



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:28 PM UTC

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](mailto: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>.

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

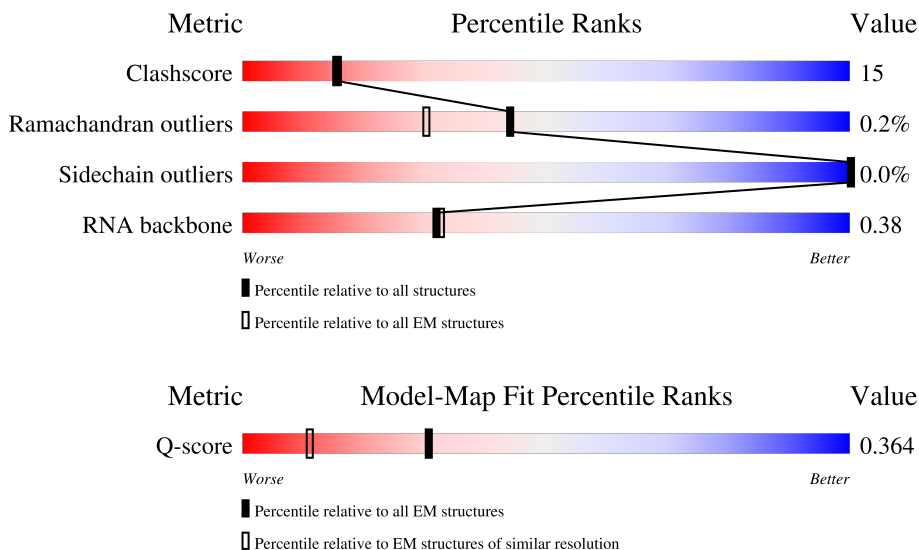
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.10 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)	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	14724 ( 2.60 - 3.60 )

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  $\geq 3$ , 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	

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Mol	Chain	Length	Quality of chain
4	5	120	
5	A	2363	
6	B	984	
7	C	340	
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	

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Mol	Chain	Length	Quality of chain
26	Y	229	
27	Z	187	
28	a	558	
29	b	293	
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 [i](#)

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
			Total	C	N	O	S		
1	e	166	1329	838	221	268	2	0	0

- Molecule 2 is a protein called Protein saf4.

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

- Molecule 3 is a RNA chain called U2snRNA.

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

- Molecule 4 is a RNA chain called U5snRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 ppl1.

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
			Total	C	N	O	S		
34	y	200	1606	1000	279	323	4	0	0

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

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

- Molecule 36 is a protein called UNK1.

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

- Molecule 37 is a protein called UNK2.

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

- Molecule 38 is a RNA chain called U6snRNA.

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

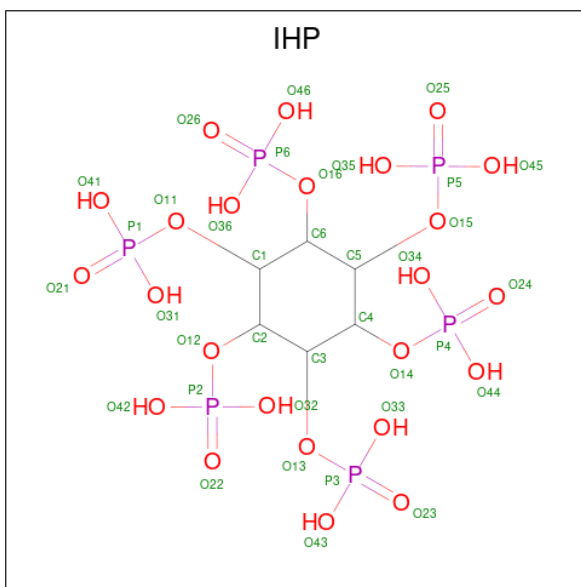
- Molecule 39 is a RNA chain called pre-mRNA.

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

- Molecule 40 is a protein called UNK3.

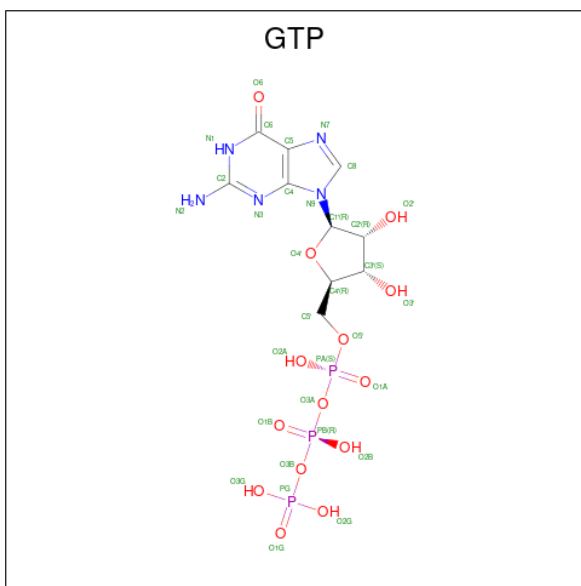
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	f	22	110	66	22	22	0	0

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>) (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	0
			32	10	5	14	3	

- 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	Mg	0
			1	1	
43	6	3	Total	Mg	0
			3	3	

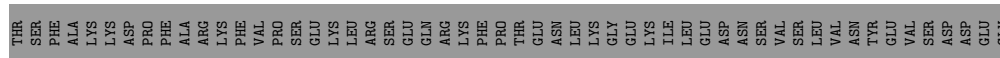
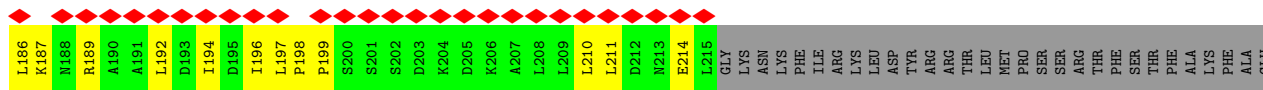
- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

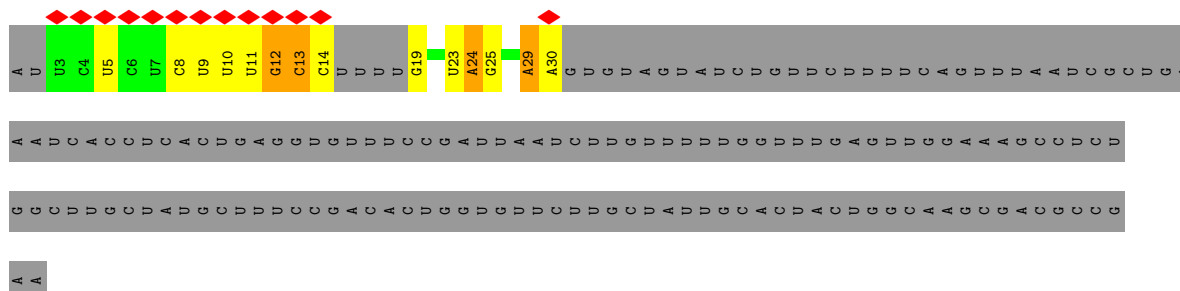
- Molecule 45 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

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

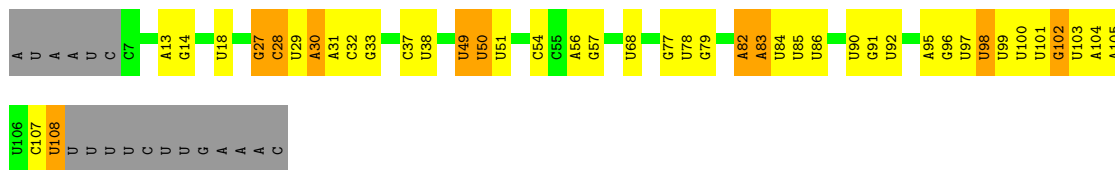




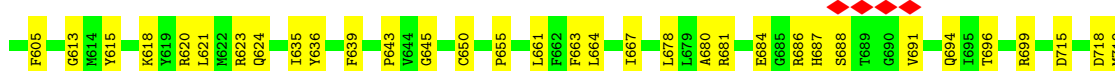
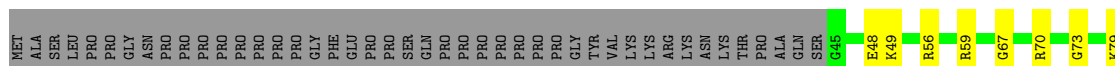
• Molecule 3: U2snRNA



