



wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 02:26 pm BST

PDB ID : 9ESI / pdb_00009esi
EMDB ID : EMD-19942
Title : Structure of a B-state intermediate committed to discard (Bd-II state)
Authors : Soni, K.; Wild, K.; Sinning, I.
Deposited on : 2024-03-26
Resolution : 3.10 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:

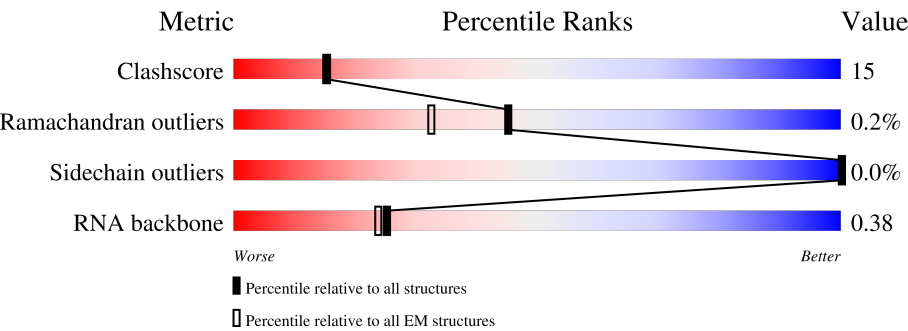
EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

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 3.10 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.




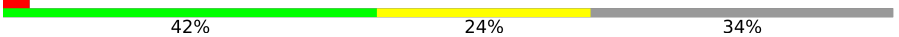
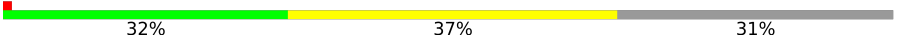


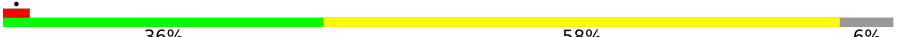




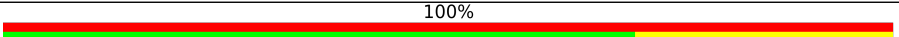


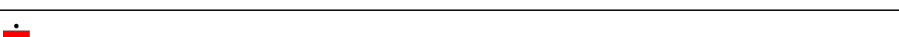
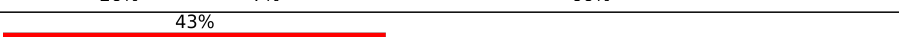
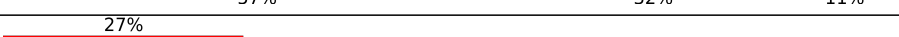



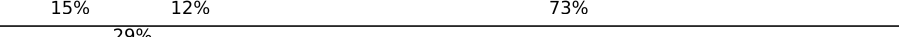
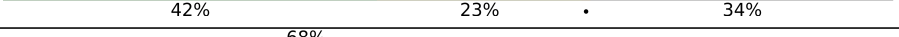




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	e	384	
2	p	299	
3	2	186	
4	5	120	
5	A	2363	
6	B	984	
7	C	340	



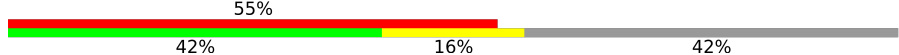
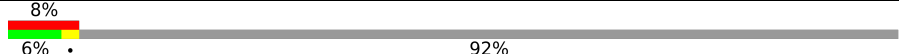
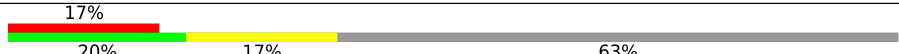

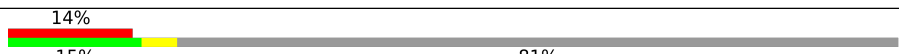

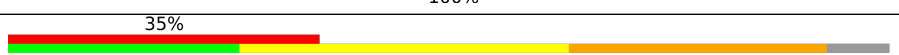
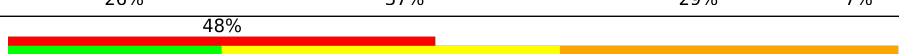

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Mol	Chain	Length	Quality of chain
8	D	97	
9	E	147	
10	F	117	
11	G	115	
12	H	84	
13	I	78	
14	J	77	
15	K	473	
16	L	557	
17	M	354	
18	N	1284	
19	O	146	
20	P	388	
21	Q	265	
22	R	674	
23	S	488	
23	T	488	
23	U	488	
23	V	488	
24	W	757	
25	X	790	
26	Y	229	
27	Z	187	
28	a	558	
29	b	293	

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Mol	Chain	Length	Quality of chain
30	c	887	
31	d	155	
32	m	797	
33	n	361	
34	y	534	
35	z	647	
36	r	346	
37	q	56	
38	6	99	
39	1	29	
40	f	22	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 98220 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 Stress response protein bis1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	e	166	Total	C	N	O	S	0	0
			1329	838	221	268	2		

- Molecule 2 is a protein called Protein saf4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	p	60	Total	C	N	O	0	0
			487	304	89	94		

- Molecule 3 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	24	Total	C	N	O	P	0	0
			500	224	79	173	24		

- Molecule 4 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	102	Total	C	N	O	P	0	0
			2149	963	358	726	102		

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1986	Total	C	N	O	S	0	0
			16424	10532	2887	2938	67		

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	918	Total	C	N	O	S	0	0
			7298	4650	1251	1362	35		

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	301	Total	C	N	O	S	0	0
			2328	1460	415	442	11		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	96	Total	C	N	O	S	0	0
			760	470	147	136	7		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	97	Total	C	N	O	S	0	0
			726	462	129	130	5		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	81	Total	C	N	O	S	0	0
			638	407	109	118	4		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	102	Total	C	N	O	S	0	0
			819	516	150	149	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	80	Total	C	N	O	S	0	0
			652	422	113	115	2		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	73	Total	C	N	O	S	0	0
			574	373	95	104	2		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	391	Total	C	N	O	S	0	0
			3053	1925	551	563	14		

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	246	Total	C	N	O	S	0	0
			1954	1221	364	363	6		

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	234	Total	C	N	O	S	0	0
			1818	1131	329	343	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	1284	Total	C	N	O	S	0	0
			10461	6715	1732	1969	45		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	271	Total	C	N	O	S	0	0
			2178	1354	397	416	11		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	603	Total	C	N	O	S	0	0
			5108	3280	892	913	23		

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	132	Total	C	N	O	S	0	0
			1055	664	181	207	3		
23	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		
23	U	430	Total	C	N	O	S	0	0
			2870	1806	492	563	9		
23	V	131	Total	C	N	O	S	0	0
			1044	655	180	206	3		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	498	Total	C	N	O	S	0	0
			4126	2577	750	788	11		

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	654	Total	C	N	O	S	0	0
			5467	3534	918	996	19		

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	98	Total	C	N	O	0	0
			845	522	157	166		

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	155	Total	C	N	O	S	0	0
			1232	766	220	243	3		

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	152	Total	C	N	O	S	0	0
			1035	644	185	205	1		

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	104	Total	C	N	O	S	0	0
			822	503	148	169	2		

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	204	Total	C	N	O	S	0	0
			1678	1071	280	315	12		

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	154	Total	C	N	O	S	0	0
			1179	750	202	223	4		

- Molecule 32 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	m	461	Total	C	N	O	S	0	0
			3813	2488	616	693	16		

- Molecule 33 is a protein called Uncharacterized protein C17A2.08c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	30	Total	C	N	O	S	0	0
			248	153	44	50	1		

- Molecule 34 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	y	200	Total	C	N	O	S	0	0
			1606	1000	279	323	4		

- Molecule 35 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	626	Total	C	N	O	S	0	0
			4980	3193	835	933	19		

- Molecule 36 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	r	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 37 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	q	56	Total	C	N	O	0	0
			295	182	57	56		

- Molecule 38 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	92	Total	C	N	O	P	0	0
			1970	882	365	631	92		

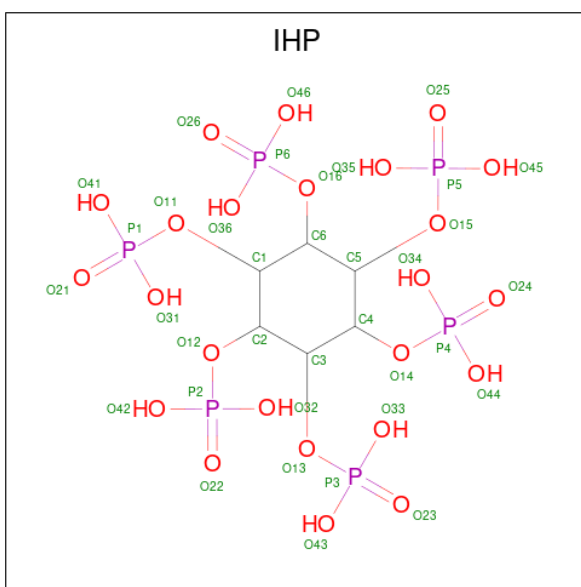
- Molecule 39 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	29	Total	C	N	O	P	0	0
			605	272	91	213	29		

- Molecule 40 is a protein called UNK3.

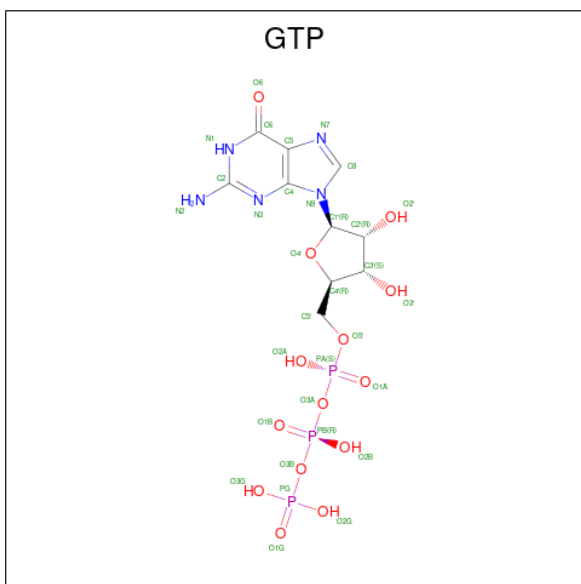
Mol	Chain	Residues	Atoms				AltConf	Trace
40	f	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

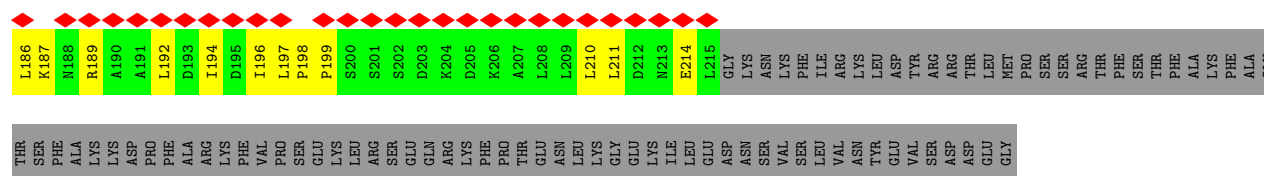
Mol	Chain	Residues	Atoms		AltConf
43	B	1	Total 1	Mg 1	0
43	6	3	Total 3	Mg 3	0

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

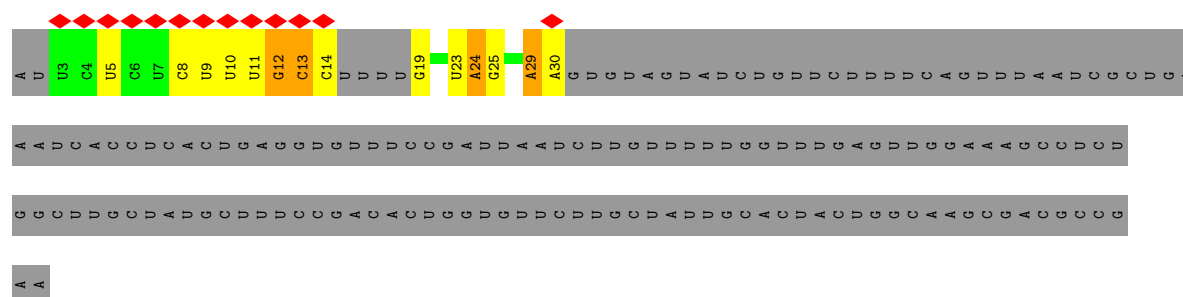
Mol	Chain	Residues	Atoms		AltConf
44	M	2	Total 2	Zn 2	0
44	O	3	Total 3	Zn 3	0
44	P	1	Total 1	Zn 1	0

- Molecule 45 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

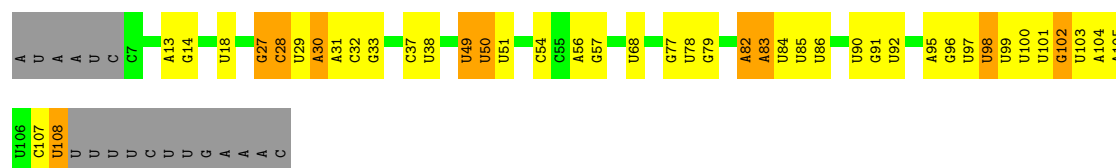
Mol	Chain	Residues	Atoms		AltConf
45	6	1	Total 1	K 1	0



