



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:52 AM UTC

PDB ID : 8I0U / pdb_00008i0u
EMDB ID : EMD-35110
Title : The cryo-EM structure of human Bact-IV complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2023-01-11
Resolution : 3.30 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:

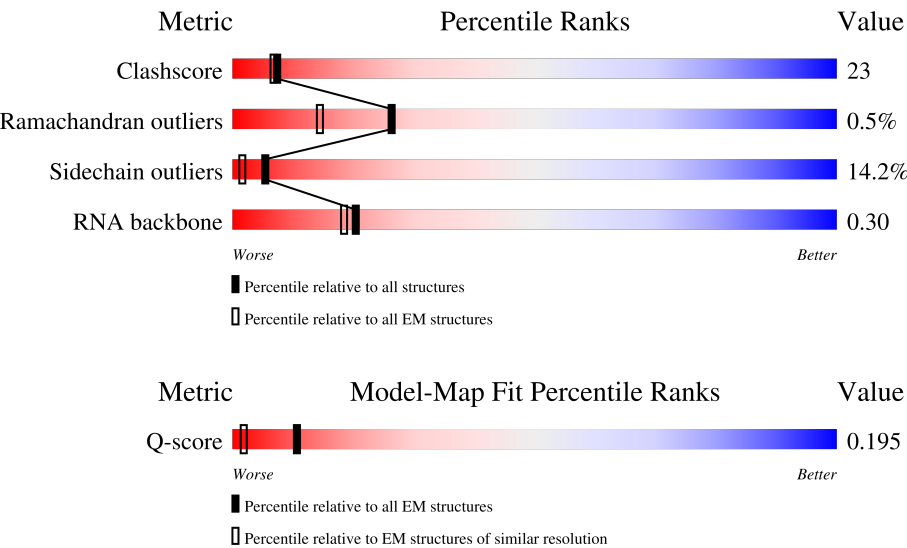
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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	15087 (2.80 - 3.80)

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	10% 52% 28% 5% 16%
2	B	117	6% 31% 35% 18% 16%
3	C	972	45% 38% 6% 12%

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Mol	Chain	Length	Quality of chain
4	E	357	
5	F	107	
6	G	220	
7	H	188	
8	I	855	
9	J	848	
10	K	343	
11	L	802	
12	M	243	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	166	
19	T	514	
20	U	2752	
21	V	908	
22	W	579	
23	X	1041	
24	Y	492	
25	Z	225	
26	y	301	
27	a	240	
27	m	240	

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Mol	Chain	Length	Quality of chain
28	b	119	
28	n	119	
29	c	118	
29	h	118	
30	d	86	
30	i	86	
31	e	92	
31	j	92	
32	f	76	
32	k	76	
33	g	126	
33	l	126	
34	q	504	
34	r	504	
34	s	504	
34	t	504	
35	1	1304	
36	3	1217	
37	p	225	
38	w	501	
39	2	895	
40	4	424	
41	7	110	
42	5	86	
43	o	255	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 106396 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	1969	Total	C	N	O	S	0	0
			16331	10528	2863	2872	68		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2066	925	347	696	98		

- 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
			6724	4298	1122	1272	32		

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

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

- Molecule 5 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 6 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	79	Total	C	N	O	P	0	0
			1587	708	248	552	79		

- Molecule 7 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	167	Total	C	N	O	P	0	0
			3539	1581	607	1184	167		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	672	Total	C	N	O	0	0
			3387	2043	672	672		

- Molecule 9 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	561	Total	C	N	O	S	0	0
			3773	2350	709	708	6		

- Molecule 10 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	24	Total	C	N	O	S	0	0
			185	114	32	36	3		

- Molecule 11 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	387	Total	C	N	O	S	0	0
			2584	1596	494	489	5		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	114	Total	C	N	O	S	0	0
			971	605	181	183	2		

- Molecule 13 is a protein called Protein BUD31 homolog.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	290	Total	C	N	O	0	0
			1447	862	292	293		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	101	Total	C	N	O	S	0	0
			876	537	175	162	2		

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1322	Total	C	N	O	0	0
			5288	2644	1322	1322		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	380	Total	C	N	O	P	S	0	0
			2915	1791	552	558	2	12		

- Molecule 18 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	158	Total	C	N	O	0	0
			770	454	158	158		

- Molecule 19 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	462	Total	C	N	O	S	0	0
			2959	1842	537	567	13		

- Molecule 22 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	501	Total	C	N	O		0	0
			2473	1471	501	501			

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	786	Total	C	N	O	S	0	0
			6357	4010	1133	1184	30		

- Molecule 24 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	320	Total	C	N	O	S	0	0
			2556	1616	420	508	12		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	155	Total	C	N	O		0	0
			772	462	155	155			

- Molecule 26 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	79	Total	C	N	O		0	0
			316	158	79	79			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	86	Total	C	N	O		0	0
			344	172	86	86			
27	m	82	Total	C	N	O		0	0
			413	249	82	82			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	82	Total	C	N	O	0	0
			328	164	82	82		
28	n	80	Total	C	N	O	0	0
			402	242	80	80		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	97	Total	C	N	O	0	0
			388	194	97	97		
29	h	95	Total	C	N	O	0	0
			482	292	95	95		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	d	74	Total	C	N	O	0	0
			296	148	74	74		
30	i	72	Total	C	N	O	0	0
			359	215	72	72		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	79	Total	C	N	O	0	0
			316	158	79	79		
31	j	81	Total	C	N	O	0	0
			403	241	81	81		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	f	74	Total	C	N	O	0	0
			296	148	74	74		
32	k	73	Total	C	N	O	0	0
			364	218	73	73		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	g	81	Total	C	N	O	0	0
			324	162	81	81		
33	l	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 34 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 35 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	816	Total	C	N	O	S	0	0
			6486	4163	1119	1165	39		

- Molecule 36 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	167	Total	C	N	O	0	0
			841	507	167	167		

- Molecule 38 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	121	Total	C	N	O	S	0	0
			999	637	178	180	4		

- Molecule 39 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2	250	Total	C	N	O	S	0	0
			1803	1131	339	326	7		

- Molecule 40 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	151	Total	C	N	O		0	0
			743	441	151	151			

- Molecule 41 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	7	81	Total	C	N	O	S	0	0
			613	376	109	115	13		

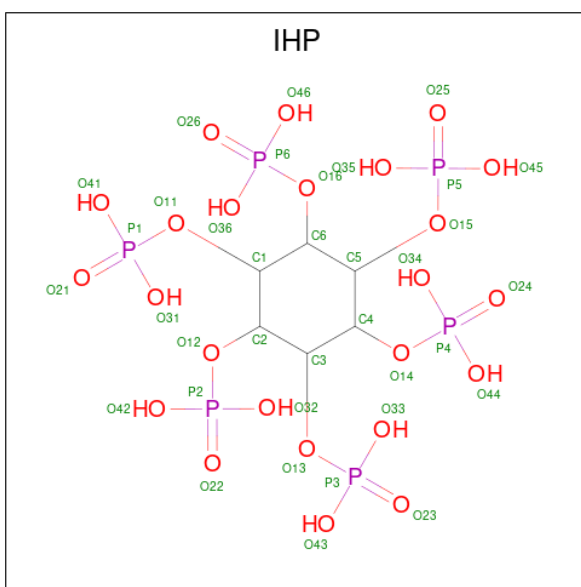
- Molecule 42 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5	77	Total	C	N	O	S	0	0
			635	403	110	117	5		

- Molecule 43 is a protein called U2 small nuclear ribonucleoprotein A'.

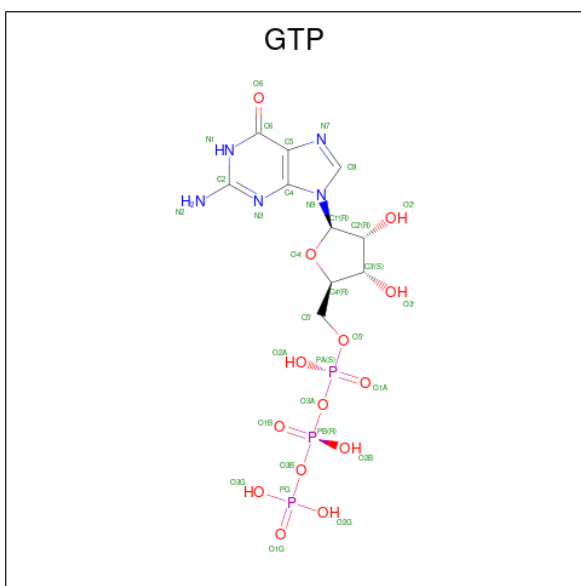
Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	162	Total	C	N	O		0	0
			816	492	162	162			

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	C	1	Total 1	Mg 1	0
46	F	6	Total 6	Mg 6	0

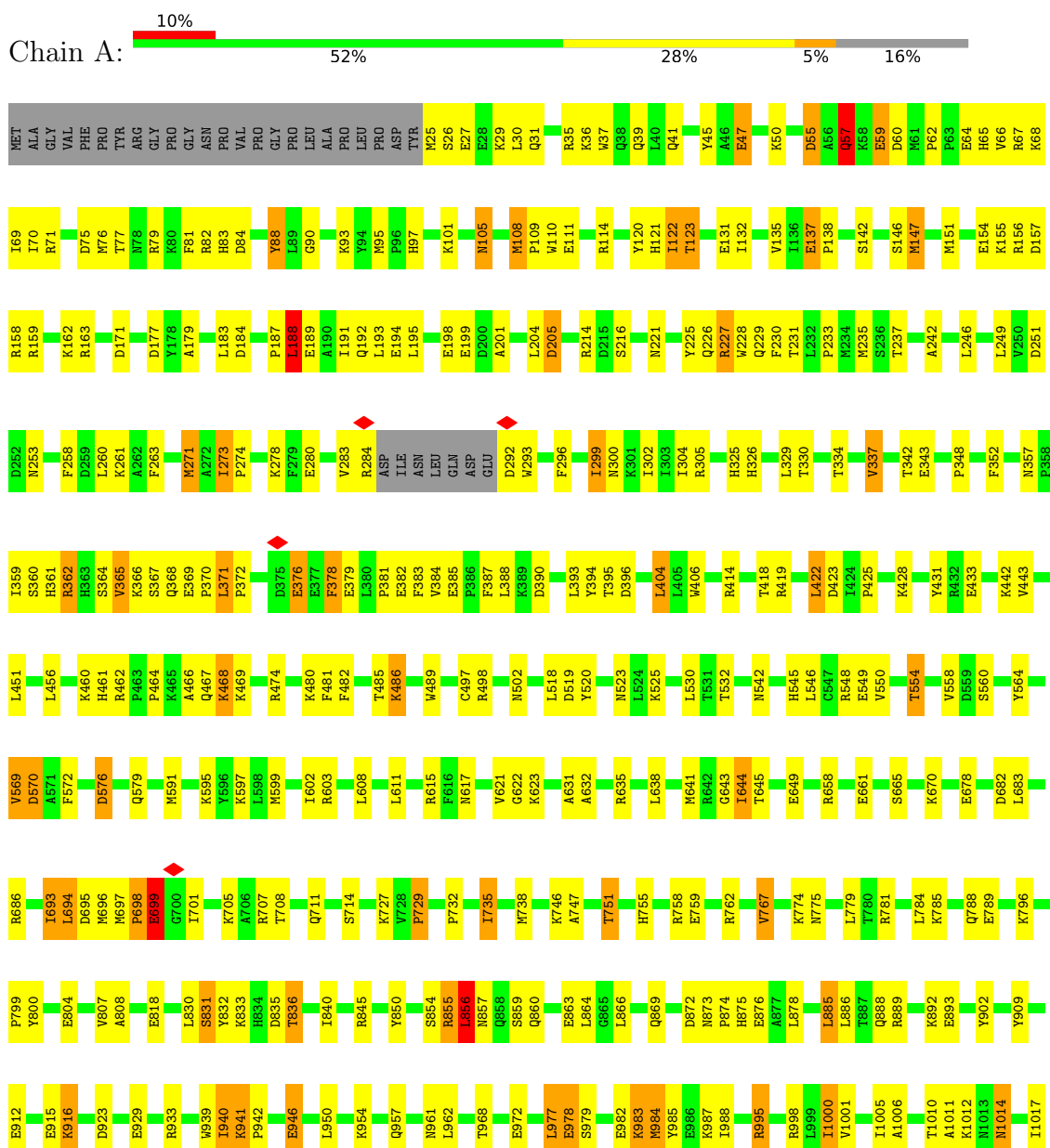
- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	K	1	Total 1	Zn 1	0
47	N	3	Total 3	Zn 3	0
47	7	3	Total 3	Zn 3	0

3 Residue-property plots

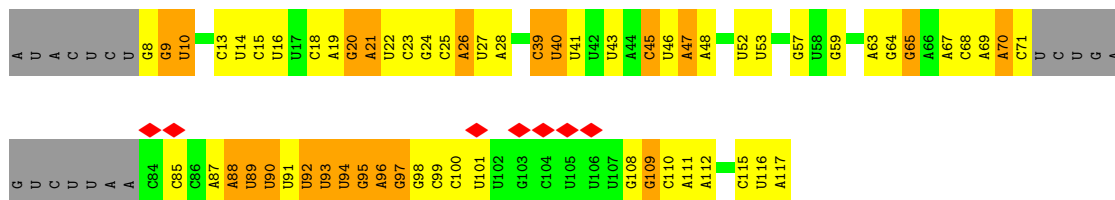
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

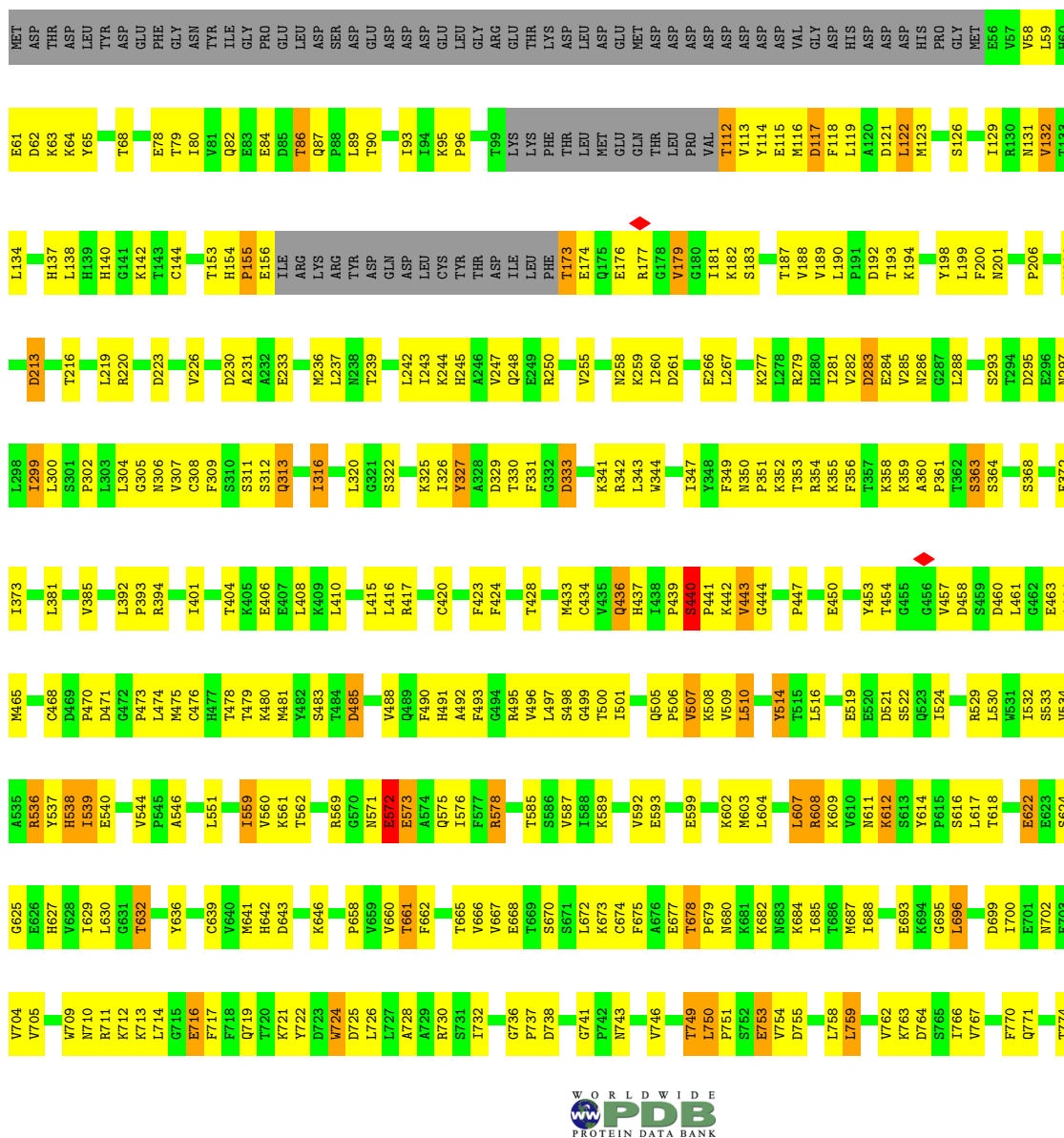


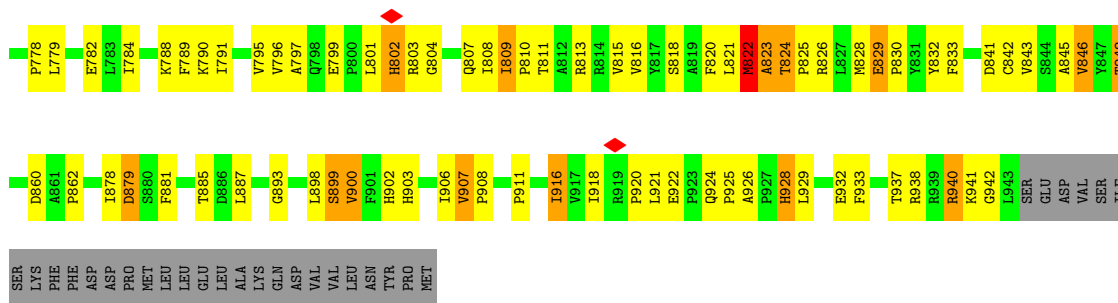
LYS	VAL	HIS	D1990	Y1930	F1810	E1745	Y1659	T1568	K1463	Q1373	R1224	M1143	M1018
GLU	LEU	GLY	Y1991	N1811	N1811	R1746	Y1660	I1571	V1481	P1374	C1228	K1144	Y1019
MET	LYS	ASP	G1992	A1932	P1812	K1749	W1661	S1572	E1482	F1229	F1229	M1147	K1020
PRO	PHE	ILE	K1993	F1933	R1813	S1755	D1663	L1573	E1489	S1251	S1251	V1147	D1021
LEU	ILE	THR	N1994	S1934	G1815	S1756	I1664	R1578	F1490	G1252	G1252	M1148	N1023
GLY	CYS	THR	N1995	R1935	G1816	S1757	R1667	A1579	K1491	S1253	S1253	R1151	I1030
TRP	ILE	THR	N1996	L1936	L1817	P1758	D1670	H1580	T1493	E1254	E1254	A1152	G1033
ILE	THR	THR	N1997	I1937	L1818	T1759	V1671	W1582	T1493	S1377	S1377	R1160	Q1034
HIS	ASP	THR	V1997	L1938	F1818	G1U	D1672	Q1583	K1498	E1378	E1378	R1163	Q1035
THR	LEU	THR	N1998	I1939	L1819	PRO	D1673	Q1584	V1498	D1381	D1381	S1164	S1038
GLN	ARG	ASN	N1998	L1940	K1820	TVR	S1673	H1585	L1501	S1382	S1382	V1165	Y1043
PRO	ALA	TYR	N1998	R1941	I1821	LEU	I1676	H1586	F1502	L1391	L1284	T1167	L1046
ASN	GLN	GLU	A2000	L1942	I1822	SER	R1681	V1590	K1505	Q1394	N1293	Q1169	V1047
GLU	ILE	THR	S2001	L1943	H1823	Q1766	F1684	Q1599	ALA	E1395	E1395	S1173	M1048
THR	GLY	PHE	T2002	H1944	T1824	N1767	F1684	E1600	GLY	A1396	PHE	F1174	L1050
LEU	THR	THR	T2003	V1945	S1825	Y1768	D1690	L1601	GLU	I1397	I1299	T1178	R1057
GLN	GLY	THR	L2002	L1946	V1826	G1769	N1691	E1606	GLU	A1398	I1301	S1179	E1060
PRO	VAL	THR	S2005	N1947	W1827	E1770	M1692	E1607	SER	Q1399	I1403	K1180	Q1075
GLN	VAL	THR	E2006	D1948	A1828	L1771	S1693	T1608	MET	R1401	G1302	D1181	D1076
ASP	SER	GLU	T2007	R1949	G1834	F1772	S1697	E1607	LYS	L1402	L1403	N1184	T1079
VAL	TRP	ARG	R2008	R1950	Q1830	S1773	P1698	I1606	ALA	T1404	F1311	L1185	R1090
THR	PRO	ARG	D2009	K1951	K1831	Q1775	T1699	N1623	GLU	K1306	E1407	L1186	Y1091
ASP	VAL	ARG	T2010	W1952	R1890	Q1775	F1698	E1624	LYS	K1306	E1407	C1190	I1092
HIS	ALA	ARG	L2011	L1953	L1891	Q1775	P1699	S1625	LYS	L1403	L1403	G1194	I1095
ALA	PRO	ALA	L2012	L1954	F1892	Q1775	V1701	N1623	K1516	L1403	L1403	K1199	D1104
ILE	VAL	SER	G2013	K1955	Q1894	I1776	L1702	S1625	K1517	T1404	F1311	R1195	L1109
MET	GLY	ALA	M2014	K1956	A1895	W1778	I1703	D1628	L1518	D1407	E1407	G1194	R1112
ALA	GLU	ASN	E2015	P1956	A1896	W1778	I1703	D1628	T1519	L1408	E1408	R1195	H1117
ASP	ASN	LEU	ILE	D1957	C1896	F1779	D1706	L1629	N1520	E1409	E1409	E1206	F1117
ASN	ARG	LEU	SER	K1958	L1897	Y1780	H1712	L1630	A1521	L1328	L1328	F1207	N1121
GLY	CYS	HIS	ALA	T1959	K1898	W1780	S1713	L1631	Q1522	S1329	S1329	T1208	N1122
THR	VAL	LEU	ALA	F1960	V1899	D1781	A1714	F1632	R1523	D1413	D1413	H1209	E1123
TRP	VAL	ARG	PRO	T1960	W1839	D1782	T1715	A1633	S1524	R1414	R1414	K1210	E1123
ASP	MET	THR	SER	I1961	E1900	T1783	G1716	S1634	G1525	G1415	G1415	D1211	G1127
GLY	VAL	ASN	GLN	T1962	K1901	W1784	N1717	Y1635	L1526	P1336	P1336	G1212	G1127
GLU	GLY	ASN	GLN	E1963	F1902	N1784	W1718	K1636	N1527	Q1337	Q1337	V1213	N1130
THR	TRP	TYR	GLN	P1964	G1903	E1843	F1719	W1637	Q1528	S1338	S1338	N1215	K1131
LYS	GLY	ILE	GLN	H1965	D1904	E1844	P1720	N1638	I1529	W1342	W1342	L1216	W1134
THR	THR	THR	THR	H1966	L1905	Y1786	P1720	V1639	I1529	I1419	I1419	Q1217	W1134
GLY	GLY	THR	THR	H1967	I1906	R1787	K1723	S1640	R1532	T1346	T1346	K1222	R1139
GLN	GLN	THR	THR	W1968	L1907	V1788	P1724	R1641	R1544	D1347	D1347	E1222	M1140
THR	THR	THR	THR	P1969	L1908	T1789	P1724	P1642	R1544	W1436	W1436	E1206	
GLY	GLY	THR	THR	T1970	A1909	I1790	L1725	S1643	V1549	G1349	G1349	F1207	
THR	PRO	GLU	THR	L1971	I1910	H1791	I1726	L1644	Q1552	I1351	I1351	H1209	
GLY	GLY	THR	THR	T1972	S1951	K1792	W1730	S1648	Q1552	H1352	H1352	K1210	
THR	GLY	THR	THR	D1973	S1951	T1793	M1734	K1649	V1553	E1369	E1369	D1211	
GLN	GLY	THR	THR	E1974	L1852	F1794	M1734	D1650	Q1554	H1359	H1359	W1213	
GLY	GLY	THR	THR	E1975	P1853	E1795	N1737	W1652	L1555	E1360	E1360	N1215	
THR	ILE	THR	THR	W1976	V1854	G1796	P1738	M1682	T1568	E1361	E1361	K1216	
LEU	LEU	THR	THR	L1977	E1855	N1797	A1739	T1655	I1569	Q1457	Q1457	Q1217	
PRO	PRO	THR	THR	I1977	E1856	L1798	L1740	T1656	H1460	D1362	D1362	L1216	
ALA	GLY	THR	THR	K1978	L1916	L1798	Y1741	T1657	F1561	Q1363	Q1363	Q1217	
TYR	TYR	THR	THR	F1917	F1917	T1799	Y1741	T1657	F1561	L1368	L1368	K1222	
LYS	ASN	THR	THR	N1918	N1918	T1800	Y1741	T1657	F1561	L1368	L1368	K1222	
THR	THR	THR	THR	N1919	N1919	T1800	Y1741	T1657	F1561	L1368	L1368	K1222	
ARG	ARG	THR	THR	L1919	L1919	T1800	Y1741	T1657	F1561	L1368	L1368	K1222	
THR	THR	THR	THR	Y1920	Y1920	T1800	Y1741	T1657	F1561	L1368	L1368	K1222	
VAL	VAL	THR	THR	D1921	D1921	P1802	P1802	P1802	P1802	P1802	P1802	P1802	P1802
ASN	ASN	THR	THR	L1983	L1983	I1861	I1861	I1861	I1861	I1861	I1861	I1861	I1861
LYS	LYS	THR	THR	W1923	W1923	G1805	G1805	G1805	G1805	G1805	G1805	G1805	G1805
GLY	GLY	THR	THR	L1924	L1924	A1806	A1806	A1806	A1806	A1806	A1806	A1806	A1806
THR	THR	THR	THR	K1925	K1925	I1807	I1807	I1807	I1807	I1807	I1807	I1807	I1807
GLY	GLY	THR	THR	T1926	T1926	F1808	F1808	F1808	F1808	F1808	F1808	F1808	F1808
THR	THR	THR	THR	I1927	I1927	M1868	M1868	M1868	M1868	M1868	M1868	M1868	M1868
LYS	LYS	THR	THR	S1928	S1928	S1929	S1929	S1929	S1929	S1929	S1929	S1929	S1929