• Molecule 4: U5snRNA

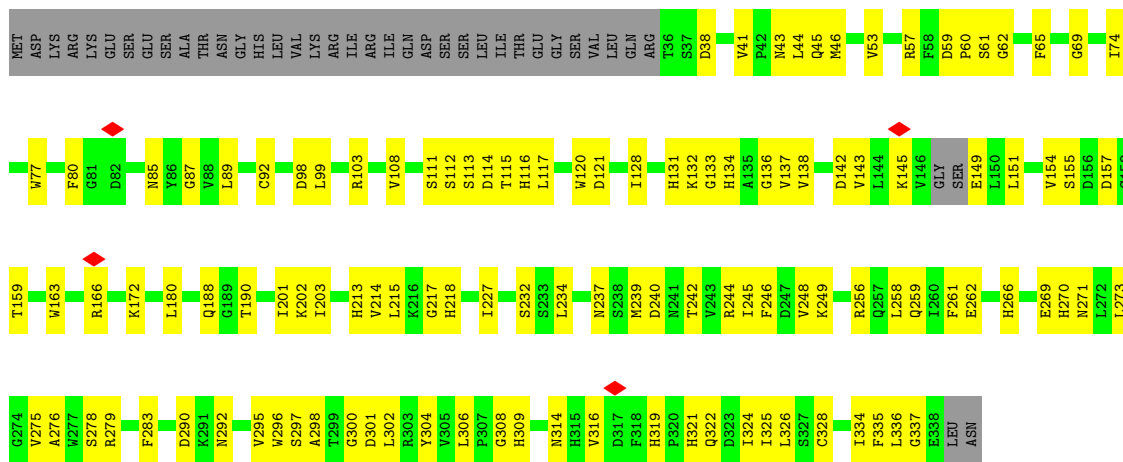


• Molecule 5: Pre-mRNA-splicing factor spp42



ILE	P1993	A1933	I1873	H1736	G1583	E1430	K1286	D1142	N984	K876	E722
GLU	N1994	T1934	R1874	S1737	I1584	D1451	W1287	M1145	N986	G877	R725
LYS	L1995	E1935	S1875	A1738	M1586	E1432	L1291	M1146	T986	R878	L986
GLN	D1996	P1936	L1876	Y1739	H1587	L1433	M1295	N1150	D987	Q883	Q726
ARG	Q1997	Q1937	M1741	W1662	K1588	D1434	T1296	K1153	Y988	R884	G727
GLU	D1998	Q1938	W1742	V1663	K1589	S1435	T1297	K1154	S1005	B885	K728
ASN	Q1999	M1939	I1743	R1665	T1592	W1436	Y1298	M1168	K1006	E886	I732
ALA	W2000	E1879	M1746	P1666	L1593	D1437	Y1299	M1169	V1011	H898	M746
GLN	L2001	E1880	P1747	L1669	K1594	G1438	E1300	R1176	V1012	I747	I747
THR	L2002	Q1881	P1748	L1670	L1595	G1439	E1301	R1177	L1016	P748	P748
ALA	V2003	R1882	L1749	M1671	L1596	I1440	I1303	I1182	L1017	K749	K749
VAL	E2004	Q1884	L1750	M1672	L1597	I1441	E1307	R1185	L1018	I904	I750
THR	P2005	I1885	Q1751	N1673	L1598	F1442	E1308	R1186	L1019	K905	L754
LYS	K2006	I1886	Q1752	N1674	Q1599	F1443	C1315	L1190	M1020	R906	P755
THR	L2007	P1826	S1753	D1674	I1600	Q1448	C1316	T1191	A1034	R907	F755
THR	L2007	M1754	M1754	R1674	F1601	K1449	K1318	L1191	A1035	L908	I758
ASN	L2007	M1755	M1755	D1677	R1602	D1450	K1319	E1196	K1036	M911	A788
VAL	R2008	I1757	I1757	N1677	S1603	R1451	P1360	E1197	M1037	R912	K797
THR	R2008	N1678	N1678	M1678	H1604	W1460	L1364	D1197	K1038	R913	T803
HIS	D2009	I1679	T1679	T1679	L1605	R1461	L1365	T1198	G1056	R914	K808
GLY	A1830	M1761	M1761	R1461	L1606	R1462	D1371	T1199	L1057	T913	E810
ASP	V1951	P1762	P1762	V1462	W1606	V1462	M1354	L1206	L1057	F914	E810
GLU	S1952	A1763	A1763	R1463	Q1607	R1463	M1355	D1206	I1063	I319	A788
MET	S1953	M1770	R1770	R1609	I1609	R1463	L1358	M1214	F1066	E920	K797
VAL	A2013	R1770	R1770	I1609	D1616	W1479	P1360	T1214	L1053	F921	K797
VAL	D2014	F1834	F1834	L1617	L1617	W1489	L1364	G1216	L1053	F921	K797
THR	Y2015	M1835	M1835	L1617	L1617	Q1490	L1364	G1216	L1053	F921	K797
THR	A2016	P1836	P1836	L1621	L1621	Q1490	L1364	G1216	L1053	F921	K797
THR	A2016	Y1836	Y1836	L1621	L1621	Q1490	L1364	G1216	L1053	F921	K797
THR	K2017	R1837	R1837	L1622	L1622	N1491	D1371	L1222	G1056	L928	T803
ALA	K2018	Q1838	Q1838	Q1622	Q1622	N1491	D1371	L1222	G1056	L928	T803
GLY	R2019	T1838	T1838	Q1623	Q1623	N1492	M1374	L1222	G1056	L928	T803
TYR	M2019	G1839	G1839	E1624	E1624	R1495	I1374	P1223	I1063	Y832	K808
ASN	N2020	Q1840	Q1840	E1624	E1624	R1495	I1374	P1223	I1063	Y832	K808
ASN	I2021	R1841	R1841	S1627	S1627	F1514	R1378	L1233	F1066	D935	E810
LYS	N2022	F1842	F1842	L1628	L1628	T1517	G1385	K1234	D1072	E938	R813
PHE	V2023	L1843	L1843	Q1629	Q1629	T1517	E1386	K1234	D1072	E938	R813
SER	V2023	K1844	K1844	L1630	L1630	K1538	L1392	W1237	R1080	D820	K819
SER	A2024	V1845	V1845	E1631	E1631	K1538	L1392	W1237	R1080	D820	K819
LYS	S2025	V1846	V1846	K1635	K1635	L1542	Y1393	N1239	E1083	D946	G821
THR	A2026	I1846	I1846	E1636	E1636	Q1546	E1400	M1243	G1086	W950	D827
GLU	T2027	H1847	H1847	T1637	T1637	R1547	E1400	M1243	G1086	F951	D827
ARG	N2028	T1848	T1848	Y1711	Y1711	R1547	E1400	M1243	G1086	F951	D827
ASN	S2029	E1849	E1849	D1714	D1714	S1548	S1406	R1244	L1095	W839	W839
ARG	E2030	V1850	V1850	A1715	A1715	G1549	S1406	R1244	L1095	W839	W839
ALA	VAL	W1851	W1851	Q1716	Q1716	G1549	S1406	R1244	L1095	W839	W839
ILE	ARG	S1911	S1911	S1717	S1717	Q1552	W1410	L1254	D1099	F959	P851
SER	ASP	E1912	E1912	M1718	M1718	R1556	K1416	I1255	P1107	W962	P852
SER	ASP	L1913	L1913	Y1719	Y1719	R1567	E1419	I1268	L1110	W963	V863
ILE	ILE	Q1914	Q1914	P1720	P1720	R1568	E1419	I1268	L1111	K964	V863
LEU	LEU	L1915	L1915	S1721	S1721	R1568	E1419	I1268	L1112	P965	V863
LEU	GLY	K1916	K1916	P1722	P1722	G1574	Q1423	L1271	I1115	E969	L862
PRO	GLY	R1856	R1856	L1723	L1723	F1574	M1424	L1272	I1115	P970	R868
LEU	MET	L1857	L1857	G1724	G1724	F1575	R1425	L1272	R1123	P971	L869
LEU	MET	L1857	L1857	V1725	V1725	Q1576	R1426	L1272	R1123	P971	L869
ARG	ILE	Q1918	Q1918	I1727	I1727	Q1576	R1426	L1272	R1123	P971	L869
THR	ILE	A1919	A1919	I1727	I1727	Q1576	R1426	L1272	R1123	P971	L869
THR	THR	A1919	A1919	I1727	I1727	Q1576	R1426	L1272	R1123	P971	L869
LYS	ALA	I1920	I1920	D1730	D1730	T1582	L1428	L1429	R1135	R973	S874
PRO	PRO	P1980	P1980	M1735	M1735	T1582	L1428	L1429	R1135	R973	S874
SER	SER	D1981	D1981								
LEU	LEU	K1982	K1982								
GLN	GLN	L1923	L1923								
ARG	ARG	S1983	S1983								
GLN	GLN	I1984	I1984								
GLN	GLN	K1925	K1925								
ILE	ILE	I1926	I1926								
ALA	ALA	N1927	N1927								
GLU	GLU	E1928	E1928								
GLU	GLU	M1929	M1929								
ASN	ASN	I1930	I1930								
ASN	ASN	V1991	V1991								
GLU	GLU	W1992	W1992								

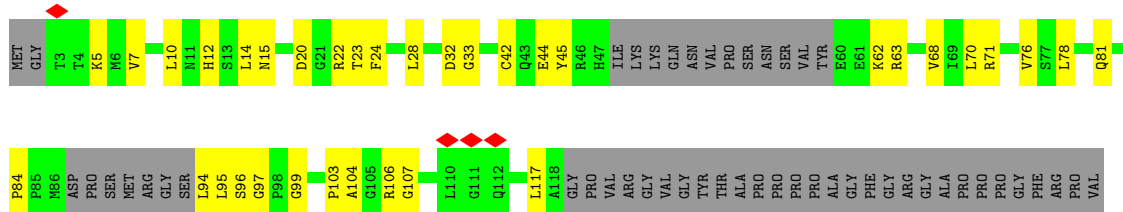




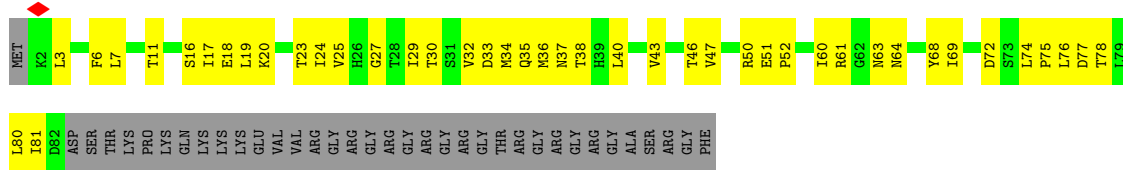
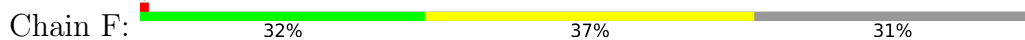
• Molecule 8: Small nuclear ribonucleoprotein Sm D3



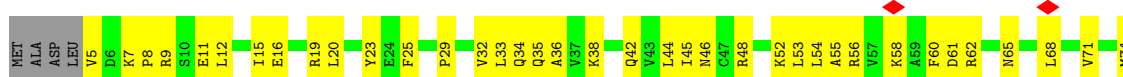
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B



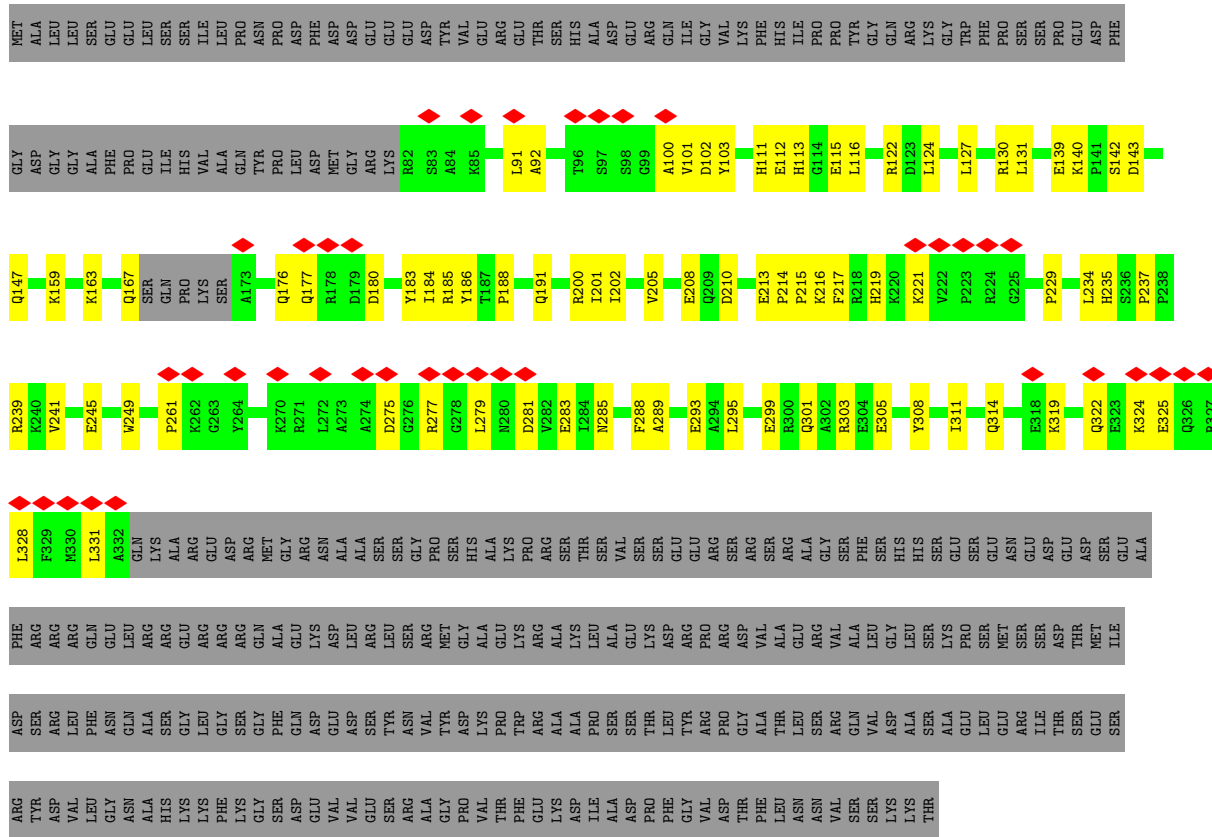
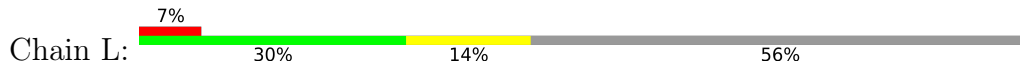
• Molecule 10: Small nuclear ribonucleoprotein Sm D1