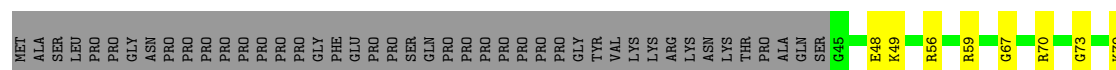
• Molecule 3: U2snRNA



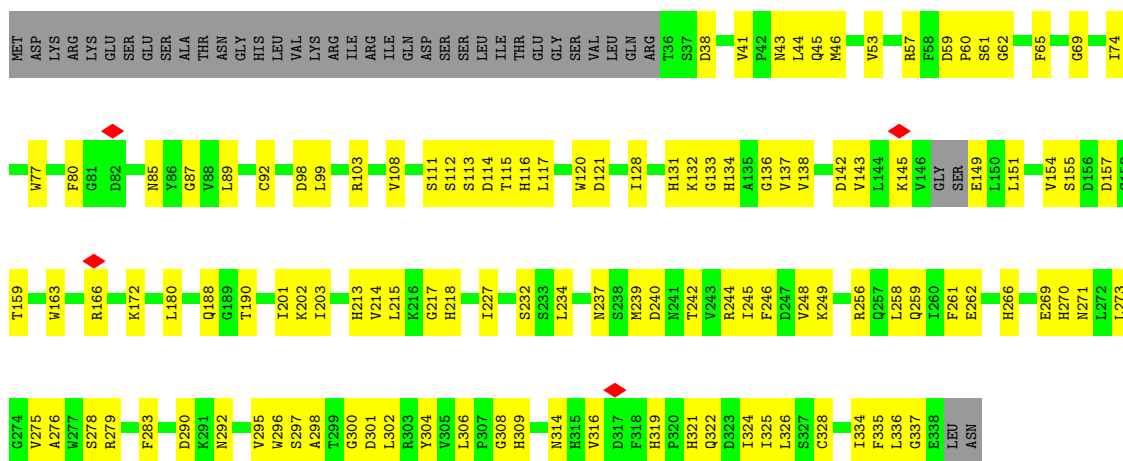
• Molecule 4: U5snRNA



• Molecule 5: Pre-mRNA-splicing factor spp42



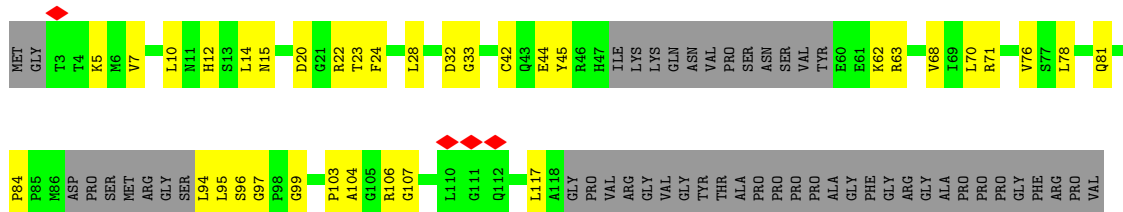
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GLU	N1994	T1934	R1874	S1737	I1584	D1431	W1287	N1145	L986	G877	R725
LYS	L1995	E1935	S1875	A1658	M1585	E1432	L1291	N1150	T986	R878	Q726
GLY	D1996	P1936	L1876	W1661	H1586	D1433	M1295	K1153	D987	Q883	G727
ARG	D1997	Q1937	P1877	N1662	G1588	S1435	T1296	K1153	V988	R884	K728
GLU	Q1998	P1937	P1878	S1663	G1589	W1436	Y1297	K1153	S1005	I732	I732
ASN	Q1999	V1939	R1665	R1665	T1592	D1437	Y1298	M1168	K1006	W746	W746
ALA	W2000	L1940	P1666	P1666	K1593	R1438	Y1299	R1176	V1011	I747	I747
VAL	L2001	F1941	L1669	L1669	L1594	G1439	E1300	R1176	L1016	P748	P748
THR	D2002	Q1881	L1670	L1670	S1595	I1444	I1303	I1182	L1017	W749	W749
ALA	V2003	P1882	D1671	D1671	L1597	T1445	E1307	R1185	R1018	K750	K750
VAL	V2003	R1883	N1672	N1672	L1598	L1446	E1307	R1185	L1019	W750	W750
THR	E2004	Q1884	N1672	N1672	Q1599	F1447	E1307	R1185	L1019	L754	L754
THR	P2005	L1885	R1673	R1673	Q1599	Q1448	C1315	M1020	R906	P755	P755
LYS	P2006	I1886	D1674	D1674	I1600	K1449	C1315	T1191	R907	P755	P755
THR	L2007	V1887	P1674	P1674	F1601	D1450	K1318	T1191	L908	I758	I758
ASN	R2008	T1888	D1677	D1677	R1602	R1451	K1318	E1196	A1034	I758	I758
VAL	D2008	N1678	N1678	N1678	S1603	R1451	R1322	E1196	K1035	S768	S768
HIS	D2009	R1889	T1679	T1679	H1604	W1460	R1322	D1197	M911	S768	S768
GLY	L2010	A1830	P1762	P1762	L1605	R1461	M1354	T1198	R912	R783	R783
ASP	I2011	G1891	A1763	A1763	W1606	V1462	M1354	D1206	N1037	A788	A788
MET	L2012	M1892	N1682	N1682	K1608	R1463	L1358	D1206	K1043	K797	K797
VAL	A2013	L1893	F1834	F1834	I1609	R1463	L1358	M1214	M1049	T803	T803
THR	D2014	L1894	Y1684	Y1684	D1616	W1479	L1364	T1215	L1053	K808	K808
THR	Y2015	P1895	W1685	W1685	L1617	W1489	L1364	G1216	L1057	A809	A809
THR	A2016	L1896	D1687	D1687	L1621	Q1490	D1371	G1056	L1057	E810	E810
SER	K2017	Y1957	V1688	V1688	Q1622	N1491	D1371	L1222	I1063	R813	R813
ALA	K2018	L1898	Q1689	Q1689	Q1623	N1492	L1374	P1223	I1063	Q814	Q814
TYR	N2019	H1899	L1690	L1690	E1624	R1495	L1378	L1233	F1066	K819	K819
GLU	N2020	L1900	R1691	R1691	S1627	F1514	R1378	K1234	D1072	G821	G821
ASN	N2020	L1901	D1696	D1696	L1628	T1517	G1385	D1235	D1072	D827	D827
GLU	I2021	L1902	S1697	S1697	Q1629	E1386	E1386	G1236	D1072	W839	W839
LYS	V2023	F1903	S1789	S1789	I1630	K1538	M1391	W1238	E1083	R843	R843
SER	A2024	P1904	N1791	N1791	E1631	L1542	Y1393	N1239	G1086	P851	P851
LYS	S2025	N1905	Y1792	Y1792	K1635	Q1546	E1400	N1248	L1095	P852	P852
THR	L2026	I1846	Y1793	Y1793	E1636	R1547	S1406	R1254	D1099	L862	L862
GLU	T2027	H1847	A1793	A1793	T1637	G1549	S1406	R1254	P1107	V863	V863
TRP	N2028	T1848	E1794	E1794	Y1711	Q1552	W1410	V1256	P1107	P965	P965
ARG	N2028	L1908	S1797	S1797	K1642	Q1552	W1410	V1256	P1107	P965	P965
ASN	S2029	K1909	N1798	N1798	M1646	R1556	E1419	I1288	L1115	E969	E969
ALA	E2030	G1910	Q1799	Q1799	N1647	R1567	E1419	I1271	L1115	P970	P970
ILE	VAL	T1971	I1912	I1912	C1650	G1574	Q1423	L1272	R1123	P971	P971
SER	ARG	E1972	L1913	L1913	A1651	F1576	R1425	S1275	R1123	L973	L973
ILE	ILE	T1973	Q1914	Q1914	D1652	Q1576	R1425	K1282	R1135	W878	W878
SER	LEU	T1974	L1915	L1915	L1653	Q1576	R1425	K1282	R1135	W878	W878
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PRO	GLY	L1976	Q1918	Q1918	L1655	Q1576	R1425	K1282	R1135	W878	W878
LEU	MET	I1977	F1917	F1917	L1656	Q1576	R1425	K1282	R1135	W878	W878
ARG	THR	I1978	Q1918	Q1918	L1656	Q1576	R1425	K1282	R1135	W878	W878
THR	ILE	L1978	A1919	A1919	L1656	Q1576	R1425	K1282	R1135	W878	W878
LYS	THR	R1979	A1919	A1919	L1656	Q1576	R1425	K1282	R1135	W878	W878
ALA	ALA	P1980	I1920	I1920	L1656	Q1576	R1425	K1282	R1135	W878	W878
PRO	PRO	D1981	I1921	I1921	L1656	Q1576	R1425	K1282	R1135	W878	W878
SER	SER	D1981	K1922	K1922	L1656	Q1576	R1425	K1282	R1135	W878	W878
LEU	LEU	D1982	L1923	L1923	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLN	GLN	S1983	L1923	L1923	L1656	Q1576	R1425	K1282	R1135	W878	W878
ARG	ARG	L1984	K1864	K1864	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLN	GLN	D1924	T1865	T1865	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLN	GLN	K1925	T1865	T1865	L1656	Q1576	R1425	K1282	R1135	W878	W878
ILE	ILE	I1926	A1866	A1866	L1656	Q1576	R1425	K1282	R1135	W878	W878
ALA	ALA	T1986	E1867	E1867	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLU	GLU	K1987	E1868	E1868	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLU	GLU	E1988	L1928	L1928	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLU	GLU	N1989	L1929	L1929	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLU	GLU	H1990	L1930	L1930	L1656	Q1576	R1425	K1282	R1135	W878	W878
GLU	GLU	V1991	L1931	L1931	L1656	Q1576	R1425	K1282	R1135	W878	W878
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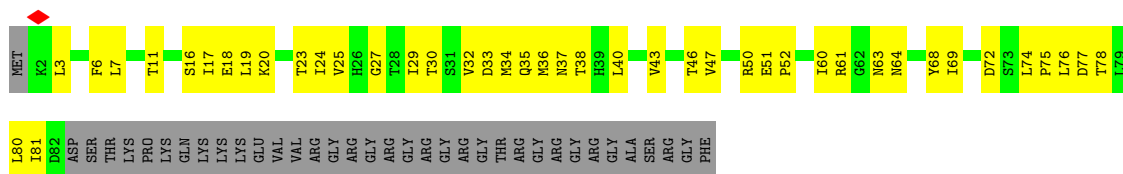
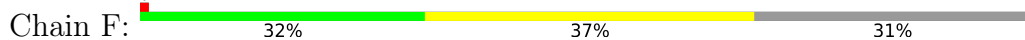
- Molecule 8: Small nuclear ribonucleoprotein Sm D3



- Molecule 9: Small nuclear ribonucleoprotein-associated protein B



- Molecule 10: Small nuclear ribonucleoprotein Sm D1



- Molecule 11: Small nuclear ribonucleoprotein Sm D2





- Molecule 12: Small nuclear ribonucleoprotein E



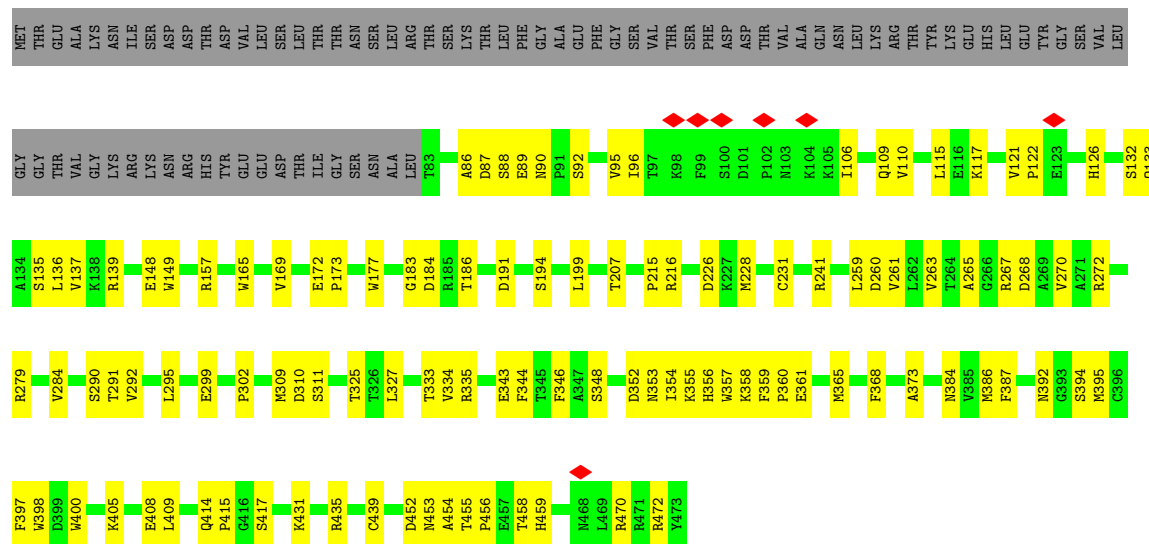
- Molecule 13: Small nuclear ribonucleoprotein F



- Molecule 14: Small nuclear ribonucleoprotein G



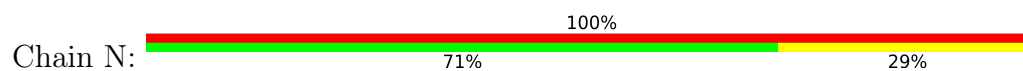
- Molecule 15: Pre-mRNA-splicing factor prp5



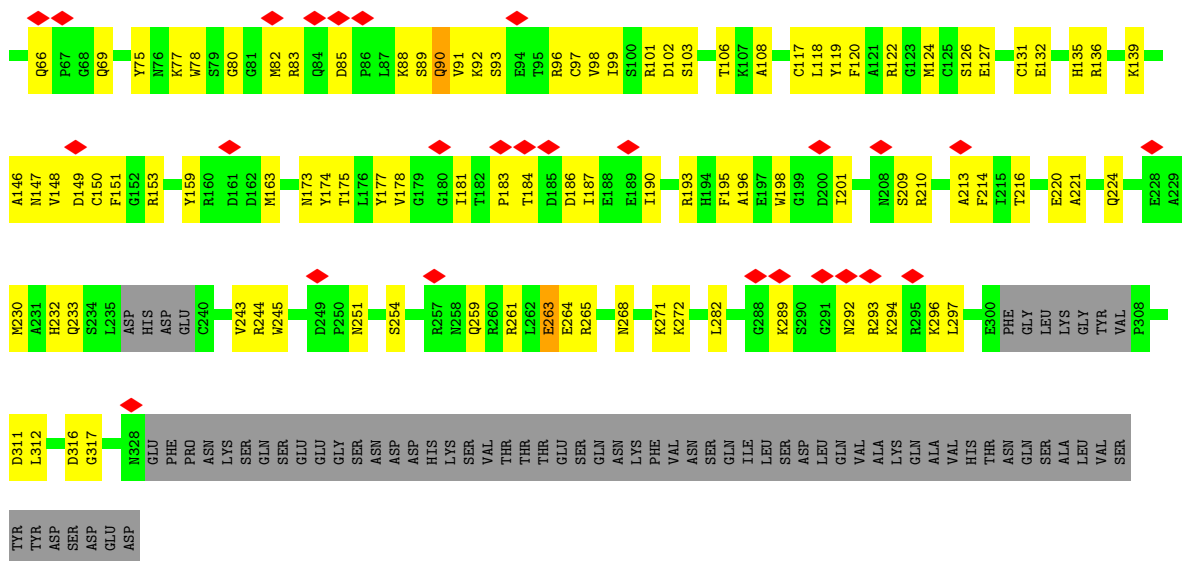
- Molecule 16: Pre-mRNA-processing protein 45



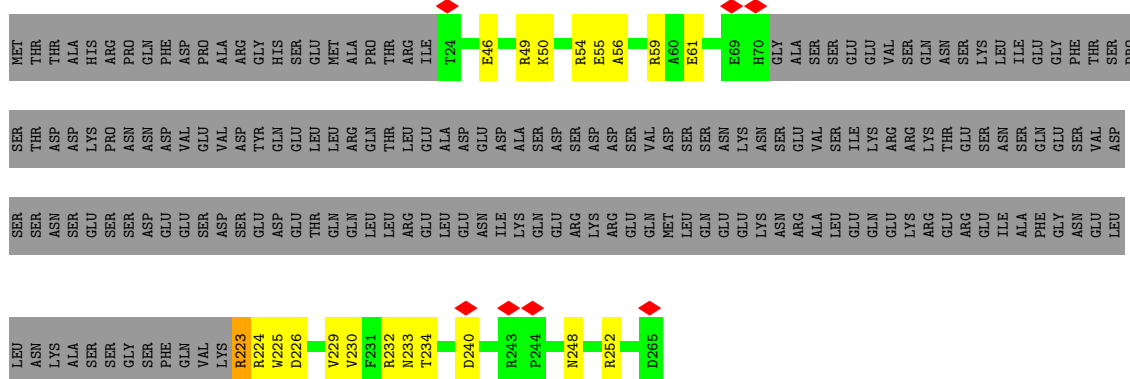
● Molecule 18: Pre-mRNA-splicing factor cwf11



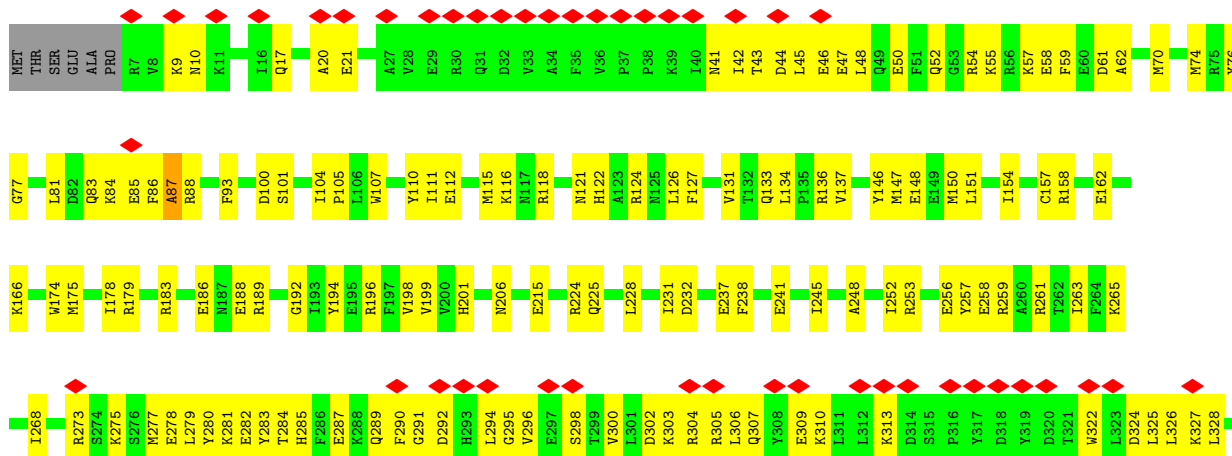
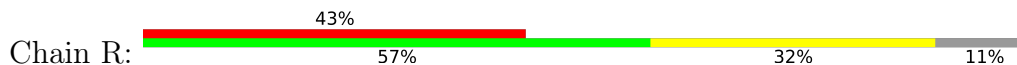
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R723	N663	P603	L543	F483	T423	F483	V303	H243	P183	M123	W63	L3
L724	S664	K604	H544	K484	A424	Y364	Y304	P244	S184	I124	Q64	Y4
Y725	T665	Q605	G545	V485	I425	A365	H305	V245	I185	Q125	R65	K5
T726	V666	L606	N546	T486	Q426	L366	L306	T246	V186	F126	V66	N6
Y727	A667	K607	A547	S487	Y427	K367	Q307	E247	E187	I127	N67	K7
N728	R668	F608	L548	V488	L428	V368	L308	D248	K188	T128	T68	K8
D729	N669	M609	D549	A489	S429	D369	T309	S249	F189	L129	E69	K9
K730	L670	F610	P550	P490	L430	F370	L310	C250	P190	C130	M70	Q10
Q731	F671	A611	L551	P491	S431	E371	F311	F251	F191	F131	S71	I11
L732	N672	L612	E552	Q492	F432	F372	S312	Y252	H192	Q132	L72	I12
E733	T673	W613	G553	L493	L373	L373	D313	T253	N193	F133	N73	N13
S734	V674	L614	V554	G494	H434	K374	F314	A254	L194	S134	H74	Y14
I735	E675	S615	T555	Q495	R435	N375	Q315	L255	L195	I75	I75	A15
L736	Q676	P616	D556	V496	Q436	V376	K316	R256	S196	N136	N76	N16
R737	L677	E617	F557	L497	Q437	F377	K316	M257	E197	L77	L77	S17
G738	D678	A618	T558	P498	S438	I378	L318	S258	W198	K138	T78	N18
S739	S679	N619	T559	Q499	K439	N379	G319	L259	I199	L139	C79	W19
Q740	V680	K620	A560	F500	A440	T380	D320	Y260	H200	R140	M80	Q20
P741	L681	Y621	T561	V501	Y441	Y381	L321	Y261	S201	L81	Q21	Q21
G742	P682	W622	I562	K502	K442	D382	V322	D262	L202	L142	L82	N22
L743	N683	L623	C563	C503	F323	R383	F323	S263	L203	L143	L83	E23
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Y747	P687	L627	V567	L507	R447	V387	S328	F267	I207	T147	K87	F27
G748	S688	L628	G568	S508	S448	N388	S328	K268	S208	N148	Y88	Q28
P749	N689	W629	M569	R509	L449	D389	L329	K269	Y209	I149	E89	Q29
T750	L690	S630	F570	P510	Y450	Y390	Q330	M270	A210	S150	Y90	T30
R751	S691	L631	Q571	G511	A451	D391	Q331	T271	Q211	I151	I91	M31
G752	T692	W632	S572	P512	E452	E392	R332	D272	L152	L152	T92	L32
L753	N693	F633	D573	F513	L453	I393	Q333	D273	N153	W93	Q33	Q33
K754	S694	R634	M574	H514	L454	I394	K334	L274	K214	S154	D94	C34
L695	H695	A635	Q575	S515	N455	N395	L335	N275	Q215	L155	L95	I35
L696	L696	K636	S576	A516	F456	F396	E336	Y276	E216	D156	I96	L36
L757	P697	E637	D577	L517	S457	T397	E337	V277	A217	N157	D97	E37
W758	K698	F638	S578	R518	E458	L398	T338	L278	K218	L158	E98	A38
F699	P699	D679	D579	D519	Q459	K399	T339	K279	V219	D159	N99	V39
K760	Y700	K640	N580	L520	Y460	D400	S340	F280	T220	K160	R100	I40
T701	T701	W641	K581	K521	R461	V401	F341	P281	P221	V161	F101	V41
L762	N702	F642	S582	N522	R462	L402	L342	F282	L222	K162	Q102	S42
E763	Q703	E643	L583	S523	L463	S523	S343	D283	L223	Y163	L103	K43
W764	N704	D644	N584	L524	S464	E404	F344	N284	A224	L164	F104	D44
L765	K705	L645	V585	K525	L465	R405	N345	T285	I225	L165	F105	A45
Q766	I706	F646	Y586	S526	K466	S406	S346	R286	I226	H166	E106	K46
S707	S707	L647	L587	P527	N467	V407	L347	G287	N227	D167	K107	Q47
A708	T708	G648	S588	F528	N468	M408	K348	N288	M228	S168	V108	V48
D709	F709	F649	P589	L529	T469	D409	S349	E289	S229	S169	I109	L49
P710	W710	G650	F590	C530	K470	Q410	L350	Y290	L230	S170	E110	S50
N711	T711	T651	Y591	L531	N471	E411	C351	E291	V231	L171	V111	L51
D712	A712	P652	Y592	I532	L472	N412	S352	K292	L232	T172	S112	L52
R713	S713	D653	H593	Y533	T473	S413	K353	E293	L233	K173	L113	H53
T714	D714	I654	S594	I594	K474	L414	C354	Q294	S234	A174	S114	E54
W715	R715	L655	L595	S535	D475	T415	Y355	K295	A235	F175	L115	L55
L716	H716	A656	A596	K536	N476	N416	L356	I296	F236	D176	N116	K56
F717	T717	P657	D537	V537	F477	Y417	R357	T297	P237	S177	L117	L57
L718	L718	P658	L598	H538	F478	F418	T358	N298	T238	Y178	S118	F58
S778	L719	N659	S479	E539	L419	L419	S359	D299	R239	K179	E119	E59
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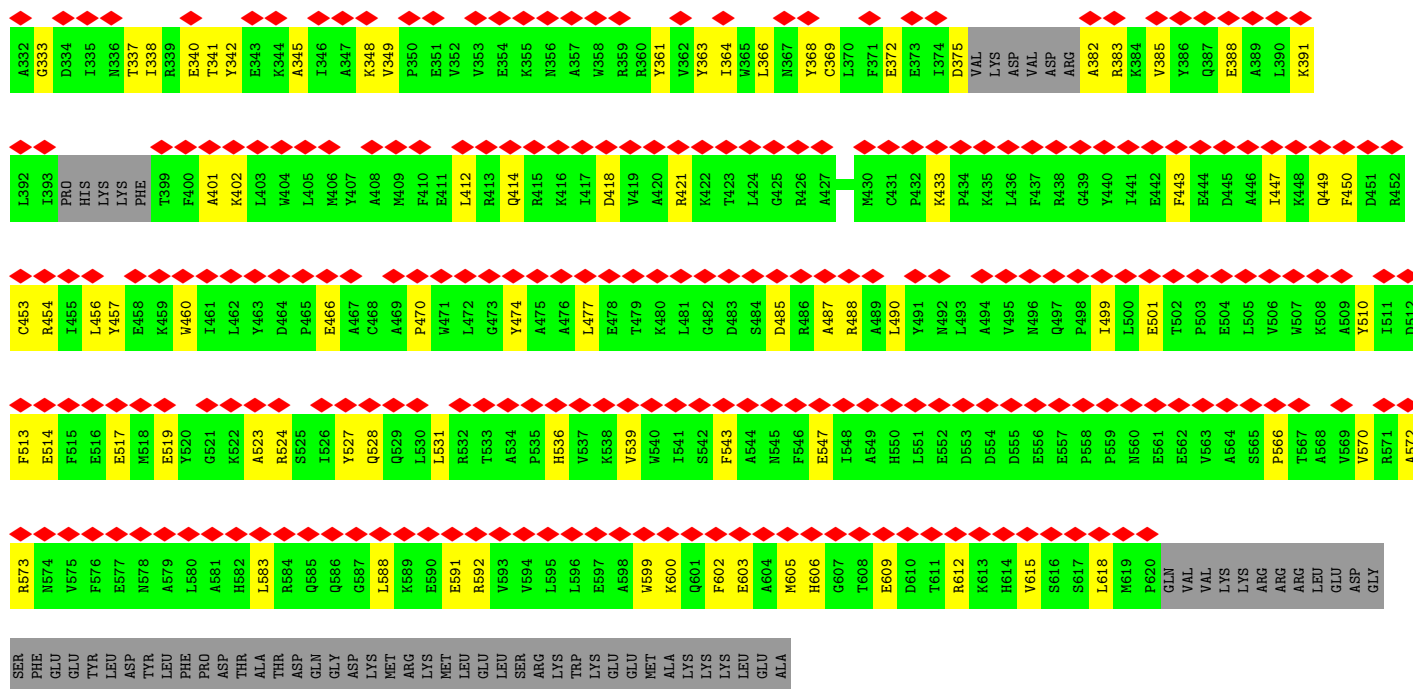