- Molecule 2: U5 snRNA

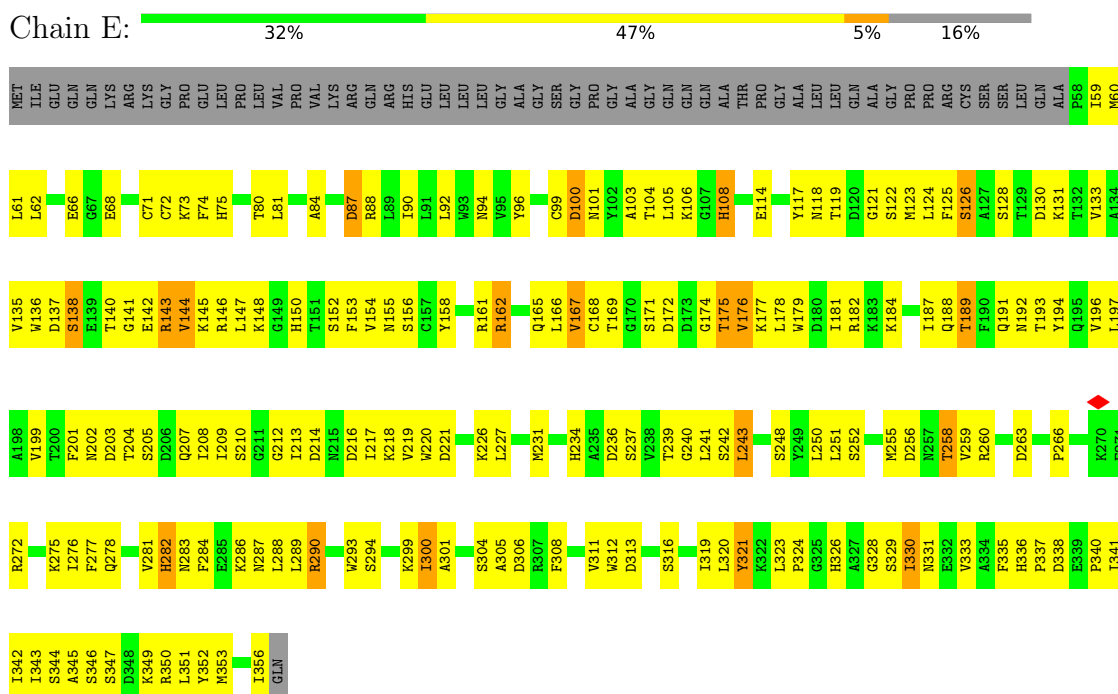


- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

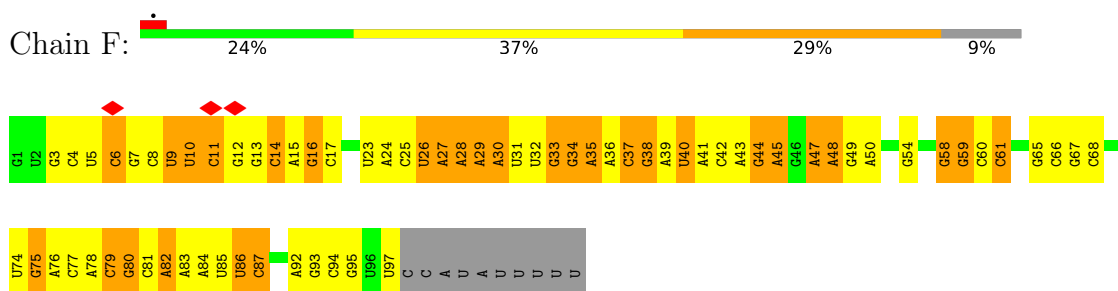




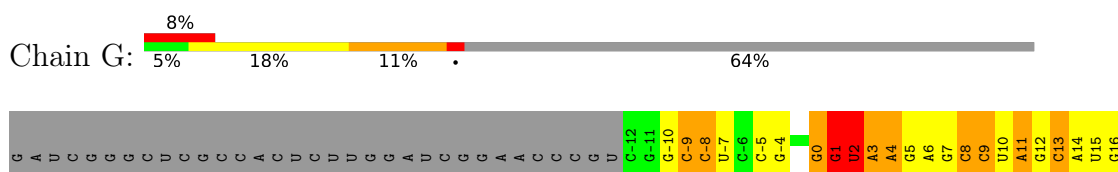
• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

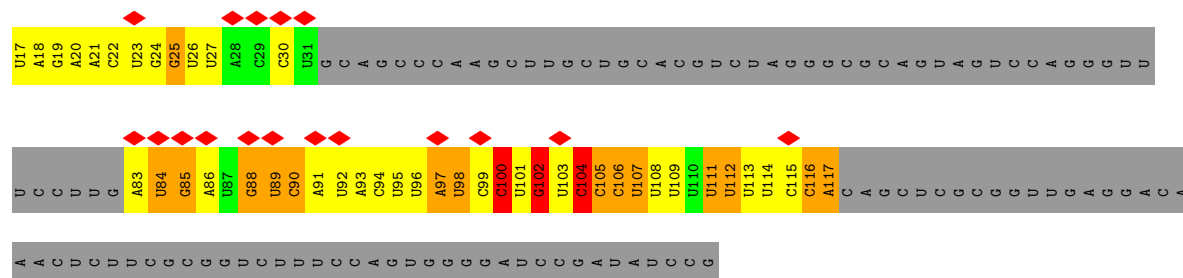


• Molecule 5: U6 snRNA

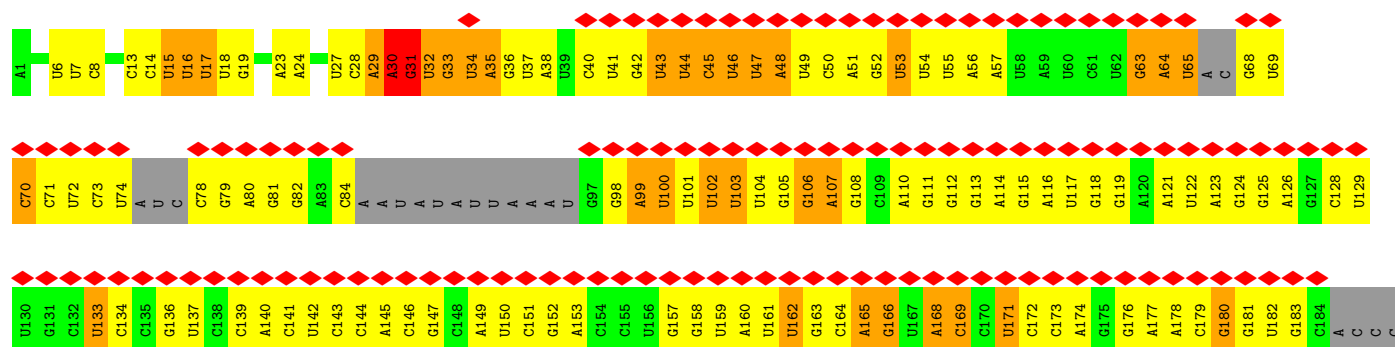


• Molecule 6: Pre-mRNA

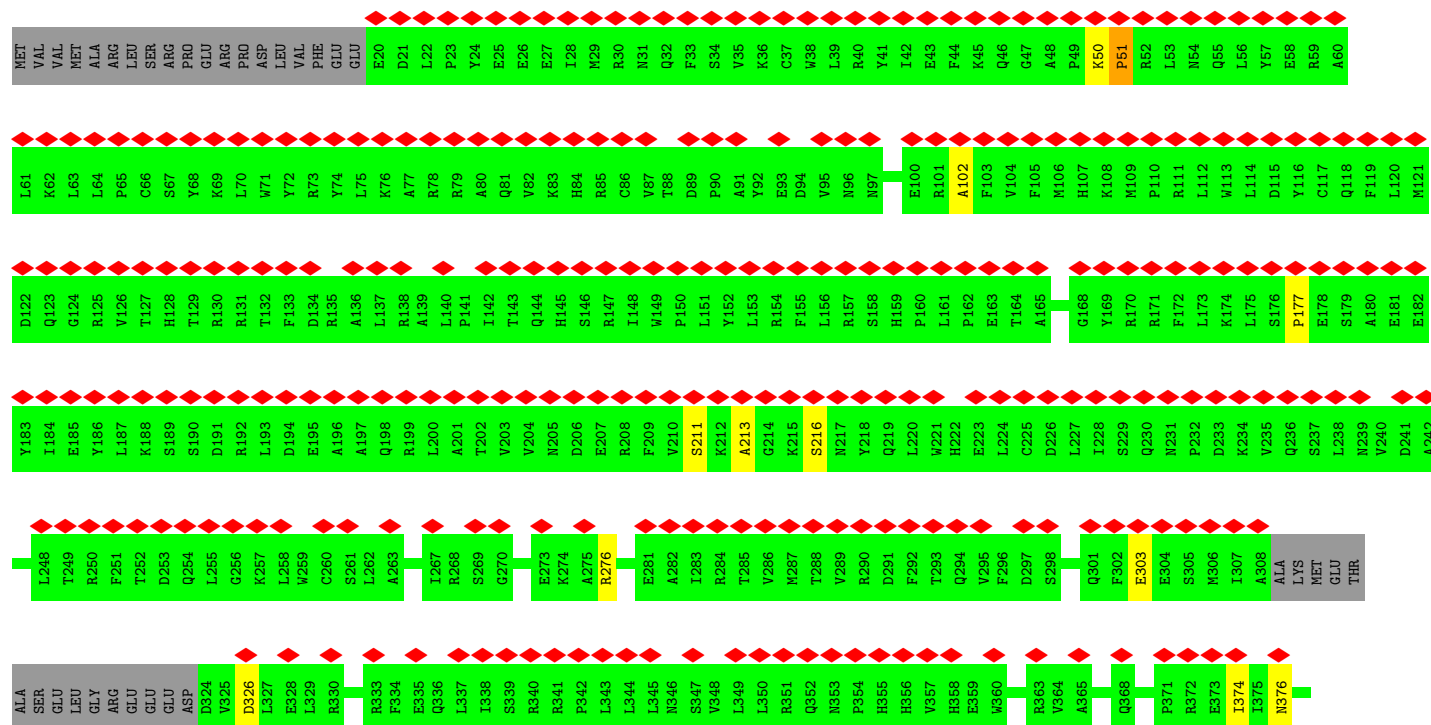
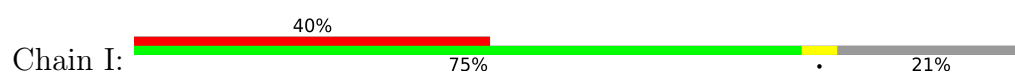


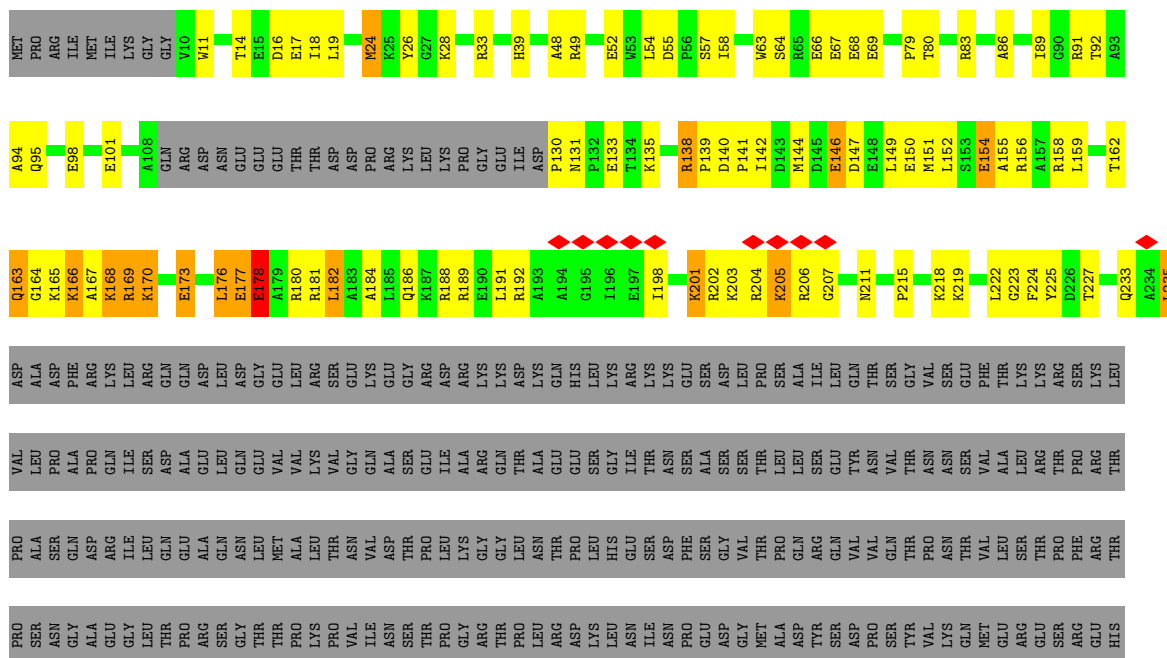


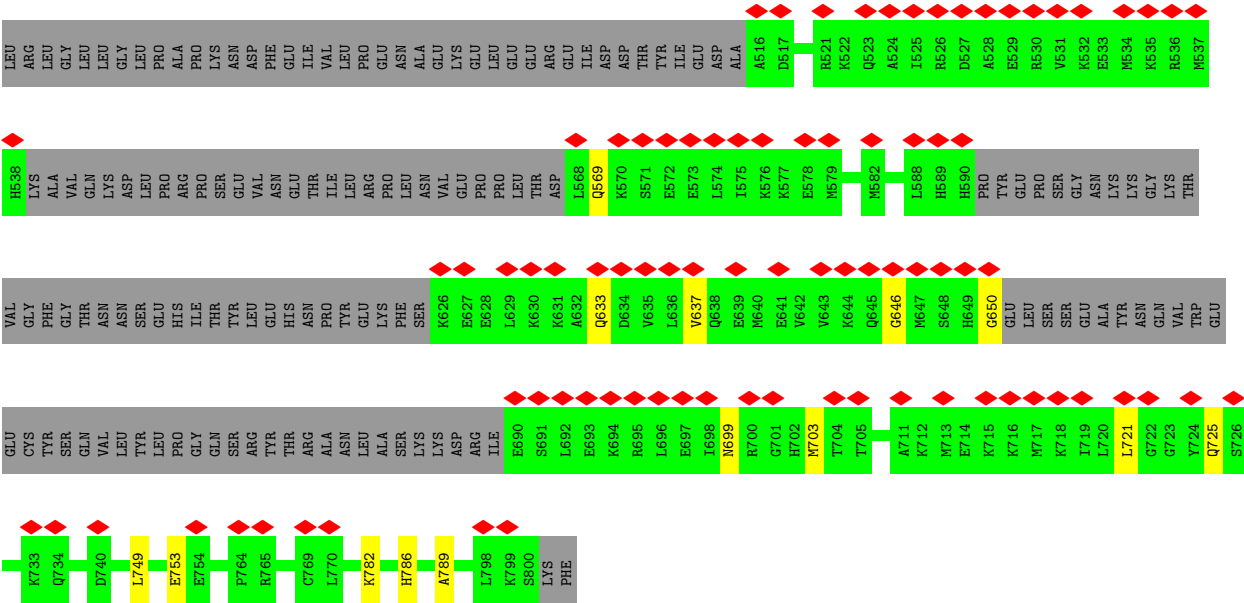
• Molecule 7: U2 snRNA



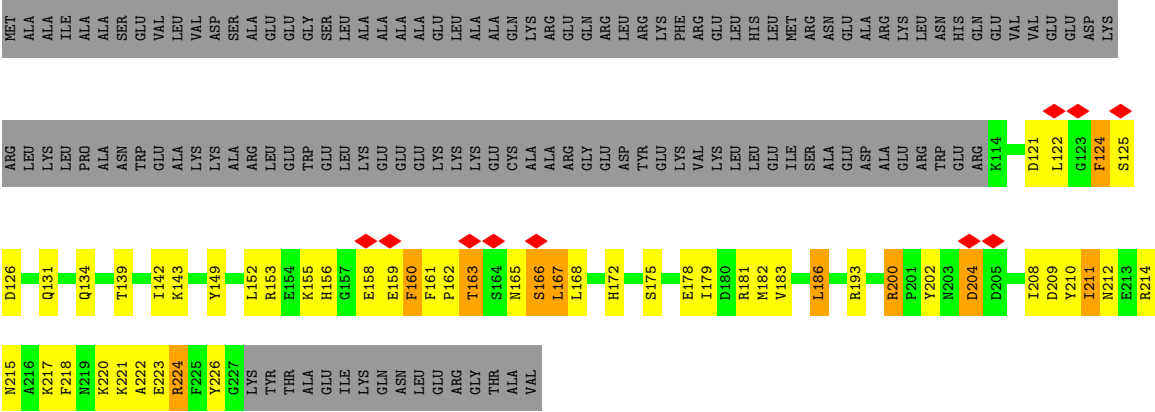
• Molecule 8: Pre-mRNA-splicing factor SYF1



