



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 01:09 PM JST

PDB ID : 5Z56
EMDB ID : EMD-6889
Title : cryo-EM structure of a human activated spliceosome (mature Bact) at 5.1 angstrom.
Authors : Zhang, X.; Yan, C.; Zhan, X.; Li, L.; Lei, J.; Shi, Y.
Deposited on : 2018-01-17
Resolution : 5.10 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:

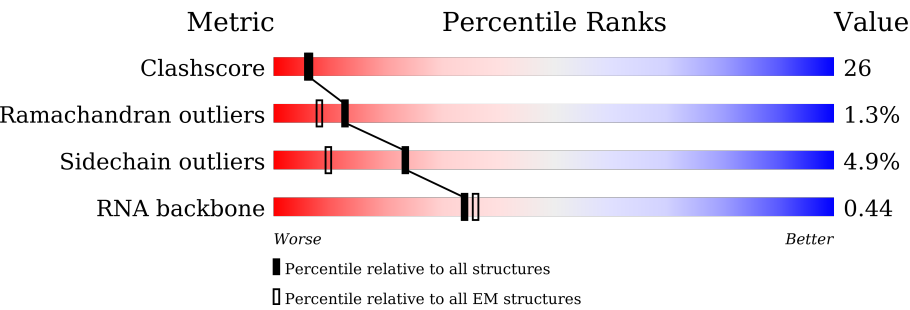
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 5.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 $\leq 5\%$. 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	<div><div>21%</div><div>55%</div><div>36%</div><div>.</div><div>.</div></div>
2	B	117	<div><div>18%</div><div>29%</div><div>26%</div><div>14%</div><div>.</div><div>28%</div></div>
3	C	972	<div><div>10%</div><div>49%</div><div>31%</div><div>7%</div><div>.</div><div>12%</div></div>
4	D	2136	<div><div>75%</div><div>79%</div><div>.</div><div>19%</div></div>
5	E	357	<div><div>26%</div><div>58%</div><div>22%</div><div>.</div><div>16%</div></div>
6	a	126	<div><div>62%</div><div>64%</div><div>36%</div></div>
6	h	126	<div><div>63%</div><div>63%</div><div>37%</div></div>

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Mol	Chain	Length	Quality of chain
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	
22	2	895	
23	3	1217	
24	4	424	
25	5	125	

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Mol	Chain	Length	Quality of chain
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	M	343	
35	N	144	
36	O	420	
37	P	229	
38	R	540	
39	S	166	
40	T	514	
41	U	2752	
42	V	908	
43	W	579	
44	X	396	
45	Y	322	
46	Z	619	
47	z	472	

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Mol	Chain	Length	Quality of chain
48	x	1041	
49	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
50	IHP	A	3000	-	-	X	-
51	GTP	C	1500	-	-	X	-
53	ZN	O	502	-	-	X	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 117278 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2232	Total	C	N	O	S	0	0
			18450	11885	3217	3269	79		

- Molecule 2 is a RNA chain called U5 snRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a RNA chain called U6 snRNA.

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

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

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

- Molecule 15 is a RNA chain called U2 snRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	437	Total	C	N	O	S	0	0
			2369	1448	460	458	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	u	106	Total	C	N	O	0	0
			530	318	106	106		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	v	167	Total	C	N	O	S	0
			946	571	193	180	2	0

- 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
			7702	4900	1347	1415	40	0

- 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
			1252	809	213	226	4	0

- 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
			9220	5854	1566	1755	45	0

- 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
			807	512	142	150	3	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	85	Total	C	N	O	S	0	0
			645	396	114	122	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	C	N	O	0	0
			2778	1650	564	564		

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

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

- Molecule 34 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	36	Total	C	N	O	S	0	0
			267	167	45	52	3		

- Molecule 35 is a protein called Protein BUD31 homolog.

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

- Molecule 36 is a protein called Pre-mRNA-splicing factor RBM22.

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

- Molecule 37 is a protein called Spliceosome-associated protein CWC15 homolog.

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

- Molecule 38 is a protein called Skip.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	309	Total	C	N	O	S	0	0
			2316	1456	413	435	12		

- Molecule 39 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 40 is a protein called Pleiotropic regulator 1.

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

- Molecule 41 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 42 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

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

- Molecule 43 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	481	Total	C	N	O		0	0
			2374	1412	481	481			

- Molecule 44 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	X	159	Total	C	N	O	S	0	0
			1021	649	173	198	1		

- Molecule 45 is a protein called RNA-binding motif protein, X-linked 2.

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

- Molecule 46 is a protein called BUD13 homolog.

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

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	177	Total	C	N	O	S	1	0
			1381	869	241	266	5		

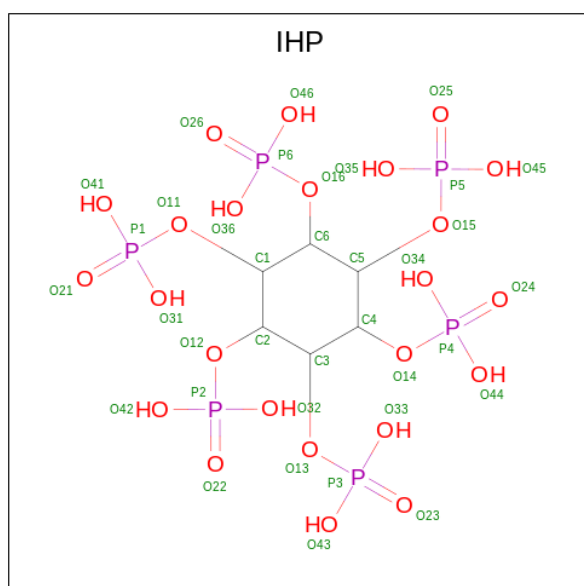
- Molecule 48 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	x	584	Total	C	N	O	0	0
			2887	1718	584	585		

- Molecule 49 is a protein called Peptidyl-prolyl cis-trans isomerase E.

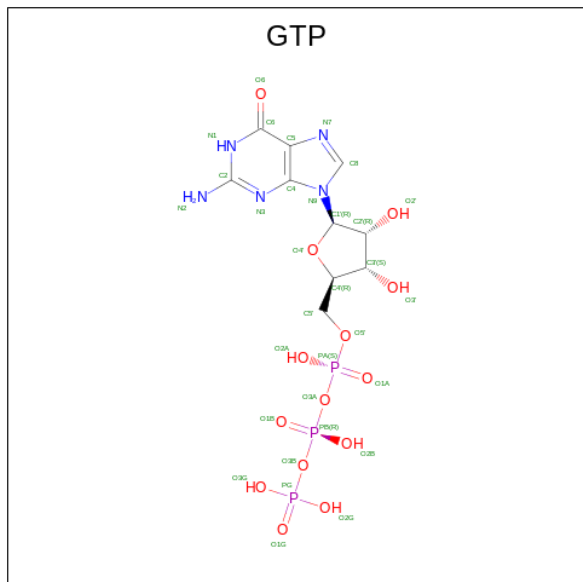
Mol	Chain	Residues	Atoms				AltConf	Trace
49	y	232	Total	C	N	O	0	0
			1133	669	232	232		

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$).



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

- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	v	1	Total	Zn	0
			1	1	
53	6	3	Total	Zn	0
			3	3	
53	M	1	Total	Zn	0
			1	1	
53	N	3	Total	Zn	0
			3	3	
53	O	3	Total	Zn	0
			3	3	

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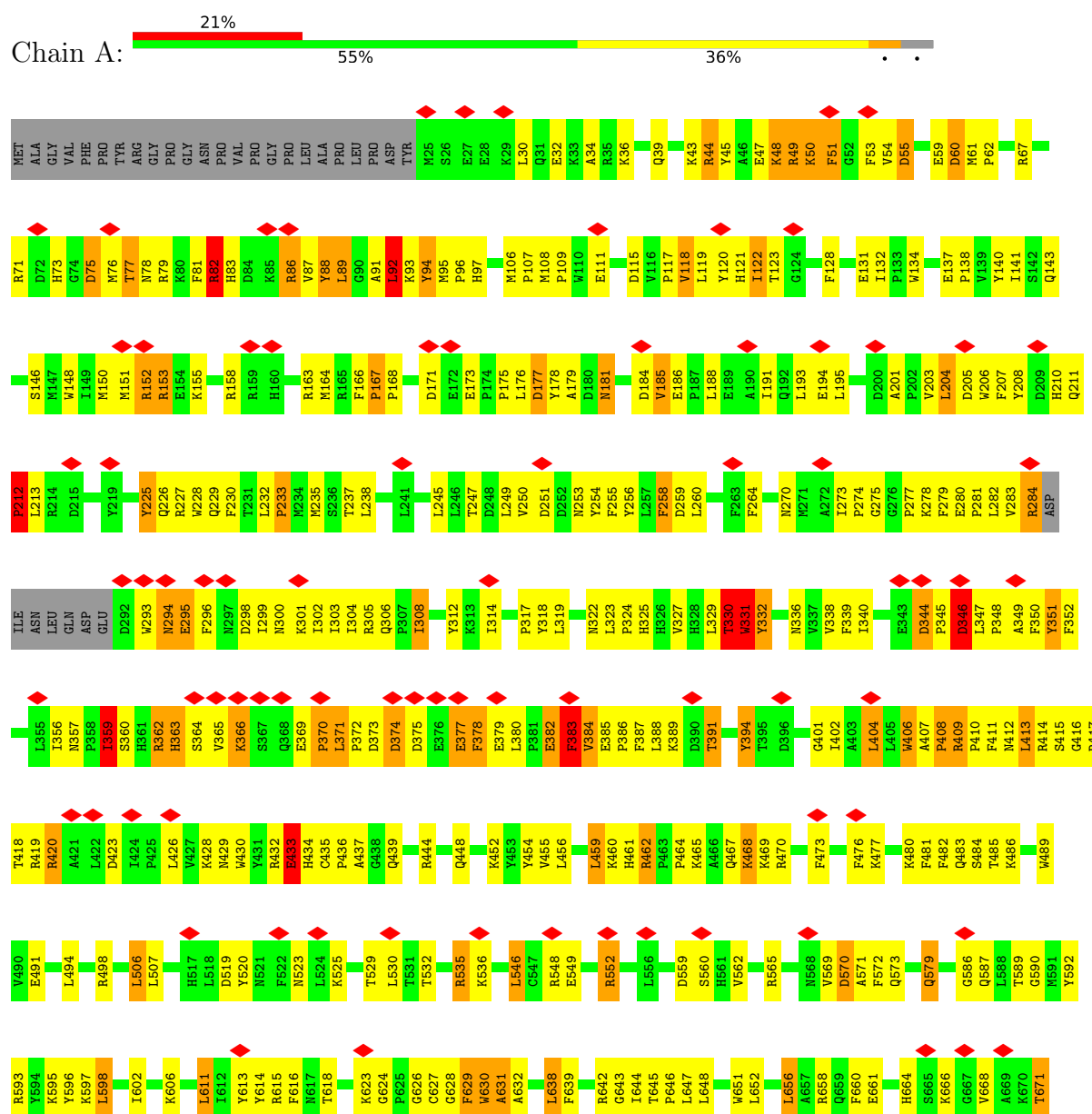
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
53	W	2	2	2	0

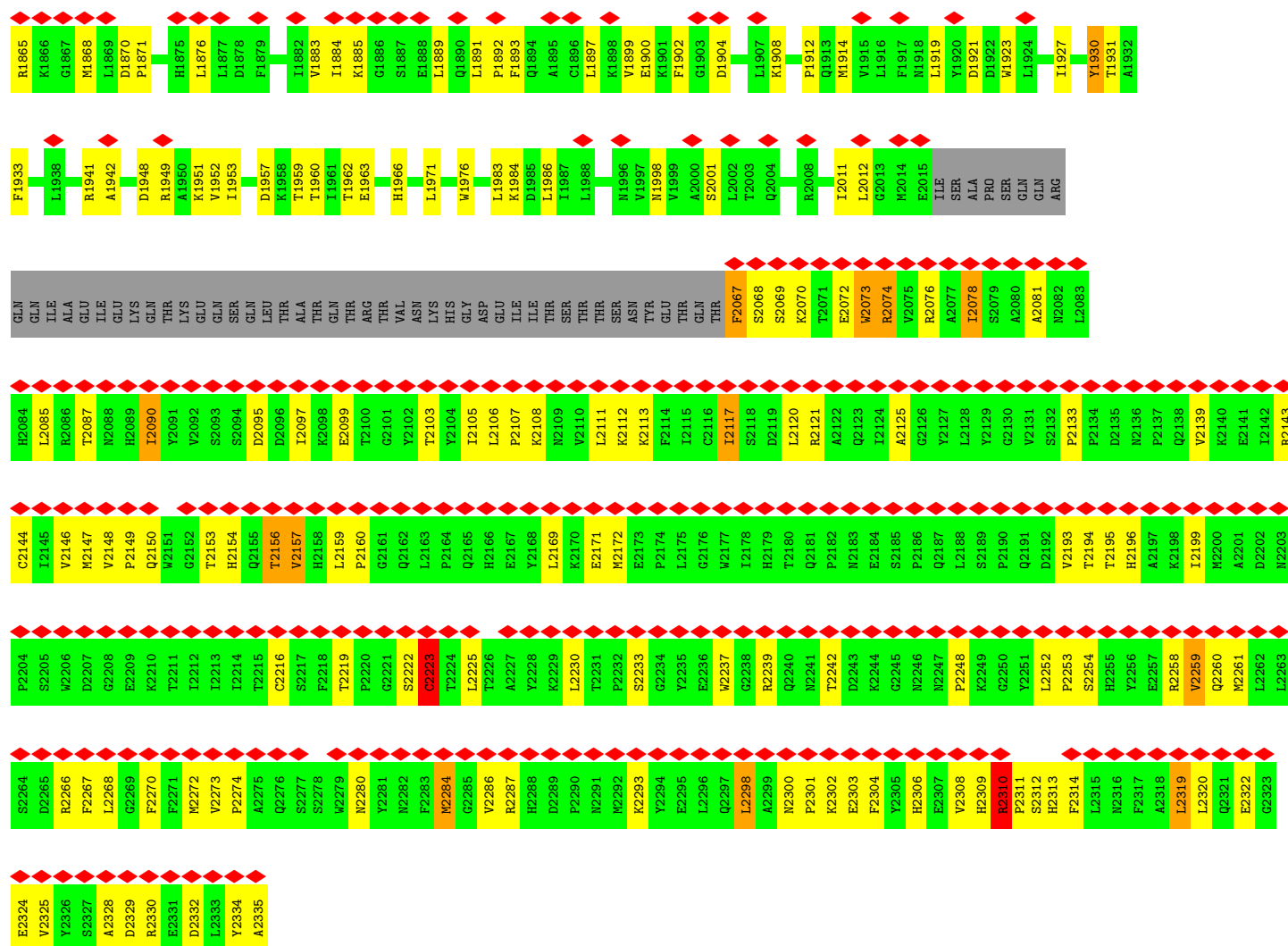
3 Residue-property plots

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

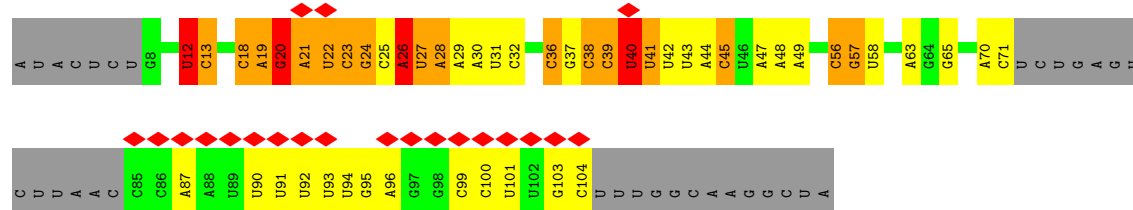
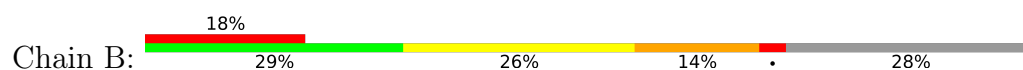
• Molecule 1: Pre-mRNA-processing-splicing factor 8



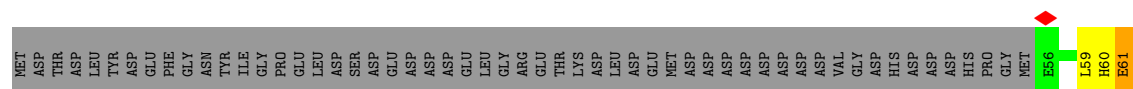




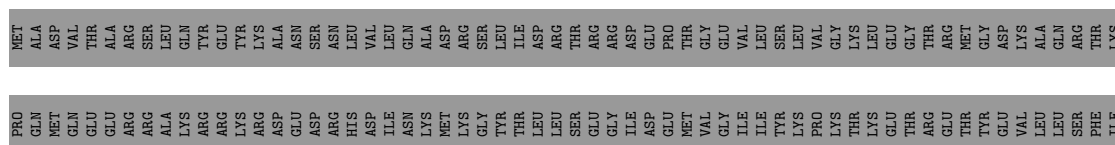
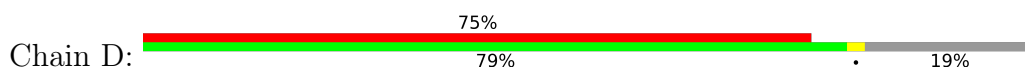
• Molecule 2: U5 snRNA



