wwPDB EM Validation Summary Report

Mar 6, 2026 – 04:13 PM UTC

PDB ID	:	5Z57 / pdb_00005z57
EMDB ID	:	EMD-6890
Title	:	Cryo-EM structure of the human activated spliceosome (late Bact) at 6.5 angstrom
Authors	:	Zhang, X.; Yan, C.; Zhan, X.; Li, L.; Lei, J.; Shi, Y.
Deposited on	:	2018-01-17
Resolution	:	6.50 Å(reported)

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

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

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

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

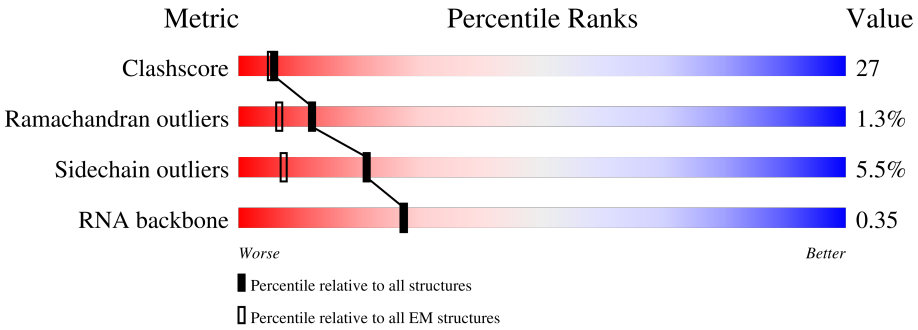
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

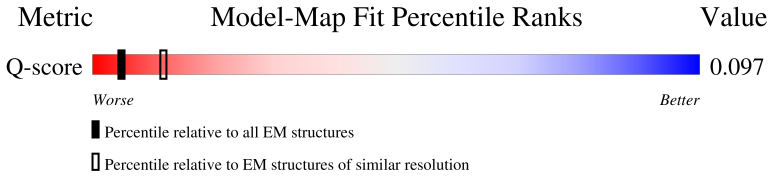
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.50 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.





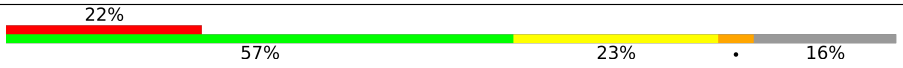
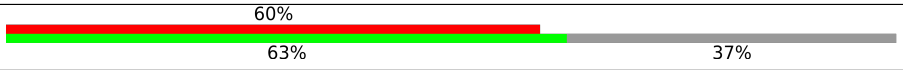
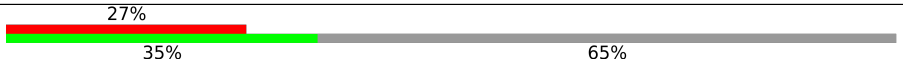
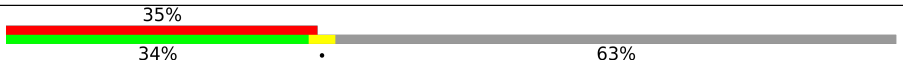
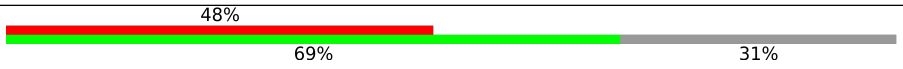
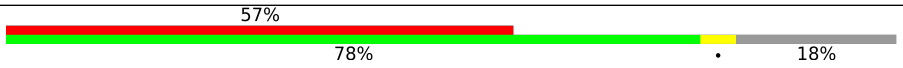
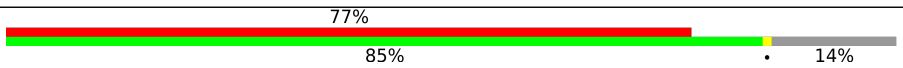
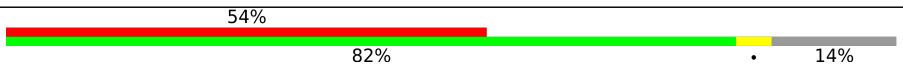
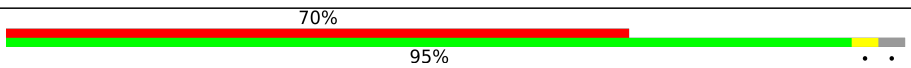
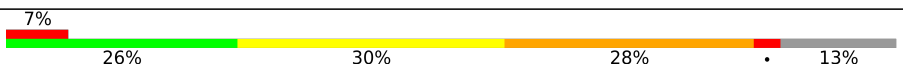
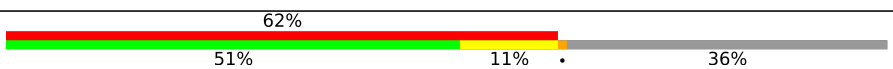
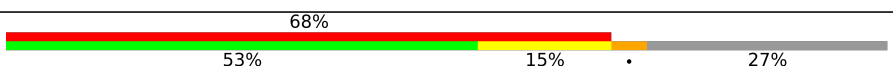
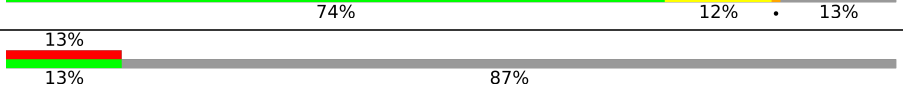
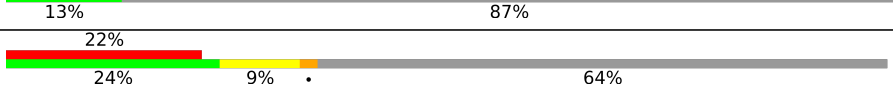
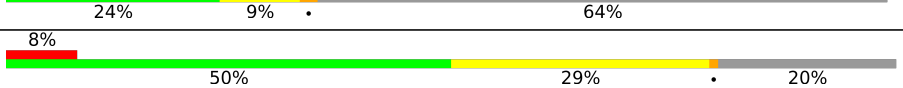
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	556 (6.00 - 7.00)

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	18% 46% 33% 5% 15%
2	B	117	13% 30% 24% 15% • 28%
3	C	972	8% 46% 34% 8% • 12%

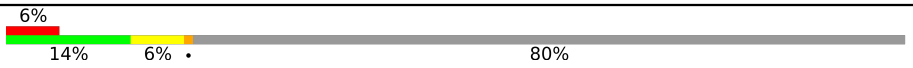
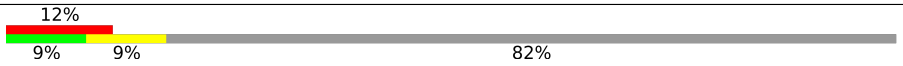
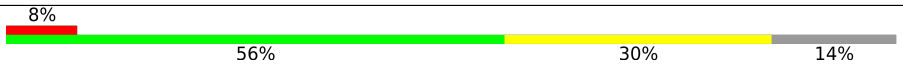
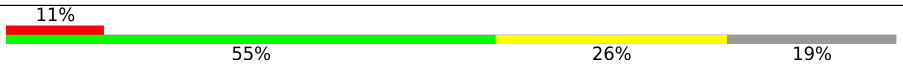
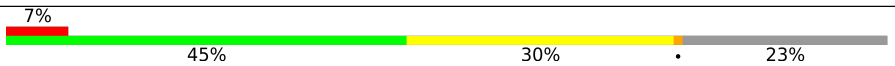
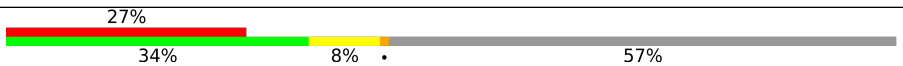
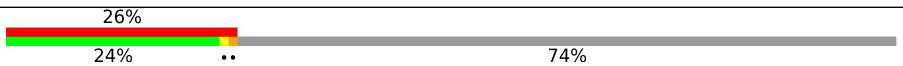
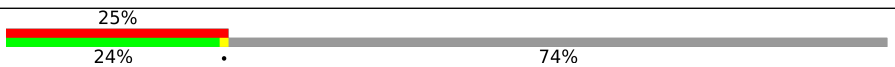
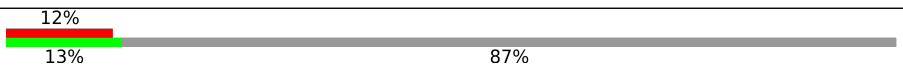
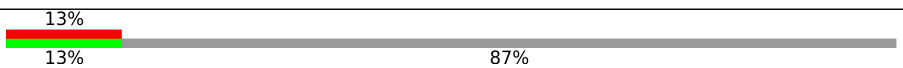
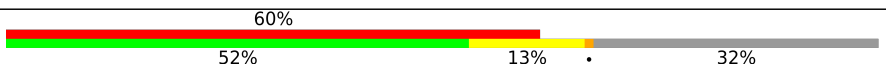
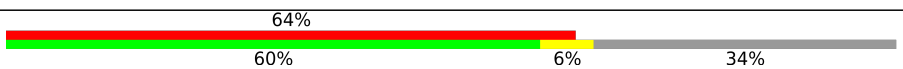
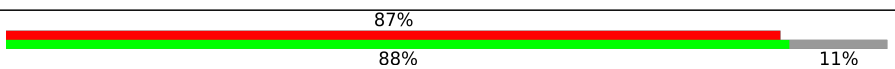
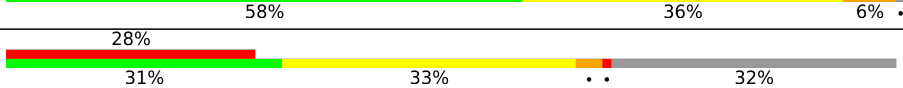
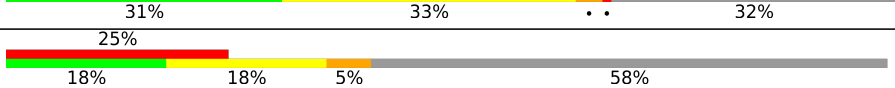
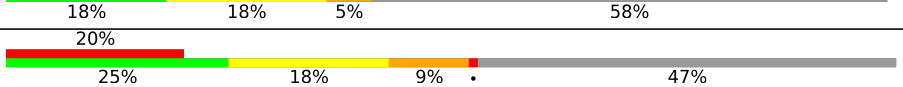
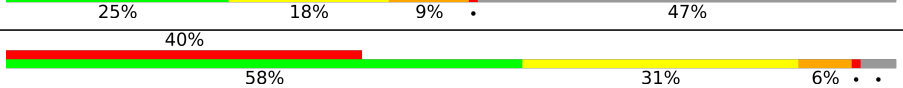
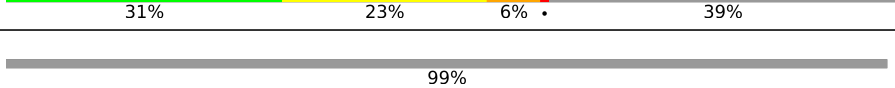
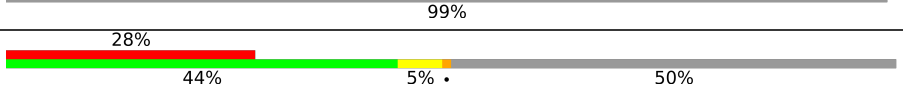
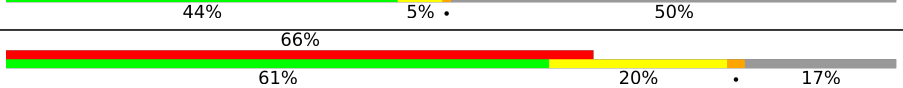
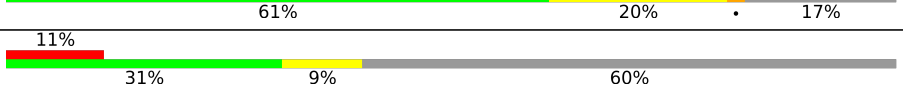
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Mol	Chain	Length	Quality of chain
4	D	2136	
5	E	357	
6	a	126	
6	h	126	
7	b	231	
7	i	231	
8	c	119	
8	j	119	
9	d	118	
9	k	118	
10	f	86	
10	m	86	
11	e	92	
11	l	92	
12	g	76	
12	n	76	
13	F	107	
14	G	274	
15	H	188	
16	o	255	
17	p	225	
18	w	501	
19	u	793	
20	v	464	
21	1	1304	

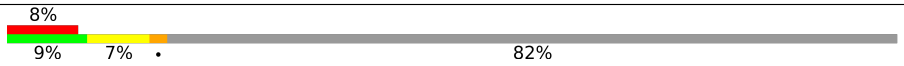
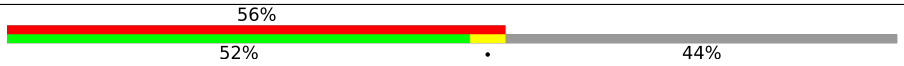
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Mol	Chain	Length	Quality of chain
22	2	895	
23	3	1217	
24	4	424	
25	5	125	
26	6	110	
27	7	86	
28	J	848	
29	L	802	
30	q	504	
30	r	504	
30	s	504	
30	t	504	
31	K	225	
32	I	855	
33	Q	1485	
34	N	144	
35	O	420	
36	P	229	
37	R	540	
38	S	166	
39	T	514	
40	U	2752	
41	V	908	
42	W	579	
43	X	396	

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Mol	Chain	Length	Quality of chain
44	Y	322	
45	Z	619	
46	x	1041	
47	y	301	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	IHP	A	2401	-	-	X	-
50	GTP	C	1500	-	-	X	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 113433 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
			Total	C	N	O	S		
1	A	1978	16399	10552	2875	2897	75	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	84	1768	792	295	597	84	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	860	6716	4294	1120	1270	32	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	1722	8528	5084	1722	1722	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	299	2338	1470	410	445	13	0	0

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	a	81	399	237	81	81	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	h	80	Total 393	C 233	N 80	O 80	0	0

- Molecule 7 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	b	82	Total 405	C 241	N 82	O 82	0	0
7	i	86	Total 422	C 250	N 86	O 86	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	c	82	Total 406	C 242	N 82	O 82	0	0
8	j	82	Total 406	C 242	N 82	O 82	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	d	97	Total 480	C 286	N 97	O 97	0	0
9	k	85	Total 422	C 252	N 85	O 85	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	f	74	Total 361	C 213	N 74	O 74	0	0
10	m	74	Total 361	C 213	N 74	O 74	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	79	Total 391	C 233	N 79	O 79	0	0
11	l	79	Total 391	C 233	N 79	O 79	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	g	74	Total 363	C 215	N 74	O 74	0	0
12	n	68	Total 334	C 198	N 68	O 68	0	0

- Molecule 13 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	93	Total 1988	C 889	N 363	O 643	P 93	0	0

- Molecule 14 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	77	Total 1545	C 689	N 240	O 539	P 77	0	0

- Molecule 15 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	136	Total 2886	C 1289	N 499	O 962	P 136	0	0

- Molecule 16 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	o	162	Total 804	C 480	N 162	O 162	0	0

- Molecule 17 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
17	p	165	Total 813	C 483	N 165	O 165	0	0

- Molecule 18 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	438	Total 2373	C 1450	N 461	O 459	S 3	0	0

- Molecule 19 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	u	104	Total	C	N	O	0	0
			520	312	104	104		

- Molecule 20 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	165	Total	C	N	O	S	0	0
			936	565	191	178	2		

- Molecule 21 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1	1038	Total	C	N	O	S	0	0
			7702	4900	1347	1415	40		

- Molecule 22 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	183	Total	C	N	O	S	0	0
			1252	809	213	226	4		

- Molecule 23 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3	1177	Total	C	N	O	S	0	0
			9195	5834	1561	1755	45		

- Molecule 24 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	4	78	Total	C	N	O	0	0
			527	345	83	99		

- Molecule 25 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5	108	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 26 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	89	Total	C	N	O	S	0	0
			670	410	119	128	13		

- Molecule 27 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	66	Total	C	N	O	S	0	0
			540	343	94	98	5		

- Molecule 28 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J	522	Total	C	N	O	S	0	0
			3463	2156	653	648	6		

- Molecule 29 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	342	Total	C	N	O	S	0	0
			2260	1430	406	420	4		

- Molecule 30 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	q	132	Total	C	N	O	0	0
			659	395	132	132		
30	r	131	Total	C	N	O	0	0
			654	392	131	131		
30	s	67	Total	C	N	O	0	0
			335	201	67	67		
30	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 31 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	K	152	Total	C	N	O	S	0	0
			979	611	177	189	2		

- Molecule 32 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	I	564	Total 2778	C 1650	N 564	O 564	0	0

- Molecule 33 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	1317	Total 6528	C 3894	N 1317	O 1317	0	0

- Molecule 34 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	N	143	Total 1184	C 746	N 217	O 209	S 12	0	0

- Molecule 35 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	O	285	Total 2273	C 1428	N 401	O 424	S 20	0	0

- Molecule 36 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	P	96	Total 829	C 508	N 162	O 157	S 2	0	0

- Molecule 37 is a protein called Skip.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	288	Total 2188	C 1375	N 392	O 409	S 12	0	0

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S	159	Total 1236	C 787	N 215	O 227	S 7	0	0

- Molecule 39 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	313	Total	C	N	O	S	0	0
			2457	1552	447	450	8		

- Molecule 40 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	U	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 41 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	V	452	Total	C	N	O	0	0
			2243	1339	452	452		

- Molecule 42 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	W	483	Total	C	N	O	0	0
			2384	1418	483	483		

- Molecule 43 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	X	158	Total	C	N	O	S	0	0
			1012	645	172	194	1		

- Molecule 44 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Y	105	Total	C	N	O	S	0	0
			743	470	127	144	2		

- Molecule 45 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Z	113	Total	C	N	O	0	0
			755	474	147	134		

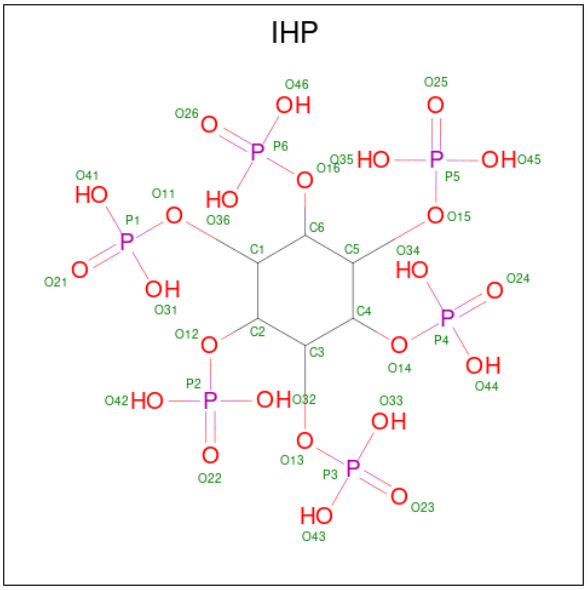
- Molecule 46 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	x	583	Total	C	N	O	0	0
			2882	1715	583	584		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase E.

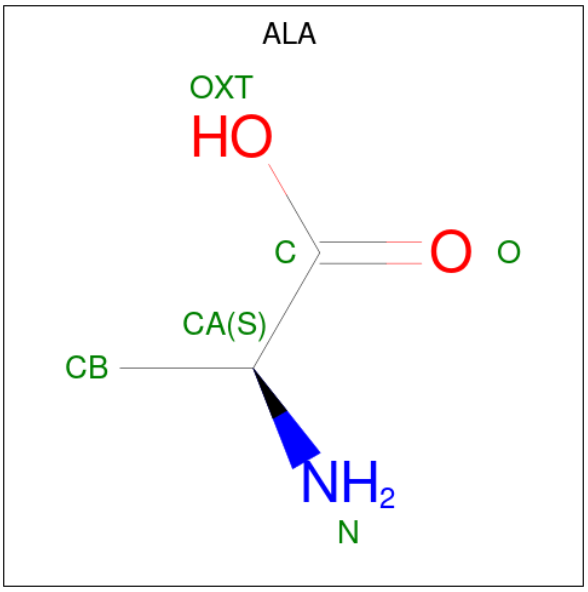
Mol	Chain	Residues	Atoms				AltConf	Trace
47	y	232	Total	C	N	O	0	0
			1133	669	232	232		

- Molecule 48 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



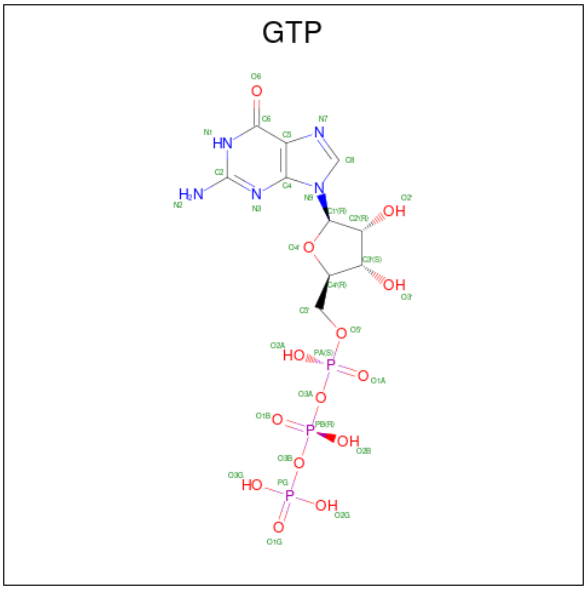
Mol	Chain	Residues	Atoms				AltConf
48	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 49 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
49	A	1	5	3	1	1	0

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	C	1	32	10	5	14	3	0

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
51	C	1	Total Mg 1 1	0
51	F	5	Total Mg 5 5	0

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

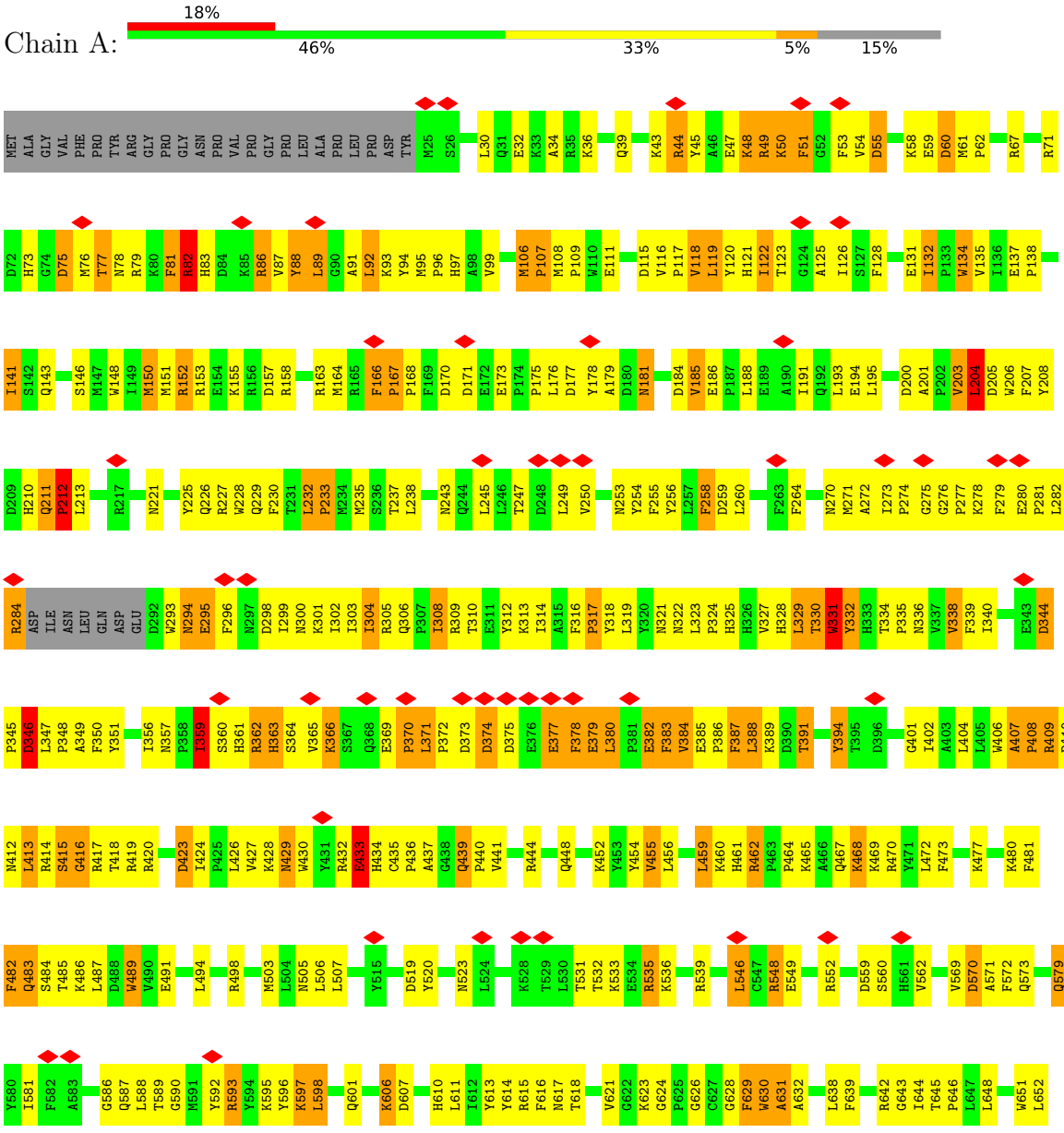
Mol	Chain	Residues	Atoms	AltConf
52	v	1	Total Zn 1 1	0
52	6	3	Total Zn 3 3	0
52	N	3	Total Zn 3 3	0
52	O	3	Total Zn 3 3	0

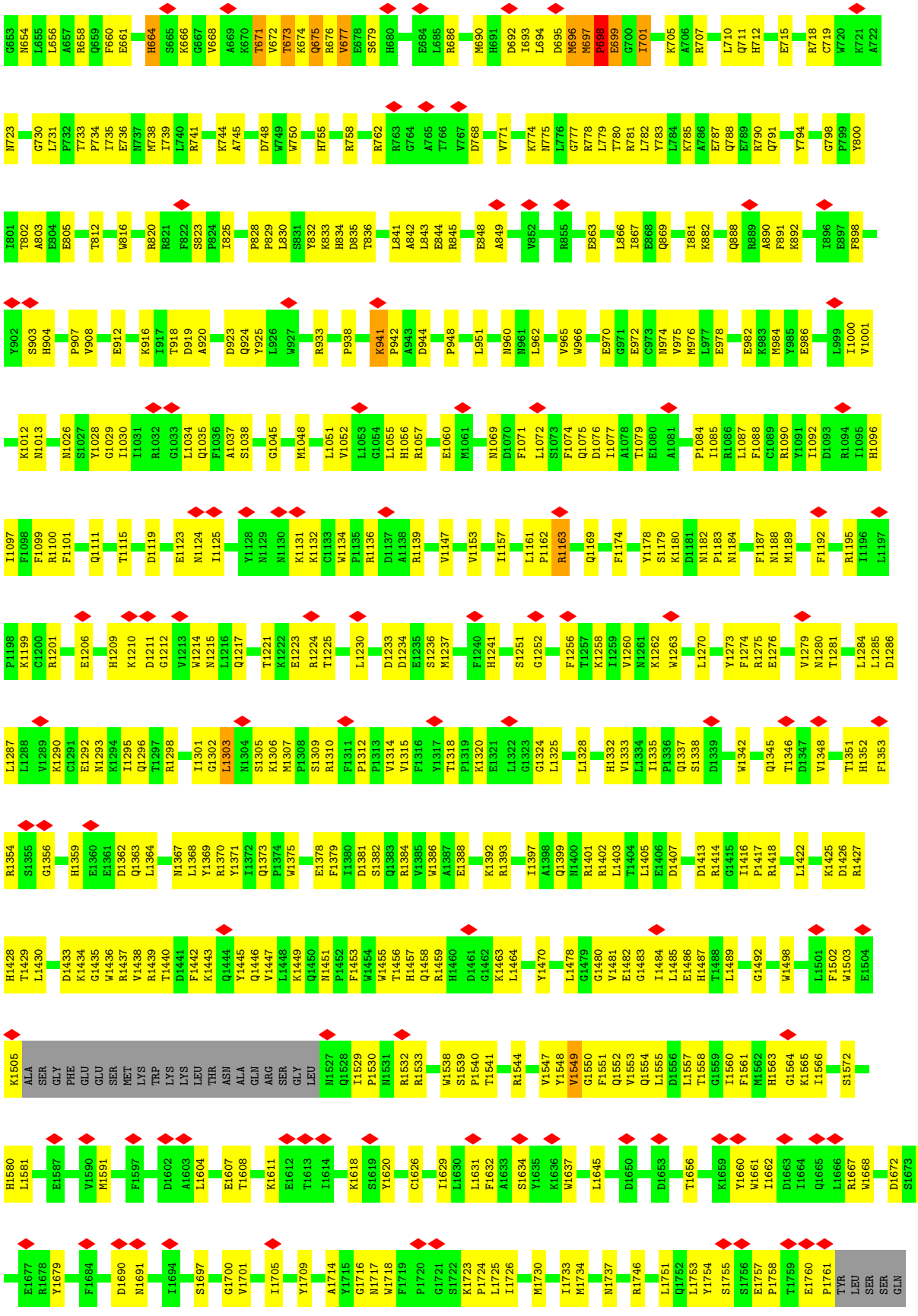
3 Residue-property plots (i)

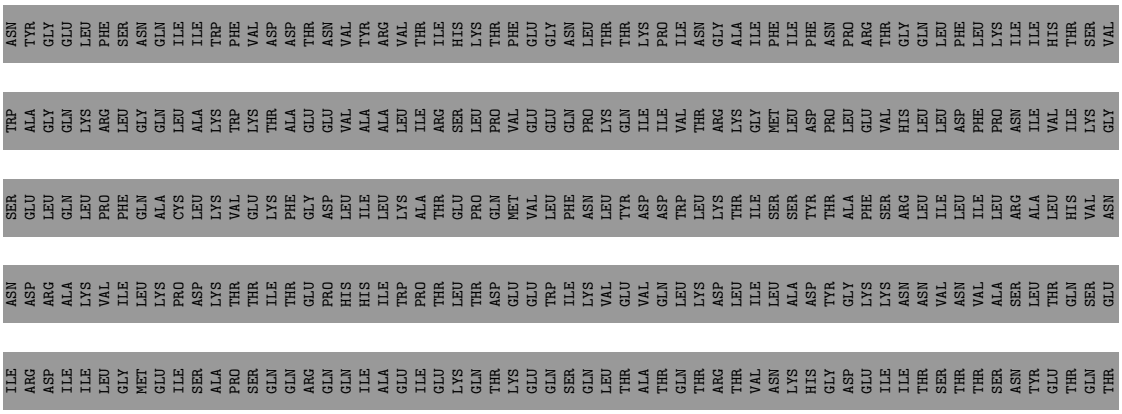
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain A:



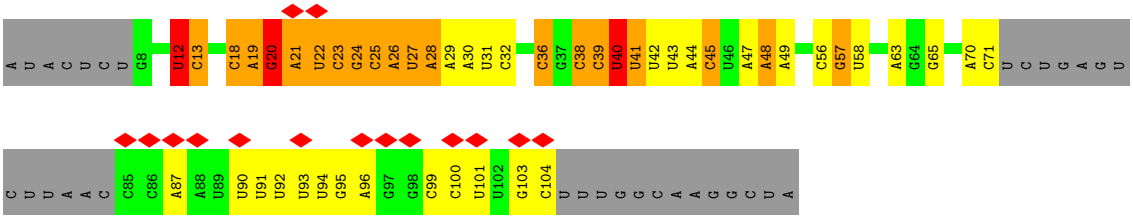

G653 N654 L655 L656 A657 R658 Q659 F660 E661 H664 S665 K666 G667 V668 A669 K670 T671 V672 T673 K674 Q675 R676 V677 E678 S679 H680 E684 L685 R686 M690 H691 D692 I693 L694 D695 M696 M697 P698 E699 G700 I701 K705 A706 R707 L710 Q711 H712 E715 R718 C719 W720 K721 A722
W723 G730 L731 P732 T733 P734 I735 E736 N737 M738 T739 L740 R741 K744 A745 D748 W749 W750 H755 R758 R762 R763 G764 A765 T766 V767 D768 V771 K774 N775 L776 G777 R778 L779 T780 R781 L782 Y783 L784 K785 A786 E787 Q788 E789 R790 Q791 Y794 G798 P799 Y800
I801 T802 A803 E804 E805 T812 W816 R820 R821 F822 S823 P824 I825 P828 P829 L830 S831 Y832 K833 H834 D835 T836 L841 A842 L843 E844 R845 E848 A849 V852 R855 E863 L866 I867 E868 Q869 I881 K882 Q888 R889 A890 F891 K892 T896 E897 F898
Y902 S903 H904 P907 V908 E912 K916 I917 T918 D919 A920 D923 Q924 Y925 L926 W927 R933 P938 K941 P942 A943 D944 P948 L951 N960 N961 L962 V965 W966 E970 G971 E972 C973 N974 V975 M976 L977 E978 E982 K983 M984 Y985 E986 L999 I1000 V1001
K1012 N1013 N1026 S1027 Y1028 G1029 I1030 I1031 R1032 G1033 L1034 Q1035 F1036 A1037 S1038 G1045 M1048 L1051 V1052 L1053 G1054 L1055 H1056 R1057 E1060 M1061 N1069 D1070 F1071 L1072 S1073 F1074 Q1075 D1076 I1077 A1078 T1079 E1080 A1081 P1084 I1085 R1086 L1087 F1088 C1089 R1090 Y1091 I1092 D1093 R1094 I1095 H1096
I1097 F1098 F1099 R1100 F1101 Q1111 T1115 D1119 E1123 N1124 I1125 Y1128 N1129 N1130 K1131 K1132 C1133 W1134 P1135 R1136 D1137 A1138 R1139 V1147 V1153 I1157 L1161 P1162 R1163 Q1169 F1174 Y1178 S1179 K1180 D1181 N1182 P1183 N1184 F1187 N1188 M1189 F1192 R1195 I1196 L1197
P1198 K1199 C1200 R1201 E1206 H1209 K1210 D1211 G1212 V1213 W1214 N1215 L1216 Q1217 T1221 K1222 E1223 R1224 T1225 L1230 D1233 D1234 E1235 S1236 M1237 F1240 H1241 S1251 G1252 F1256 T1257 K1258 I1259 V1260 N1261 K1262 W1263 L1270 Y1273 F1274 R1275 E1276 V1279 N1280 T1281 L1284 L1285 D1286
L1287 L1288 V1289 K1290 C1291 E1292 N1293 K1294 I1295 Q1296 T1297 R1298 I1301 G1302 L1303 N1304 S1305 K1306 M1307 P1308 S1309 R1310 F1311 P1312 P1313 V1314 V1315 F1316 Y1317 T1318 P1319 K1320 E1321 L1322 G1323 G1324 L1325 L1328 H1332 V1333 L1334 I1335 P1336 Q1337 S1338 D1339 W1342 Q1345 T1346 D1347 V1348 T1351 H1352 F1353
R1354 S1355 G1356 H1359 E1360 E1361 D1362 Q1363 L1364 N1367 L1368 Y1369 R1370 Y1371 I1372 Q1373 P1374 W1375 E1378 F1379 T1380 D1381 S1382 Q1383 R1384 V1385 W1386 A1387 E1388 K1392 R1393 I1397 A1398 Q1399 N1400 R1401 R1402 L1403 T1404 L1405 E1406 D1407 D1413 R1414 G1415 I1416 P1417 R1418 L1422 K1425 D1426 R1427
H1428 T1429 L1430 D1433 K1434 G1435 W1436 R1437 V1438 R1439 T1440 D1441 F1442 K1443 Q1444 Y1445 Q1446 V1447 L1448 K1449 Q1450 N1451 P1452 F1453 W1454 W1455 T1456 H1457 Q1458 R1459 H1460 D1461 G1462 K1463 L1464 Y1470 L1478 G1479 G1480 V1481 E1482 G1483 I1484 L1485 E1486 H1487 T1488 L1489 G1492 W1498 L1501 F1502 W1503 E1504
K1505 ALA SER GLY PHE GLU GLU SER MET LYS TRP LYS LYS LEU THR ASN ALA GLN ARG SER GLY LEU N1527 Q1528 I1529 P1530 N1531 R1532 R1533 W1538 S1539 P1540 T1541 R1544 V1547 Y1548 V1549 G1550 F1551 Q1552 V1553 G1554 L1555 D1556 L1557 T1558 G1559 I1560 F1561 M1562 H1563 G1564 K1565 I1566 S1572
H1580 L1581 E1587 V1590 M1591 F1597 D1602 A1603 L1604 E1607 T1608 K1611 E1612 T1613 I1614 K1618 S1619 Y1620 C1626 I1629 L1630 L1631 F1632 A1633 S1634 V1635 K1636 W1637 L1645 D1650 D1653 T1656 K1659 Y1660 W1661 I1662 D1663 I1664 Q1665 L1666 R1667 W1668 D1672 S1673 H1674
E1677 R1678 Y1679 F1684 D1690 N1691 I1694 S1697 G1700 V1701 I1705 Y1709 A1714 Y1715 G1716 N1717 W1718 F1719 P1720 G1721 S1722 K1723 P1724 L1725 I1726 M1730 I1733 M1734 N1737 R1746 L1751 Q1752 L1753 Y1754 S1755 S1756 E1757 P1758 T1759 E1760 P1761 TYR LEU SER SER GLN



