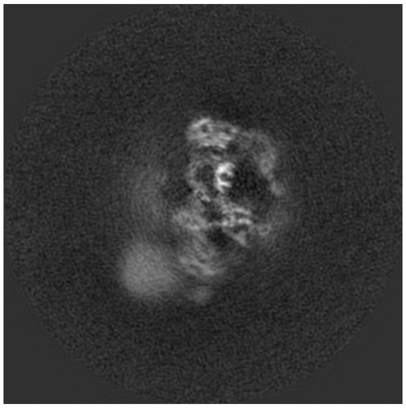
The images above show the map projected in three orthogonal directions.

6.2 Central slices

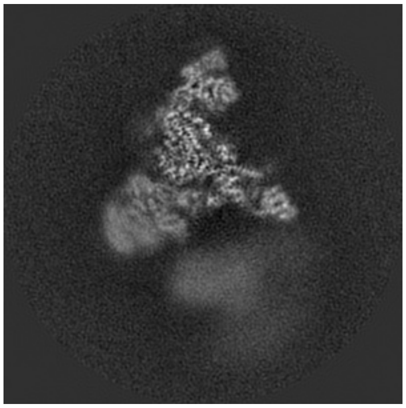
6.2.1 Primary map



X Index: 216

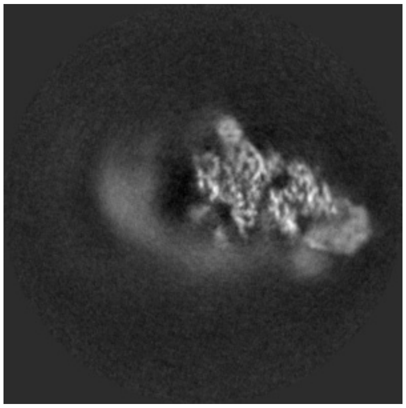


Y Index: 216

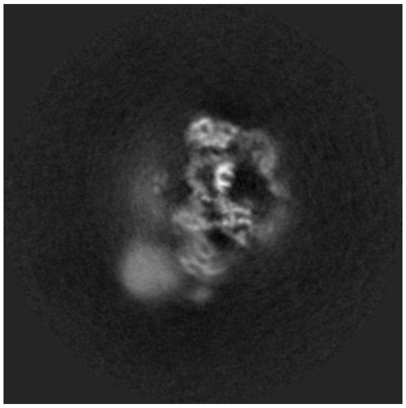


Z Index: 216

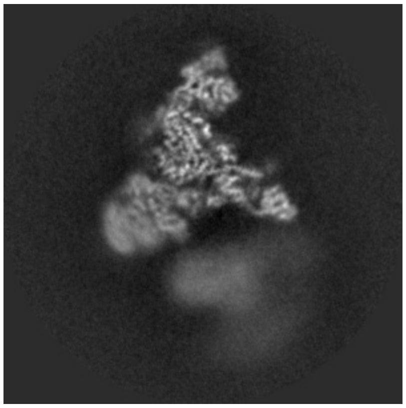
6.2.2 Raw map



X Index: 216



Y Index: 216

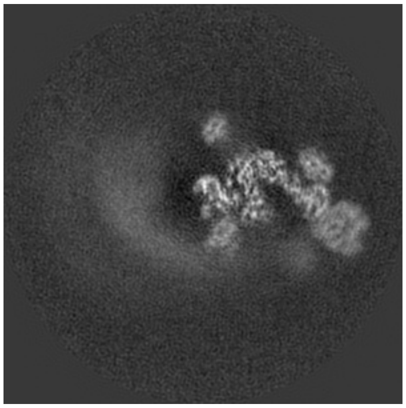


Z Index: 216

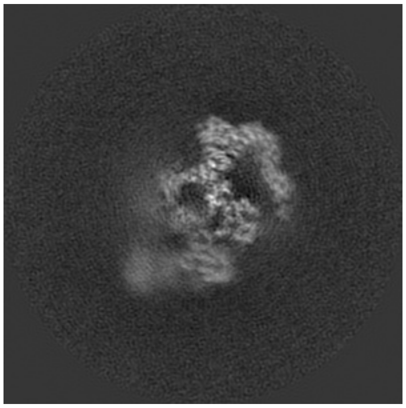
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