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

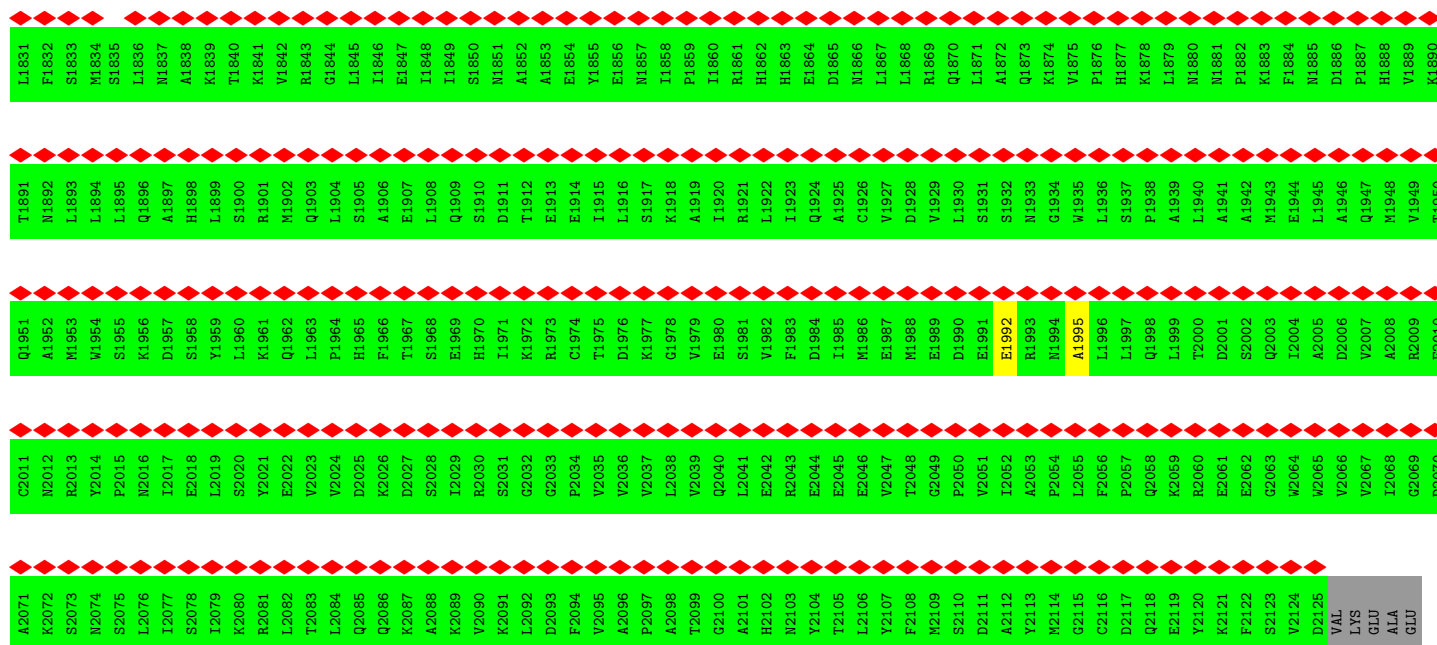


- Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

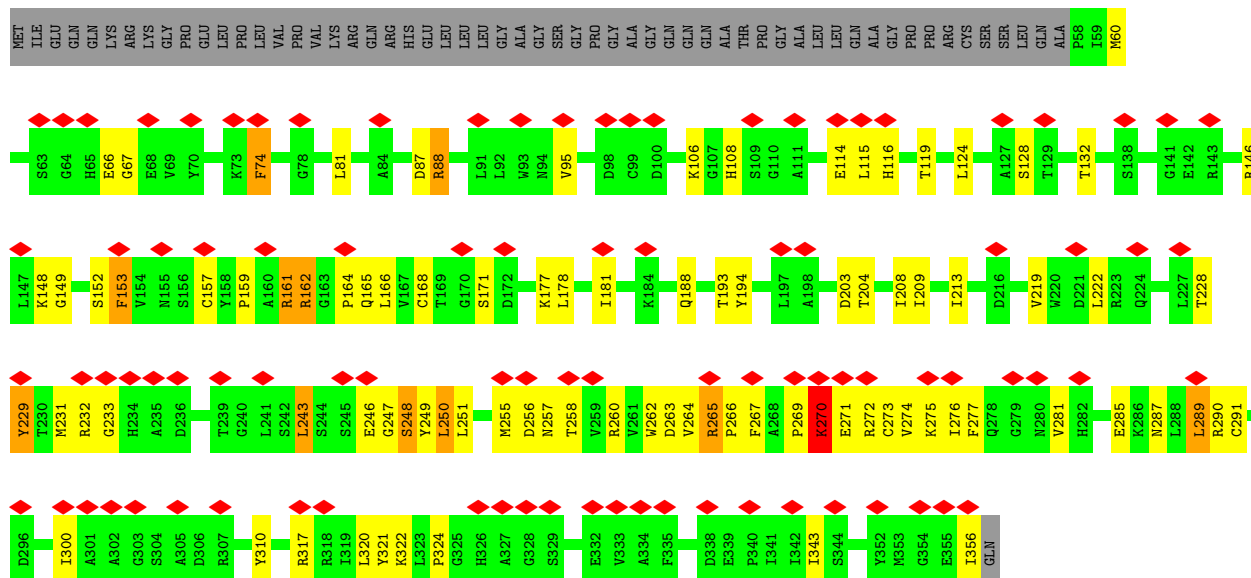




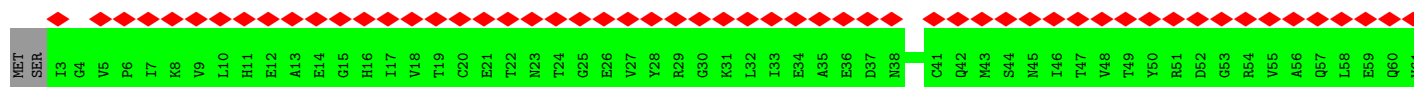
Y1771	K1711	C1651	H1591	N1531	C1471	E1411	P1351	L1291	E1231	G1171	K1110	P1047
N1772	D1712	V1652	C1592	I1532	S1472	T1412	T1352	P1292	V1232	K1172	T1111	V1048
L1773	F1713	G1653	T1593	S1533	R1473	S1413	G1353	E1293	I1233	T1173	L1112	K1049
Q1774	F1714	M1654	E1594	H1534	M1474	T1414	S1354	K1294	L1234	I1174	N1113	E1050
G1775	K1715	N1655	D1595	Q1535	R1475	D1415	G1355	Y1295	H1235	K1175	L1114	S1051
L1776	K1716	V1656	D1596	Q1536	R1476	L1416	G1356	P1296	H1236	K1176	C1115	I1052
S1777	F1717	A1657	L1597	T1537	I1477	K1417	T1357	P1297	E1237	Y1177	K1116	E1053
H1778	L1718	A1658	I1598	R1538	S1478	L1418	C1358	P1298	Y1238	V1178	M1117	S1056
R1779	Y1719	P1659	L1599	L1539	S1479	L1419	G1359	T1299	F1239	L1179	I1118	A1057
H1780	E1720	H1660	Y1600	L1540	Q1480	G1420	A1360	E1300	L1240	L1180	D1119	K1058
L1781	P1721	V1661	L1601	S1541	I1481	K1421	E1361	L1301	L1241	F1181	K1120	I1059
S1782	L1722	I1662	E1602	M1542	E1482	G1422	F1362	L1302	K1242	P1182	R1121	M1060
D1783	P1723	I1663	L1603	A1543	R1483	N1423	A1363	D1303	A1243	K1183	M1122	V1061
H1784	V1724	M1664	K1604	K1544	P1484	I1424	I1364	L1304	K1244	L1184	W1123	L1062
L1785	E1725	D1665	S1605	P1545	I1485	I1425	L1365	Q1305	Y1245	E1185	Q1124	L1063
S1786	S1726	T1666	D1606	V1546	R1486	I1426	R1366	P1306	A1246	L1186	S1125	Q1064
E1787	H1727	Q1667	S1607	Y1547	I1487	S1427	M1367	L1307	Q1247	S1187	M1126	A1065
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V1789	D1729	Y1669	L1609	A1549	A1489	P1429	L1369	V1309	E1249	H1189	L1129	I1067
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Q1791	C1731	G1671	E1611	T1551	S1491	K1431	S1371	A1311	L1251	Q1191	Q1131	Q1069
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V1810	D1750	H1690	R1630	R1570	S1510	F1451	Y1390	P1330	W1270	W1210	R1152	G1089
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P1812	V1752	N1692	V1632	T1572	F1512	V1453	D1392	Q1332	S1272	E1212	Y1154	L1091
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L1815	L1755	L1695	L1635	D1575	H1515	V1456	K1396	V1335	W1275	H1215	N1157	A1094
G1816	T1756	Q1696	F1636	I1576	P1516	H1457	F1397	F1336	L1276	G1216	I1095	F1096
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I1818	T1758	D1698	S1638	T1578	V1518	I1459	Q1399	T1338	C1278	S1218	N1159	E1097
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A1820	L1760	G1700	A1640	C1580	P1520	G1461	R1400	Y1340	T1280	A1220	G1162	V1099
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V1822	R1762	C1702	Q1642	E1582	P1522	N1463	K1403	S1342	L1282	W1222	L1164	G1103
Y1823	R1763	V1703	V1643	D1583	L1523	K1464	K1404	D1343	P1283	I1223	I1165	G1103
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V1826	T1765	M1705	V1645	Q1585	L1525	V1466	V1406	M1345	S1285	V1225	M1167	A1105
L1827	Q1766	C1706	A1646	H1586	H1526	L1467	V1407	N1346	F1286	E1226	P1168	Q1106
T1828	N1767	Q1707	S1647	Q1587	I1527	E1468	L1407	F1347	R1287	D1227	K1169	L1107
N1769	P1768	R1648	R1648	R1588	Q1528	V1469	L1408	V1348	H1288	V1228	M1170	
I1829	Y1770	S1709	S1649	F1589	G1529	I1470	T1409	G1349	L1289	D1229		
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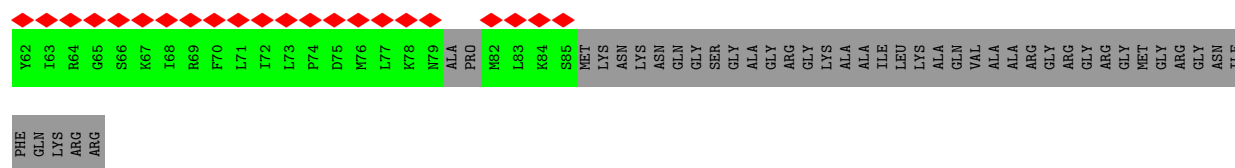


• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

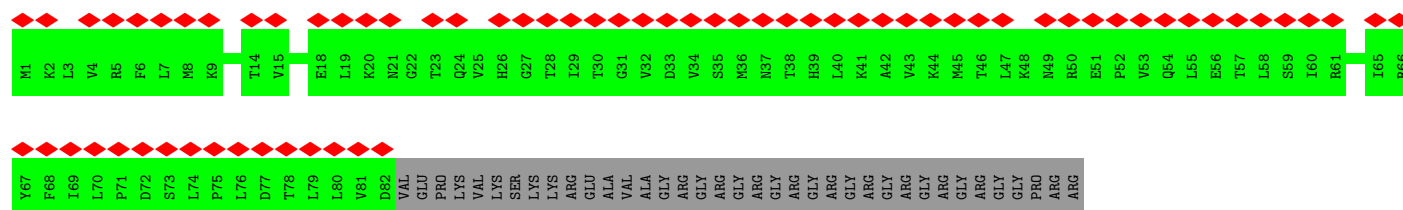


• Molecule 6: Small nuclear ribonucleoprotein Sm D3

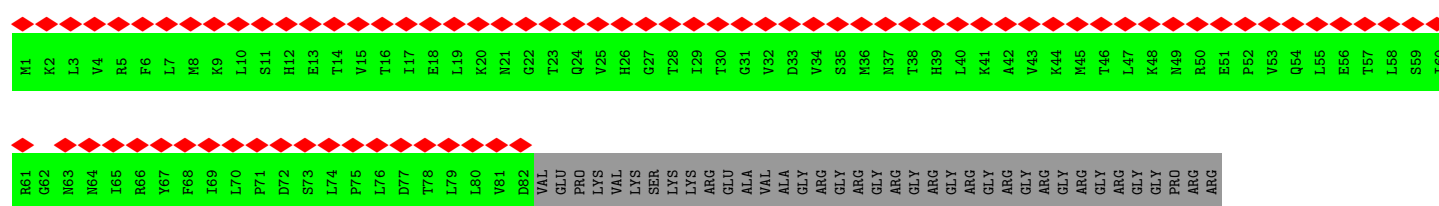




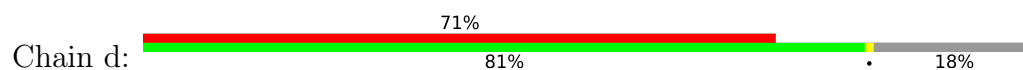
- Molecule 8: Small nuclear ribonucleoprotein Sm D1



- Molecule 8: Small nuclear ribonucleoprotein Sm D1



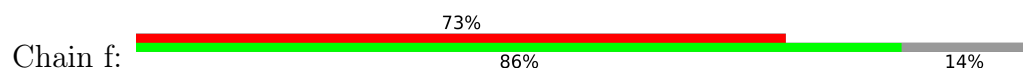
- Molecule 9: Small nuclear ribonucleoprotein Sm D2

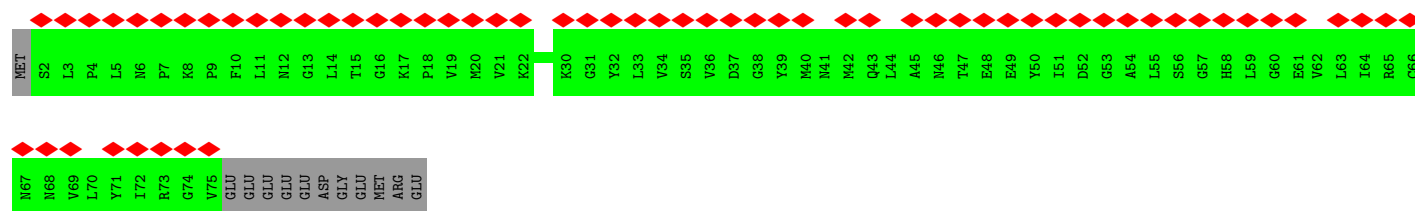


- Molecule 9: Small nuclear ribonucleoprotein Sm D2

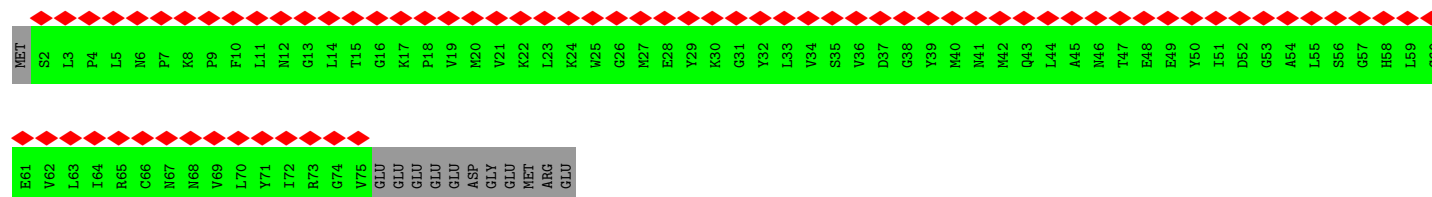
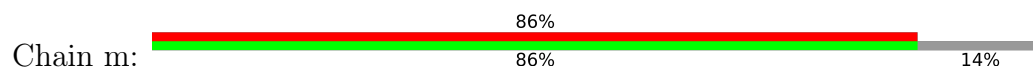


- Molecule 10: Small nuclear ribonucleoprotein F

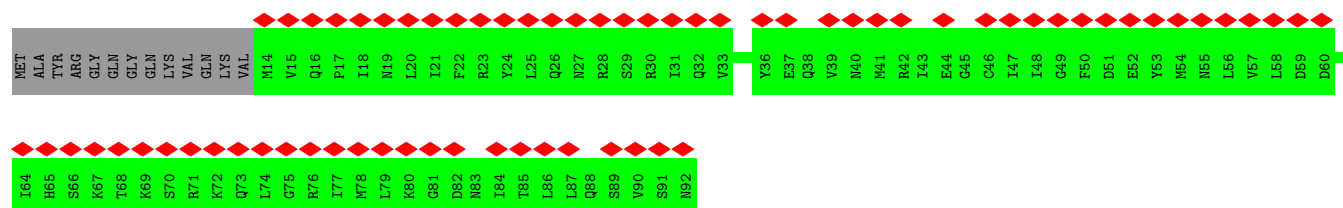
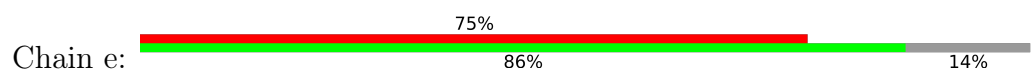




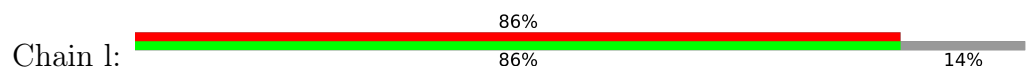
• Molecule 10: Small nuclear ribonucleoprotein F



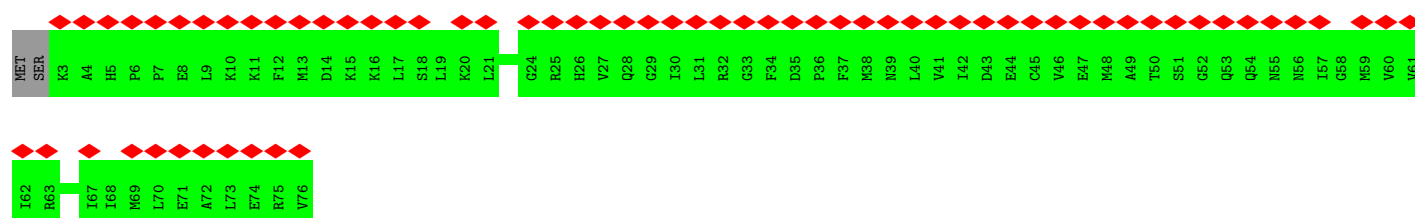
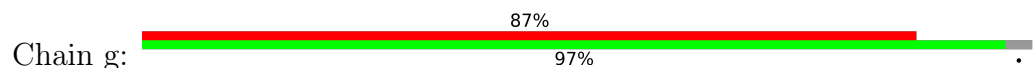
• Molecule 11: Small nuclear ribonucleoprotein E



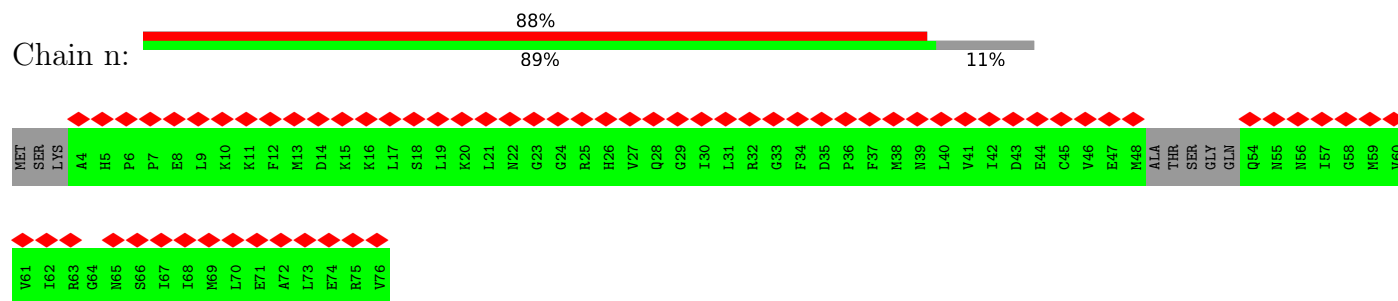
• Molecule 11: Small nuclear ribonucleoprotein E



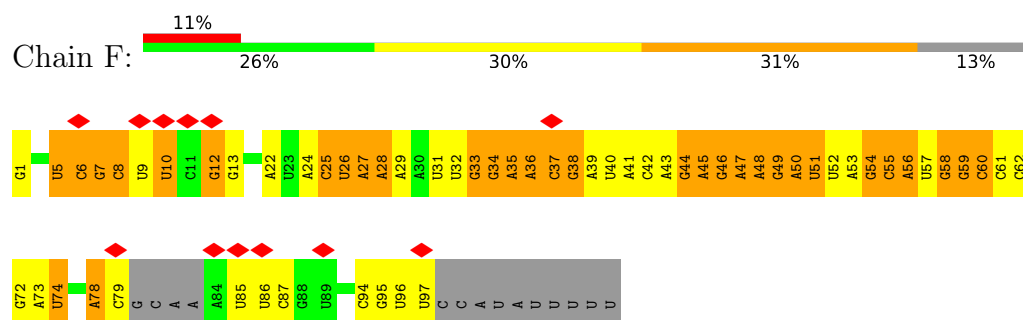
• Molecule 12: Small nuclear ribonucleoprotein G



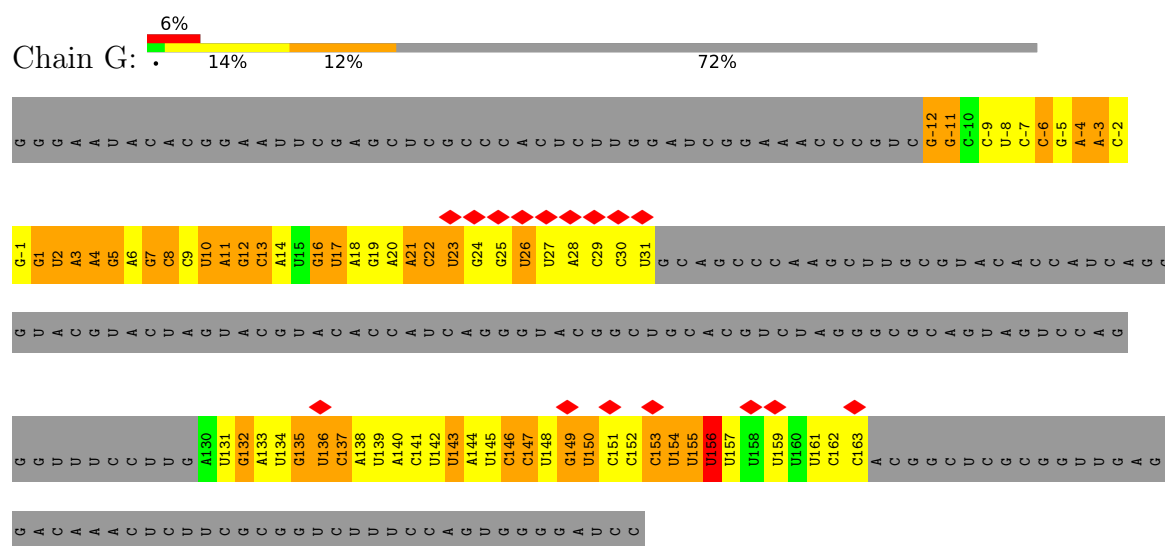
- Molecule 12: Small nuclear ribonucleoprotein G



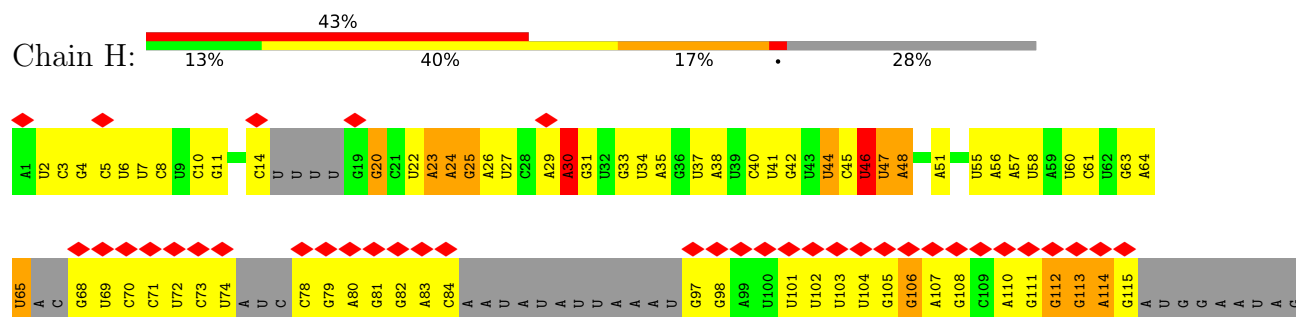
- Molecule 13: U6 snRNA

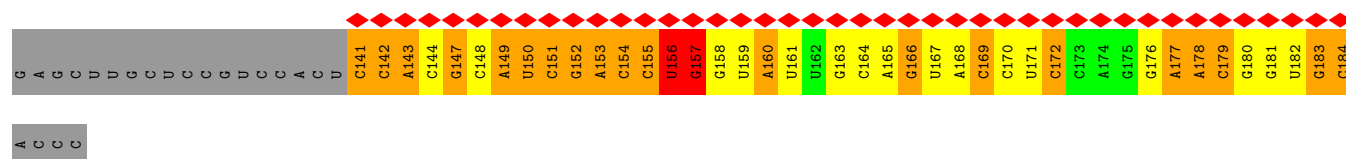


- Molecule 14: pre-mRNA

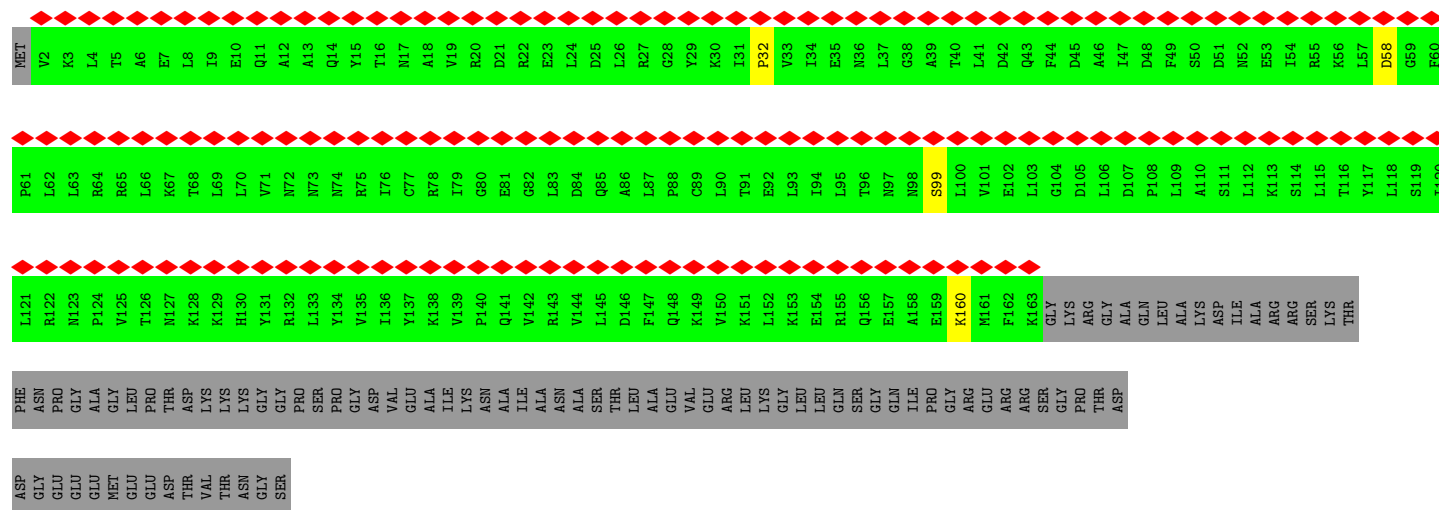


- Molecule 15: U2 snRNA

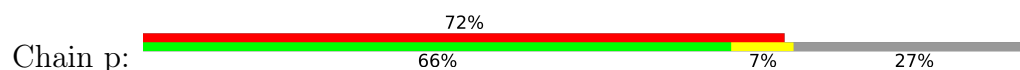




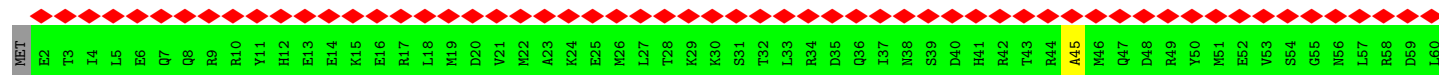
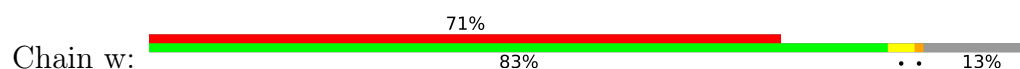
• Molecule 16: U2 small nuclear ribonucleoprotein A'