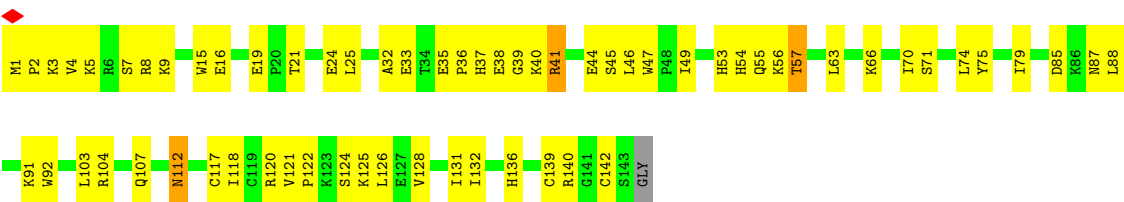




• Molecule 12: Pre-mRNA-splicing factor SYF2

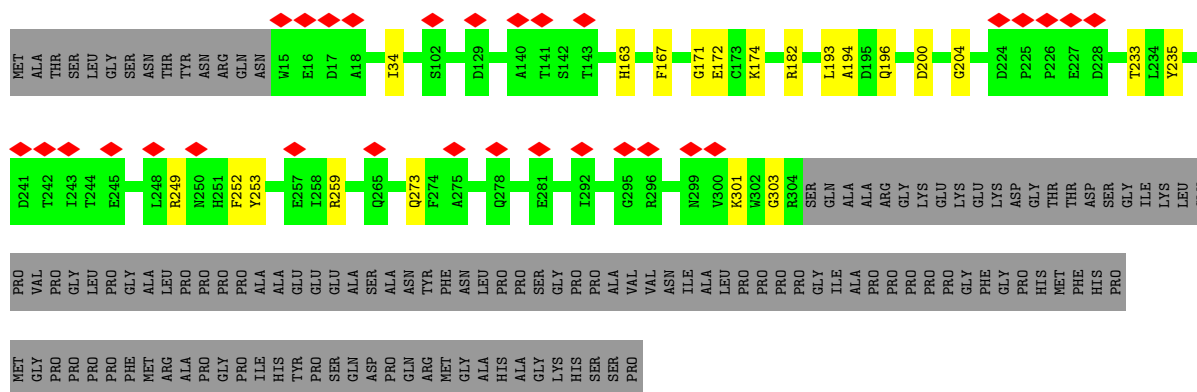


• Molecule 13: Protein BUD31 homolog

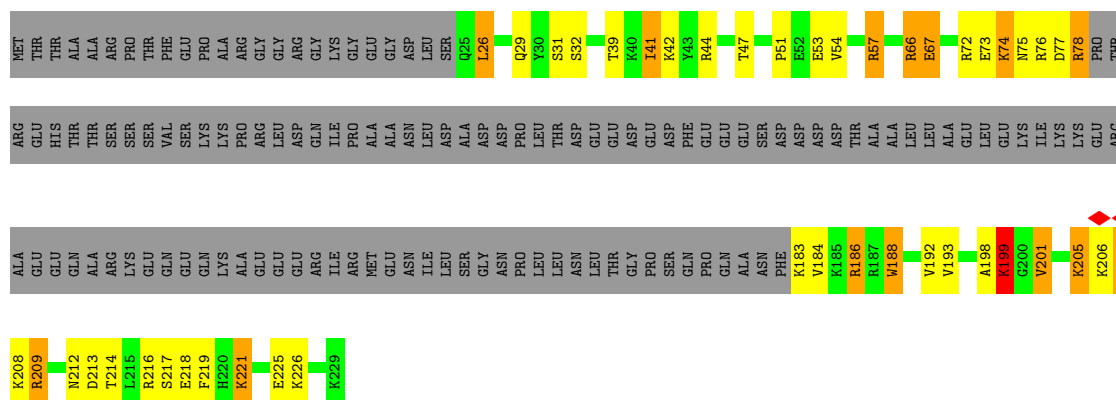
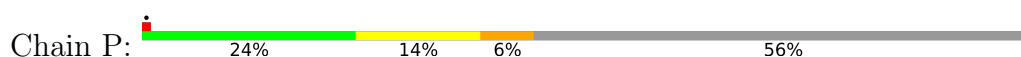


• Molecule 14: Pre-mRNA-splicing factor RBM22

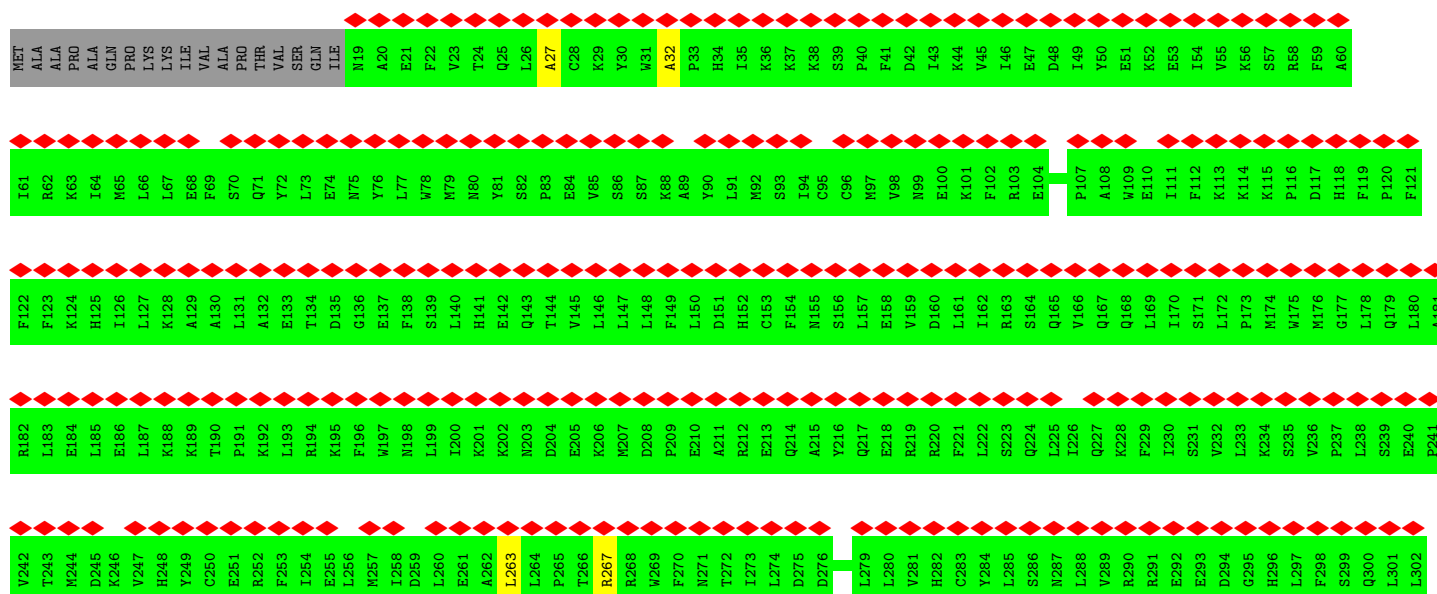
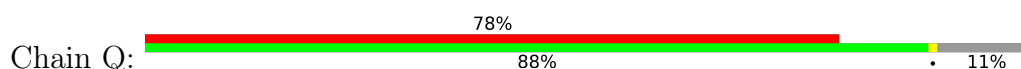




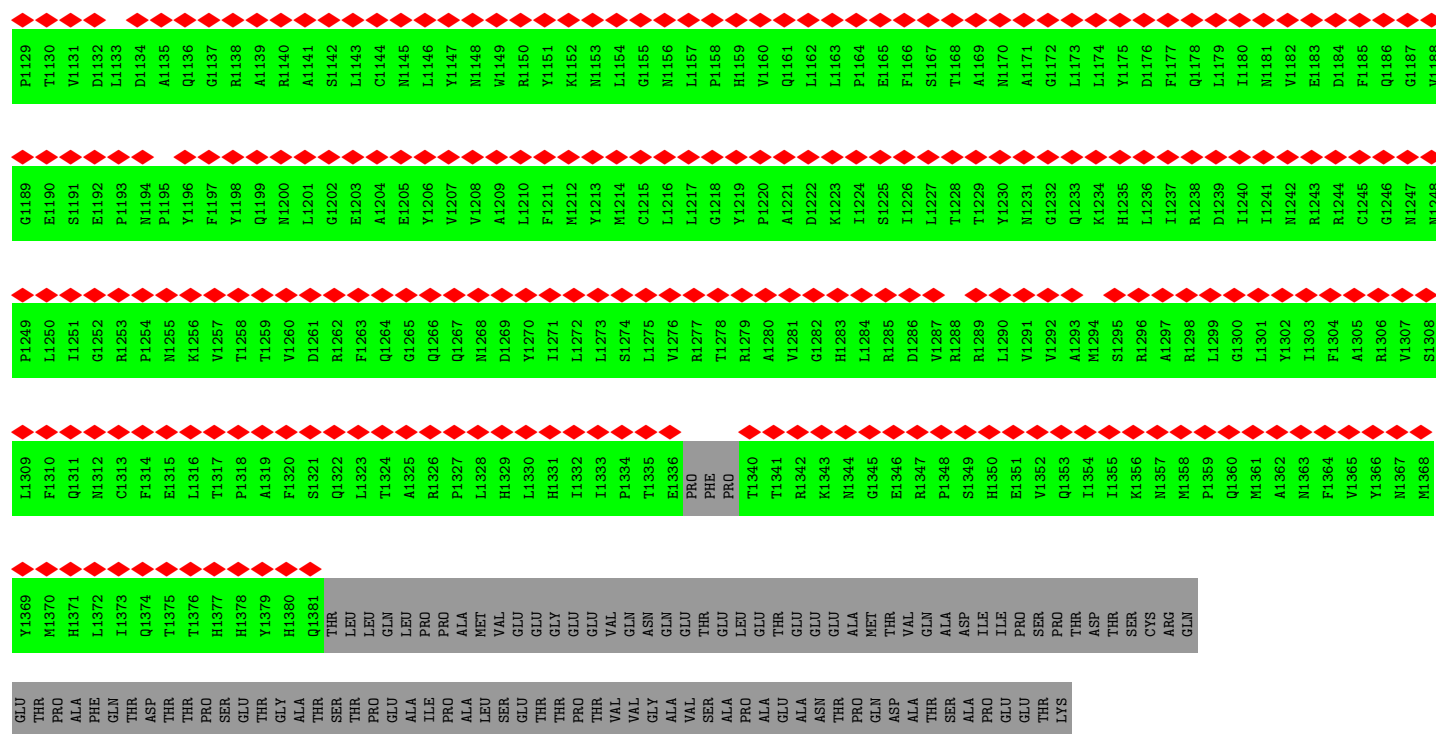
• Molecule 15: Spliceosome-associated protein CWC15 homolog



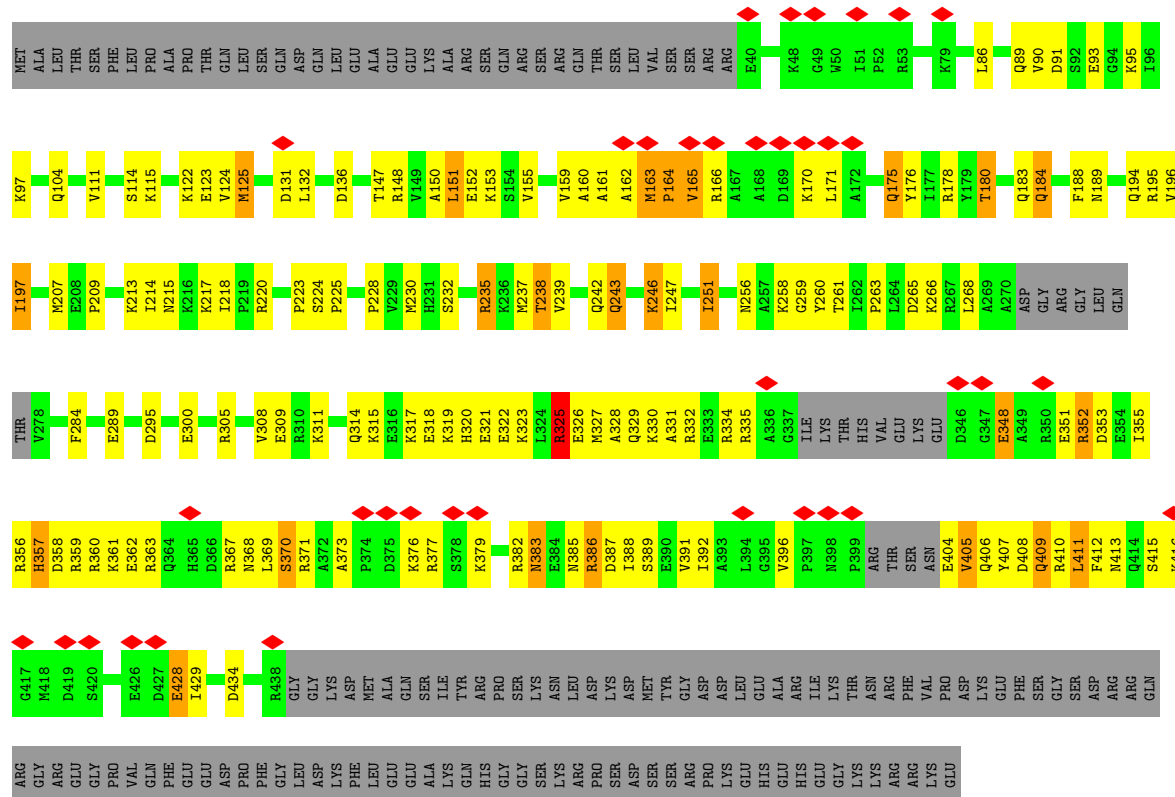
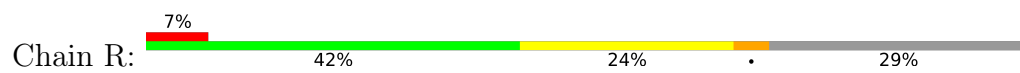
• Molecule 16: RNA helicase aquarius



L1068	E1069	E1070	E1071	T1072	F1073	P1074	P1075	L1076	L1077	L1078	Q1079	M1080	P1081	Q1082	D1083	G1084	F1085	S1086	L1087	L1088	K1089	R1090	W1091	I1092	M1093	I1094	G1095	D1096	Q1099	L1100	P1101	P1102	V1103	I1104	K1105	N1106	M1107	A1108	F1109	Q1110	K1111	Y1112	S1113	M1114	M1115	E1116	Q1117	S1118	L1119	F1120	T1121	F1123	R1124	R1125	G1127	V1128			
H1000	I1001	K1002	T1006	Q1007	L1008	E1009	E1010	F1011	E1015	L1016	L1017	R1018	S1019	Q1020	L1021	D1022	R1023	S1024	K1025	Y1026	L1027	L1028	E1031	A1032	K1033	A1036	M1037	T1038	C1039	A1043	L1044	A1045	R1046	H1047	D1048	L1049	V1050	K1051	L1052	G1053	F1054	K1055	Y1056	D1057	N1058	I1059	L1060	M1061	E1062	E1063	A1064	A1065	Q1066	I1067					
L937	Y938	Q939	V940	M941	S942	R943	W944	E945	E946	Y947	L948	S949	K950	V951	K952	N953	LYS	GLY	SER	THR	LEU	P959	D960	V961	T962	E963	V964	S965	T966	H971	E972	Y973	F974	A975	N976	A977	PRO	GLN	PRO	L981	F982	K983	G984	R985	S986	Y987	E988	E989	D990	M991	E992	I993	A994	E995	G996	C997	F998	R999	
H875	L876	L879	G880	H881	GLY	GLU	E884	E885	L886	E887	T888	E889	K890	D891	F892	S893	R894	G896	R897	V898	N899	Y900	V901	L902	A903	R904	R905	I906	E907	L908	L909	E910	E911	V912	K913	R914	L915	Q916	K917	S918	L919	N956	Q920	V921	P922	G923	D924	A925	S926	Y927	T928	C929	E930	T931	Y934	F935	F936		
G813	M814	Q815	P816	L817	L818	T819	M820	V821	E822	G823	P824	P825	G826	T827	G828	K829	A833	V834	Q835	L836	L837	S838	N839	I840	Y841	H842	N843	F844	P845	E846	Q847	R848	T849	L850	L851	V852	T853	H854	S855	L856	Q857	A858	L859	N860	Q861	L862	F863	K864	L865	H866	H867	A868	L869	D870	L871	D872			
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	H722	R723	L724	K725	A726	S727	F728	P729	G730	H731	N732	W733	K734	V735	T736	V737	E738	D739	P740	A741	L742	Q743	ILE	PRO	P746	F747	R748	I749	T750	F751	P752
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	R658	R659	K660	P661	K662	E663	F666	K667	A668	V669	L670	E671	T672	I673	R674	N675	L676	M677	N678	T679	D680	C681	V682	V683	P684	D685	W686	L687	H688	D689	I690	I691	L692		
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	Q598	G599	M600	L601	D602	D603	K604	G605	R606	V607	I608	GLU	ASP	GLY	PRO	GLU	P614	R615	L618	R619	G620	E621	S622	R623	T624	F625	R626	V627	F628	L629	D630		
I433	W434	D435	E436	M437	I438	V439	P440	T441	E442	Y443	Y444	S445	G446	E447	G448	C449	L450	A451	L452	P453	K454	L455	M456	L457	Q458	F459	L460	T461	L462	H463	D464	Y465	L466	L467	V468	M469	F470	M471	L472	F473	R474	L475	E476	E554	S477	T478	Y479	E480	I481	R482	Q483	D487	K493	P494	W495	Q496	S497	GLU	
L372	S373	S374	N375	T376	L377	H378	A381	S382	Y383	L384	C385	L386	L387	P388	T389	L390	P391	K392	N393	E394	D395	T396	T397	F398	D399	K400	E401	F402	L403	L404	E405	L406	L407	V408	S409	R410	E412	R413	R414	I415	S416	Q417	E357	I418	Q419	Q420	L421	M422	Q423	M424	P425	Y427	P428	T429	E430	K431	I432		
TYR	G500	G501	V502	W503	G506	W507	I514	V515	A516	F517	T518	V519	V520	E521	V522	A523	K524	P525	N526	I527	G528	E529	N530	W531	P532	T533	R534	V535	R536	A537	D538	V539	T540	I541	N542	L543	I549	K550	D551	E552	W553	E554	G555	L556	R557	K558	H559	D560	V561	C562	F563	L564	I565	R568	P569				



• Molecule 17: SNW domain-containing protein 1



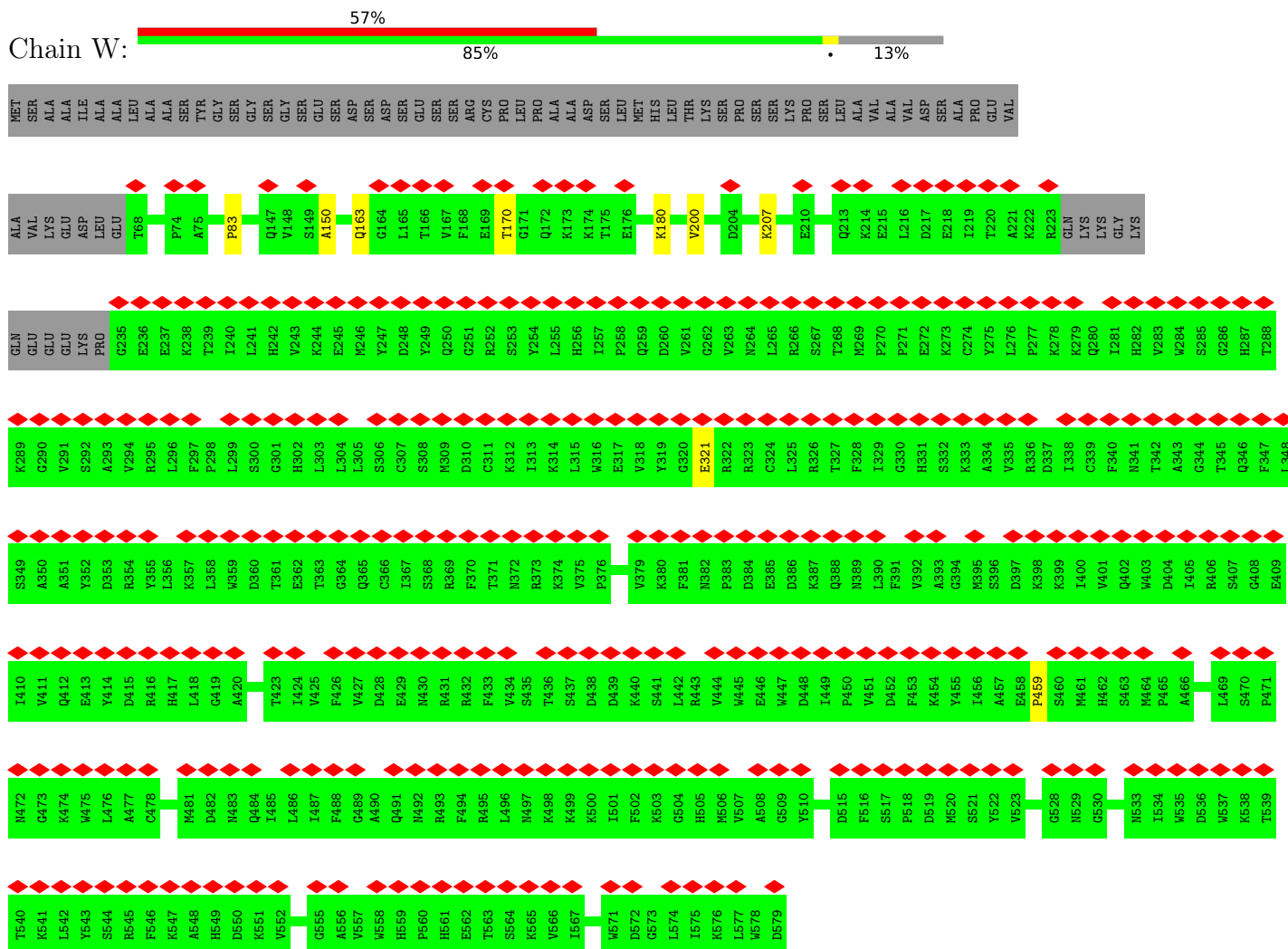
• Molecule 18: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:

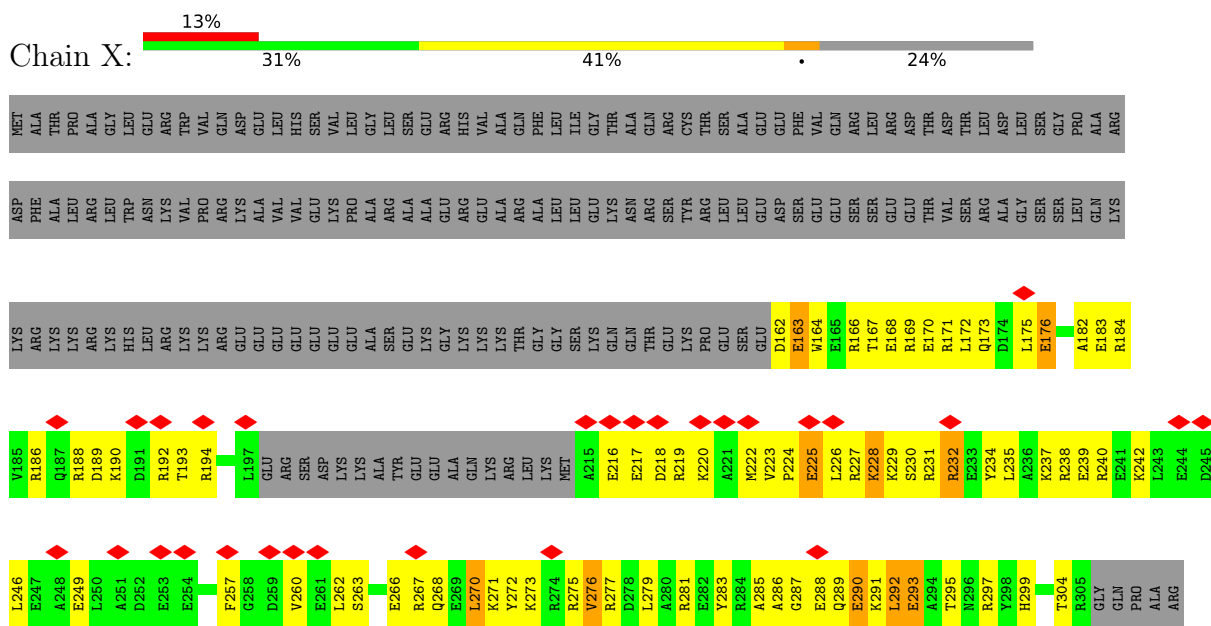


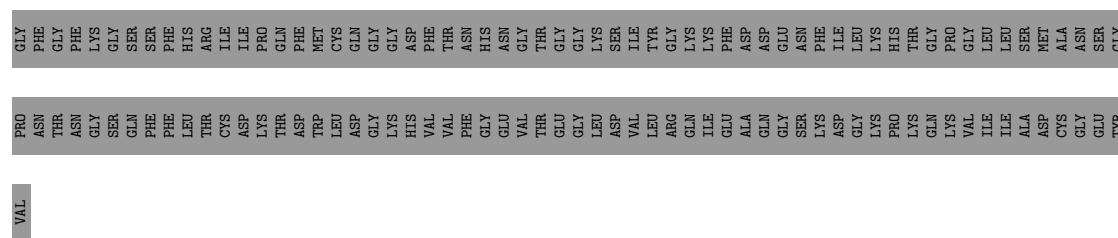
- Molecule 21: Pre-mRNA-splicing factor CWC22 homolog



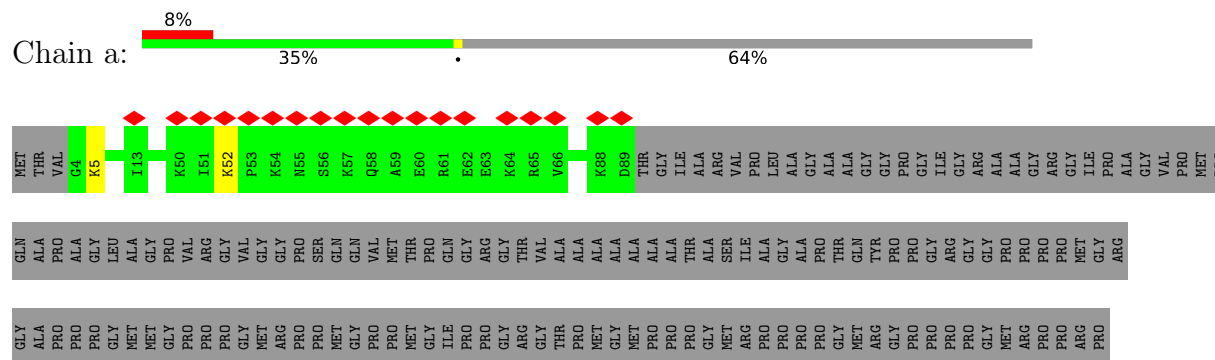


- Molecule 23: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

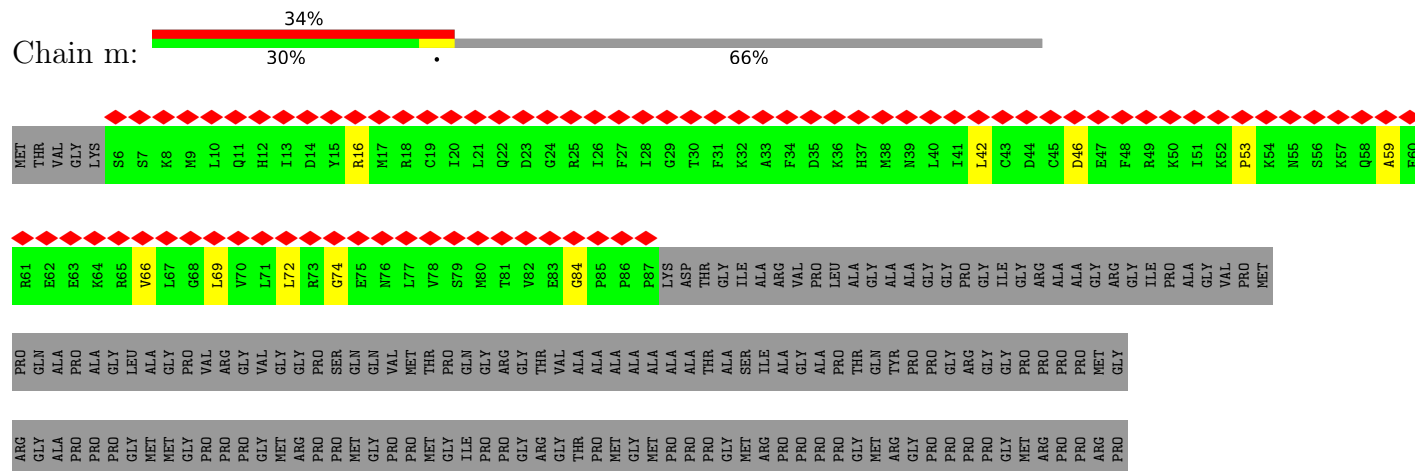




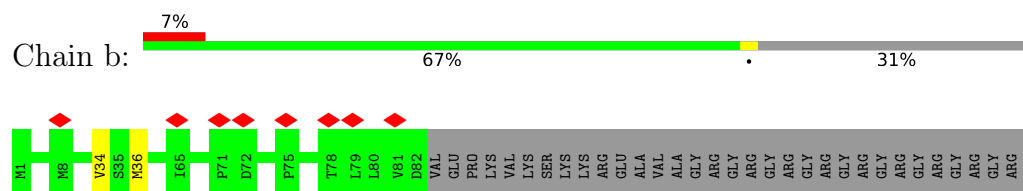
• Molecule 27: Small nuclear ribonucleoprotein-associated proteins B and B'



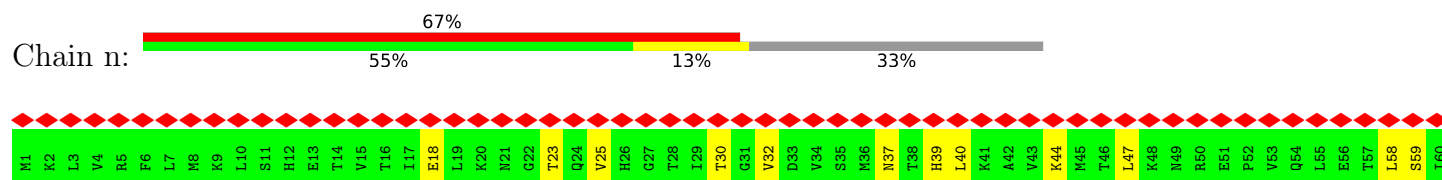
• Molecule 27: Small nuclear ribonucleoprotein-associated proteins B and B'

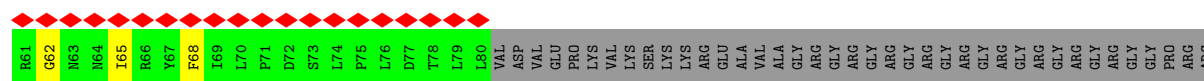


• Molecule 28: Small nuclear ribonucleoprotein Sm D1

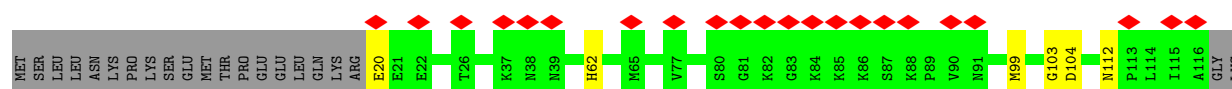


• Molecule 28: Small nuclear ribonucleoprotein Sm D1

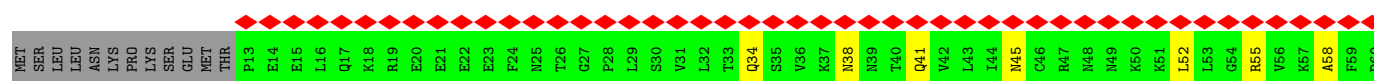
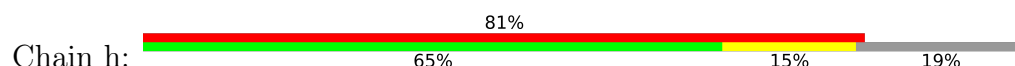




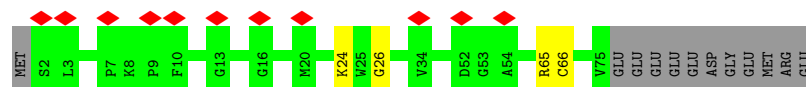
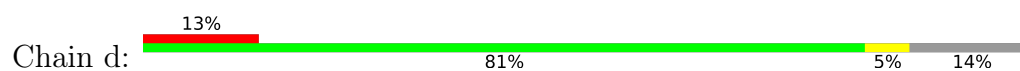
• Molecule 29: Small nuclear ribonucleoprotein Sm D2



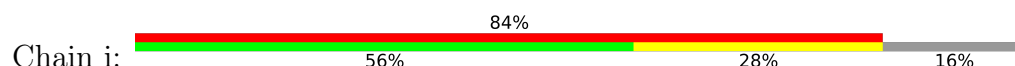
• Molecule 29: Small nuclear ribonucleoprotein Sm D2



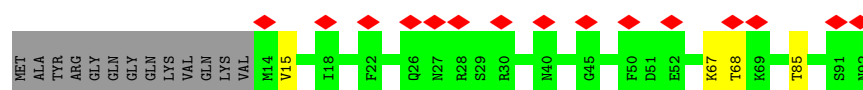
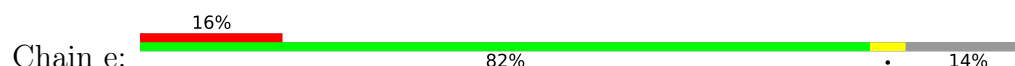
• Molecule 30: Small nuclear ribonucleoprotein F



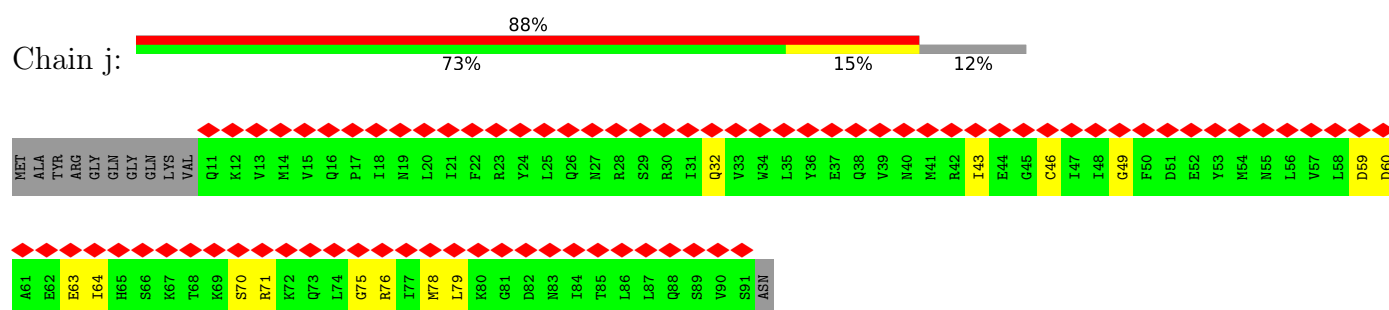
• Molecule 30: Small nuclear ribonucleoprotein F



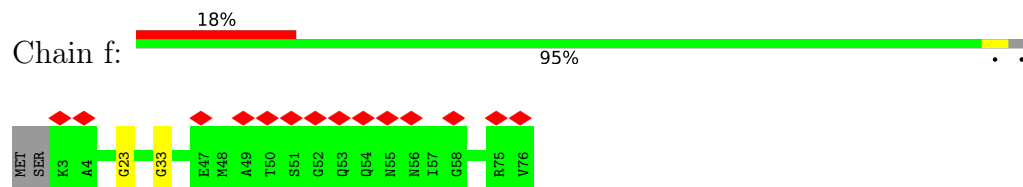
• Molecule 31: Small nuclear ribonucleoprotein E



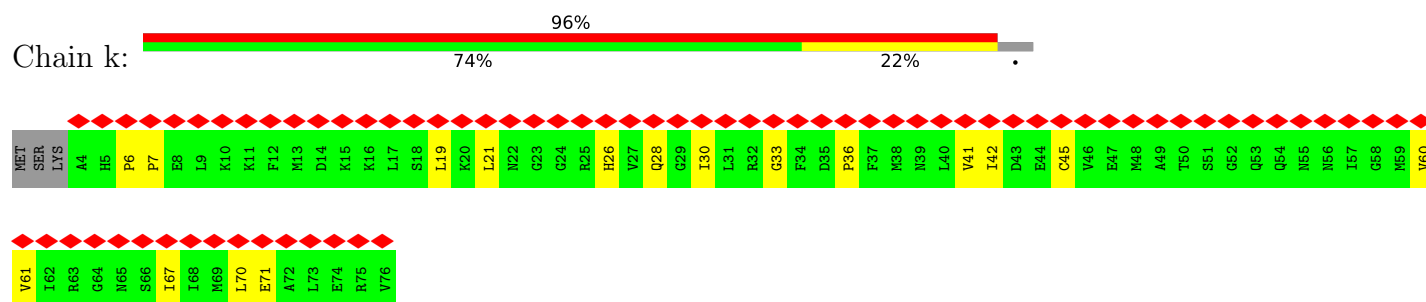
• Molecule 31: Small nuclear ribonucleoprotein E



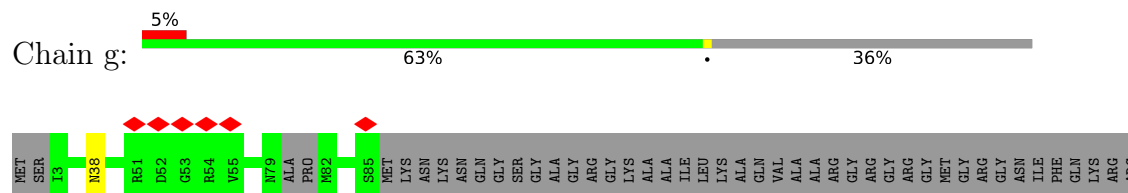
- Molecule 32: Small nuclear ribonucleoprotein G



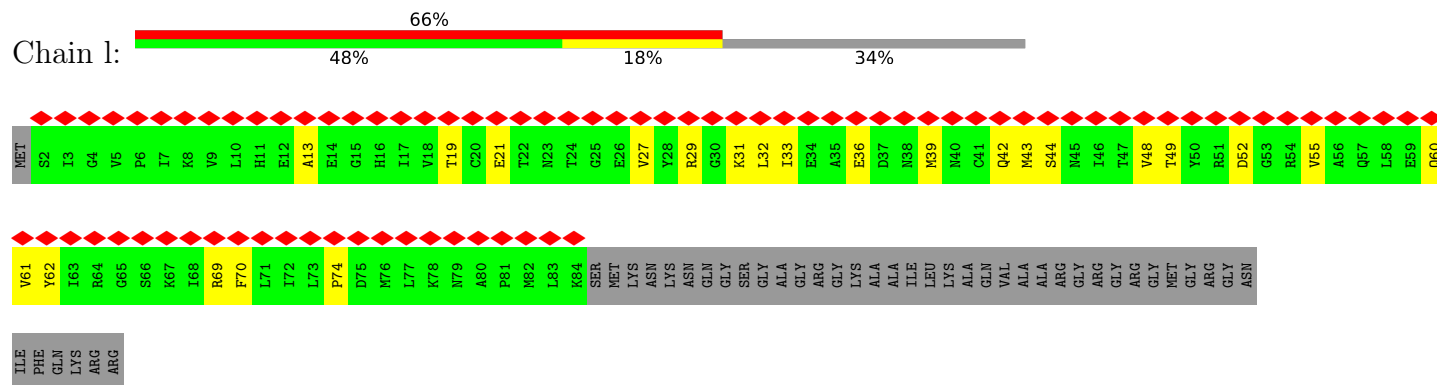
- Molecule 32: Small nuclear ribonucleoprotein G



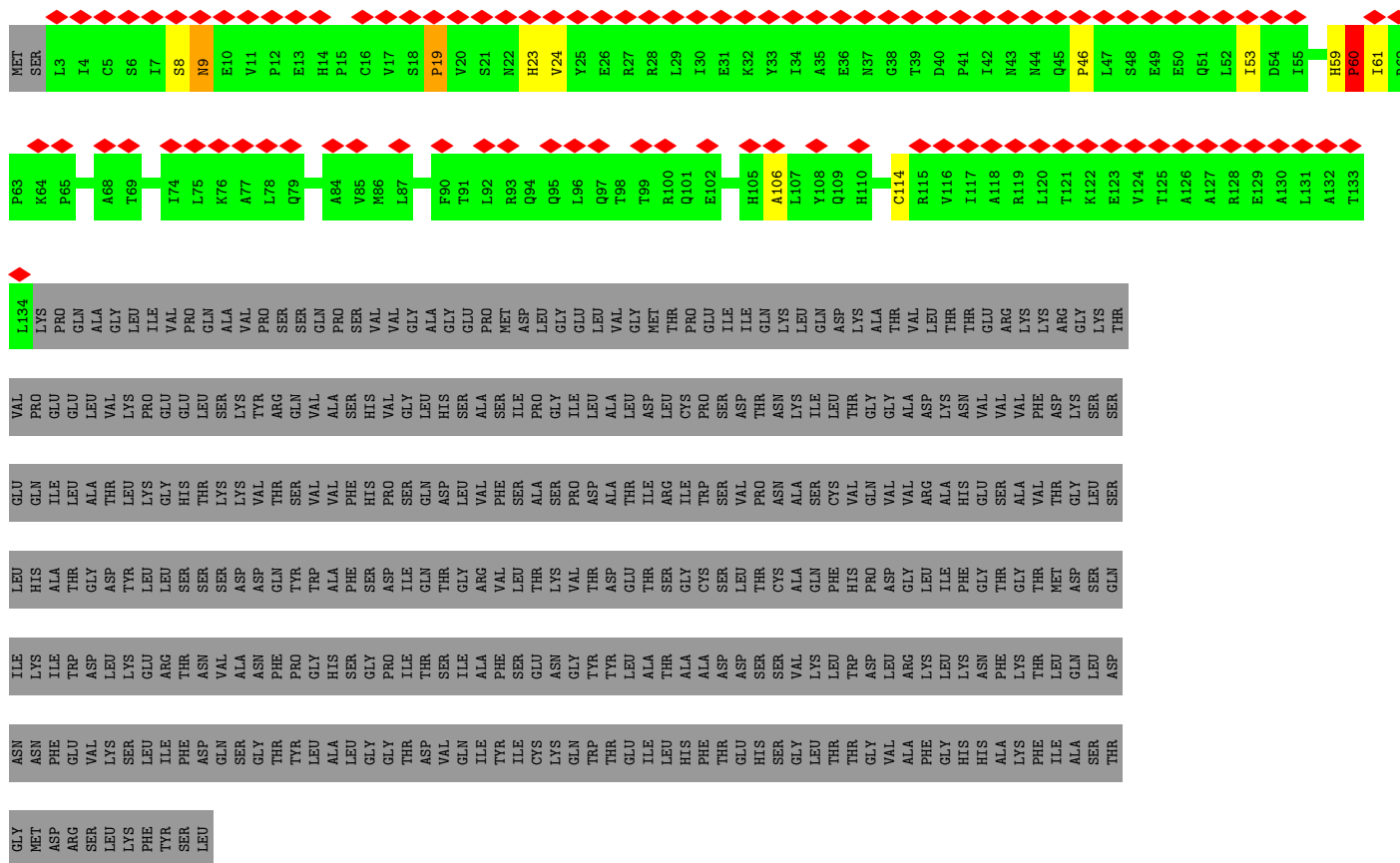
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