• Molecule 2: U5 snRNA

Chain B:

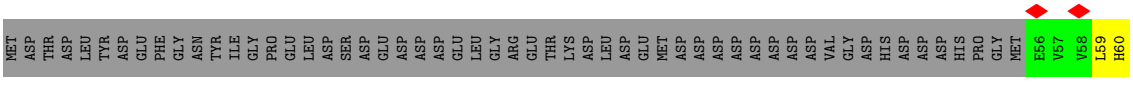


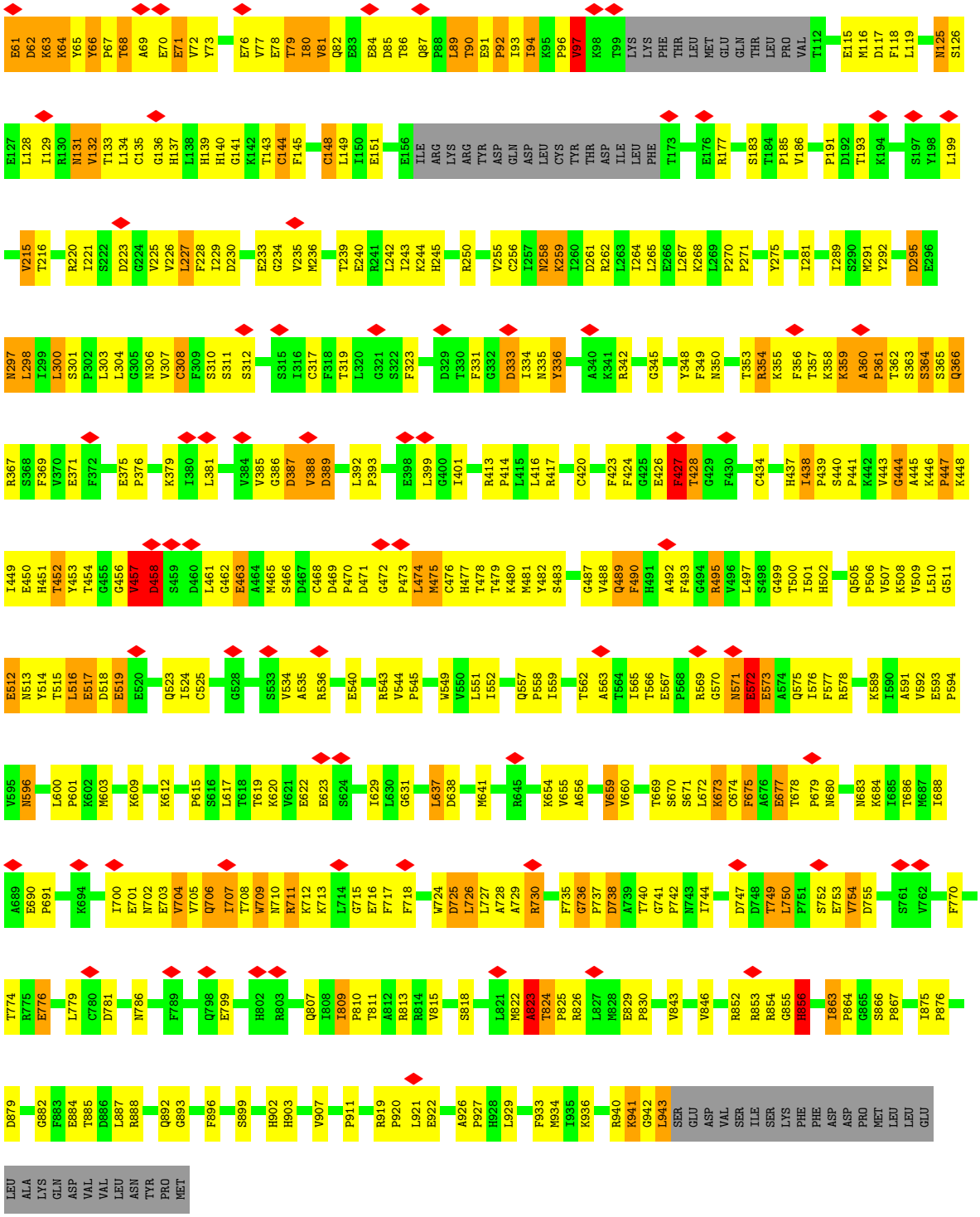


• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:



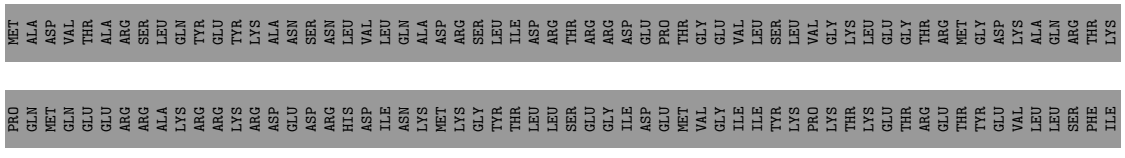


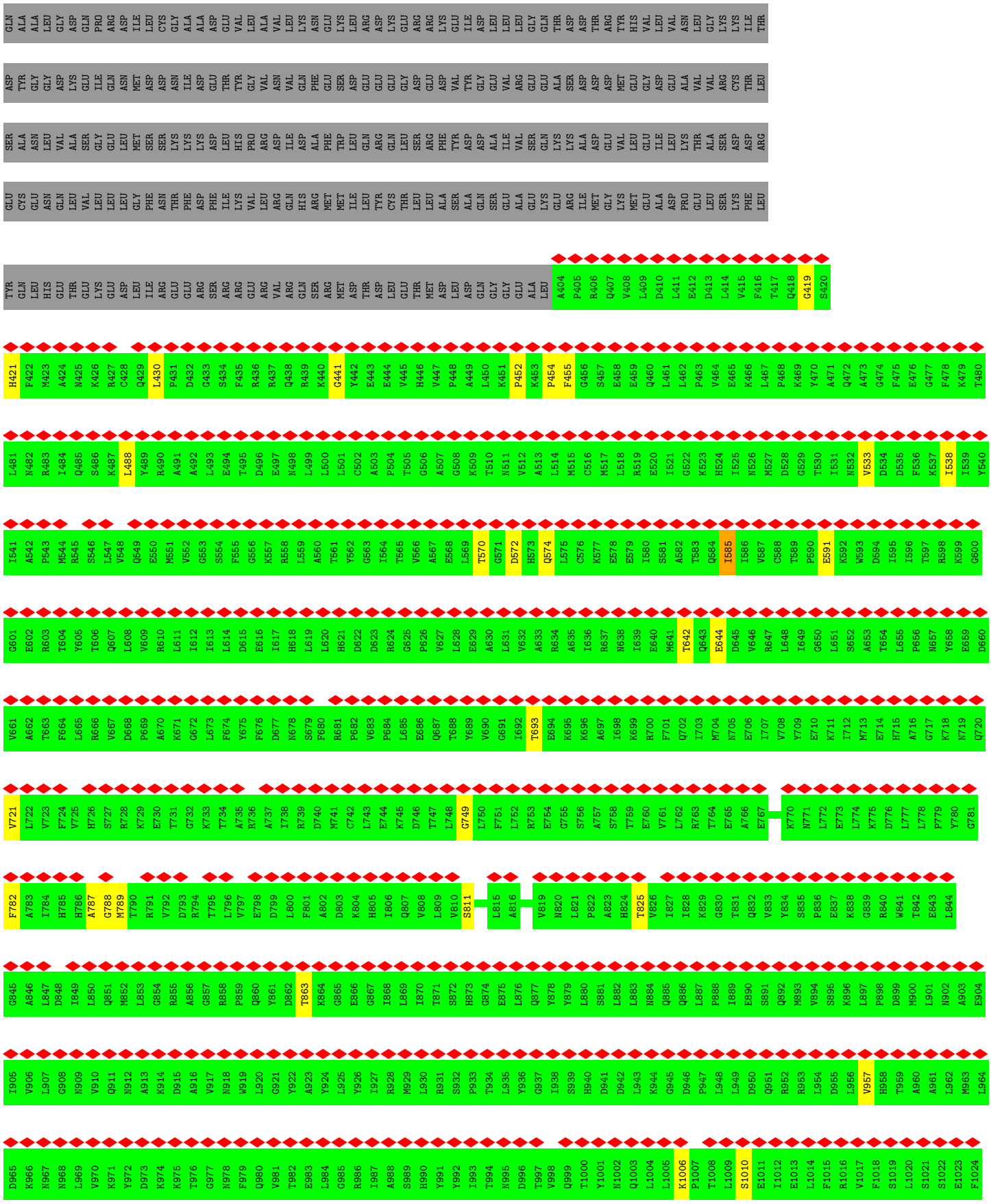


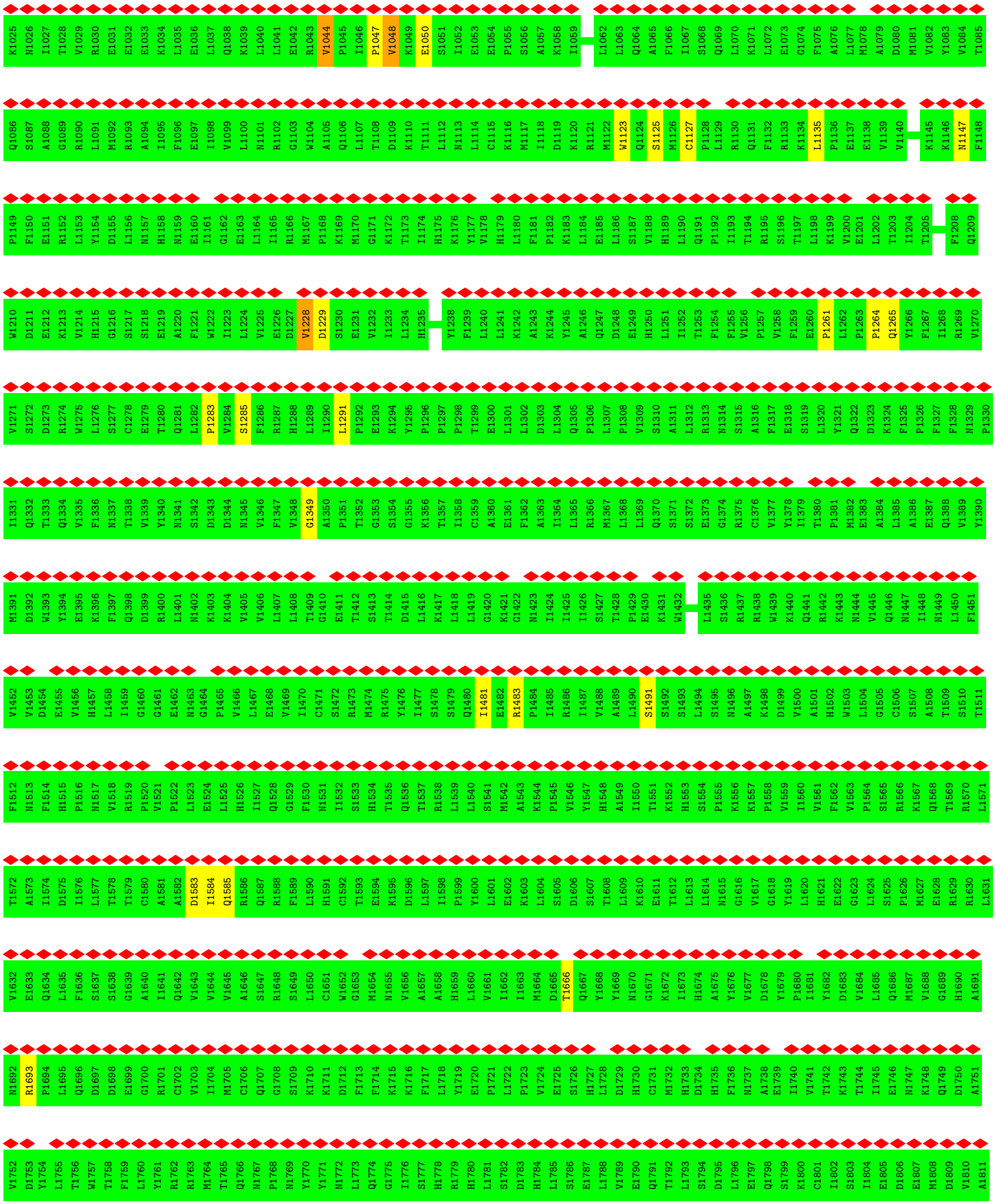
• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

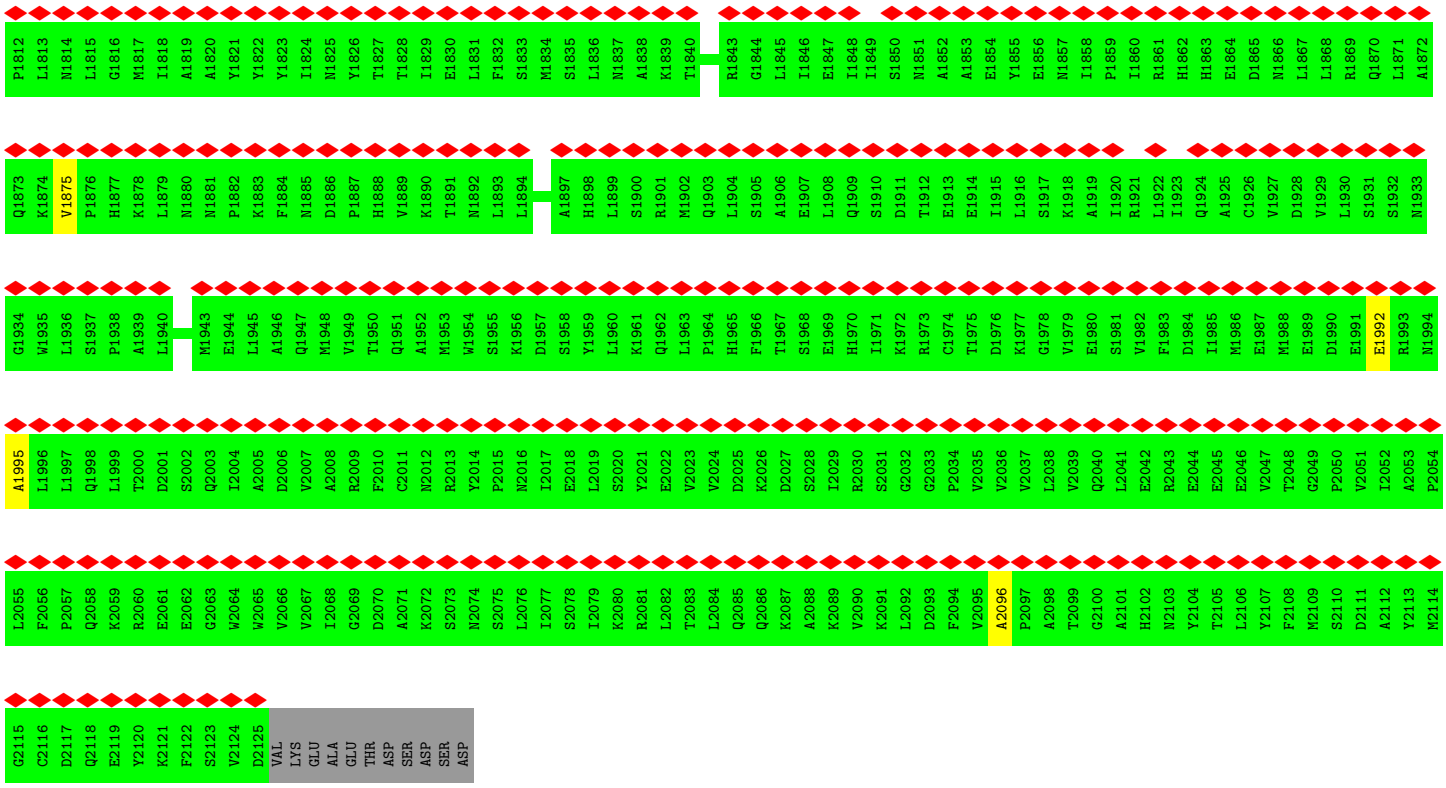
Chain D:






GLN ALA ALA LEU GLY ASP GLN PRO ARG ASP ILE LEU CYS GLY ALA ALA ASP GLU VAL LEU ALA VAL LEU LYS ASN GLU LYS LEU ARG ASP LYS GLU ARG ARG LYS GLU ILE ASP LEU LEU LEU GLY GLN THR ASP THR ARG TYR HIS VAL LEU VAL ASN LEU GLY LYS THR ILE LEU
ASP TYR GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN ILE ASP GLU THR TYR GLY VAL ASN VAL GLN PHE GLU SER ASP GLU GLU GLU GLY ASP GLU ASP VAL TYR GLY GLU VAL GLU ILE GLU LEU ALA VAL LEU GLY ASP GLU VAL ASN LEU GLY LYS ILE
SER ALA ASN LEU VAL ALA SER GLY GLU LEU MET SER SER LYS LYS LYS ASP LEU HIS PRO ARG ASP ILE ASP ALA PHE TRP LEU GLN ARG GLN LEU GLU SER ARG PHE TYR ASP LEU ALA ILE VAL SER GLN LYS LYS ALA ASP ILE LEU LYS THR ALA SER ASP ARG
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TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP LEU ASP GLN GLY GLY GLU ALA LEU A404 P405 R406 Q407 V408 L409 D410 L411 E412 D413 L414 V415 F416 T417 Q418 G419 S420
H421 F422 M423 A424 N425 K426 R427 C428 Q429 L430 P431 D432 G433 S434 F435 R436 R437 Q438 R439 K440 G441 Y442 E443 E444 V445 H446 V447 P448 A449 L450 K451 P452 K453 P454 F455 G456 S457 E458 E459 Q460 L461 L462 P463 V464 E465 K466 L467 P468 K469 Y470 A471 Q472 A473 G474 F475 E476 G477 F478 K479 T480
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V661 A662 T663 F664 L665 R666 V667 D668 P669 A670 K671 G672 L673 F674 Y675 F676 D677 N678 S679 F680 R681 P682 V683 P684 L685 E686 Q687 T688 Y689 V690 G691 I692 T693 E694 K695 K696 A697 I698 K699 R700 F701 Q702 I703 M704 N705 E706 I707 V708 Y709 E710 K711 I712 M713 E714 H715 A716 G717 K718 N719 Q720
V721 L722 V723 F724 V725 H726 S727 R728 K729 E730 T731 G732 K733 T734 A735 R736 A737 I738 R739 D740 M741 C742 L743 E744 K745 D746 T747 L748 G749 L750 F751 L752 R753 E754 G755 S756 A757 S758 T759 E760 V761 L762 R763 T764 E765 A766 E767 K770 N771 L772 E773 L774 K775 D776 L777 L778 P779 Y780 G781
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G845 A846 L847 D848 I849 L850 Q851 M852 L853 G854 R855 A856 G857 R858 P859 Q860 Y861 D862 T863 K864 G865 E866 G867 I868 L869 I870 T871 S872 H873 G874 E875 L876 Q877 Y878 Y879 L880 S881 L882 L883 N884 Q885 Q886 L887 P888 I889 E890 S891 Q892 M893 V894 S895 K896 L897 P898 D899 M900 L901 N902 A903 E904
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D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 L984 G985 R986 I987 A988 S989 H990 Y991 Y992 I993 T994 N995 D996 T997 V998 Q999 T1000 Y1001 N1002 Q1003 L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 L1014 F1015 R1016 V1017 F1018 S1019 L1020 S1021 S1022 E1023 F1024

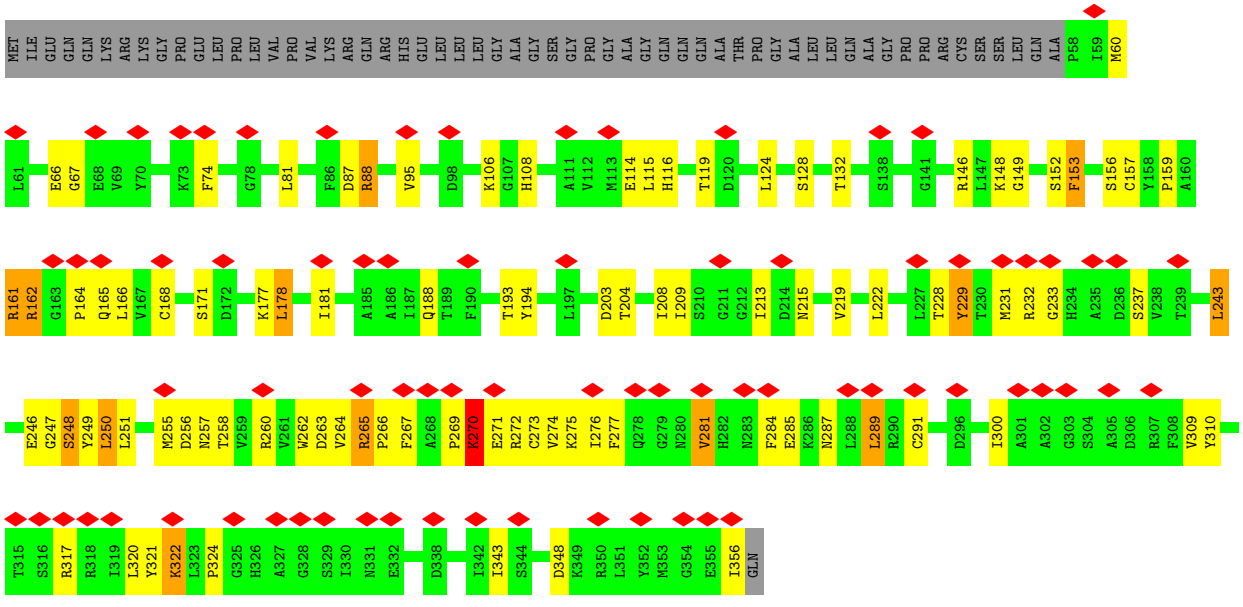

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Q1086 S1087 A1088 G1089 R1090 L1091 M1092 R1093 A1094 I1095 F1096 E1097 I1098 V1099 L1100 N1101 R1102 G1103 W1104 A1105 Q1106 L1107 T1108 D1109 K1110 T1111 L1112 N1113 L1114 C1115 K1116 M1117 I1118 D1119 K1120 R1121 M1122 W1123 Q1124 S1125 M1126 C1127 P1128 L1129 R1130 Q1131 F1132 R1133 K1134 L1135 P1136 E1137 E1138 V1139 V1140 K1145 K1146 N1147 F1148
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• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:

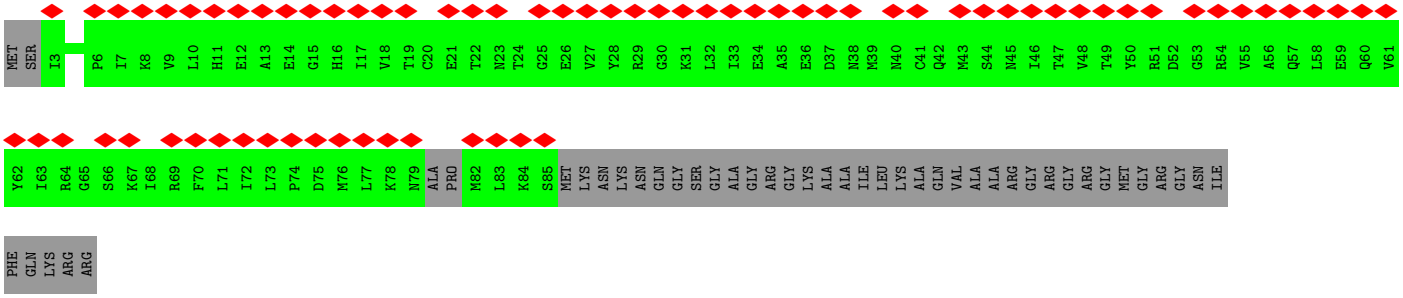




• Molecule 6: Small nuclear ribonucleoprotein Sm D3

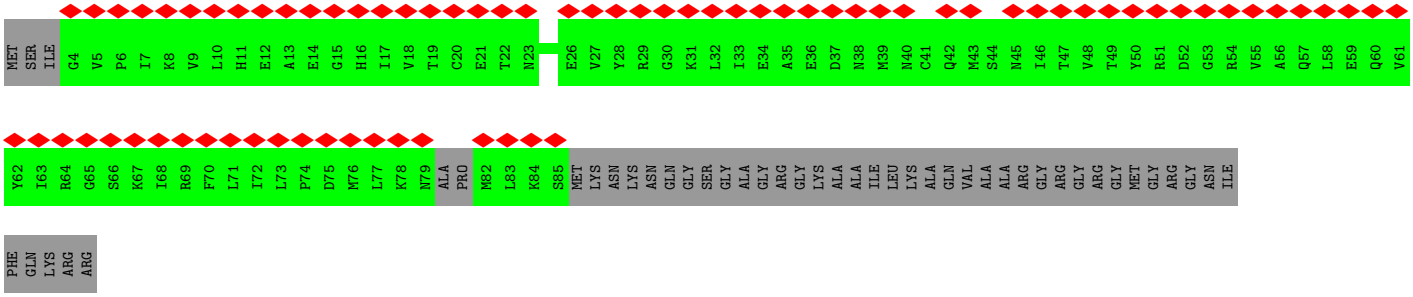
Chain a:





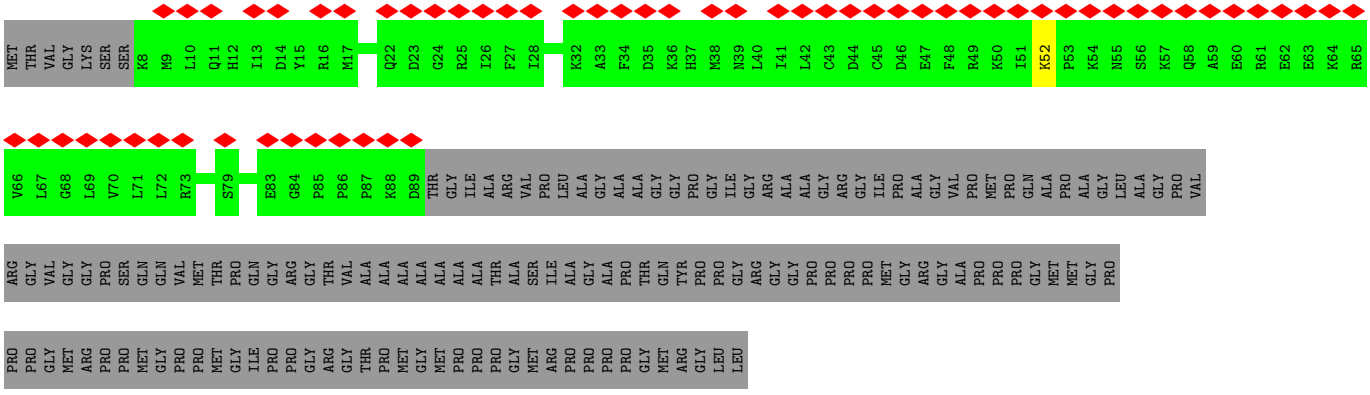
• Molecule 6: Small nuclear ribonucleoprotein Sm D3





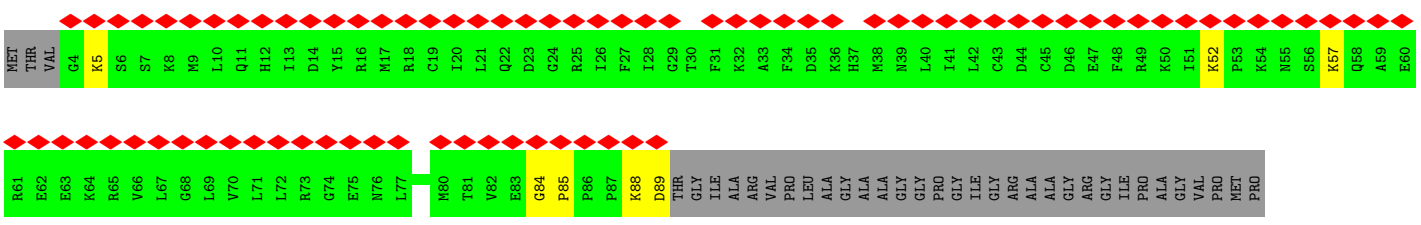
• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'

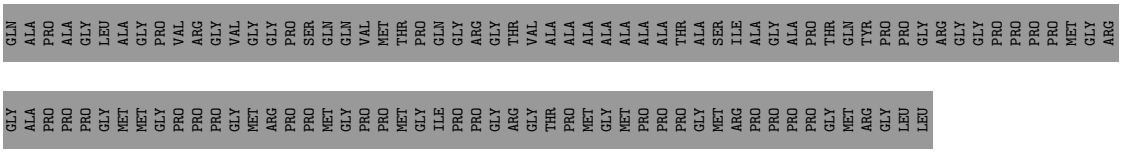




• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'

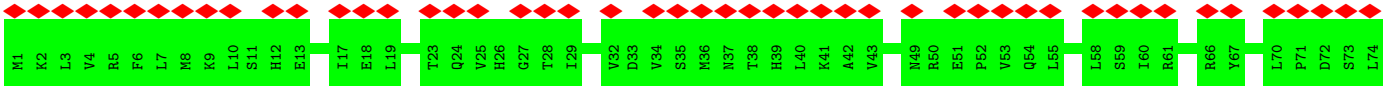


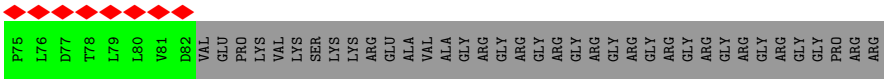




• Molecule 8: Small nuclear ribonucleoprotein Sm D1

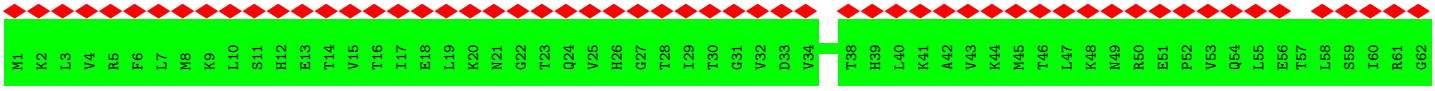






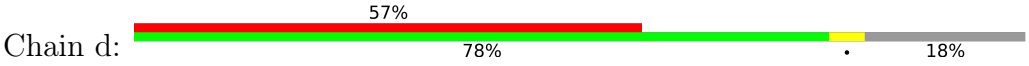
• Molecule 8: Small nuclear ribonucleoprotein Sm D1