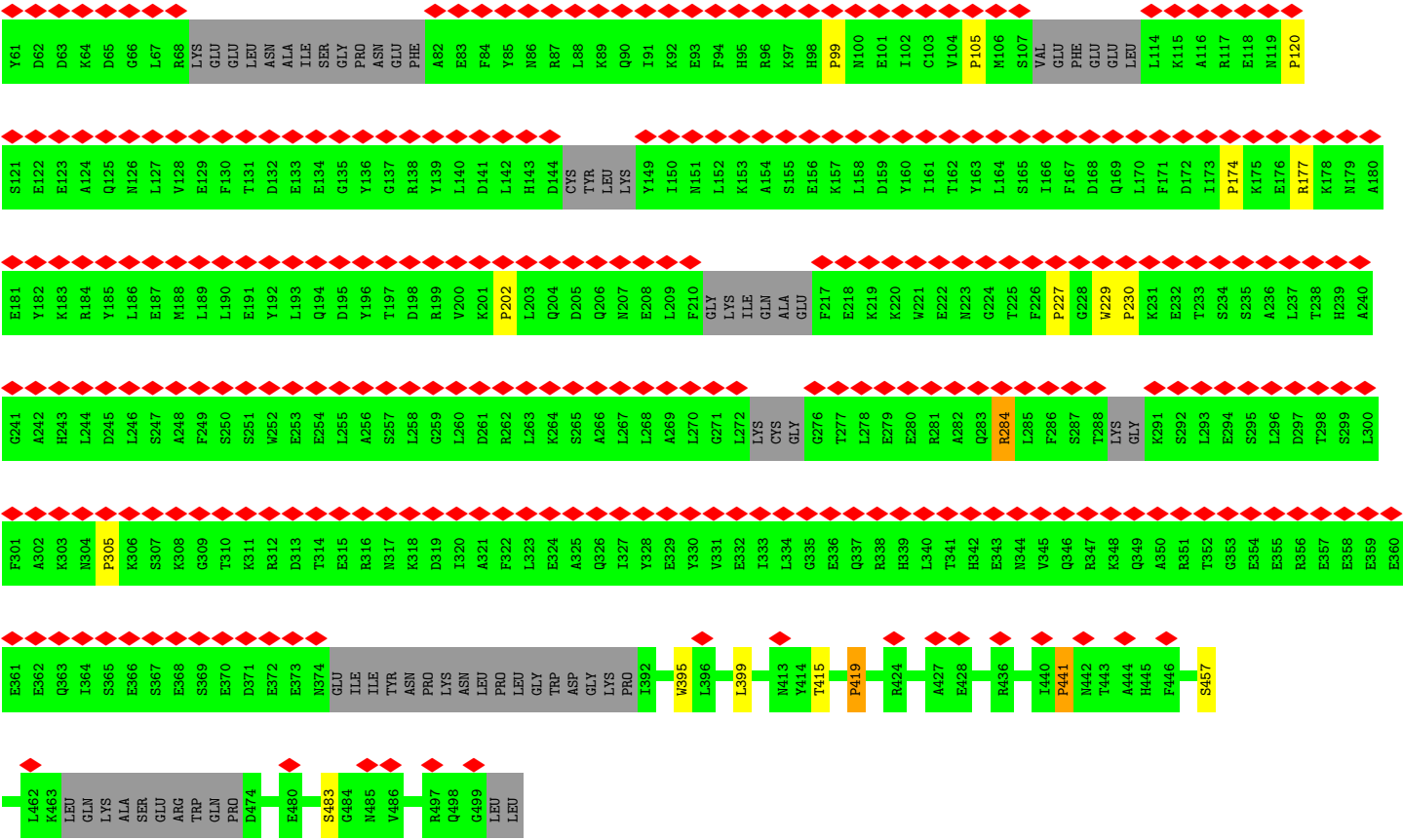


• Molecule 17: U2 small nuclear ribonucleoprotein B''

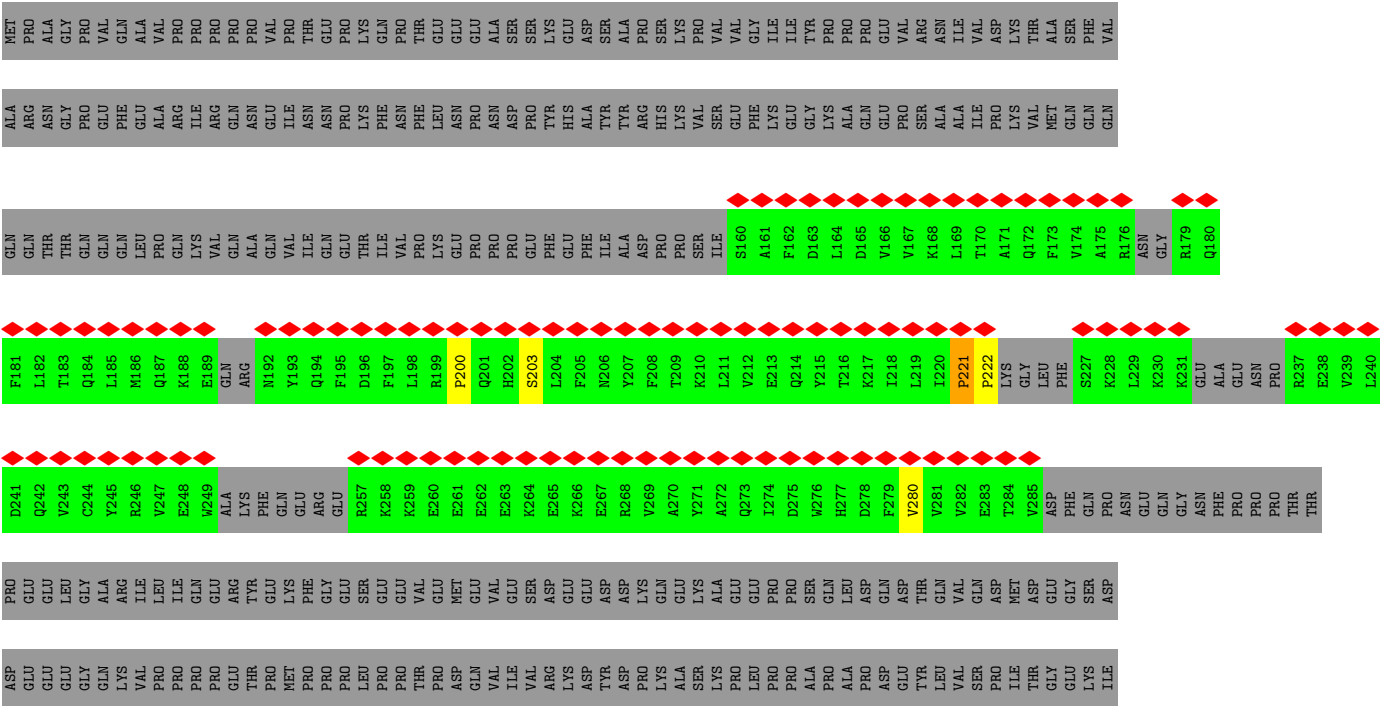


• Molecule 18: Splicing factor 3A subunit 3



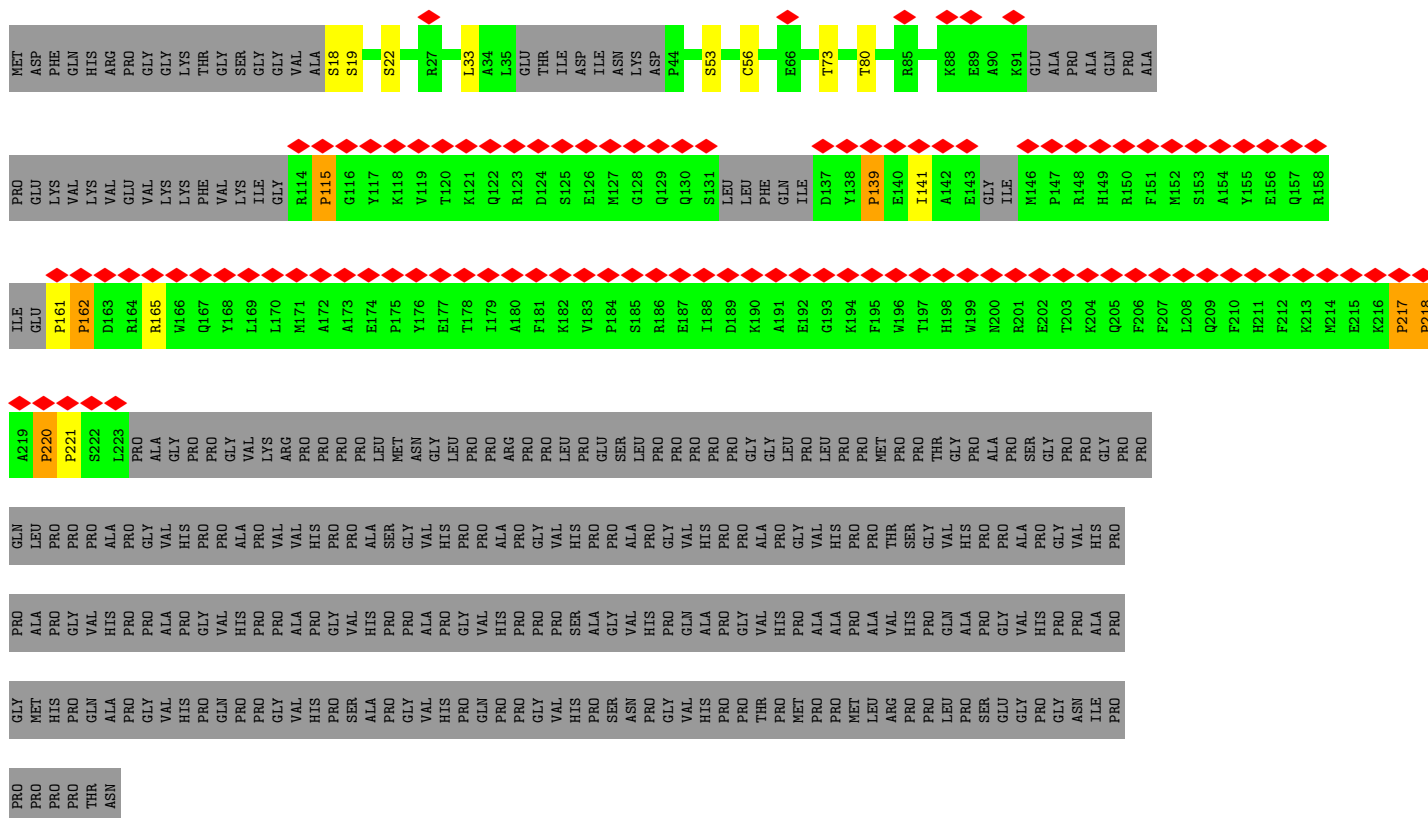


• Molecule 19: Splicing factor 3A subunit 1



[illegible]

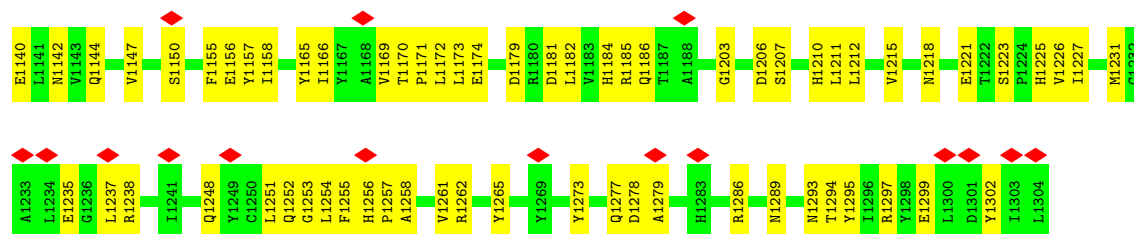
- Molecule 20: Splicing factor 3A subunit 2



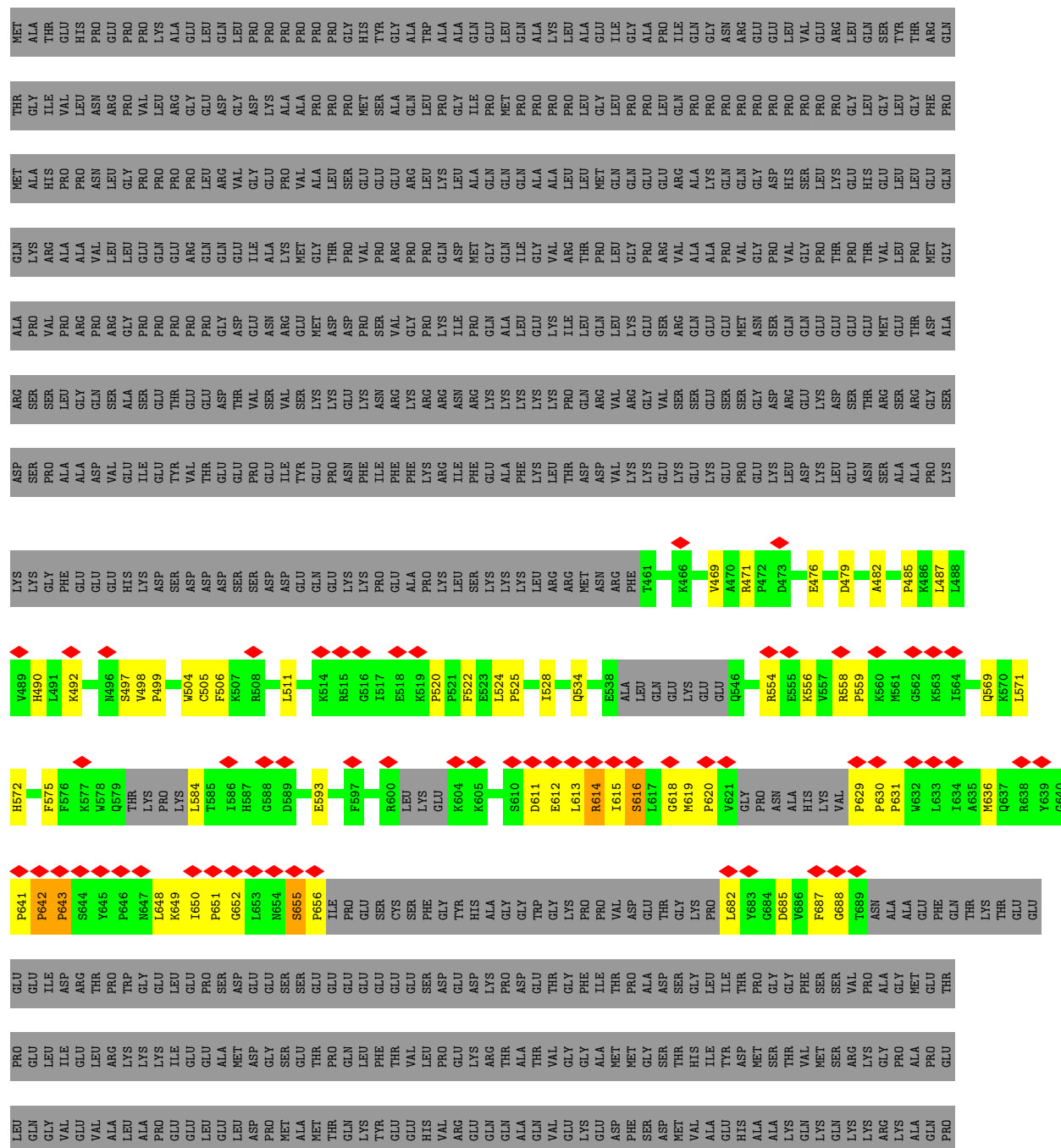
- Molecule 21: Splicing factor 3B subunit 1





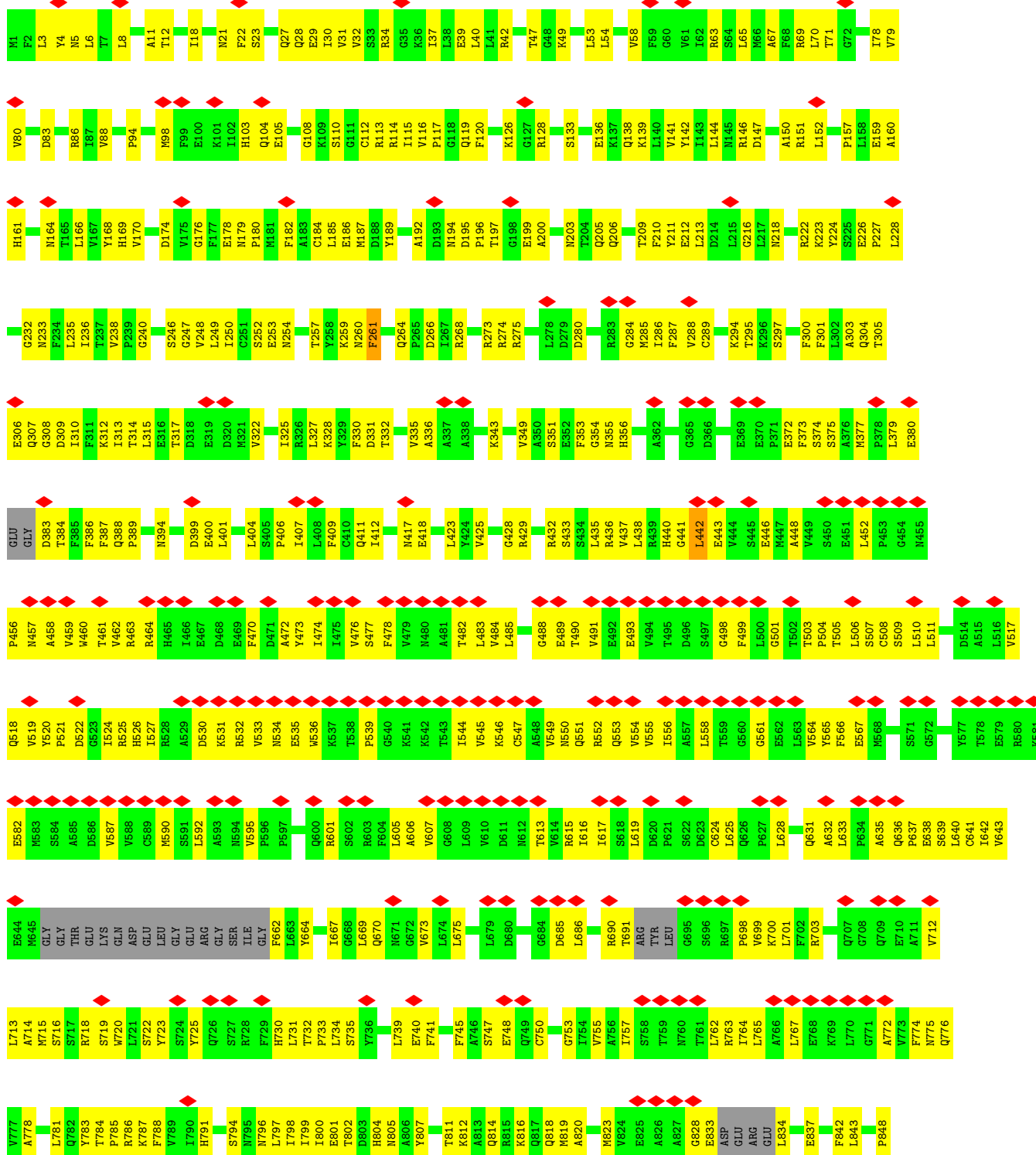


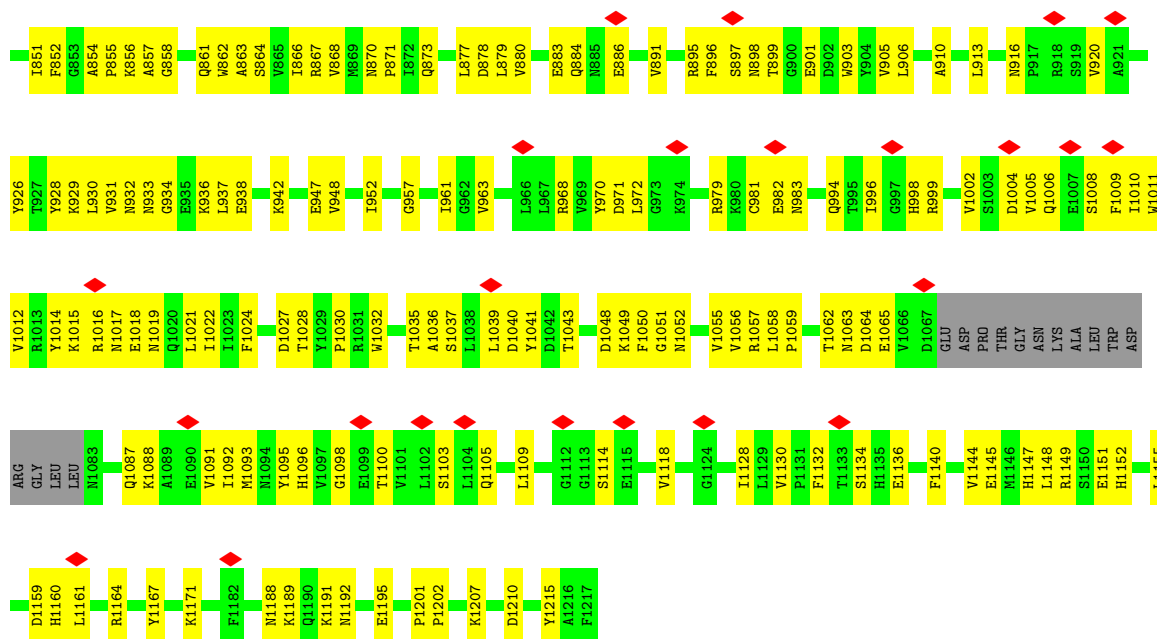
• Molecule 22: Splicing factor 3B subunit 2