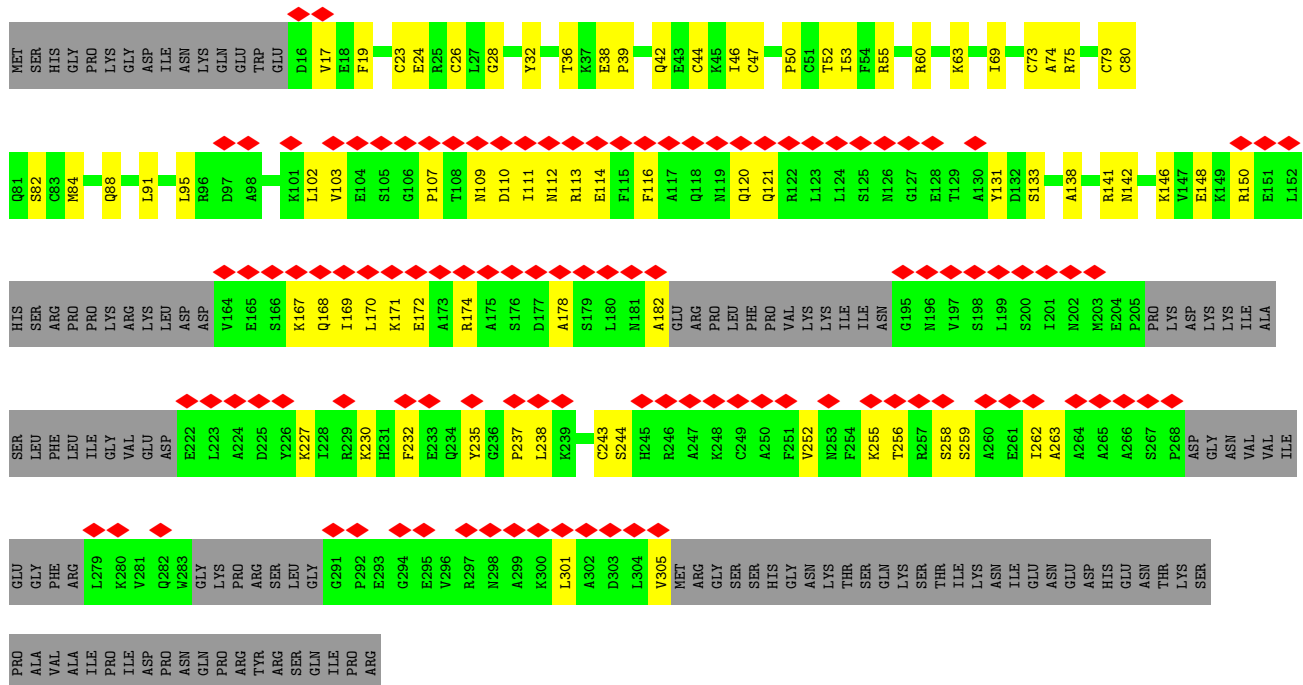
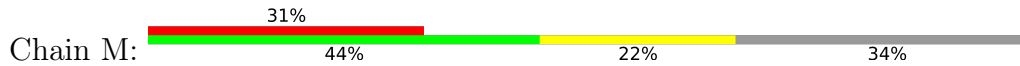
• Molecule 11: Small nuclear ribonucleoprotein Sm D2







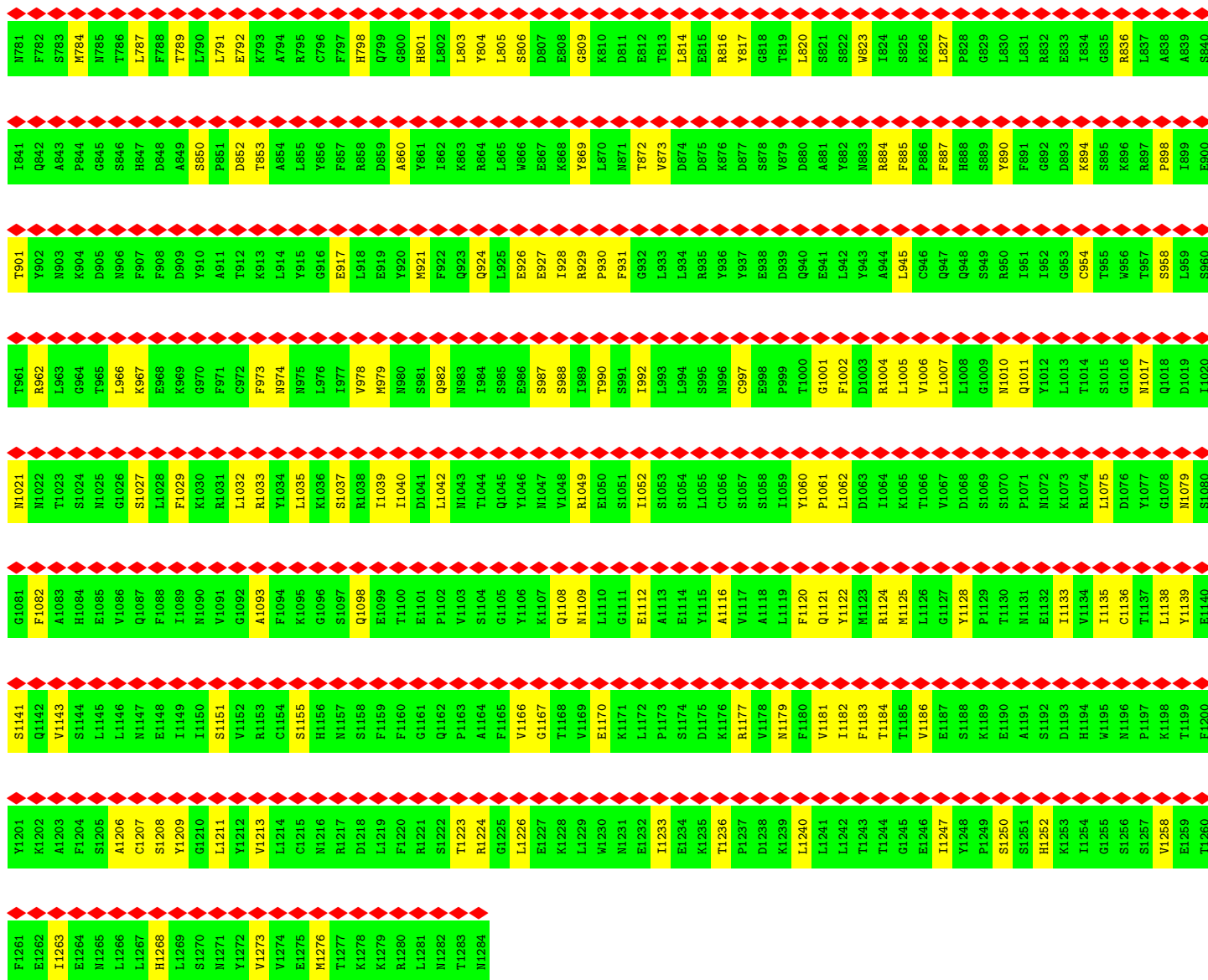
● Molecule 17: Pre-mRNA-splicing factor cwf5



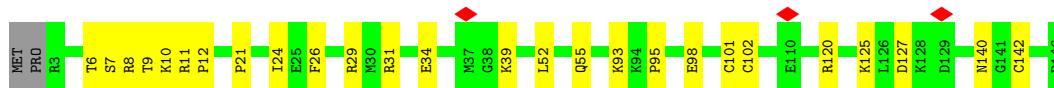
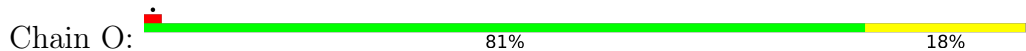
• Molecule 18: Pre-mRNA-splicing factor cwf11



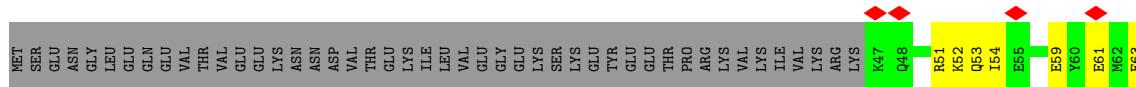
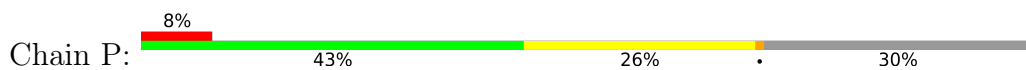
M1	V2	L3	Y4	K5	N6	K7	K8	K9	Q10	I11	I12	M13	Y14	A15	N16	S17	M18	W19	G20	Q21	N22	E23	G24	V25	E26	F27	Q28	E29	T30	M31	L32	Q33	C34	I35	L36	E37	A38	V39	I40	V41	S42	K43	D44	A45	K46	Q47	V48	L49	S50	L51	L52	H53	E54	L55	K56	L57	F58	E59	N60	
F61	L62	W63	Q64	R65	V66	N67	T68	E69	M70	S71	L72	W73	H74	I75	N76	L77	T78	C79	M80	L81	Q82	L83	Y84	K85	S86	K87	Y88	E89	I89	Y90	I91	T92	M93	D94	L95	I96	D97	E98	N99	R100	F101	Q102	L103	F104	F105	K106	K107	V108	I109	S110	V111	S112	L113	E114	L115	N116	L117	S118	E119	V120
V121	Y122	M123	I124	Q125	F126	I127	T128	L129	C130	F131	Q132	F133	S134	M135	I136	L137	K138	L139	R140	K141	L142	V143	Y144	Q145	L146	T147	M148	E149	S150	I151	L152	M153	D154	L155	D156	M157	L158	D159	K160	V161	Q162	L163	A164	I165	H166	D167	S168	S169	S170	L171	T172	K173	A174	F175	D176	Y177	K178	K179	E180	
K181	R182	P183	S184	I185	V186	E187	K188	F189	P190	L191	H192	N193	L194	L195	S196	M197	W198	I199	H200	S201	L202	L203	I204	K205	S206	I207	S208	Y209	A210	Q211	T212	E213	K214	Q215	E216	K217	K218	V219	T220	P221	L222	L223	A224	I225	I226	M227	M228	S229	E230	L230	V231	L232	L233	S234	A235	F236	Y237	T238	R239	R240
F241	A242	H243	P244	I245	V246	E247	D248	S249	C250	F251	Y252	T253	A254	L255	R256	S257	M258	L259	Y260	Y261	D262	S263	N264	E265	L266	F267	K268	K269	M270	T271	D272	D273	L274	M275	Y276	V277	L278	K279	F280	P281	F282	D283	N284	I285	R286	G287	N288	E289	Y290	E291	K292	E293	Q294	K295	I296	R297	N298	D299	E300	
L301	V302	Y303	Y304	H305	L306	Q307	L308	S309	L310	F311	S312	D313	F314	Q315	K316	E317	L318	G319	D320	L321	S322	F323	C324	T325	Q326	T327	S328	L329	Q330	Q331	R332	Q333	K334	L335	E336	E337	I338	T339	S340	F341	L342	S343	F344	A345	S346	L347	K348	S349	L350	C351	S352	K353	C354	Y355	L356	R357	T358	S359	F360	
P361	E362	K363	Y364	A365	L366	K367	V368	D369	F370	E371	F372	L373	K374	N375	V376	F377	I378	N379	T380	Y381	D382	R383	T384	R385	L386	V387	N388	D389	Y390	D391	E392	I393	L394	N395	F396	T397	L398	K399	D400	V401	G403	A404	R405	S406	V407	M408	D409	Q410	E411	N412	S413	L414	T415	N416	Y417	F418	L419	L420		
Q421	M422	T423	A424	I425	T426	Y427	L428	S429	L430	S431	F432	F433	M434	R435	Q436	Q437	S438	Q439	A440	Y441	K442	K443	L444	L445	L446	R447	S448	L449	Y450	A451	A452	L453	L454	M455	F456	S457	E458	Q459	Y460	R461	L462	L463	S464	I465	K466	M467	A468	T469	K470	M471	L472	T473	K474	D475	N476	F477	R478	S479	L480	
M481	M482	F483	K484	V485	T486	S487	V488	A489	P490	P491	Q492	I493	G494	Q495	V496	L497	P498	Q499	F500	Y501	K502	C503	Q504	M505	G506	L507	S508	R509	P510	G511	P512	F513	H514	S515	A516	L517	R518	D519	L520	R521	N522	S523	L524	K525	S526	P527	F528	L529	C530	L531	I532	Y533	L534	S535	E536	K536	D537	M538	E539	Y540
K541	L542	L543	H544	G545	N546	A547	L548	D549	P550	L551	E552	G553	V554	T555	D556	F557	T558	I559	A560	T561	I562	C563	N564	D565	V566	W567	G568	M569	F570	G571	S572	D573	M574	Q575	S576	D577	S578	D579	N580	K581	S582	L583	N584	V585	Y586	L587	S588	P589	F590	Y591	L592	H593	D594	L595	A596	G597	L598	G599	E600	
Y601	R602	P603	K604	Q605	L606	K607	F608	N609	F610	A611	L612	W613	L614	S615	D616	E617	A618	N619	K620	Y621	M622	L623	D624	L625	N626	I627	L628	W629	L630	L631	L632	N633	R634	A635	K636	E637	F638	P639	K640	W641	F642	E643	D644	L645	F646	L647	Q648	F649	Q650	T651	P652	D653	T654	L655	C656	A656	F657	L658	N659	A660
G661	L662	N663	S664	I665	V666	A667	R668	N669	L670	F671	N672	T673	W674	E675	Q676	L677	G678	S679	V680	L681	P682	N683	C684	H685	W686	P687	G688	N689	L690	S691	T692	E693	S694	L695	L696	L697	K698	F699	Y700	T701	N702	Q703	N704	K705	L706	S707	A708	D709	W710	T711	A712	S713	D714	R715	H716	F717	L718	L719	P720	
S721	N722	R723	L724	T725	V726	Y727	N728	D729	K730	Q731	L732	E733	S734	T735	L736	R737	S738	S739	Q740	P741	G742	L743	T744	M745	W746	Y747	G748	P749	T750	R751	G752	G753	K754	H755	V756	L757	C758	C759	K760	L761	L762	E763	W764	L765	Q766	D767	T768	S769	P770	M771	D772	R773	T774	V775	W776	L777	S778	D779	S780	