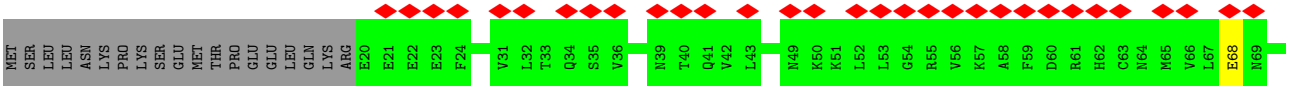


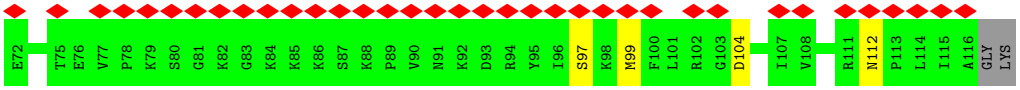




• Molecule 9: Small nuclear ribonucleoprotein Sm D2

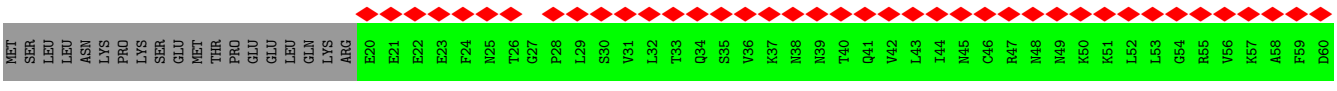


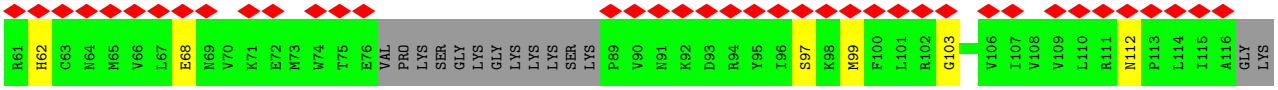




• Molecule 9: Small nuclear ribonucleoprotein Sm D2

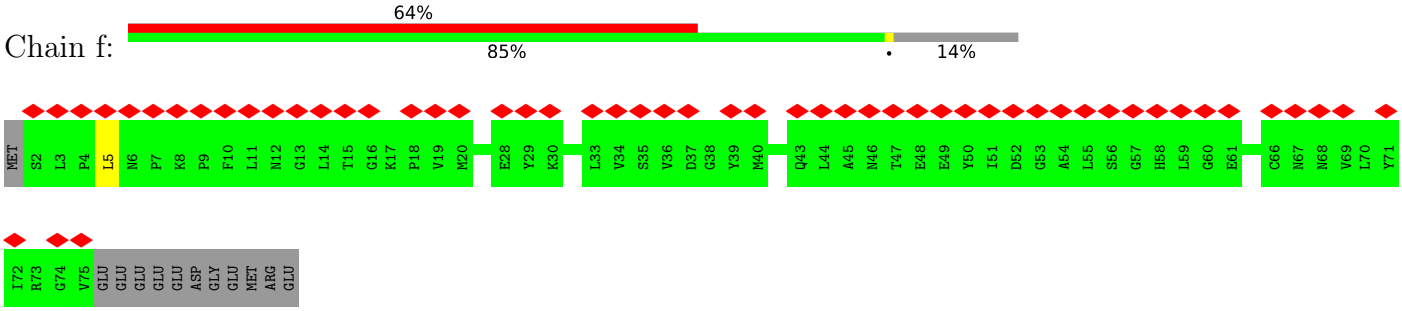






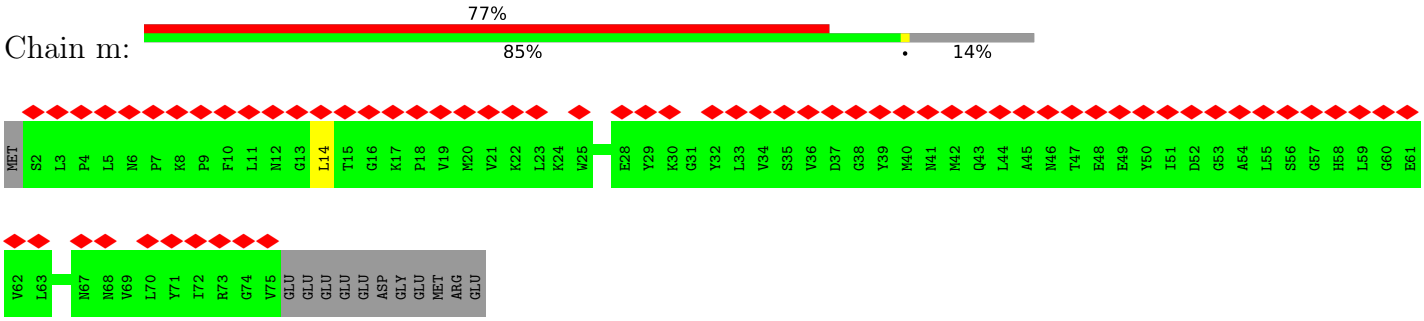
• Molecule 10: Small nuclear ribonucleoprotein F

Chain f:



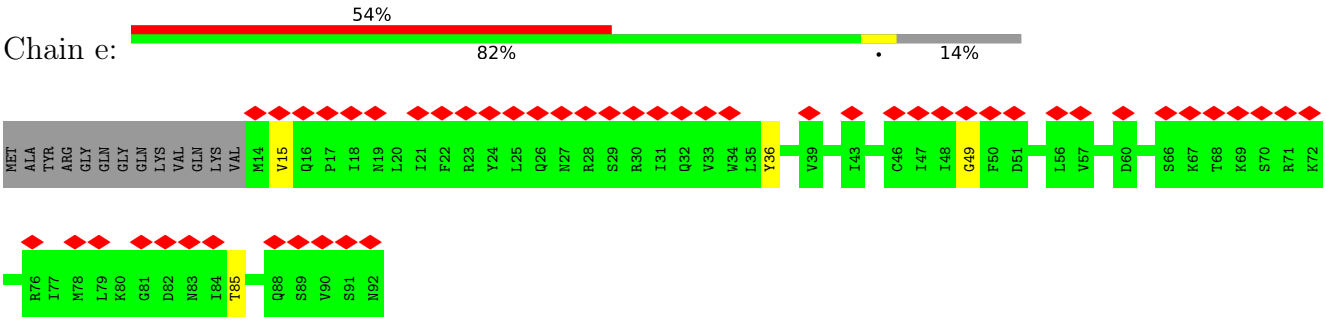
• Molecule 10: Small nuclear ribonucleoprotein F

Chain m:



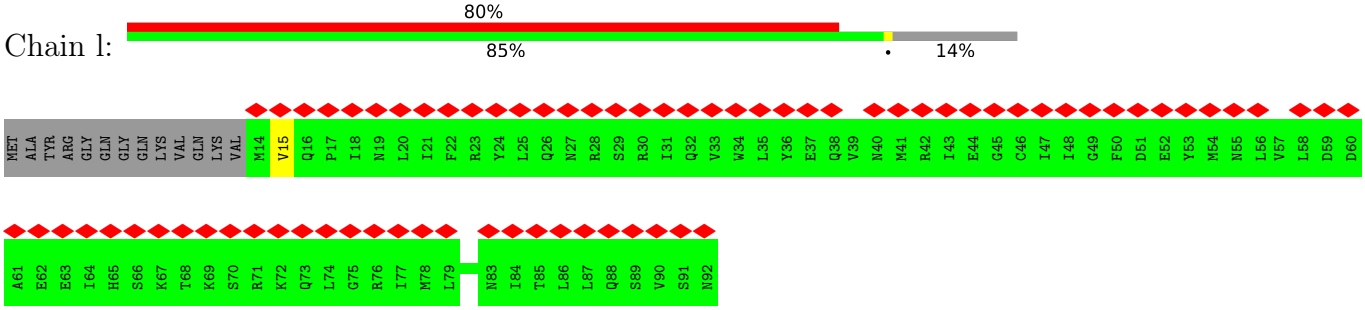
• Molecule 11: Small nuclear ribonucleoprotein E

Chain e:



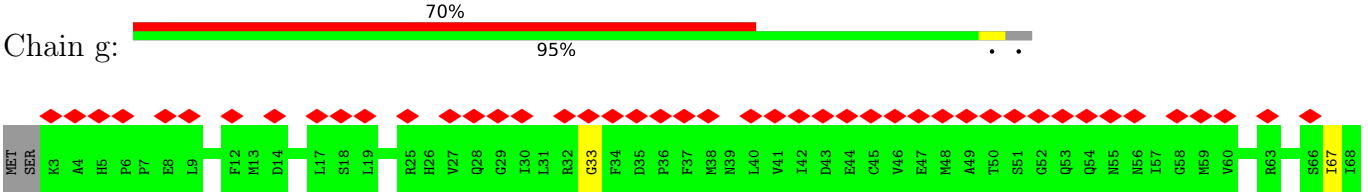
• Molecule 11: Small nuclear ribonucleoprotein E

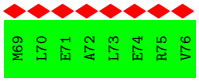
Chain l:



• Molecule 12: Small nuclear ribonucleoprotein G

Chain g:

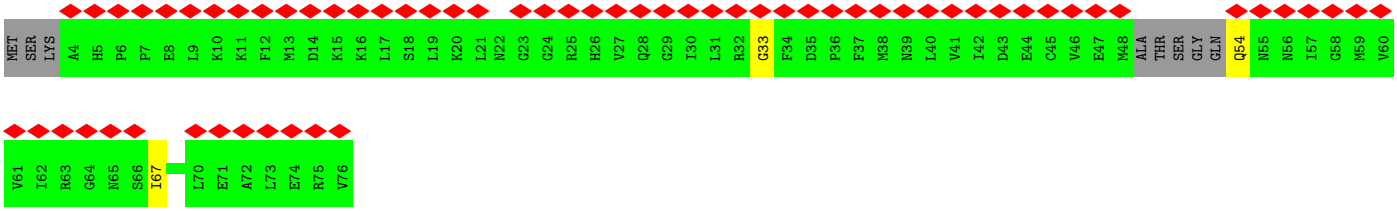




• Molecule 12: Small nuclear ribonucleoprotein G

Chain n:

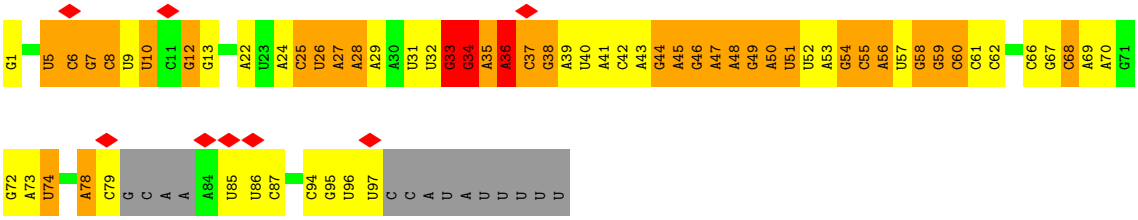




• Molecule 13: U6 snRNA

Chain F:

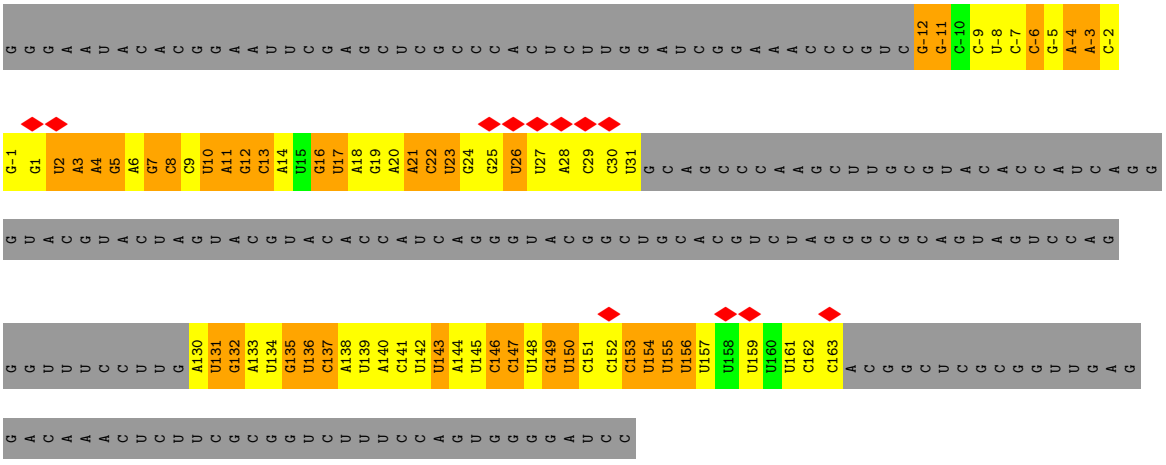




• Molecule 14: pre-mRNA

Chain G:

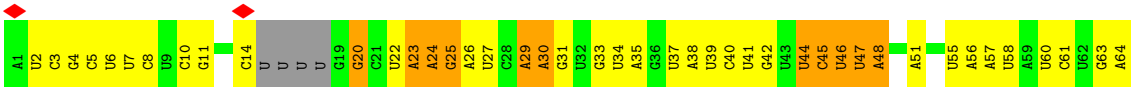


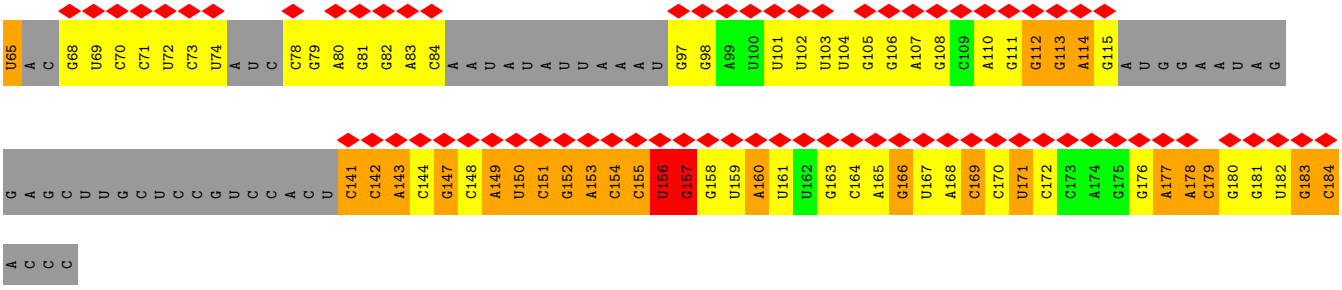


• Molecule 15: U2 snRNA

Chain H:



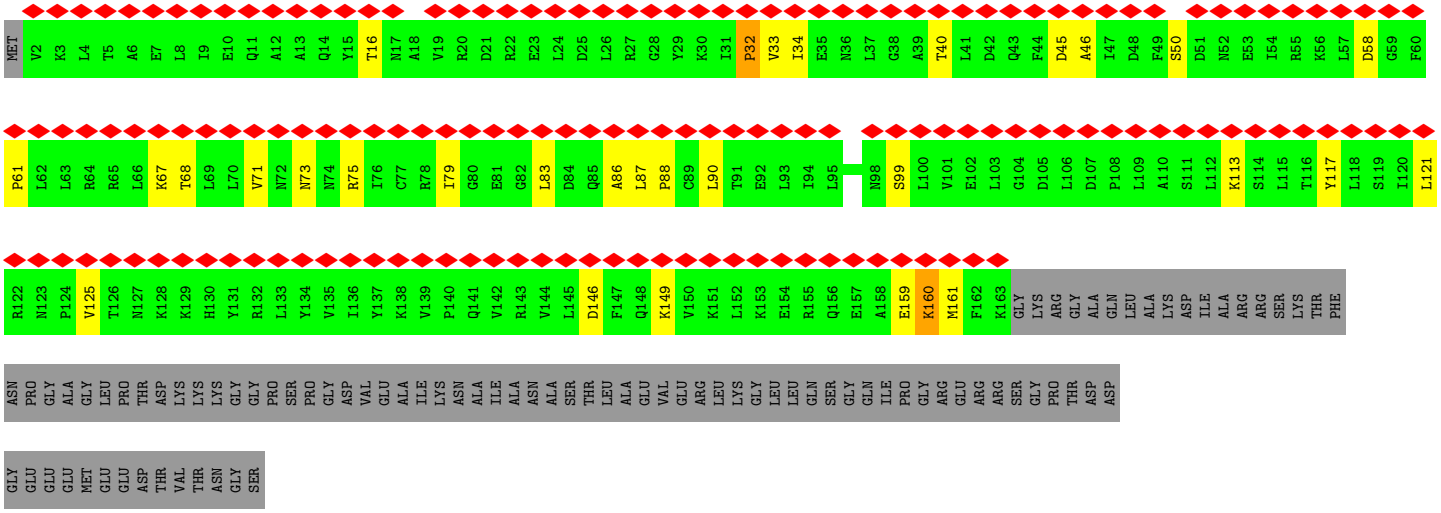




• Molecule 16: U2 small nuclear ribonucleoprotein A'

Chain o:

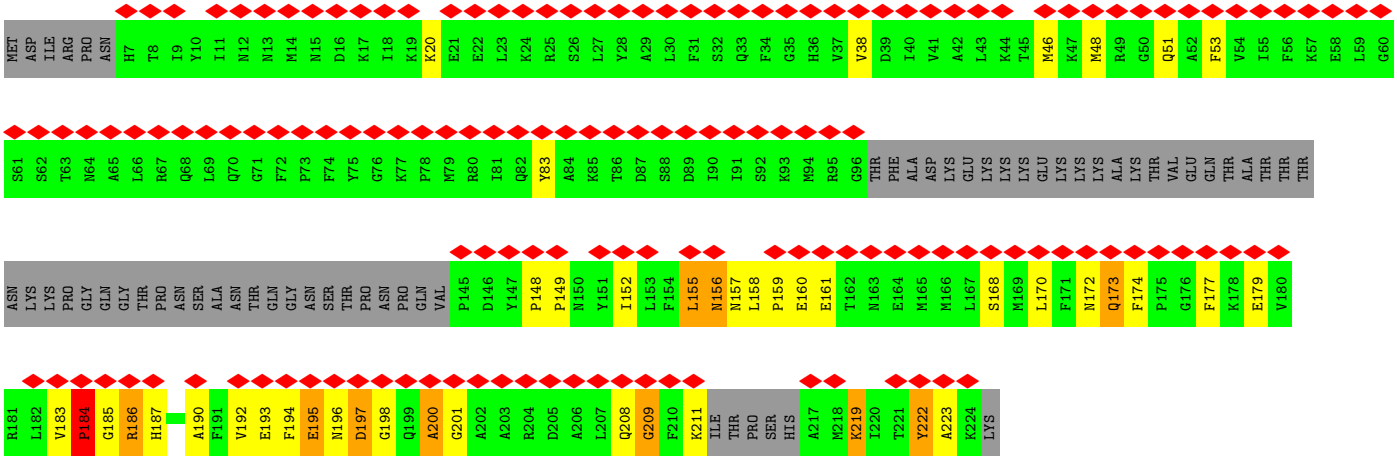




• Molecule 17: U2 small nuclear ribonucleoprotein B"

Chain p:

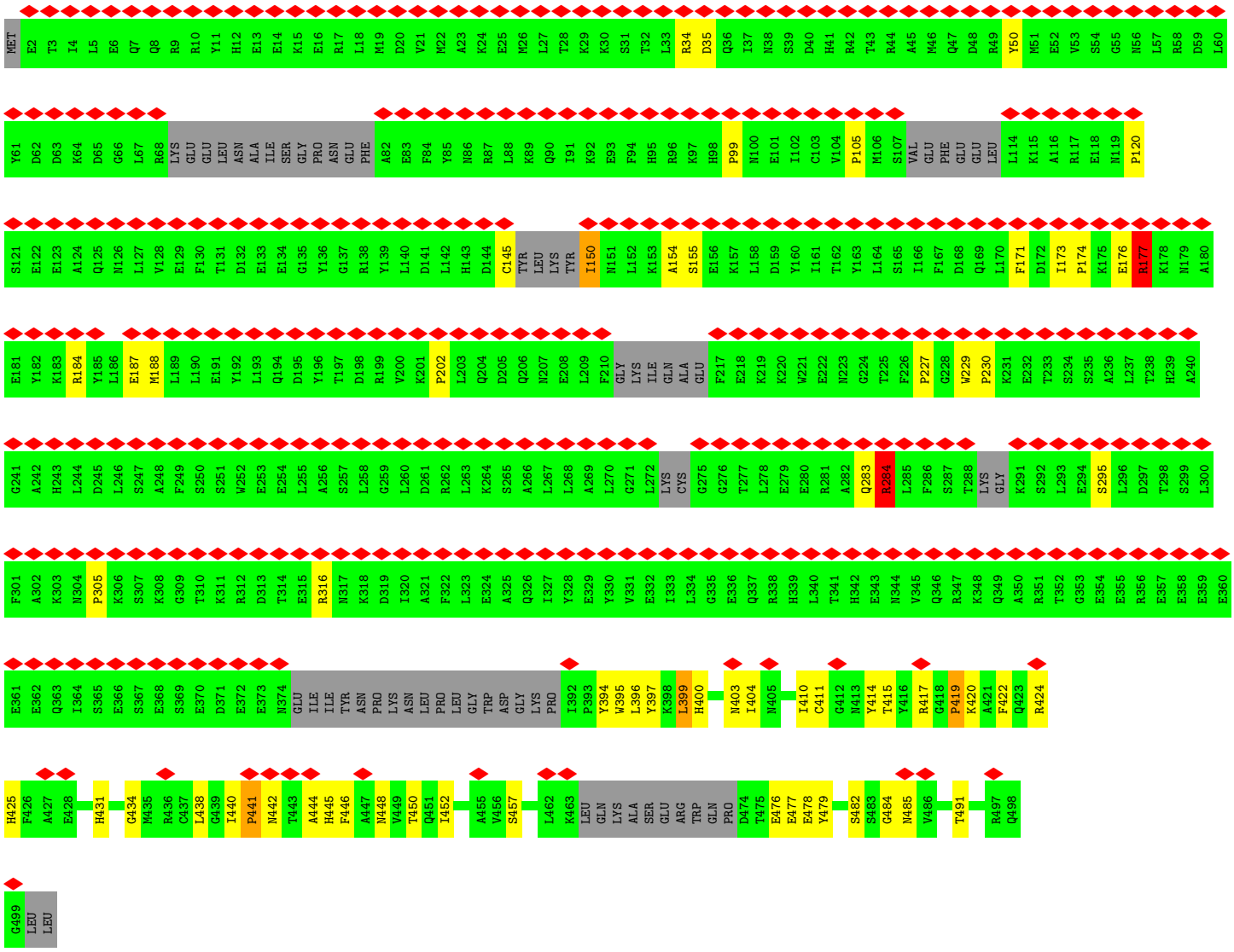




• Molecule 18: Splicing factor 3A subunit 3

Chain w:

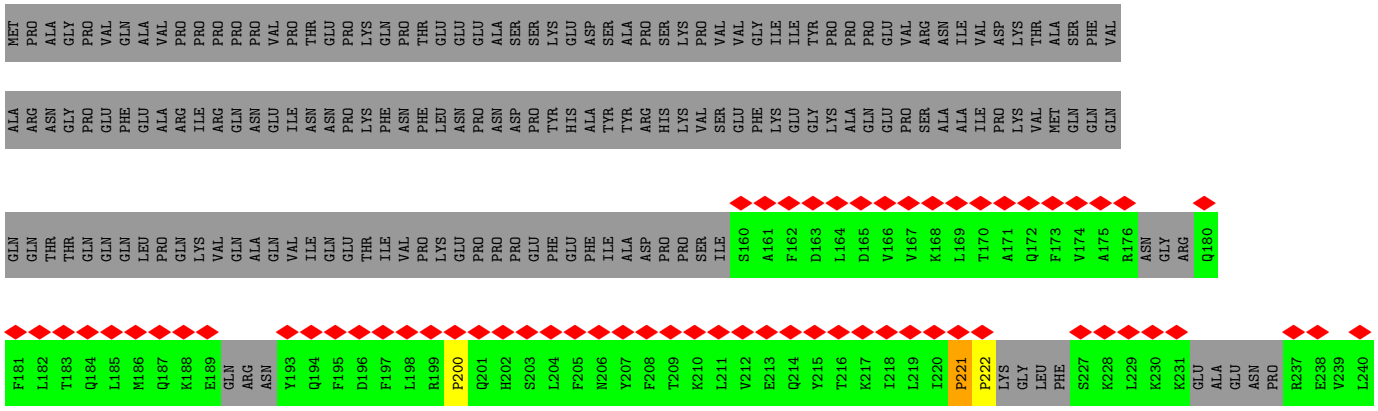


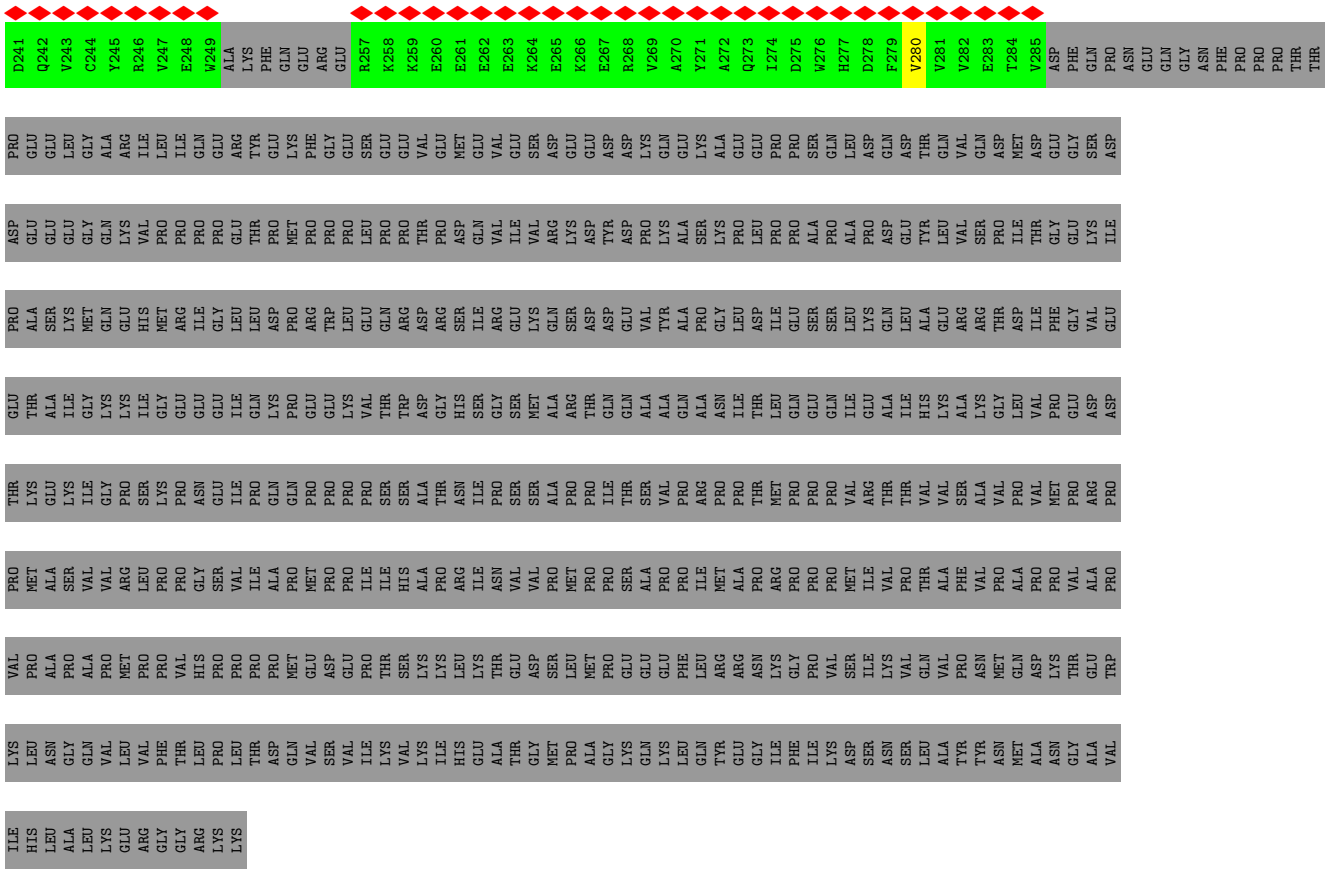


• Molecule 19: Splicing factor 3A subunit 1

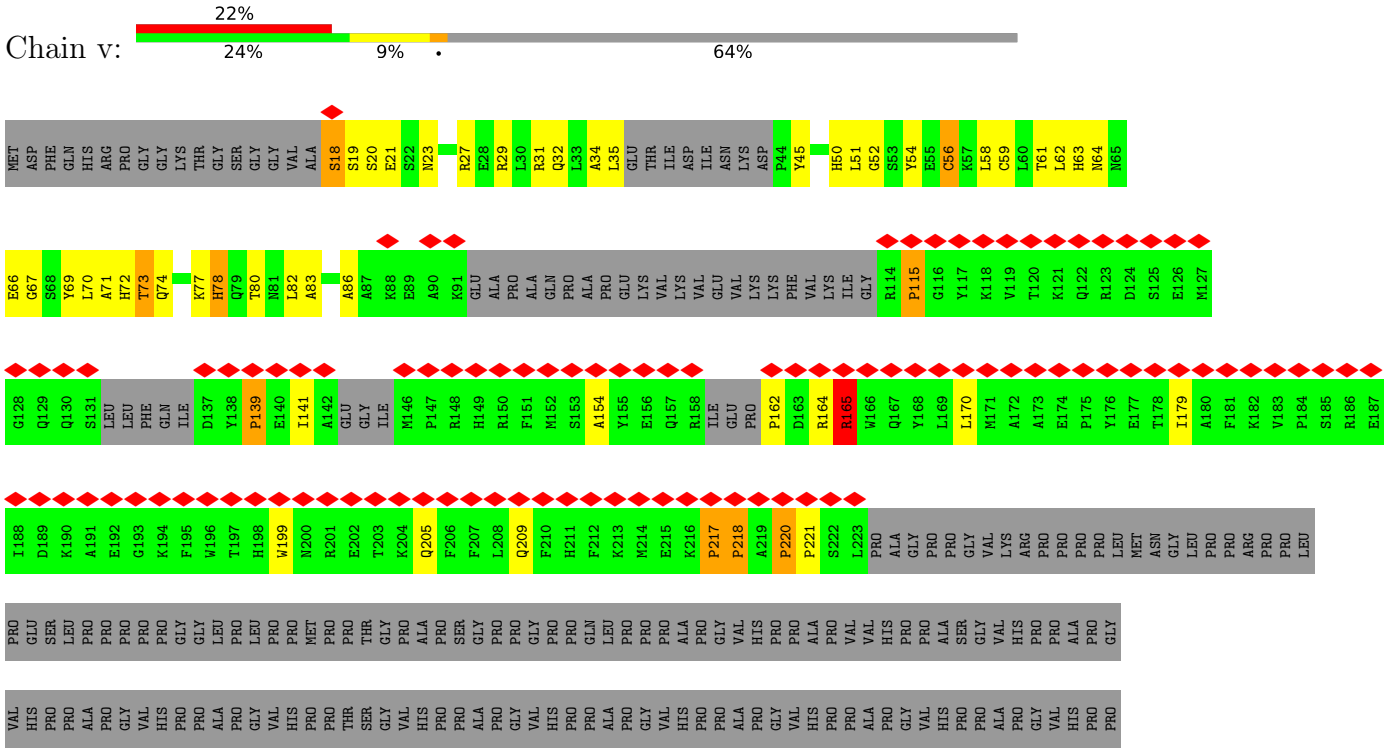
Chain u:

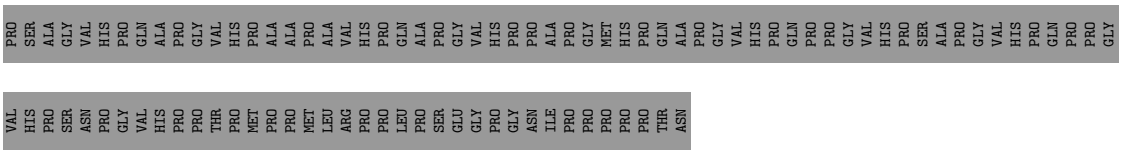






• Molecule 20: Splicing factor 3A subunit 2

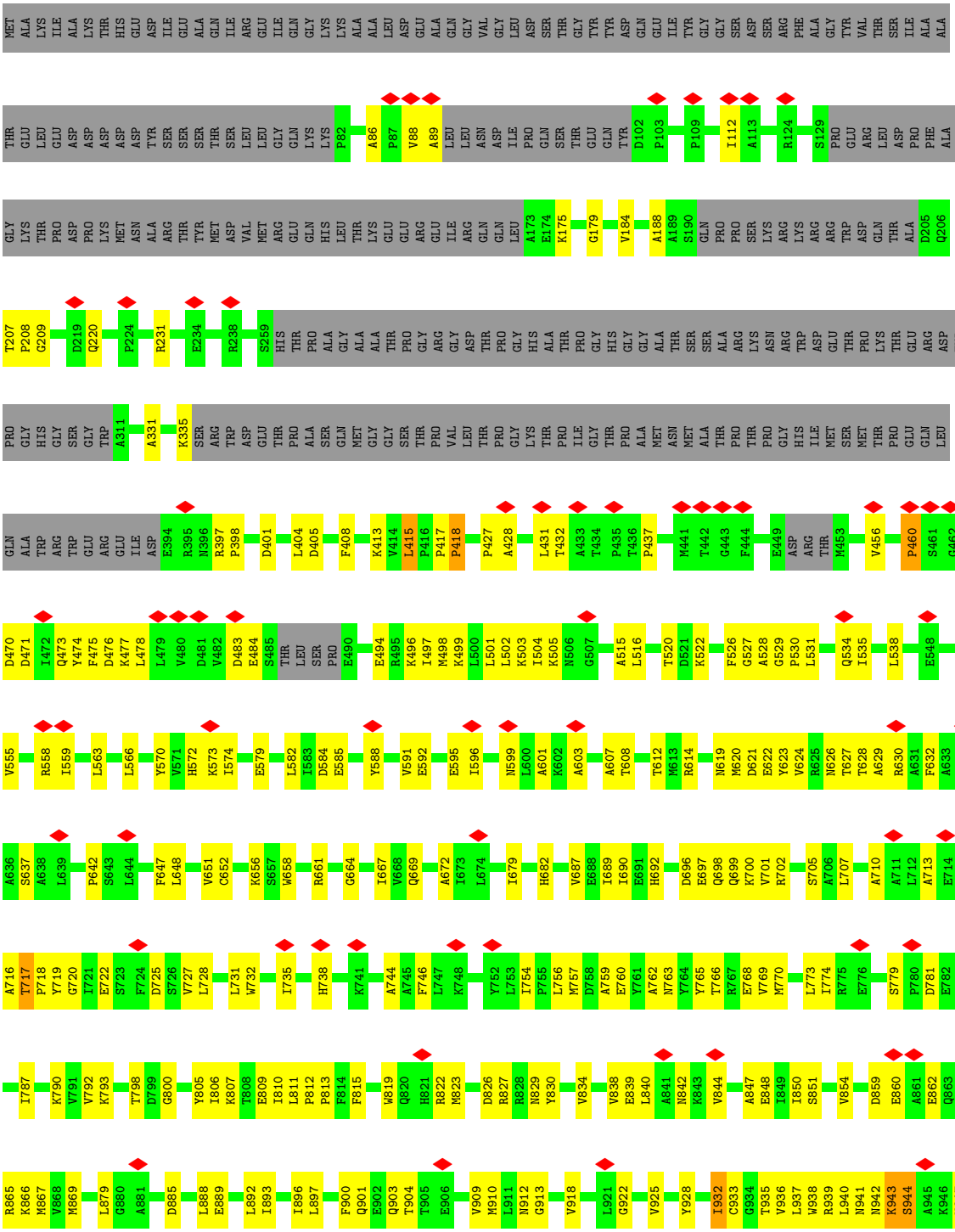


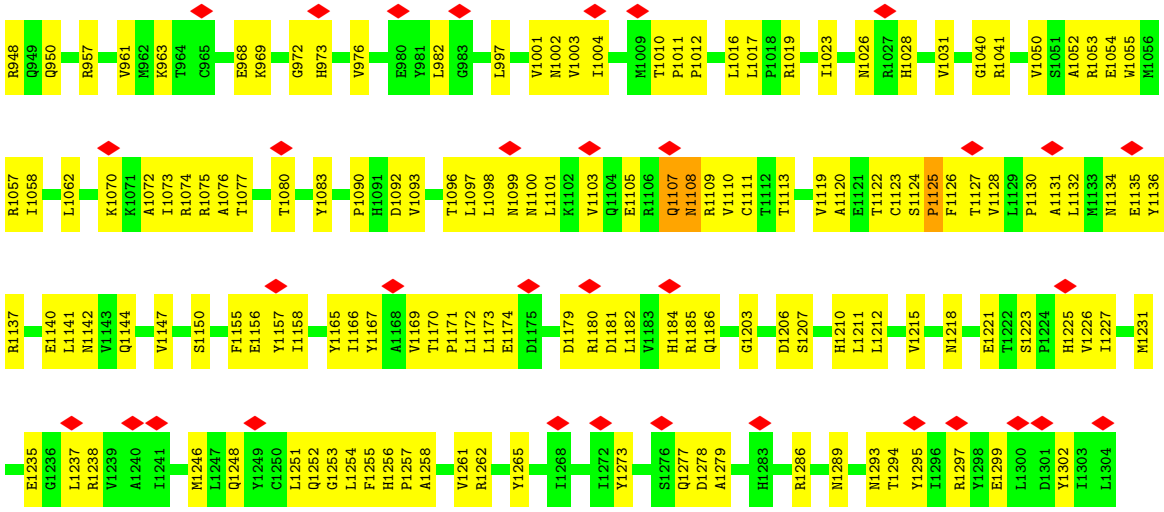


• Molecule 21: Splicing factor 3B subunit 1

Chain 1:



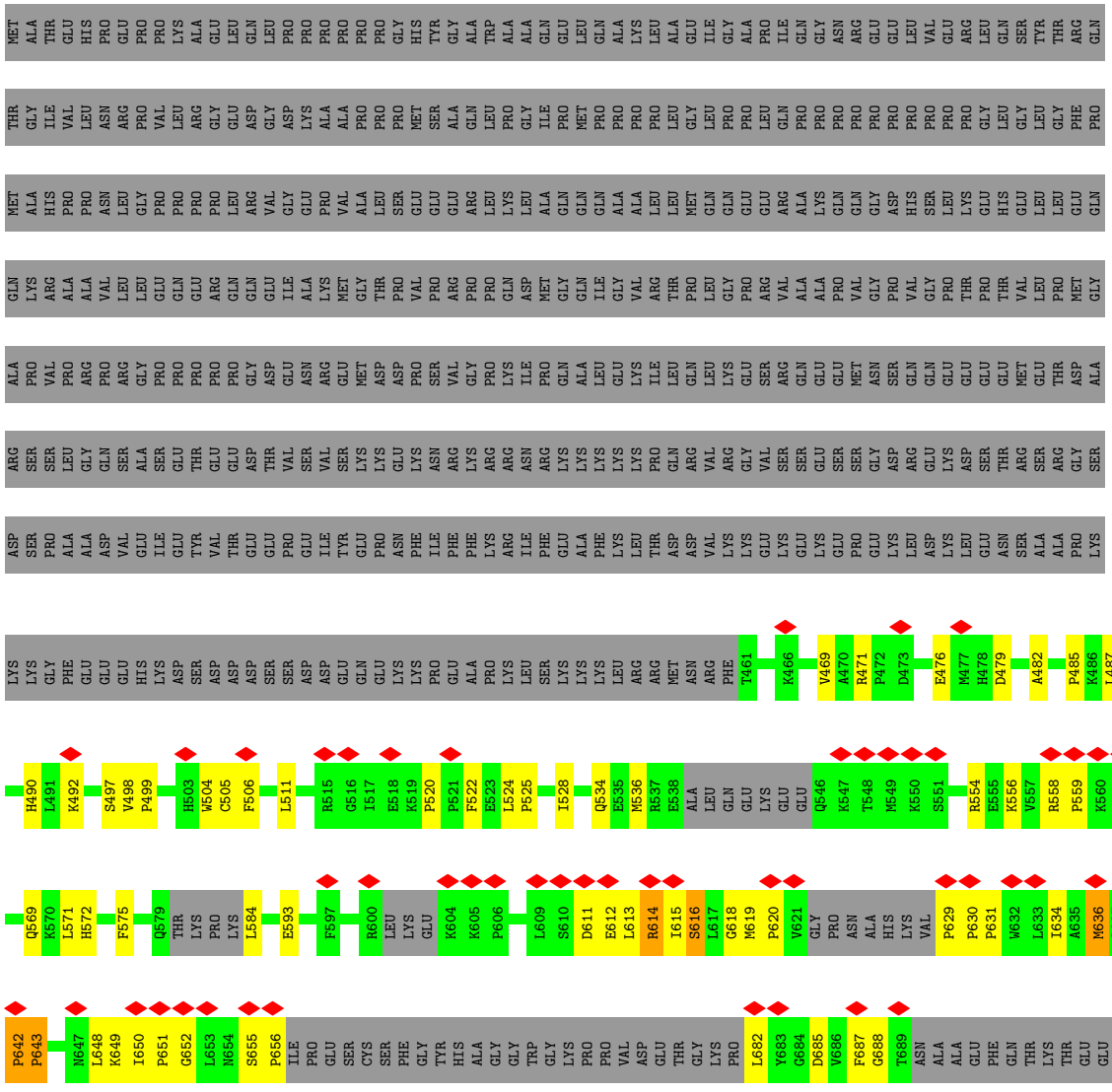


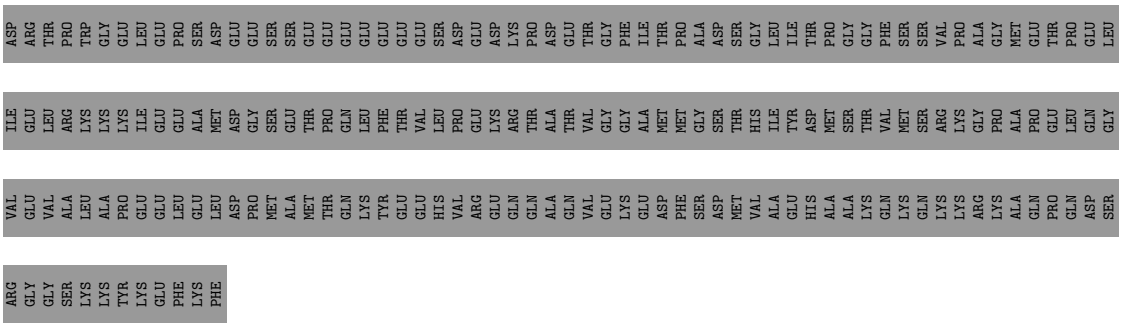


• Molecule 22: Splicing factor 3B subunit 2

Chain 2:



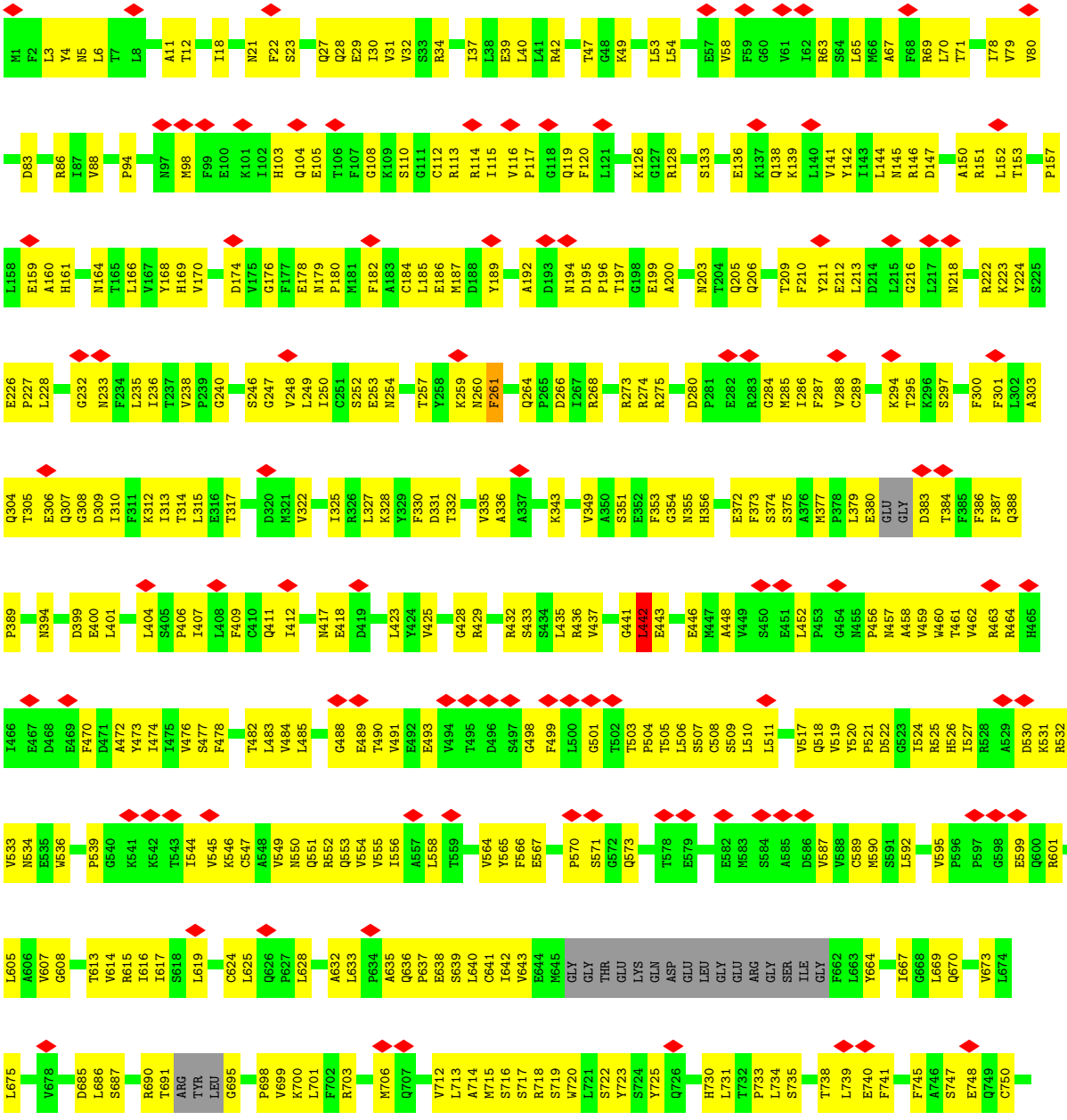


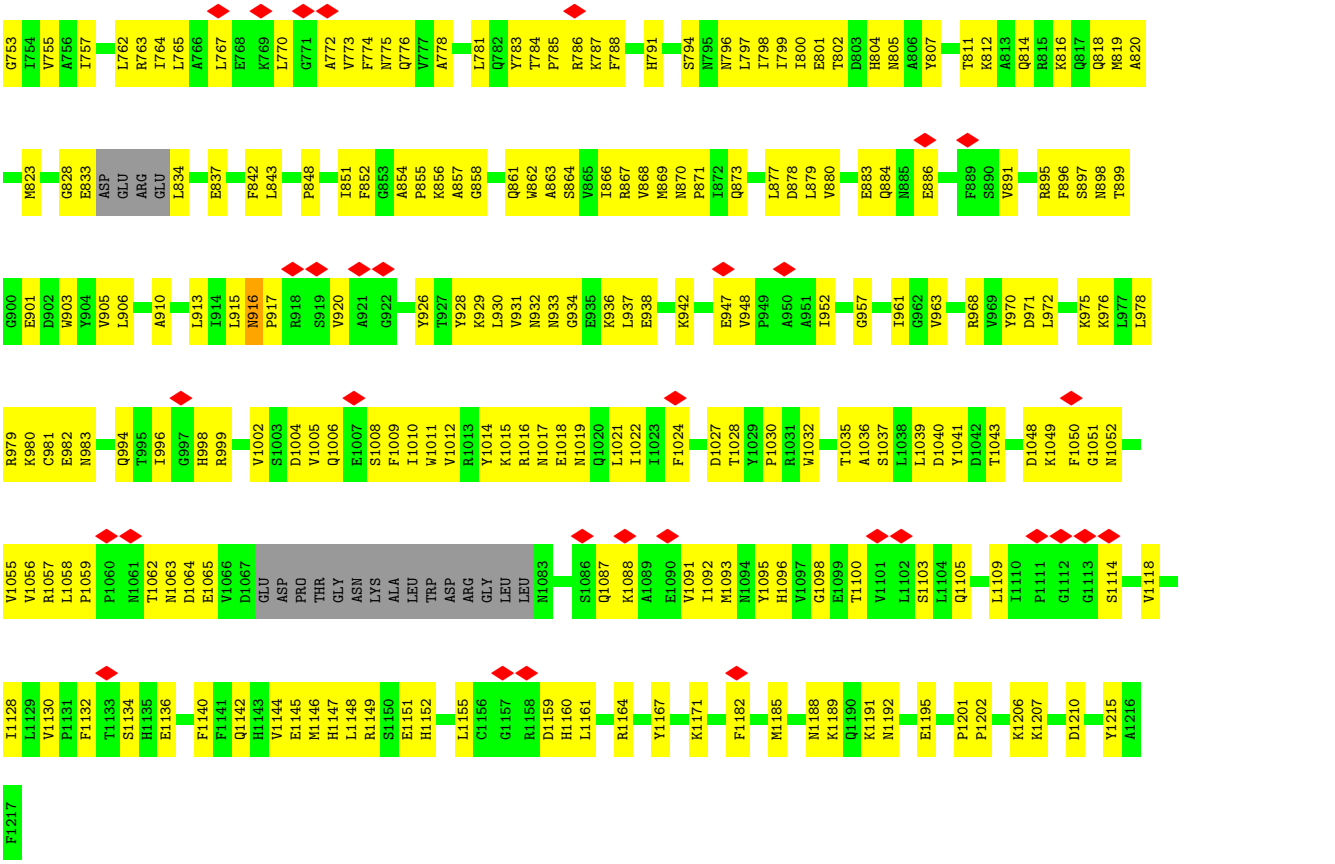


• Molecule 23: Splicing factor 3B subunit 3

Chain 3:



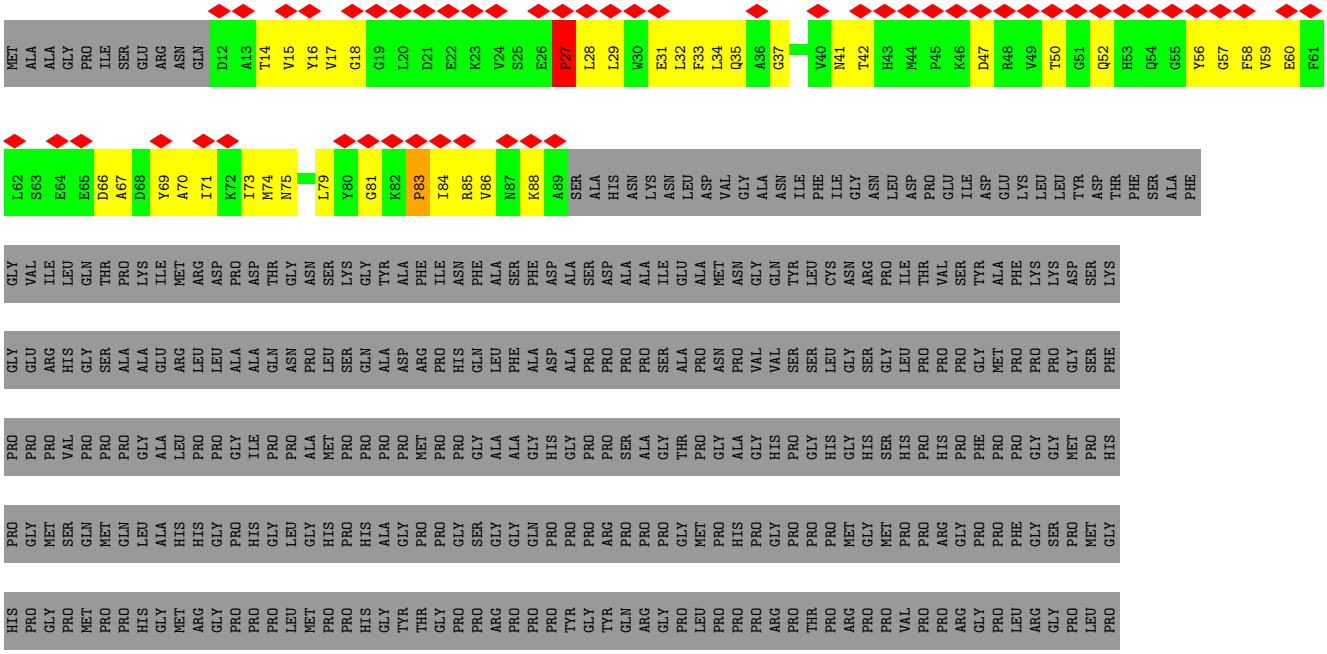




• Molecule 24: Splicing factor 3B subunit 4

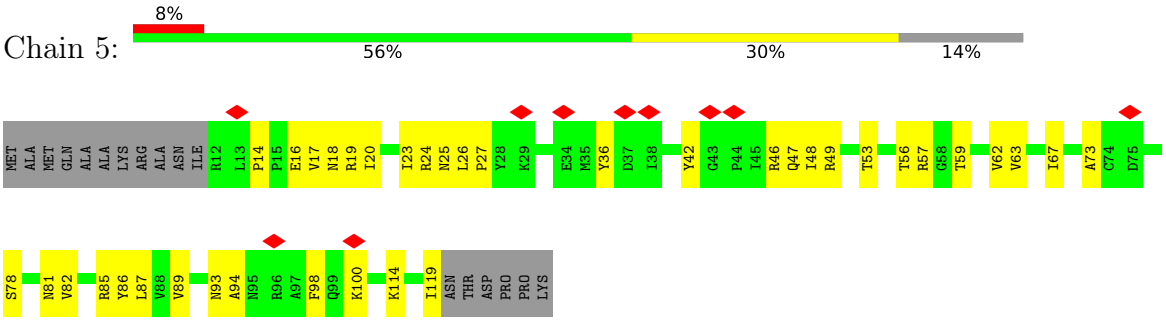
Chain 4:



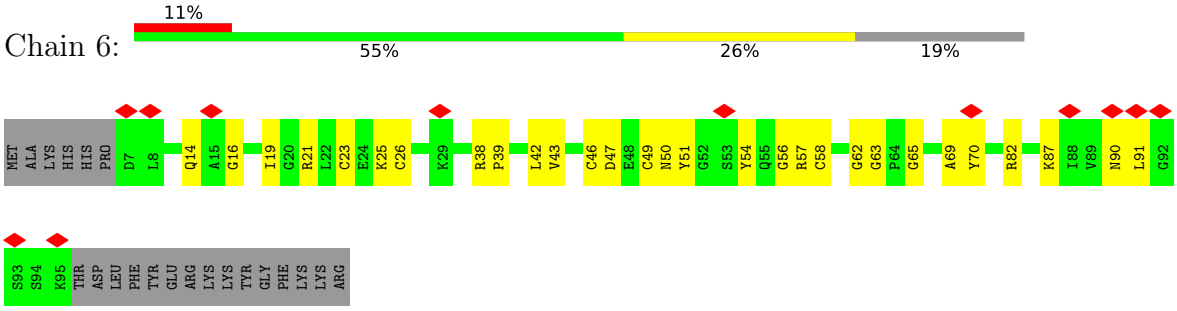




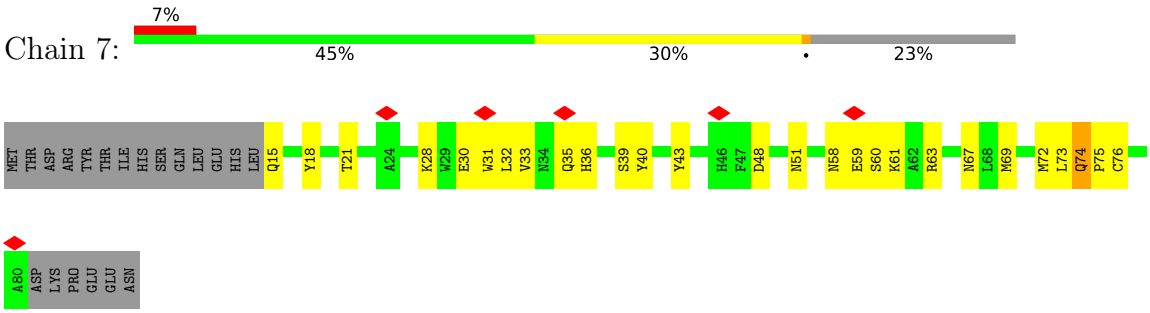
• Molecule 25: Splicing factor 3B subunit 6



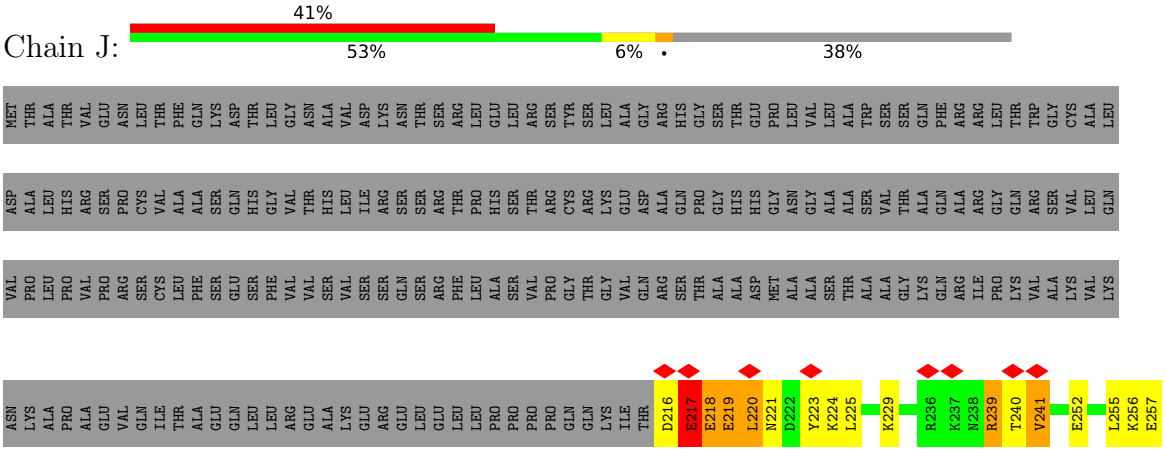
• Molecule 26: PHD finger-like domain-containing protein 5A

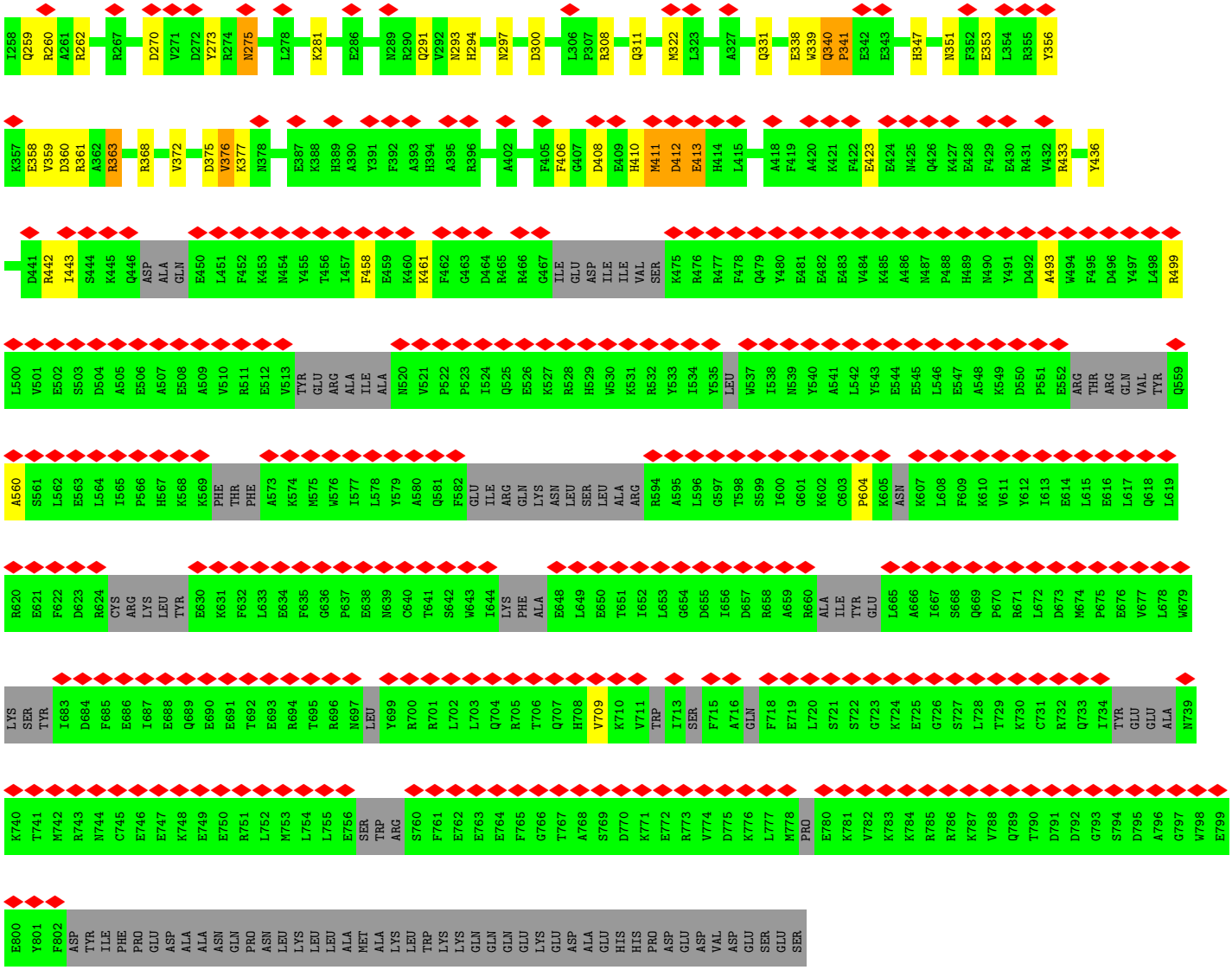


• Molecule 27: Splicing factor 3B subunit 5



• Molecule 28: Crooked neck-like protein 1

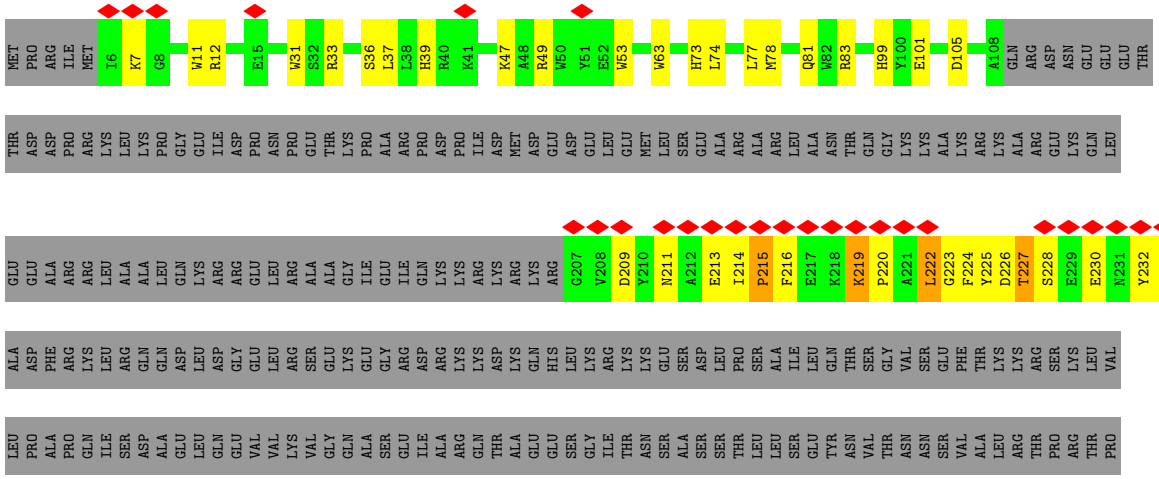


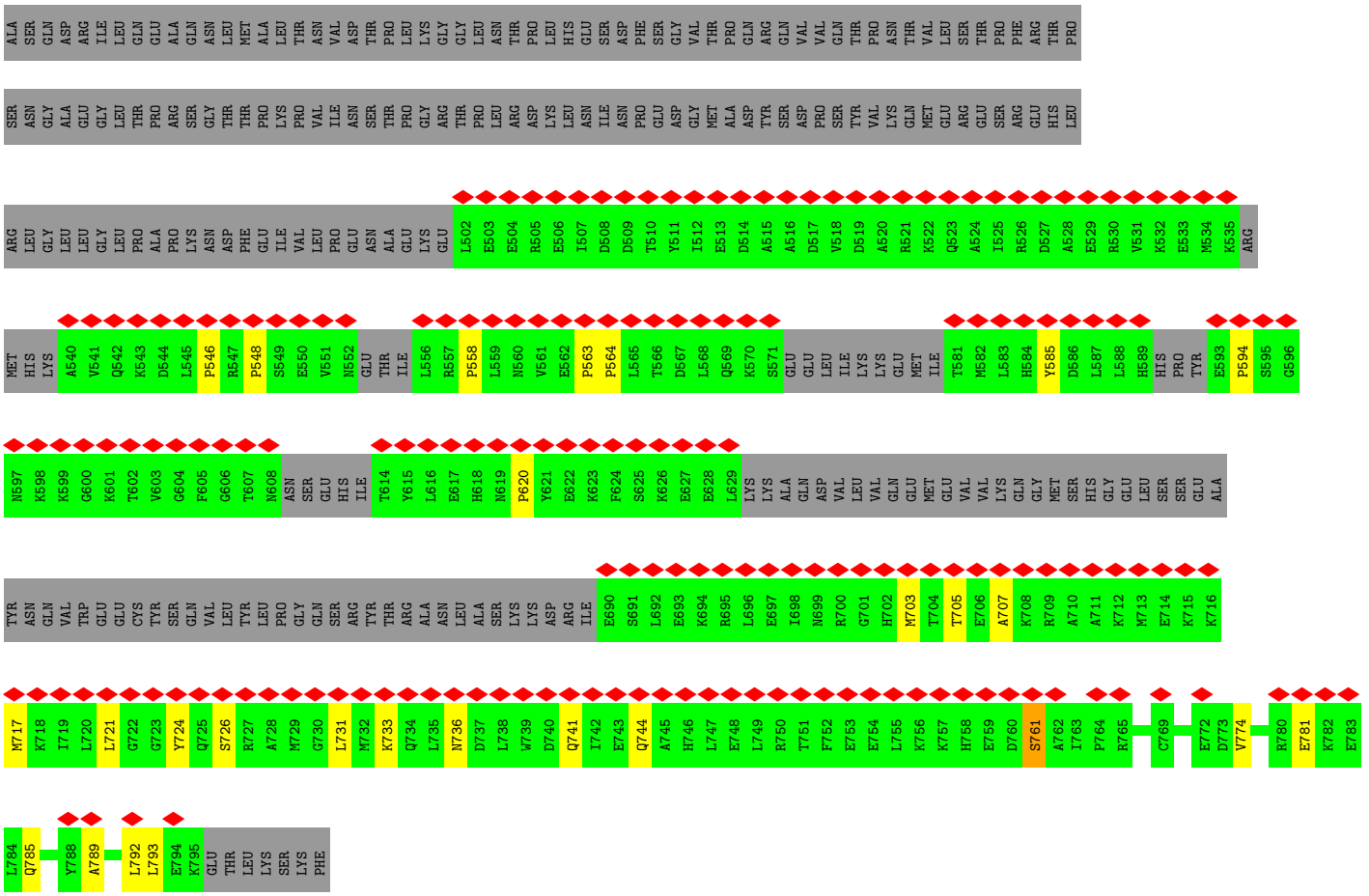


• Molecule 29: Cell division cycle 5-like protein

Chain L:



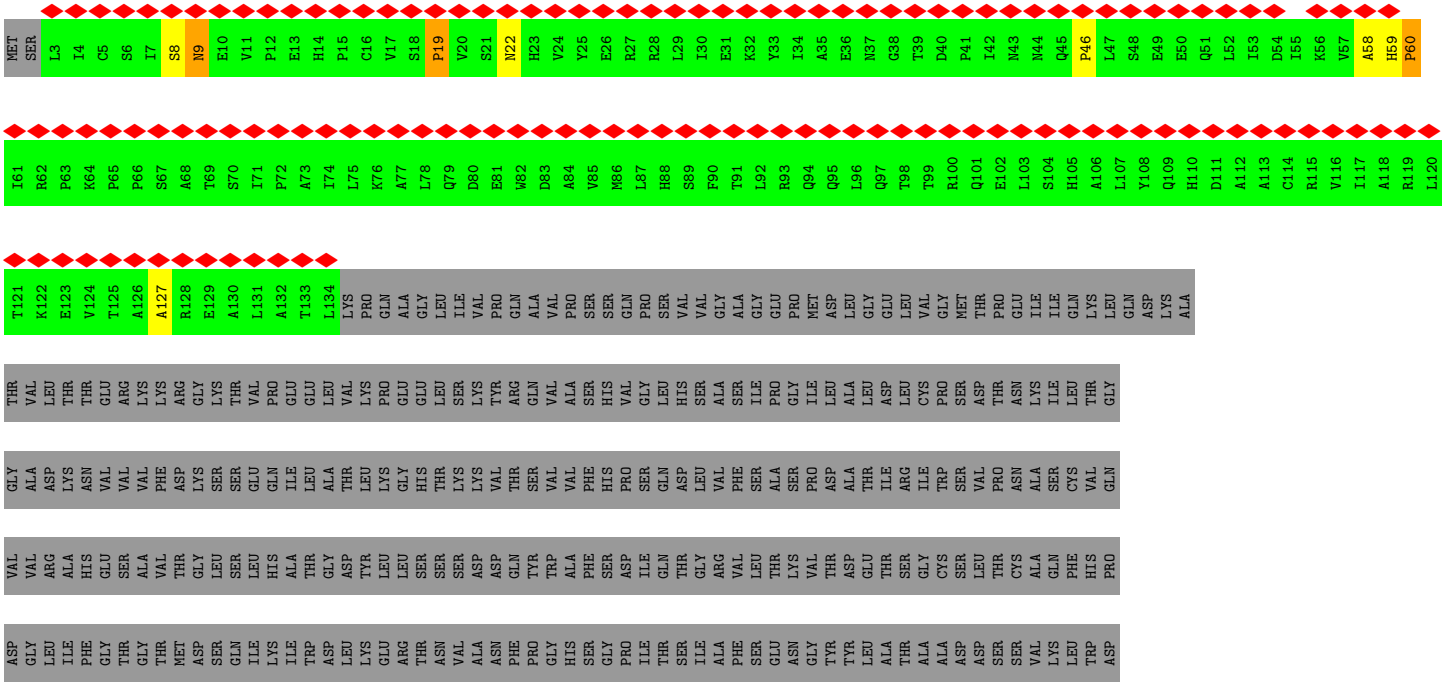


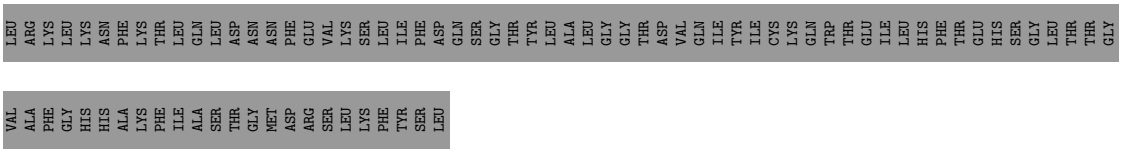


• Molecule 30: Pre-mRNA-processing factor 19

Chain q:





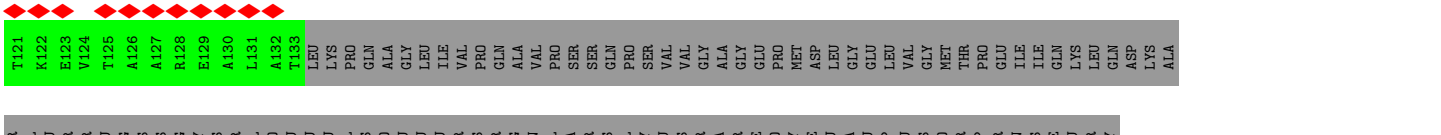


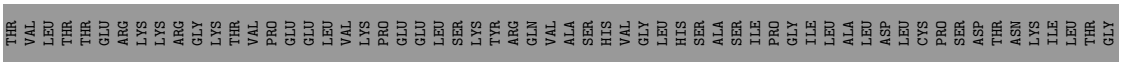
• Molecule 30: Pre-mRNA-processing factor 19

Chain r:

















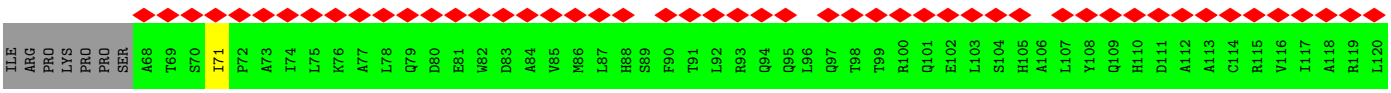


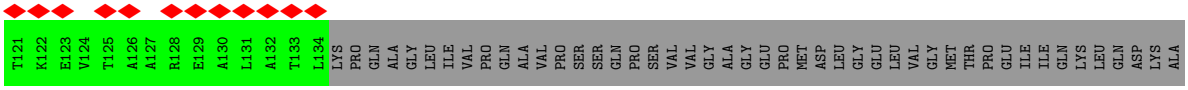
• Molecule 30: Pre-mRNA-processing factor 19

Chain s:

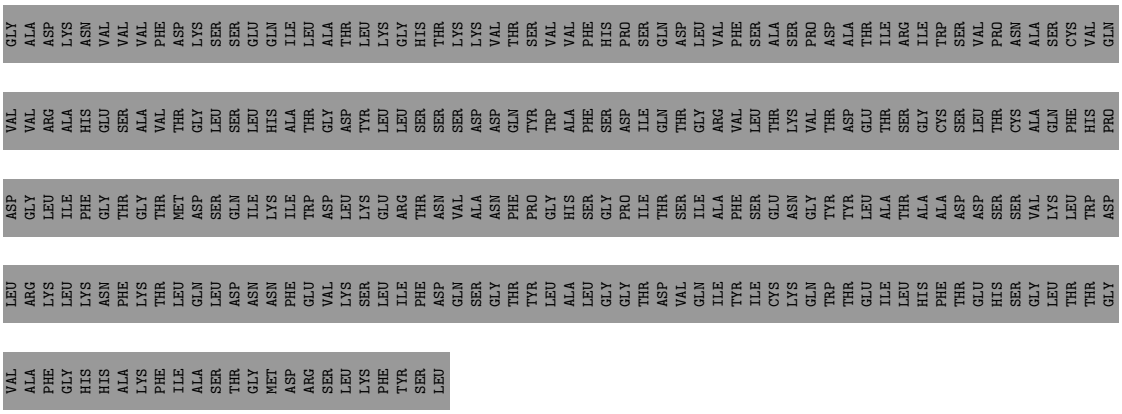








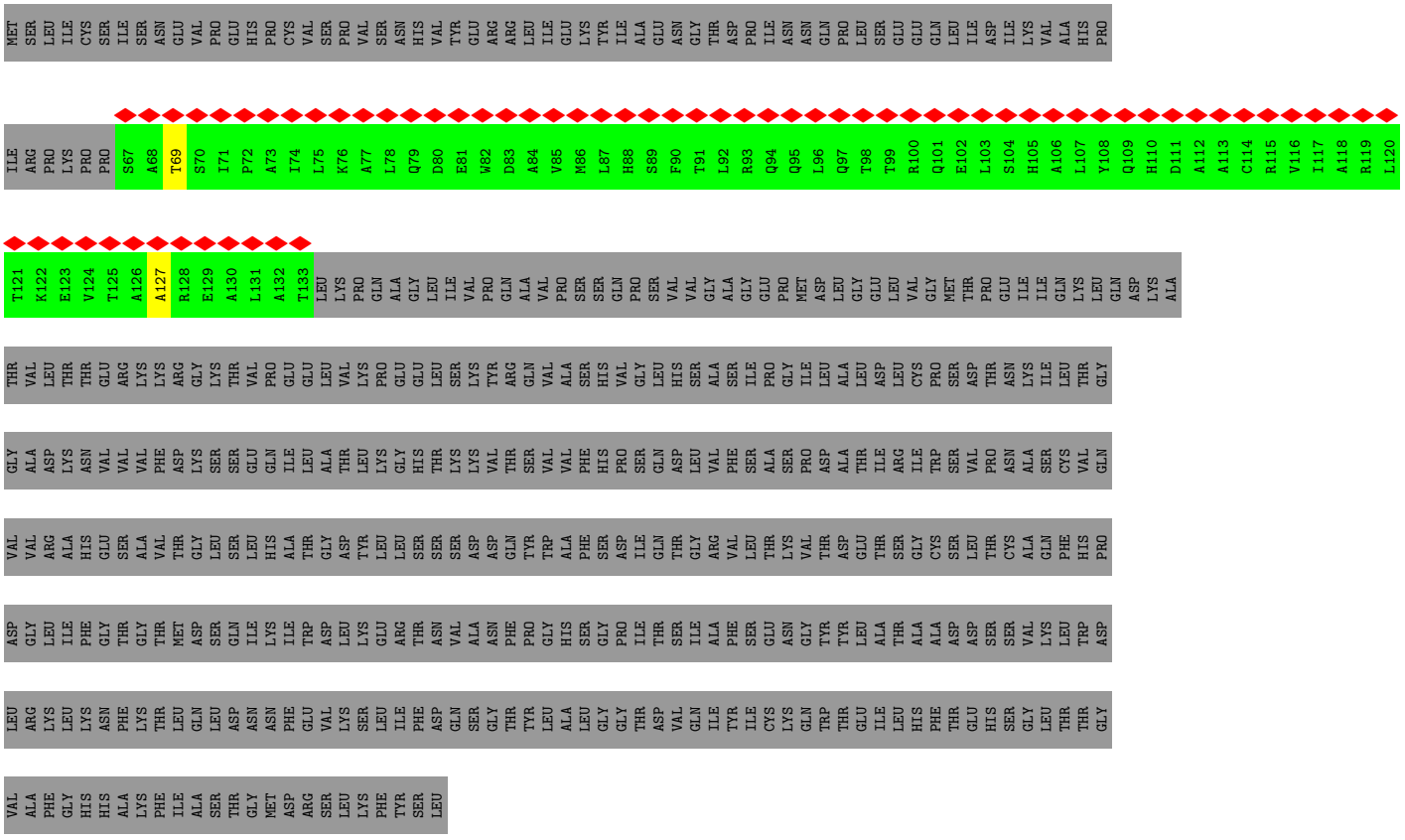




• Molecule 30: Pre-mRNA-processing factor 19

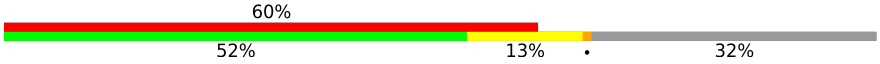
Chain t:

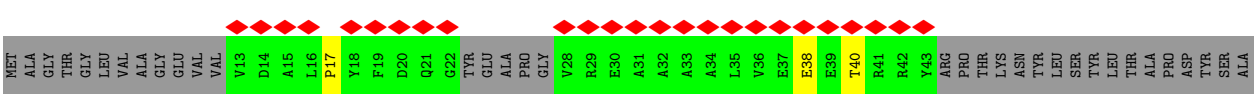


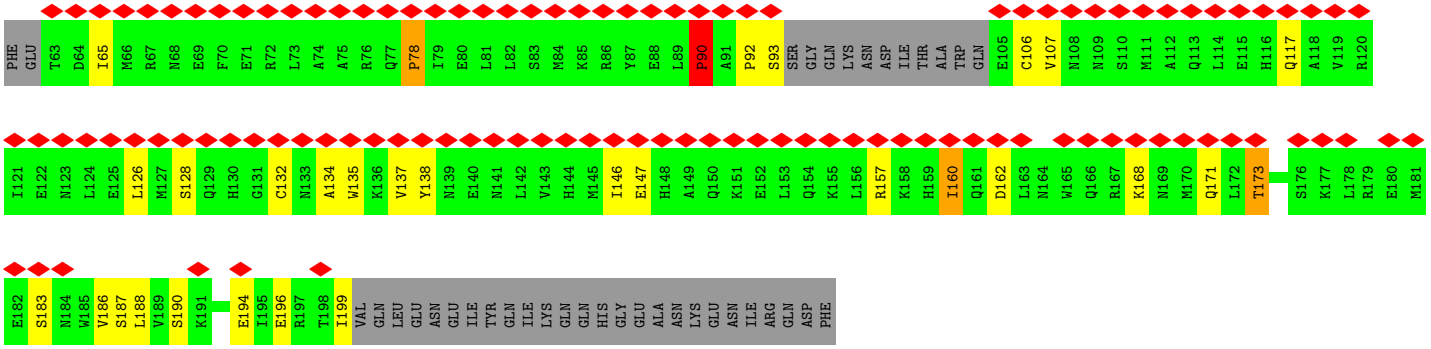


• Molecule 31: Pre-mRNA-splicing factor SPF27

Chain K:



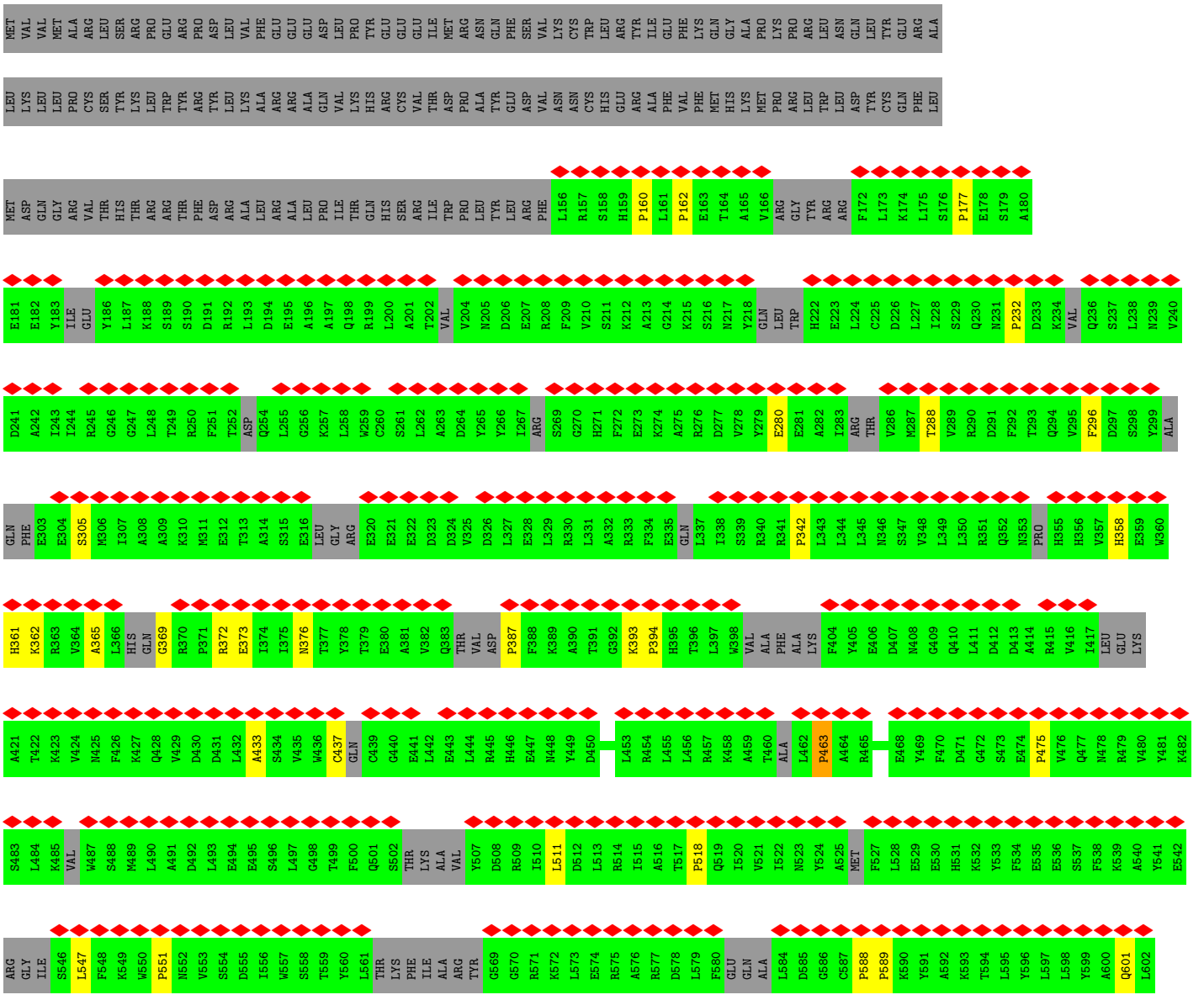


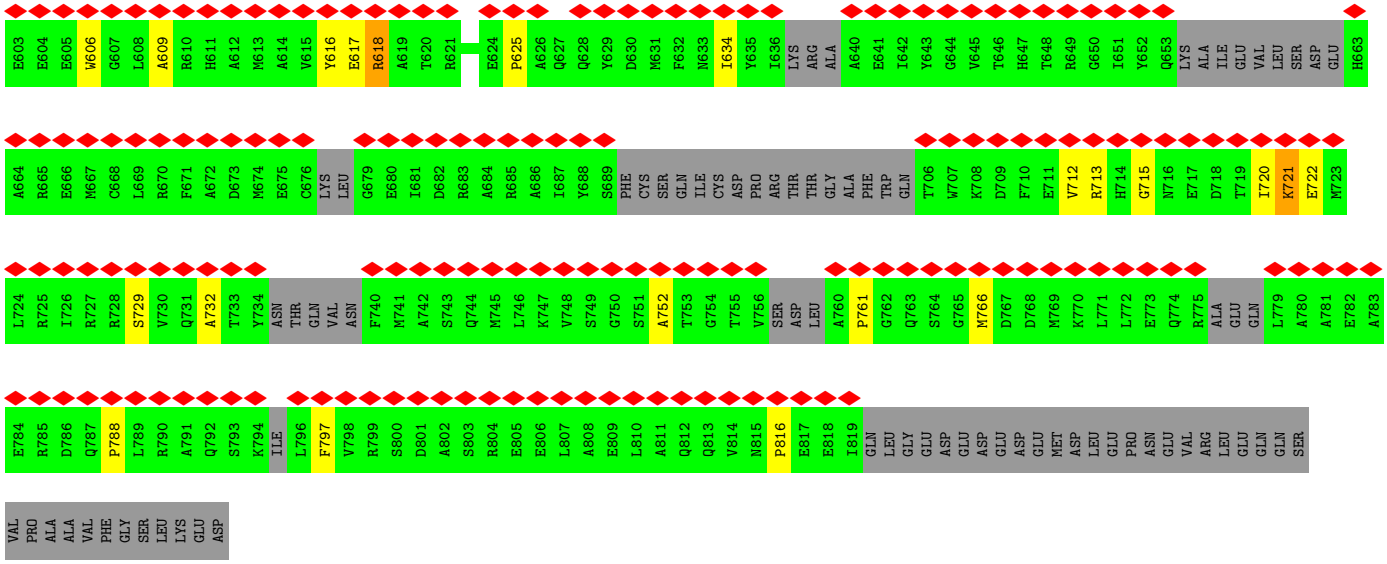


• Molecule 32: Pre-mRNA-splicing factor SYF1

Chain I:



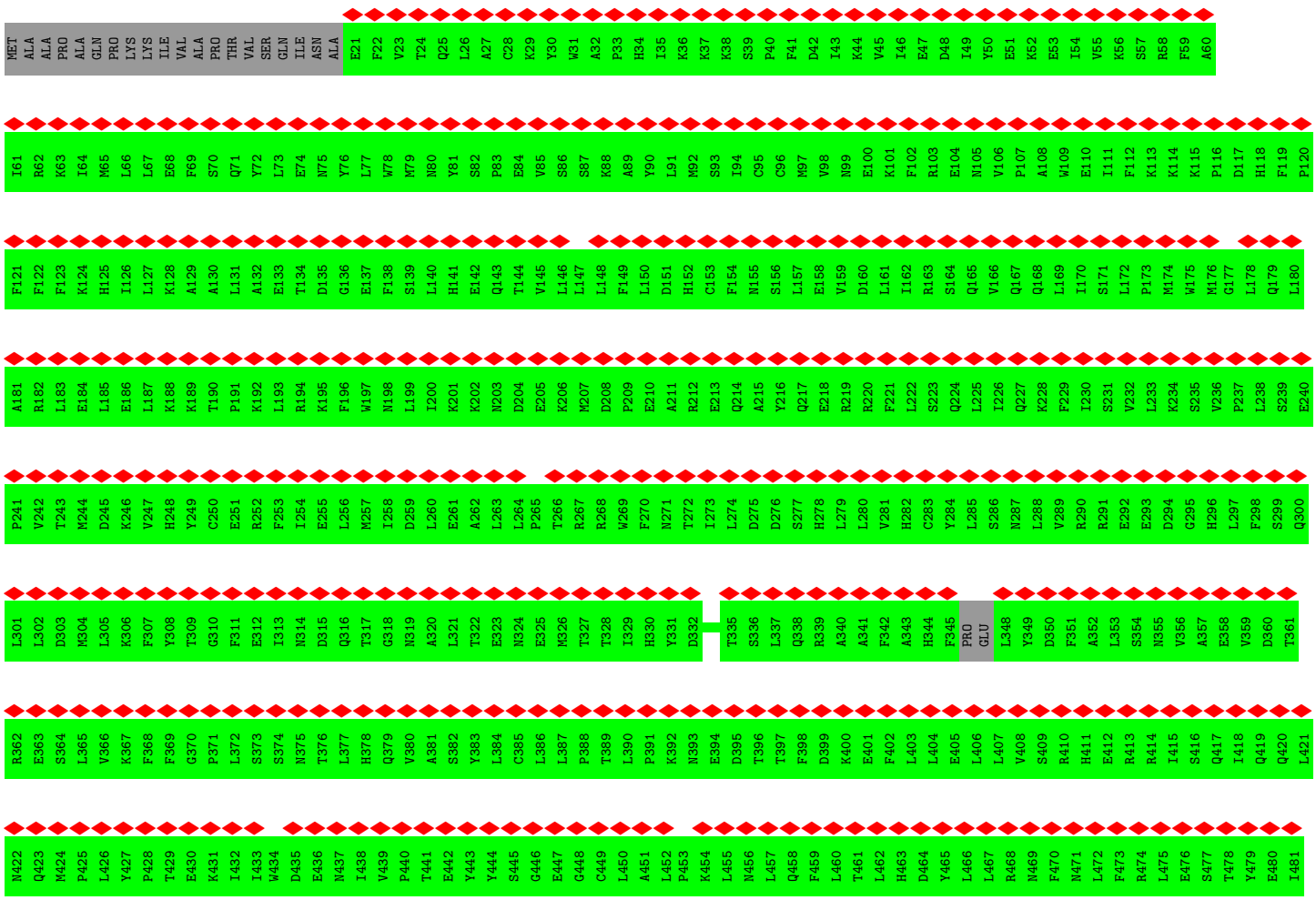


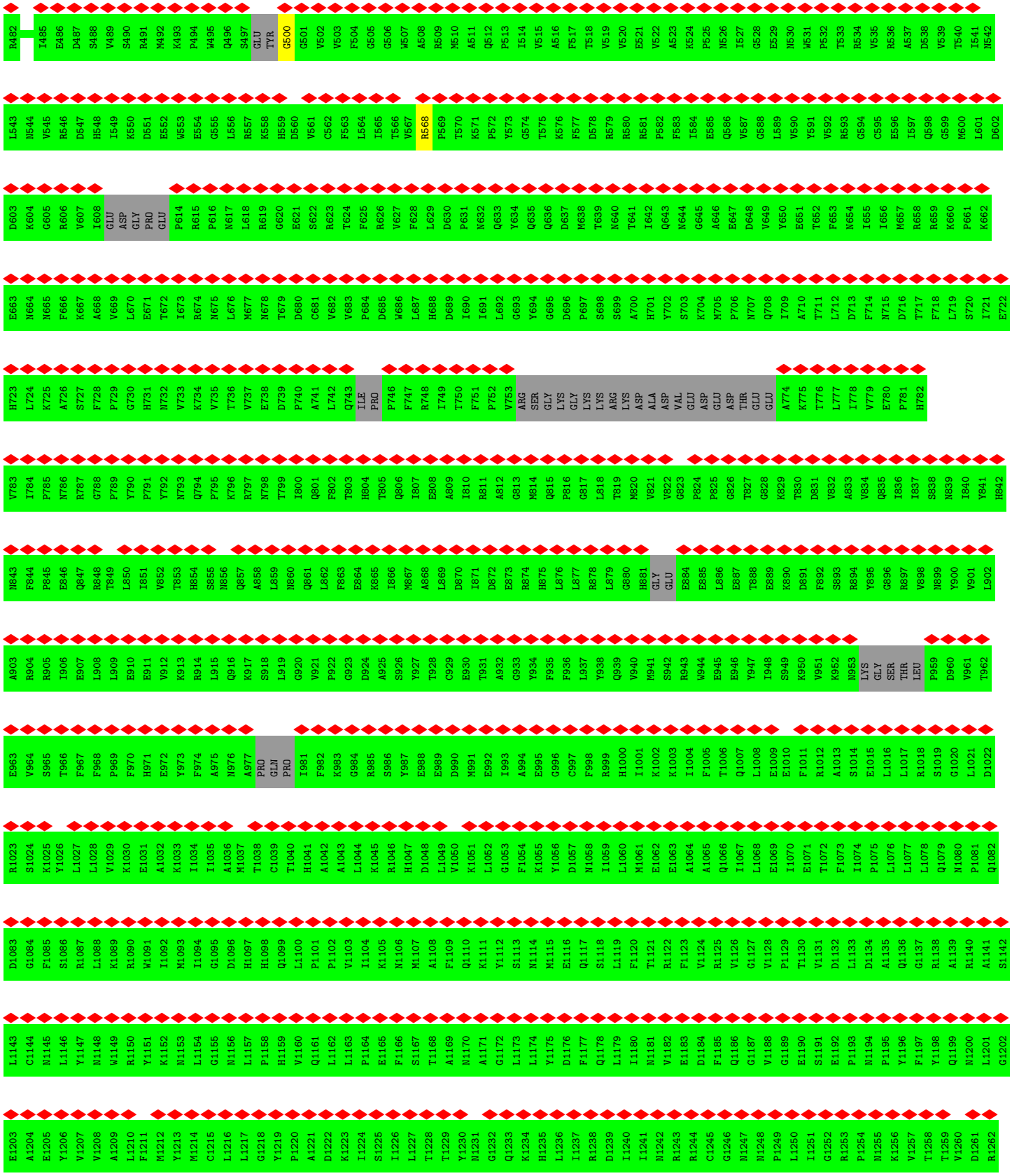


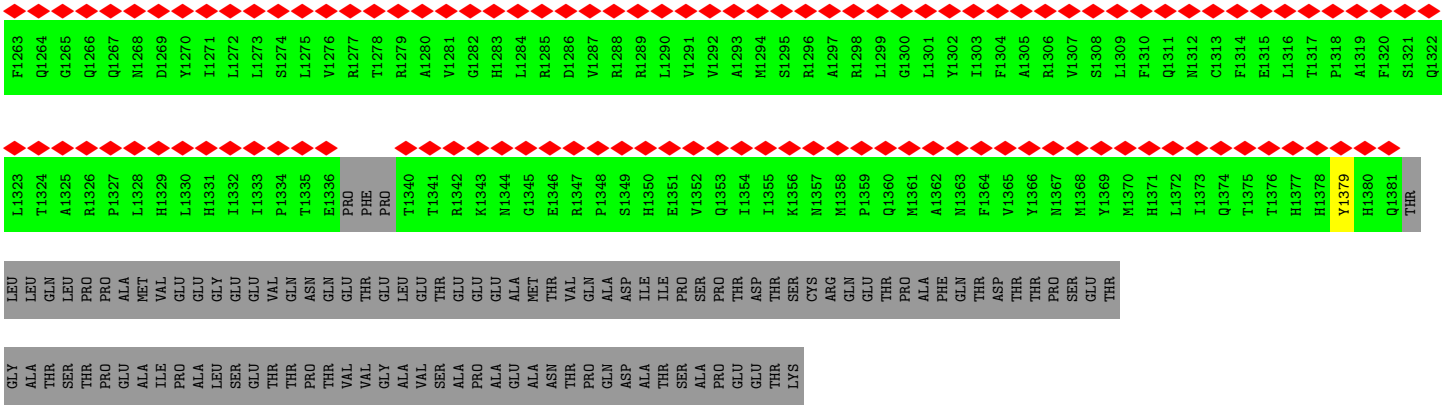
• Molecule 33: Intron-binding protein aquarius

Chain Q:





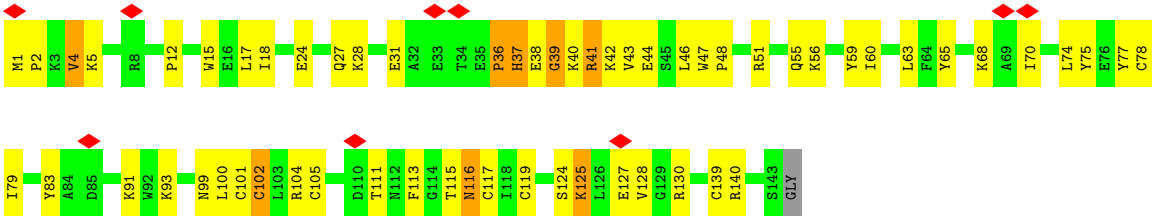

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L543 N544 V545 R546 D547 H548 I549 K550 D551 E552 W553 E554 G555 L556 R557 K558 H559 D560 V561 C562 F563 L564 I565 T566 V567 R568 P569 T570 K571 P572 Y573 G574 T575 K576 F577 D578 R579 R580 R581 P582 F583 I584 E585 Q586 V587 G588 L589 V590 Y591 V592 R593 G594 C595 E596 I597 Q598 G599 M600 L601 D602
D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 I656 M657 R658 R659 K660 P661 K662
E663 N664 N665 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 E681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720 I721 E722
H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU GLU A774 K775 T776 L777 I778 V779 E780 P781 H782
V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840 Y841 H842
N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 R878 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900 V901 L902
A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 T931 A932 G933 Y934 F935 P936 L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960 V961 T962
E963 V964 S965 T966 F967 F968 P969 F970 H971 E972 Y973 F974 A975 N976 A977 PRO GLN PRO I981 F982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999 H1000 I1001 K1002 K1003 I1004 F1005 T1006 Q1007 L1008 E1009 E1010 F1011 R1012 A1013 S1014 E1015 L1016 L1017 R1018 S1019 G1020 L1021 D1022
R1023 S1024 K1025 Y1026 L1027 L1028 V1029 K1030 E1031 A1032 K1033 I1034 I1035 A1036 M1037 T1038 C1039 T1040 H1041 A1042 A1043 L1044 K1045 R1046 H1047 D1048 L1049 V1050 K1051 L1052 G1053 F1054 K1055 Y1056 D1057 N1058 I1059 L1060 M1061 E1062 E1063 A1064 A1065 Q1066 I1067 L1068 E1069 I1070 E1071 T1072 F1073 I1074 P1075 L1076 L1077 L1078 Q1079 N1080 P1081 Q1082
D1083 G1084 F1085 S1086 R1087 L1088 K1089 R1090 W1091 I1092 M1093 I1094 G1095 D1096 H1097 H1098 Q1099 L1100 P1101 P1102 V1103 I1104 K1105 N1106 M1107 A1108 F1109 Q1110 K1111 Y1112 S1113 N1114 M1115 E1116 Q1117 S1118 L1119 F1120 T1121 R1122 F1123 V1124 R1125 V1126 G1127 V1128 P1129 T1130 V1131 D1132 L1133 D1134 A1135 Q1136 G1137 R1138 A1139 R1140 A1141 S1142
L1143 C1144 N1145 L1146 Y1147 N1148 W1149 R1150 Y1151 K1152 N1153 L1154 G1155 N1156 L1157 P1158 H1159 V1160 Q1161 L1162 L1163 P1164 E1165 F1166 S1167 T1168 A1169 N1170 A1171 G1172 L1173 L1174 Y1175 D1176 F1177 Q1178 L1179 I1180 N1181 V1182 E1183 D1184 F1185 Q1186 G1187 V1188 G1189 E1190 S1191 E1192 P1193 N1194 P1195 Y1196 F1197 Y1198 Q1199 N1200 L1201 G1202
E1203 A1204 E1205 Y1206 V1207 V1208 A1209 L1210 F1211 M1212 Y1213 M1214 C1215 L1216 L1217 G1218 Y1219 P1220 A1221 D1222 K1223 I1224 S1225 I1226 L1227 T1228 T1229 Y1230 N1231 G1232 Q1233 K1234 H1235 L1236 I1237 R1238 D1239 I1240 I1241 N1242 R1243 R1244 C1245 G1246 N1247 N1248 P1249 L1250 I1251 G1252 R1253 P1254 N1255 K1256 V1257 T1258 T1259 V1260 D1261 R1262



• Molecule 34: Protein BUD31 homolog

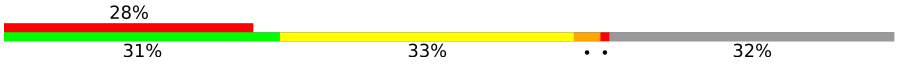
Chain N:

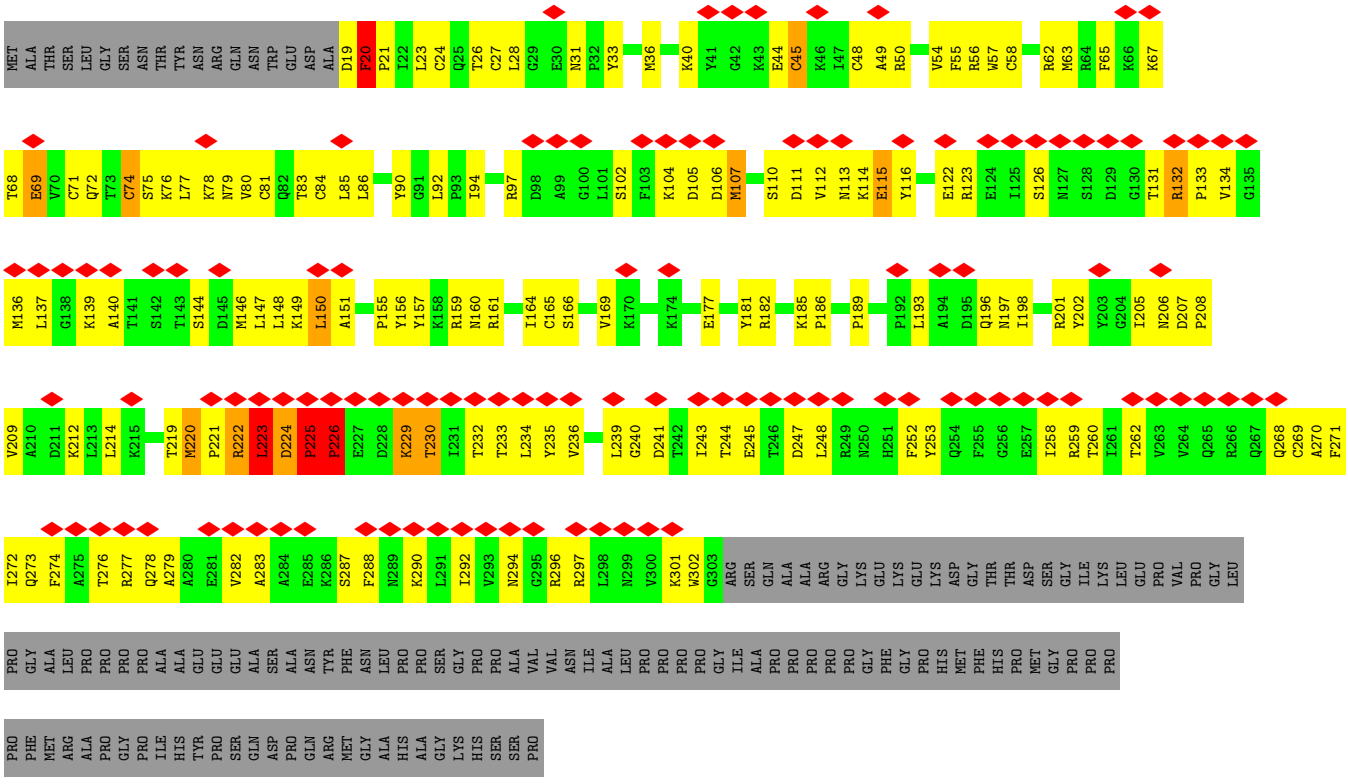




• Molecule 35: Pre-mRNA-splicing factor RBM22

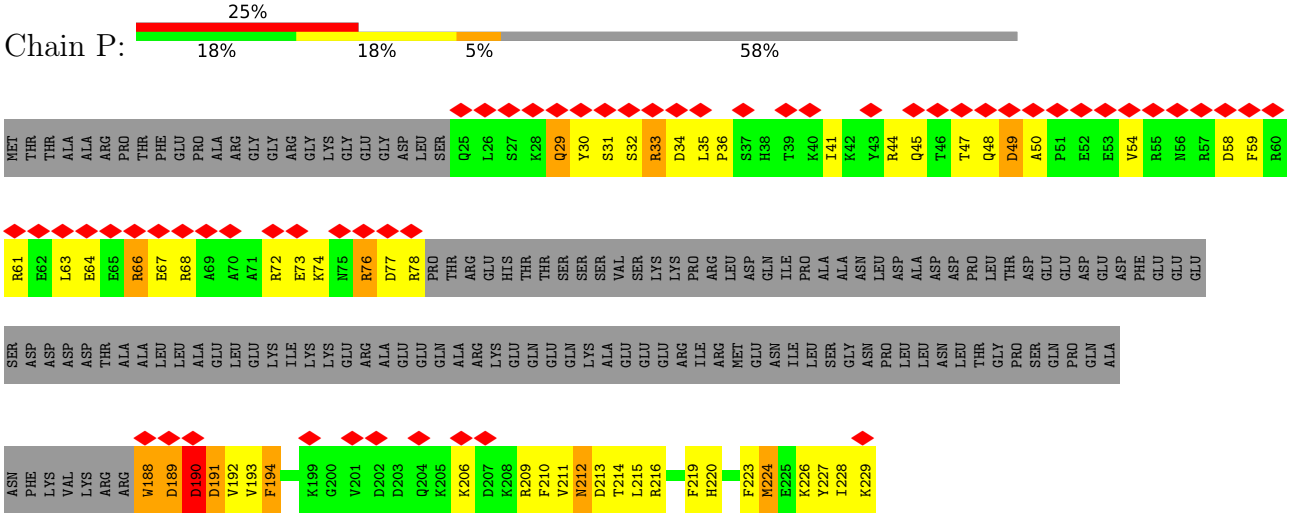
Chain O:





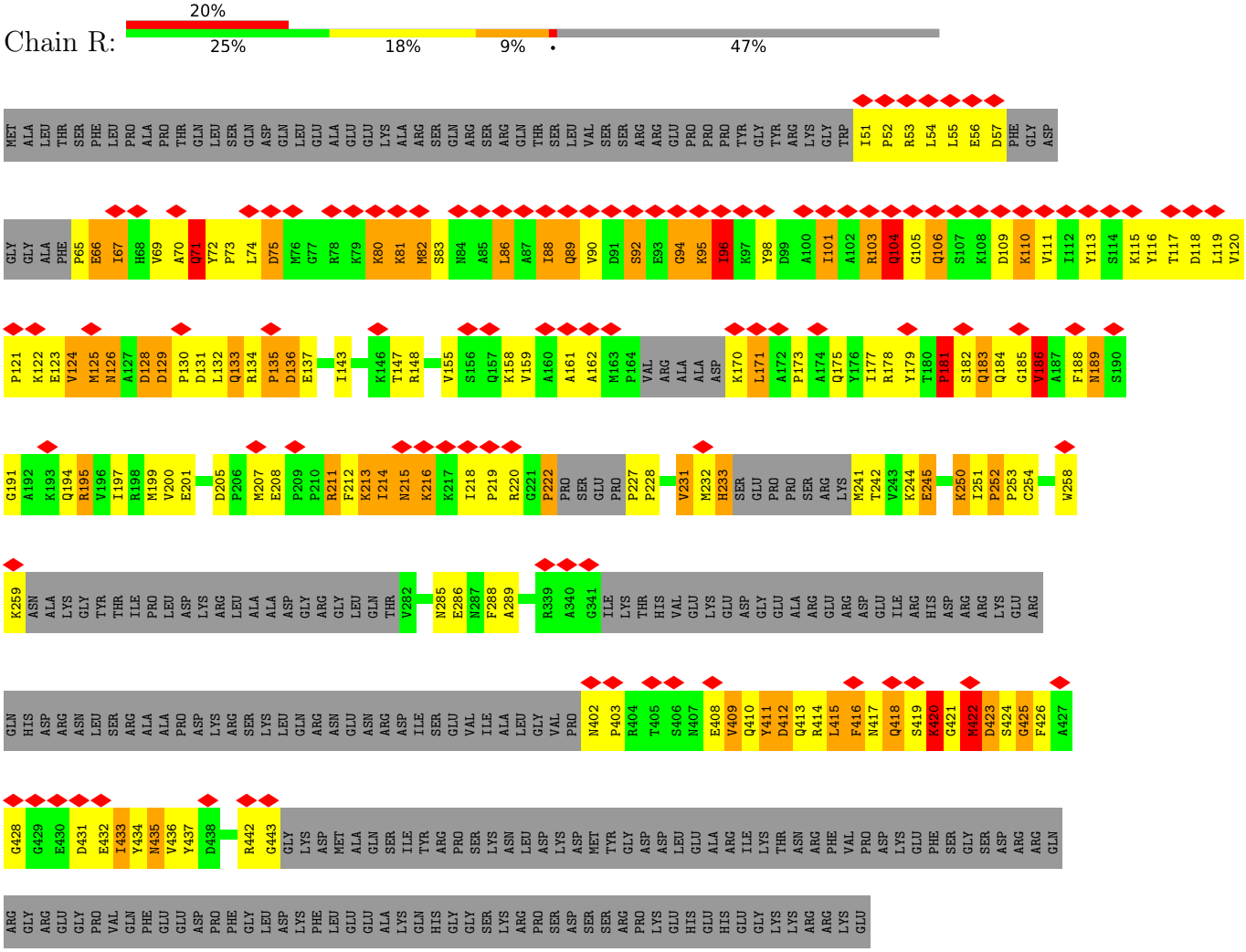
• Molecule 36: Spliceosome-associated protein CWC15 homolog

Chain P:



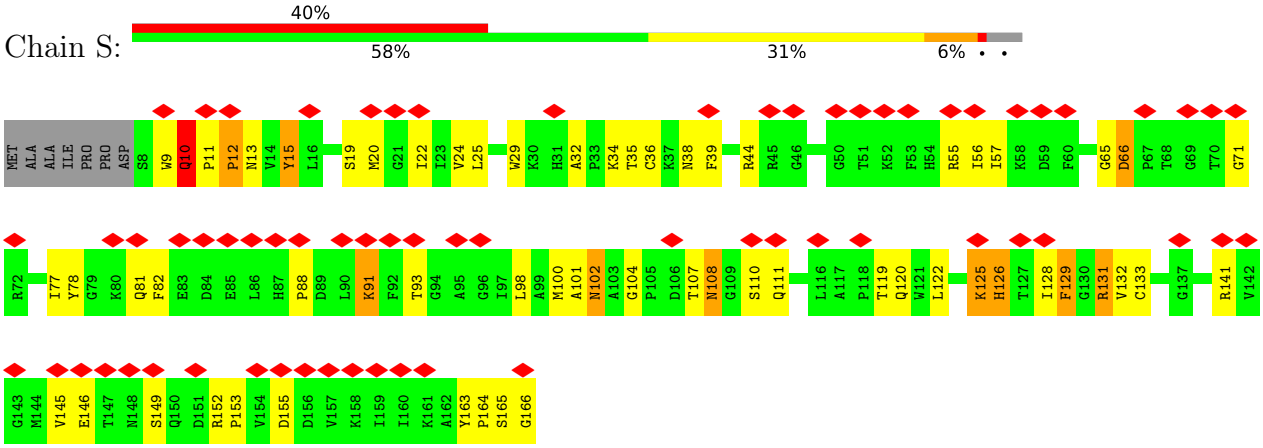
• Molecule 37: Skip

Chain R:



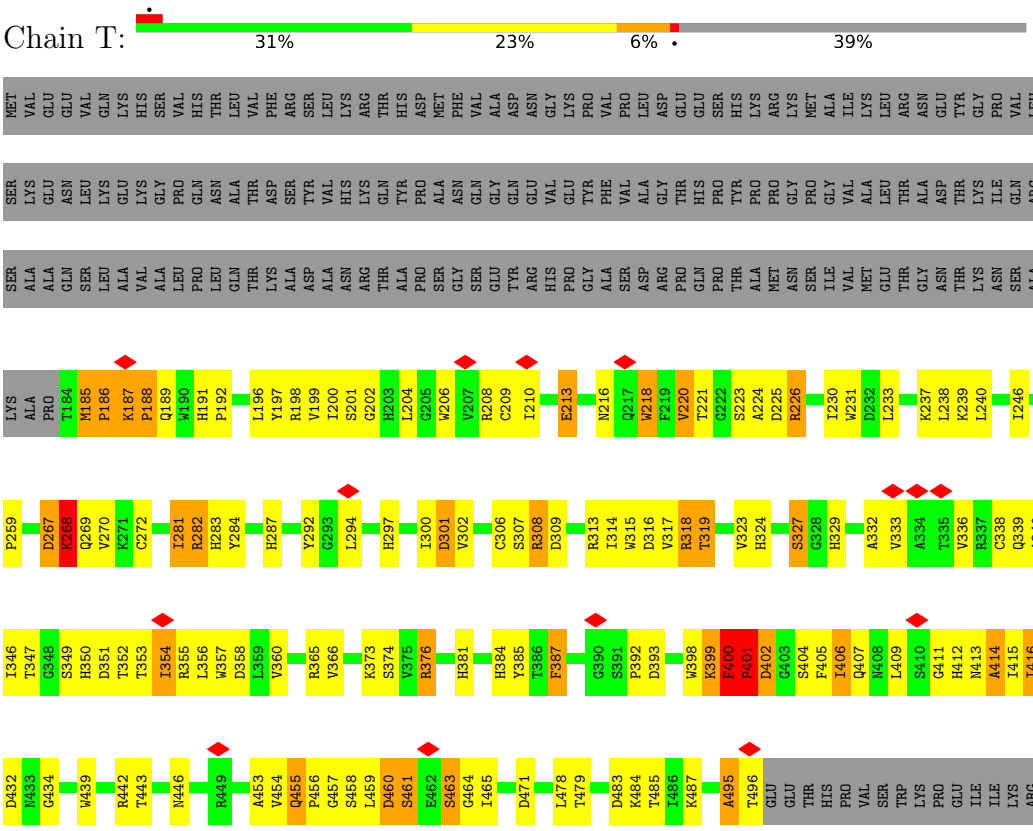
• Molecule 38: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:



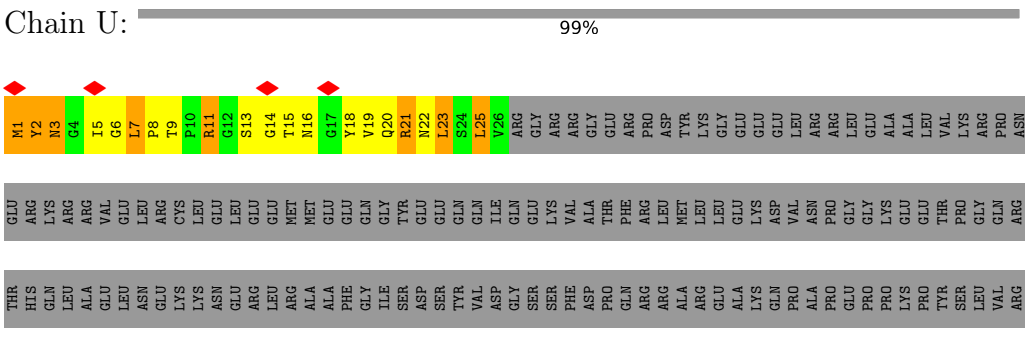
• Molecule 39: Pleiotropic regulator 1

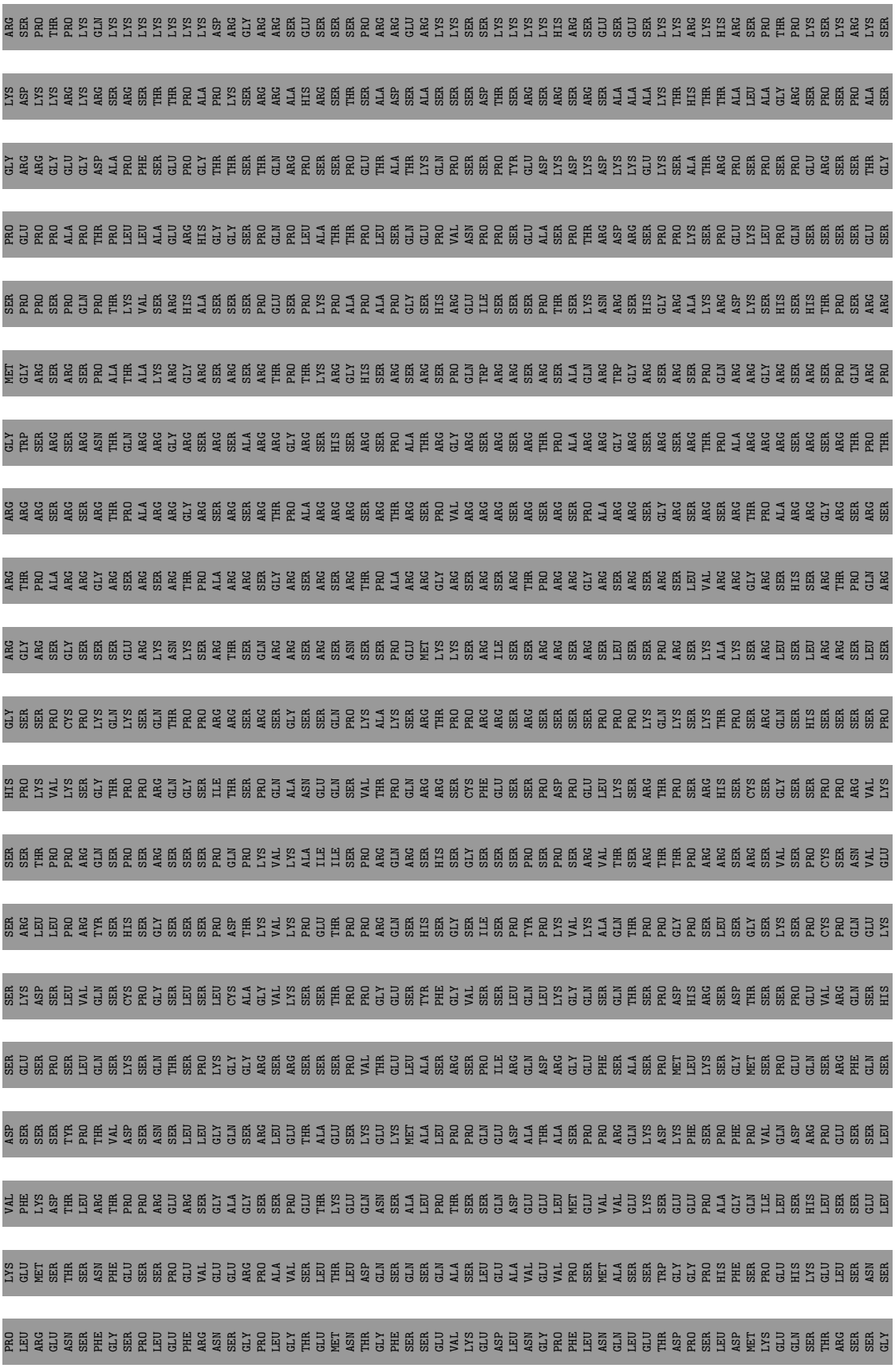
Chain T:

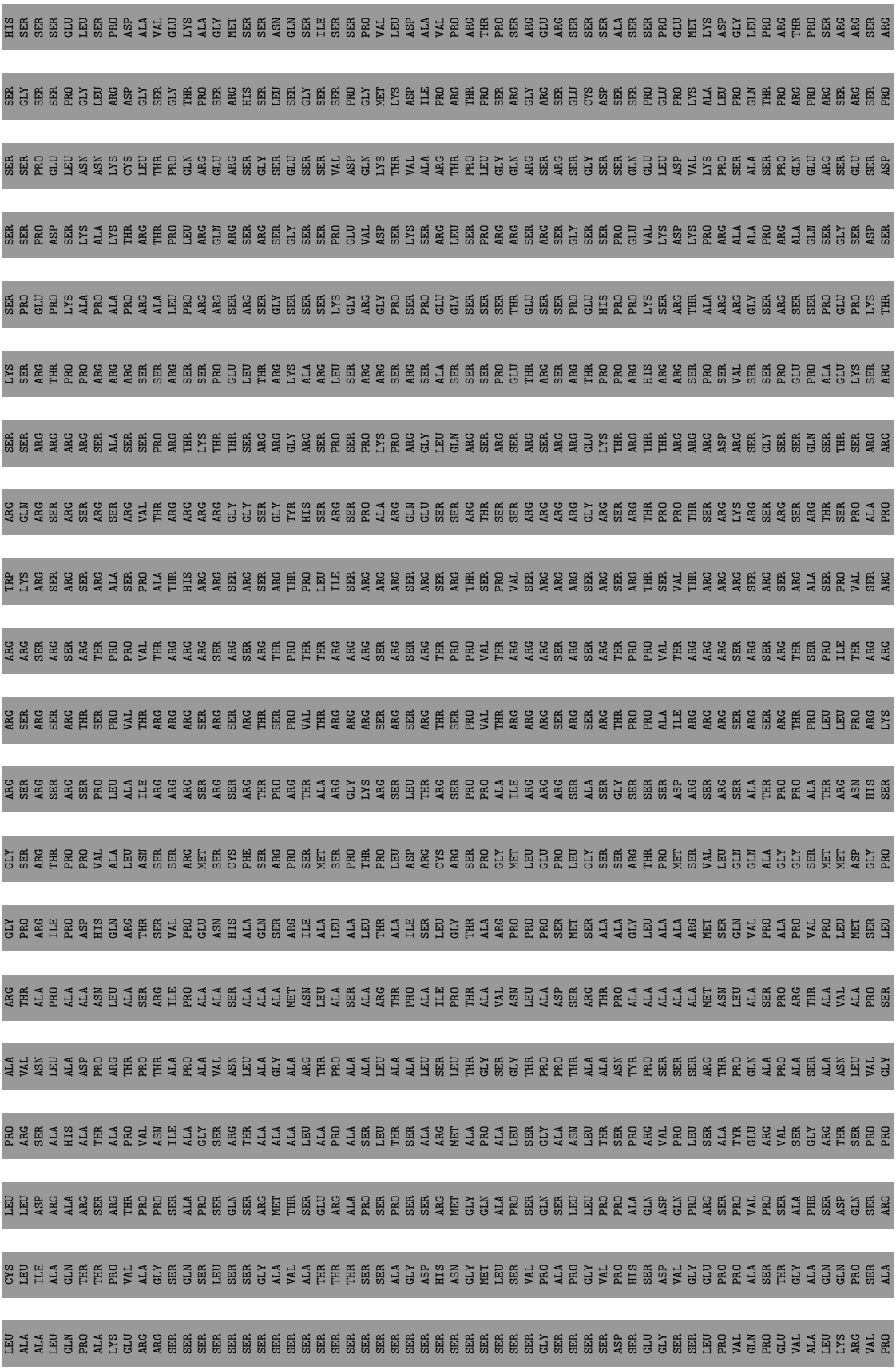


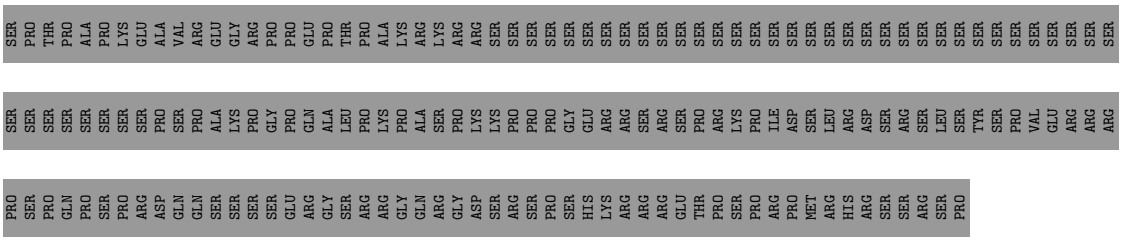
• Molecule 40: Serine/arginine repetitive matrix protein 2

Chain U:



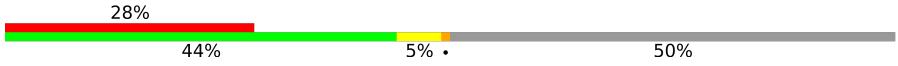

ARG SER PRO THR PRO LYS GLN LYS LYS LYS LYS LYS LYS LYS LYS ASP ARG GLY ARG ARG SER GLU SER SER SER PRO ARG ARG GLU ARG LYS LYS SER SER SER LYS LYS LYS HIS ARG SER GLU SER GLU SER PRO LYS SER LYS ARG LYS SER
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GLY ARG ARG GLY GLU GLY ASP ALA PRO PHE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

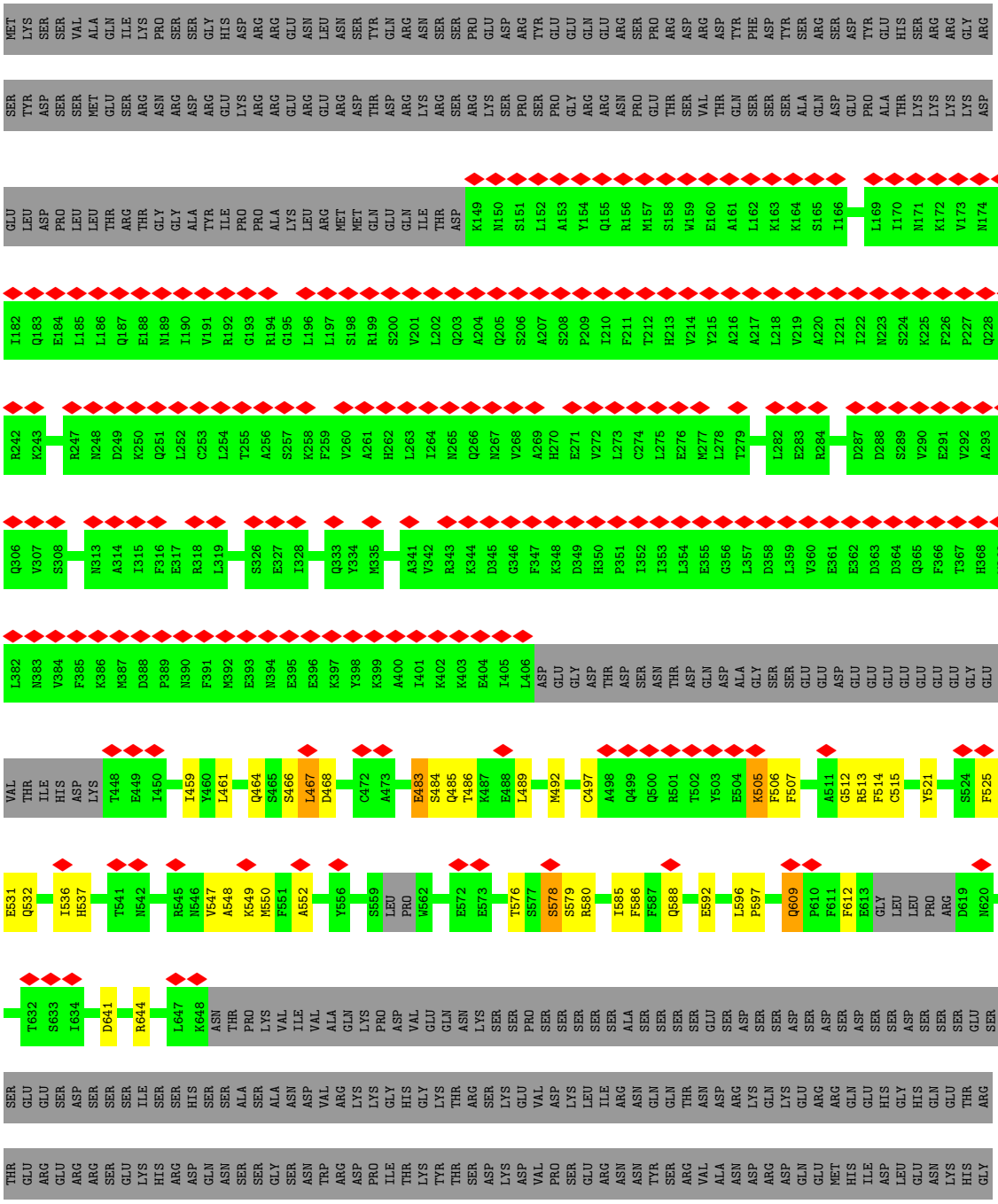

HIS SER SER SER GLU LEU SER PRO ASP ALA VAL GLU LYS ALA GLY MET SER SER ASN GLN SER ILE SER SER PRO VAL LEU ASP ALA VAL PRO ARG THR PRO SER ARG GLU ARG SER SER SER ALA SER SER PRO GLU MET LYS ASP GLY LEU PRO ARG THR PRO SER ARG GLU ARG SER SER SER
SER GLY SER SER PRO GLY LEU ARG ASP GLY SER GLY THR PRO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

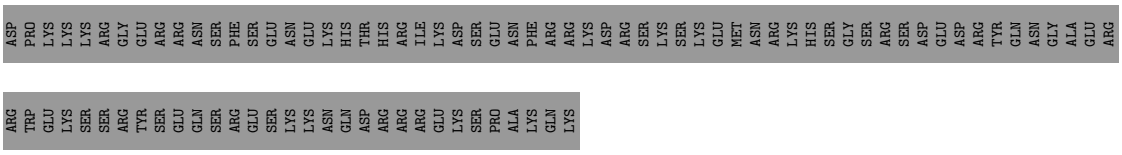


• Molecule 41: Pre-mRNA-splicing factor CWC22 homolog

Chain V:





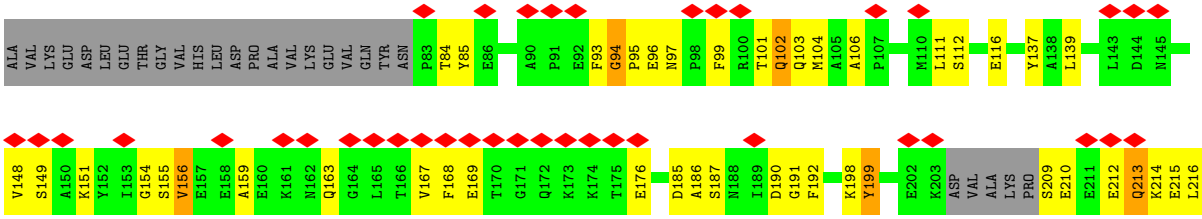


• Molecule 42: Pre-mRNA-processing factor 17

Chain W:



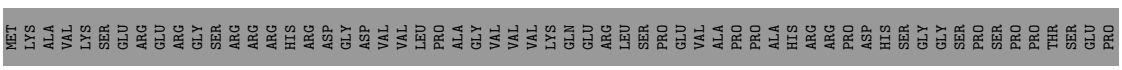




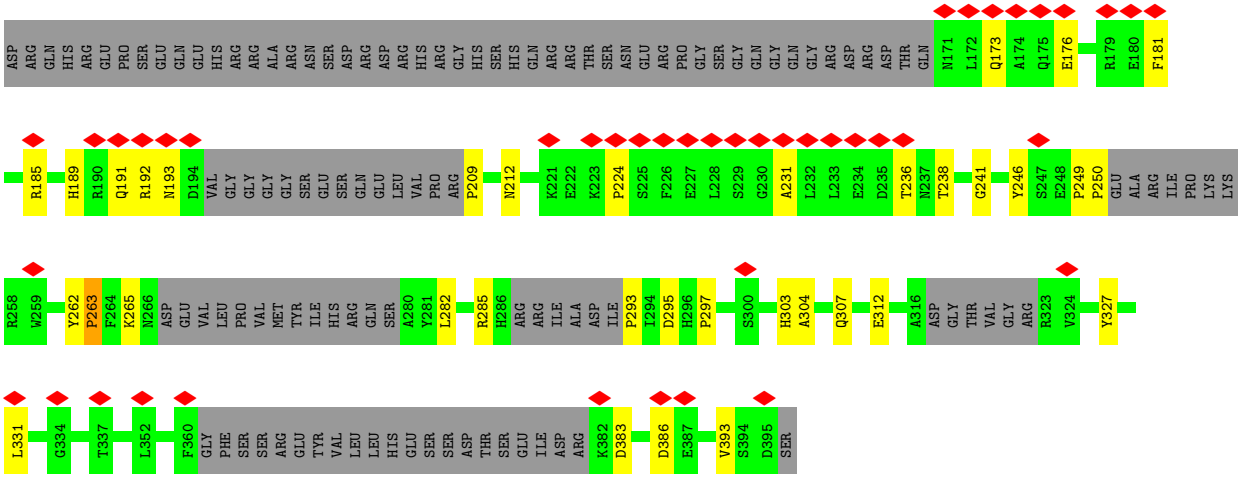
• Molecule 43: Smad nuclear-interacting protein 1

Chain X:





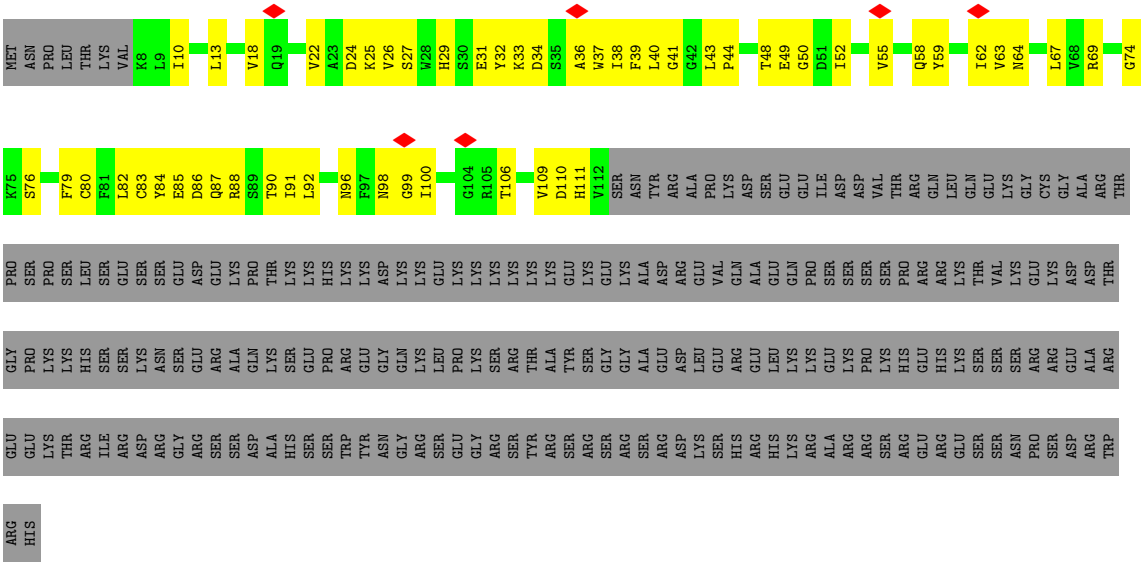




• Molecule 44: RNA-binding motif protein, X-linked 2

Chain Y:

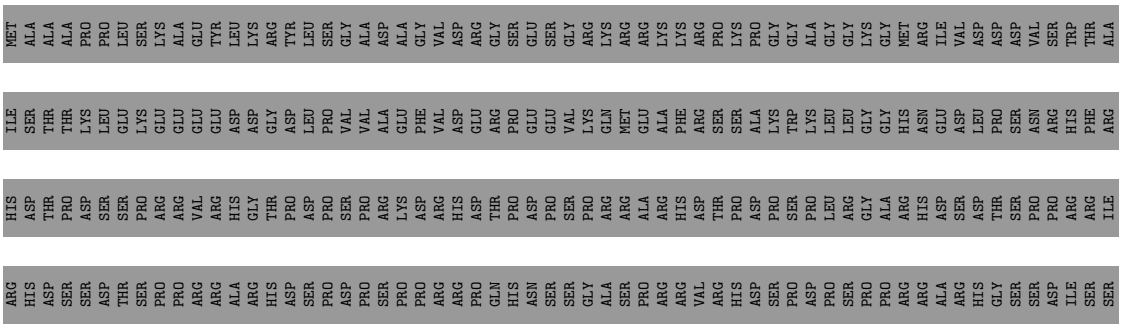


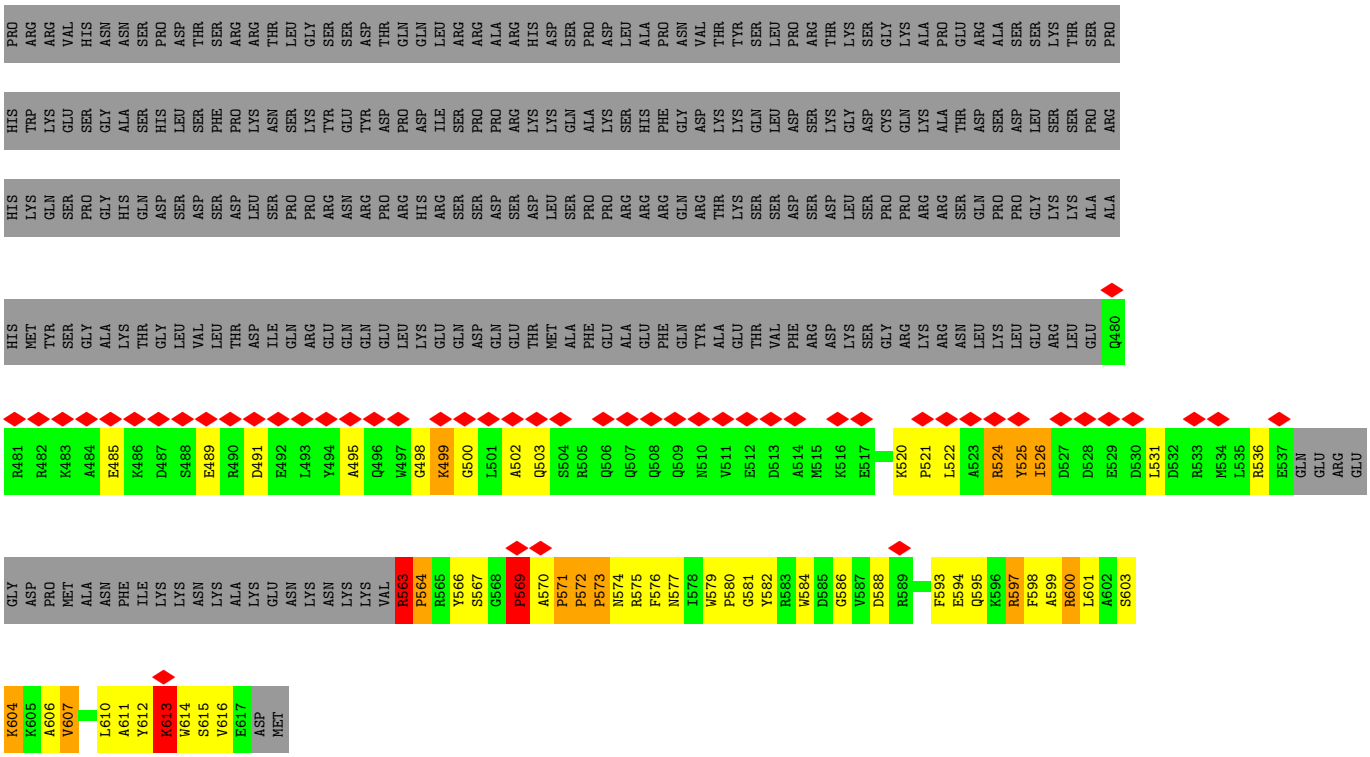


• Molecule 45: BUD13 homolog

Chain Z:

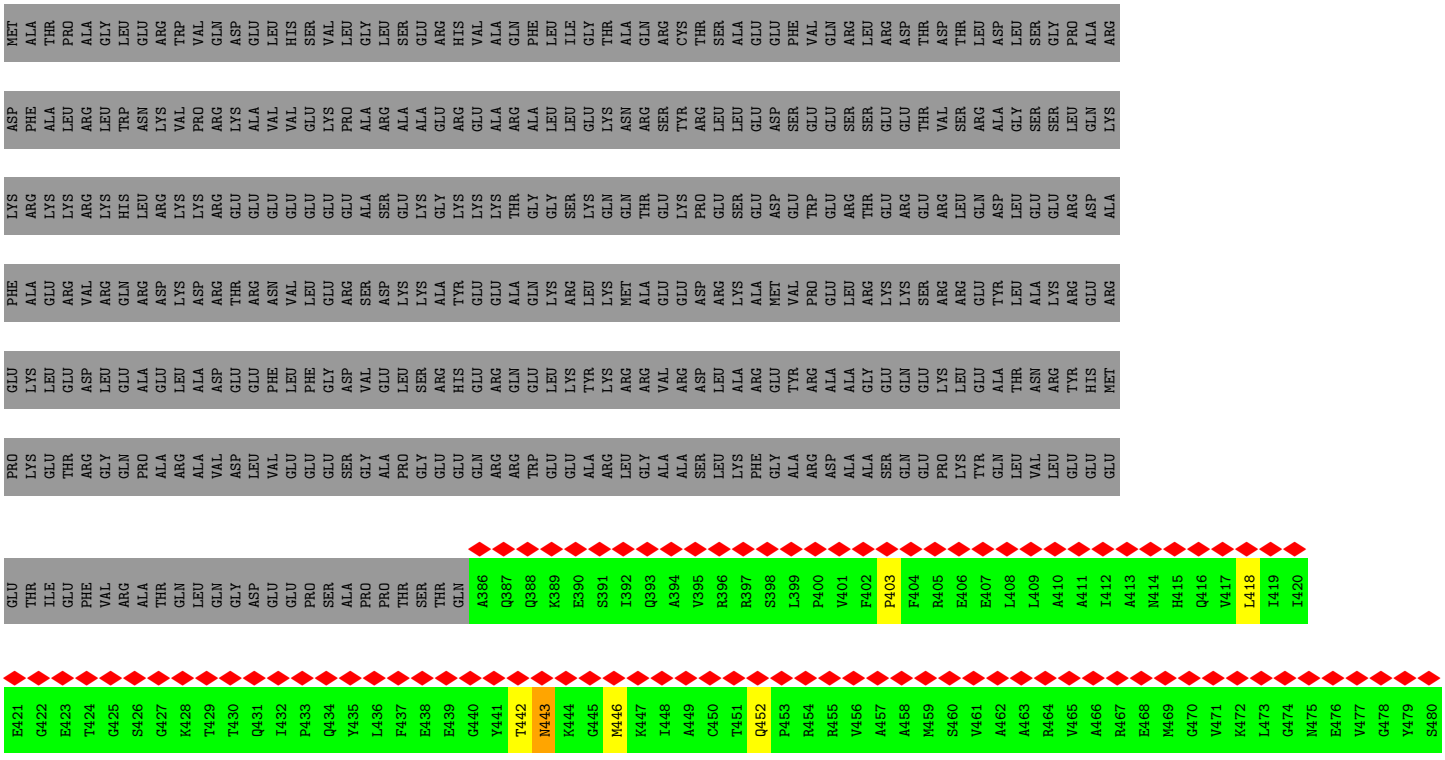


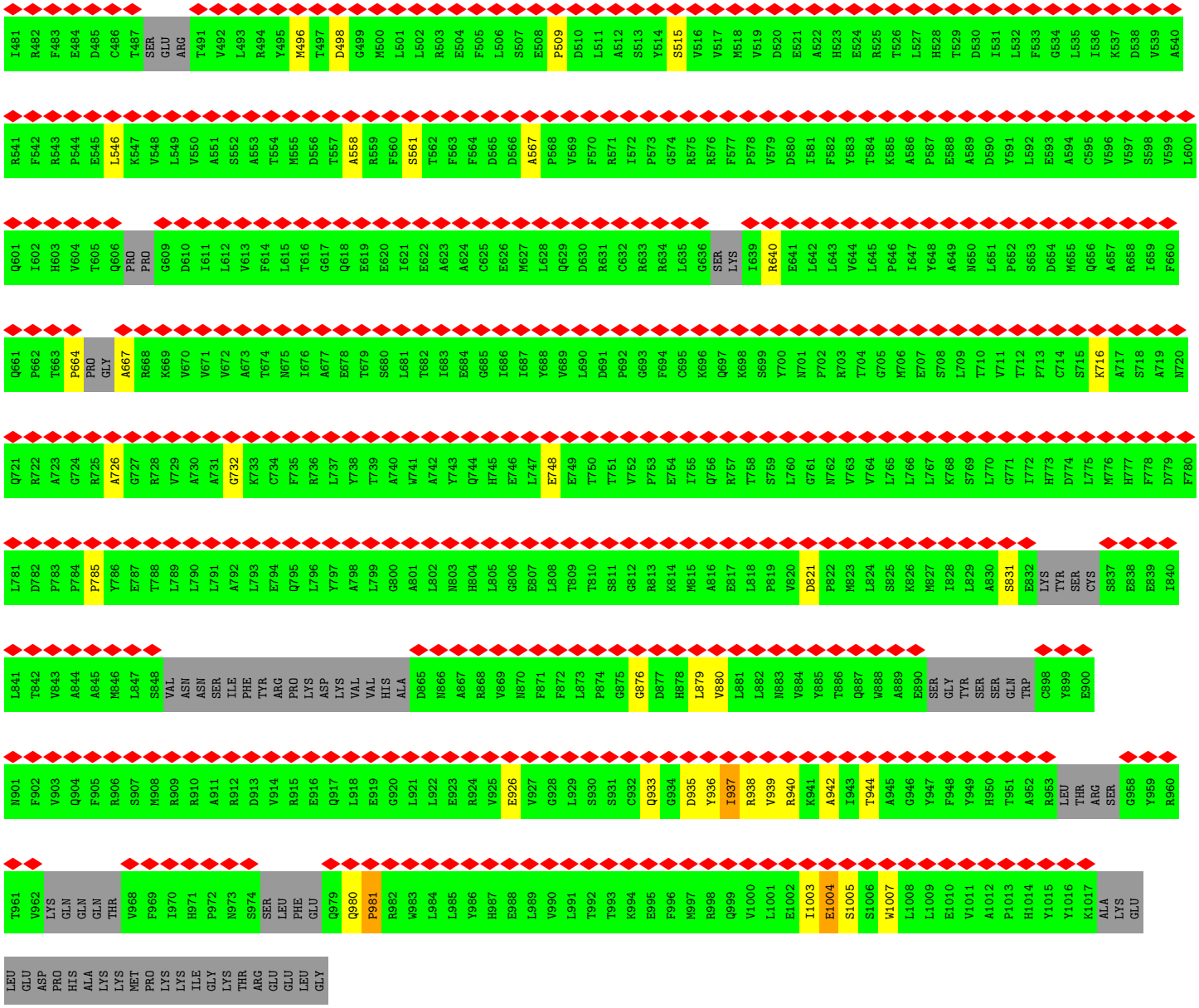




• Molecule 46: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16



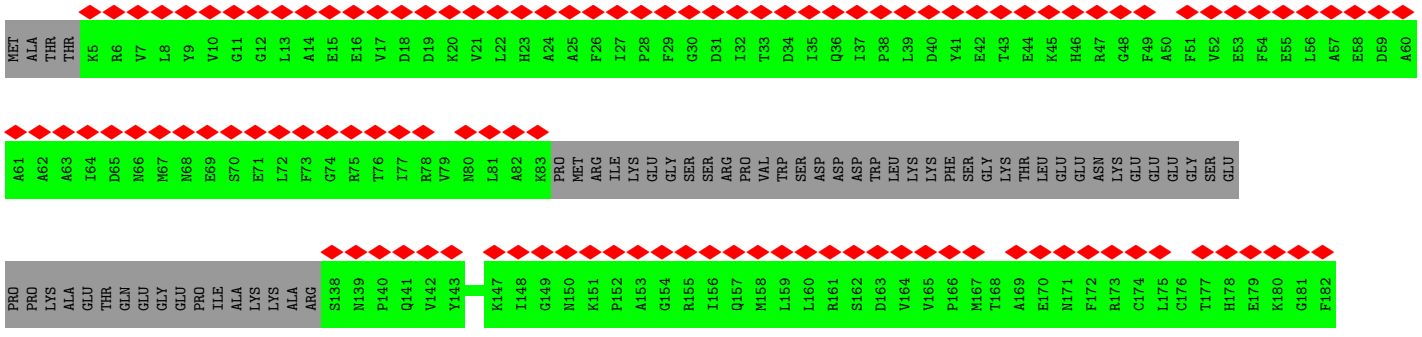


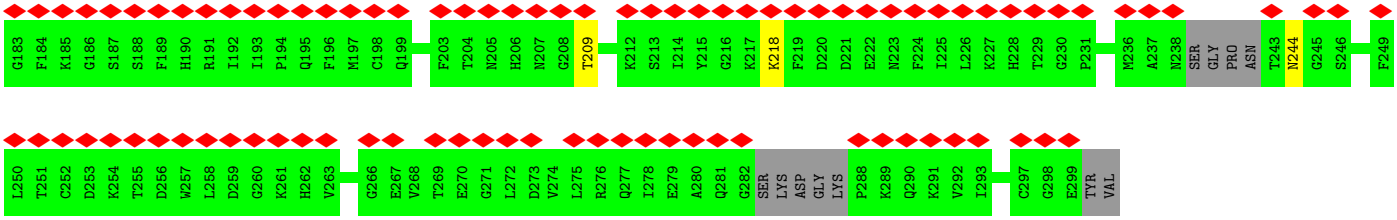


• Molecule 47: Peptidyl-prolyl cis-trans isomerase E

Chain y:






G183 F184 K185 G186 S187 S188 F189 H190 R191 I192 I193 P194 Q195 F196 M197 C198 Q199
F203 T204 N205 H206 N207 G208 T209
K212 S213 I214 Y215 G216 K217 K218 F219 D220 D221 E222 N223 F224 I225 L226 K227 H228 T229 G230 P231
M236 A237 N238 SER GLY PRO ASN T243 N244 G245 S246 F249
L250 T251 C252 D253 K254 T255 D256 W257 L258 D259 G260 K261 H262 V263
G266 E267 V268 T269 E270 G271 L272 D273 V274 L275 R276 Q277 I278 E279 A280 Q281 G282 SER LYS ASP GLY LYS P288 K289 Q290 K291 V292 I293
C297 G298 E299 TYR VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14316	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.142	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0323	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IHP, ZN, GTP

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	0.88	38/16867 (0.2%)	0.99	49/22888 (0.2%)
2	B	0.67	1/1970 (0.1%)	0.95	7/3060 (0.2%)
3	C	1.08	13/6864 (0.2%)	1.27	40/9334 (0.4%)
4	D	0.55	0/8527	1.11	27/11887 (0.2%)
5	E	0.87	0/2392	1.00	6/3242 (0.2%)
6	a	0.77	0/397	0.99	0/549
6	h	0.77	0/391	0.99	0/540
7	b	0.83	0/404	1.12	2/561 (0.4%)
7	i	0.84	0/421	1.15	3/583 (0.5%)
8	c	0.88	0/405	1.11	0/563
8	j	0.87	0/405	1.11	0/563
9	d	1.12	0/479	1.25	1/666 (0.2%)
9	k	1.14	0/420	1.23	1/583 (0.2%)
10	f	1.20	0/360	1.25	0/497
10	m	1.21	1/360 (0.3%)	1.25	0/497
11	e	1.03	0/390	1.24	1/542 (0.2%)
11	l	1.02	0/390	1.23	0/542
12	g	0.86	0/362	1.08	1/501 (0.2%)
12	n	0.85	0/332	1.08	1/458 (0.2%)
13	F	0.35	0/2224	0.66	5/3462 (0.1%)
14	G	0.25	0/1717	0.54	0/2664
15	H	0.51	7/3217 (0.2%)	0.77	8/4997 (0.2%)
16	o	0.93	0/803	2.15	35/1119 (3.1%)
17	p	1.60	3/810 (0.4%)	2.10	25/1122 (2.2%)
18	w	0.62	6/2380 (0.3%)	0.98	14/3274 (0.4%)
19	u	0.36	0/514	0.95	3/710 (0.4%)
20	v	0.88	4/935 (0.4%)	1.08	10/1266 (0.8%)
21	1	0.27	0/7826	0.61	3/10617 (0.0%)
22	2	0.59	4/1277 (0.3%)	0.92	9/1724 (0.5%)
23	3	0.23	0/9381	0.55	5/12732 (0.0%)
24	4	1.08	2/535 (0.4%)	1.28	5/724 (0.7%)
25	5	0.20	0/823	0.53	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	6	0.20	0/678	0.59	0/909
27	7	0.22	0/556	0.49	0/751
28	J	0.80	1/3500 (0.0%)	1.13	3/4750 (0.1%)
29	L	0.58	4/2283 (0.2%)	0.88	8/3088 (0.3%)
30	q	0.62	0/658	0.97	3/919 (0.3%)
30	r	0.58	0/653	0.99	3/912 (0.3%)
30	s	0.49	0/334	0.91	0/466
30	t	0.56	0/334	0.82	0/466
31	K	0.98	11/981 (1.1%)	1.03	6/1317 (0.5%)
32	I	0.54	0/2745	0.91	18/3765 (0.5%)
33	Q	0.37	0/6518	0.85	3/9075 (0.0%)
34	N	1.15	1/1210 (0.1%)	1.17	4/1622 (0.2%)
35	O	1.05	5/2321 (0.2%)	1.11	10/3135 (0.3%)
36	P	0.98	0/841	1.27	4/1117 (0.4%)
37	R	0.87	7/2224 (0.3%)	1.16	10/2992 (0.3%)
38	S	0.81	0/1268	1.14	9/1714 (0.5%)
39	T	1.44	13/2522 (0.5%)	1.42	26/3438 (0.8%)
40	U	1.44	2/196 (1.0%)	1.54	4/265 (1.5%)
41	V	0.89	1/2239 (0.0%)	1.17	3/3118 (0.1%)
42	W	0.88	2/2381 (0.1%)	1.33	27/3310 (0.8%)
43	X	0.21	0/1012	0.57	0/1351
44	Y	0.24	0/753	0.58	0/1014
45	Z	0.65	6/772 (0.8%)	1.11	9/1056 (0.9%)
46	x	0.59	1/2871 (0.0%)	0.82	11/3981 (0.3%)
47	y	0.55	0/1129	0.91	0/1558
All	All	0.75	133/115557 (0.1%)	1.00	422/159679 (0.3%)

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	6
3	C	0	3
4	D	0	1
9	d	0	1
9	k	0	1
21	1	0	9
22	2	0	1
23	3	0	4
27	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	N	0	1
37	R	0	1
39	T	0	2
43	X	0	1
All	All	0	32

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	106	CYS	CB-SG	-11.61	1.43	1.81
31	K	132	CYS	CB-SG	-8.70	1.52	1.81
3	C	387	ASP	CA-C	-8.61	1.48	1.52
17	p	156	ASN	C-N	-8.31	1.22	1.33
1	A	316	PHE	C-N	-8.15	1.25	1.34

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	T	187	LYS	CA-C-N	13.13	132.89	119.76
39	T	187	LYS	C-N-CA	13.13	132.89	119.76
24	4	83	PRO	CA-CB-CG	10.35	124.17	104.50
35	O	225	PRO	N-CA-C	10.32	123.29	110.70
42	W	278	LYS	CB-CA-C	-9.96	95.82	111.17

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	PHE	Peptide
1	A	346	ASP	Peptide
1	A	408	PRO	Peptide
1	A	433	GLU	Peptide
1	A	697	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16399	0	16176	1449	0
2	B	1768	0	897	120	0
3	C	6716	0	6691	916	0
4	D	8528	0	3745	82	0
5	E	2338	0	2272	156	0
6	a	399	0	173	0	0
6	h	393	0	170	0	0
7	b	405	0	170	0	0
7	i	422	0	177	10	0
8	c	406	0	170	0	0
8	j	406	0	170	0	0
9	d	480	0	200	2	0
9	k	422	0	175	2	0
10	f	361	0	158	1	0
10	m	361	0	158	0	0
11	e	391	0	163	3	0
11	l	391	0	163	1	0
12	g	363	0	160	1	0
12	n	334	0	143	3	0
13	F	1988	0	1005	185	0
14	G	1545	0	786	208	0
15	H	2886	0	1463	277	0
16	o	804	0	350	9	0
17	p	813	0	366	14	0
18	w	2373	0	1301	97	0
19	u	520	0	214	0	0
20	v	936	0	591	82	0
21	1	7702	0	7389	336	0
22	2	1252	0	1040	61	0
23	3	9195	0	9091	501	0
24	4	527	0	438	41	0
25	5	807	0	729	28	0
26	6	670	0	654	21	0
27	7	540	0	509	24	0
28	J	3463	0	2544	116	0
29	L	2260	0	1776	100	0
30	q	659	0	296	7	0
30	r	654	0	294	6	0
30	s	335	0	168	0	0
30	t	335	0	168	1	0
31	K	979	0	739	12	0
32	I	2778	0	1238	22	0
33	Q	6528	0	2814	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	N	1184	0	1190	75	0
35	O	2273	0	2244	257	0
36	P	829	0	814	200	0
37	R	2188	0	2102	412	0
38	S	1236	0	1210	140	0
39	T	2457	0	2416	253	0
40	U	193	0	196	44	0
41	V	2243	0	971	50	0
42	W	2384	0	1055	134	0
43	X	1012	0	733	17	0
44	Y	743	0	613	67	0
45	Z	755	0	591	115	0
46	x	2882	0	1308	23	0
47	y	1133	0	519	2	0
48	A	36	0	6	10	0
49	A	5	0	4	2	0
50	C	32	0	12	11	0
51	C	1	0	0	0	0
51	F	5	0	0	0	0
52	6	3	0	0	0	0
52	N	3	0	0	0	0
52	O	3	0	0	2	0
52	v	1	0	0	0	0
All	All	113433	0	84078	5291	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 27.

The worst 5 of 5291 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)
44:Y:37:TRP:CH2	45:Z:498:GLY:HA2	1.23	1.65
1:A:1758:PRO:HA	21:1:938:TRP:CD1	1.28	1.59
1:A:2270:PHE:HB3	4:D:1264:PRO:CB	1.34	1.56
3:C:149:LEU:HD13	3:C:427:PHE:CD2	1.38	1.54
1:A:2270:PHE:CG	4:D:1264:PRO:CB	1.89	1.54

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1970/2335 (84%)	1835 (93%)	108 (6%)	27 (1%)	9 40
3	C	854/972 (88%)	777 (91%)	57 (7%)	20 (2%)	5 28
4	D	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	43 78
5	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3 22
6	a	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
6	h	76/126 (60%)	75 (99%)	1 (1%)	0	100 100
7	b	80/231 (35%)	78 (98%)	2 (2%)	0	100 100
7	i	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
8	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
8	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
9	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
9	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
10	f	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
10	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
11	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
11	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
12	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
12	n	64/76 (84%)	62 (97%)	2 (3%)	0	100 100
16	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9 42
17	p	159/225 (71%)	138 (87%)	9 (6%)	12 (8%)	1 10
18	w	420/501 (84%)	380 (90%)	37 (9%)	3 (1%)	18 56
19	u	92/793 (12%)	86 (94%)	4 (4%)	2 (2%)	5 29
20	v	153/464 (33%)	124 (81%)	22 (14%)	7 (5%)	2 16
21	1	1022/1304 (78%)	897 (88%)	119 (12%)	6 (1%)	21 59
22	2	171/895 (19%)	154 (90%)	17 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	3	1165/1217 (96%)	1081 (93%)	80 (7%)	4 (0%)	36 72
24	4	76/424 (18%)	69 (91%)	6 (8%)	1 (1%)	9 42
25	5	106/125 (85%)	90 (85%)	16 (15%)	0	100 100
26	6	87/110 (79%)	80 (92%)	7 (8%)	0	100 100
27	7	64/86 (74%)	55 (86%)	9 (14%)	0	100 100
28	J	483/848 (57%)	452 (94%)	24 (5%)	7 (1%)	9 40
29	L	324/802 (40%)	304 (94%)	18 (6%)	2 (1%)	21 59
30	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3 22
30	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	7 38
30	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8 40
30	t	65/504 (13%)	64 (98%)	0	1 (2%)	8 40
31	K	144/225 (64%)	134 (93%)	6 (4%)	4 (3%)	4 24
32	I	498/855 (58%)	479 (96%)	11 (2%)	8 (2%)	7 38
33	Q	1297/1485 (87%)	1271 (98%)	26 (2%)	0	100 100
34	N	141/144 (98%)	126 (89%)	12 (8%)	3 (2%)	5 30
35	O	283/420 (67%)	247 (87%)	26 (9%)	10 (4%)	3 20
36	P	92/229 (40%)	82 (89%)	8 (9%)	2 (2%)	5 29
37	R	274/540 (51%)	234 (85%)	25 (9%)	15 (6%)	1 14
38	S	157/166 (95%)	144 (92%)	10 (6%)	3 (2%)	6 32
39	T	311/514 (60%)	282 (91%)	17 (6%)	12 (4%)	2 18
40	U	24/2752 (1%)	20 (83%)	3 (12%)	1 (4%)	2 17
41	V	444/908 (49%)	412 (93%)	27 (6%)	5 (1%)	11 46
42	W	477/579 (82%)	421 (88%)	32 (7%)	24 (5%)	1 16
43	X	144/396 (36%)	134 (93%)	10 (7%)	0	100 100
44	Y	103/322 (32%)	92 (89%)	11 (11%)	0	100 100
45	Z	109/619 (18%)	93 (85%)	10 (9%)	6 (6%)	1 14
46	x	561/1041 (54%)	536 (96%)	20 (4%)	5 (1%)	14 51
47	y	224/301 (74%)	217 (97%)	7 (3%)	0	100 100
All	All	16082/29057 (55%)	14914 (93%)	957 (6%)	211 (1%)	12 42

5 of 211 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	92	LEU
1	A	167	PRO
1	A	188	LEU
1	A	331	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1773/2108 (84%)	1661 (94%)	112 (6%)	16 37
3	C	745/866 (86%)	676 (91%)	69 (9%)	8 26
5	E	256/300 (85%)	244 (95%)	12 (5%)	23 45
18	w	49/446 (11%)	47 (96%)	2 (4%)	27 49
20	v	30/382 (8%)	28 (93%)	2 (7%)	15 36
21	1	735/1104 (67%)	735 (100%)	0	100 100
22	2	94/776 (12%)	90 (96%)	4 (4%)	26 47
23	3	1012/1051 (96%)	1011 (100%)	1 (0%)	88 89
24	4	39/336 (12%)	37 (95%)	2 (5%)	21 42
25	5	74/109 (68%)	74 (100%)	0	100 100
26	6	76/95 (80%)	76 (100%)	0	100 100
27	7	57/77 (74%)	57 (100%)	0	100 100
28	J	205/751 (27%)	193 (94%)	12 (6%)	18 39
29	L	131/709 (18%)	123 (94%)	8 (6%)	17 38
31	K	54/196 (28%)	46 (85%)	8 (15%)	3 13
34	N	130/130 (100%)	124 (95%)	6 (5%)	24 45
35	O	250/361 (69%)	240 (96%)	10 (4%)	28 49
36	P	90/203 (44%)	78 (87%)	12 (13%)	4 14
37	R	215/463 (46%)	162 (75%)	53 (25%)	1 4
38	S	129/134 (96%)	121 (94%)	8 (6%)	16 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	T	268/441 (61%)	251 (94%)	17 (6%)	16 37
40	U	21/2432 (1%)	16 (76%)	5 (24%)	1 4
43	X	51/349 (15%)	44 (86%)	7 (14%)	3 14
44	Y	57/291 (20%)	56 (98%)	1 (2%)	51 68
45	Z	47/545 (9%)	38 (81%)	9 (19%)	1 8
46	x	1/897 (0%)	1 (100%)	0	100 100
All	All	6589/15552 (42%)	6229 (94%)	360 (6%)	21 41

5 of 360 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	K	173	THR
37	R	158	LYS
35	O	45	CYS
37	R	56	GLU
37	R	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
37	R	435	ASN
38	S	150	GLN
43	X	307	GLN
3	C	706	GLN
3	C	596	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	91/107 (85%)	38 (41%)	12 (13%)
14	G	76/274 (27%)	48 (63%)	9 (11%)
15	H	130/188 (69%)	33 (25%)	4 (3%)
2	B	82/117 (70%)	19 (23%)	10 (12%)
All	All	379/686 (55%)	138 (36%)	35 (9%)

5 of 138 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	G	151	C
14	G	153	C
15	H	46	U
13	F	25	C
13	F	7	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
50	GTP	C	1500	51	33,34,34	1.45	5 (15%)	50,54,54	2.04	10 (20%)
48	IHP	A	2401	-	36,36,36	1.04	2 (5%)	60,60,60	1.74	15 (25%)
49	ALA	A	2402	-	3,4,5	0.67	0	2,4,6	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GTP	C	1500	51	-	8/22/38/38	0/3/3/3
48	IHP	A	2401	-	-	6/30/54/54	0/1/1/1
49	ALA	A	2402	-	-	0/1/2/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	1500	GTP	C5-N7	-3.76	1.31	1.39
50	C	1500	GTP	C6-N1	-3.32	1.32	1.38
50	C	1500	GTP	PA-O3A	3.16	1.62	1.59
48	A	2401	IHP	P5-O45	-2.95	1.43	1.54
48	A	2401	IHP	P2-O12	2.73	1.64	1.59

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C	1500	GTP	C5-C4-N3	-7.07	117.14	128.39
50	C	1500	GTP	C2-N3-C4	5.94	122.54	112.30
50	C	1500	GTP	N9-C4-N3	5.74	137.44	125.95
48	A	2401	IHP	O35-P5-O15	-4.53	88.19	105.85
48	A	2401	IHP	O45-P5-O35	4.13	123.30	107.80

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	A	2401	IHP	C4-C5-O15-P5
48	A	2401	IHP	C6-C5-O15-P5
50	C	1500	GTP	PB-O3B-PG-O3G
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C	1500	GTP	11	0

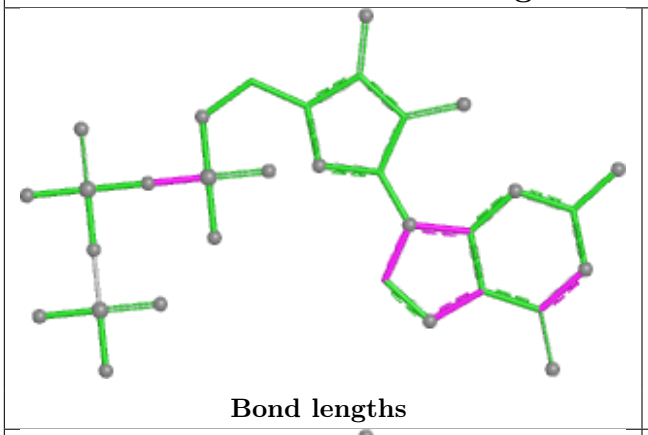
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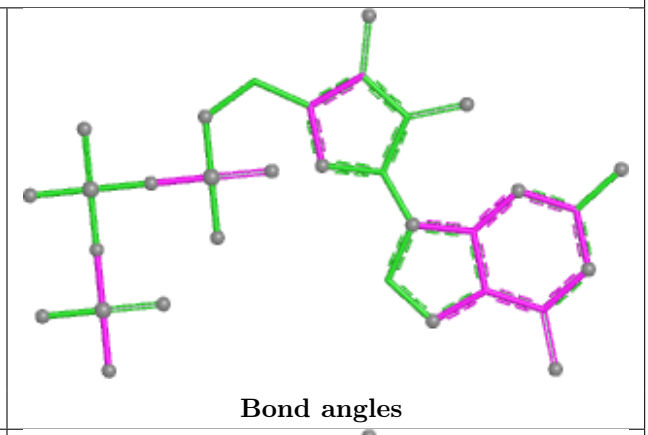
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	A	2401	IHP	10	0
49	A	2402	ALA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