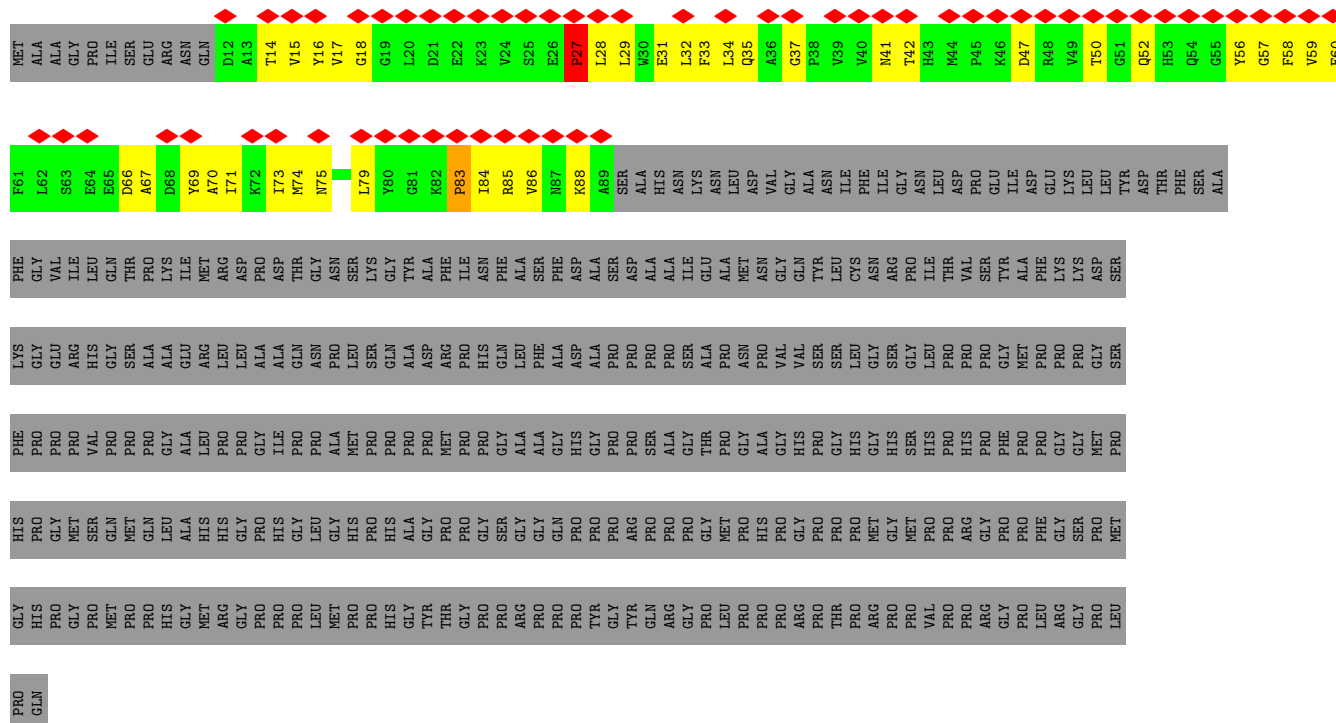
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ASP
SER
ARG
GLY
GLY
SER
LYS
LYS
LYS
TYR
GLU
PHE
LYS
PHE

• Molecule 23: Splicing factor 3B subunit 3





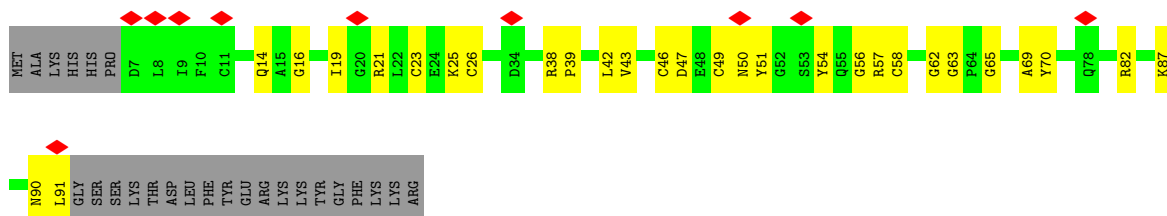
• Molecule 24: Splicing factor 3B subunit 4



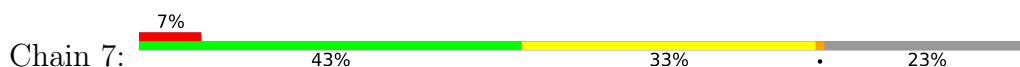
• Molecule 25: Splicing factor 3B subunit 6



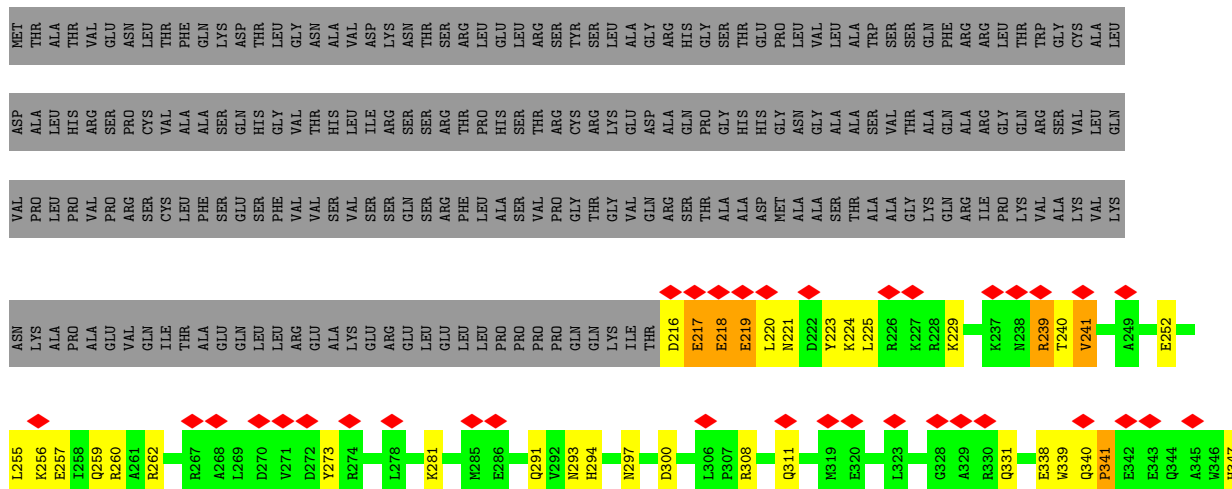
- Molecule 26: PHD finger-like domain-containing protein 5A

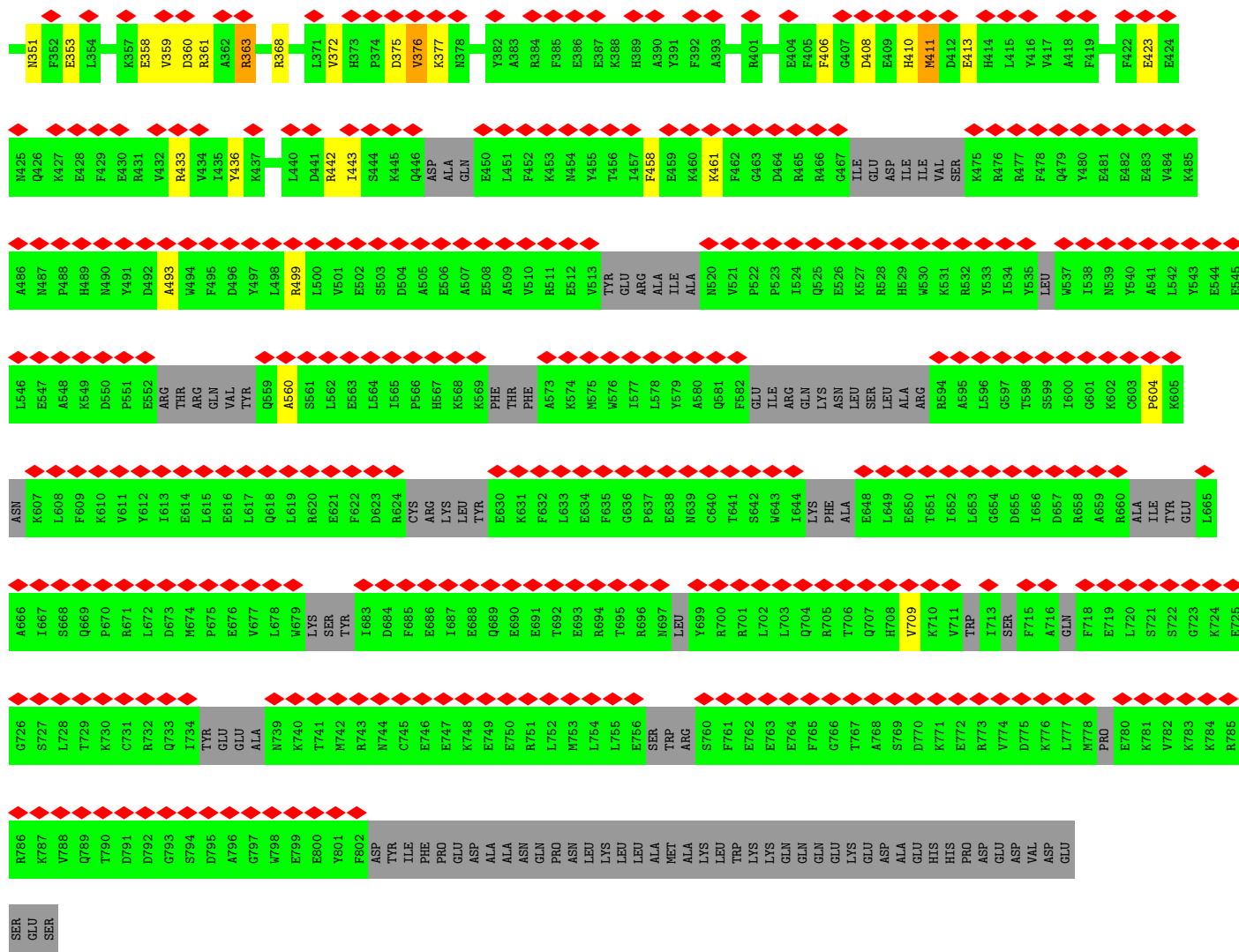


- Molecule 27: Splicing factor 3B subunit 5

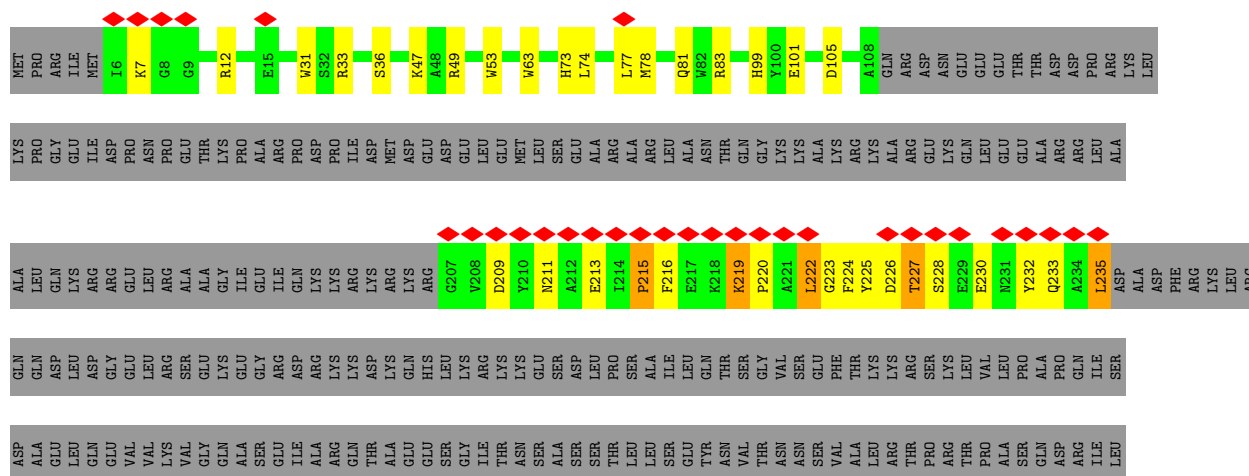
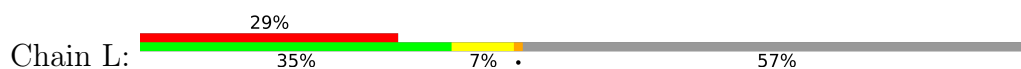


- Molecule 28: Crooked neck-like protein 1

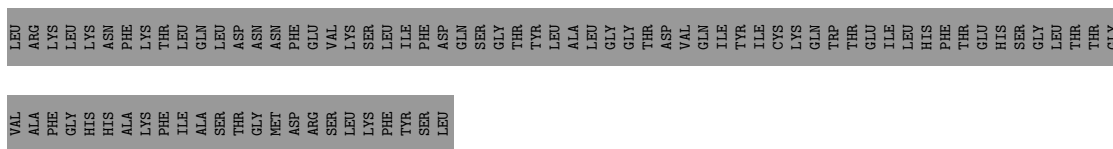




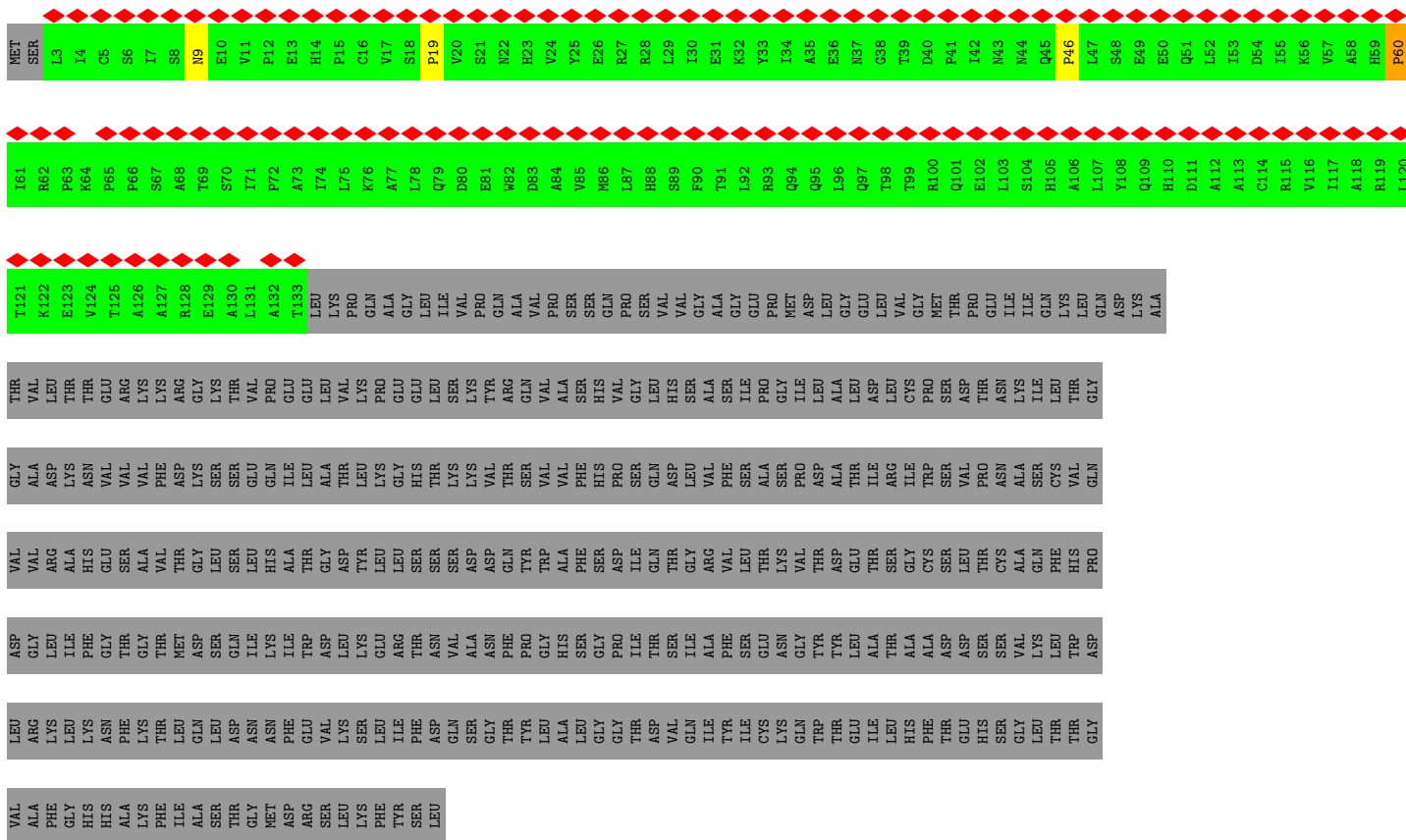
• Molecule 29: Cell division cycle 5-like protein