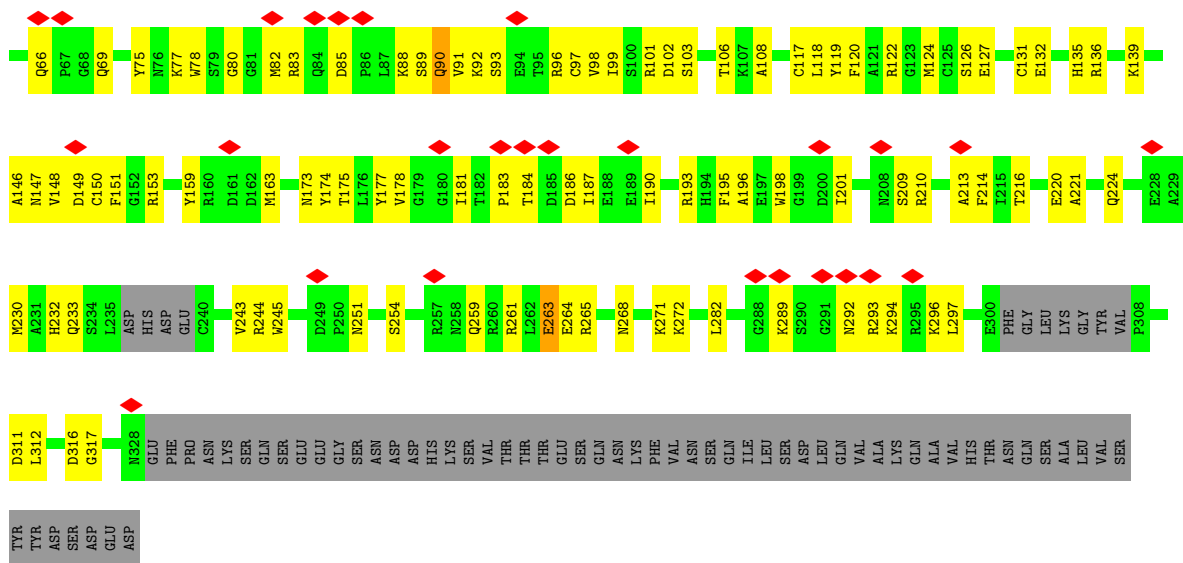


• Molecule 19: Pre-mRNA-splicing factor cwf14

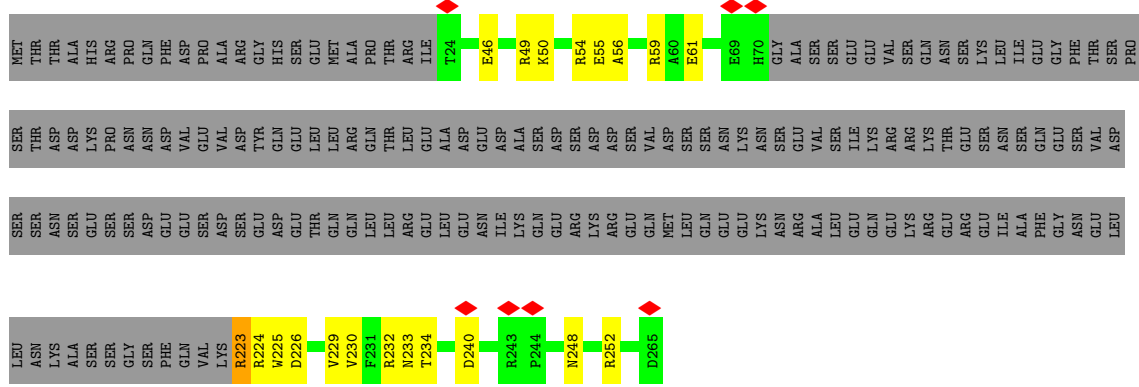


• Molecule 20: Pre-mRNA-splicing factor cwf2

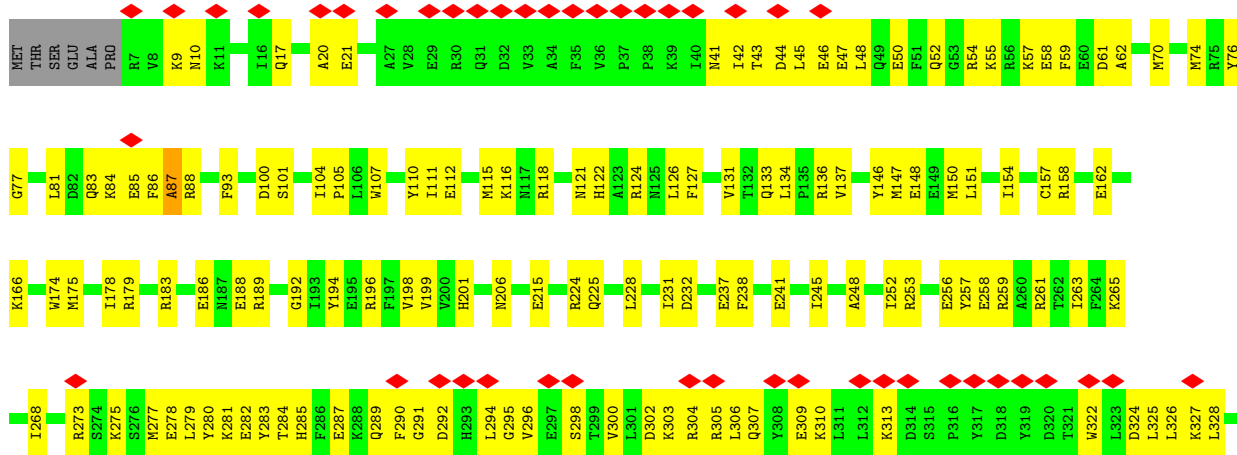




• Molecule 21: Pre-mRNA-splicing factor cwf15

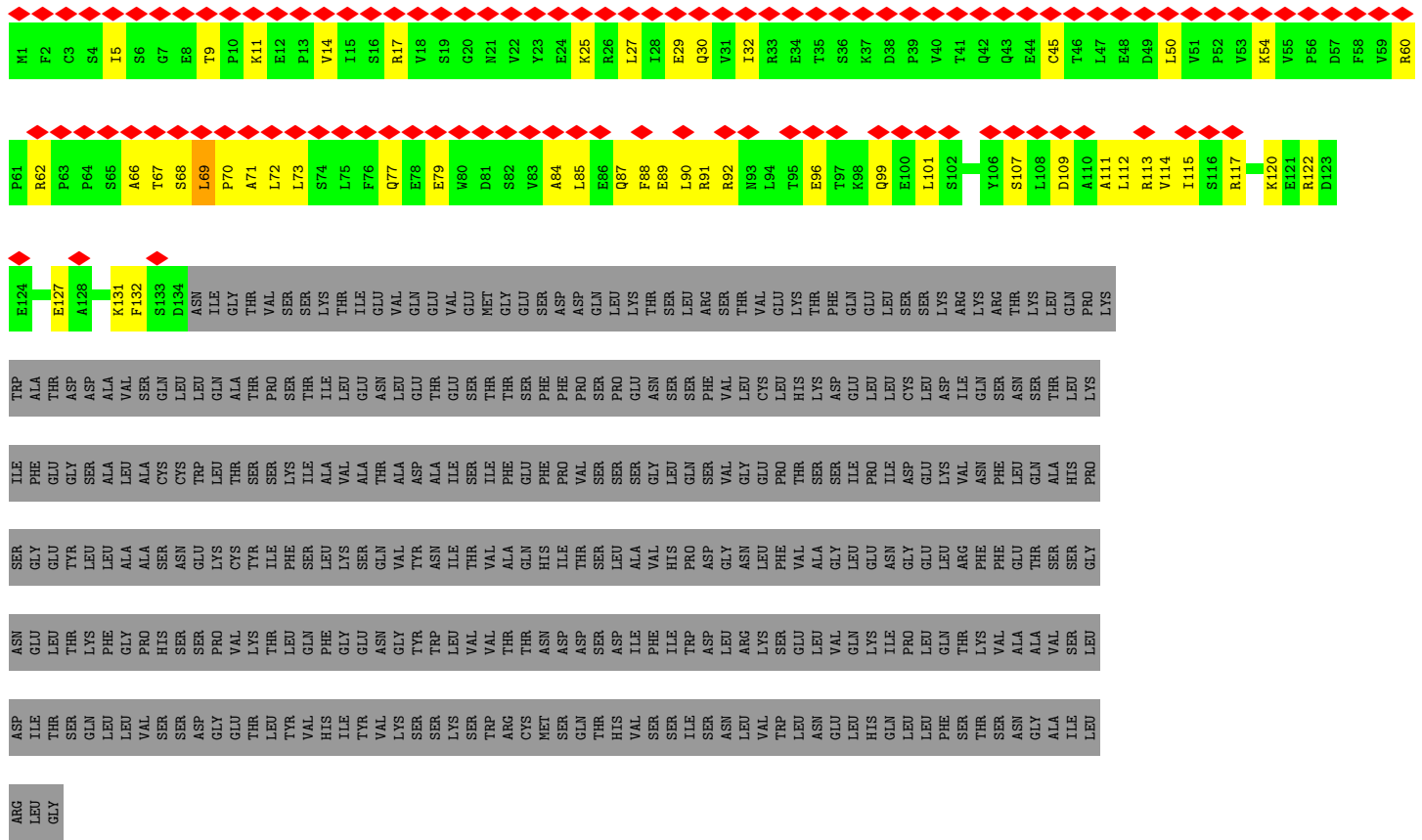


• Molecule 22: Pre-mRNA-splicing factor cwf4

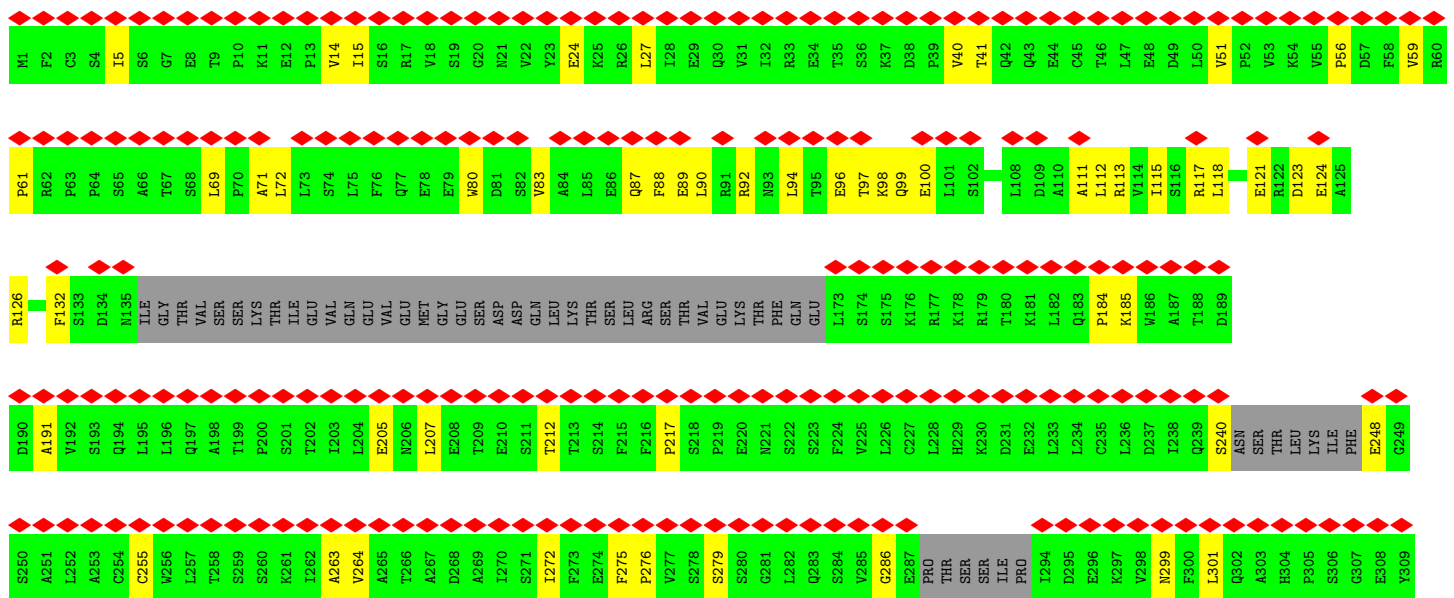
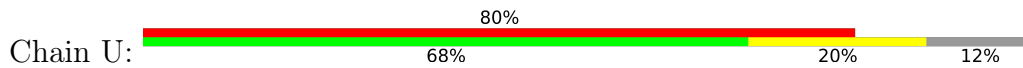