• Molecule 21: Pre-mRNA-splicing factor cwf15

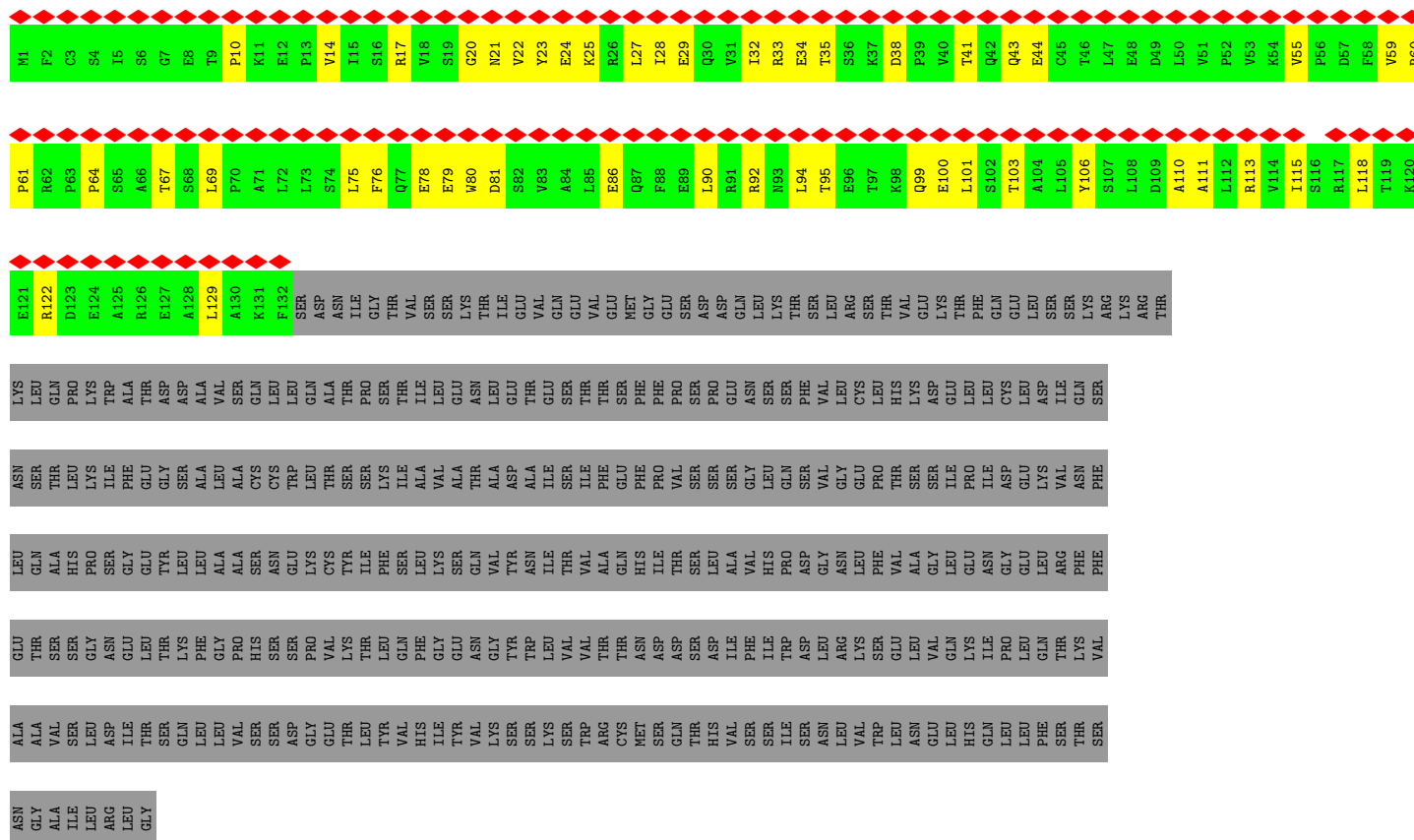


• Molecule 22: Pre-mRNA-splicing factor cwf4

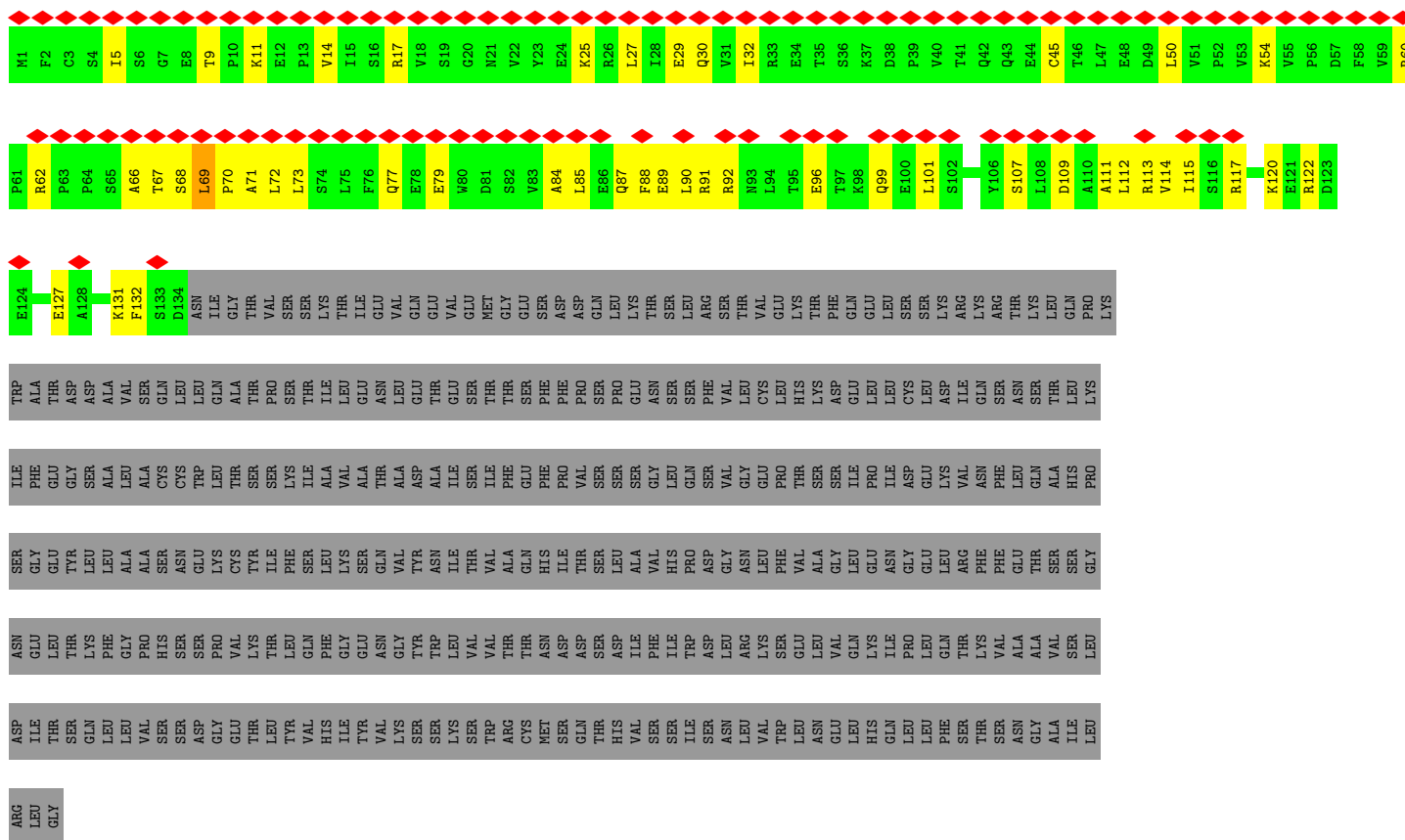




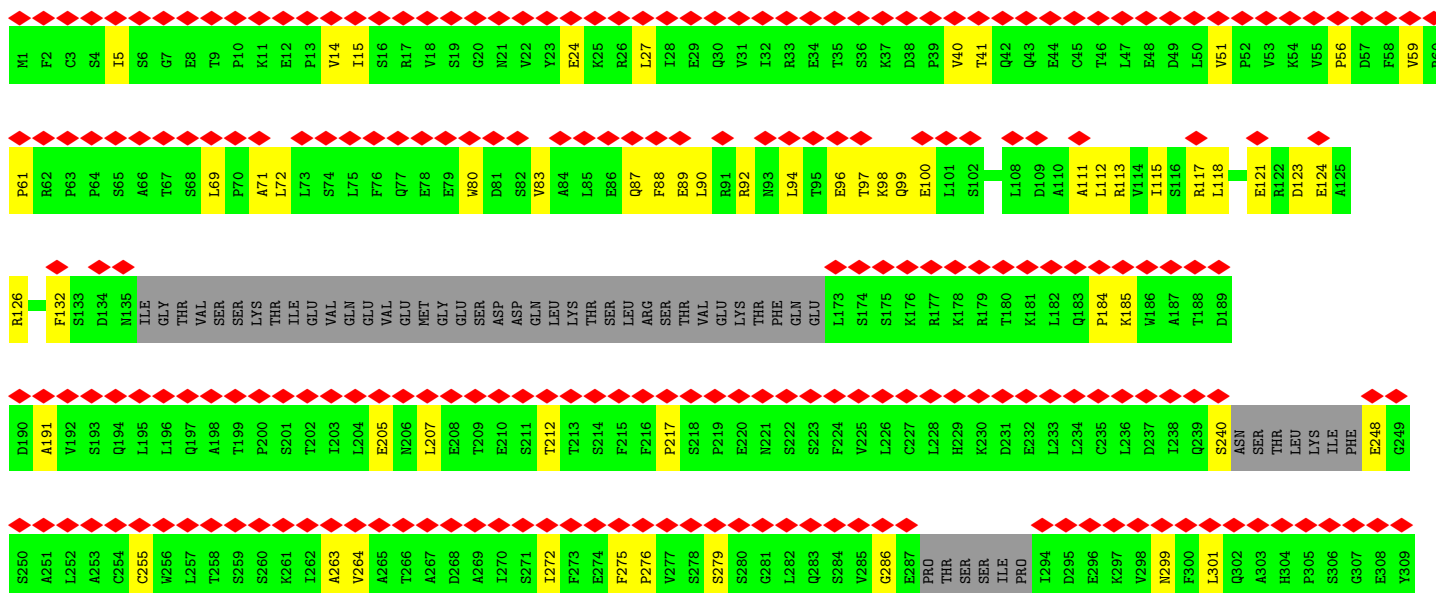
• Molecule 23: Pre-mRNA-processing factor 19

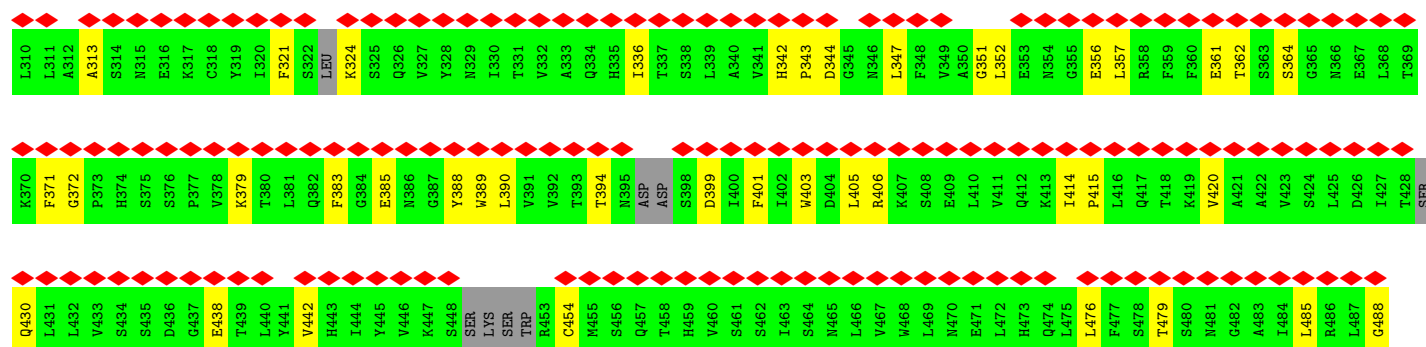


Chain T:

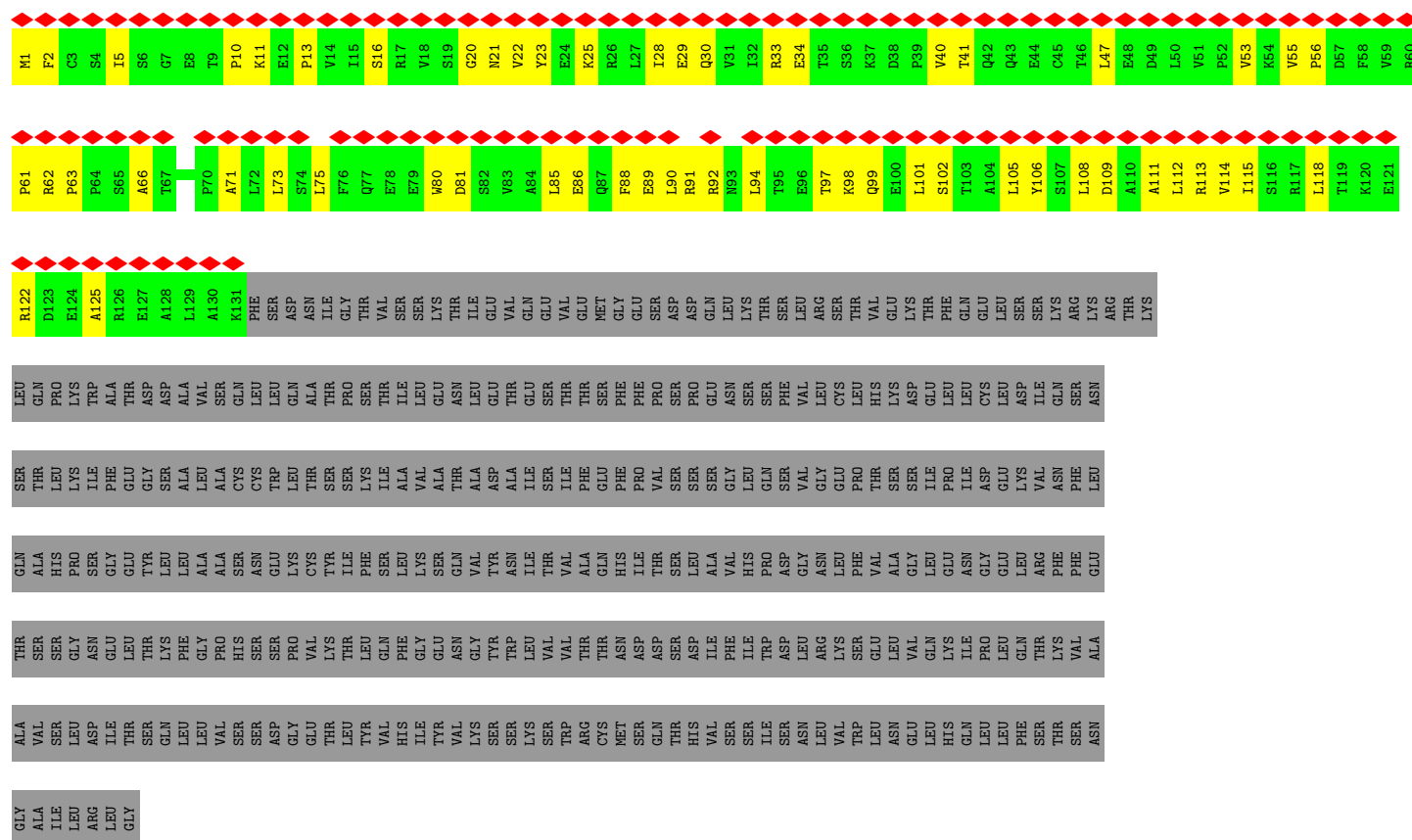


Chain U:



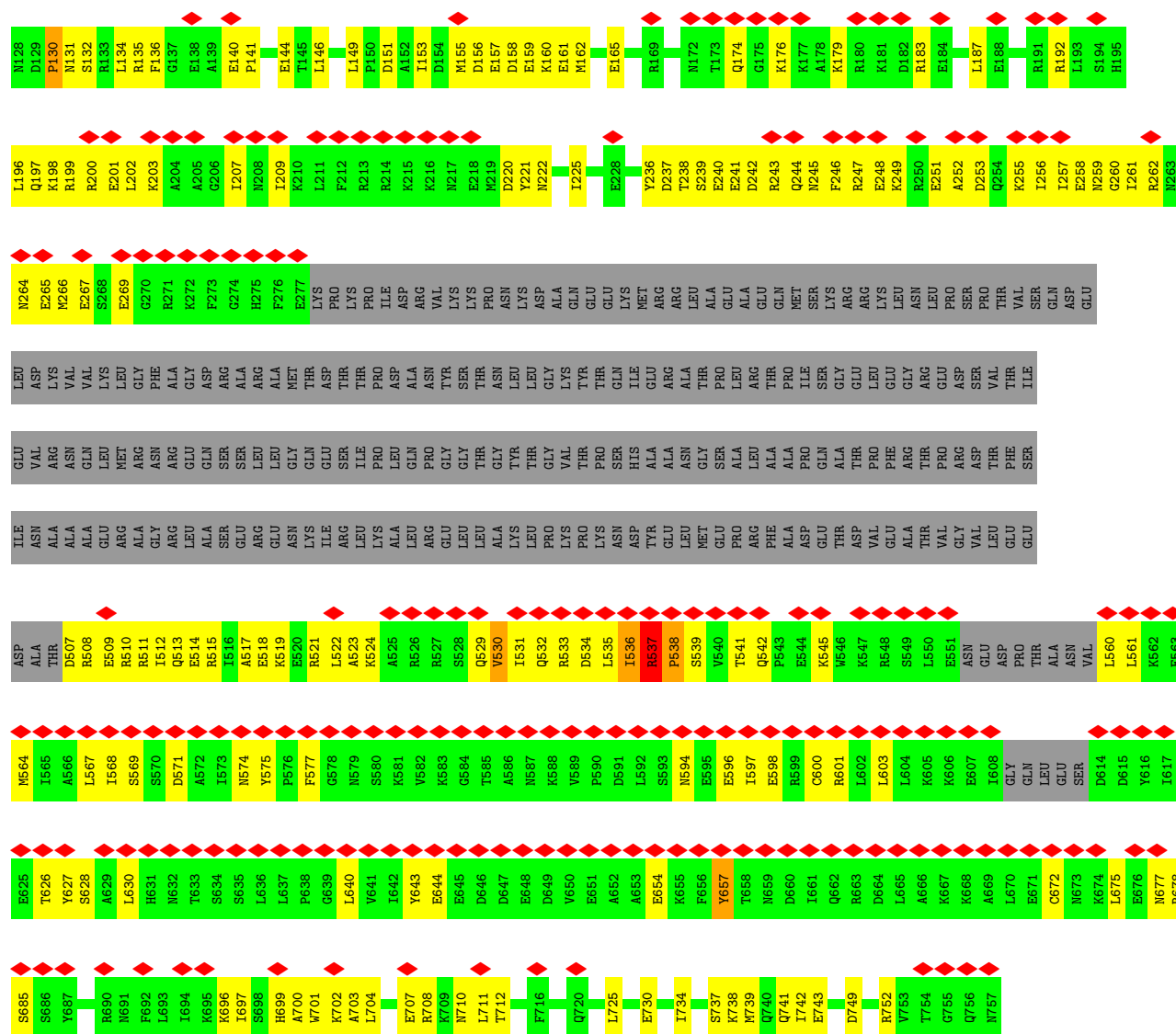


• Molecule 23: Pre-mRNA-processing factor 19

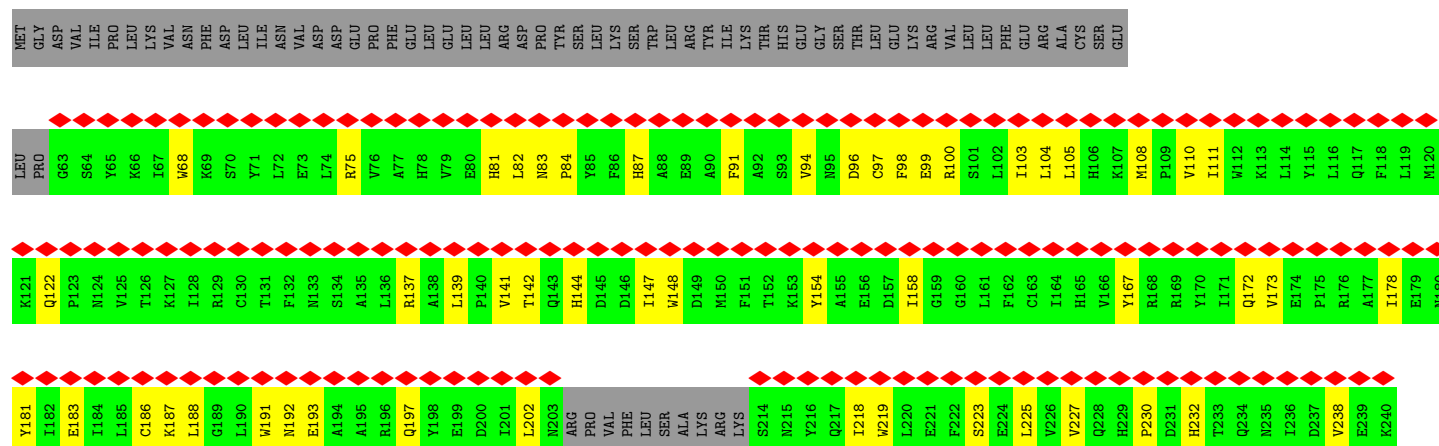


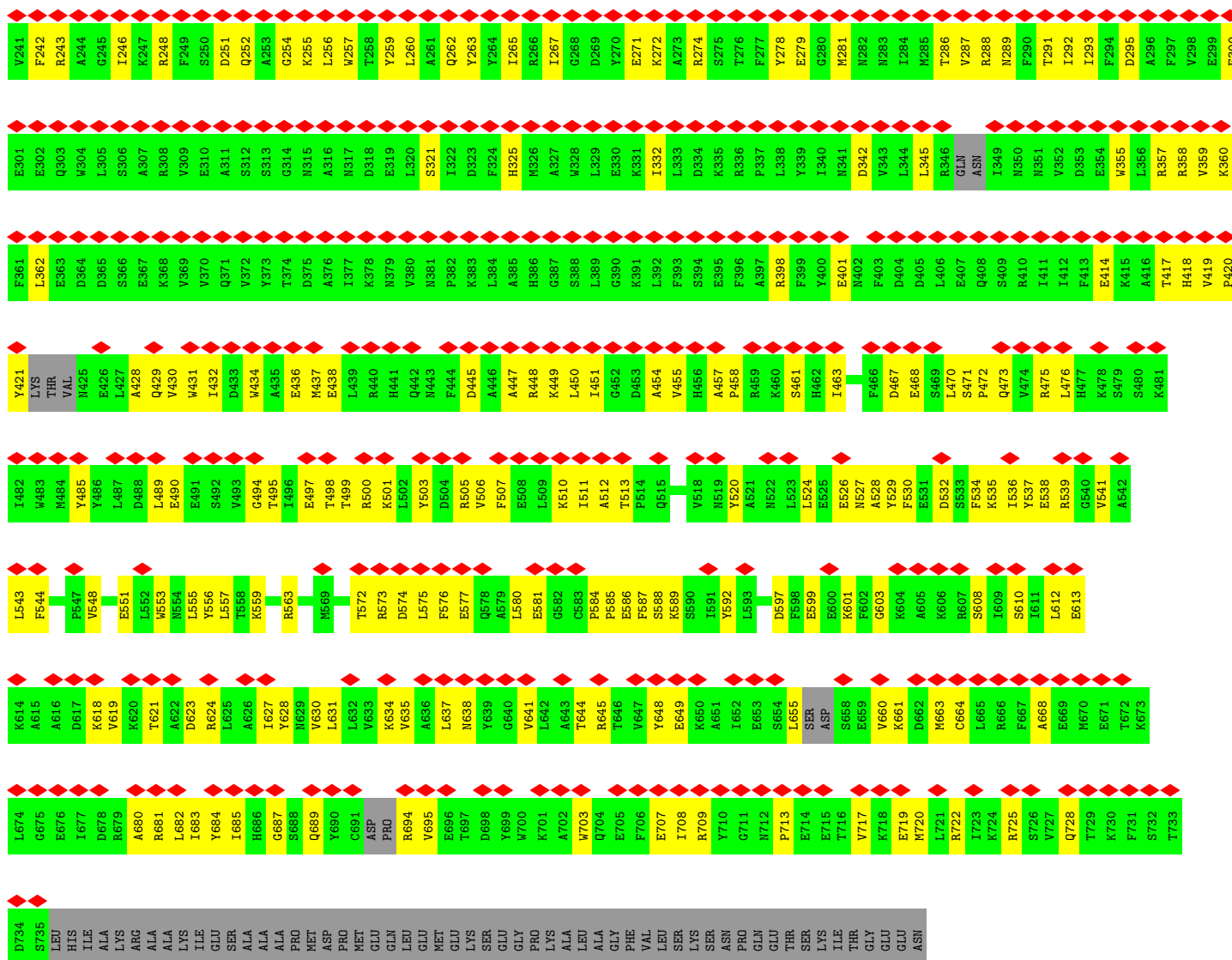
• Molecule 24: Pre-mRNA-splicing factor cdc5



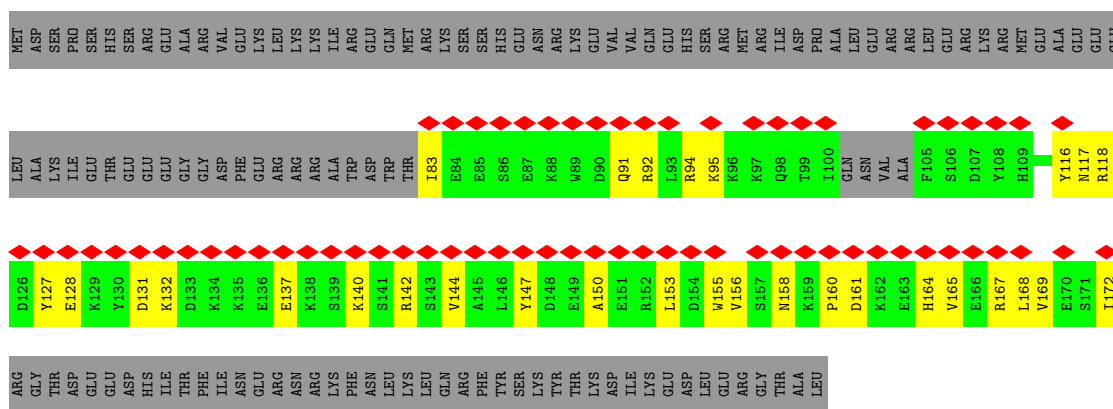


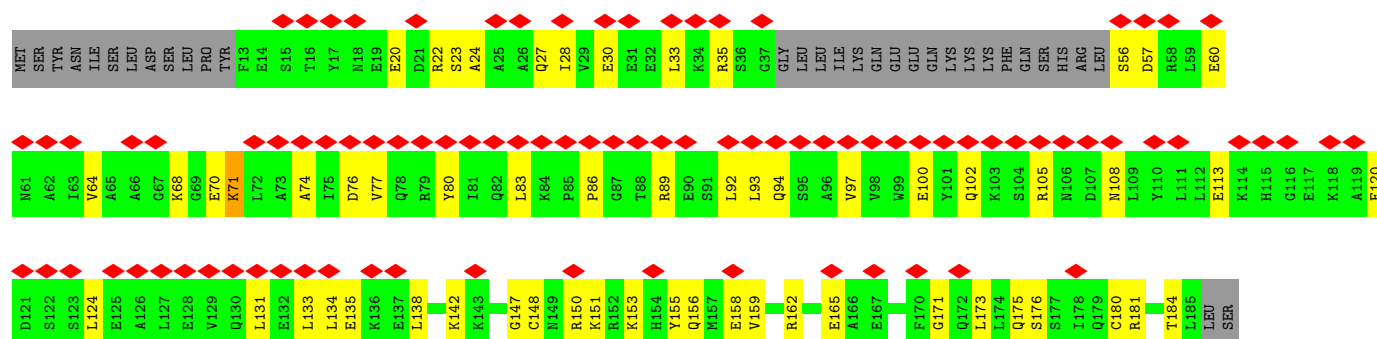
• Molecule 25: Pre-mRNA-splicing factor cwf3



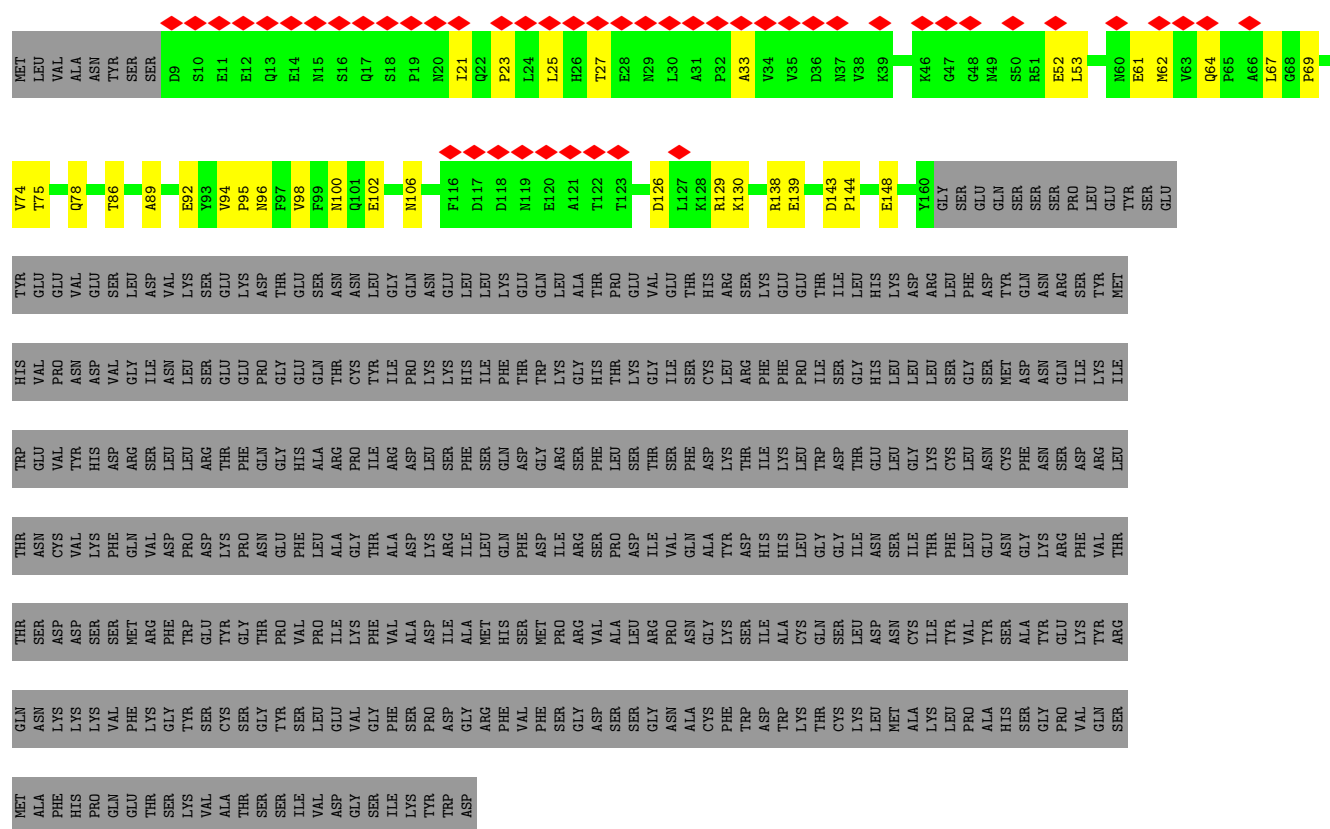


• Molecule 26: Pre-mRNA-splicing factor syf2

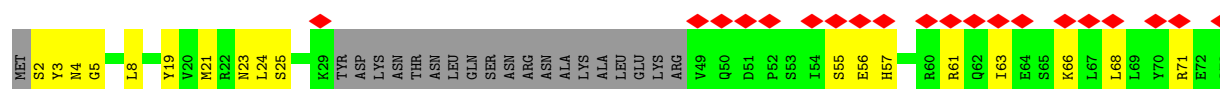




• Molecule 28: Pre-mRNA-processing factor 17



• Molecule 29: Pre-mRNA-splicing factor cwf21



[illegible]

- Molecule 31: Peptidyl-prolyl cis-trans isomerase ppi1



Figure 1: Schematic representation of the 16S rRNA gene structure. The diagram shows a linear sequence of 16S rRNA genes, with each gene represented by a yellow bar. The genes are labeled with their accession numbers: F102, F103, L106, L112, K115, H116, F119, V128, R131, R136, D141, L147, I150, K151, L155, M157, A2, N3, V4, L6, Q7, T8, S9, L10, G11, K12, I13, L14, L17, E20, H21, A22, P23, C26, Q27, N28, F29, Y30, T31, L32, Y37, Y38, D39, R45, I52, Q53, R52, Q53, G54, T55, D70, K71, D74, S78, L88, S89, M90, A91, N92, A93, G94, and V95. Red diamonds indicate the positions of the 16S rRNA genes that are part of the 16S rRNA gene cluster. The genes are arranged in two rows, with the top row containing genes F102 through V95 and the bottom row containing genes A2 through G94. The genes are connected by lines, indicating their relative positions in the genome.

- Molecule 32: G-patch domain-containing protein C1486.03

[illegible][illegible]

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

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

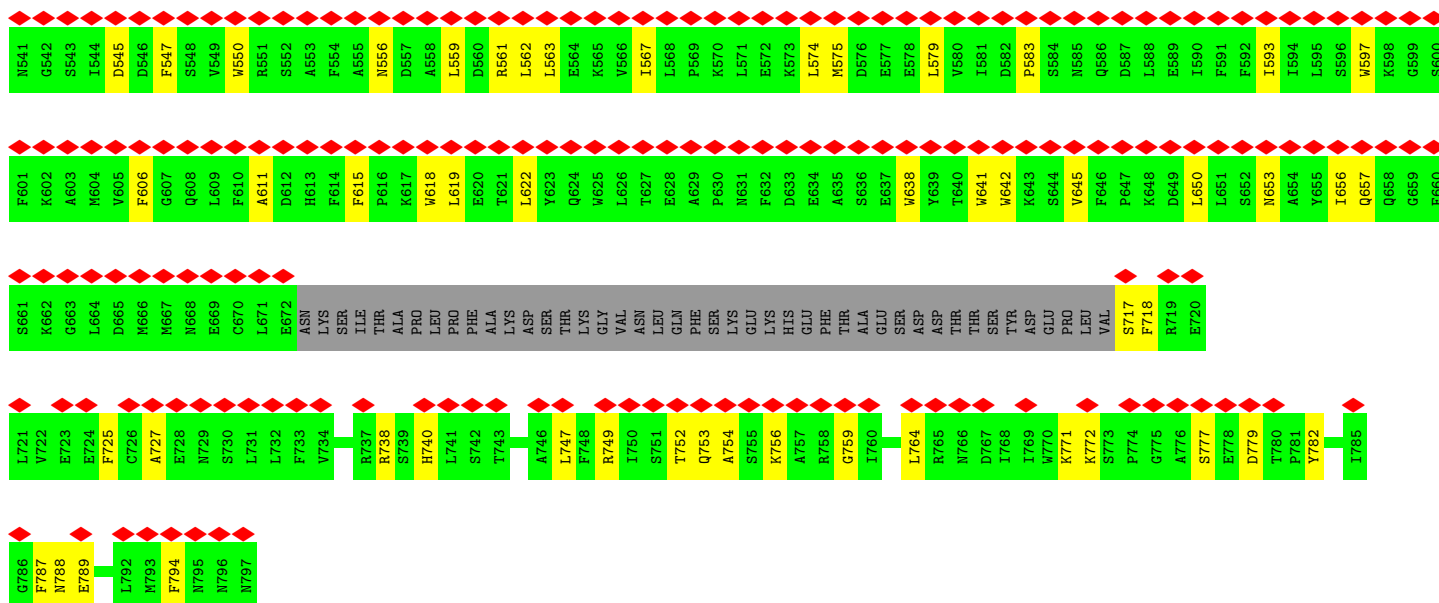
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S301	R302	L303	E304	K305	L306	L307	G308	K309	V310	M311	E312	V313	K314	S315	R316	S317	M318	E319	F320	T321	V322	P323	E324	A325	E326	T327	D328	V329	I330	E331	K332	R333	L334	P335	K336	L337	N338	N339	L340	L341	E342	T343	L344	P345	V346	E347	F348	S349	E350	A351	S352	N353	H354	F355	E356	L357	D358	S359	H360
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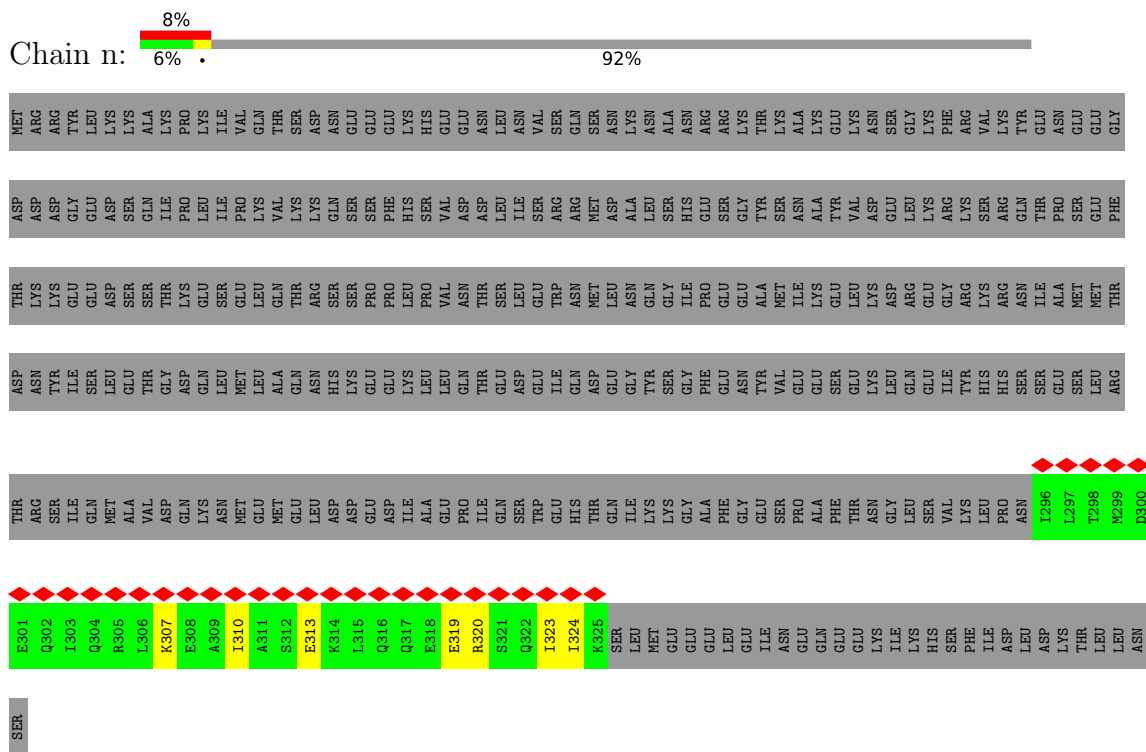
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GLU	LEU	GLU	GLY	GLN	SER	SEU
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S432						
F433						
M434						
M435						
F436						
V437						
W438						
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L476						
L477						
Q478						
D479						
N480						