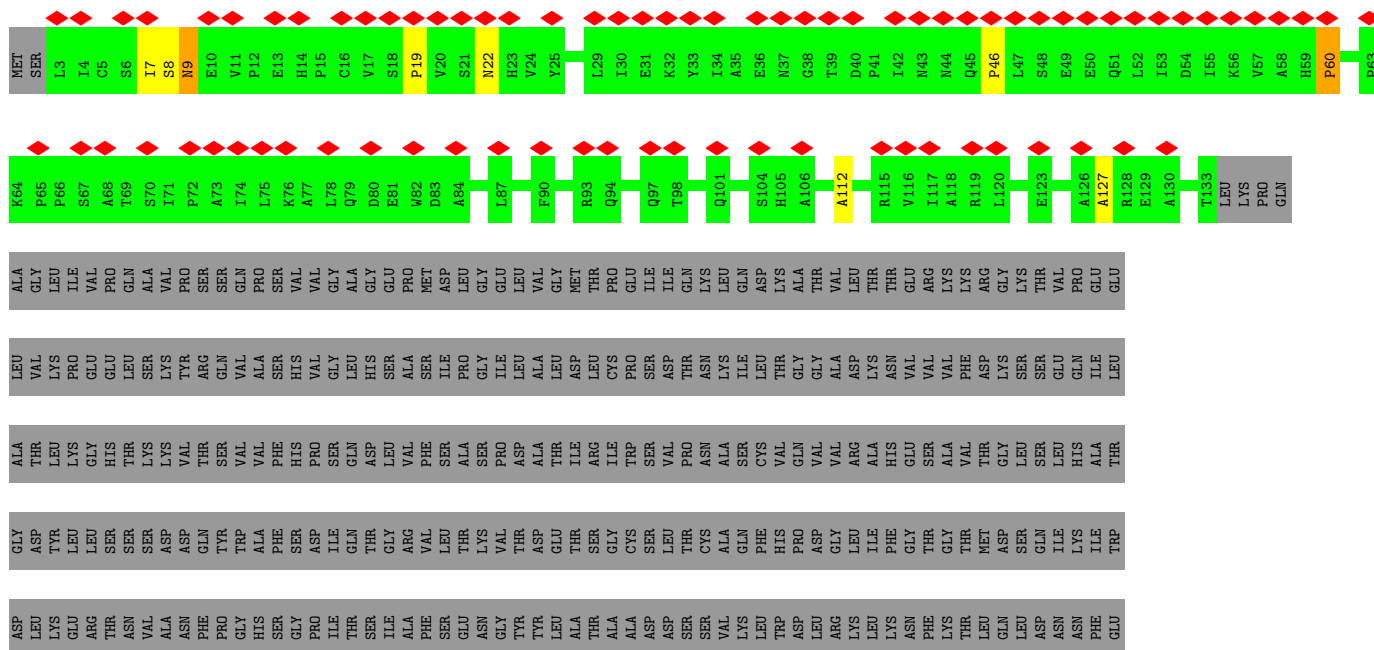
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



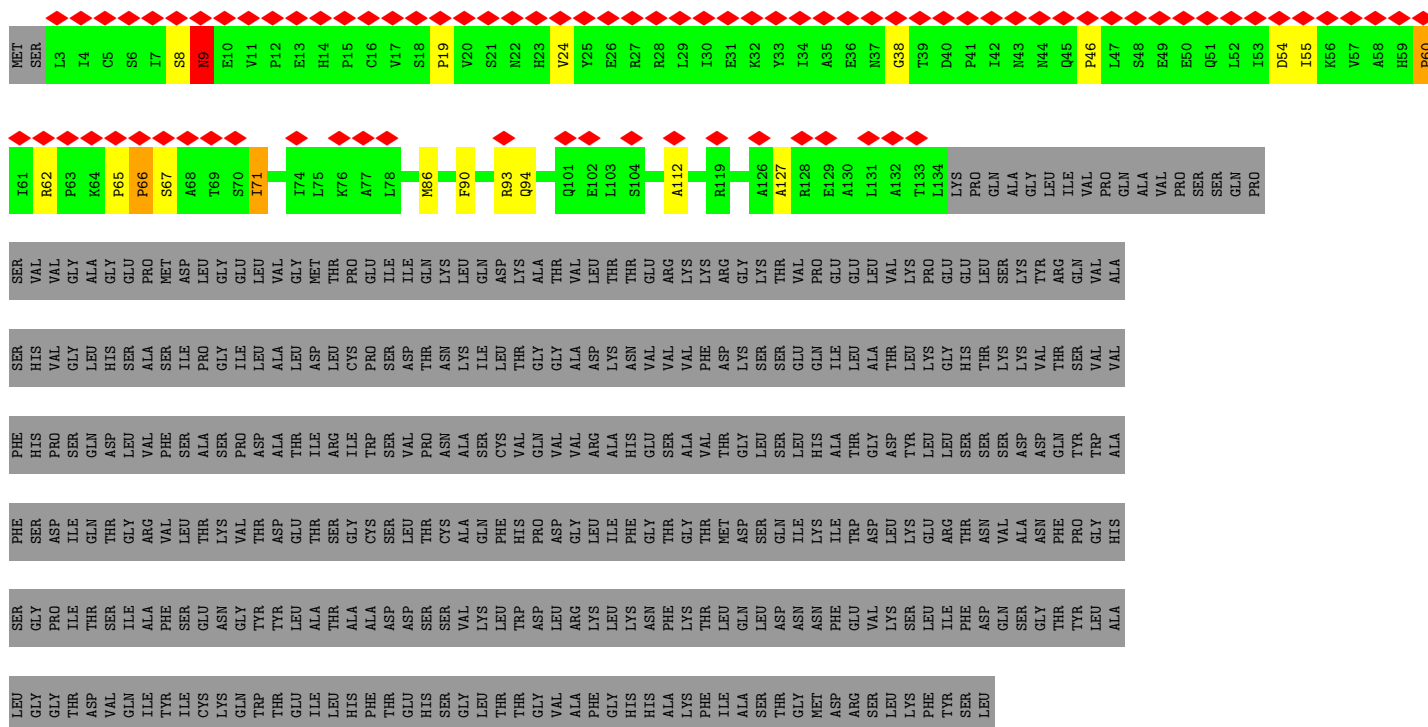
- Molecule 34: Pre-mRNA-processing factor 19



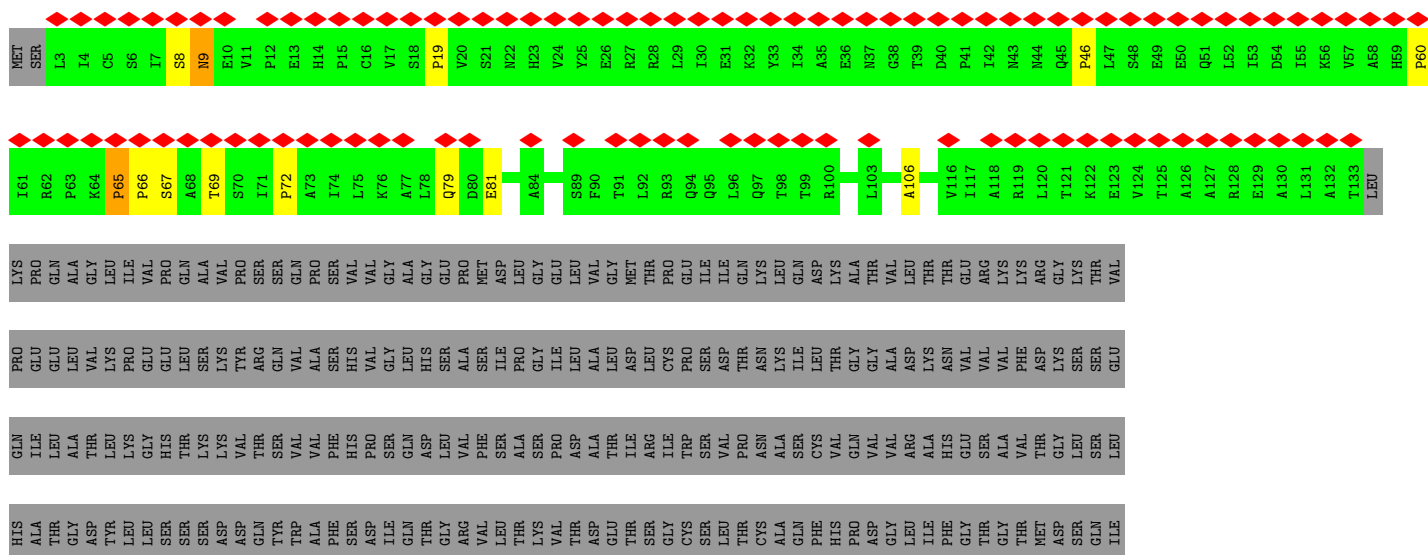
- Molecule 34: Pre-mRNA-processing factor 19

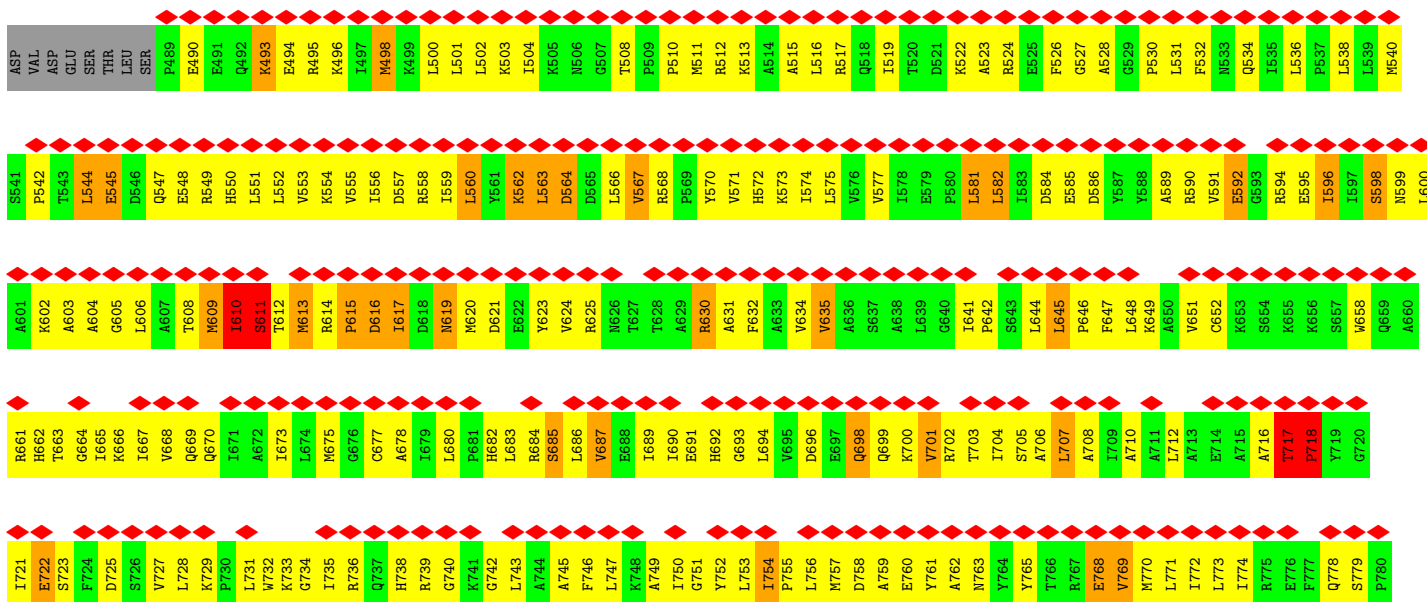


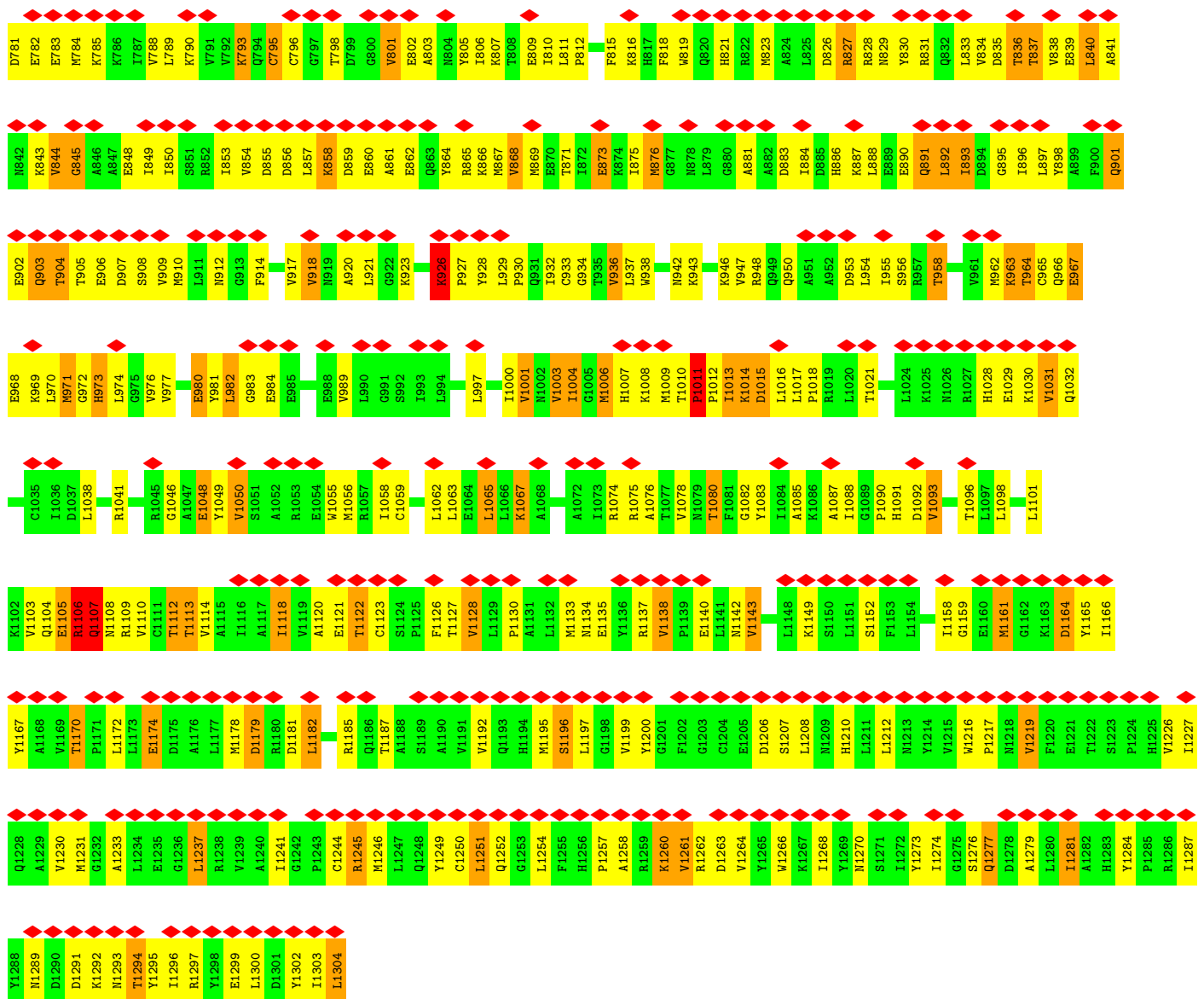
- Molecule 34: Pre-mRNA-processing factor 19



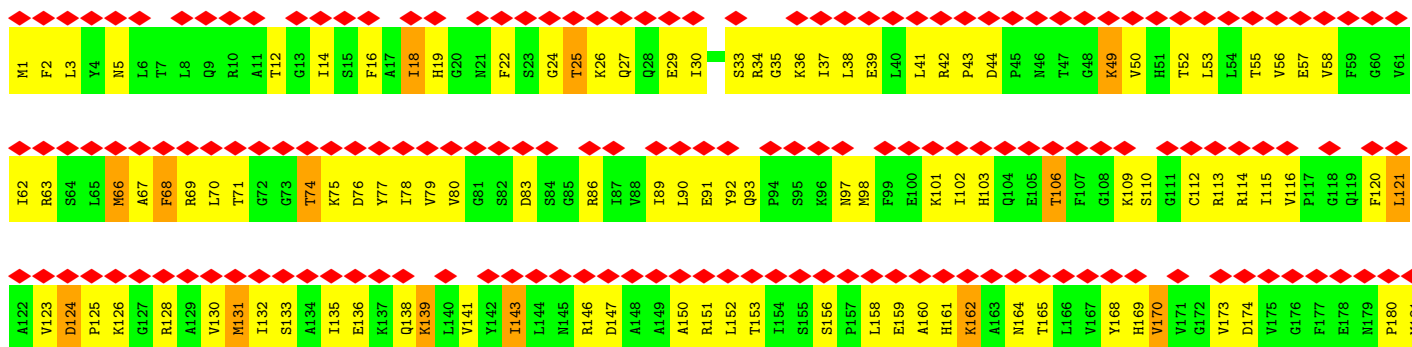
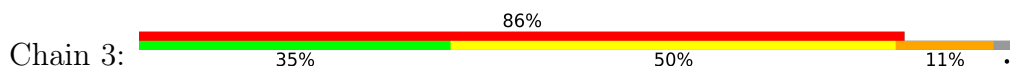
- Molecule 34: Pre-mRNA-processing factor 19







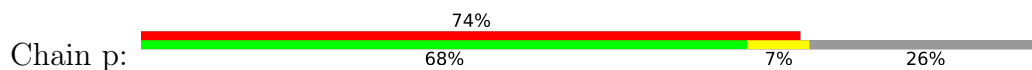
• Molecule 36: Splicing factor 3B subunit 3





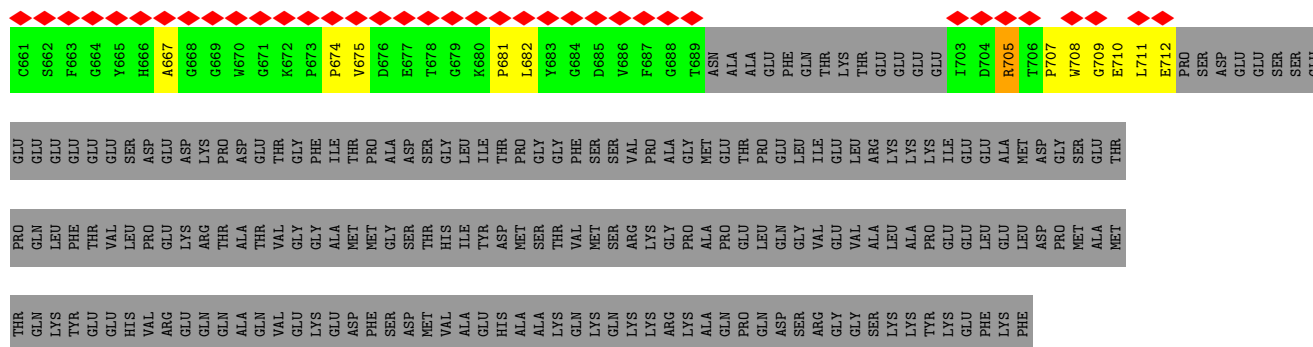


• Molecule 37: U2 small nuclear ribonucleoprotein B"

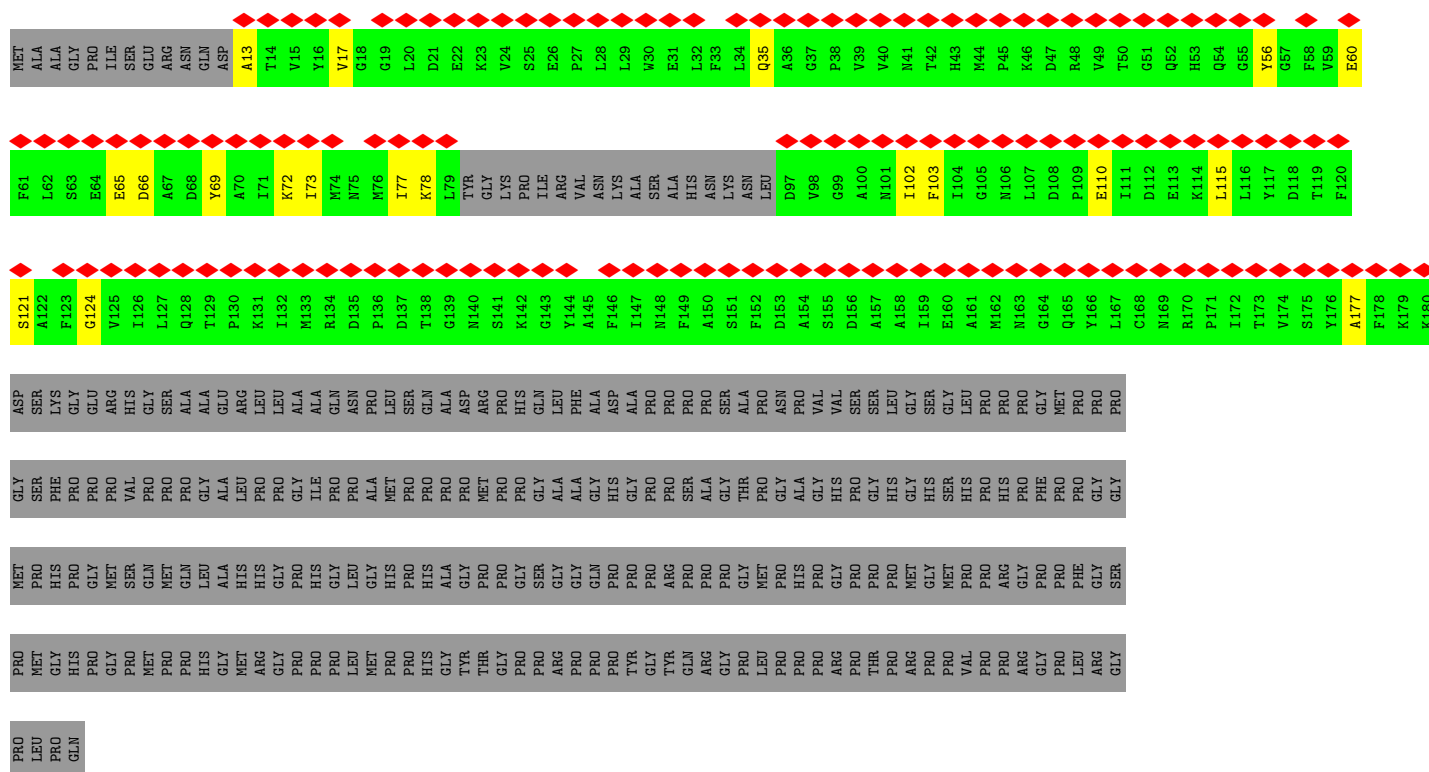


• Molecule 38: Splicing factor 3A subunit 3

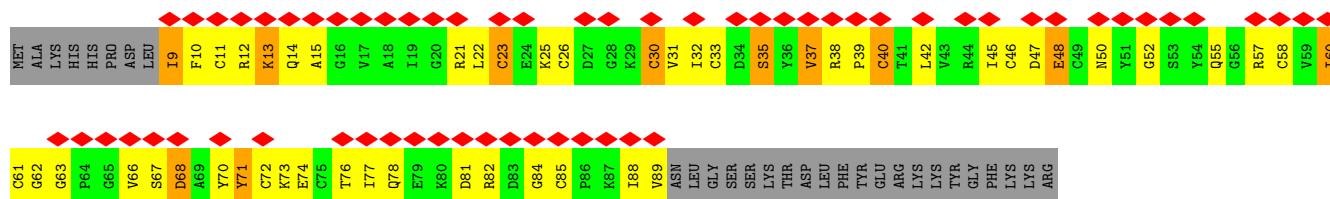
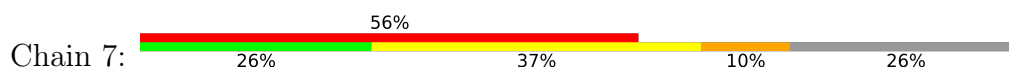