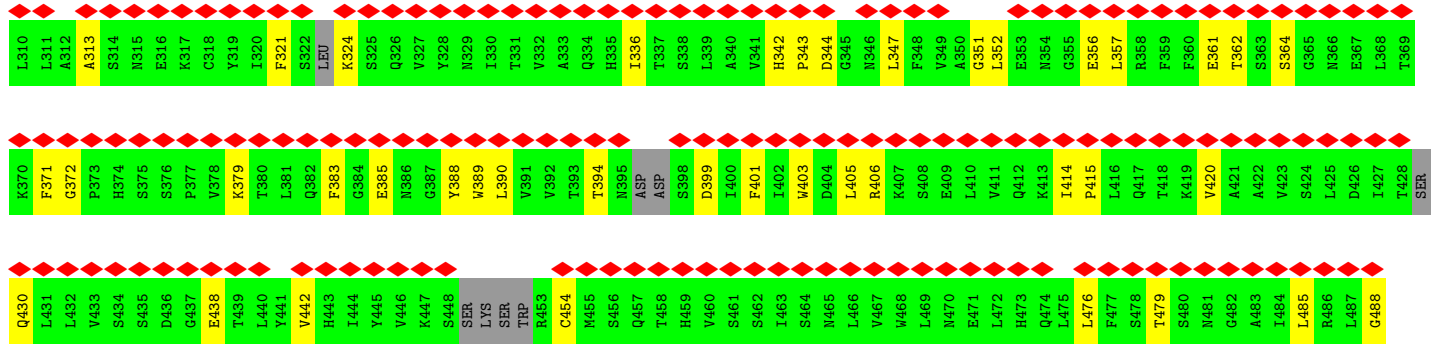


• Molecule 23: Pre-mRNA-processing factor 19

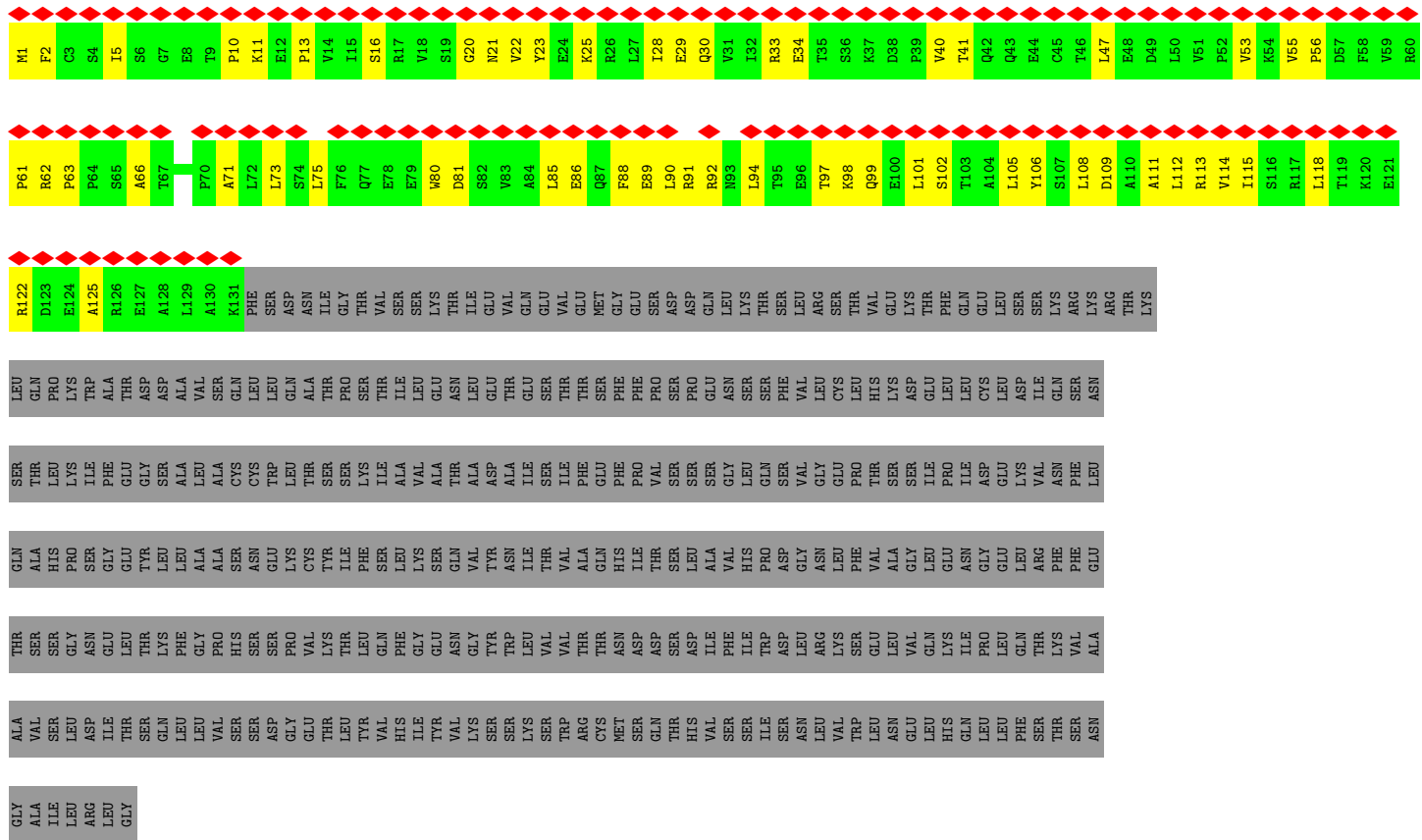


• Molecule 23: Pre-mRNA-processing factor 19

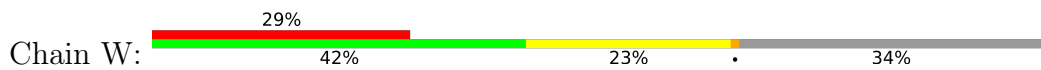


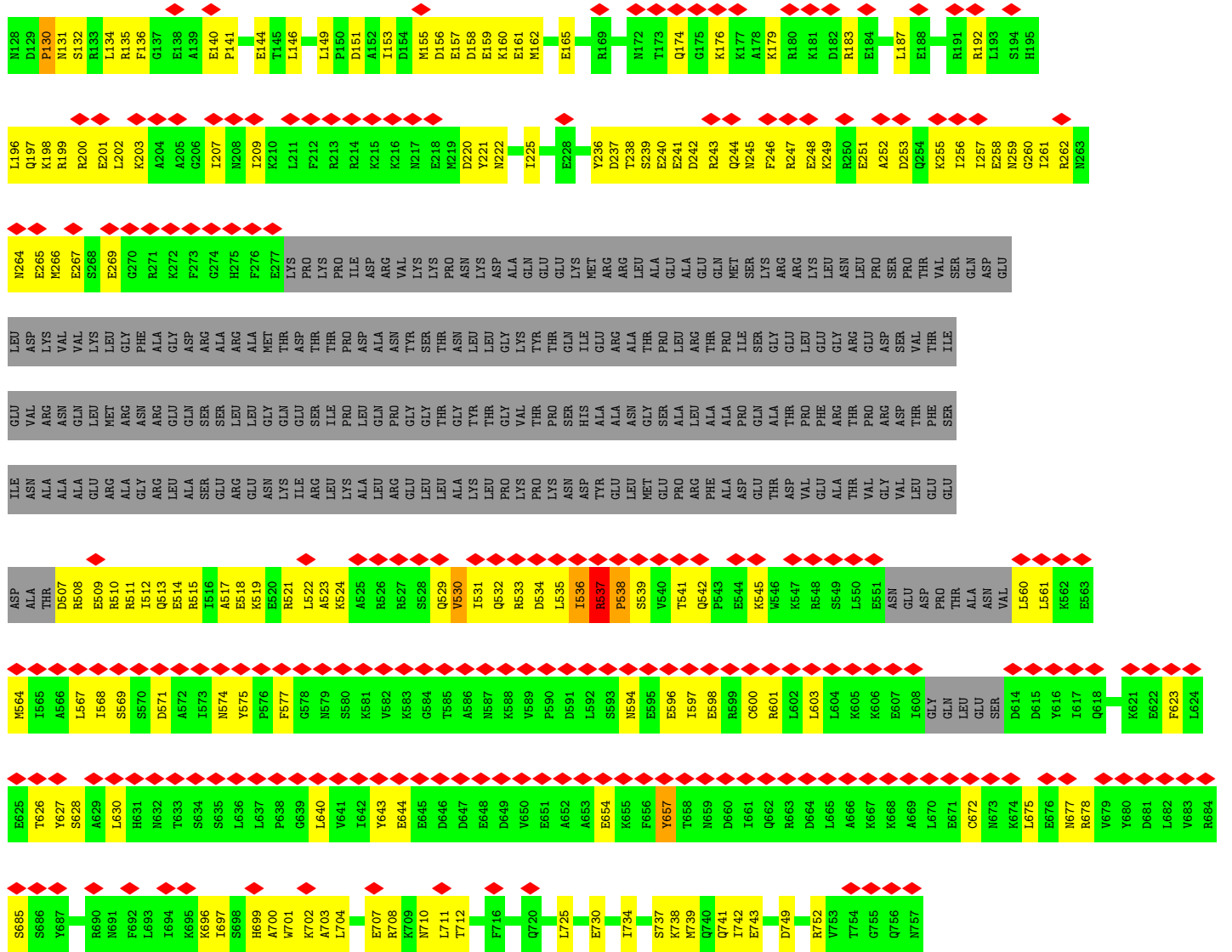


• Molecule 23: Pre-mRNA-processing factor 19