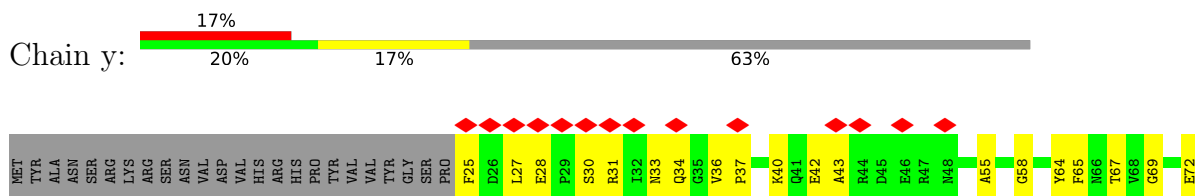
I481	L482	P483	R484	L485	K486	D487	A488	V489	S490	K491	W492	N493	P494	K495	L496	K497	L498	K499	K500	N501	D502	S503	L504	H505	H506	G507	I508	F509	P510	W511	L512	P513	Y514	L515	E516	K517	H518	A519	D520	S521	L522	L523	Q524	Q525	S526	V526	L527	V528	Q529	F530	S531	L532	I533	L534	S535	P536	W537	K538	I539	F540
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

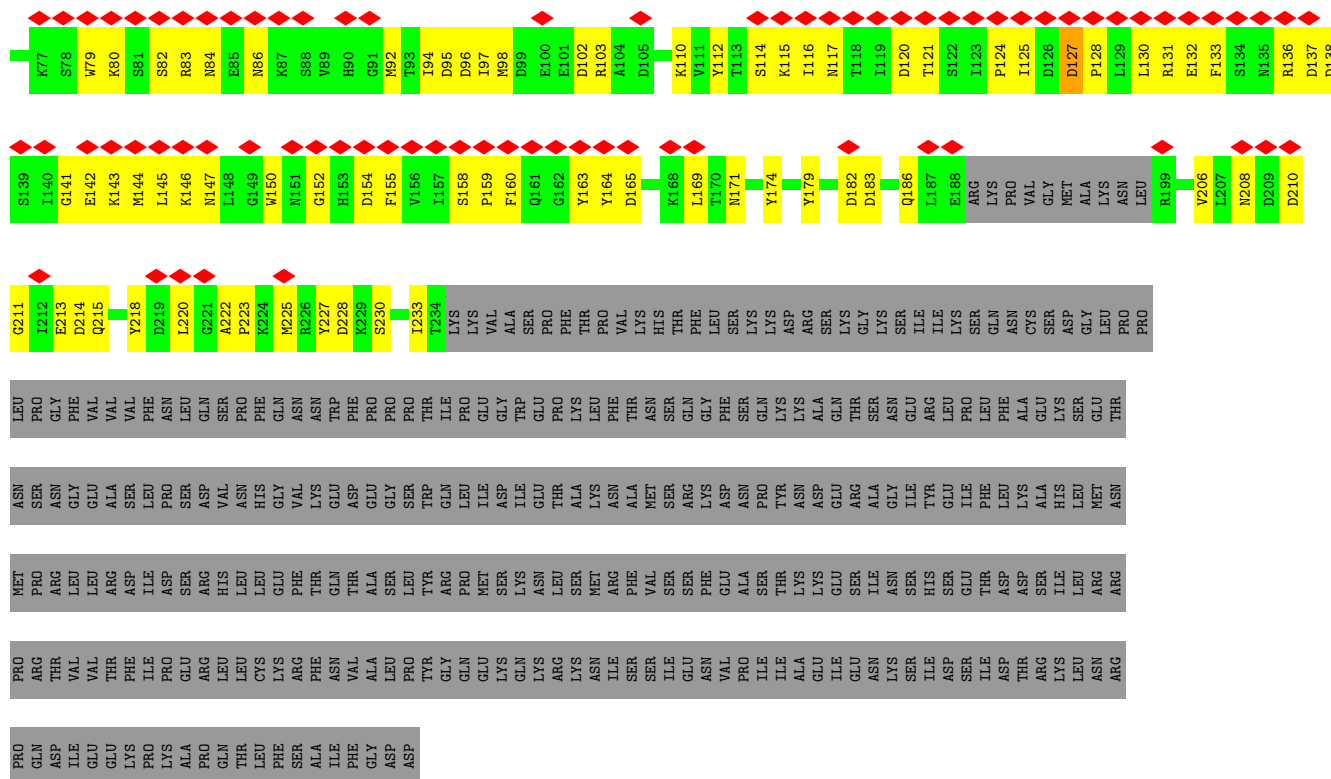


- Molecule 33: Uncharacterized protein C17A2.08c

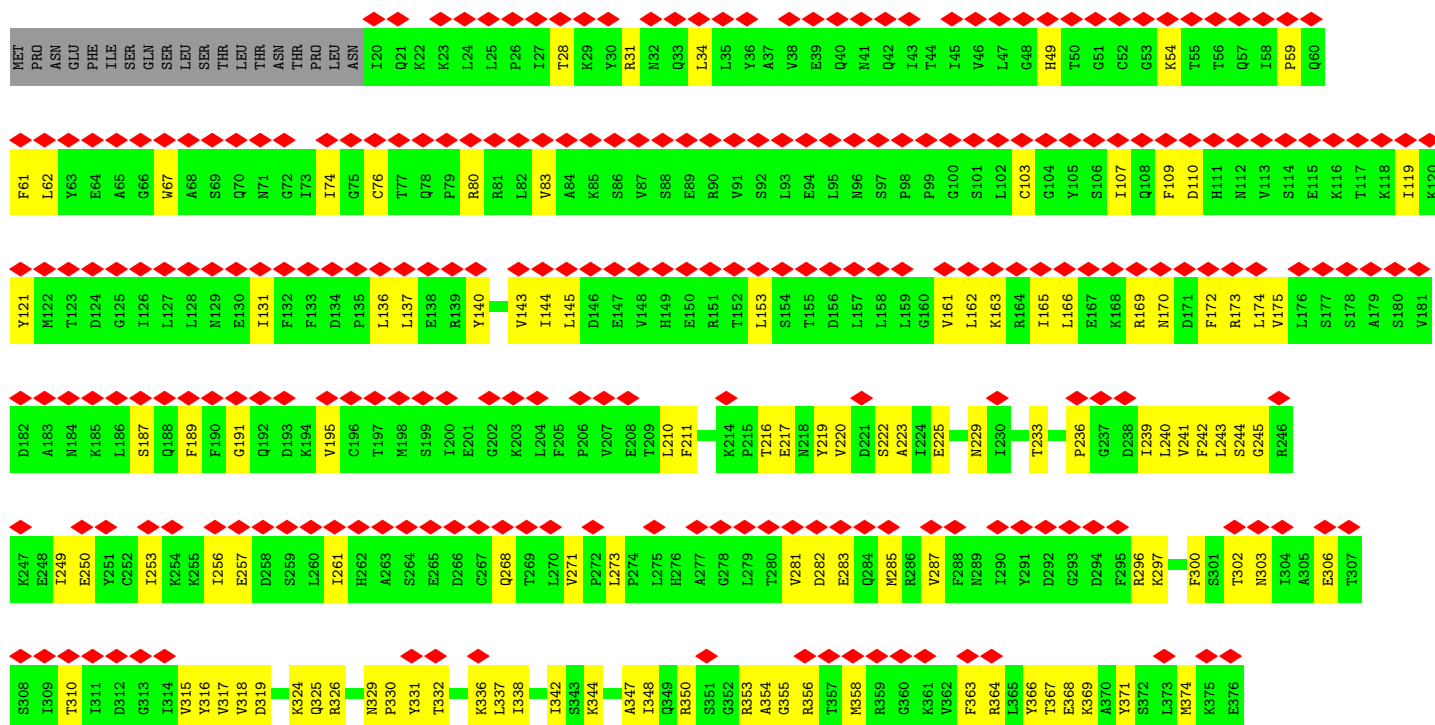


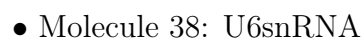
- Molecule 34: Uncharacterized protein C20H4.06c

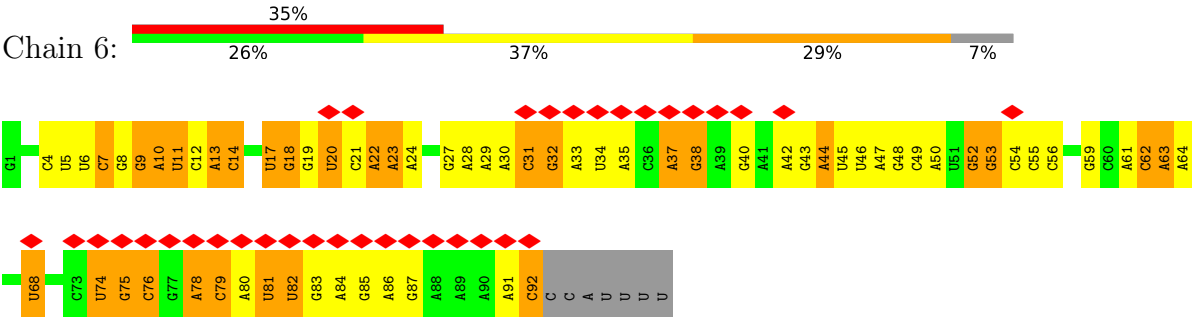




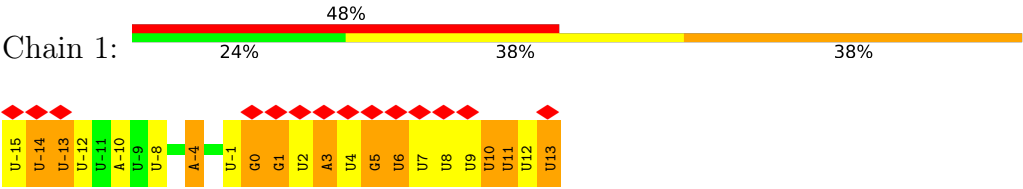
• Molecule 35: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09



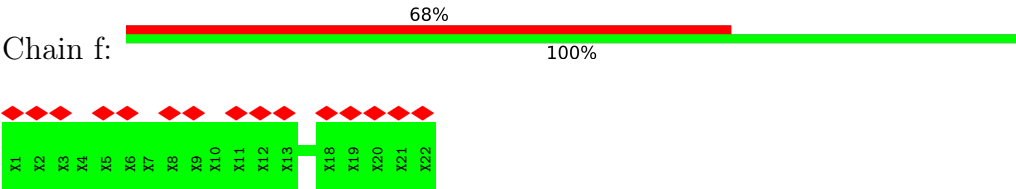




● Molecule 39: pre-mRNA



● Molecule 40: UNK3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	37.664	Depositor
Minimum map value	-23.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.904	Depositor
Recommended contour level	3.2	Depositor
Map size (\AA)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.822, 0.822, 0.822	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	e	0.24	0/1354	0.43	0/1831
2	p	0.18	0/491	0.43	0/654
3	2	0.24	0/554	0.29	0/856
4	5	0.44	0/2397	0.33	0/3727
5	A	0.45	0/16857	0.46	2/22848 (0.0%)
6	B	0.42	0/7459	0.44	0/10117
7	C	0.28	0/2376	0.41	0/3216
8	D	0.40	0/772	0.40	0/1038
9	E	0.30	0/737	0.46	0/993
10	F	0.31	0/646	0.57	0/875
11	G	0.25	0/829	0.47	0/1111
12	H	0.29	0/662	0.47	0/894
13	I	0.28	0/585	0.60	0/794
14	J	0.37	0/578	0.46	0/774
15	K	0.47	0/3130	0.49	0/4251
16	L	0.32	0/1991	0.46	0/2684
17	M	0.25	0/1841	0.44	0/2468
18	N	0.13	0/10690	0.33	0/14463
19	O	0.40	0/1199	0.48	0/1609
20	P	0.33	0/2222	0.57	1/2991 (0.0%)
21	Q	0.36	0/767	0.46	0/1028
22	R	0.26	0/5235	0.45	0/7067
23	S	0.20	0/1072	0.50	0/1453
23	T	0.19	0/1086	0.43	0/1472
23	U	0.14	0/2897	0.37	0/3914
23	V	0.19	0/1060	0.50	0/1437
24	W	0.25	0/4187	0.52	3/5613 (0.1%)
25	X	0.17	0/5599	0.44	0/7566
26	Y	0.16	0/857	0.41	0/1138
27	Z	0.20	0/1244	0.47	0/1667
28	a	0.28	0/1055	0.44	0/1443
29	b	0.27	0/829	0.38	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	c	0.40	0/1711	0.49	0/2312
31	d	0.24	0/1206	0.43	0/1636
32	m	0.15	0/3916	0.36	0/5300
33	n	0.12	0/247	0.31	0/327
34	y	0.26	0/1641	0.58	0/2211
35	z	0.19	0/5079	0.41	0/6875
37	q	0.23	0/32	0.19	0/43
38	6	0.22	0/2207	0.36	0/3438
39	1	0.33	0/673	0.47	0/1043
All	All	0.31	0/99970	0.44	6/136288 (0.0%)

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
21	Q	0	1
24	W	0	3
35	z	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	130	PRO	CA-N-CD	-6.83	102.43	112.00
24	W	626	THR	CA-C-N	-6.03	112.44	120.63
24	W	626	THR	C-N-CA	-6.03	112.44	120.63
5	A	1043	LYS	CB-CA-C	-5.86	109.80	116.54
5	A	978	TRP	CB-CG-CD2	-5.34	119.32	126.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	223	ARG	Sidechain
24	W	533	ARG	Sidechain
24	W	537	ARG	Sidechain
24	W	657	TYR	Peptide
35	z	326	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	1329	0	1293	41	0
2	p	487	0	515	23	0
3	2	500	0	257	17	0
4	5	2149	0	1085	36	0
5	A	16424	0	16380	403	0
6	B	7298	0	7336	175	0
7	C	2328	0	2276	95	0
8	D	760	0	776	22	0
9	E	726	0	750	40	0
10	F	638	0	682	42	0
11	G	819	0	845	63	0
12	H	652	0	680	33	0
13	I	574	0	591	49	0
14	J	573	0	602	19	0
15	K	3053	0	3011	95	0
16	L	1954	0	1991	79	0
17	M	1818	0	1822	64	0
18	N	10461	0	10412	246	0
19	O	1176	0	1167	23	0
20	P	2178	0	2101	110	0
21	Q	752	0	729	25	0
22	R	5108	0	5024	200	0
23	S	1055	0	1075	58	0
23	T	1069	0	1084	48	0
23	U	2870	0	2403	79	0
23	V	1044	0	1066	71	0
24	W	4126	0	4148	185	0
25	X	5467	0	5372	211	0
26	Y	845	0	842	39	0
27	Z	1232	0	1242	58	0
28	a	1035	0	837	34	0
29	b	822	0	820	29	0
30	c	1678	0	1659	62	0
31	d	1179	0	1169	38	0
32	m	3813	0	3794	90	0
33	n	248	0	262	8	0
34	y	1606	0	1502	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	z	4980	0	5047	178	0
36	r	335	0	79	10	0
37	q	295	0	85	0	0
38	6	1970	0	994	52	0
39	1	605	0	302	14	0
40	f	110	0	29	0	0
41	A	36	0	6	0	0
42	B	32	0	12	4	0
43	6	3	0	0	0	0
43	B	1	0	0	0	0
44	M	2	0	0	0	0
44	O	3	0	0	0	0
44	P	1	0	0	0	0
45	6	1	0	0	0	0
All	All	98220	0	94154	2803	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 15.