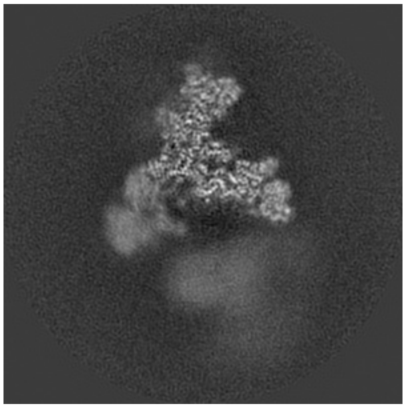
6.3.1 Primary map



X Index: 237

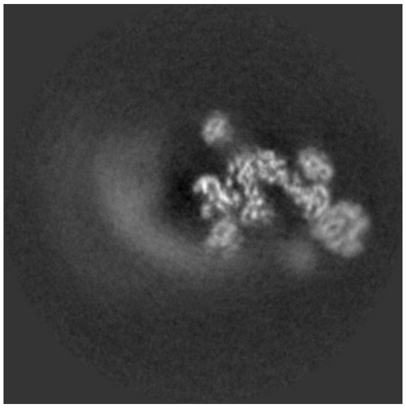


Y Index: 229

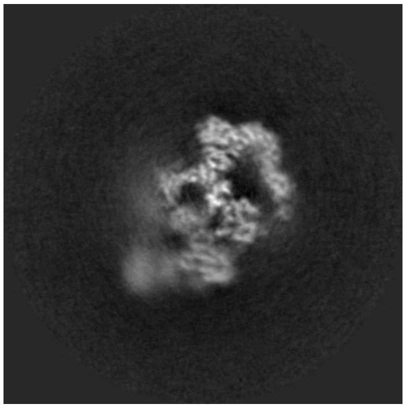


Z Index: 225

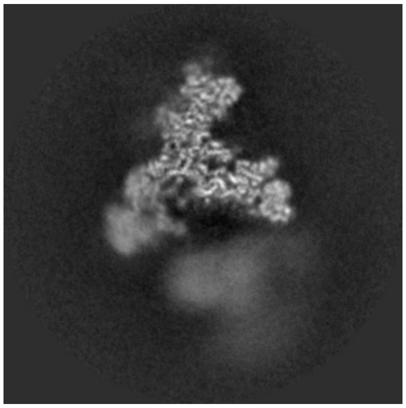
6.3.2 Raw map



X Index: 237



Y Index: 229



Z Index: 225