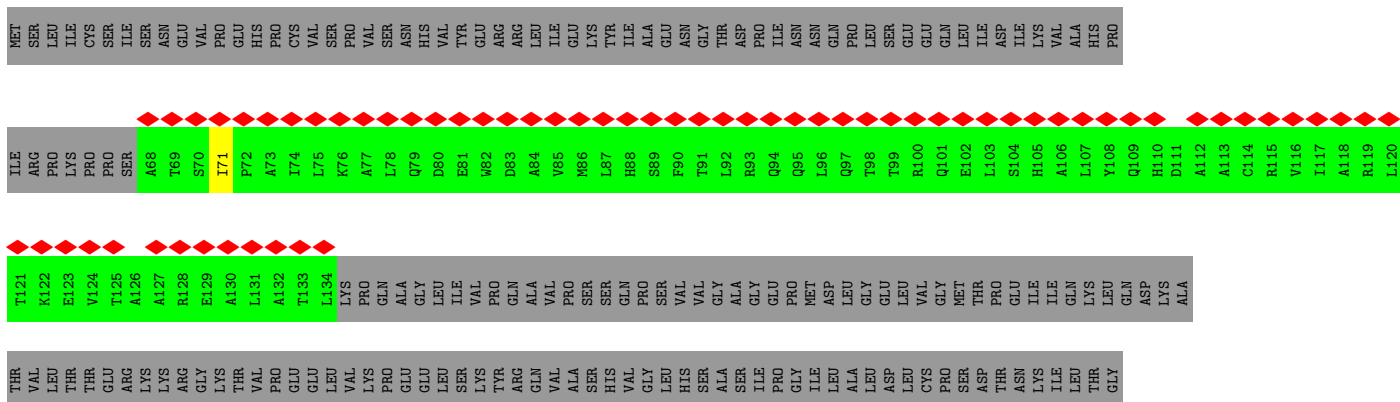


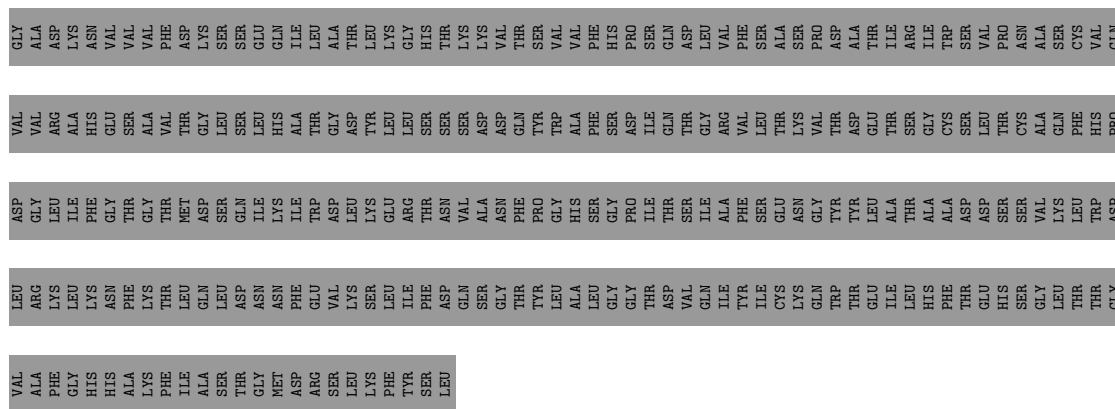


- Molecule 30: Pre-mRNA-processing factor 19

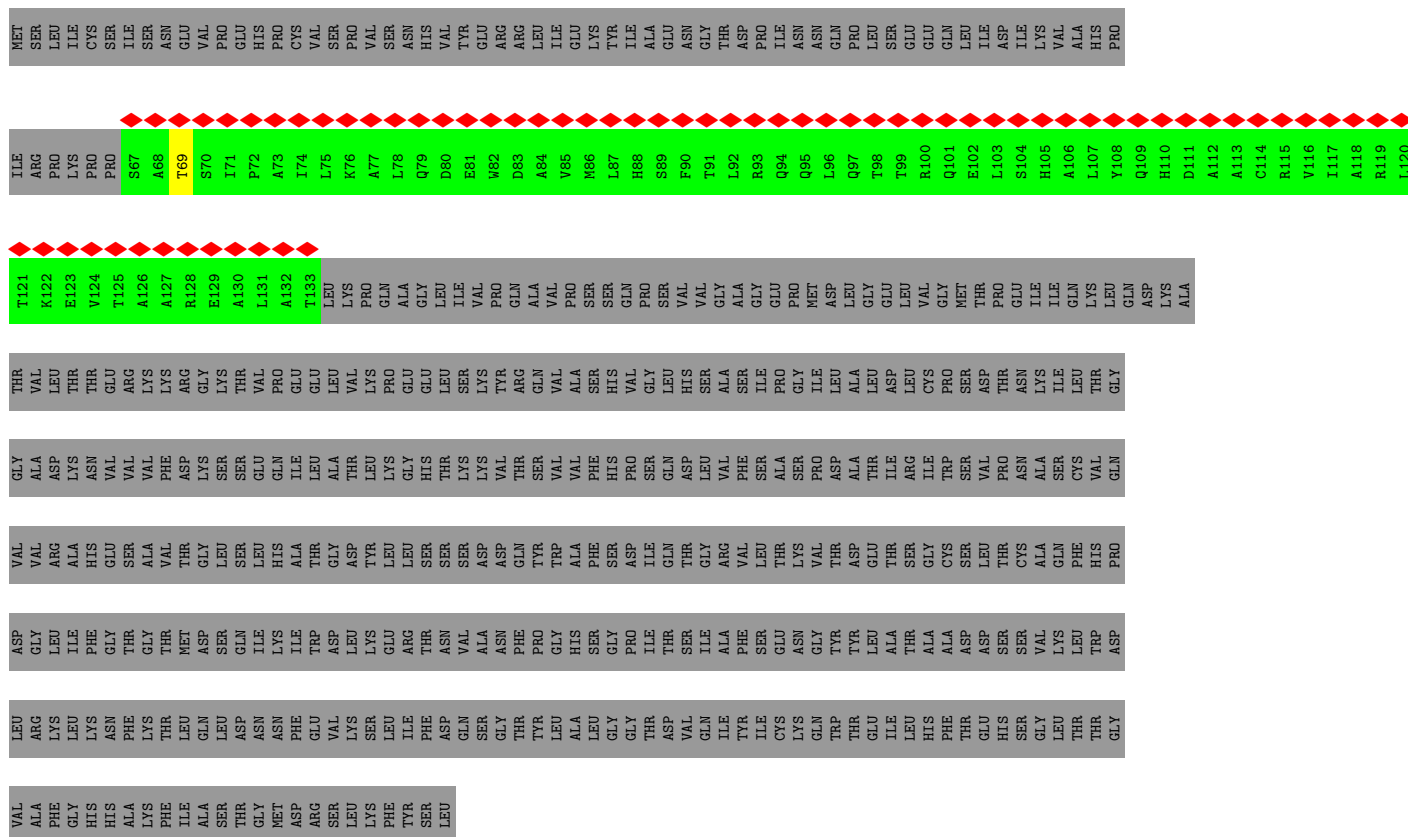


- Molecule 30: Pre-mRNA-processing factor 19



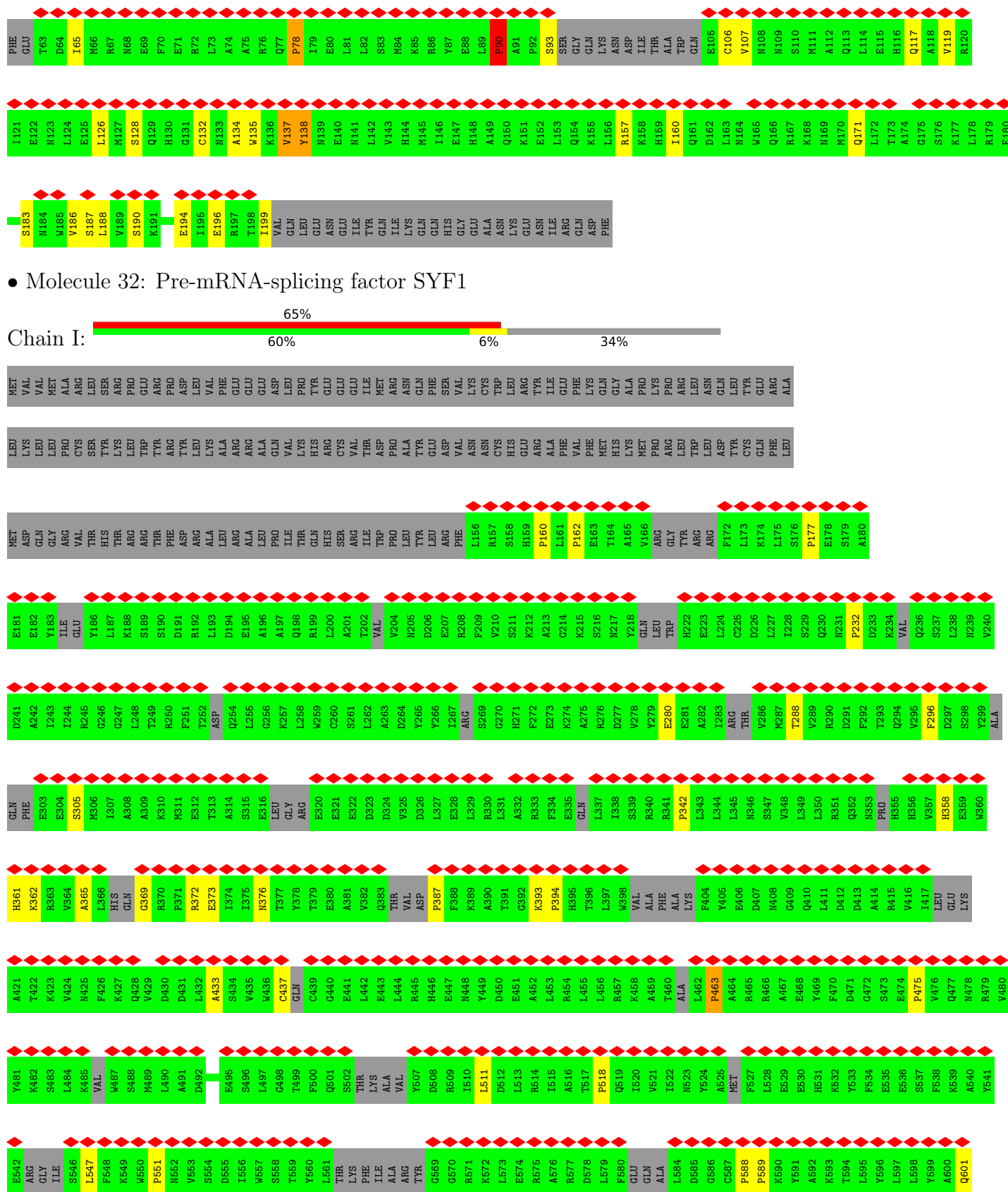


- Molecule 30: Pre-mRNA-processing factor 19

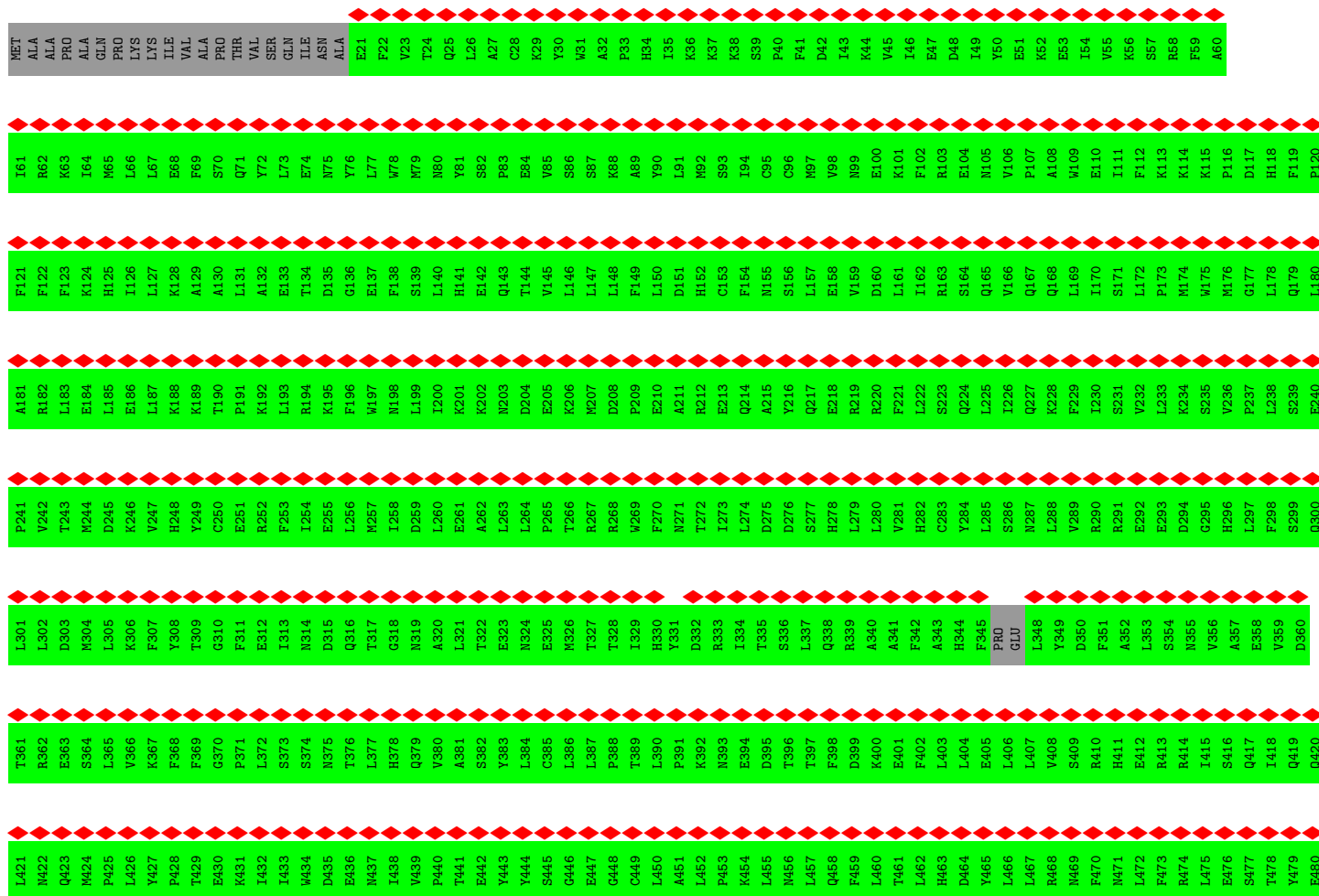
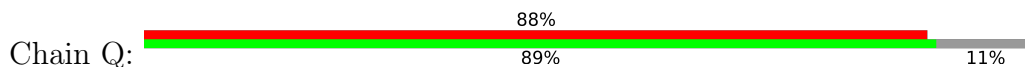


- Molecule 31: Pre-mRNA-splicing factor SPF27



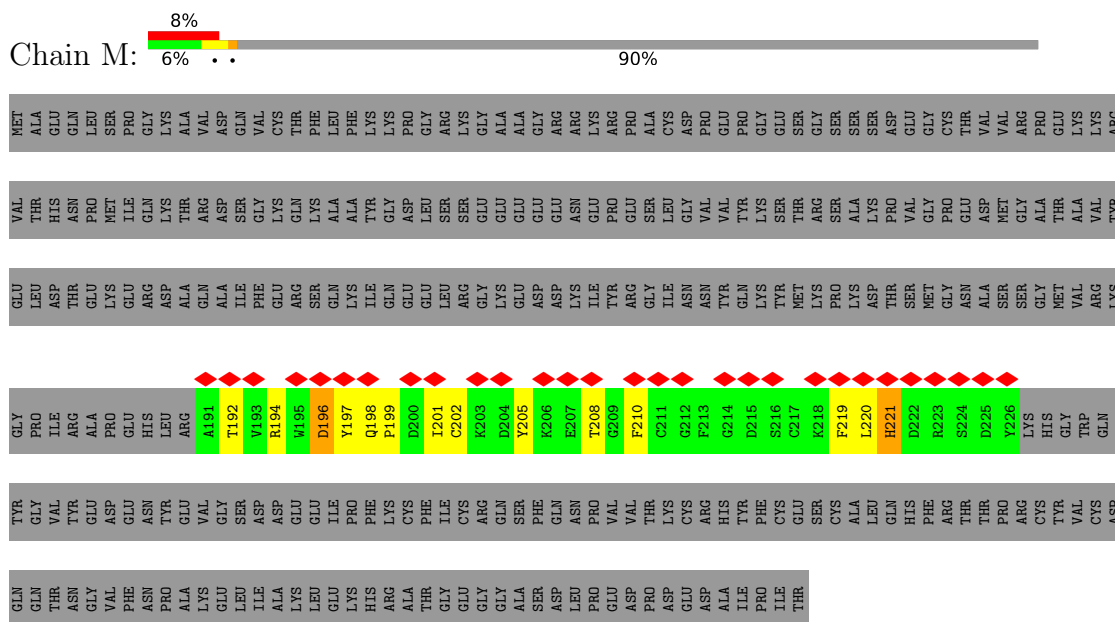


- Molecule 33: Intron-binding protein aquarius

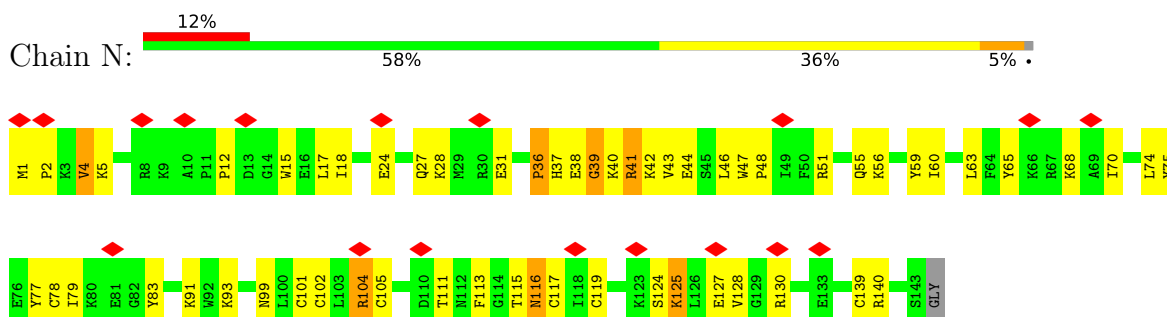


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E1203	L1143	G1083	R1023	A903	N843	V783	H723	E663	D603	L543	Q483
A1204	C1144	G1084	S1024	R904	F844	I784	L724	N664	K604	N544	D484
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V1207	Y1147	R1087	L1027	E907	Q847	R787	S727	K667	V607	D547	D487
V1208	N1148	L1088	L1028	L908	R848	G788	F728	A668	I608	H548	S488
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L1210	R1150	R1090	K1030	E910	L850	V790	G730	L670	ASP	K550	S490
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M1212	K1152	I1092	A1032	V912	V852	V792	N732	T672	GLU	E552	R492
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L1214	L1154	I1094	I1034	R914	H854	Q794	K734	R674	R615	E554	P494
C1215	G1155	G1095	I1035	L915	S855	P795	V735	N675	P616	G555	W495
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G1218	P1158	H1098	T1038	S918	A858	N798	E738	N678	R619	K558	
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Y1230	N1170	Q1110	V1050	E930	D870	I810	T750	I690	P631	T570	M510
N1231	A1171	K1111	K1051	T931	I871	R811	F751	I691	N632	K571	A511
G1232	G1172	Y1112	L1052	A932	D872	A812	P752	L692	Q633	P572	Q512
K1233	L1173	S1113	G1053	G933	E873	G813	V753	G693	Y634	Y573	P513
L1234	L1174	M1114	F1054	Y934	R874	M814	ARG	Y694	Q635	G574	I514
H1235	Y1175	M1115	K1055	F935	H875	Q815	GLY	D695	D636	T575	V515
L1236	D1176	E1116	Y1056	F936	L876	P816	GLY	P697	D637	K576	A516
I1237	F1177	Q1117	D1057	L937	L877	G817	LYS	S698	M638	F577	F517
R1238	Q1178	S1118	N1058	Y938	R878	L818	LYS	T639	T639	D578	T518
D1239	L1179	L1119	I1059	Q939	L879	T819	ARG	S699	T641	R579	V519
I1240	I1180	F1120	L1060	V940	G880	M820	LYS	A700	T641	V520	V520
I1241	M1181	T1121	M1061	M941	H881	V821	ALA	H701	I642	R581	E521
N1242	V1182	R1122	E1062	S942	GLY	V822	ASP	Y702	Q643	P582	V522
R1243	E1183	F1123	E1063	K1003	E884	G823	VAL	S703	N644	F583	A523
A1244	D1184	V1124	A1064	W944	E885	P824	GLU	K704	G645	I584	K524
C1245	F1185	R1125	A1065	E945	E886	P825	ASP	M705	A646	E585	P525
G1246	Q1186	V1126	Q1066	E946	L887	G826	GLU	P706	E647	Q586	N526
N1247	G1187	G1127	L1067	Y947	E887	T827	THR	N707	D648	I527	I527
N1248	V1188	V1128	L1068	I948	T888	G828	GLU	Q708	V649	G588	G528
P1249	H1189	P1129	E1069	S949	E889	K829		I709	Y650	L589	E529
L1250	E1190	T1130	F1070	K950	K890	T830	K775	A710	E651	V590	N530
I1251	S1191	R1012	E1071	V951	D891	D831	T776	T711	T652	Y591	W531
G1252	E1192	D1132	T1072	K952	F892	V832	L777	L712	F653	V592	P532
R1253	P1193	L1133	F1073	N953	A1013	A833	I778	D713	N654	R593	T533
P1254	N1194	D1134	I1074	LYS	R894	V834	V779	F714	I655	G594	R534
N1255	P1195	E1015	I1075	Y895	Y895	Q835		N715	I656	C595	V535
K1256	Y1196	A1135	P1075	G996	G996	I836		D716	M657	E596	R536
L1257	F1197	Q1136	L1076	SEN	R897	T837		T717	E647	I597	A537
T1258	Y1198	G1137	L1077	THR	V898	I837		F718	R658	Q598	D538
Q1259	W1199	R1138	L1078	LEU	N899	S838		L719	R659	G599	V539
L1260	W1200	P1140	Q1079	D960	Y900	T840		S720	K660	W600	T540

- Molecule 34: RING finger protein 113A

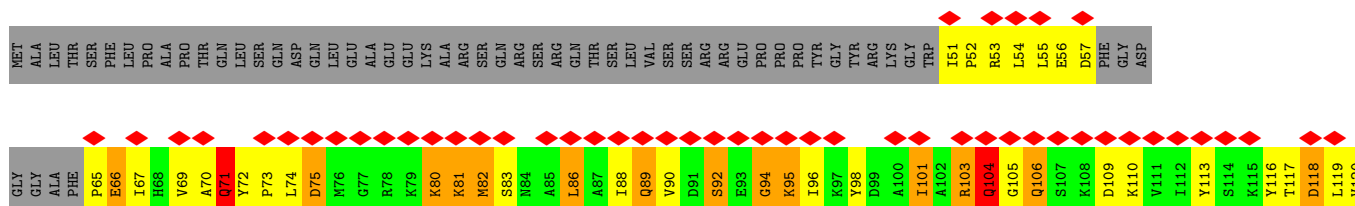


- Molecule 35: Protein BUD31 homolog



- Molecule 36: Pre-mRNA-splicing factor RBM22

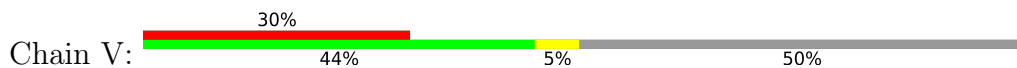


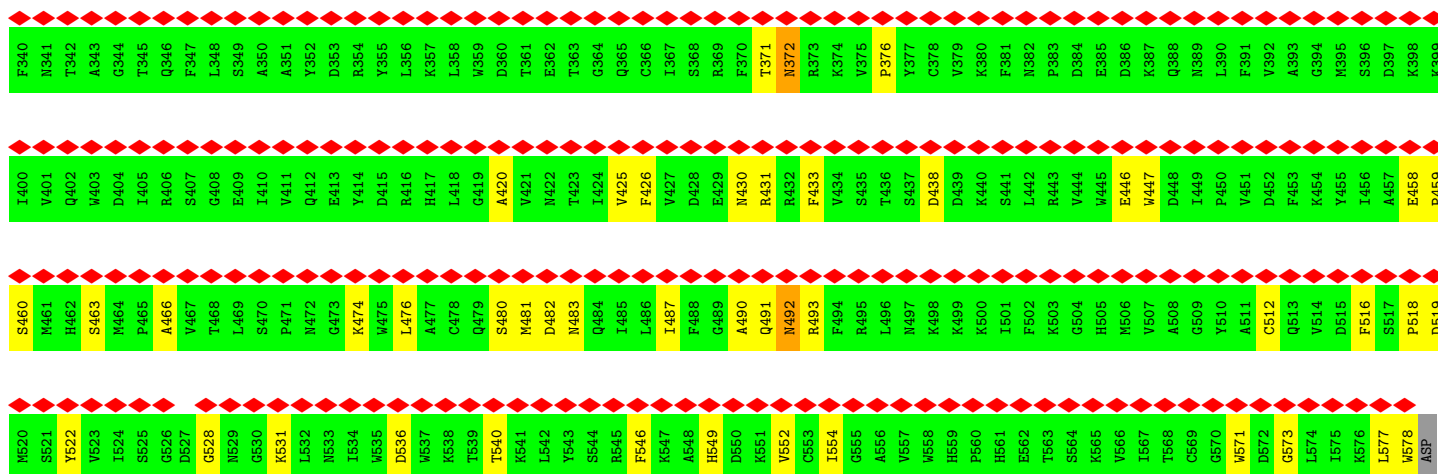




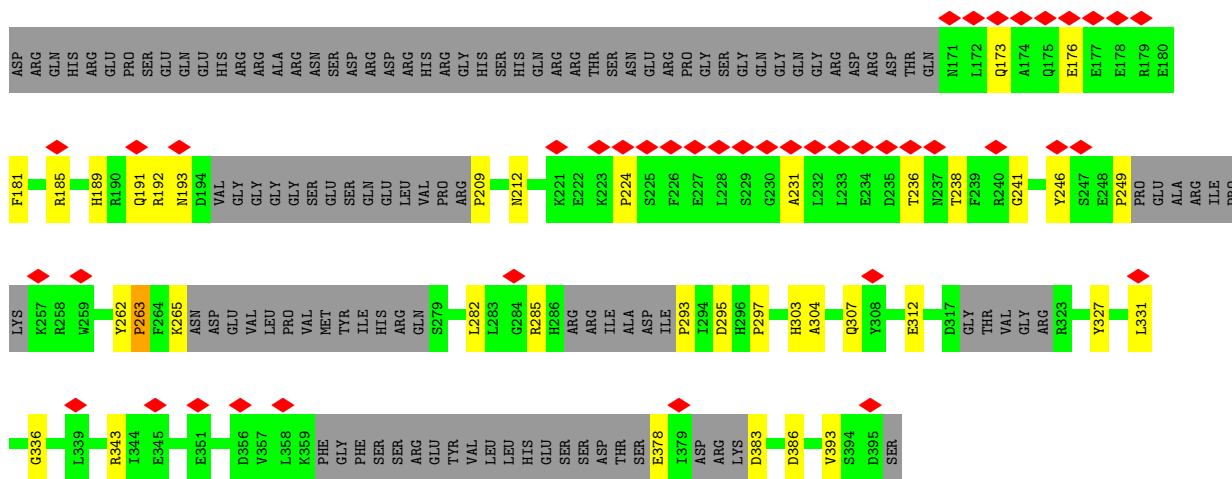
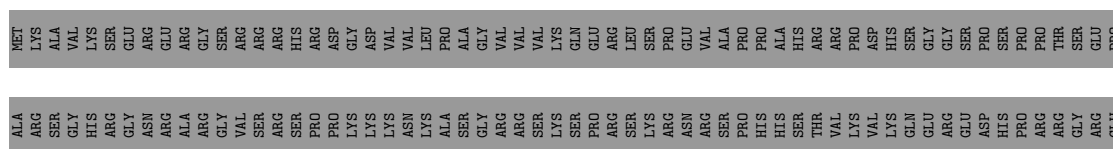
[illegible]