• Molecule 40: Splicing factor 3B subunit 4



• Molecule 41: PHD finger-like domain-containing protein 5A



• Molecule 42: Splicing factor 3B subunit 5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47352	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.422	Depositor
Minimum map value	-1.073	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.077, 1.077, 1.077	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, SEP, GTP, IHP, ZN

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	0.71	2/16774 (0.0%)	0.71	9/22749 (0.0%)
2	B	0.53	0/2303	0.44	0/3579
3	C	0.49	0/6873	0.65	3/9346 (0.0%)
4	E	0.35	0/2392	0.62	0/3242
5	F	0.57	0/2323	0.52	0/3619
6	G	0.48	1/1764 (0.1%)	0.95	14/2737 (0.5%)
7	H	0.39	1/3947 (0.0%)	0.61	7/6138 (0.1%)
8	I	0.22	0/3406	0.46	0/4767
9	J	0.59	1/3817 (0.0%)	0.75	3/5184 (0.1%)
10	K	0.63	0/188	0.72	0/248
11	L	0.52	0/2612	0.75	4/3548 (0.1%)
12	M	0.56	0/991	0.98	1/1325 (0.1%)
13	N	0.56	0/1210	0.67	0/1622
14	O	0.29	0/1447	0.50	0/2013
15	P	0.71	0/888	0.95	1/1177 (0.1%)
16	Q	0.13	0/5279	0.30	0/6583
17	R	0.51	0/2937	0.73	1/3945 (0.0%)
18	S	0.21	0/769	0.41	0/1063
19	T	0.94	0/2574	0.73	0/3511
20	U	0.37	0/424	0.55	0/582
21	V	0.26	0/2993	0.48	0/4088
22	W	0.57	0/2471	1.03	0/3437
23	X	0.35	1/6479 (0.0%)	0.66	9/8747 (0.1%)
24	Y	0.26	0/2605	0.56	0/3522
25	Z	0.59	1/768 (0.1%)	0.99	2/1067 (0.2%)
26	y	0.16	0/315	0.30	0/392
27	a	0.86	0/343	1.21	3/427 (0.7%)
27	m	0.24	0/416	0.58	0/581
28	b	0.89	0/327	1.11	0/407
28	n	0.24	0/404	0.57	0/564
29	c	1.14	0/387	1.22	1/482 (0.2%)
29	h	0.22	0/485	0.47	0/677

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	d	1.23	0/295	1.26	0/367
30	i	0.23	0/362	0.52	0/502
31	e	1.04	0/315	1.27	1/392 (0.3%)
31	j	0.22	0/403	0.50	0/561
32	f	0.87	0/295	1.05	0/367
32	k	0.24	0/366	0.54	0/509
33	g	0.80	0/322	1.01	0/399
33	l	0.23	0/417	0.56	0/581
34	q	0.62	0/658	1.04	3/919 (0.3%)
34	r	0.57	0/653	0.99	3/912 (0.3%)
34	s	0.60	1/658 (0.2%)	1.11	4/919 (0.4%)
34	t	0.62	0/653	0.94	3/912 (0.3%)
35	1	0.71	5/6609 (0.1%)	0.94	15/8947 (0.2%)
36	3	0.47	0/9408	0.73	5/12767 (0.0%)
37	p	0.22	0/847	0.49	0/1181
38	w	0.29	0/1029	0.57	0/1393
39	2	0.73	5/1833 (0.3%)	1.27	10/2469 (0.4%)
40	4	0.36	0/741	0.65	0/1027
41	7	0.46	0/621	0.74	0/833
42	5	0.65	0/654	0.78	0/885
43	o	0.22	0/821	0.55	0/1149
All	All	0.54	18/108871 (0.0%)	0.72	102/149360 (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	11
3	C	0	4
4	E	0	1
6	G	0	1
8	I	0	1
9	J	0	2
12	M	0	1
13	N	0	1
15	P	0	1
17	R	0	1
23	X	0	1
24	Y	0	1
29	c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	1	0	5
36	3	0	5
39	2	0	1
41	7	0	1
42	5	0	1
All	All	0	40

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	207	PRO	C-N	19.22	1.50	1.33
35	1	718	PRO	N-CA	17.61	1.69	1.47
23	X	701	ASN	C-N	16.48	1.51	1.34
35	1	926	LYS	C-N	14.68	1.50	1.34
39	2	642	PRO	N-CA	11.64	1.70	1.46

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2	640	GLY	CA-C-N	22.18	143.22	120.38
39	2	640	GLY	C-N-CA	22.18	143.22	120.38
9	J	207	PRO	CA-C-N	21.57	135.41	119.66
9	J	207	PRO	C-N-CA	21.57	135.41	119.66
39	2	645	TYR	CA-C-N	20.38	145.31	119.84

There are no chirality outliers.

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	PRO	Peptide
1	A	365	VAL	Peptide
1	A	433	GLU	Peptide
1	A	699	GLU	Peptide
1	A	855	ARG	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	16331	0	16276	650	0
2	B	2066	0	1047	93	0
3	C	6724	0	6696	332	0
4	E	2338	0	2275	158	0
5	F	2075	0	1048	86	0
6	G	1587	0	808	133	0
7	H	3539	0	1791	125	0
8	I	3387	0	1651	23	0
9	J	3773	0	2869	94	0
10	K	185	0	165	21	0
11	L	2584	0	2096	111	0
12	M	971	0	950	78	0
13	N	1184	0	1190	48	0
14	O	1447	0	638	31	0
15	P	876	0	875	53	0
16	Q	5288	0	1361	7	0
17	R	2915	0	2795	202	0
18	S	770	0	356	7	0
19	T	2507	0	2451	87	0
20	U	422	0	291	14	0
21	V	2959	0	2237	111	0
22	W	2473	0	1096	13	0
23	X	6357	0	6349	425	0
24	Y	2556	0	2492	150	0
25	Z	772	0	342	18	0
26	y	316	0	86	4	0
27	a	344	0	93	0	0
27	m	413	0	194	7	0
28	b	328	0	89	5	0
28	n	402	0	184	9	0
29	c	388	0	102	7	0
29	h	482	0	220	12	0
30	d	296	0	87	10	0
30	i	359	0	179	17	0
31	e	316	0	85	4	0
31	j	403	0	173	9	0
32	f	296	0	84	5	0
32	k	364	0	176	13	0
33	g	324	0	89	4	0
33	l	415	0	198	15	0
34	q	659	0	296	19	0
34	r	654	0	294	8	0
34	s	659	0	296	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	t	654	0	294	14	0
35	1	6486	0	6690	695	0
36	3	9220	0	9139	729	0
37	p	841	0	420	9	0
38	w	999	0	961	110	0
39	2	1803	0	1611	210	0
40	4	743	0	344	31	0
41	7	613	0	597	45	0
42	5	635	0	595	104	0
43	o	816	0	386	10	0
44	A	36	0	6	5	0
45	C	32	0	12	0	0
46	C	1	0	0	0	0
46	F	6	0	0	0	0
47	7	3	0	0	0	0
47	K	1	0	0	0	0
47	N	3	0	0	0	0
All	All	106396	0	84125	4419	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 23.

The worst 5 of 4419 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)
39:2:594:GLY:HA2	39:2:597:PHE:CE2	1.21	1.65
35:1:1056:MET:HG2	39:2:561:MET:SD	1.37	1.64
39:2:635:ALA:CB	40:4:73:ILE:HA	1.32	1.59
39:2:635:ALA:HB3	40:4:73:ILE:CA	1.10	1.55
39:2:641:PRO:N	39:2:641:PRO:CA	1.69	1.55

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	1961/2335 (84%)	1760 (90%)	186 (10%)	15 (1%)	16	45
3	C	854/972 (88%)	751 (88%)	100 (12%)	3 (0%)	30	60
4	E	297/357 (83%)	270 (91%)	27 (9%)	0	100	100
8	I	662/855 (77%)	575 (87%)	86 (13%)	1 (0%)	43	71
9	J	525/848 (62%)	487 (93%)	33 (6%)	5 (1%)	12	40
10	K	22/343 (6%)	18 (82%)	4 (18%)	0	100	100
11	L	375/802 (47%)	358 (96%)	16 (4%)	1 (0%)	36	65
12	M	112/243 (46%)	105 (94%)	5 (4%)	2 (2%)	6	29
13	N	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
14	O	288/420 (69%)	262 (91%)	26 (9%)	0	100	100
15	P	97/229 (42%)	89 (92%)	7 (7%)	1 (1%)	12	40
16	Q	1304/1485 (88%)	1279 (98%)	25 (2%)	0	100	100
17	R	370/536 (69%)	336 (91%)	31 (8%)	3 (1%)	16	45
18	S	156/166 (94%)	144 (92%)	12 (8%)	0	100	100
19	T	318/514 (62%)	300 (94%)	18 (6%)	0	100	100
20	U	68/2752 (2%)	63 (93%)	4 (6%)	1 (2%)	8	32
21	V	458/908 (50%)	433 (94%)	25 (6%)	0	100	100
22	W	497/579 (86%)	473 (95%)	24 (5%)	0	100	100
23	X	778/1041 (75%)	728 (94%)	49 (6%)	1 (0%)	48	75
24	Y	318/492 (65%)	296 (93%)	22 (7%)	0	100	100
25	Z	147/225 (65%)	138 (94%)	5 (3%)	4 (3%)	4	22
26	y	77/301 (26%)	76 (99%)	1 (1%)	0	100	100
27	a	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
27	m	80/240 (33%)	72 (90%)	8 (10%)	0	100	100
28	b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
28	n	78/119 (66%)	67 (86%)	11 (14%)	0	100	100
29	c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
29	h	91/118 (77%)	82 (90%)	9 (10%)	0	100	100
30	d	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
30	i	70/86 (81%)	64 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
31	j	79/92 (86%)	73 (92%)	6 (8%)	0	100	100
32	f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
32	k	71/76 (93%)	63 (89%)	8 (11%)	0	100	100
33	g	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
33	l	81/126 (64%)	70 (86%)	11 (14%)	0	100	100
34	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2	13
34	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	7	31
34	s	130/504 (26%)	114 (88%)	8 (6%)	8 (6%)	1	9
34	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3	20
35	1	814/1304 (62%)	703 (86%)	101 (12%)	10 (1%)	10	37
36	3	1165/1217 (96%)	992 (85%)	172 (15%)	1 (0%)	48	75
37	p	163/225 (72%)	147 (90%)	15 (9%)	1 (1%)	21	52
38	w	119/501 (24%)	107 (90%)	12 (10%)	0	100	100
39	2	246/895 (28%)	208 (85%)	34 (14%)	4 (2%)	7	31
40	4	147/424 (35%)	129 (88%)	18 (12%)	0	100	100
41	7	79/110 (72%)	65 (82%)	14 (18%)	0	100	100
42	5	75/86 (87%)	64 (85%)	11 (15%)	0	100	100
43	o	160/255 (63%)	136 (85%)	24 (15%)	0	100	100
All	All	14418/25294 (57%)	13114 (91%)	1231 (8%)	73 (0%)	26	55

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1417	PRO
9	J	202	GLU
17	R	164	PRO
25	Z	78	PRO
25	Z	86	ARG

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	1768/2108 (84%)	1578 (89%)	190 (11%)	6	24
3	C	747/866 (86%)	652 (87%)	95 (13%)	4	18
4	E	256/300 (85%)	219 (86%)	37 (14%)	3	14
8	I	24/749 (3%)	24 (100%)	0	100	100
9	J	239/751 (32%)	222 (93%)	17 (7%)	13	40
10	K	20/294 (7%)	16 (80%)	4 (20%)	1	6
11	L	171/709 (24%)	149 (87%)	22 (13%)	4	17
12	M	104/209 (50%)	92 (88%)	12 (12%)	5	21
13	N	130/130 (100%)	121 (93%)	9 (7%)	14	41
14	O	3/361 (1%)	3 (100%)	0	100	100
15	P	95/203 (47%)	75 (79%)	20 (21%)	1	5
17	R	282/457 (62%)	242 (86%)	40 (14%)	3	14
19	T	273/441 (62%)	244 (89%)	29 (11%)	6	24
20	U	21/2432 (1%)	17 (81%)	4 (19%)	1	7
21	V	188/838 (22%)	155 (82%)	33 (18%)	2	9
23	X	682/897 (76%)	610 (89%)	72 (11%)	6	24
24	Y	286/451 (63%)	244 (85%)	42 (15%)	3	14
27	m	4/177 (2%)	4 (100%)	0	100	100
28	n	3/101 (3%)	3 (100%)	0	100	100
29	h	5/110 (4%)	5 (100%)	0	100	100
30	i	4/74 (5%)	4 (100%)	0	100	100
31	j	1/84 (1%)	1 (100%)	0	100	100
32	k	3/66 (4%)	3 (100%)	0	100	100
33	l	3/101 (3%)	3 (100%)	0	100	100
35	1	700/1104 (63%)	577 (82%)	123 (18%)	2	9
36	3	1018/1051 (97%)	791 (78%)	227 (22%)	1	5
37	p	8/195 (4%)	8 (100%)	0	100	100
38	w	104/446 (23%)	87 (84%)	17 (16%)	2	11
39	2	151/776 (20%)	126 (83%)	25 (17%)	2	11
41	7	69/95 (73%)	53 (77%)	16 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	5	68/77 (88%)	48 (71%)	20 (29%)	0	2
43	o	6/218 (3%)	6 (100%)	0	100	100
All	All	7436/16871 (44%)	6382 (86%)	1054 (14%)	5	14

5 of 1054 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	3	945	VAL
36	3	1062	THR
36	3	943	THR
42	5	27	THR
15	P	32	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
23	X	917	GLN
36	3	179	ASN
24	Y	115	ASN
35	1	886	HIS
36	3	264	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	28 (29%)	3 (3%)
5	F	96/107 (89%)	42 (43%)	6 (6%)
6	G	77/220 (35%)	44 (57%)	12 (15%)
7	H	163/188 (86%)	69 (42%)	9 (5%)
All	All	432/632 (68%)	183 (42%)	30 (6%)

5 of 183 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	U
2	B	20	G
2	B	21	A
2	B	22	U

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	G	100	C
7	H	45	C
6	G	103	U
7	H	165	A
7	H	30	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	SEP	R	232	17	8,9,10	1.57	1 (12%)	7,12,14	1.14	0
17	SEP	R	224	17	8,9,10	1.47	1 (12%)	7,12,14	1.25	1 (14%)

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
17	SEP	R	232	17	-	3/6/8/10	-
17	SEP	R	224	17	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	232	SEP	P-O1P	3.35	1.60	1.50
17	R	224	SEP	P-O1P	3.26	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	224	SEP	OG-CB-CA	2.44	110.52	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	R	224	SEP	N-CA-CB-OG
17	R	224	SEP	C-CA-CB-OG
17	R	232	SEP	C-CA-CB-OG
17	R	232	SEP	CB-OG-P-O2P
17	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 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	$\# Z > 2$
45	GTP	C	1500	46	33,34,34	1.12	3 (9%)	50,54,54	1.96	12 (24%)
44	IHP	A	3000	-	36,36,36	1.02	1 (2%)	60,60,60	2.04	15 (25%)

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
45	GTP	C	1500	46	-	5/22/38/38	0/3/3/3
44	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C5-N7	-2.35	1.34	1.39
44	A	3000	IHP	P5-O15	2.17	1.63	1.59
45	C	1500	GTP	C5-C6	-2.03	1.37	1.44
45	C	1500	GTP	O4'-C4'	-2.01	1.40	1.45

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C	1500	GTP	C5-C4-N3	-6.08	118.72	128.39
45	C	1500	GTP	C2-N3-C4	4.85	120.65	112.30
44	A	3000	IHP	O41-P1-O31	4.76	125.65	107.80
44	A	3000	IHP	O15-C5-C4	4.72	118.81	108.76
44	A	3000	IHP	C5-C4-C3	4.57	120.46	110.43

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C3-C4-O14-P4
45	C	1500	GTP	C4'-C5'-O5'-PA
45	C	1500	GTP	C3'-C4'-C5'-O5'
45	C	1500	GTP	O4'-C4'-C5'-O5'
44	A	3000	IHP	C1-C6-O16-P6

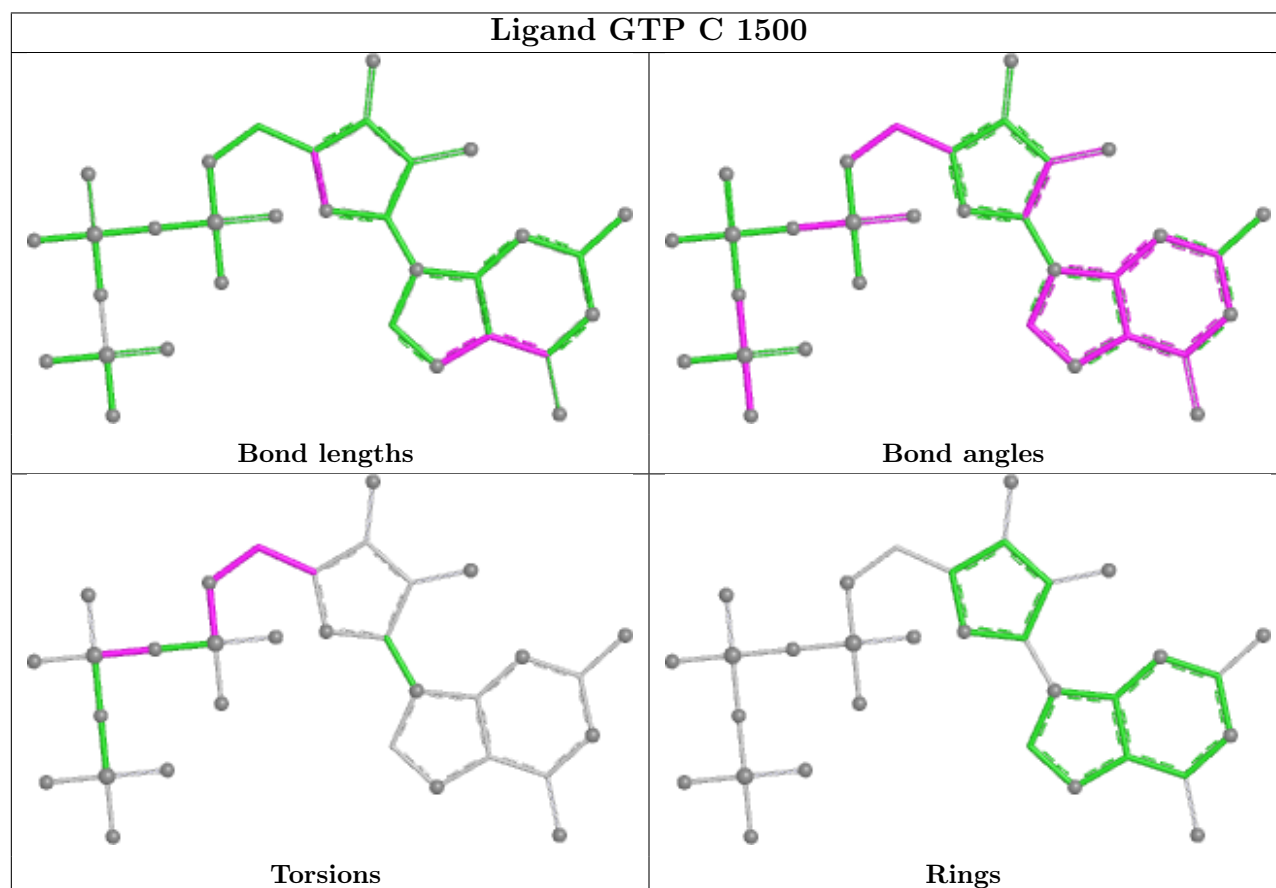
There are no ring outliers.