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

6.4.2 Raw map

X

Y

Z

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

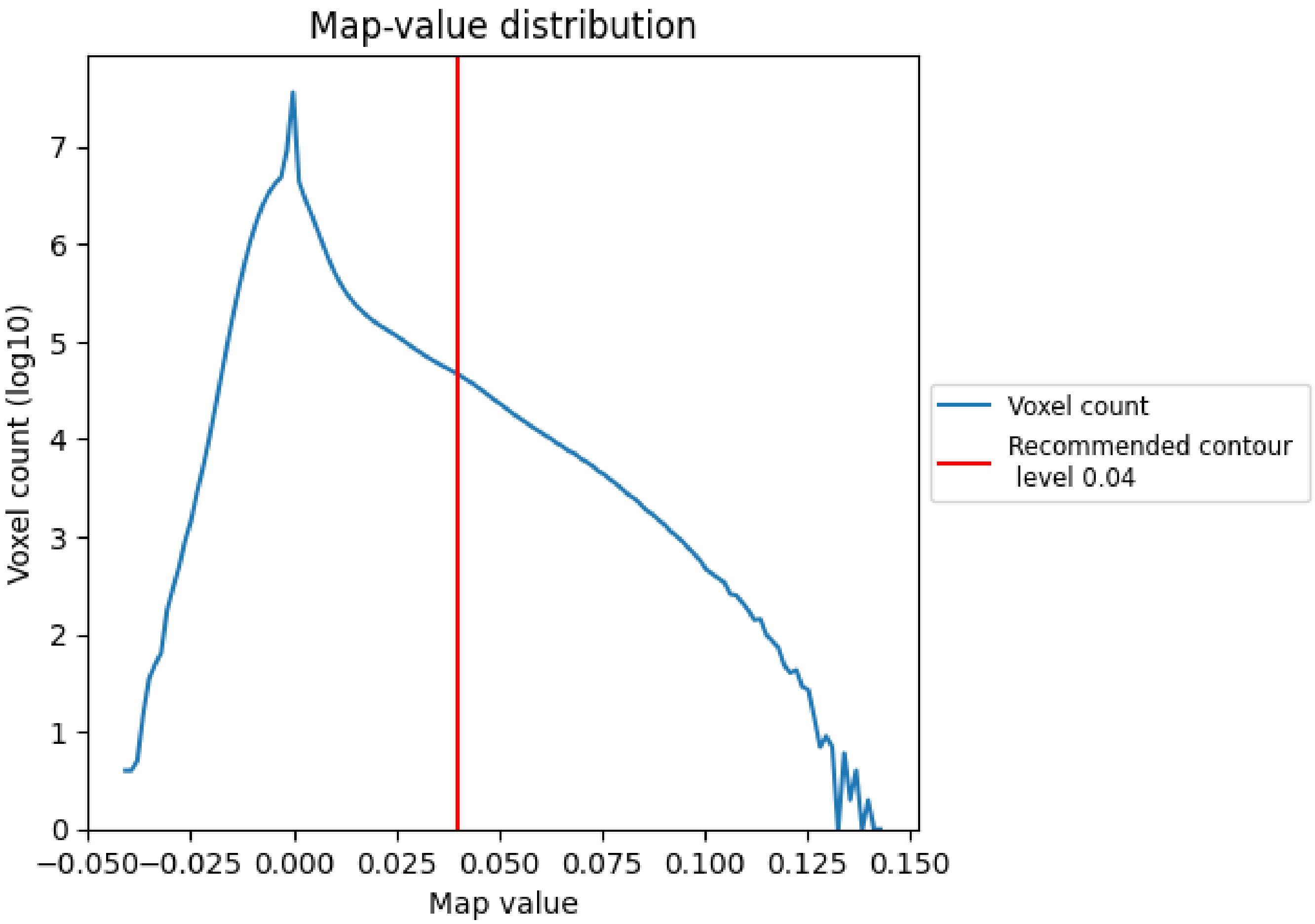
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

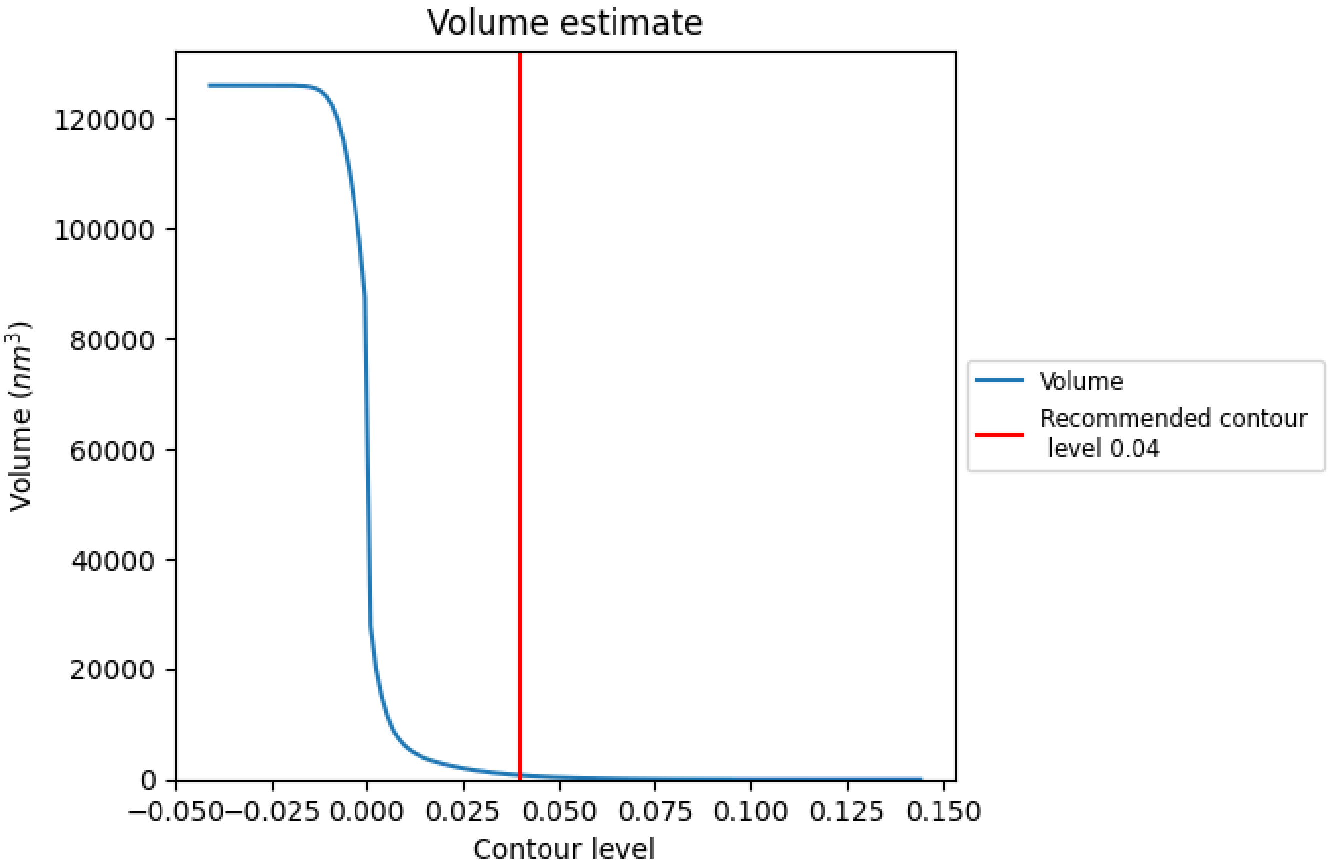
This section contains the results of statistical analysis of the map.