- Molecule 42: Pre-mRNA-splicing factor CWC22 homolog

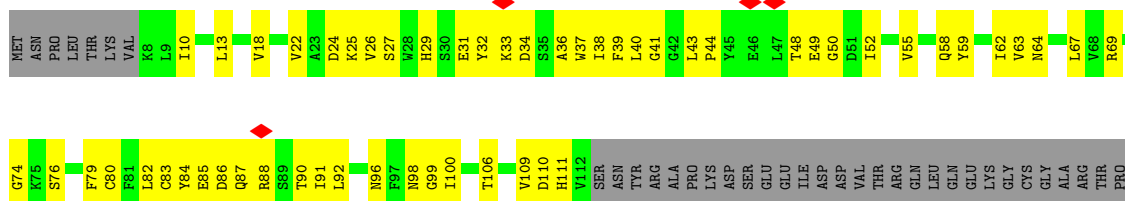
[illegible]

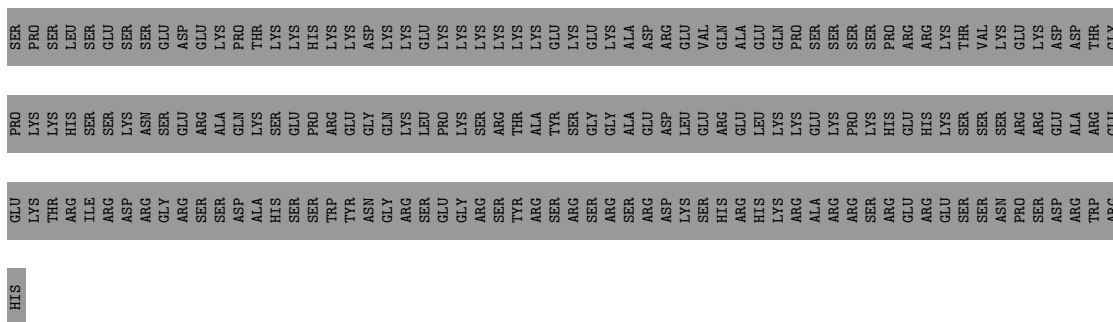


• Molecule 44: Smad nuclear-interacting protein 1

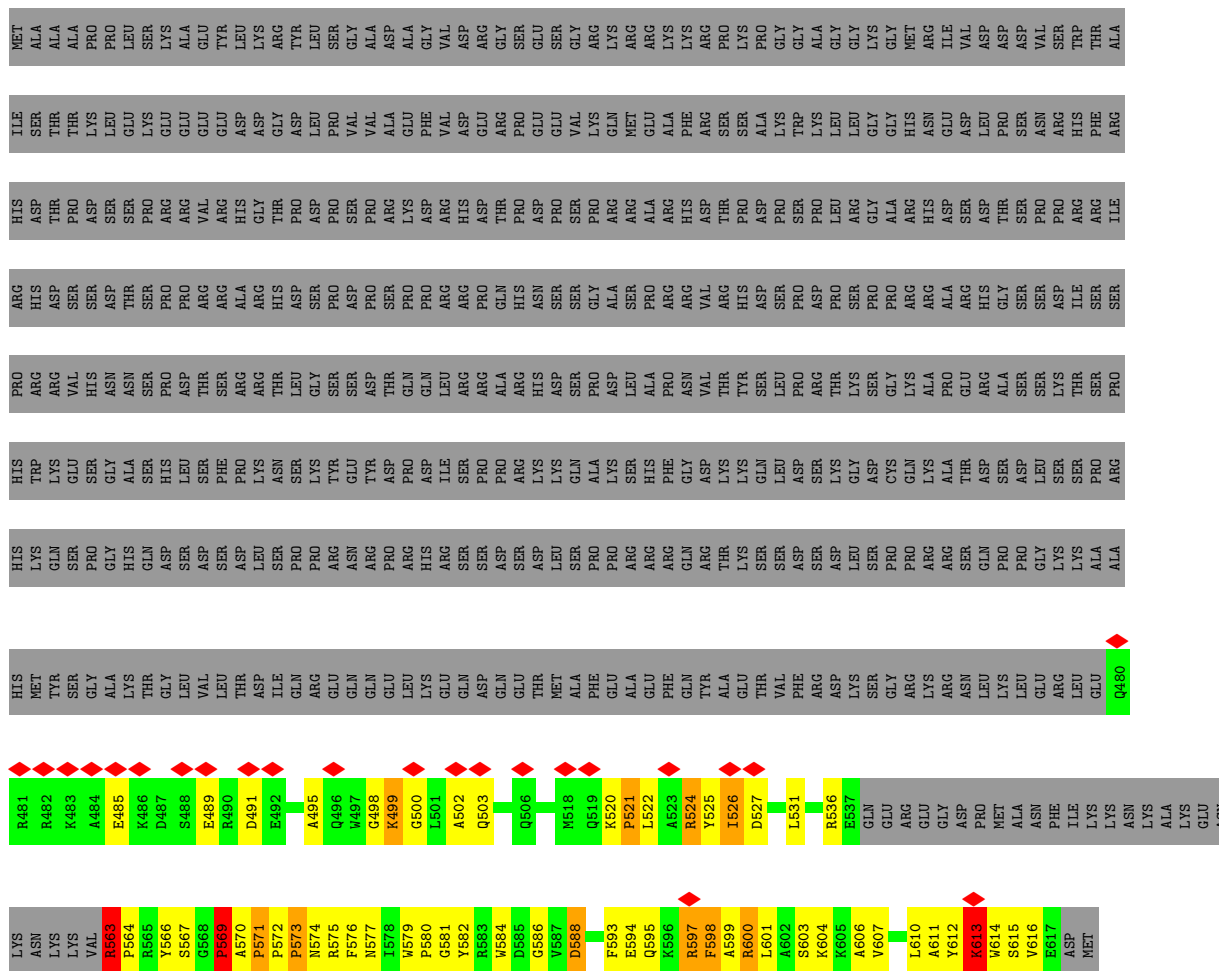


• Molecule 45: RNA-binding motif protein, X-linked 2

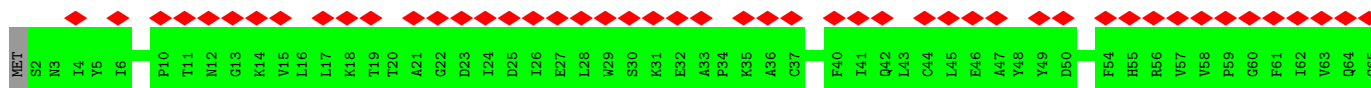


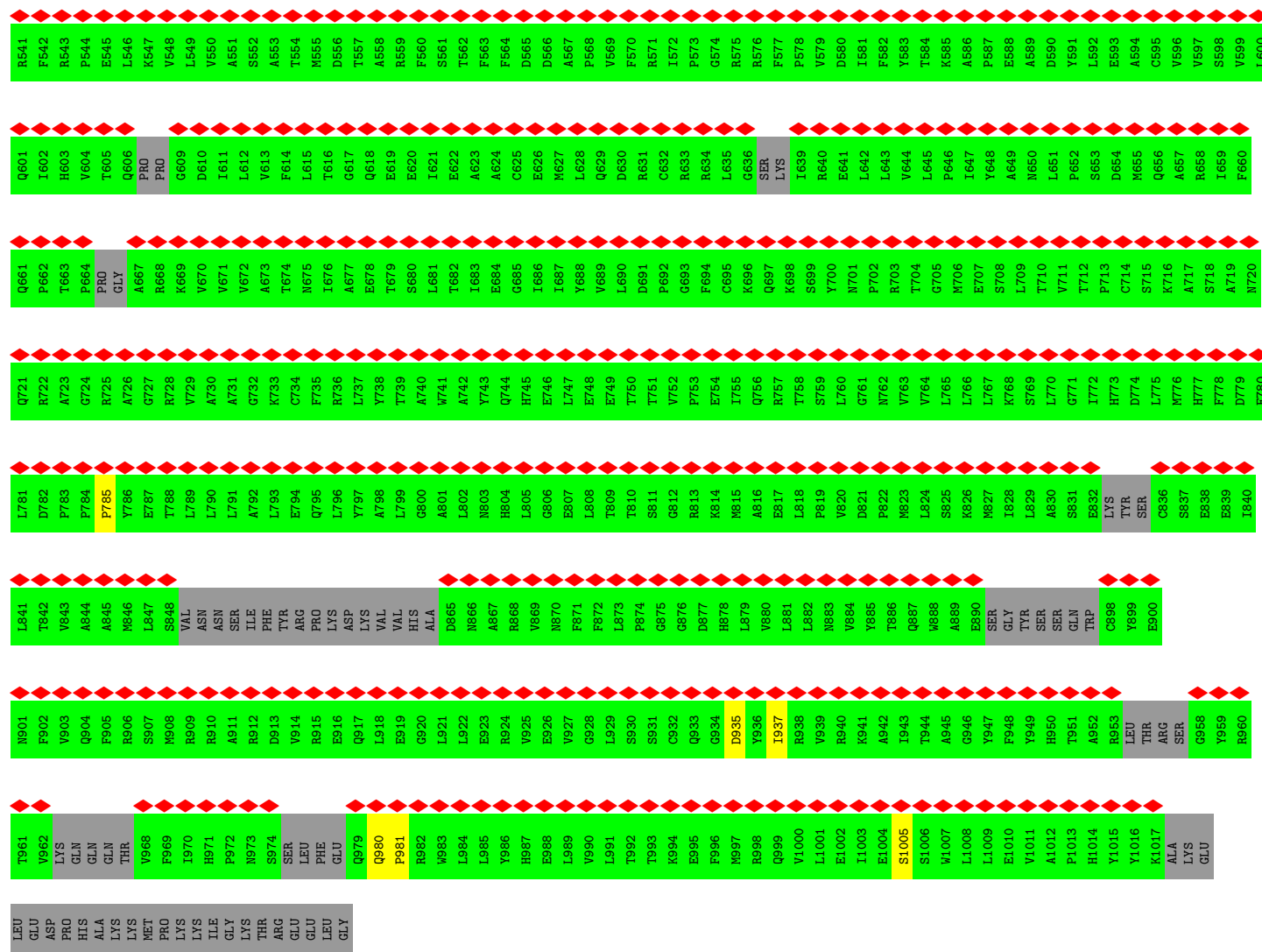


- Molecule 46: BUD13 homolog



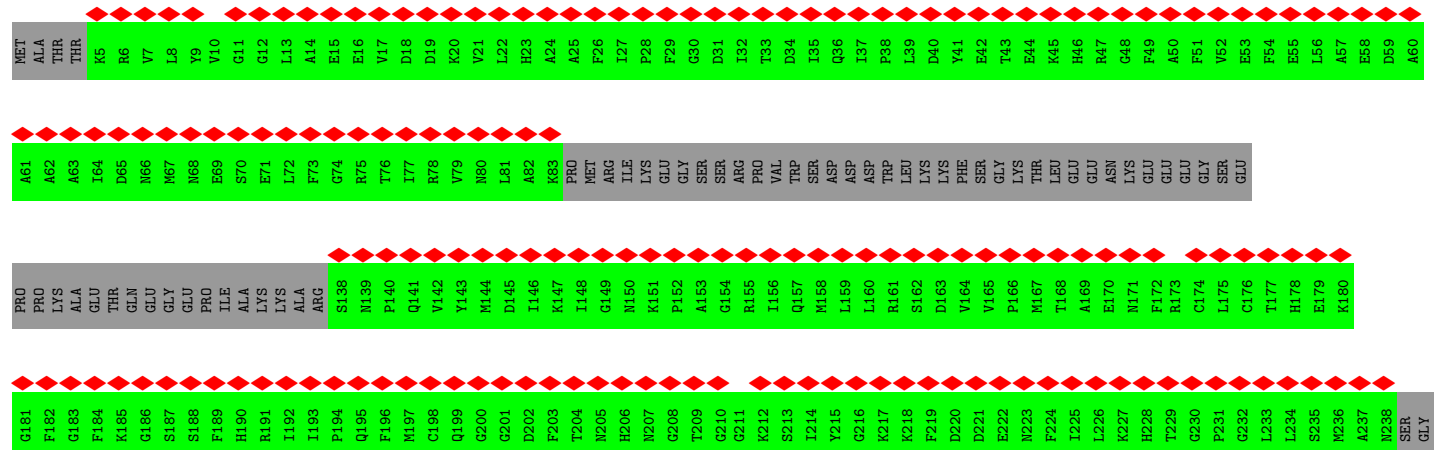
- Molecule 47: Peptidyl-prolyl cis-trans isomerase CWC27 homolog





• Molecule 49: Peptidyl-prolyl cis-trans isomerase E

Chain y:



VAL.	PRO	ASU
	N243	
	N244	
	G245	
	S246	
	Q247	
	F248	
	F249	
	L250	
	T251	
	C252	
	D253	
	K254	
	T255	
	D256	
	V257	
	L258	
	D259	
	G260	
	K261	
	H262	
	V263	
	V264	
	P265	
	G266	
	E267	
	V268	
	T269	
	E270	
	G271	
	L272	
	D273	
	V274	
	L275	
	R276	
	Q277	
	L278	
	E279	
	A280	
	Q281	
	G282	
	SER	
	LYS	
	ASP	
	GLY	
	LYS	
	P288	
	K289	
	Q290	
	K291	
	V292	
	I293	
	I294	
	A295	
	D296	
	C297	
	G298	
	E299	
	ARG	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27405	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 ($e^-/\text{\AA}^2$)	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	0.168	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0374	Depositor
Map size (\AA)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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, GTP, ZN, IHP

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	0.68	9/18964 (0.0%)	0.77	25/25741 (0.1%)
2	B	0.75	2/1970 (0.1%)	0.91	7/3060 (0.2%)
3	C	0.79	1/6864 (0.0%)	0.96	10/9334 (0.1%)
4	D	0.33	0/8527	0.59	0/11887
5	E	0.64	0/2392	0.79	0/3242
6	a	0.47	0/397	0.61	0/549
6	h	0.46	0/391	0.61	0/540
7	b	0.49	0/404	0.72	0/561
7	i	0.50	0/421	0.73	0/583
8	c	0.57	0/405	0.73	0/563
8	j	0.57	0/405	0.73	0/563
9	d	0.68	0/479	0.84	0/666
9	k	0.70	0/420	0.85	0/583
10	f	0.75	0/360	0.81	0/497
10	m	0.75	0/360	0.81	0/497
11	e	0.65	0/390	0.80	0/542
11	l	0.64	0/390	0.80	0/542
12	g	0.54	0/362	0.71	0/501
12	n	0.54	0/332	0.72	0/458
13	F	0.39	0/2224	0.86	0/3462
14	G	0.35	0/1717	0.95	1/2664 (0.0%)
15	H	0.59	7/3217 (0.2%)	1.06	18/4997 (0.4%)
16	o	0.61	0/803	1.41	2/1119 (0.2%)
17	p	1.01	1/810 (0.1%)	1.46	4/1122 (0.4%)
18	w	0.53	5/2376 (0.2%)	0.67	13/3269 (0.4%)
19	u	0.23	0/524	0.62	4/724 (0.6%)
20	v	0.73	4/945 (0.4%)	0.83	10/1280 (0.8%)
21	1	0.33	0/7826	0.51	0/10617
22	2	0.52	3/1277 (0.2%)	0.73	7/1724 (0.4%)
23	3	0.32	0/9408	0.53	0/12767
24	4	0.83	2/535 (0.4%)	0.98	4/724 (0.6%)
25	5	0.29	0/823	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	6	0.29	0/653	0.48	0/877
27	7	0.31	0/556	0.45	0/751
28	J	0.62	0/3500	0.73	0/4750
29	L	0.52	3/2283 (0.1%)	0.58	8/3088 (0.3%)
30	q	0.35	0/658	0.58	3/919 (0.3%)
30	r	0.32	0/653	0.59	3/912 (0.3%)
30	s	0.26	0/334	0.37	0/466
30	t	0.30	0/334	0.38	0/466
31	K	1.28	14/981 (1.4%)	0.69	5/1317 (0.4%)
32	I	0.39	0/2745	0.56	17/3765 (0.5%)
33	Q	0.21	0/6518	0.42	0/9075
34	M	0.29	0/272	0.48	0/363
35	N	0.88	1/1210 (0.1%)	1.00	3/1622 (0.2%)
36	O	0.80	3/2321 (0.1%)	0.94	6/3135 (0.2%)
37	P	0.83	1/841 (0.1%)	1.01	2/1117 (0.2%)
38	R	0.66	4/2353 (0.2%)	0.87	8/3167 (0.3%)
39	S	0.59	0/1268	0.80	1/1714 (0.1%)
40	T	1.05	1/2522 (0.0%)	1.11	4/3438 (0.1%)
41	U	1.03	0/196	1.09	1/265 (0.4%)
42	V	0.54	0/2239	0.67	1/3118 (0.0%)
43	W	0.55	0/2371	0.77	4/3296 (0.1%)
44	X	0.27	0/1020	0.48	0/1360
45	Y	0.31	0/753	0.48	0/1014
46	Z	0.57	2/772 (0.3%)	0.79	7/1056 (0.7%)
47	z	0.29	0/1414	0.51	0/1916
48	x	0.35	0/2876	0.53	3/3988 (0.1%)
49	y	0.35	0/1129	0.61	0/1558
All	All	0.57	63/119490 (0.1%)	0.74	181/165014 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	3	0	4
27	7	0	1
34	M	0	1
35	N	0	1
38	R	0	1
40	T	0	2
44	X	0	1
All	All	0	33

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	106	CYS	CB-SG	-23.13	1.43	1.82
31	K	132	CYS	CB-SG	-17.48	1.52	1.82
29	L	761	SER	CB-OG	8.91	1.53	1.42
31	K	128	SER	CB-OG	8.42	1.53	1.42
31	K	183	SER	CB-OG	8.28	1.53	1.42

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	83	PRO	CA-CB-CG	10.19	124.17	104.80
22	2	636	MET	CG-SD-CE	9.28	115.05	100.20
38	R	226	PRO	CA-N-CD	-8.88	99.07	111.50
31	K	90	PRO	CA-CB-CG	8.66	121.26	104.80
46	Z	569	PRO	CA-N-CD	-8.56	99.52	111.50

There are no chirality outliers.

5 of 33 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	18450	0	18276	1482	0
2	B	1768	0	897	120	0
3	C	6716	0	6691	892	0
4	D	8528	0	3745	69	0
5	E	2338	0	2272	153	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	0	0
8	c	406	0	170	0	0
8	j	406	0	170	0	0
9	d	480	0	200	0	0
9	k	422	0	175	0	0
10	f	361	0	158	0	0
10	m	361	0	158	0	0
11	e	391	0	163	0	0
11	l	391	0	163	0	0
12	g	363	0	160	0	0
12	n	334	0	143	0	0
13	F	1988	0	1005	186	0
14	G	1545	0	786	190	0
15	H	2886	0	1463	239	0
16	o	804	0	350	0	0
17	p	813	0	365	0	0
18	w	2369	0	1298	0	0
19	u	530	0	218	0	0
20	v	946	0	594	0	0
21	1	7702	0	7389	291	0
22	2	1252	0	1040	57	0
23	3	9220	0	9139	481	0
24	4	527	0	438	40	0
25	5	807	0	729	26	0
26	6	645	0	628	21	0
27	7	540	0	509	25	0
28	J	3463	0	2544	102	0
29	L	2260	0	1776	92	0
30	q	659	0	296	0	0
30	r	654	0	294	0	0
30	s	335	0	168	0	0
30	t	335	0	168	0	0
31	K	979	0	739	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	I	2778	0	1238	21	0
33	Q	6528	0	2814	6	0
34	M	267	0	225	29	0
35	N	1184	0	1190	75	0
36	O	2273	0	2244	225	0
37	P	829	0	814	192	0
38	R	2316	0	2189	420	0
39	S	1236	0	1210	135	0
40	T	2457	0	2416	251	0
41	U	193	0	196	40	0
42	V	2243	0	971	48	0
43	W	2374	0	1051	108	0
44	X	1021	0	738	19	0
45	Y	743	0	613	67	0
46	Z	755	0	591	154	0
47	z	1381	0	1298	0	0
48	x	2887	0	1310	0	0
49	y	1133	0	519	0	0
50	A	36	0	6	10	0
51	C	32	0	12	11	0
52	C	1	0	0	0	0
52	F	5	0	0	0	0
53	6	3	0	0	0	0
53	M	1	0	0	0	0
53	N	3	0	0	0	0
53	O	3	0	0	3	0
53	W	2	0	0	0	0
53	v	1	0	0	0	0
All	All	117278	0	87812	4995	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 26.