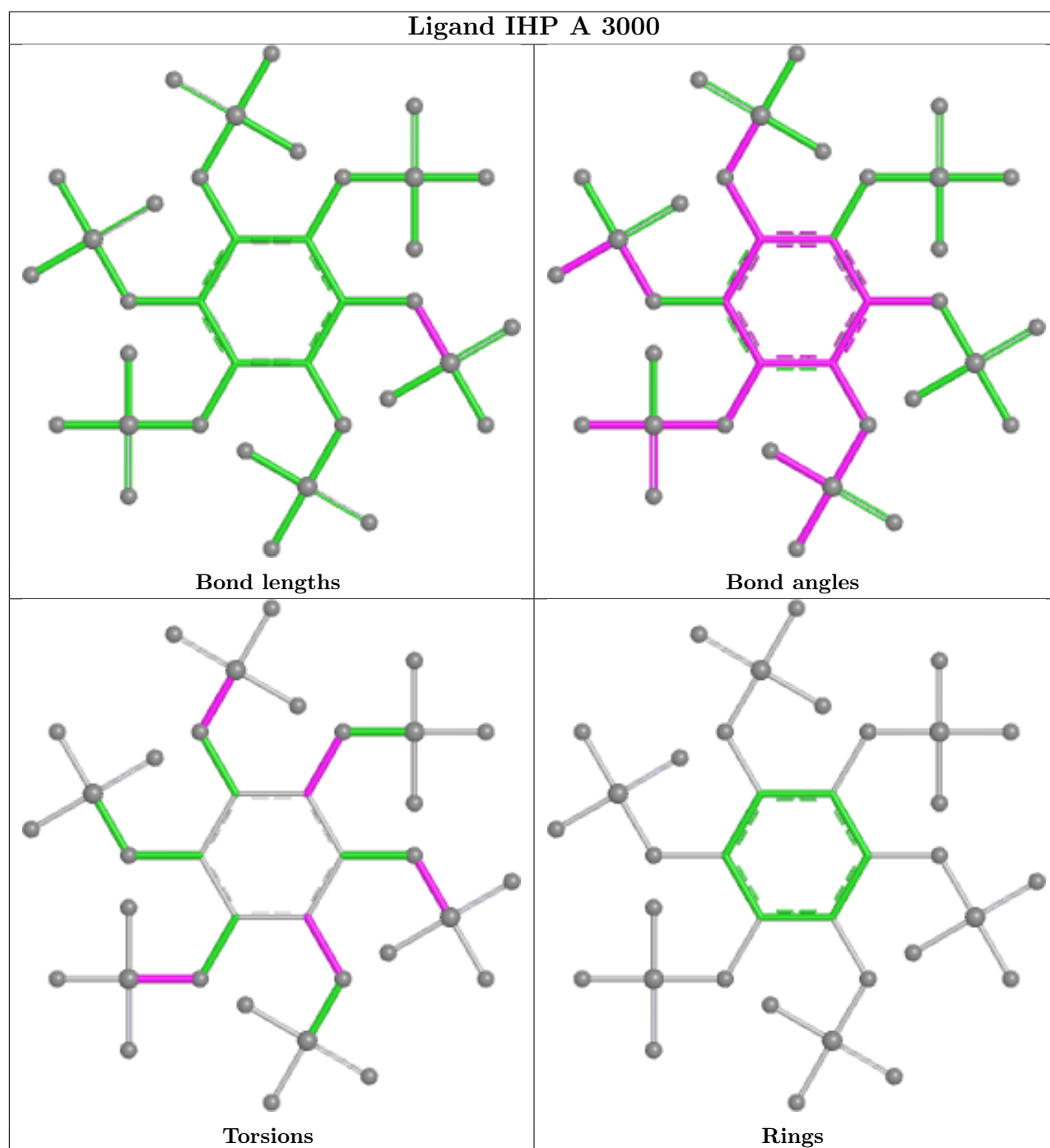
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	A	3000	IHP	5	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.

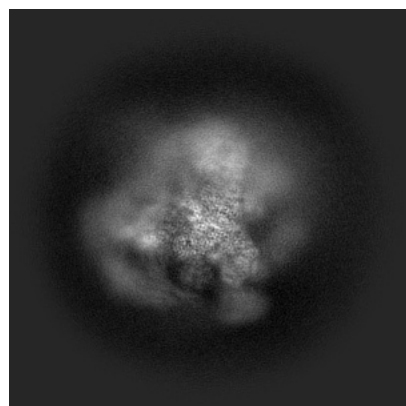
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35110. These allow visual inspection of the internal detail of the map and identification of artifacts.

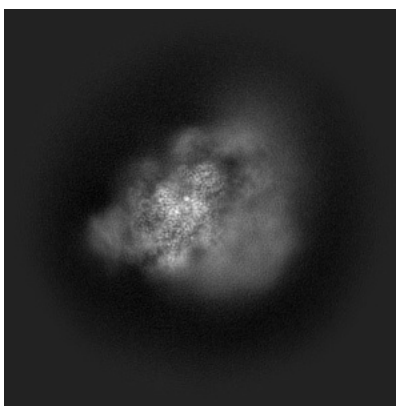
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

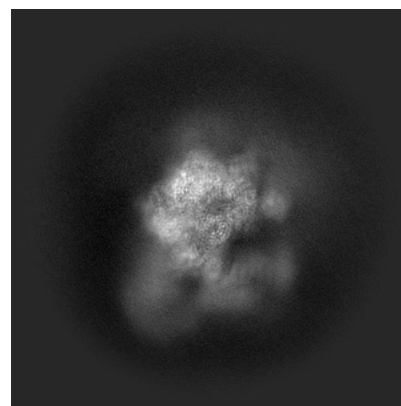
6.1.1 Primary map



X

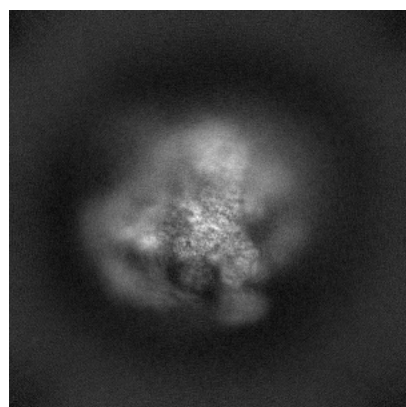


Y

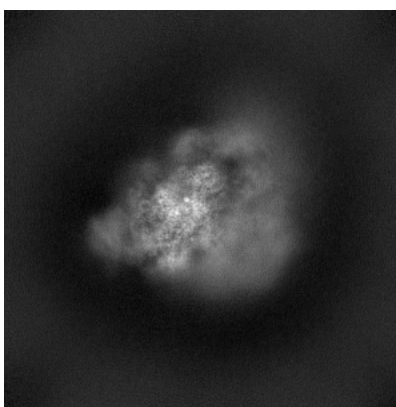


Z

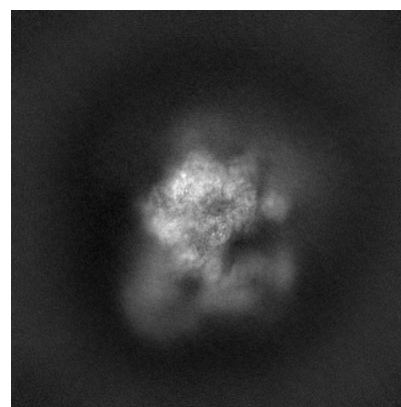
6.1.2 Raw map



X



Y

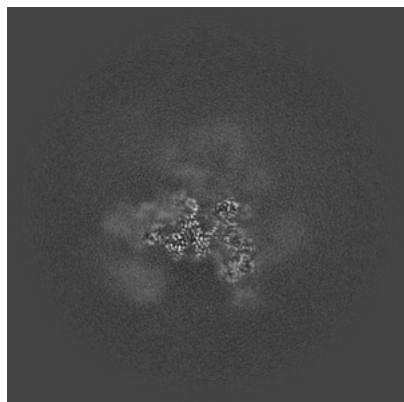


Z

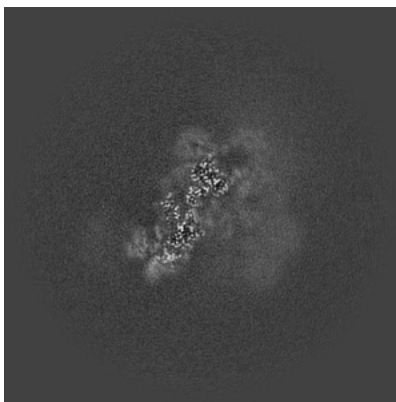
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

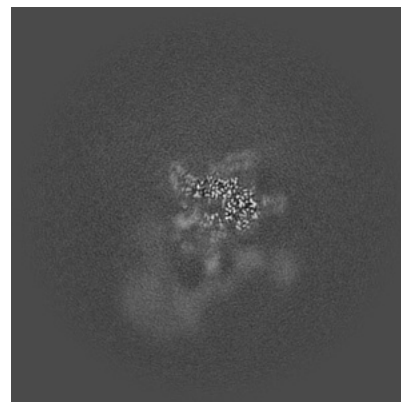
6.2.1 Primary map



X Index: 240

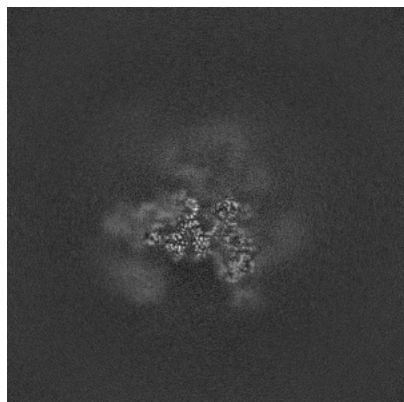


Y Index: 240

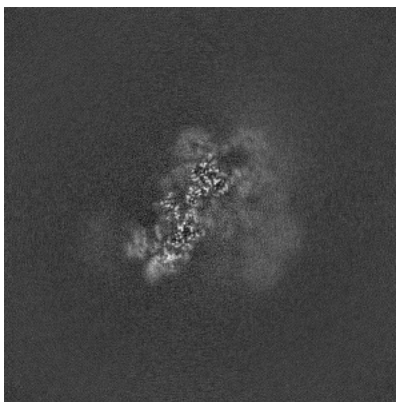


Z Index: 240

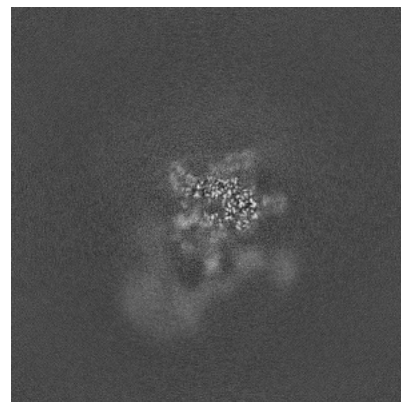
6.2.2 Raw map



X Index: 240



Y Index: 240

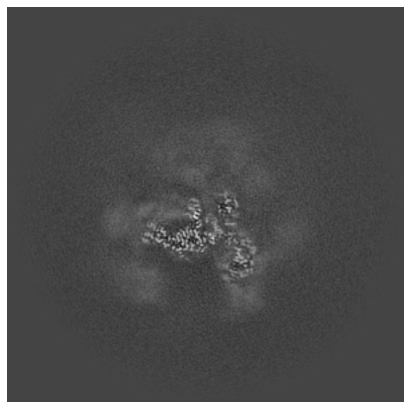


Z Index: 240

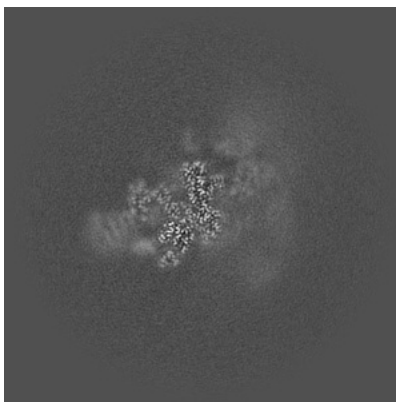
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

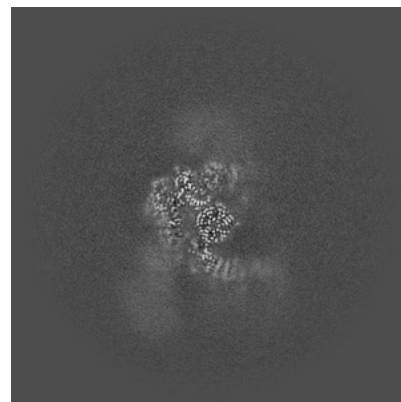
6.3.1 Primary map



X Index: 235

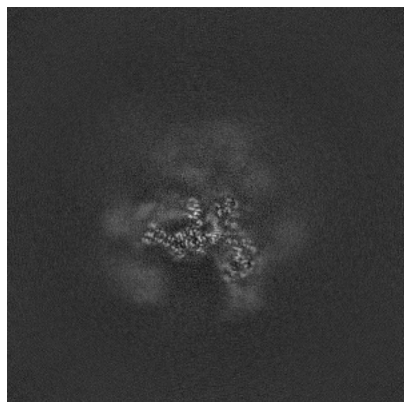


Y Index: 262

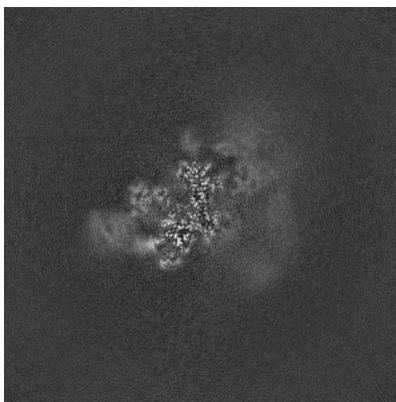


Z Index: 200

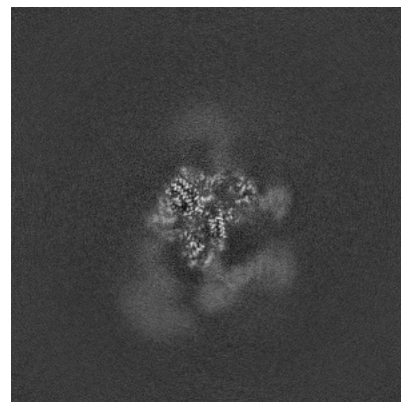
6.3.2 Raw map



X Index: 236



Y Index: 259

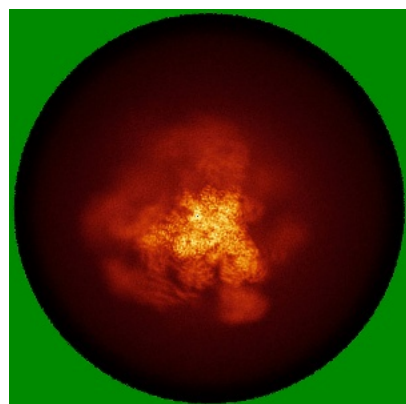


Z Index: 218

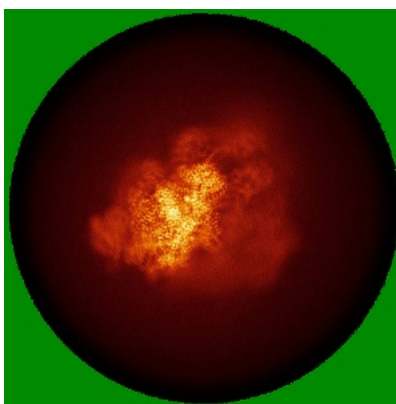
The images above show the largest variance slices of the map in three orthogonal directions.

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

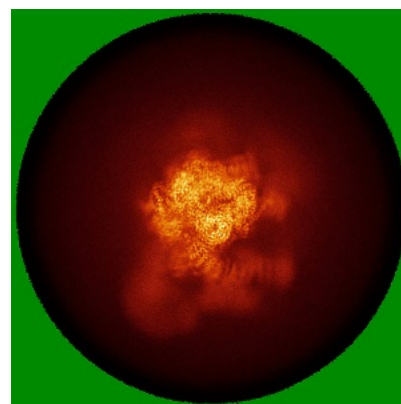
6.4.1 Primary map



X

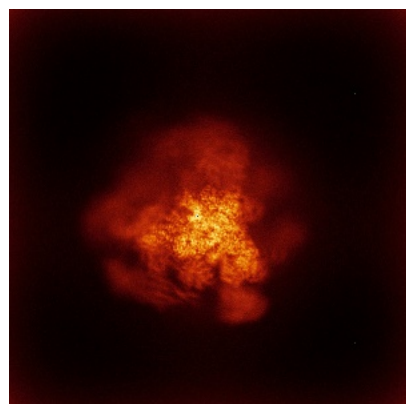


Y

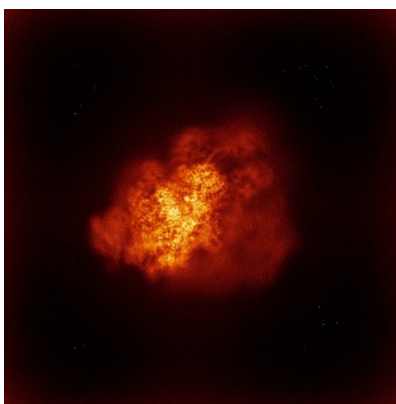


Z

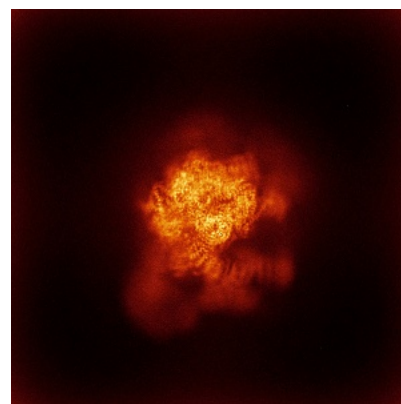
6.4.2 Raw map



X



Y

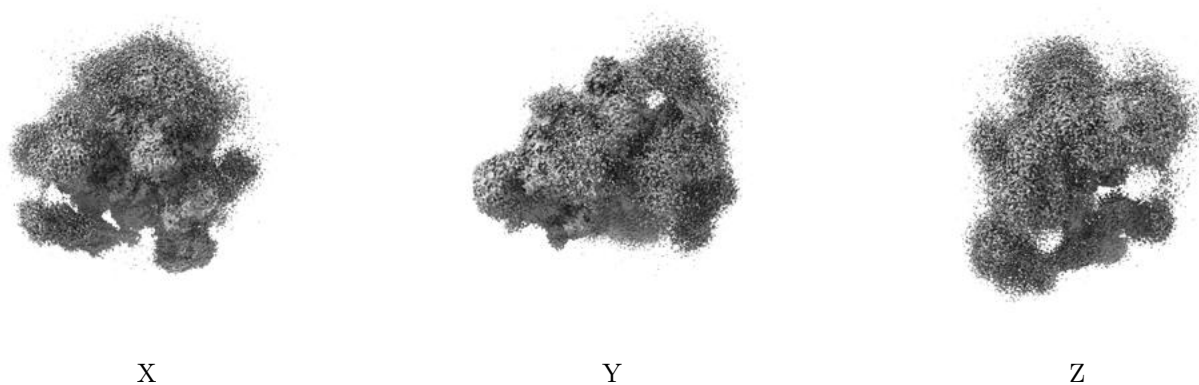


Z

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.

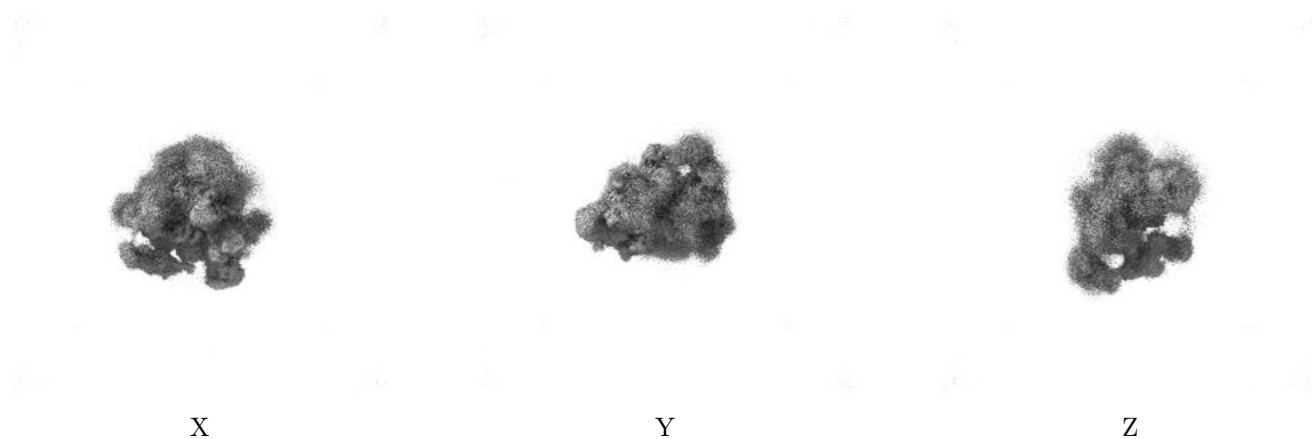
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

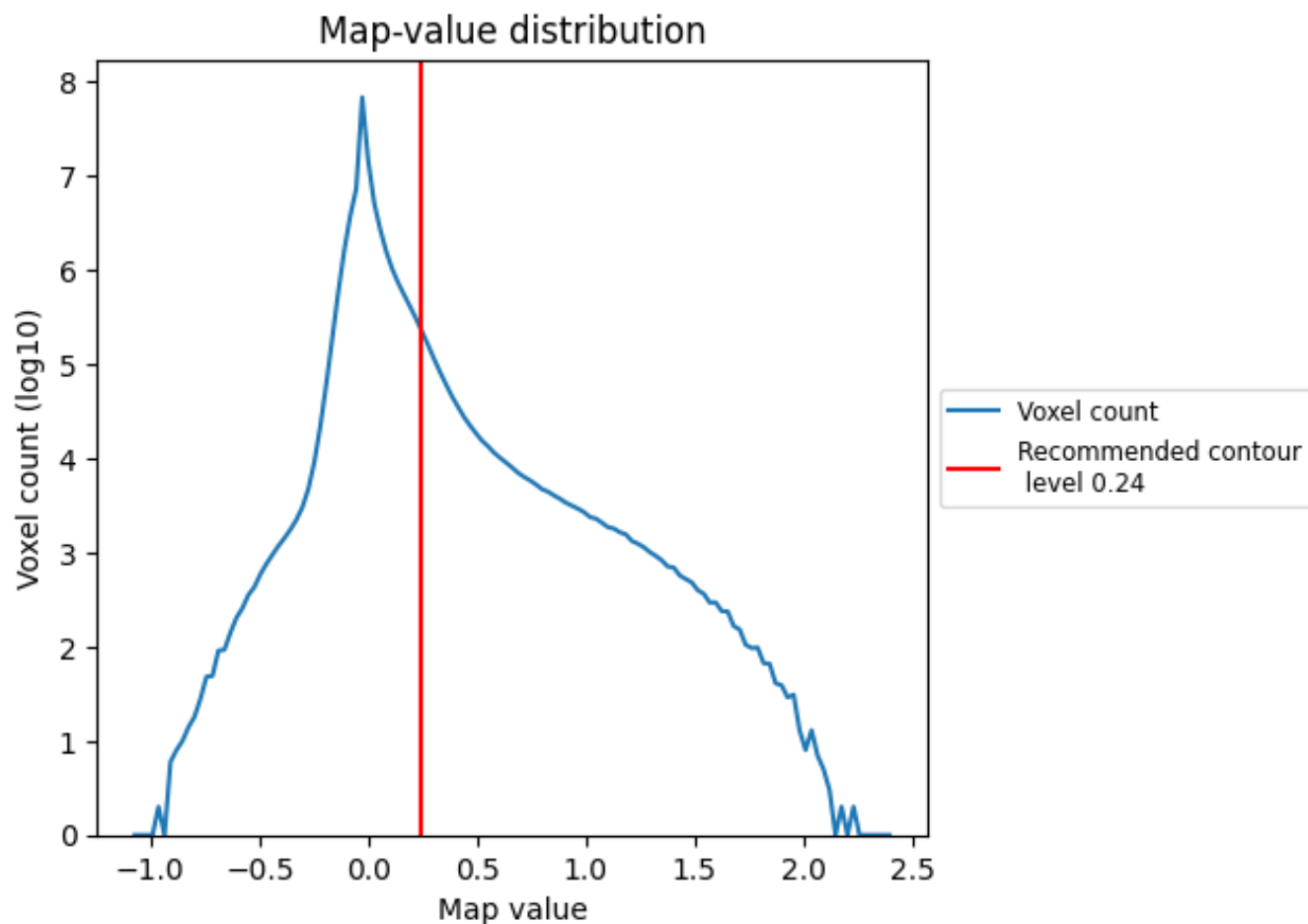
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