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.

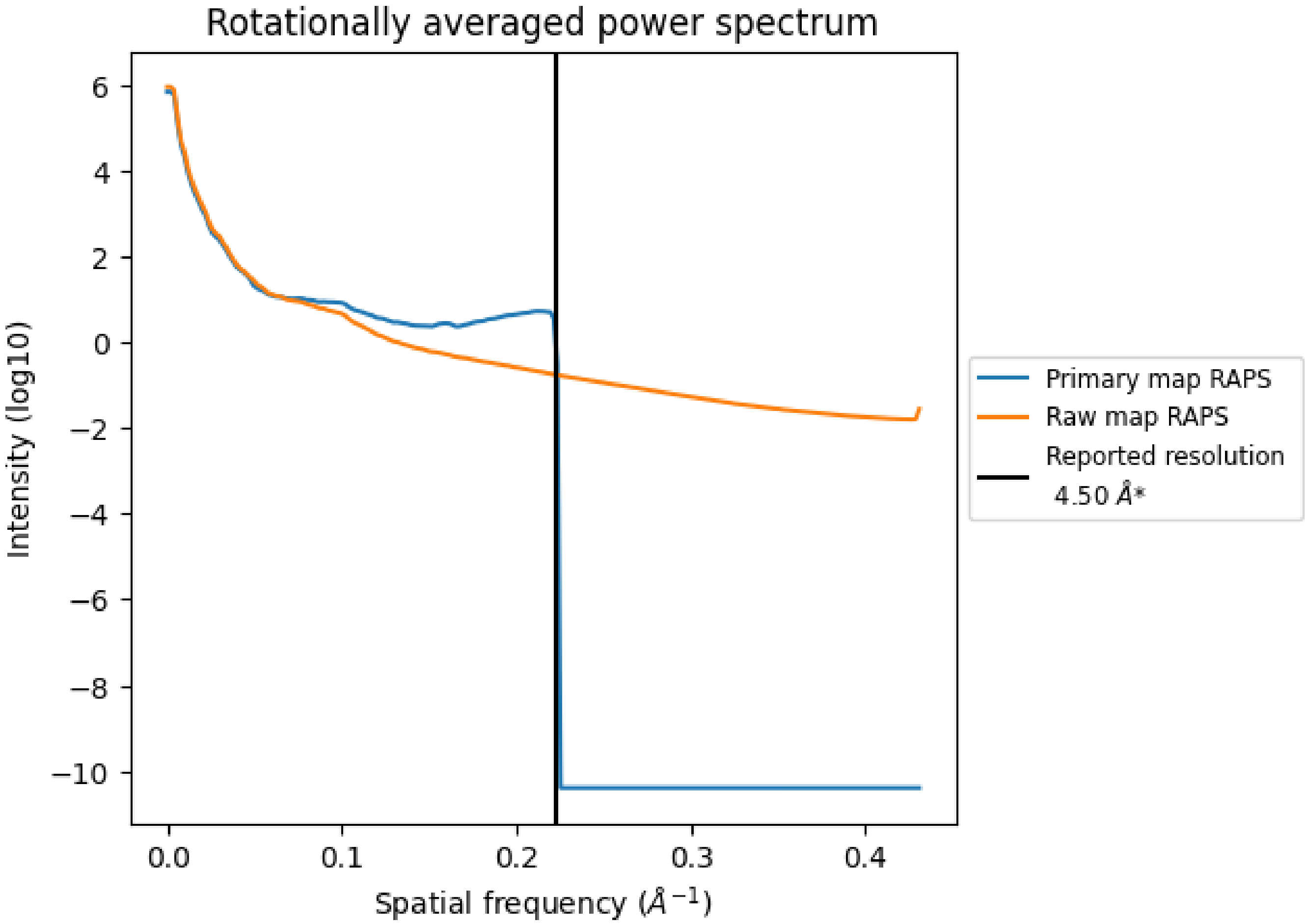
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 761 nm^3; this corresponds to an approximate mass of 688 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 ⓘ