The worst 5 of 4995 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)
45:Y:37:TRP:CH2	46:Z:498:GLY:HA2	1.23	1.65
1:A:2270:PHE:HB3	4:D:1264:PRO:CB	1.34	1.57
1:A:2270:PHE:CG	4:D:1264:PRO:CB	1.89	1.56
3:C:149:LEU:HD13	3:C:427:PHE:CD2	1.38	1.54
3:C:77:VAL:HG11	40:T:196:LEU:CG	1.39	1.52

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	2224/2335 (95%)	2081 (94%)	115 (5%)	28 (1%)	10	42
3	C	854/972 (88%)	777 (91%)	57 (7%)	20 (2%)	5	28
4	D	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	44	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%)	10	42
17	p	159/225 (71%)	138 (87%)	9 (6%)	12 (8%)	1	10
18	w	419/501 (84%)	378 (90%)	38 (9%)	3 (1%)	19	56
19	u	94/793 (12%)	87 (93%)	5 (5%)	2 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	v	155/464 (33%)	125 (81%)	22 (14%)	8 (5%)	1	15
21	1	1022/1304 (78%)	897 (88%)	119 (12%)	6 (1%)	22	59
22	2	171/895 (19%)	154 (90%)	17 (10%)	0	100	100
23	3	1165/1217 (96%)	1086 (93%)	78 (7%)	1 (0%)	48	83
24	4	76/424 (18%)	69 (91%)	6 (8%)	1 (1%)	10	42
25	5	106/125 (85%)	90 (85%)	16 (15%)	0	100	100
26	6	83/110 (76%)	76 (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%)	22	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%)	8	37
30	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	39
30	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	39
31	K	144/225 (64%)	134 (93%)	6 (4%)	4 (3%)	4	24
32	I	498/855 (58%)	479 (96%)	11 (2%)	8 (2%)	8	37
33	Q	1297/1485 (87%)	1271 (98%)	26 (2%)	0	100	100
34	M	34/343 (10%)	30 (88%)	3 (9%)	1 (3%)	3	23
35	N	141/144 (98%)	126 (89%)	12 (8%)	3 (2%)	5	29
36	O	283/420 (67%)	247 (87%)	26 (9%)	10 (4%)	3	20
37	P	92/229 (40%)	82 (89%)	8 (9%)	2 (2%)	5	29
38	R	295/540 (55%)	249 (84%)	31 (10%)	15 (5%)	1	15
39	S	157/166 (95%)	144 (92%)	10 (6%)	3 (2%)	6	32
40	T	311/514 (60%)	282 (91%)	17 (6%)	12 (4%)	2	18
41	U	24/2752 (1%)	20 (83%)	3 (12%)	1 (4%)	2	17
42	V	444/908 (49%)	412 (93%)	27 (6%)	5 (1%)	12	46
43	W	475/579 (82%)	419 (88%)	32 (7%)	24 (5%)	1	15
44	X	143/396 (36%)	133 (93%)	10 (7%)	0	100	100
45	Y	103/322 (32%)	92 (89%)	11 (11%)	0	100	100
46	Z	109/619 (18%)	93 (85%)	10 (9%)	6 (6%)	1	15
47	z	176/472 (37%)	170 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	x	562/1041 (54%)	537 (96%)	20 (4%)	5 (1%)	14	50
49	y	224/301 (74%)	217 (97%)	7 (3%)	0	100	100
All	All	16564/29872 (55%)	15374 (93%)	979 (6%)	211 (1%)	13	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 ⓘ

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	2001/2108 (95%)	1902 (95%)	99 (5%)	21	42
3	C	745/866 (86%)	677 (91%)	68 (9%)	7	24
5	E	256/300 (85%)	244 (95%)	12 (5%)	22	44
18	w	49/446 (11%)	47 (96%)	2 (4%)	26	47
20	v	30/382 (8%)	28 (93%)	2 (7%)	13	34
21	1	735/1104 (67%)	735 (100%)	0	100	100
22	2	94/776 (12%)	90 (96%)	4 (4%)	25	46
23	3	1018/1051 (97%)	1017 (100%)	1 (0%)	92	95
24	4	39/336 (12%)	37 (95%)	2 (5%)	20	41
25	5	74/109 (68%)	74 (100%)	0	100	100
26	6	73/95 (77%)	73 (100%)	0	100	100
27	7	57/77 (74%)	57 (100%)	0	100	100
28	J	205/751 (27%)	194 (95%)	11 (5%)	18	40
29	L	131/709 (18%)	122 (93%)	9 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	K	54/196 (28%)	49 (91%)	5 (9%)	7	23
34	M	25/294 (8%)	24 (96%)	1 (4%)	27	48
35	N	130/130 (100%)	125 (96%)	5 (4%)	28	49
36	O	250/361 (69%)	239 (96%)	11 (4%)	24	46
37	P	90/203 (44%)	77 (86%)	13 (14%)	2	13
38	R	220/463 (48%)	170 (77%)	50 (23%)	0	5
39	S	129/134 (96%)	119 (92%)	10 (8%)	10	29
40	T	268/441 (61%)	251 (94%)	17 (6%)	15	36
41	U	21/2432 (1%)	16 (76%)	5 (24%)	0	4
44	X	52/349 (15%)	46 (88%)	6 (12%)	4	17
45	Y	57/291 (20%)	56 (98%)	1 (2%)	54	71
46	Z	47/545 (9%)	39 (83%)	8 (17%)	1	9
47	z	146/416 (35%)	146 (100%)	0	100	100
48	x	1/897 (0%)	1 (100%)	0	100	100
All	All	6997/16262 (43%)	6655 (95%)	342 (5%)	23	42

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	O	229	LYS
38	R	409	VAL
37	P	76	ARG
38	R	118	ASP
39	S	108	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
21	1	1277	GLN
47	z	127	HIS
28	J	221	ASN
47	z	112	GLN
40	T	217	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	91/107 (85%)	37 (40%)	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%)	137 (36%)	35 (9%)

5 of 137 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 21 ligands modelled in this entry, 19 are monoatomic - leaving 2 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	$\# Z > 2$
51	GTP	C	1500	52	26,34,34	1.18	1 (3%)	32,54,54	1.81	8 (25%)
50	IHP	A	3000	-	36,36,36	1.01	2 (5%)	54,60,60	1.62	12 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	GTP	C	1500	52	-	7/18/38/38	0/3/3/3
50	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	C	1500	GTP	C6-N1	-3.52	1.32	1.37
50	A	3000	IHP	P5-O45	-2.86	1.43	1.54
50	A	3000	IHP	P2-O12	2.65	1.64	1.59

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	A	3000	IHP	O45-P5-O35	4.10	123.30	107.64
50	A	3000	IHP	O35-P5-O15	-3.97	88.19	105.99
51	C	1500	GTP	C5-C6-N1	3.79	120.64	113.95
51	C	1500	GTP	PA-O3A-PB	-3.79	119.84	132.83
51	C	1500	GTP	O6-C6-C5	-3.73	117.08	124.37

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

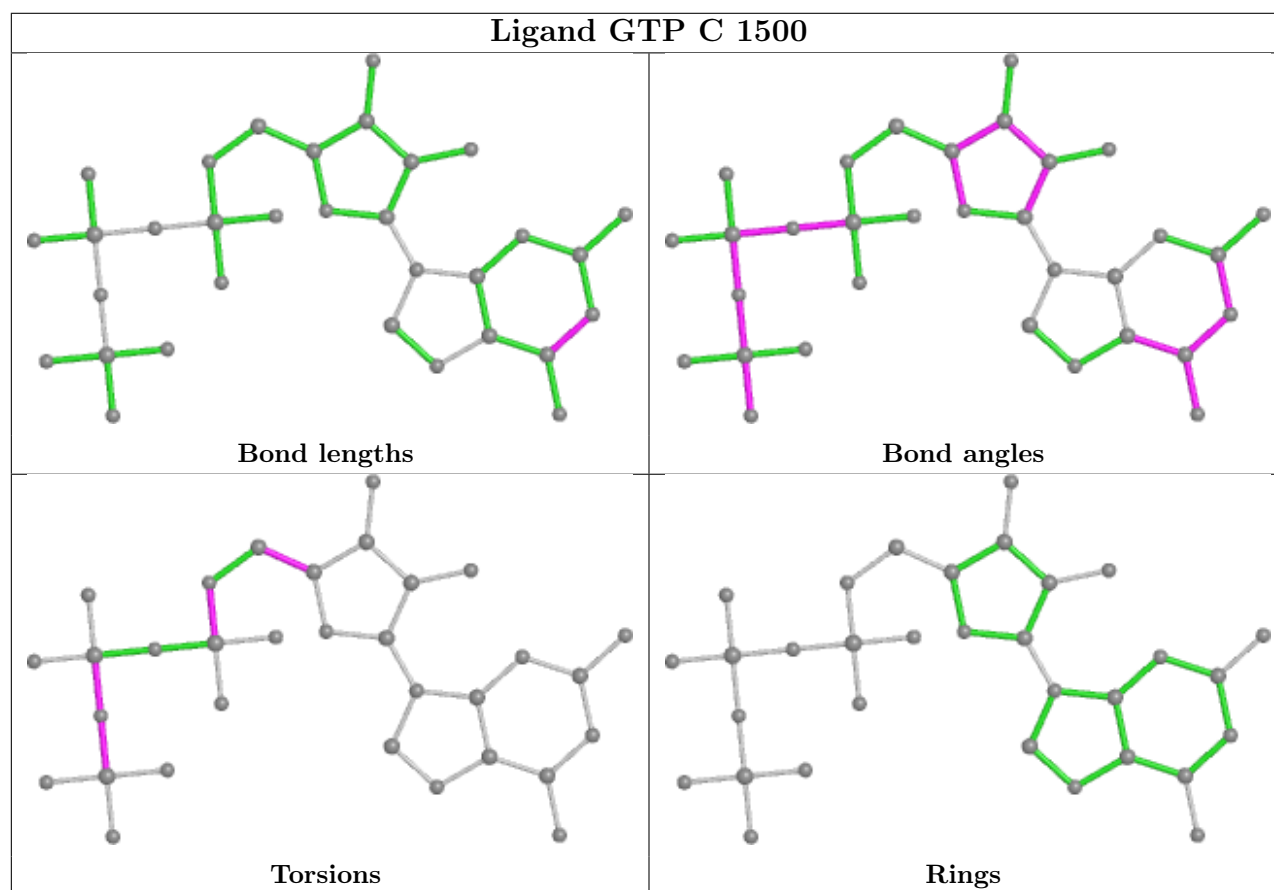
Mol	Chain	Res	Type	Atoms
50	A	3000	IHP	C4-C5-O15-P5
50	A	3000	IHP	C6-C5-O15-P5
51	C	1500	GTP	PB-O3B-PG-O3G
51	C	1500	GTP	C5'-O5'-PA-O3A
51	C	1500	GTP	C5'-O5'-PA-O1A

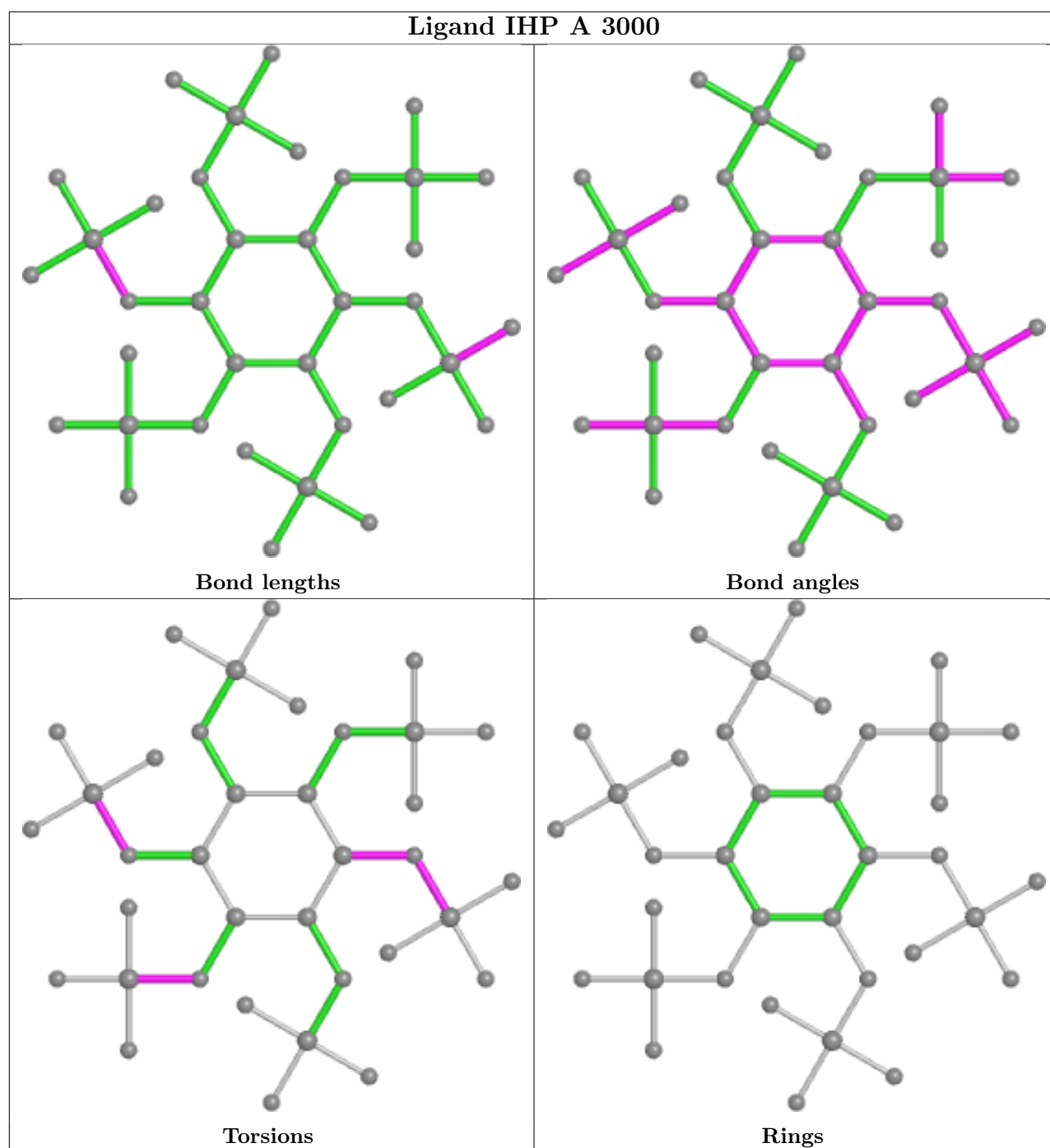
There are no ring outliers.

2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	C	1500	GTP	11	0
50	A	3000	IHP	10	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 than 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.





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.

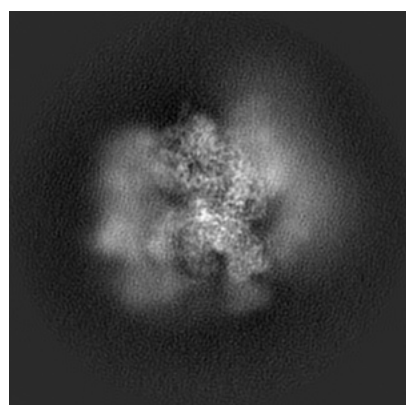
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6889. These allow visual inspection of the internal detail of the map and identification of artifacts.

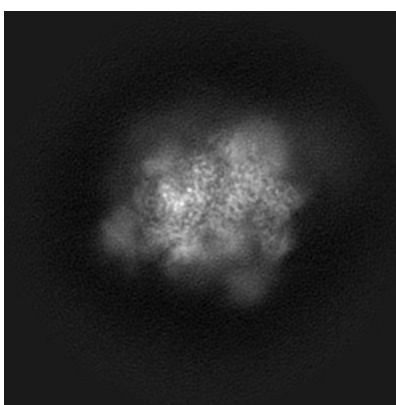
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

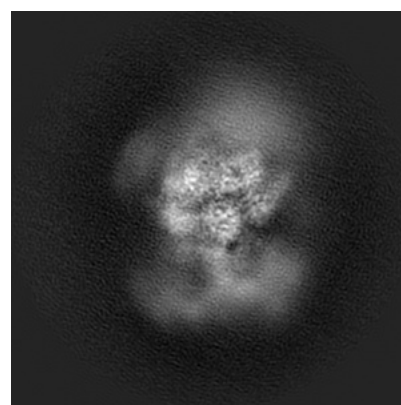
6.1.1 Primary map



X



Y

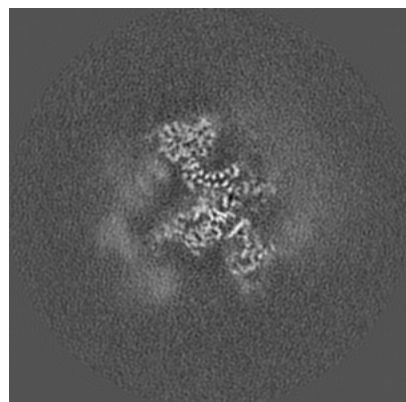


Z

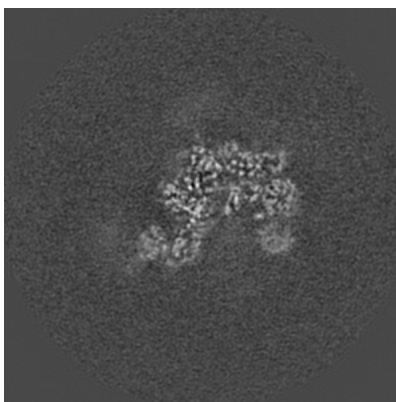
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

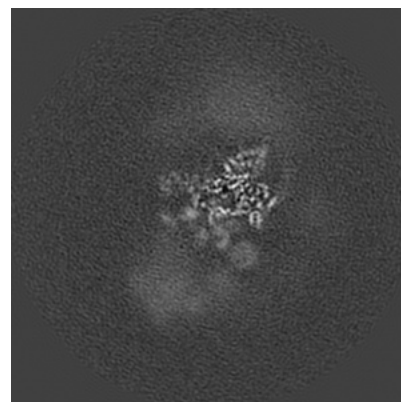
6.2.1 Primary map



X Index: 200



Y Index: 200

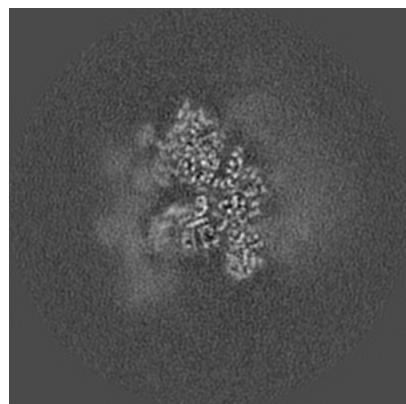


Z Index: 200

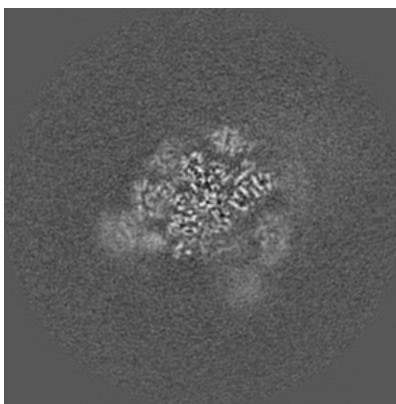
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

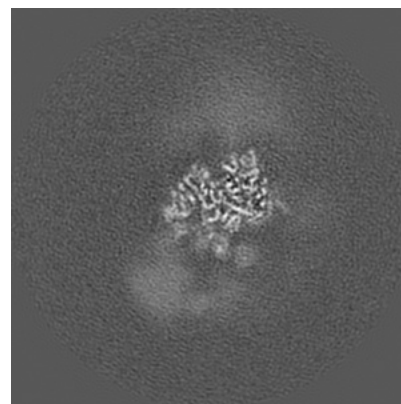
6.3.1 Primary map



X Index: 212



Y Index: 225

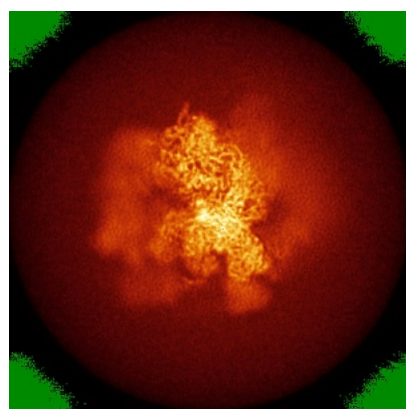


Z Index: 192

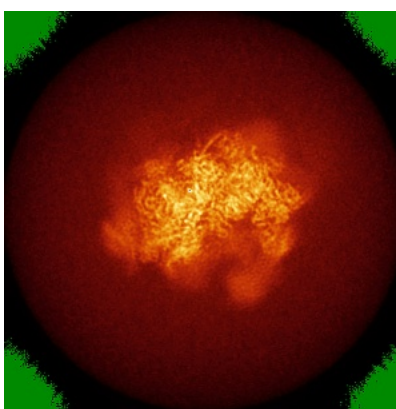
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

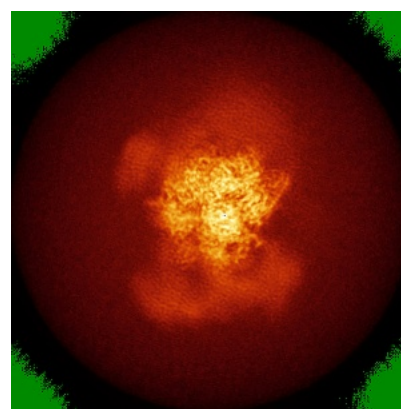
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0374. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