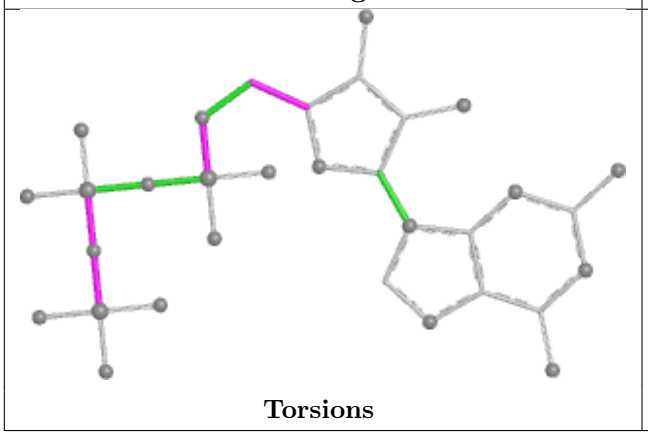
Ligand GTP C 1500



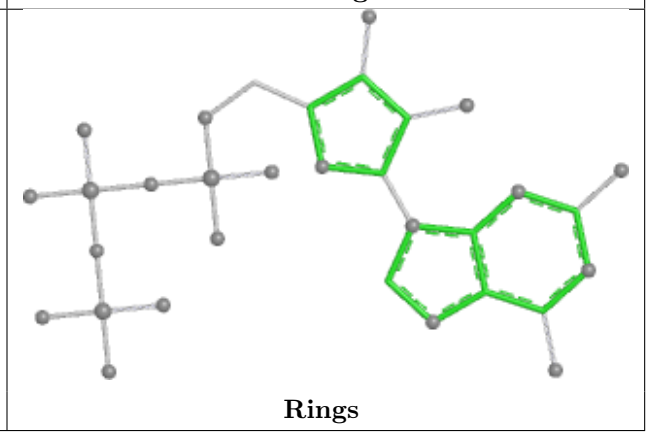
Bond lengths



Bond angles

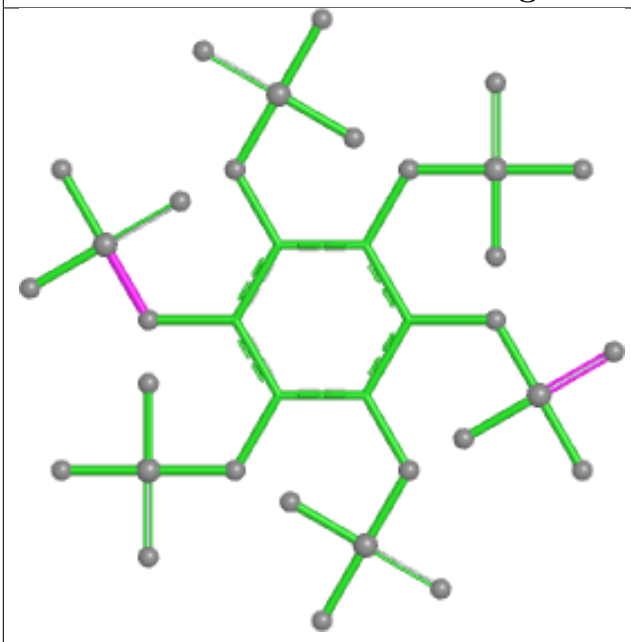


Torsions

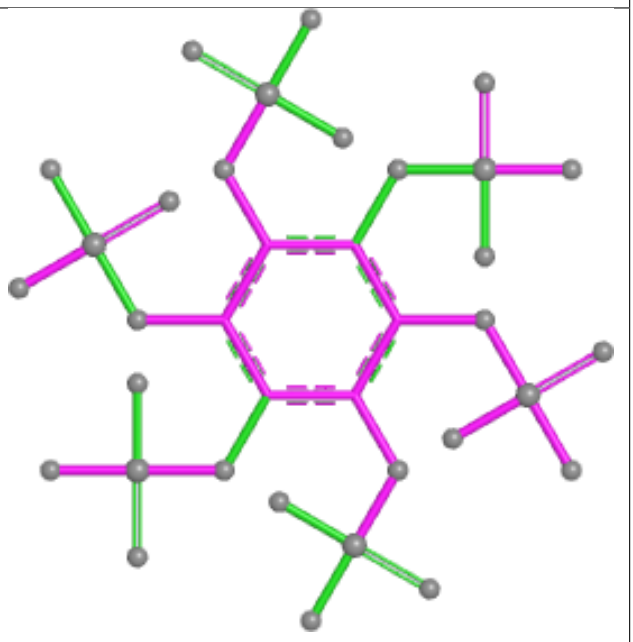


Rings

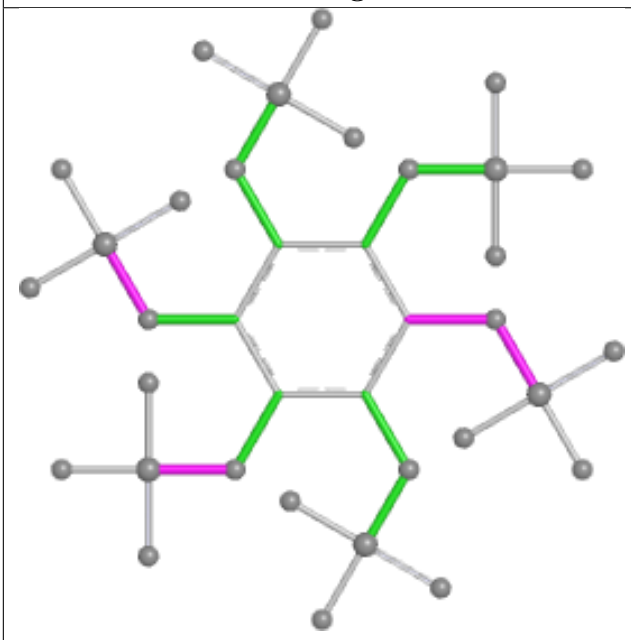
Ligand IHP A 2401



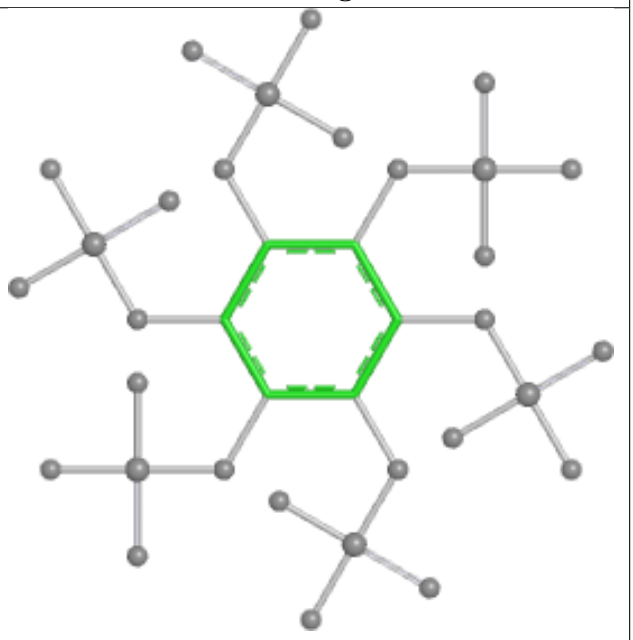
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

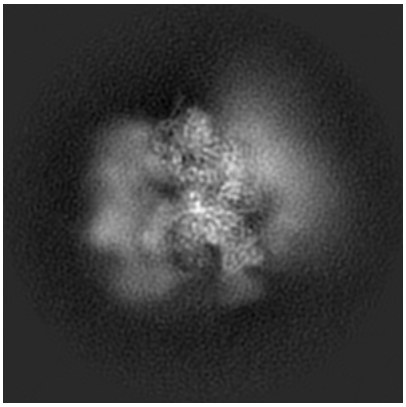
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6890. These allow visual inspection of the internal detail of the map and identification of artifacts.

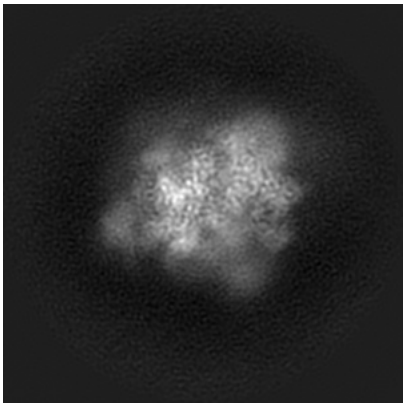
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

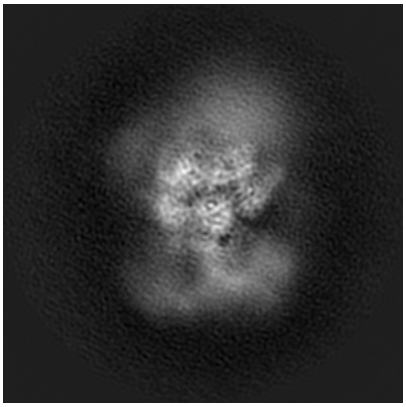
6.1.1 Primary map



X



Y

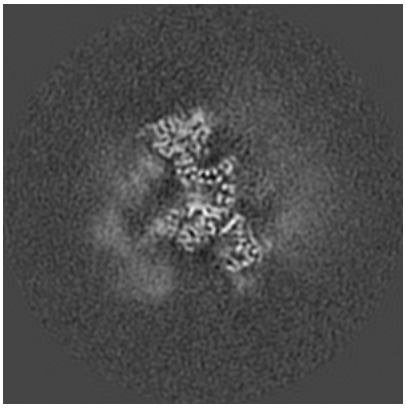


Z

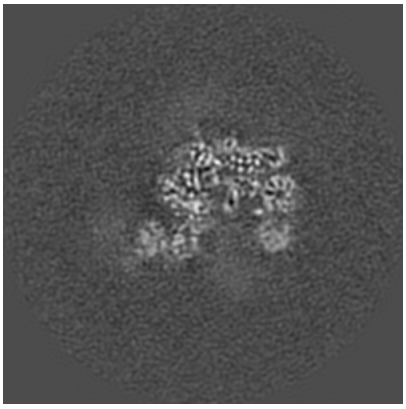
The images above show the map projected in three orthogonal directions.

6.2 Central slices

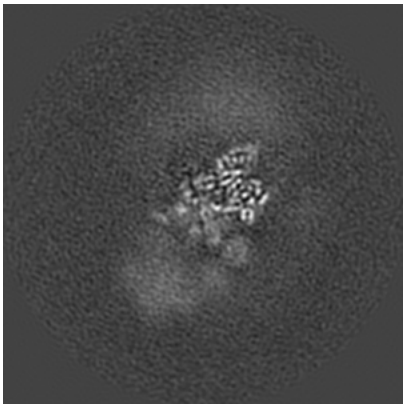
6.2.1 Primary map



X Index: 200



Y Index: 200

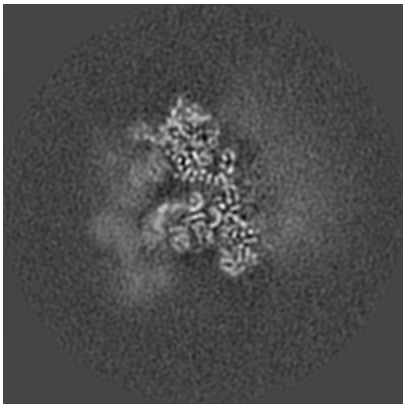


Z Index: 200

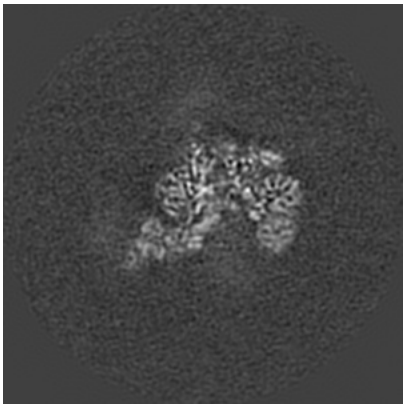
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

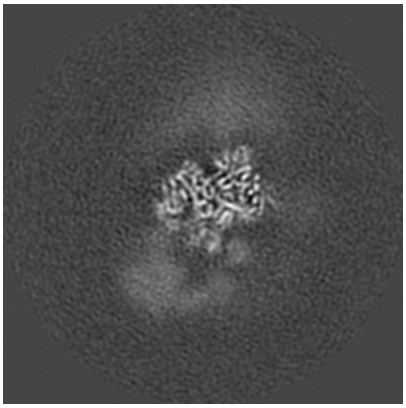
6.3.1 Primary map



X Index: 210



Y Index: 195

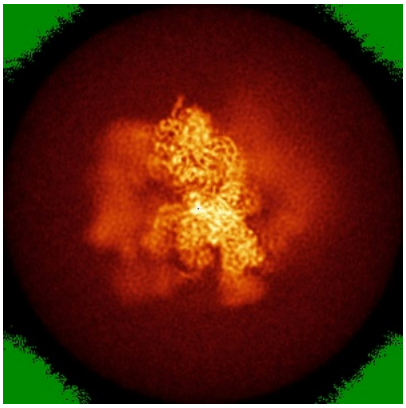


Z Index: 192

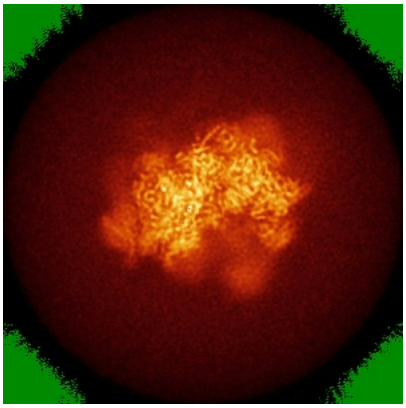
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

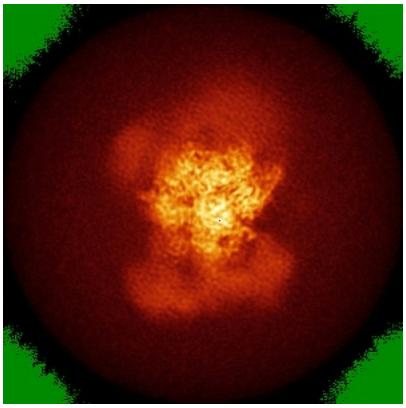
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0323. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

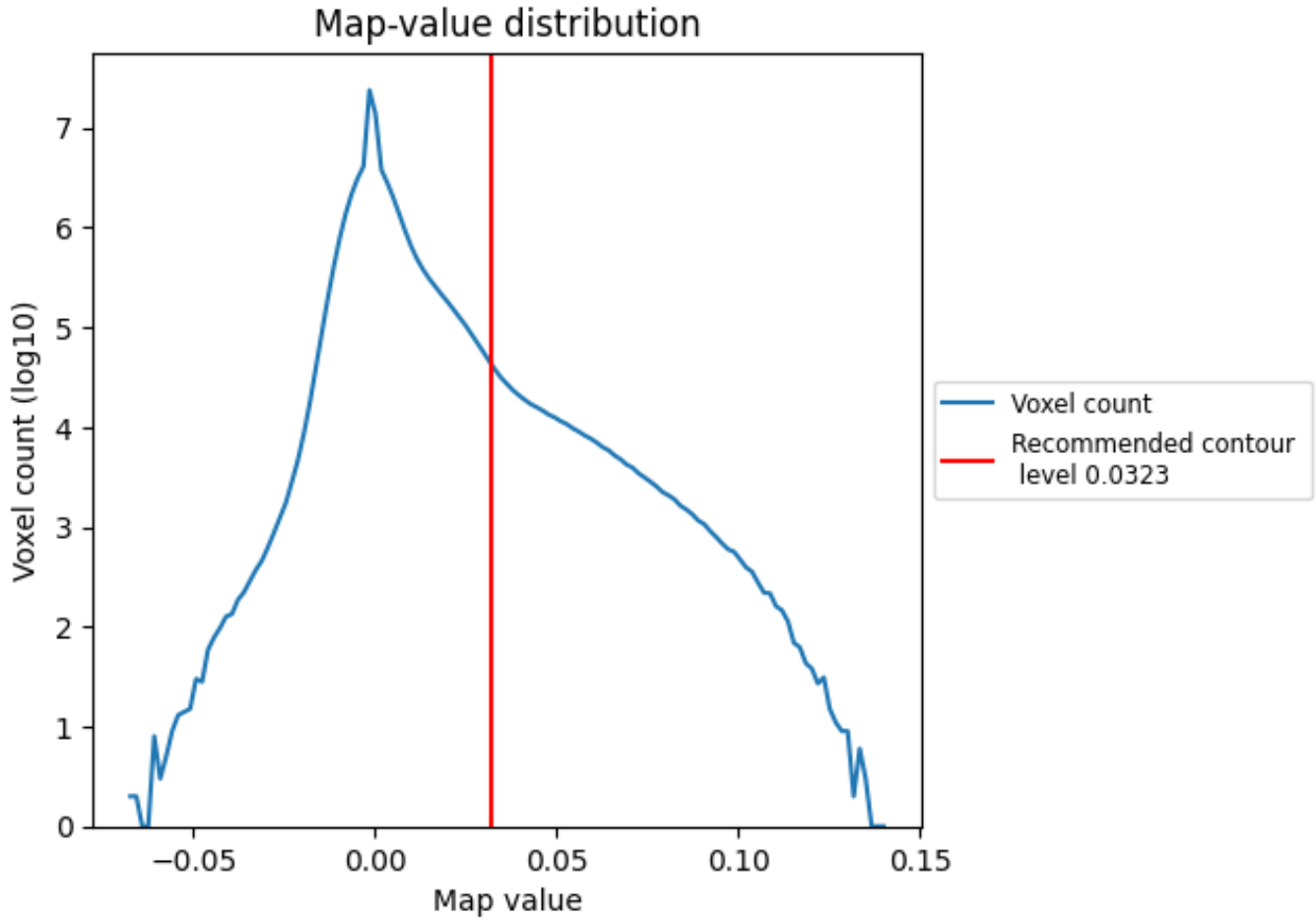
6.6 Mask visualisation (i)

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

7 Map analysis

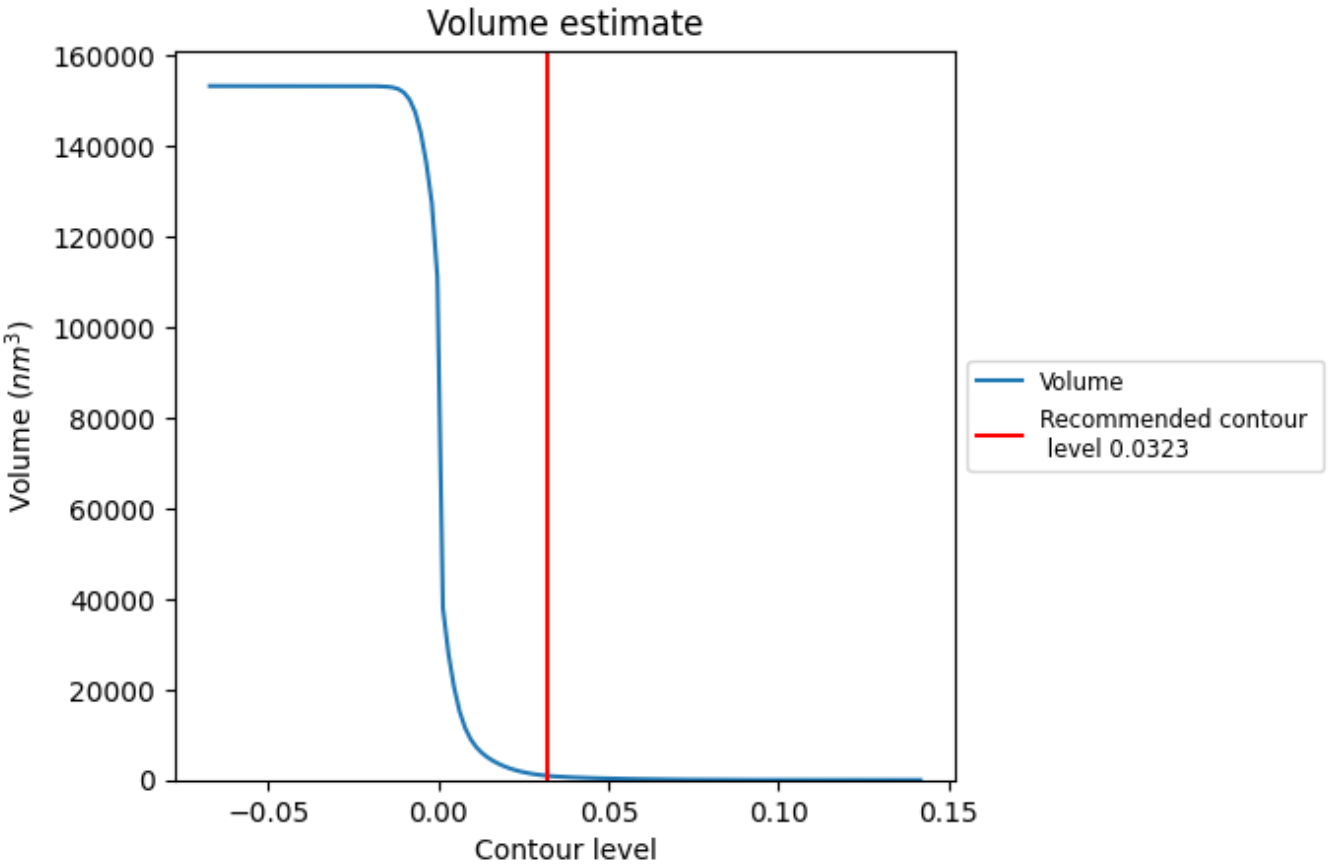
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

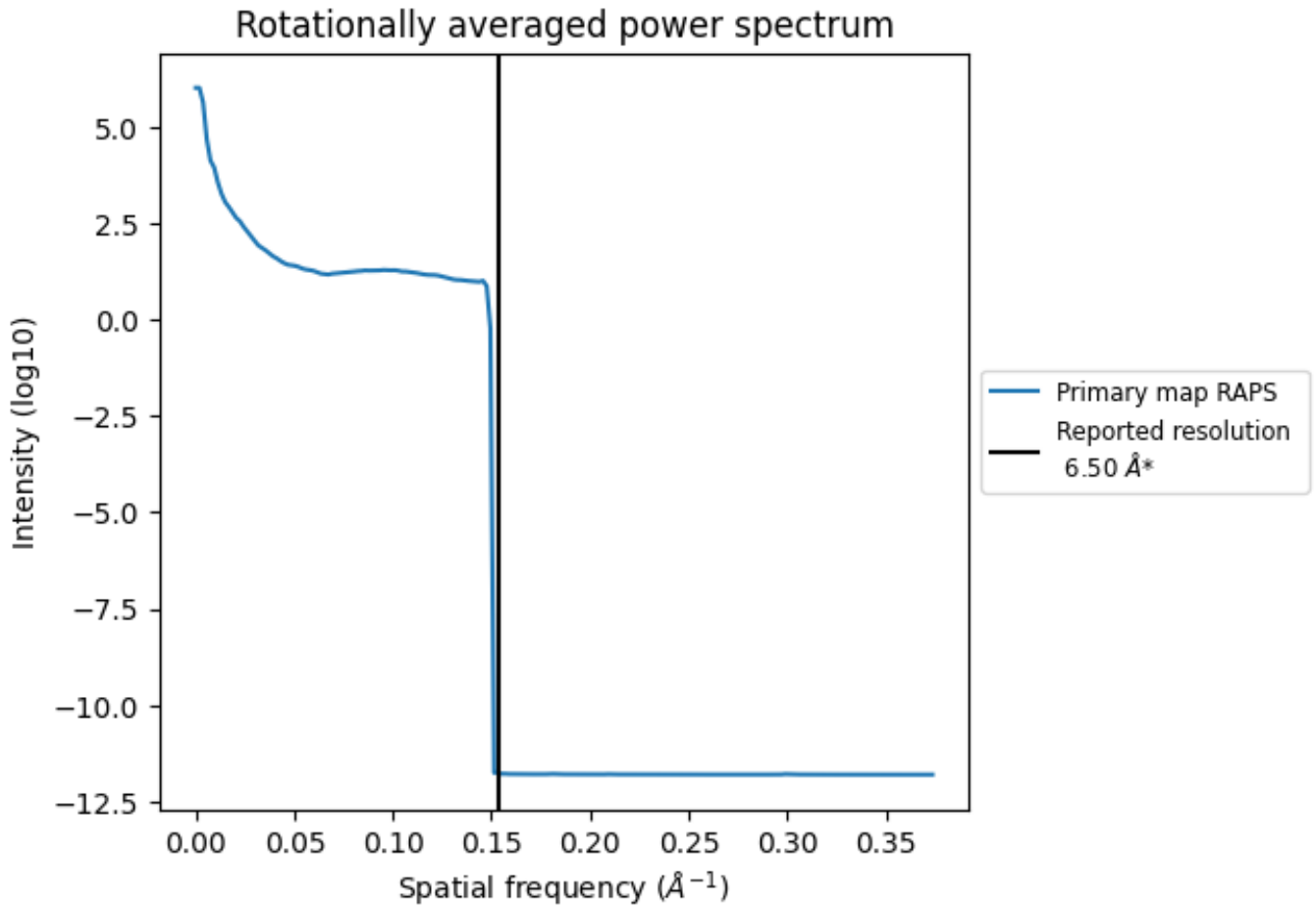
7.2 Volume estimate (i)



The volume at the recommended contour level is 909 nm^3; this corresponds to an approximate mass of 821 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.154 $Å^{-1}$

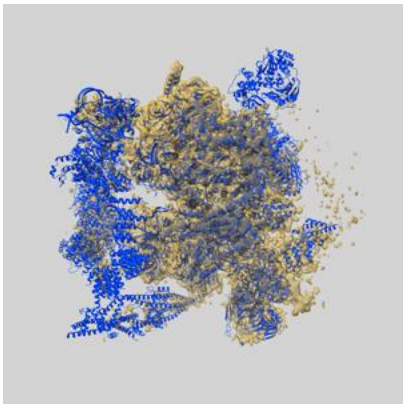
8 Fourier-Shell correlation (i)

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

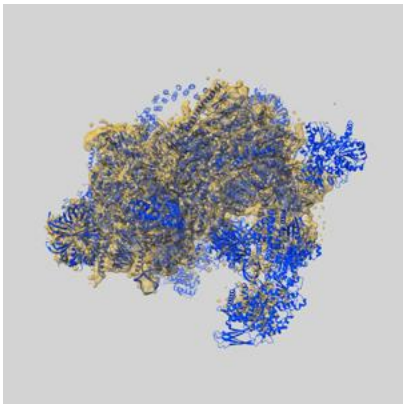
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6890 and PDB model 5Z57. Per-residue inclusion information can be found in section 3 on page 16.

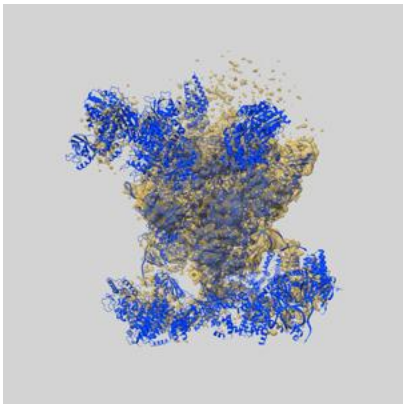
9.1 Map-model overlay



X



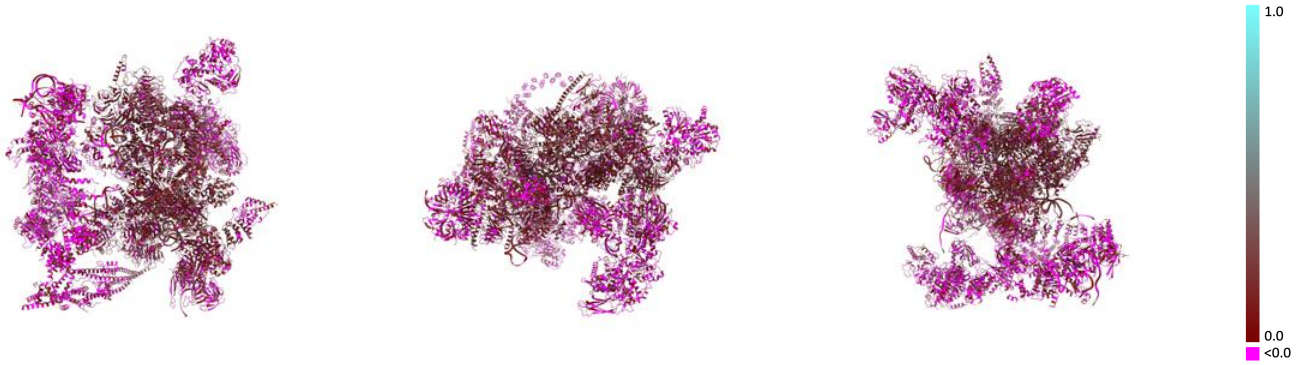
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0323 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

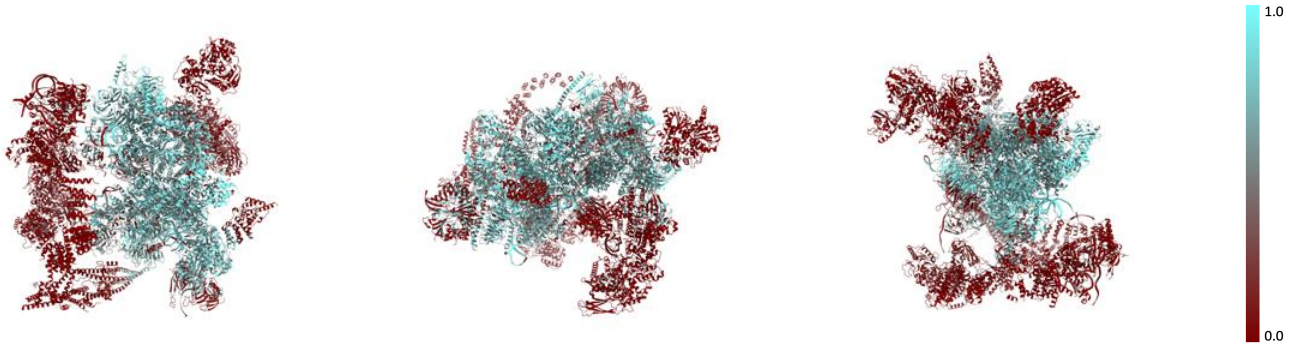
9.2 Q-score mapped to coordinate model



X Y Z

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

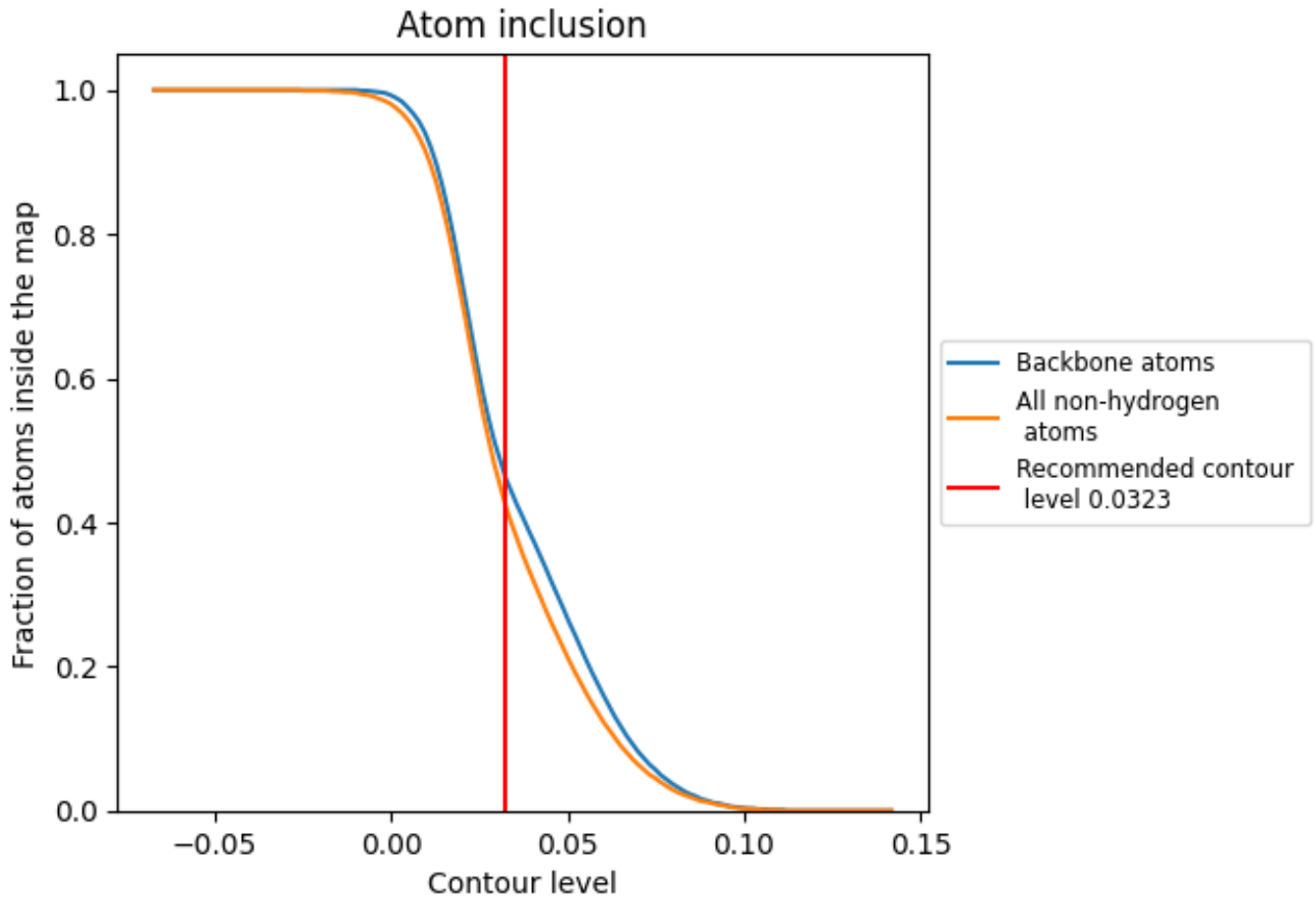
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0323).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 42% 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 (0.0323) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4240	0.0970
1	0.6630	0.1660
2	0.6030	0.1390
3	0.6990	0.1390
4	0.3290	0.0210
5	0.7030	0.1570
6	0.6660	0.1340
7	0.6700	0.1450
A	0.5700	0.1360
B	0.7770	0.1670
C	0.6930	0.1510
D	0.0490	0.0190
E	0.6060	0.1060
F	0.8090	0.1690
G	0.7570	0.1610
H	0.4220	0.0840
I	0.0380	0.0050
J	0.3450	0.0650
K	0.1220	0.0430
L	0.3250	0.0880
N	0.6690	0.1380
O	0.4910	0.1160
P	0.3290	0.1440
Q	0.0240	0.0100
R	0.4890	0.1440
S	0.4900	0.1130
T	0.7380	0.1470
U	0.6680	0.1850
V	0.4080	0.1230
W	0.1940	0.0690
X	0.6450	0.1400
Y	0.7100	0.1780
Z	0.4450	0.1540
a	0.1400	0.0070
b	0.2860	0.0520



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Chain	Atom inclusion	Q-score
c	0.3200	0.0290
d	0.3120	0.0350
e	0.3480	0.0300
f	0.2800	0.0180
g	0.2810	0.0330
h	0.0590	-0.0130
i	0.0690	0.0440
j	0.0910	0.0080
k	0.0640	0.0180
l	0.0790	-0.0210
m	0.1190	-0.0100
n	0.0870	0.0230
o	0.0310	0.0290
p	0.1010	0.0230
q	0.0210	-0.0080
r	0.0460	0.0430
s	0.1100	0.0360
t	0.0000	0.0240
u	0.0130	0.0250
v	0.3530	0.0880
w	0.2140	0.0530
x	0.0000	0.0020
y	0.1290	0.0030