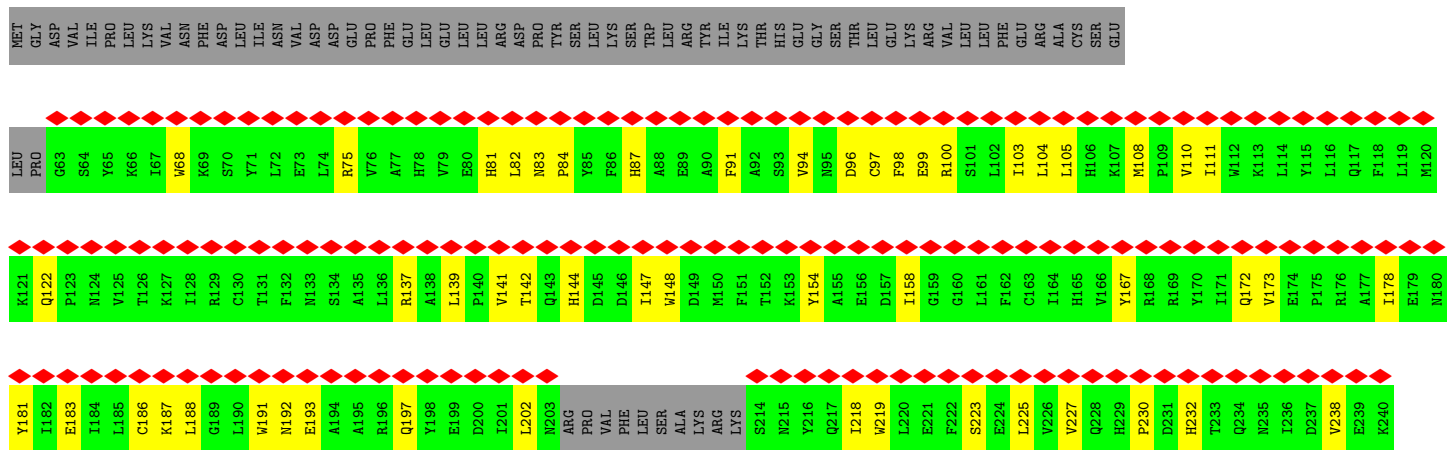


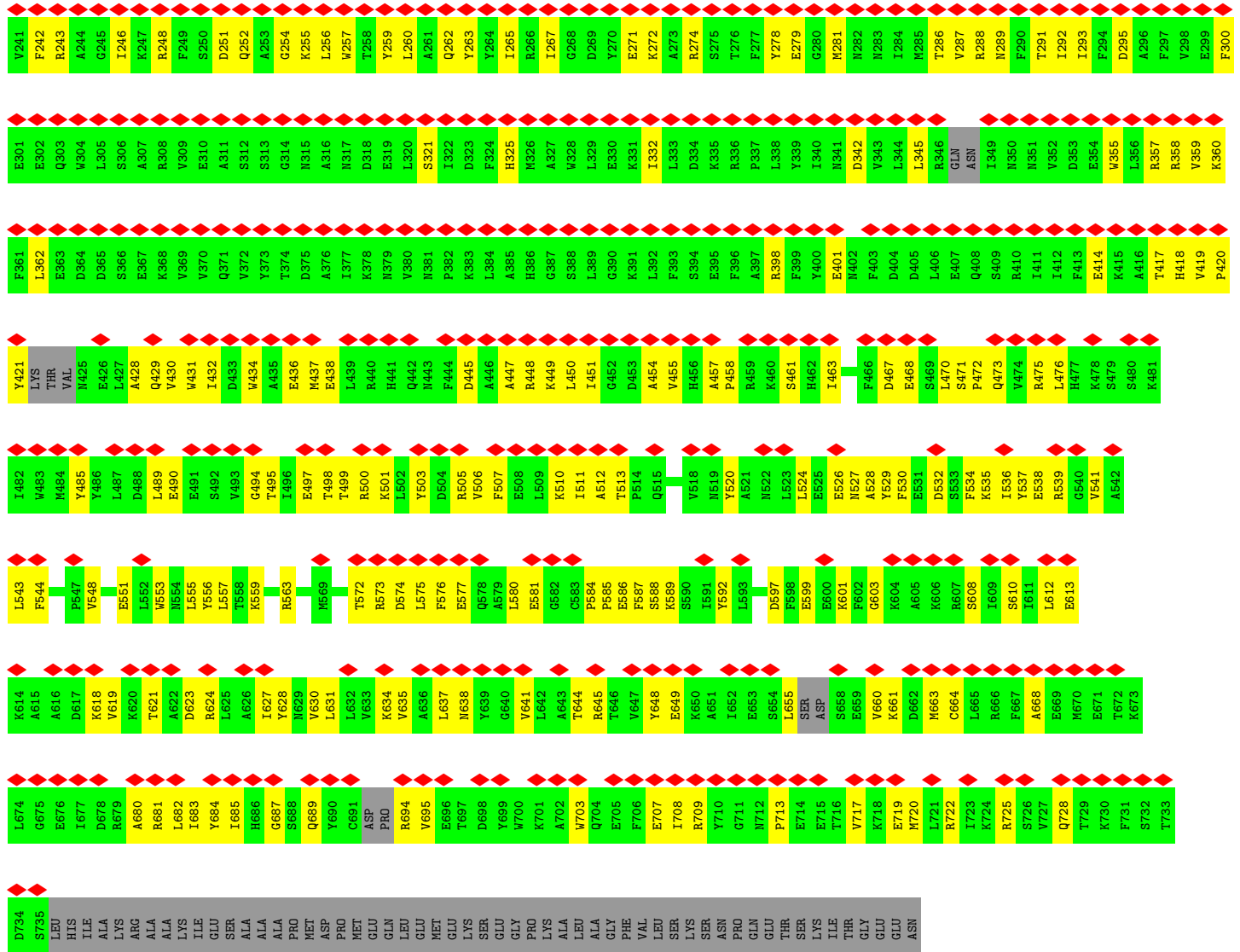
• Molecule 24: Pre-mRNA-splicing factor cdc5



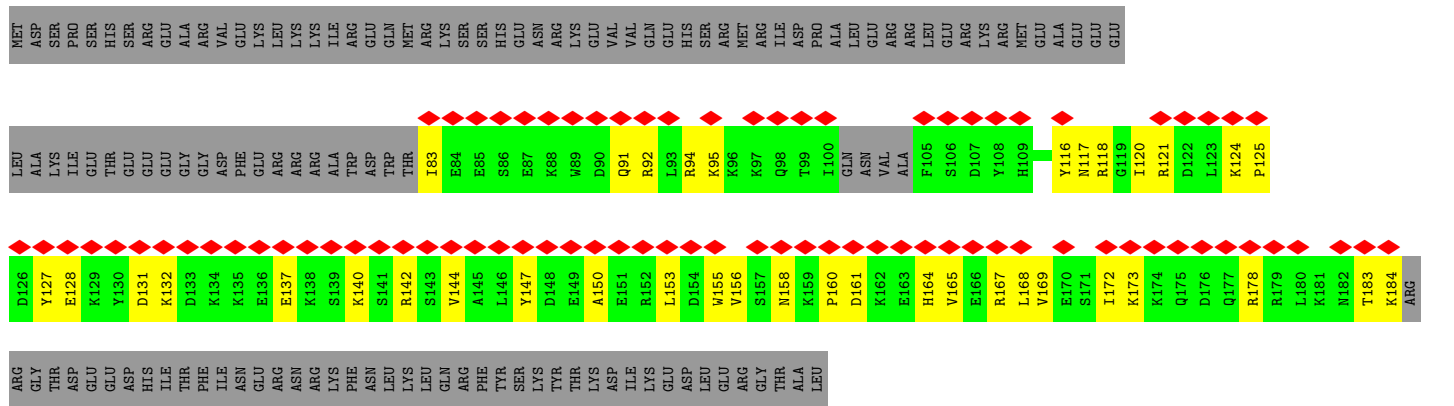


● Molecule 25: Pre-mRNA-splicing factor cwf3



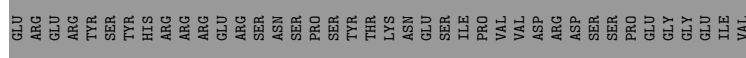
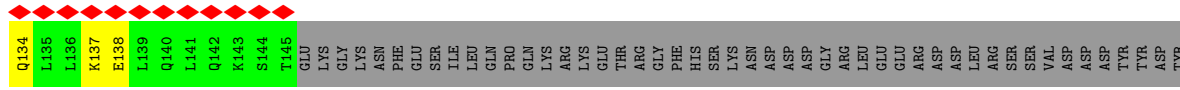
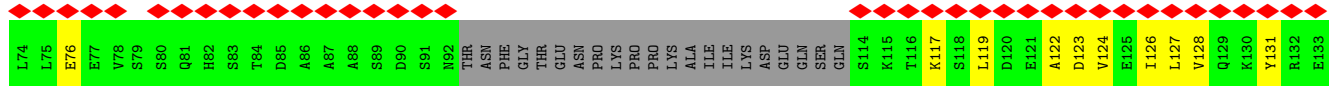