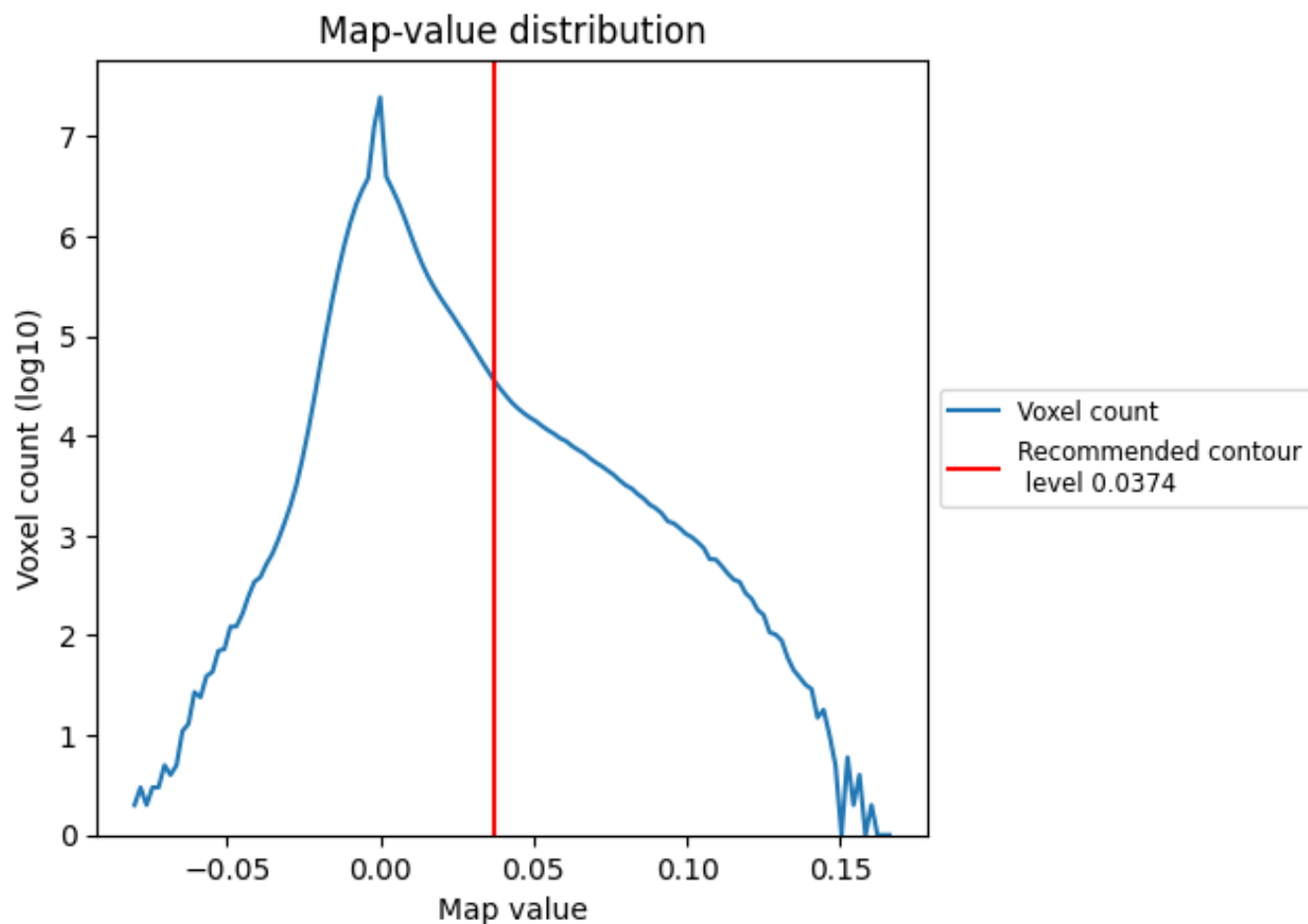
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

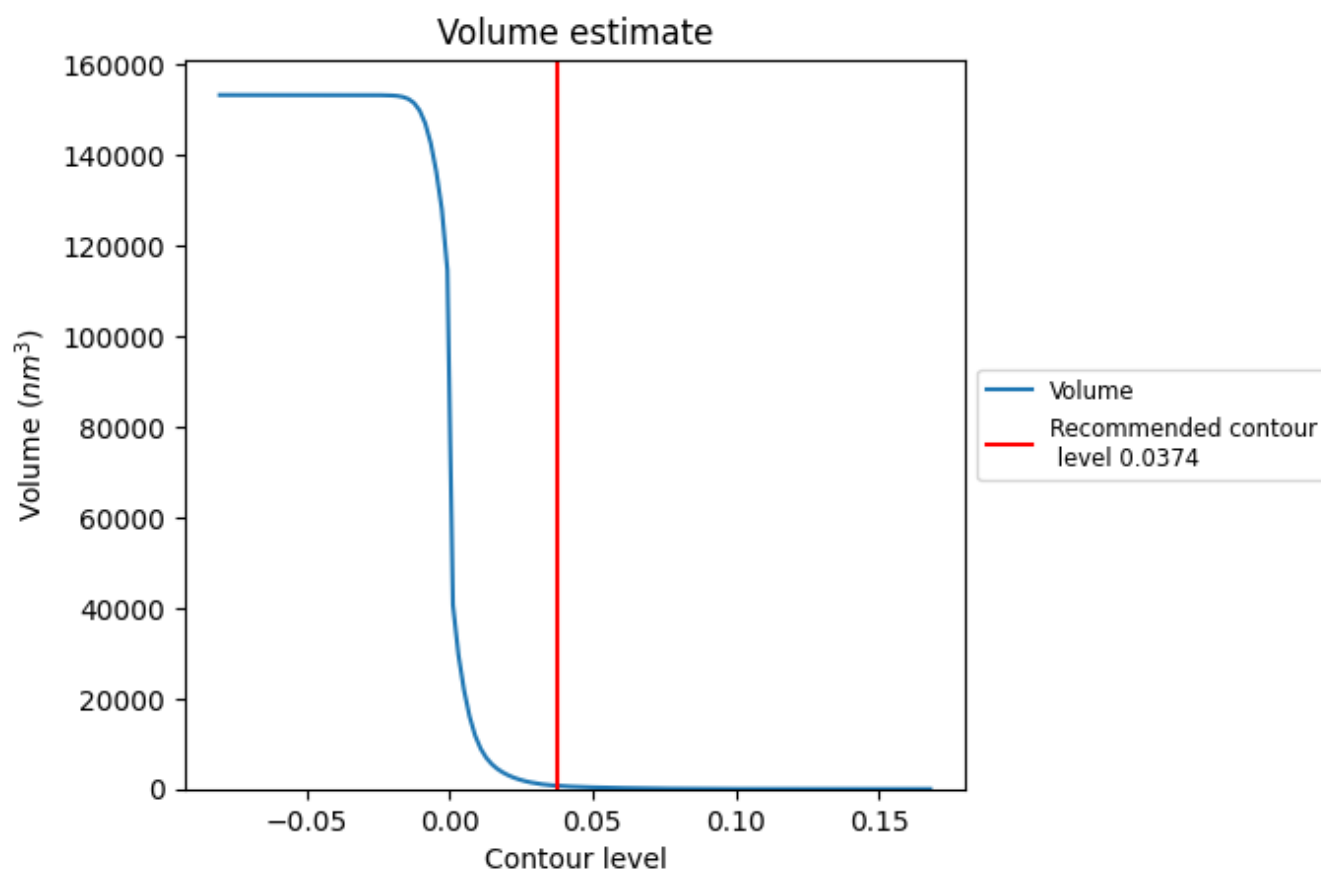
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

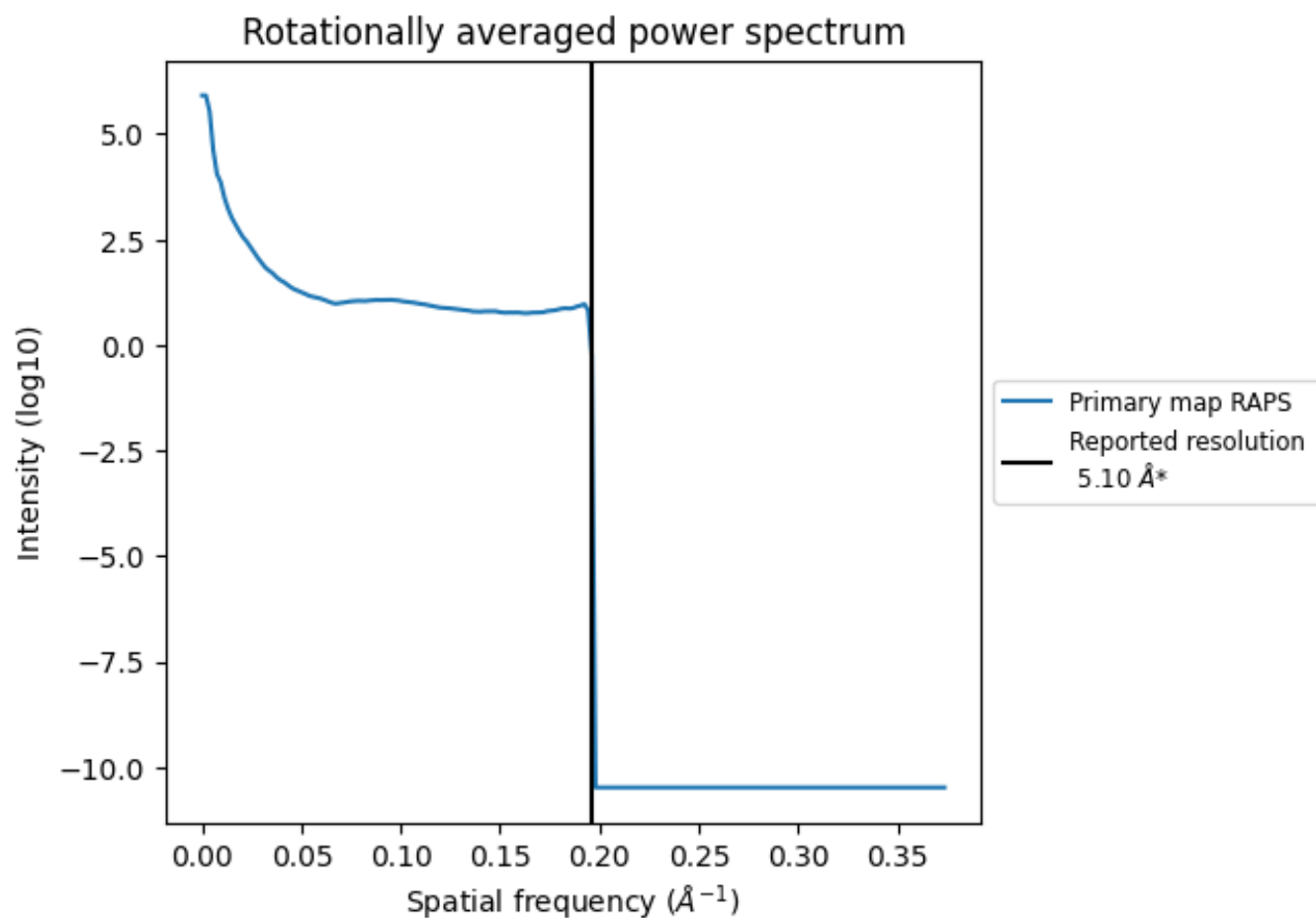
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 725 nm³; this corresponds to an approximate mass of 654 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.196 \AA^{-1}

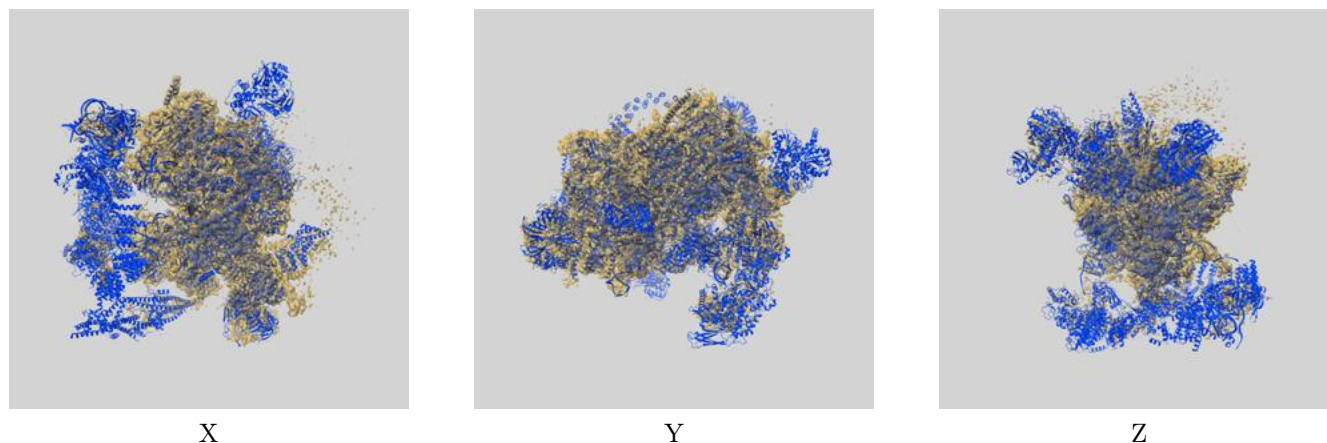
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

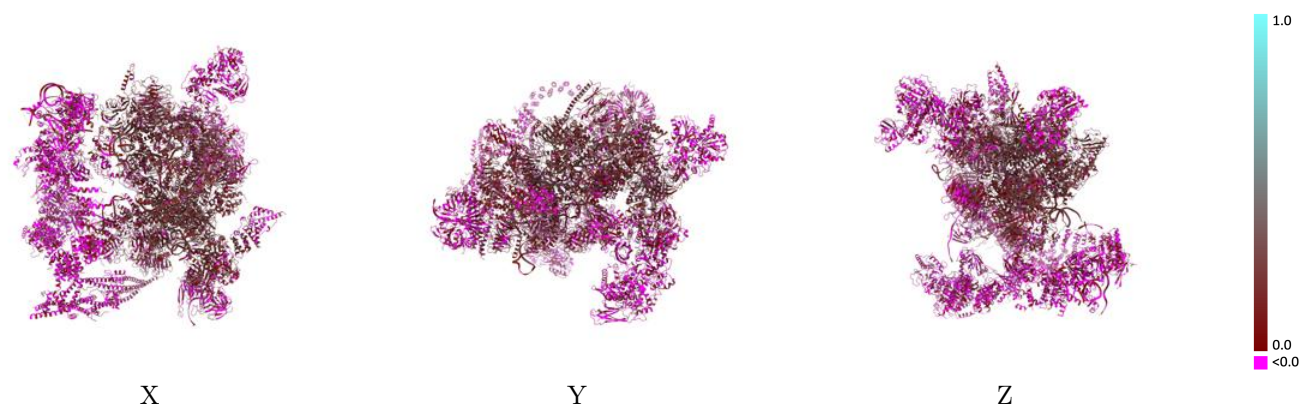
This section contains information regarding the fit between EMDB map EMD-6889 and PDB model 5Z56. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



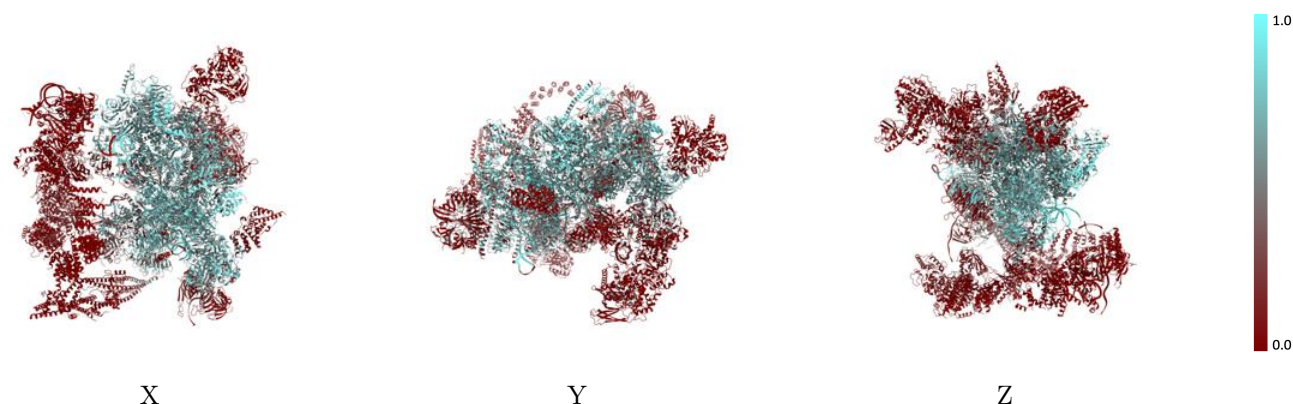
The images above show the 3D surface view of the map at the recommended contour level 0.0374 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



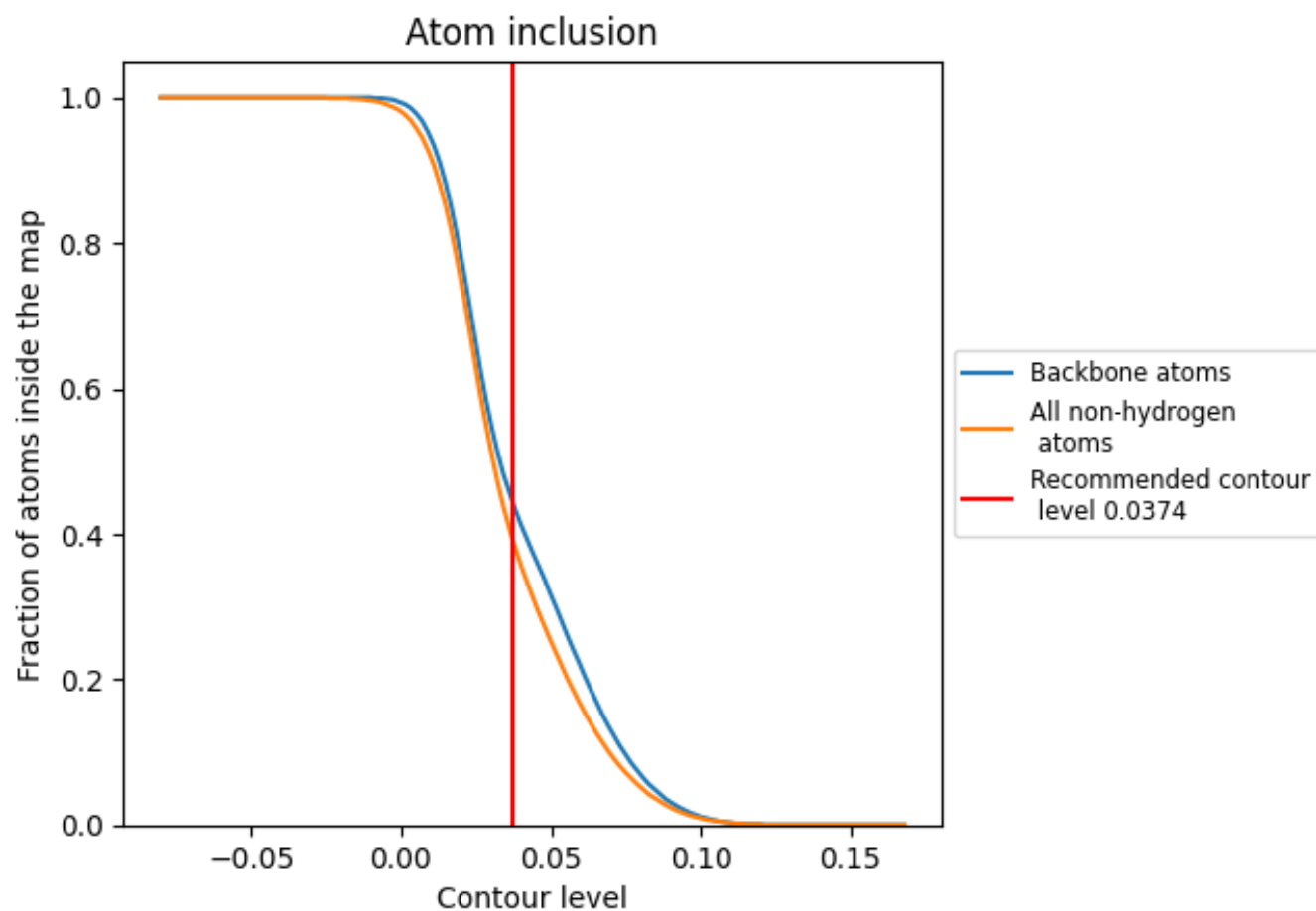
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0374).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 39% 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 (0.0374) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3900	 0.1310
1	 0.6320	 0.2170
2	 0.5230	 0.1780
3	 0.6060	 0.1710
4	 0.2310	 0.0610
5	 0.6450	 0.2070
6	 0.6670	 0.2070
7	 0.6700	 0.2160
A	 0.5630	 0.2060
B	 0.7040	 0.1870
C	 0.6430	 0.1910
D	 0.1000	 0.0630
E	 0.5400	 0.1430
F	 0.7610	 0.2100
G	 0.7270	 0.2080
H	 0.3810	 0.1180
I	 0.0210	 0.0120
J	 0.2700	 0.0700
K	 0.0710	 0.0420
L	 0.2920	 0.1050
M	 0.2260	 0.1790
N	 0.6190	 0.1720
O	 0.4390	 0.1590
P	 0.2840	 0.1630
Q	 0.0090	 -0.0050
R	 0.4890	 0.2030
S	 0.3280	 0.0920
T	 0.6900	 0.1960
U	 0.4870	 0.2470
V	 0.3750	 0.1280
W	 0.1590	 0.0700
X	 0.6110	 0.1900
Y	 0.7010	 0.2550
Z	 0.6410	 0.2540
a	 0.0550	 0.0050



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Chain	Atom inclusion	Q-score
b	 0.0960	 0.0920
c	 0.1870	 -0.0010
d	 0.1830	 0.0510
e	 0.1690	 0.0540
f	 0.1690	 -0.0090
g	 0.1180	 0.0210
h	 0.0280	 0.0350
i	 0.0090	 0.0050
j	 0.0370	 -0.0030
k	 0.0240	 0.0350
l	 0.0050	 -0.0000
m	 0.0220	 0.0220
n	 0.0270	 0.0070
o	 0.0110	 0.0180
p	 0.0320	 0.0150
q	 0.0020	 -0.0120
r	 0.0120	 0.0120
s	 0.0480	 0.0470
t	 0.0030	 -0.0040
u	 0.0020	 0.0250
v	 0.3360	 0.1070
w	 0.1970	 0.0420
x	 0.0010	 -0.0010
y	 0.0470	 0.0010
z	 0.1700	 0.1660