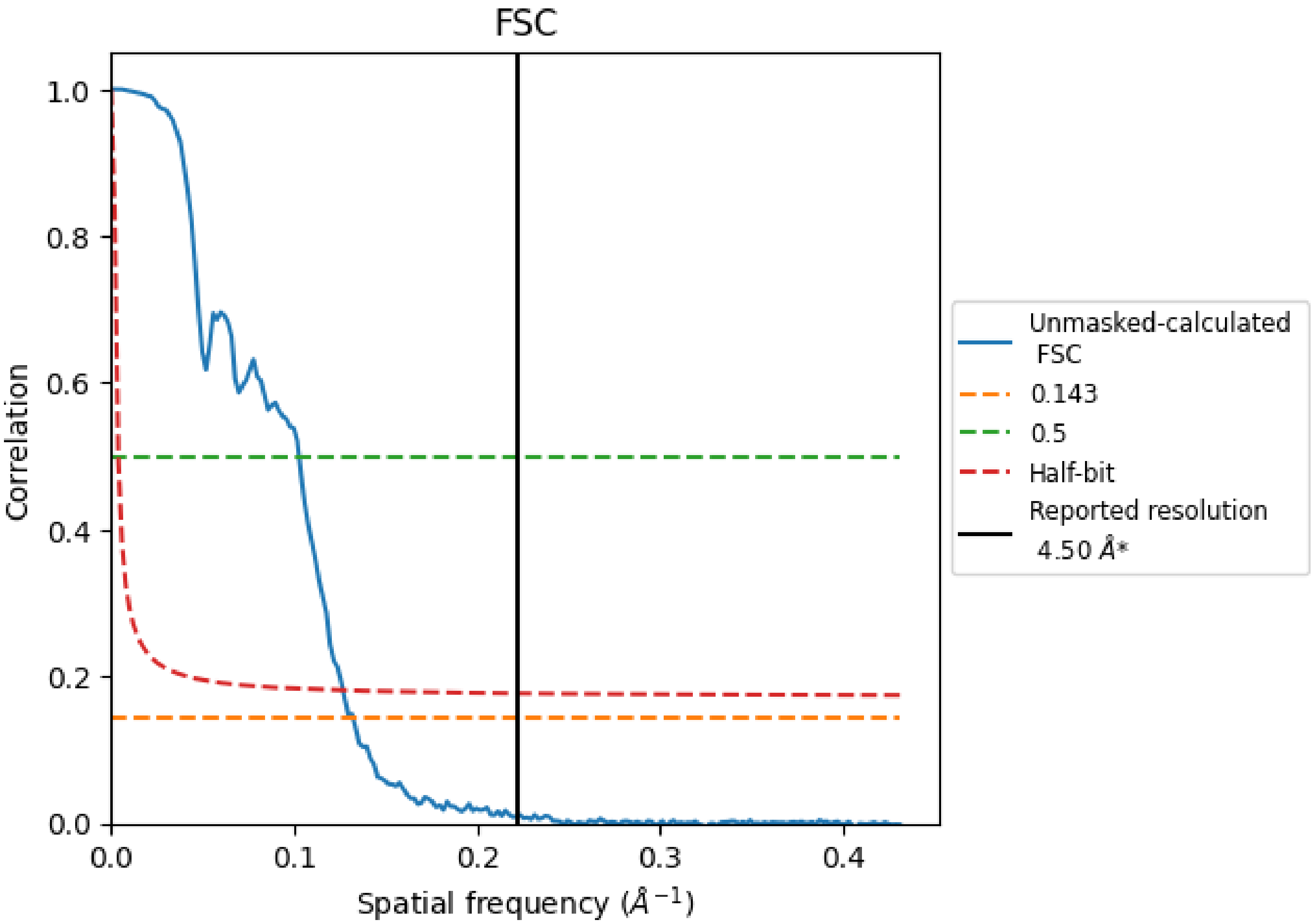


*Reported resolution corresponds to spatial frequency of 0.222 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates ⓘ

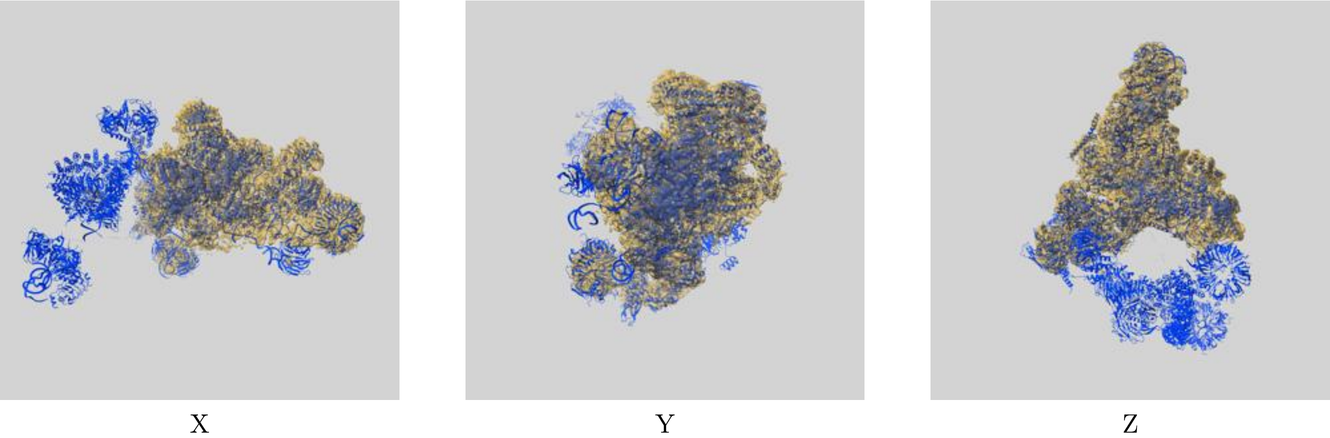
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.56	9.74	7.