The worst 5 of 2803 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)
20:P:82:MET:HG2	38:6:32:G:H21	1.06	1.18
35:z:379:GLU:HG3	35:z:384:ASN:ND2	1.58	1.18
20:P:82:MET:HG2	38:6:32:G:N2	1.63	1.11
35:z:379:GLU:CG	35:z:384:ASN:HD21	1.68	1.06
20:P:118:LEU:HD11	20:P:153:ARG:NH2	1.71	1.04

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	e	156/384 (41%)	146 (94%)	10 (6%)	0	100	100
2	p	58/299 (19%)	55 (95%)	3 (5%)	0	100	100
5	A	1984/2363 (84%)	1893 (95%)	90 (4%)	1 (0%)	48	79
6	B	916/984 (93%)	867 (95%)	49 (5%)	0	100	100
7	C	297/340 (87%)	278 (94%)	19 (6%)	0	100	100
8	D	94/97 (97%)	93 (99%)	1 (1%)	0	100	100
9	E	91/147 (62%)	88 (97%)	3 (3%)	0	100	100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100	100
11	G	98/115 (85%)	92 (94%)	6 (6%)	0	100	100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
13	I	71/78 (91%)	68 (96%)	3 (4%)	0	100	100
14	J	71/77 (92%)	68 (96%)	3 (4%)	0	100	100
15	K	389/473 (82%)	359 (92%)	30 (8%)	0	100	100
16	L	242/557 (43%)	226 (93%)	14 (6%)	2 (1%)	16	48
17	M	222/354 (63%)	215 (97%)	7 (3%)	0	100	100
18	N	1282/1284 (100%)	1261 (98%)	21 (2%)	0	100	100
19	O	142/146 (97%)	136 (96%)	6 (4%)	0	100	100
20	P	265/388 (68%)	247 (93%)	17 (6%)	1 (0%)	30	63
21	Q	86/265 (32%)	82 (95%)	3 (4%)	1 (1%)	11	38
22	R	597/674 (89%)	585 (98%)	11 (2%)	1 (0%)	44	74
23	S	130/488 (27%)	121 (93%)	9 (7%)	0	100	100
23	T	132/488 (27%)	127 (96%)	4 (3%)	1 (1%)	16	48
23	U	414/488 (85%)	399 (96%)	15 (4%)	0	100	100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
24	W	488/757 (64%)	450 (92%)	33 (7%)	5 (1%)	13	42
25	X	642/790 (81%)	608 (95%)	33 (5%)	1 (0%)	44	74
26	Y	94/229 (41%)	89 (95%)	4 (4%)	1 (1%)	12	39
27	Z	151/187 (81%)	145 (96%)	5 (3%)	1 (1%)	19	51
28	a	150/558 (27%)	138 (92%)	12 (8%)	0	100	100
29	b	98/293 (33%)	92 (94%)	6 (6%)	0	100	100
30	c	202/887 (23%)	194 (96%)	8 (4%)	0	100	100
31	d	152/155 (98%)	138 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	m	455/797 (57%)	447 (98%)	7 (2%)	1 (0%)	44	74
33	n	28/361 (8%)	27 (96%)	1 (4%)	0	100	100
34	y	196/534 (37%)	168 (86%)	25 (13%)	3 (2%)	8	33
35	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	44	74
37	q	3/56 (5%)	3 (100%)	0	0	100	100
All	All	11306/17429 (65%)	10784 (95%)	502 (4%)	20 (0%)	45	74

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	Y	144	VAL
34	y	115	LYS
23	T	69	LEU
24	W	536	ILE
5	A	1115	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	149/346 (43%)	149 (100%)	0	100	100
2	p	56/274 (20%)	56 (100%)	0	100	100
5	A	1798/2138 (84%)	1798 (100%)	0	100	100
6	B	821/881 (93%)	821 (100%)	0	100	100
7	C	257/292 (88%)	257 (100%)	0	100	100
8	D	85/86 (99%)	85 (100%)	0	100	100
9	E	80/118 (68%)	80 (100%)	0	100	100
10	F	76/102 (74%)	76 (100%)	0	100	100
11	G	91/101 (90%)	91 (100%)	0	100	100
12	H	73/76 (96%)	73 (100%)	0	100	100
13	I	64/69 (93%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	J	63/67 (94%)	63 (100%)	0	100	100
15	K	333/405 (82%)	333 (100%)	0	100	100
16	L	211/477 (44%)	211 (100%)	0	100	100
17	M	198/306 (65%)	198 (100%)	0	100	100
18	N	1188/1188 (100%)	1188 (100%)	0	100	100
19	O	130/132 (98%)	130 (100%)	0	100	100
20	P	231/340 (68%)	231 (100%)	0	100	100
21	Q	79/240 (33%)	79 (100%)	0	100	100
22	R	532/597 (89%)	532 (100%)	0	100	100
23	S	121/443 (27%)	121 (100%)	0	100	100
23	T	123/443 (28%)	123 (100%)	0	100	100
23	U	222/443 (50%)	220 (99%)	2 (1%)	75	88
23	V	120/443 (27%)	120 (100%)	0	100	100
24	W	443/656 (68%)	443 (100%)	0	100	100
25	X	586/707 (83%)	586 (100%)	0	100	100
26	Y	94/214 (44%)	94 (100%)	0	100	100
27	Z	132/163 (81%)	132 (100%)	0	100	100
28	a	79/496 (16%)	79 (100%)	0	100	100
29	b	95/275 (34%)	95 (100%)	0	100	100
30	c	188/816 (23%)	188 (100%)	0	100	100
31	d	128/129 (99%)	128 (100%)	0	100	100
32	m	425/719 (59%)	425 (100%)	0	100	100
33	n	28/335 (8%)	28 (100%)	0	100	100
34	y	173/478 (36%)	173 (100%)	0	100	100
35	z	564/585 (96%)	564 (100%)	0	100	100
37	q	2/2 (100%)	2 (100%)	0	100	100
All	All	10038/15582 (64%)	10036 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	U	184	PRO
23	U	415	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
18	N	1108	GLN
22	R	367	ASN
35	z	108	GLN
20	P	111	ASN
21	Q	68	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	22/186 (11%)	5 (22%)	0
38	6	91/99 (91%)	44 (48%)	7 (7%)
39	1	28/29 (96%)	19 (67%)	2 (7%)
4	5	101/120 (84%)	22 (21%)	2 (1%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

5 of 90 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	11	U
3	2	12	G
3	2	13	C
3	2	24	A
3	2	29	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	6	52	G
38	6	74	U
39	1	1	G
39	1	0	G
38	6	29	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 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$
42	GTP	B	1001	43	26,34,34	1.45	3 (11%)	32,54,54	1.75	8 (25%)
41	IHP	A	2401	-	36,36,36	1.54	13 (36%)	54,60,60	1.48	10 (18%)

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
42	GTP	B	1001	43	-	0/18/38/38	0/3/3/3
41	IHP	A	2401	-	-	4/30/54/54	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	B	1001	GTP	C5-C6	-4.74	1.37	1.47
42	B	1001	GTP	C2'-C1'	-2.47	1.50	1.53
41	A	2401	IHP	P1-O31	-2.46	1.45	1.54
41	A	2401	IHP	P3-O33	-2.36	1.45	1.54
41	A	2401	IHP	P6-O46	-2.35	1.45	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	B	1001	GTP	PB-O3B-PG	-5.21	114.95	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	B	1001	GTP	C5-C6-N1	3.71	120.51	113.95
42	B	1001	GTP	C2-N1-C6	-3.26	119.09	125.10
41	A	2401	IHP	C5-C6-C1	3.18	117.38	110.41
42	B	1001	GTP	PA-O3A-PB	-3.16	121.99	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

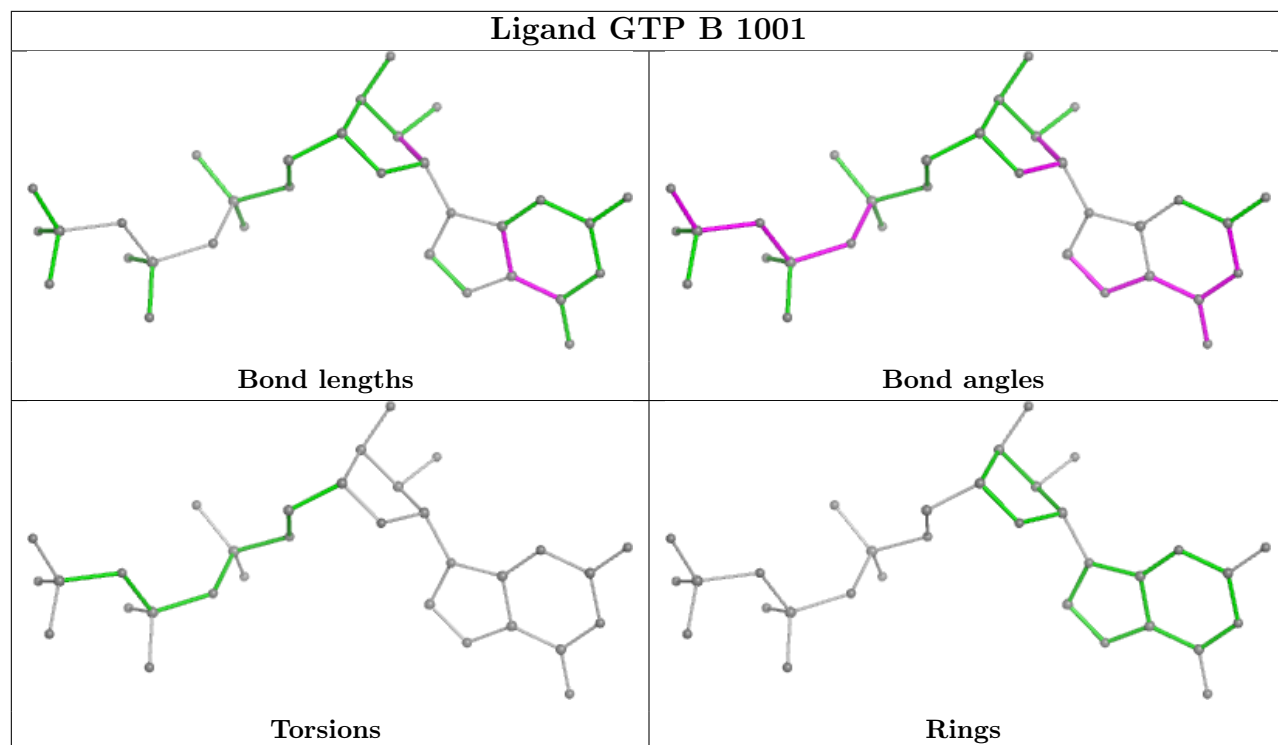
Mol	Chain	Res	Type	Atoms
41	A	2401	IHP	C6-O16-P6-O26
41	A	2401	IHP	C1-O11-P1-O41
41	A	2401	IHP	C6-O16-P6-O36
41	A	2401	IHP	C5-O15-P5-O35

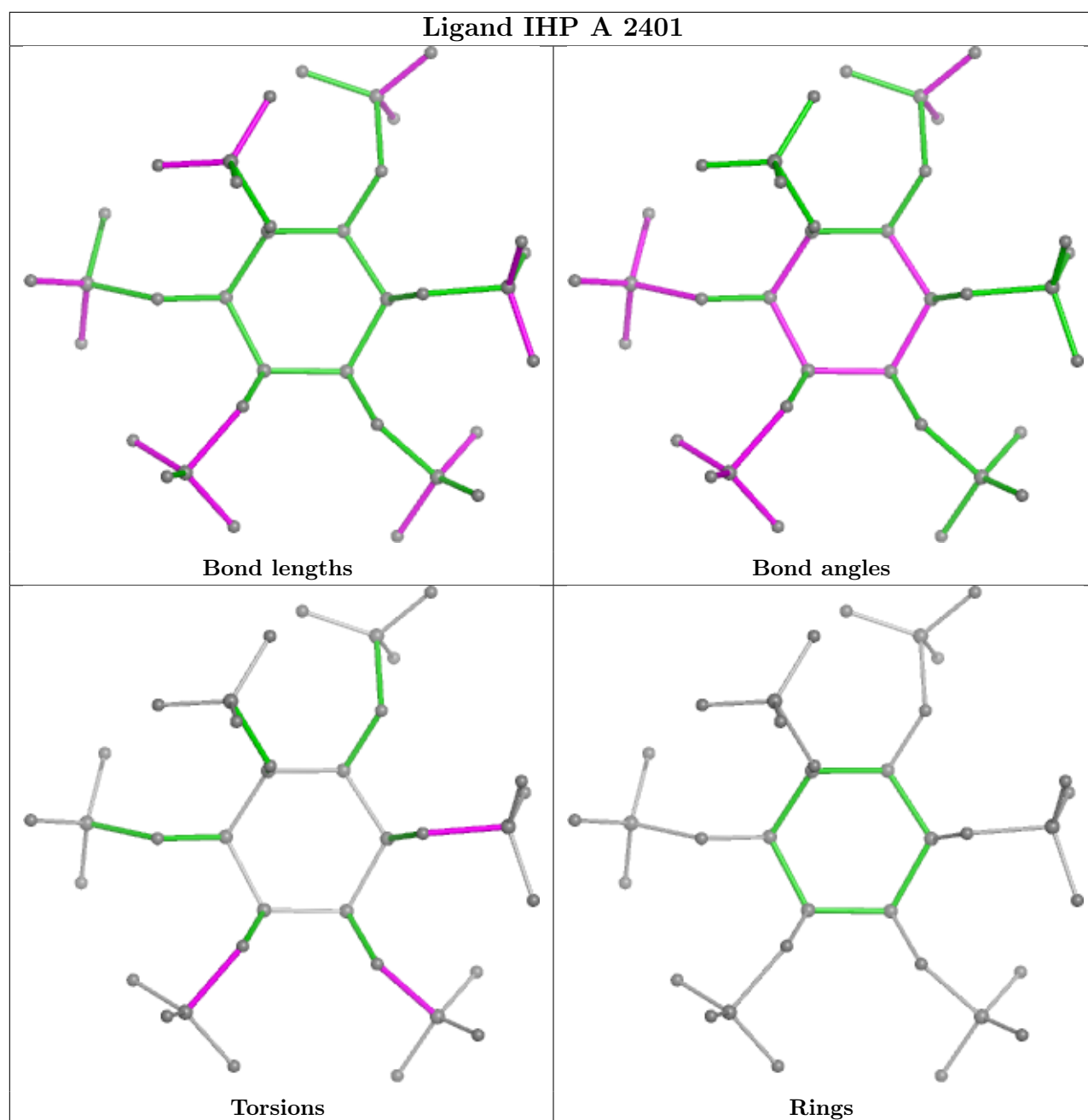
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	B	1001	GTP	4	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.

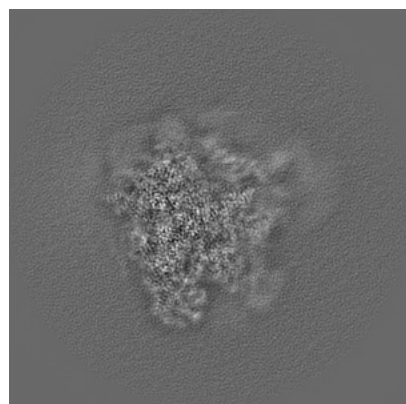
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19942. These allow visual inspection of the internal detail of the map and identification of artifacts.

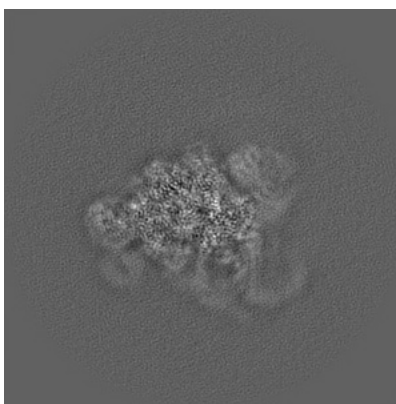
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

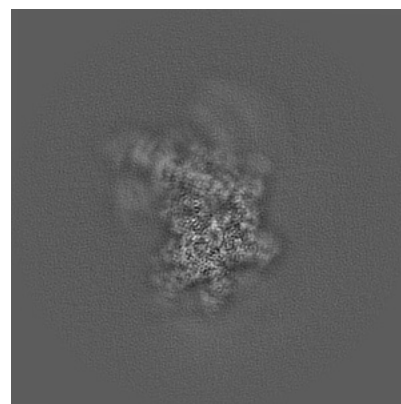
6.1.1 Primary map



X

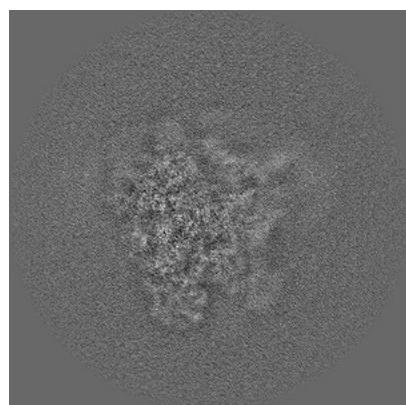


Y

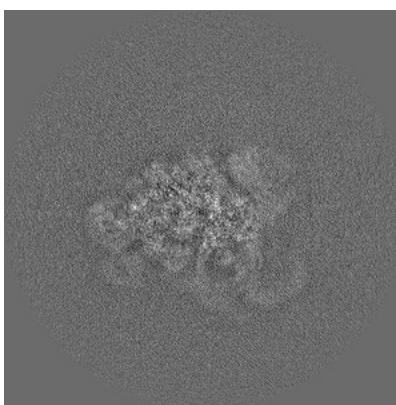


Z

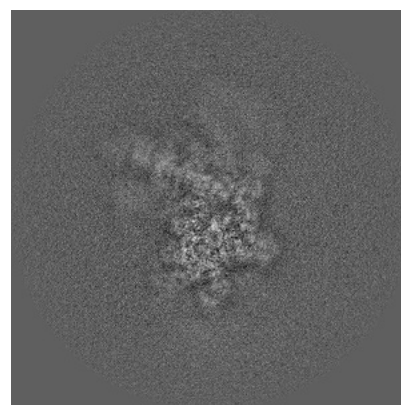
6.1.2 Raw map



X



Y

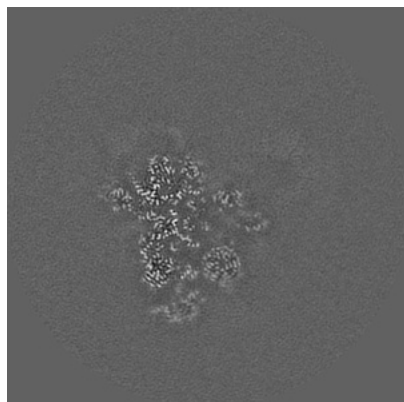


Z

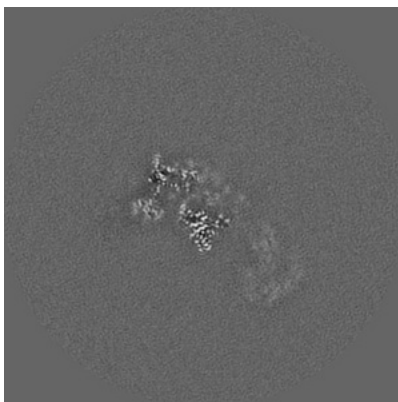
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