• Molecule 26: Pre-mRNA-splicing factor syf2

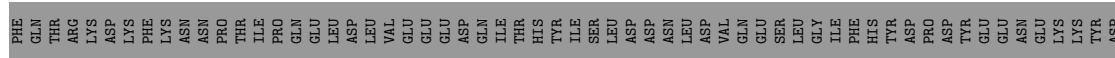
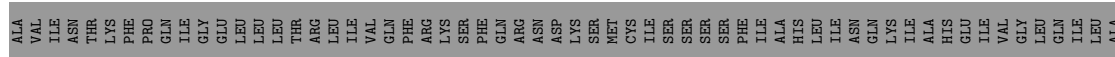
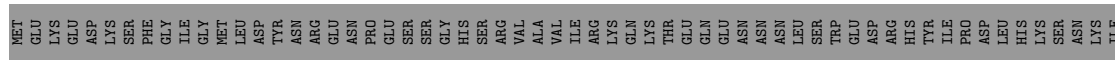


• Molecule 27: Pre-mRNA-splicing factor cwf7

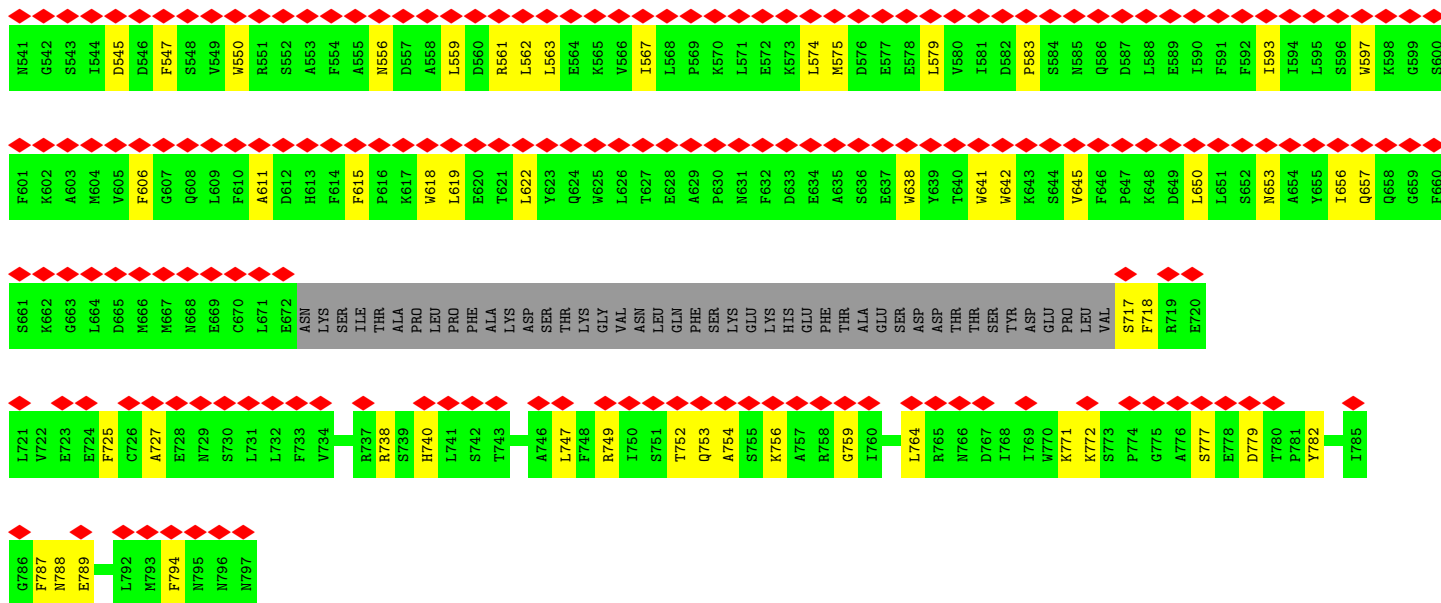




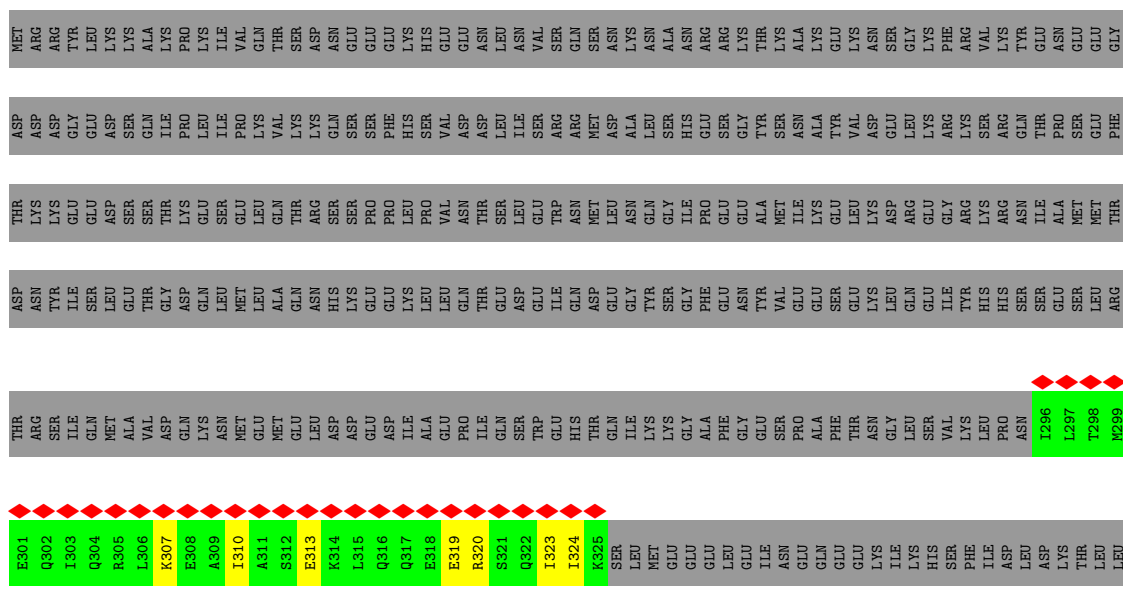
● Molecule 30: Pre-mRNA-splicing factor cwf22