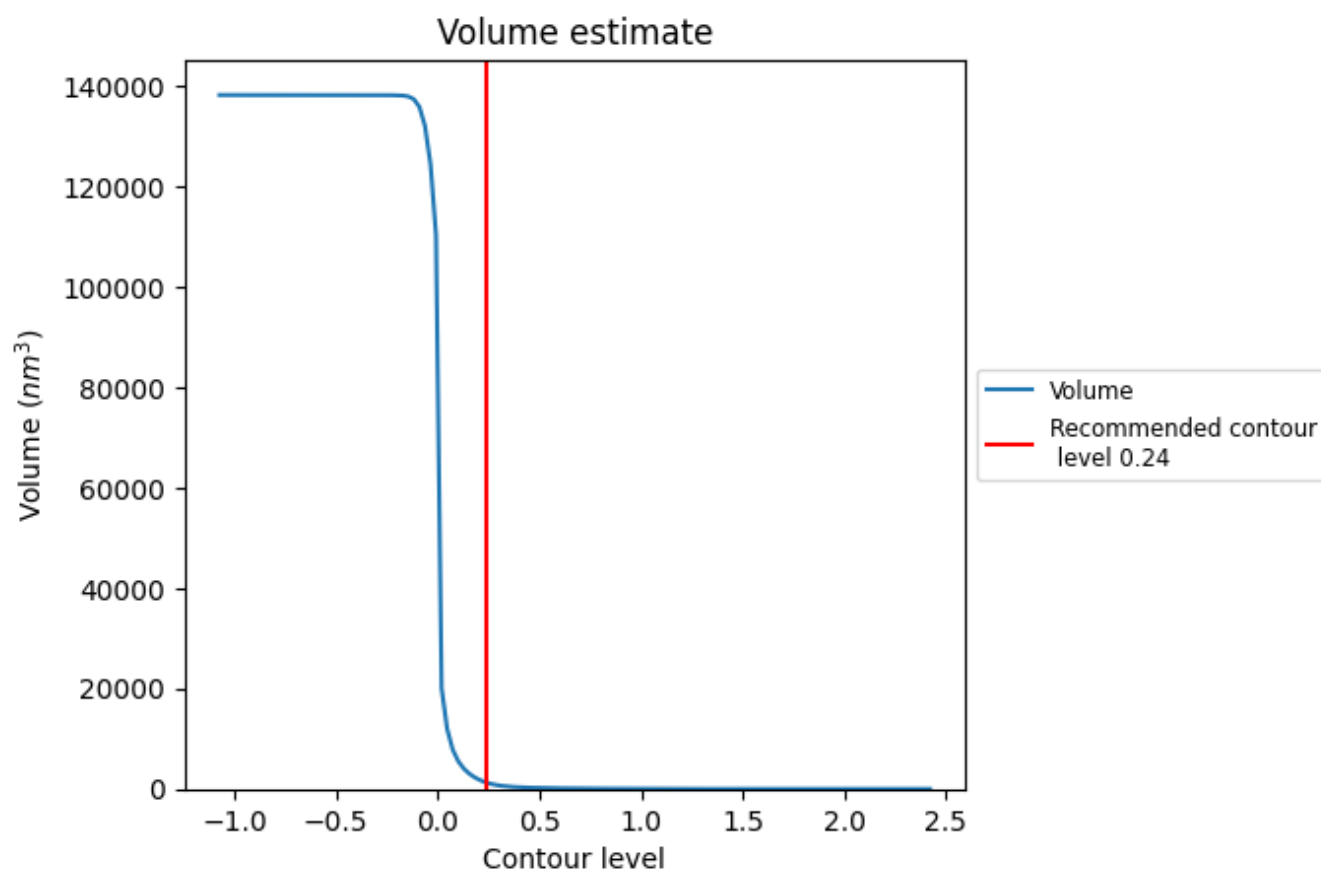
This section contains the results of statistical analysis of the map.

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.

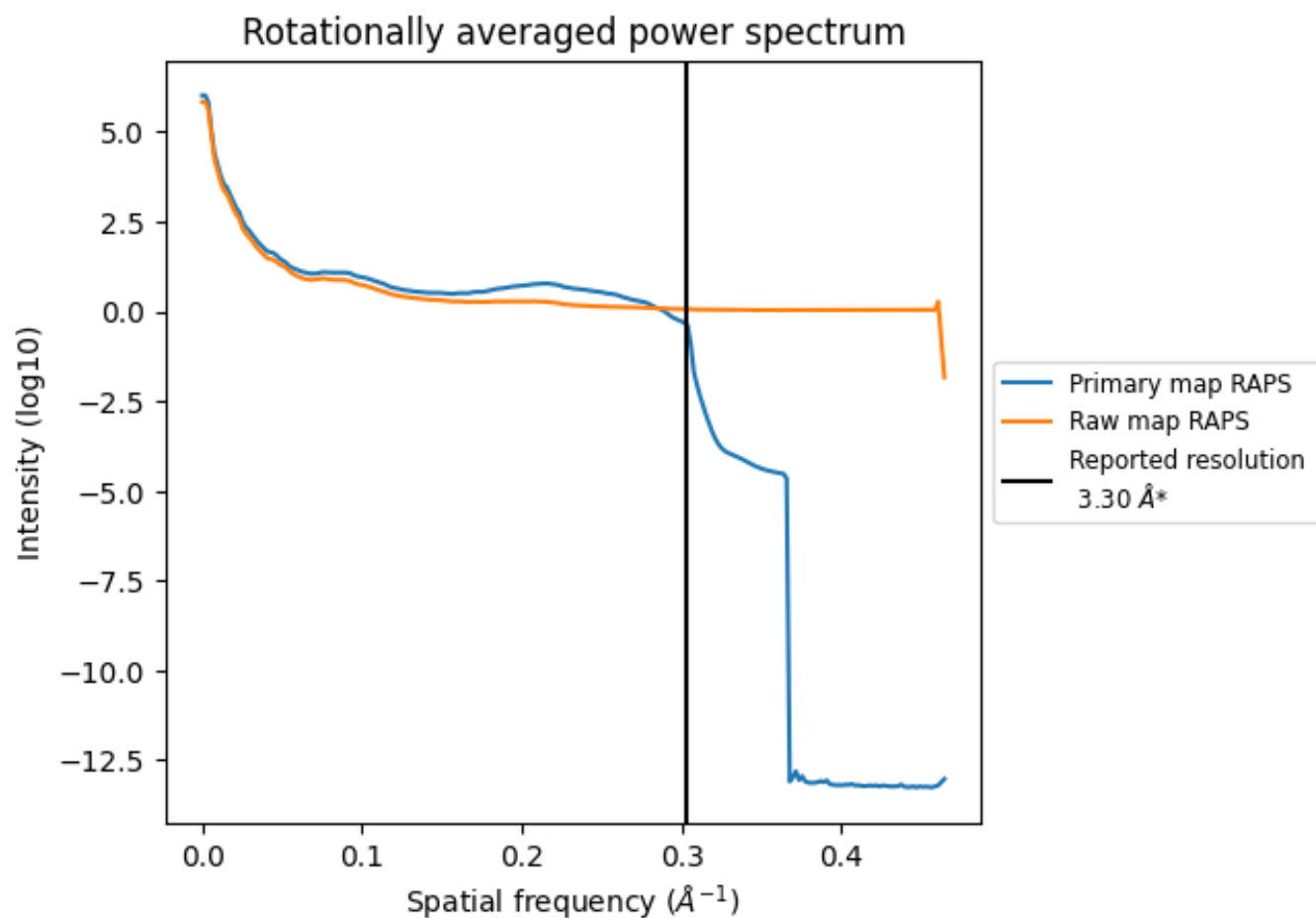
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1270 nm^3 ; this corresponds to an approximate mass of 1147 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 ⓘ

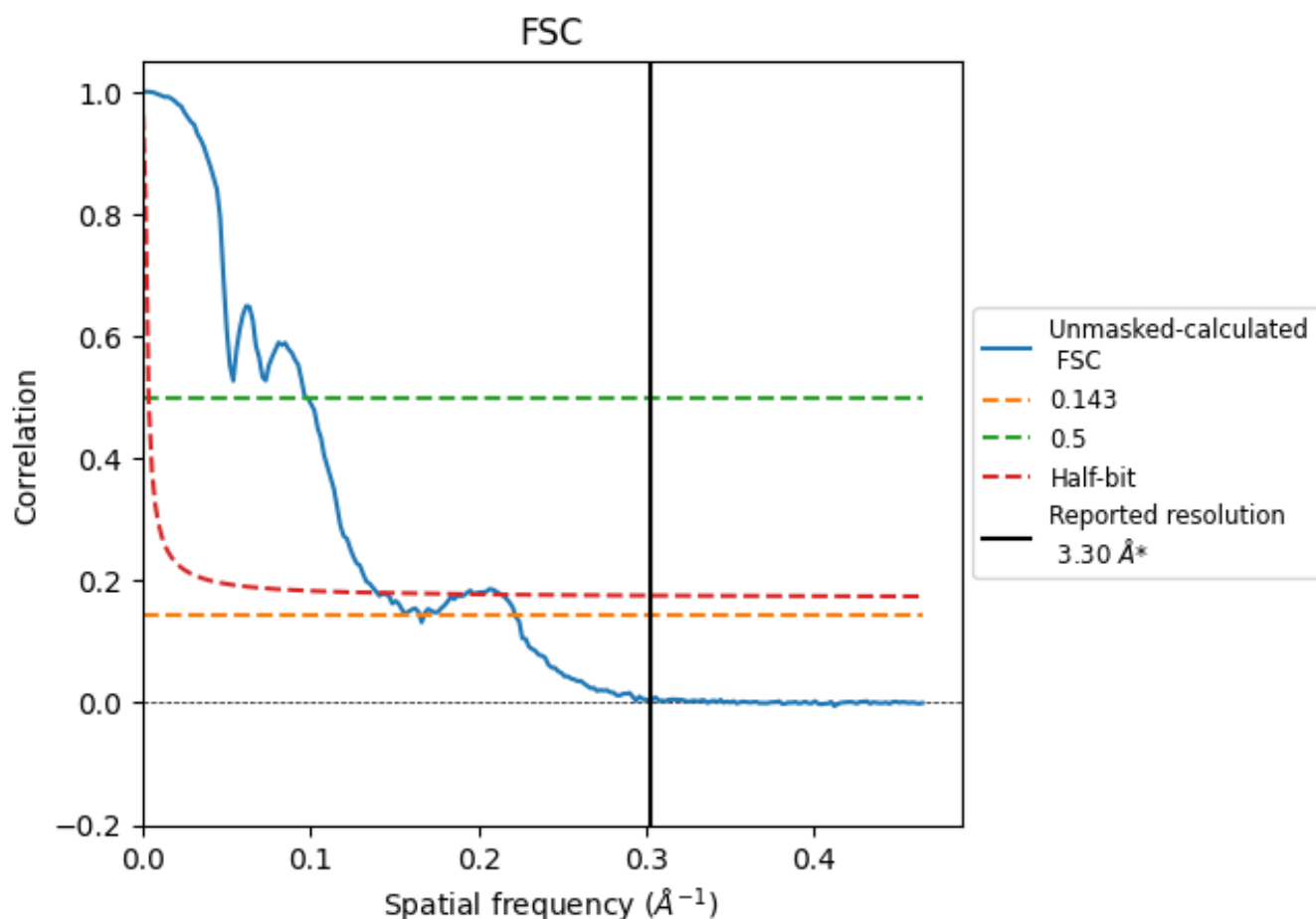


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

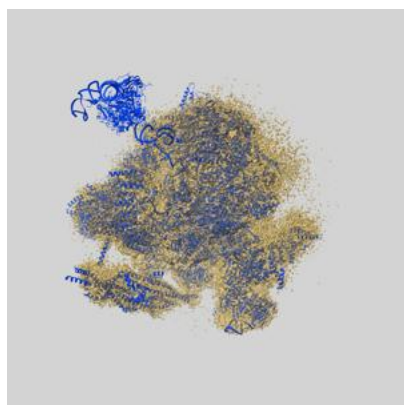
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.06	10.25	7.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.06 differs from the reported value 3.3 by more than 10 %

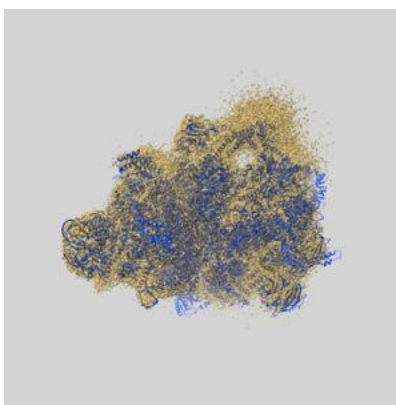
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35110 and PDB model 8I0U. Per-residue inclusion information can be found in section 3 on page 14.

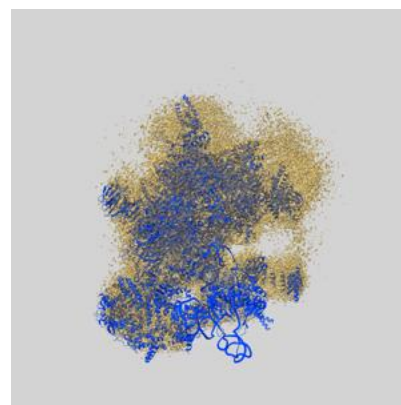
9.1 Map-model overlay [i](#)



X



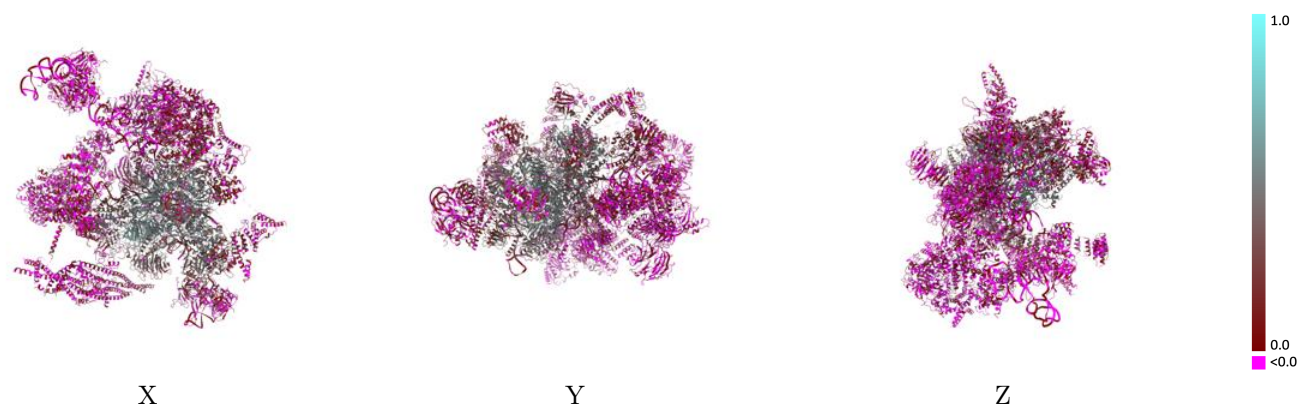
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

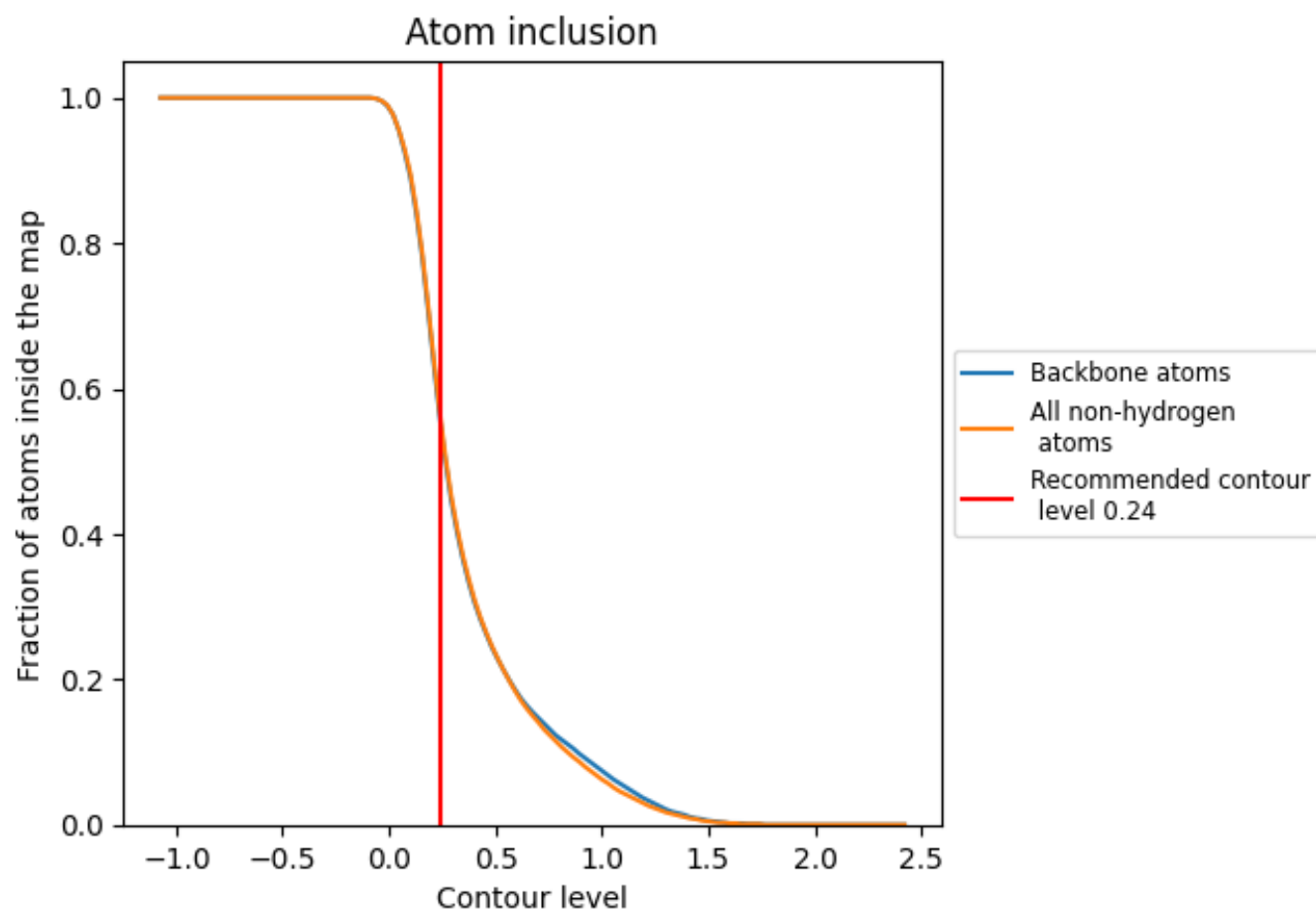


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5640	 0.1950
1	 0.3010	 0.0610
2	 0.1370	 0.0270
3	 0.1540	 0.0140
4	 0.0820	 0.0730
5	 0.1900	 0.0420
7	 0.2500	 0.0280
A	 0.8410	 0.4130
B	 0.8840	 0.2950
C	 0.9260	 0.3690
E	 0.9220	 0.3010
F	 0.8990	 0.3120
G	 0.7160	 0.1670
H	 0.2260	 0.0480
I	 0.4770	 0.0620
J	 0.7680	 0.2640
K	 0.5190	 0.1250
L	 0.7490	 0.2670
M	 0.7880	 0.2730
N	 0.9310	 0.4230
O	 0.8600	 0.3210
P	 0.8790	 0.4120
Q	 0.1160	 0.0130
R	 0.8110	 0.3270
S	 0.8680	 0.1710
T	 0.9810	 0.5470
U	 0.6150	 0.2860
V	 0.5210	 0.1380
W	 0.3650	 0.0840
X	 0.6580	 0.1520
Y	 0.7070	 0.1480
Z	 0.5870	 0.0830
a	 0.7410	 0.1220
b	 0.8170	 0.0700
c	 0.6830	 0.0420



Continued on next page...

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Chain	Atom inclusion	Q-score
d	 0.7370	 0.0720
e	 0.7220	 0.0200
f	 0.7030	 0.0640
g	 0.8890	 0.1830
h	 0.0000	 -0.0280
i	 0.0000	 0.0130
j	 0.0000	 0.0080
k	 0.0000	 -0.0330
l	 0.0020	 0.0010
m	 0.0000	 0.0040
n	 0.0000	 0.0480
o	 0.0000	 -0.0050
p	 0.0020	 0.0130
q	 0.2560	 0.0050
r	 0.4110	 0.0430
s	 0.3380	 0.0280
t	 0.2160	 0.0160
w	 0.1590	 0.0060
y	 0.1270	 0.0130