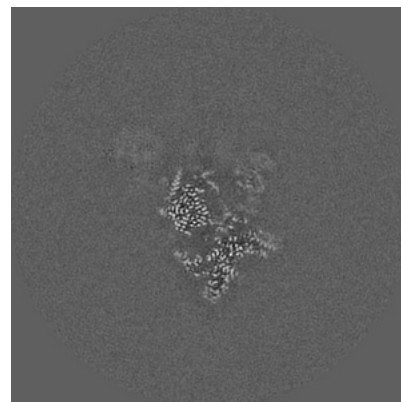
6.2.1 Primary map



X Index: 280

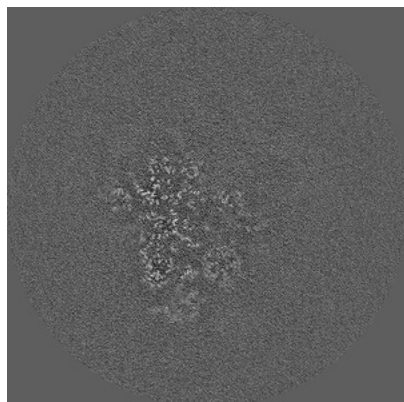


Y Index: 280

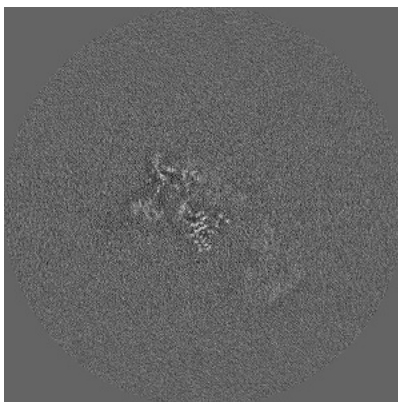


Z Index: 280

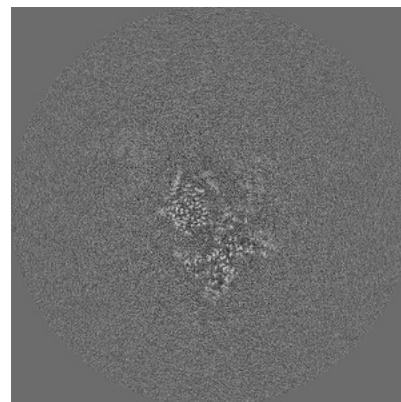
6.2.2 Raw map



X Index: 280



Y Index: 280

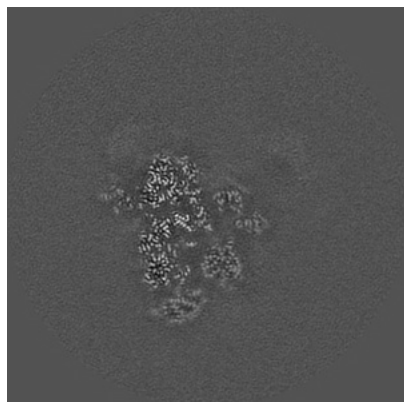


Z Index: 280

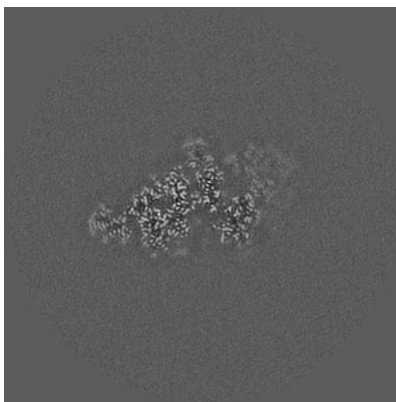
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

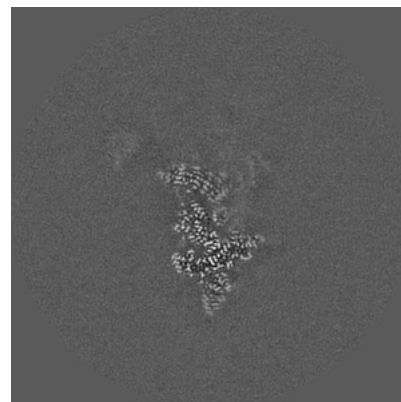
6.3.1 Primary map



X Index: 276

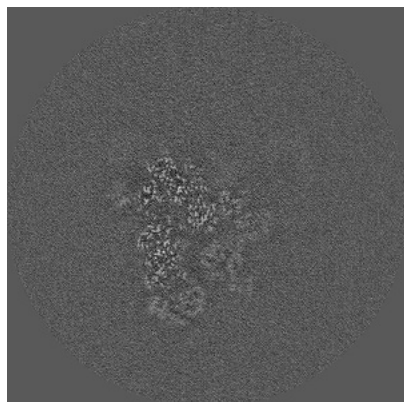


Y Index: 219

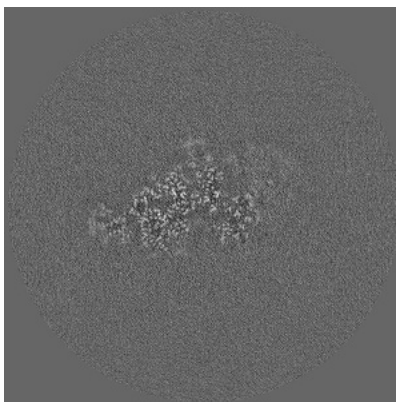


Z Index: 295

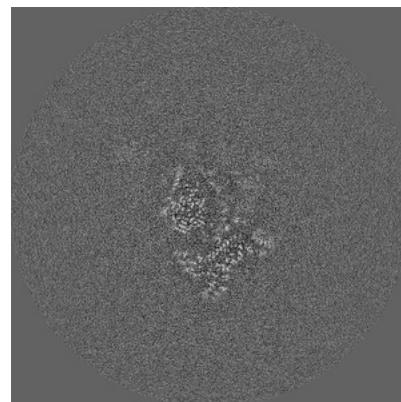
6.3.2 Raw map



X Index: 269



Y Index: 219

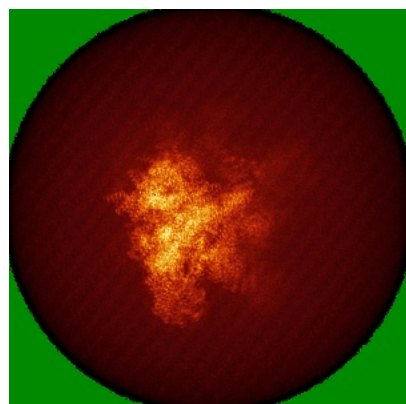


Z Index: 282

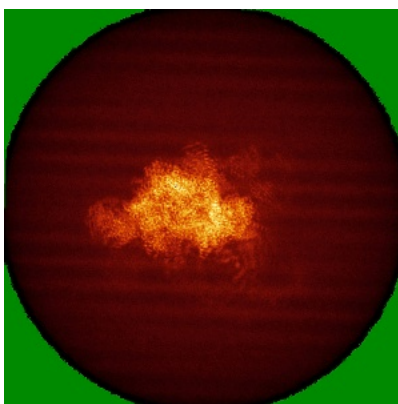
The images above show the largest variance slices of the map in three orthogonal directions.

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

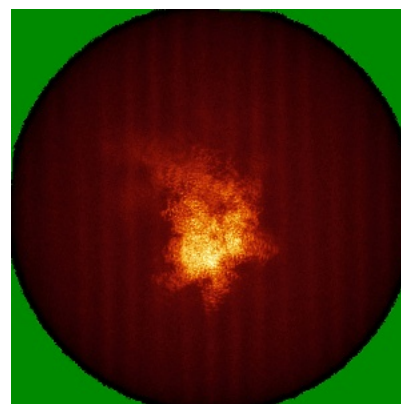
6.4.1 Primary map



X

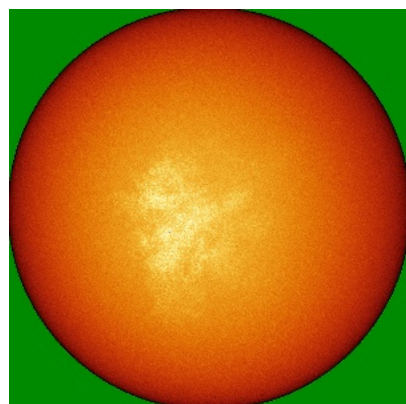


Y

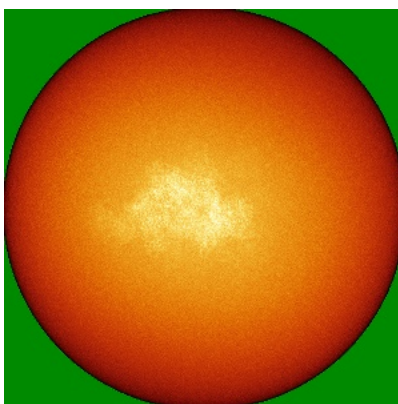


Z

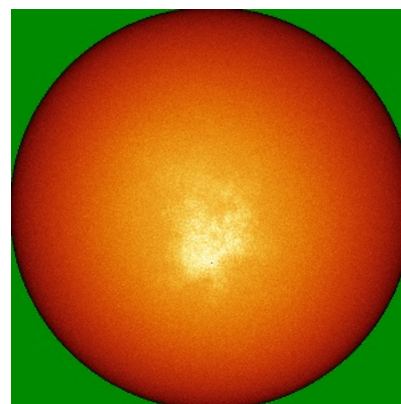
6.4.2 Raw map



X



Y

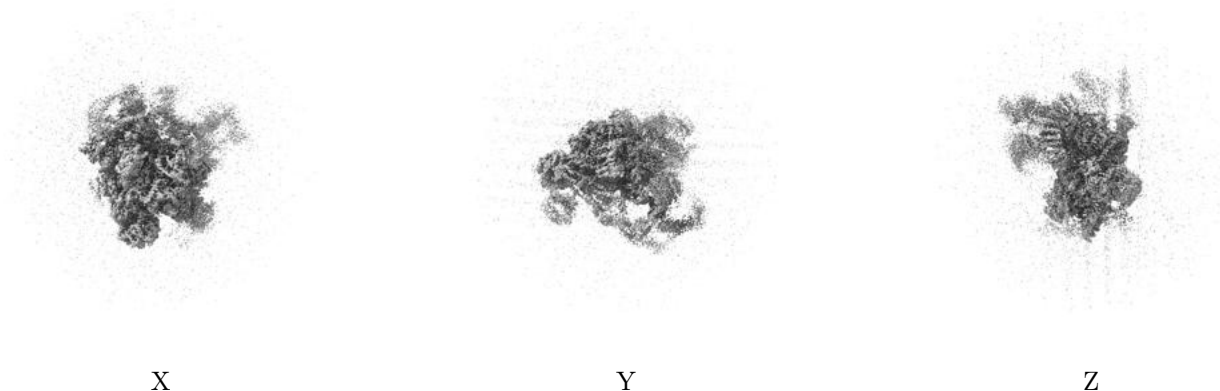


Z

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.

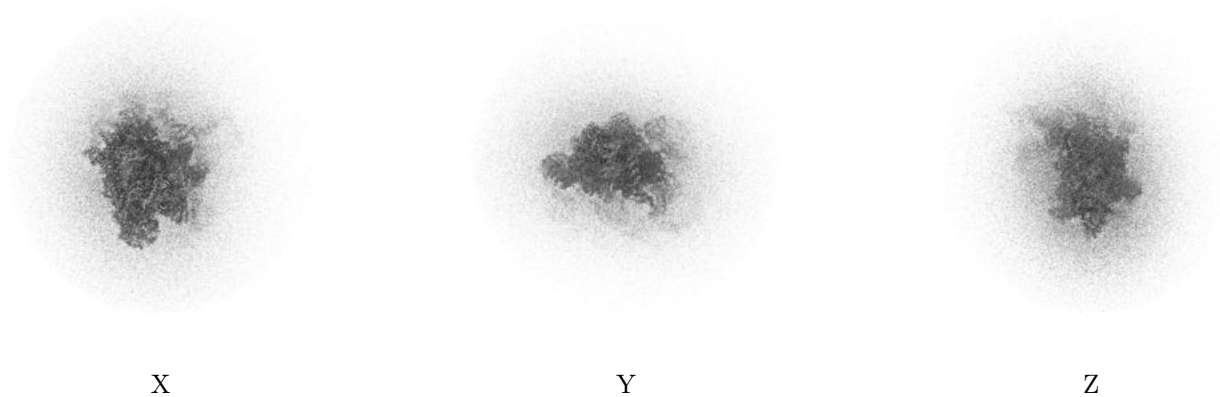
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.2. 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.

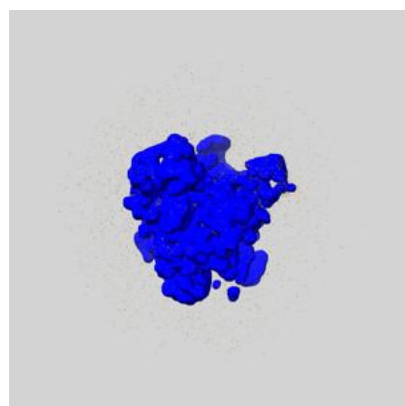
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

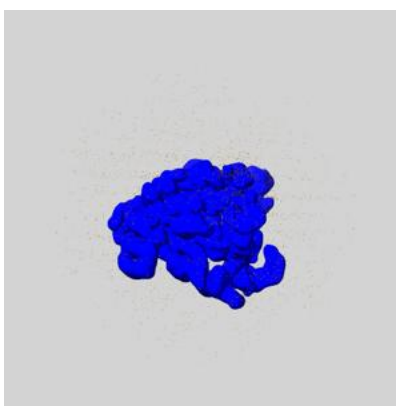
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

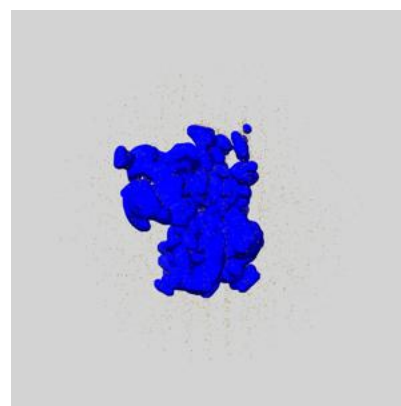
6.6.1 emd_19942_msk_1.map [i](#)



X



Y

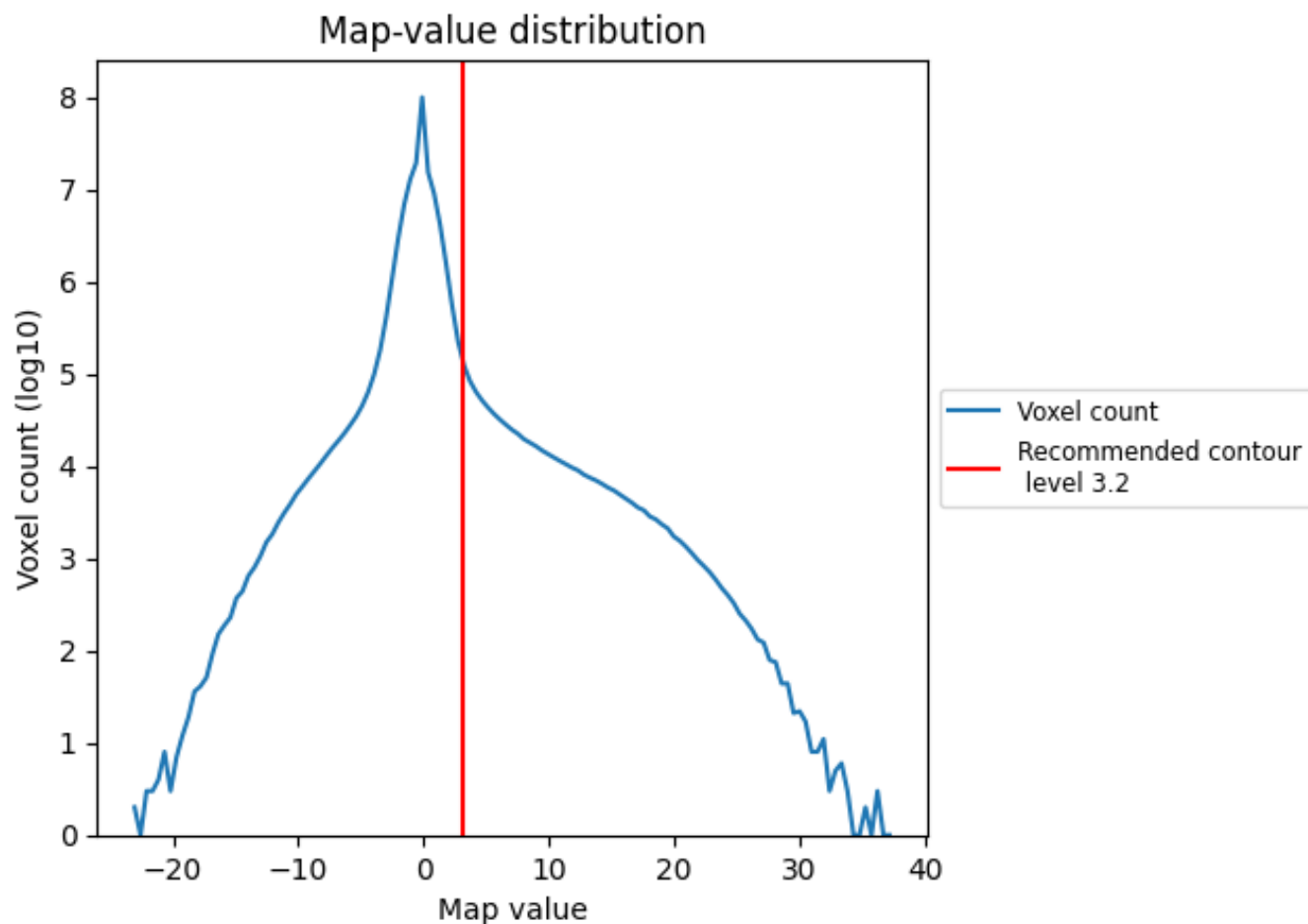


Z

7 Map analysis [i](#)

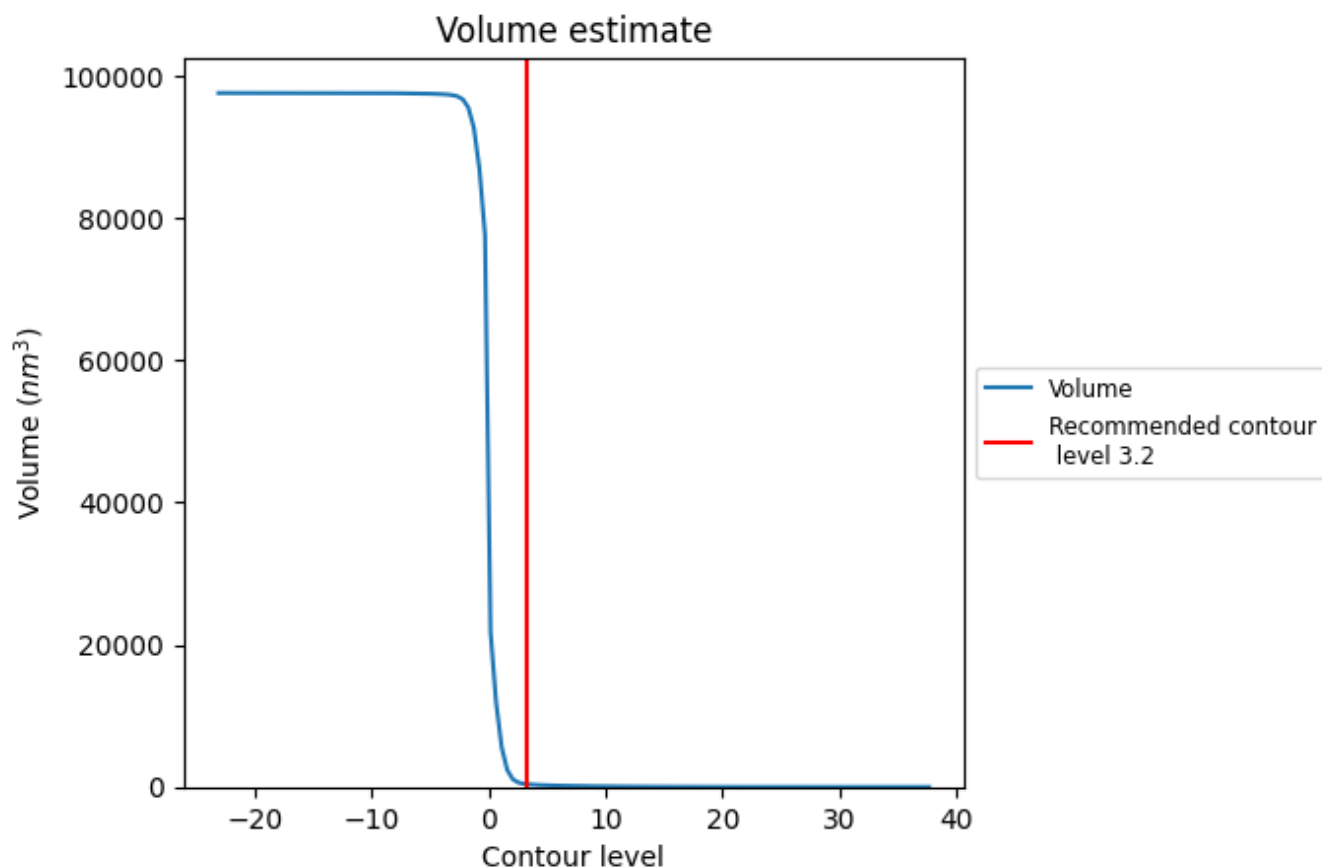
This section contains the results of statistical analysis of the map.