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.56 differs from the reported value 4.5 by more than 10 %

9 Map-model fit (i)

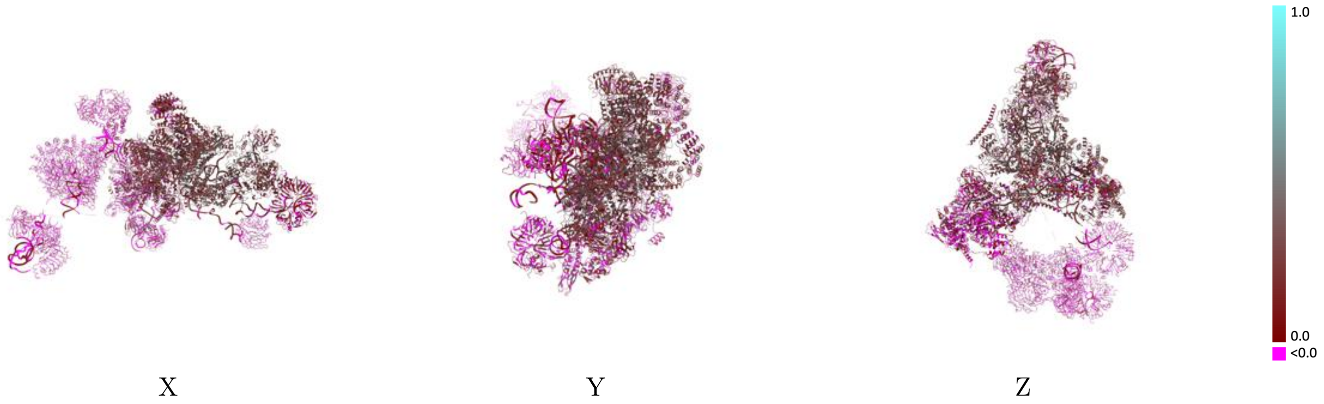
This section contains information regarding the fit between EMDB map EMD-3766 and PDB model 5O9Z. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)