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.

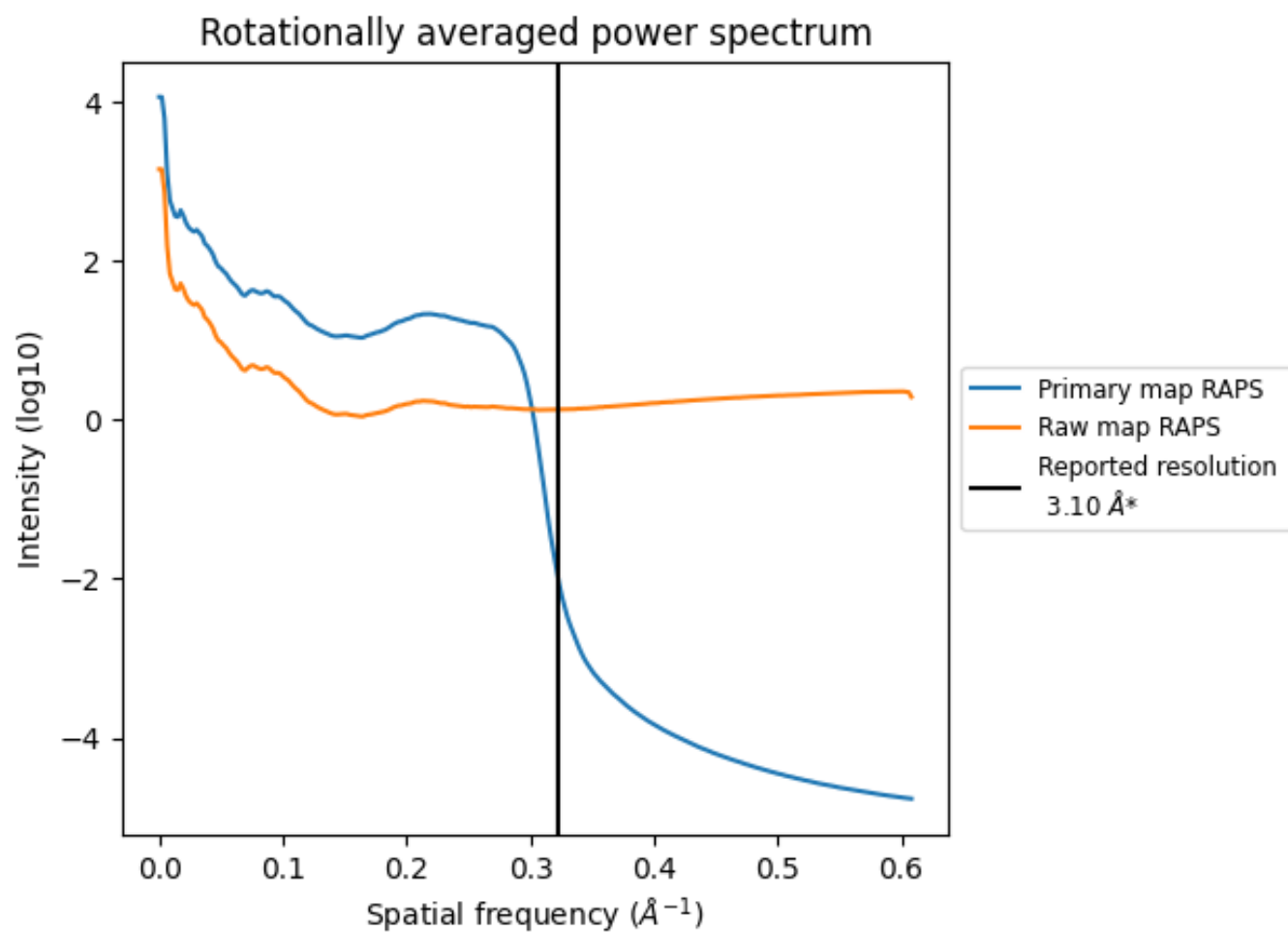
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm^3 ; this corresponds to an approximate mass of 375 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 ⓘ

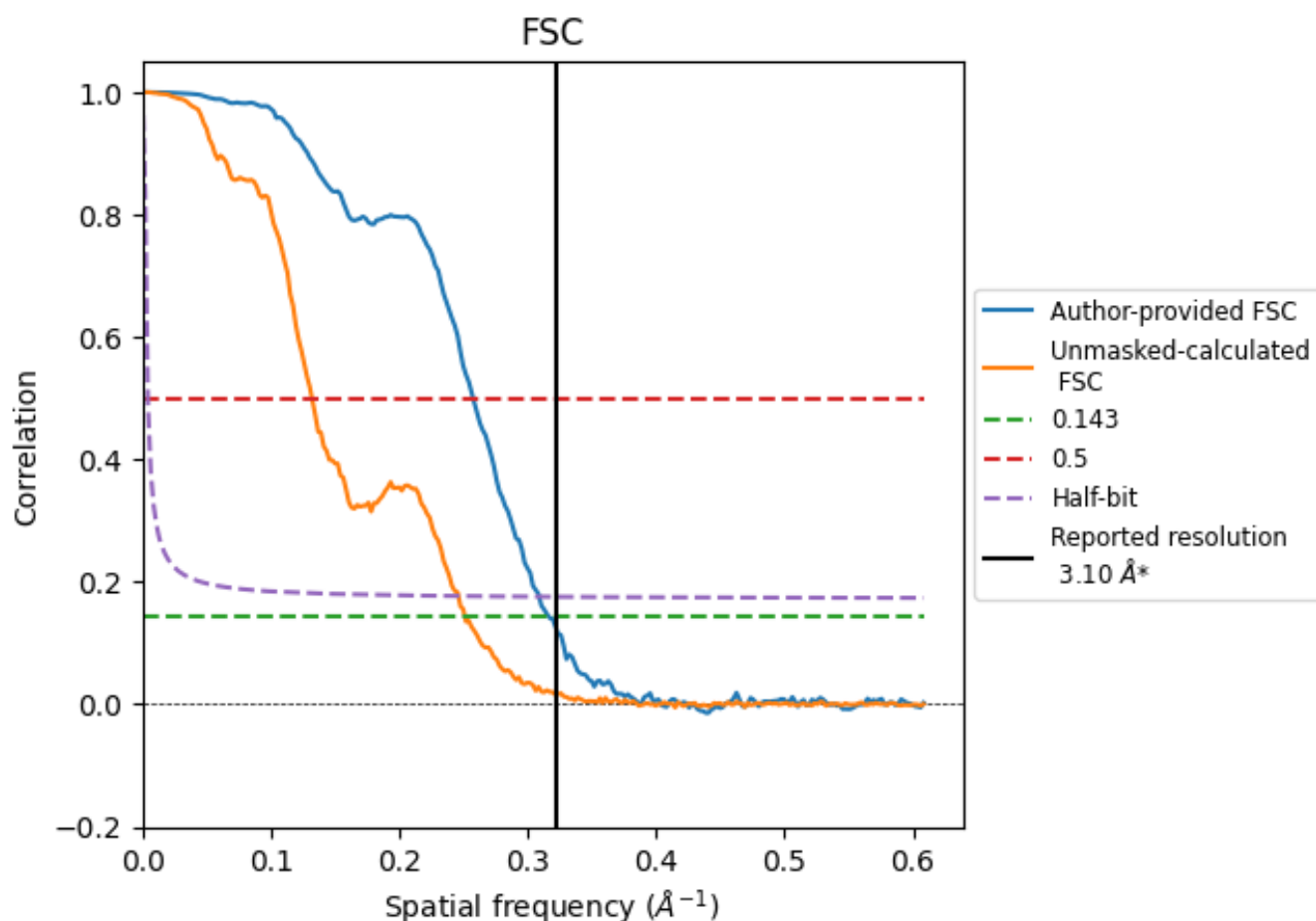


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

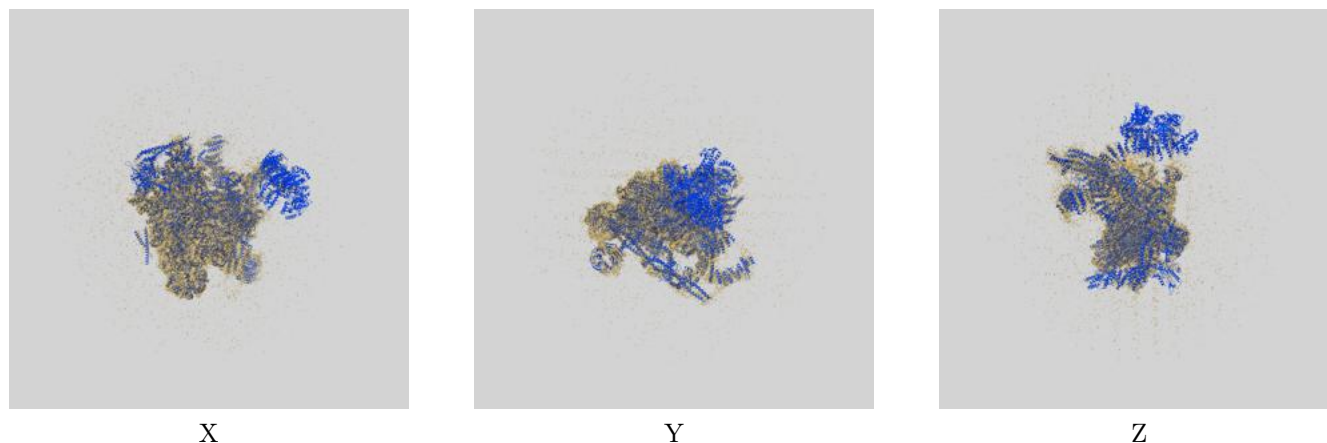
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.88	3.24
Unmasked-calculated*	3.98	7.58	4.06

*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 3.98 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

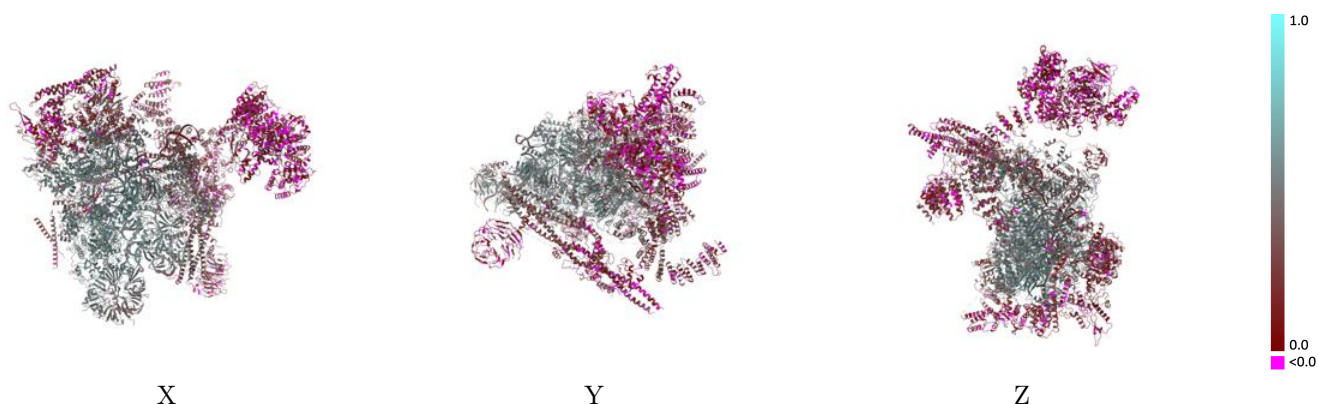
This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9ESI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



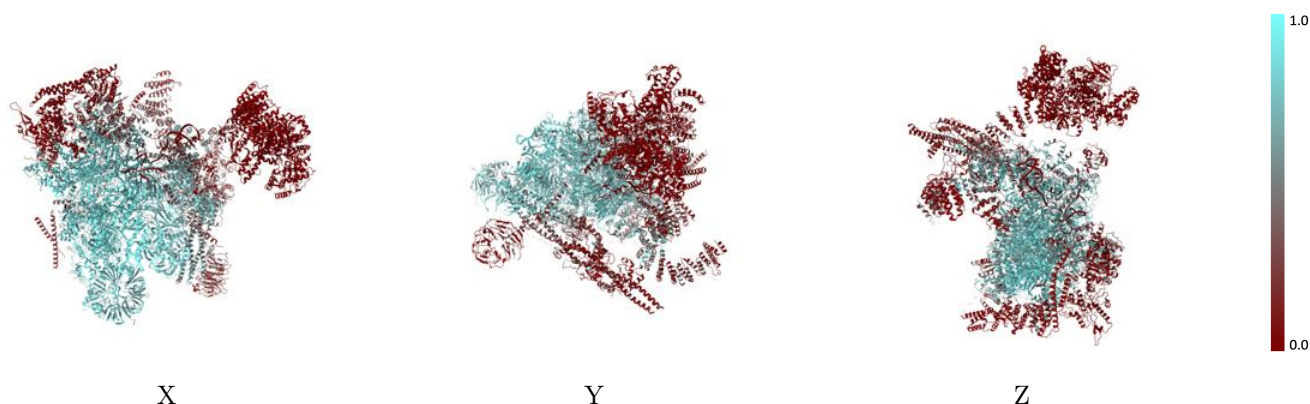
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



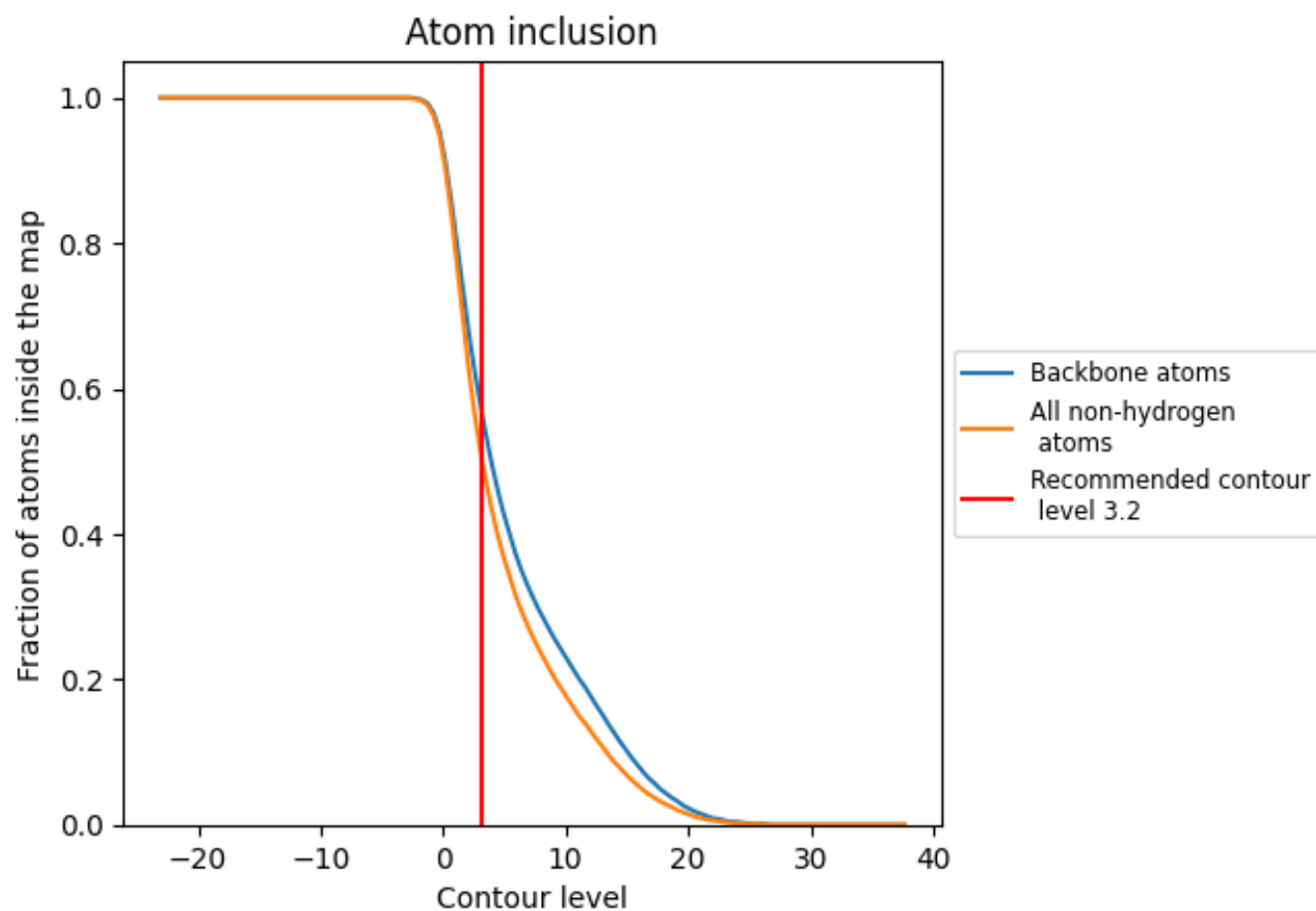
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 50% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4990	 0.3640
1	 0.5170	 0.4200
2	 0.4320	 0.3200
5	 0.9380	 0.5360
6	 0.5180	 0.4060
A	 0.7590	 0.4960
B	 0.8490	 0.5310
C	 0.7990	 0.5030
D	 0.8680	 0.5490
E	 0.7970	 0.5080
F	 0.7330	 0.4680
G	 0.7130	 0.4240
H	 0.7930	 0.5050
I	 0.7390	 0.4490
J	 0.8260	 0.5340
K	 0.8780	 0.5480
L	 0.7030	 0.4700
M	 0.4680	 0.3830
N	 0.0050	 0.1040
O	 0.8500	 0.5400
P	 0.6750	 0.4450
Q	 0.7790	 0.5310
R	 0.4450	 0.3280
S	 0.0530	 0.1340
T	 0.2000	 0.2100
U	 0.1300	 0.1600
V	 0.0770	 0.1340
W	 0.4690	 0.3200
X	 0.1770	 0.1980
Y	 0.1780	 0.3150
Z	 0.3780	 0.2660
a	 0.6470	 0.4370
b	 0.3050	 0.3220
c	 0.8220	 0.5050
d	 0.7110	 0.4720



Continued on next page...

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Chain	Atom inclusion	Q-score
e	 0.4730	 0.4550
f	 0.3910	 0.3230
m	 0.0830	 0.1860
n	 0.0210	 0.1600
p	 0.3440	 0.3510
q	 0.3880	 0.4780
r	 0.3490	 0.2780
y	 0.4500	 0.3500
z	 0.2880	 0.2760