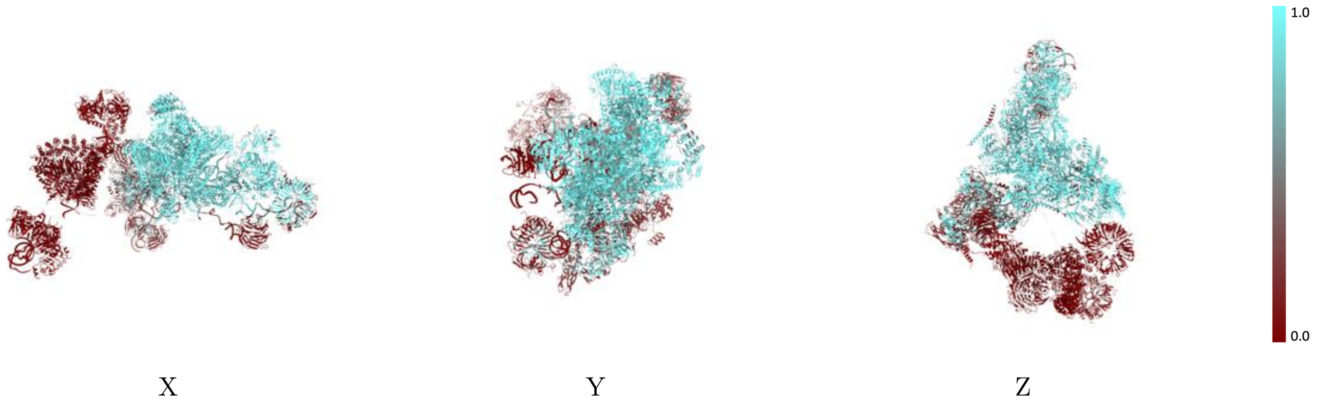
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



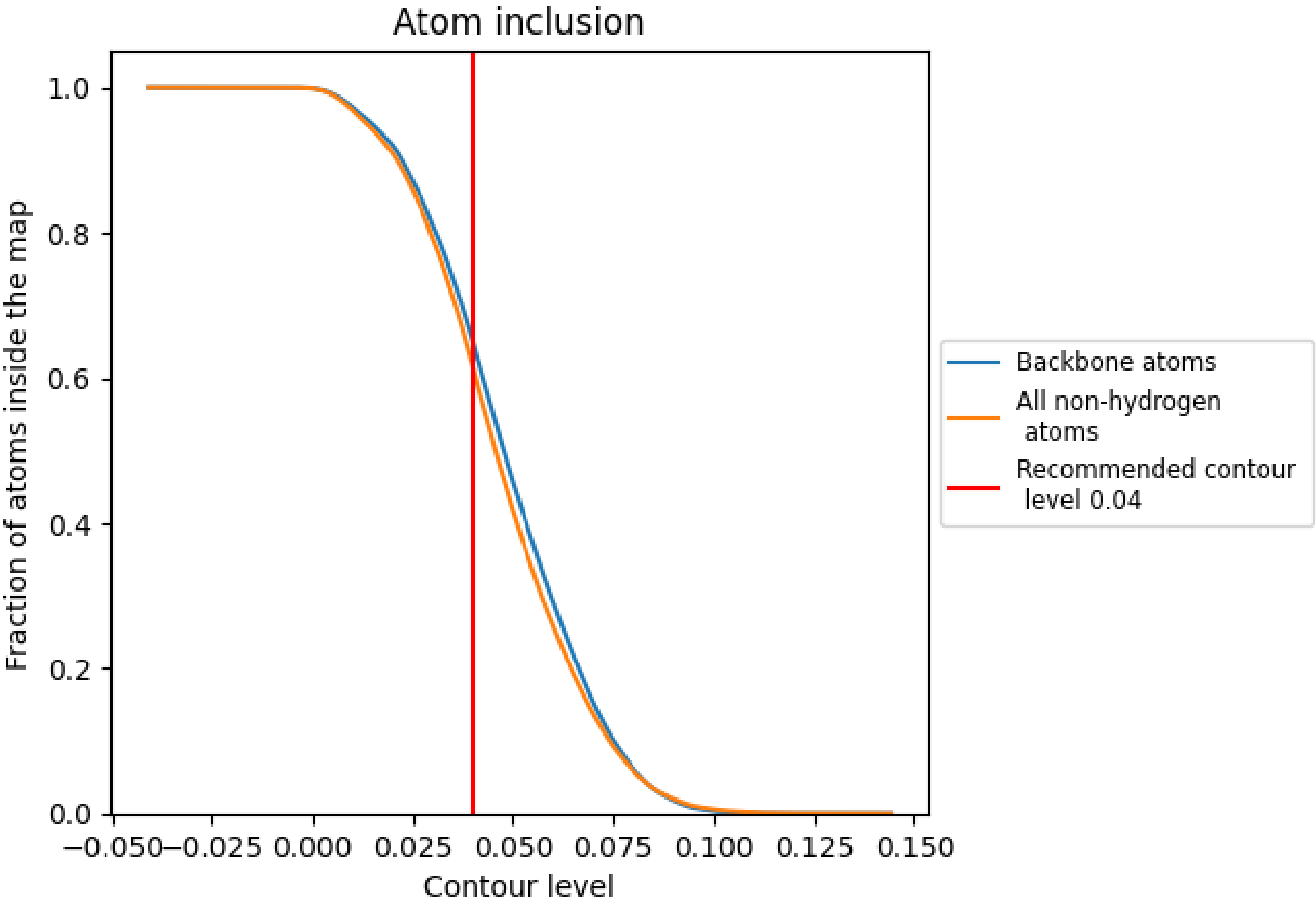
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 65% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6147	0.1700
1	0.0000	-0.0190
2	0.0033	0.0020
4	0.5472	0.1530
5	0.7514	0.1460
6	0.5125	0.1590
A	0.8732	0.2930
B	0.9022	0.2720
C	0.4551	0.1010
D	0.0795	0.0160
E	0.8719	0.2380
F	0.9357	0.2270
G	0.8541	0.2100
H	0.8559	0.2640
I	0.8641	0.2710
J	0.9084	0.3400
K	0.5333	0.1580
L	0.0022	0.0000
M	0.8448	0.1800
N	0.8881	0.2410
O	0.9104	0.3320
P	0.8668	0.2450
Q	0.8439	0.2290
R	0.0000	-0.0450
S	0.0000	-0.0040
T	0.0000	0.0150
U	0.0000	0.0180
V	0.0000	-0.0160
W	0.0000	0.0150
X	0.0000	-0.0380
Y	0.4815	0.1140
Z	0.0000	0.0200
a	0.6463	0.0580
b	0.5220	0.0720
c	0.6753	0.1070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	🟦 0.6977	🟫 0.1330
e	🟦 0.7256	🟫 0.1590
f	🟦 0.6740	🟫 0.1190
g	⬛ 0.4968	🟥 0.0860
h	🟫 0.3127	🟥 0.0490
i	🟫 0.1808	🟥 0.0130
j	🟫 0.1778	🟪 -0.0180
k	🟫 0.1126	🟪 -0.0050
l	🟫 0.2011	🟪 -0.0270
m	🟫 0.1994	🟥 0.0790
n	🟫 0.2379	🟪 -0.0190
o	🟥 0.0000	🟥 0.0070
p	🟥 0.0000	🟪 -0.0560
q	🟥 0.0000	🟥 0.0160
r	🟥 0.0000	🟥 0.0060
s	🟥 0.0000	🟥 0.0340
t	🟥 0.0000	🟥 0.0120
u	🟥 0.0000	🟥 0.0350
v	🟥 0.0000	🟥 0.0080
w	🟥 0.0009	🟥 0.0070
x	🟥 0.0000	🟥 0.0850
y	🟥 0.0000	🟪 -0.0320
z	🟥 0.0000	🟥 0.0070