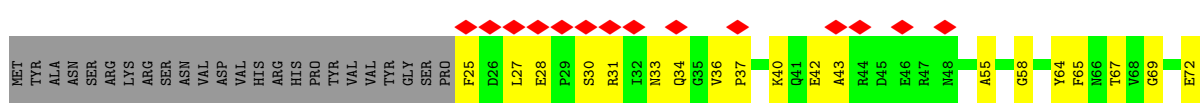


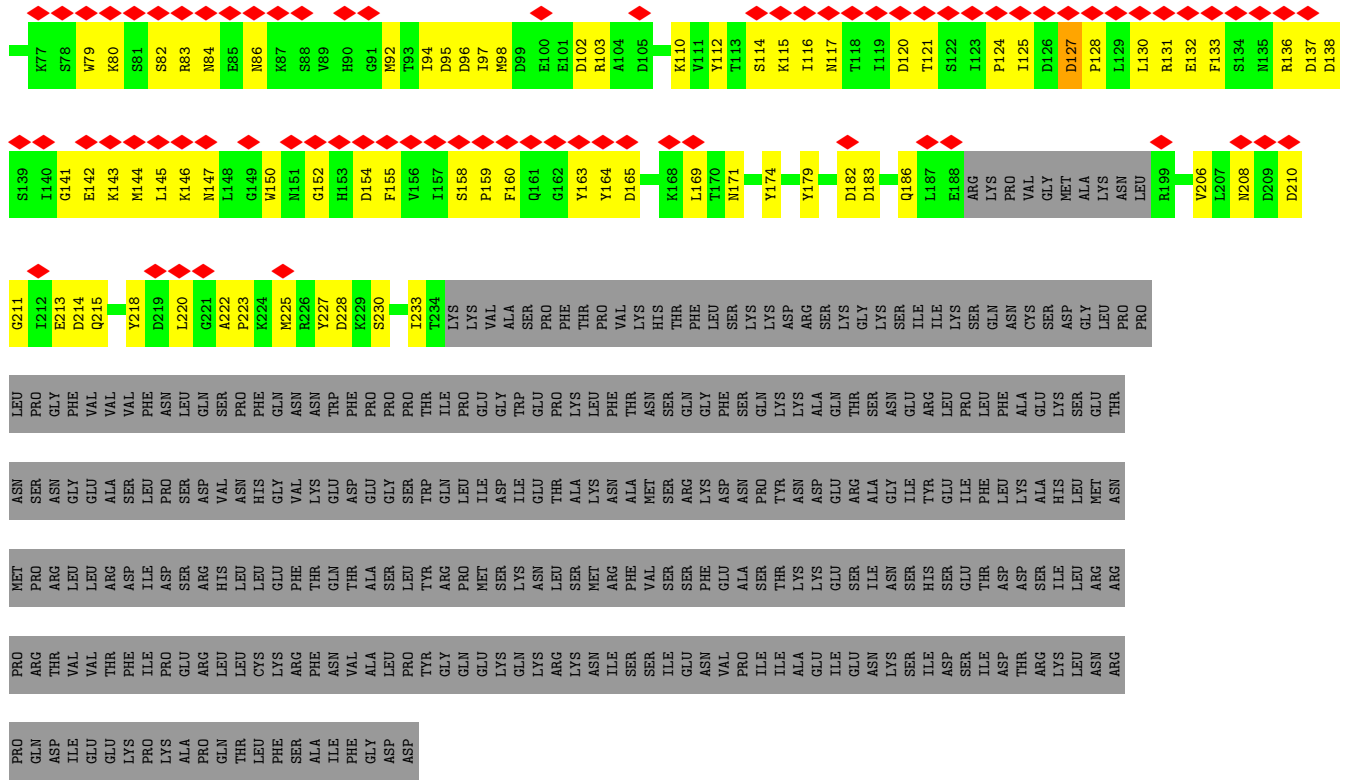


• Molecule 33: Uncharacterized protein C17A2.08c

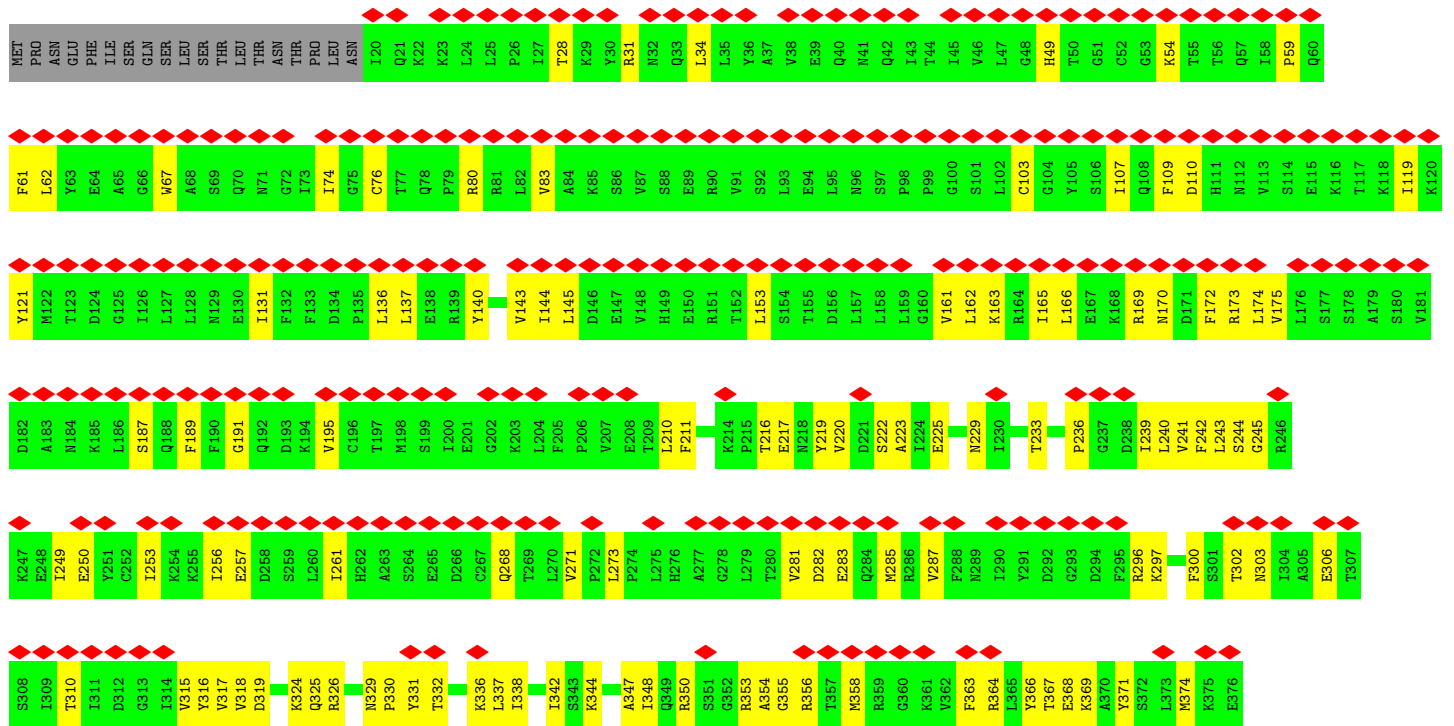


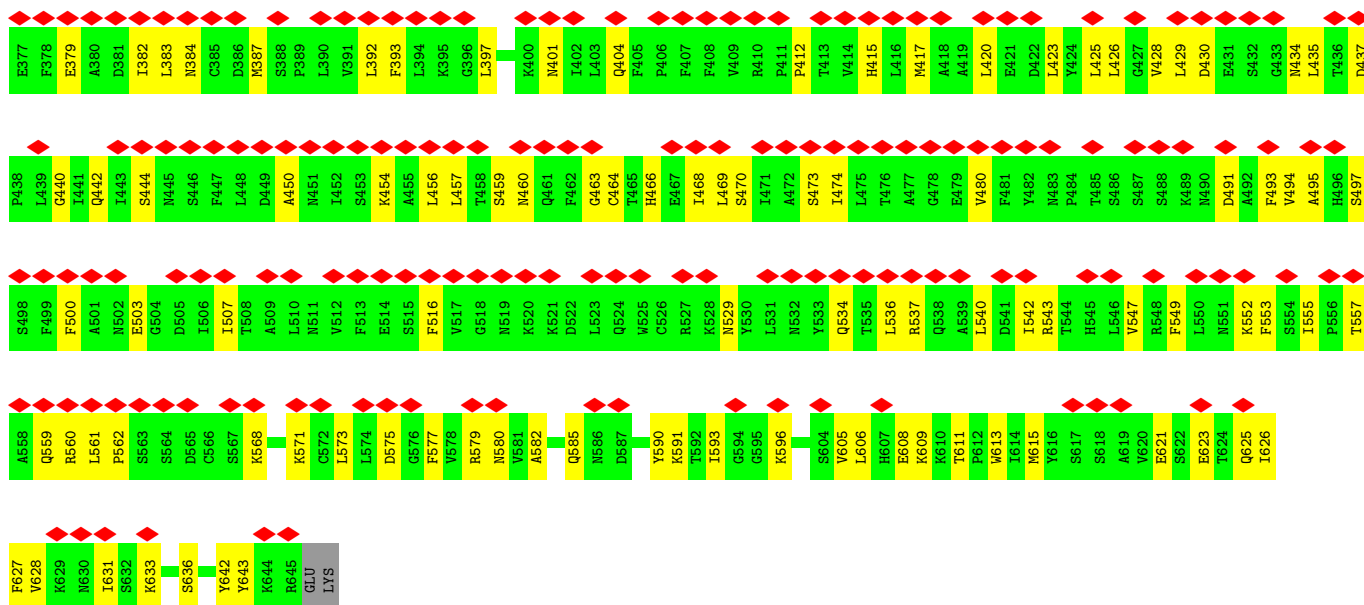
• Molecule 34: Uncharacterized protein C20H4.06c



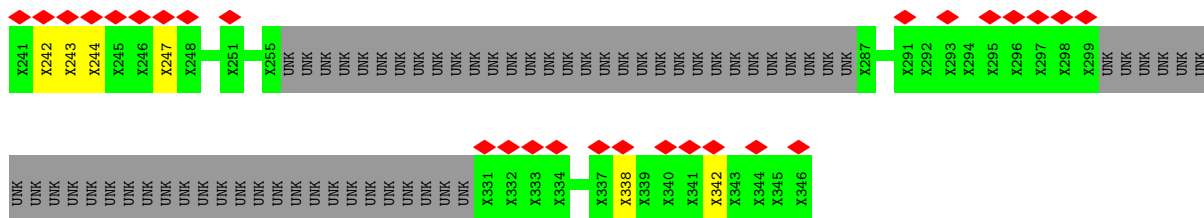
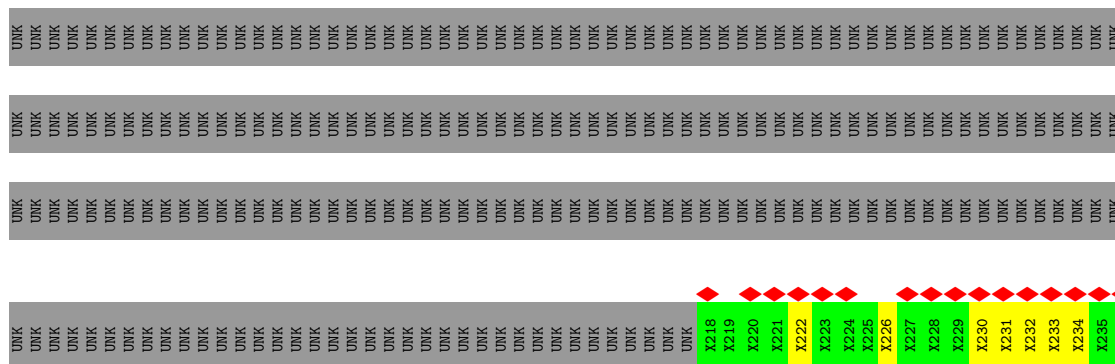


● Molecule 35: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09

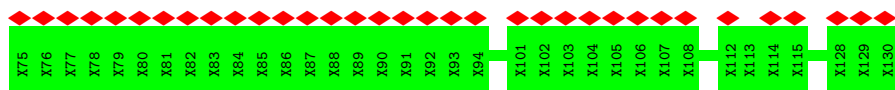




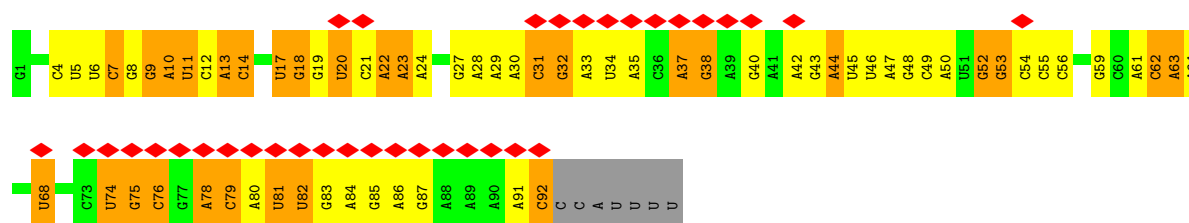
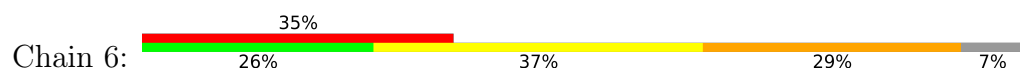
• Molecule 36: UNK1



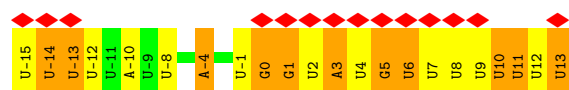
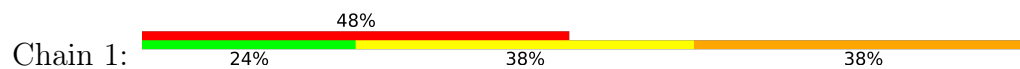
• Molecule 37: UNK2



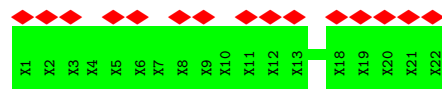
• Molecule 38: U6snRNA



• 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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	0.822, 0.822, 0.822	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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 [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	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	78
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	47
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	61
21	Q	86/265 (32%)	82 (95%)	3 (4%)	1 (1%)	10	37
22	R	597/674 (89%)	585 (98%)	11 (2%)	1 (0%)	43	73
23	S	130/488 (27%)	121 (93%)	9 (7%)	0	100	100
23	T	132/488 (27%)	127 (96%)	4 (3%)	1 (1%)	16	47
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%)	12	41
25	X	642/790 (81%)	608 (95%)	33 (5%)	1 (0%)	43	73
26	Y	94/229 (41%)	89 (95%)	4 (4%)	1 (1%)	11	39
27	Z	151/187 (81%)	145 (96%)	5 (3%)	1 (1%)	18	49
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%)	43	73
33	n	28/361 (8%)	27 (96%)	1 (4%)	0	100	100
34	y	196/534 (37%)	168 (86%)	25 (13%)	3 (2%)	8	32
35	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	43	73
37	q	3/56 (5%)	3 (100%)	0	0	100	100
All	All	11306/17429 (65%)	10784 (95%)	502 (4%)	20 (0%)	44	73

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 [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	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%)	70	80
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 [i](#)

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	33,34,34	1.01	1 (3%)	50,54,54	1.59	9 (18%)
41	IHP	A	2401	-	36,36,36	1.58	13 (36%)	60,60,60	1.52	12 (20%)

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	-	0/22/38/38	0/3/3/3
41	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	A	2401	IHP	P1-O31	-2.54	1.45	1.54
41	A	2401	IHP	P3-O33	-2.43	1.45	1.54
41	A	2401	IHP	P6-O46	-2.42	1.45	1.54
41	A	2401	IHP	P5-O45	-2.40	1.45	1.54
41	A	2401	IHP	P3-O43	-2.40	1.45	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	B	1001	GTP	C5-C4-N3	-5.02	120.39	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	B	1001	GTP	C2-N3-C4	4.58	120.19	112.30
42	B	1001	GTP	C2-N1-C6	-3.32	119.09	125.11
42	B	1001	GTP	N9-C4-N3	3.29	132.54	125.95
41	A	2401	IHP	C5-C6-C1	3.17	117.38	110.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

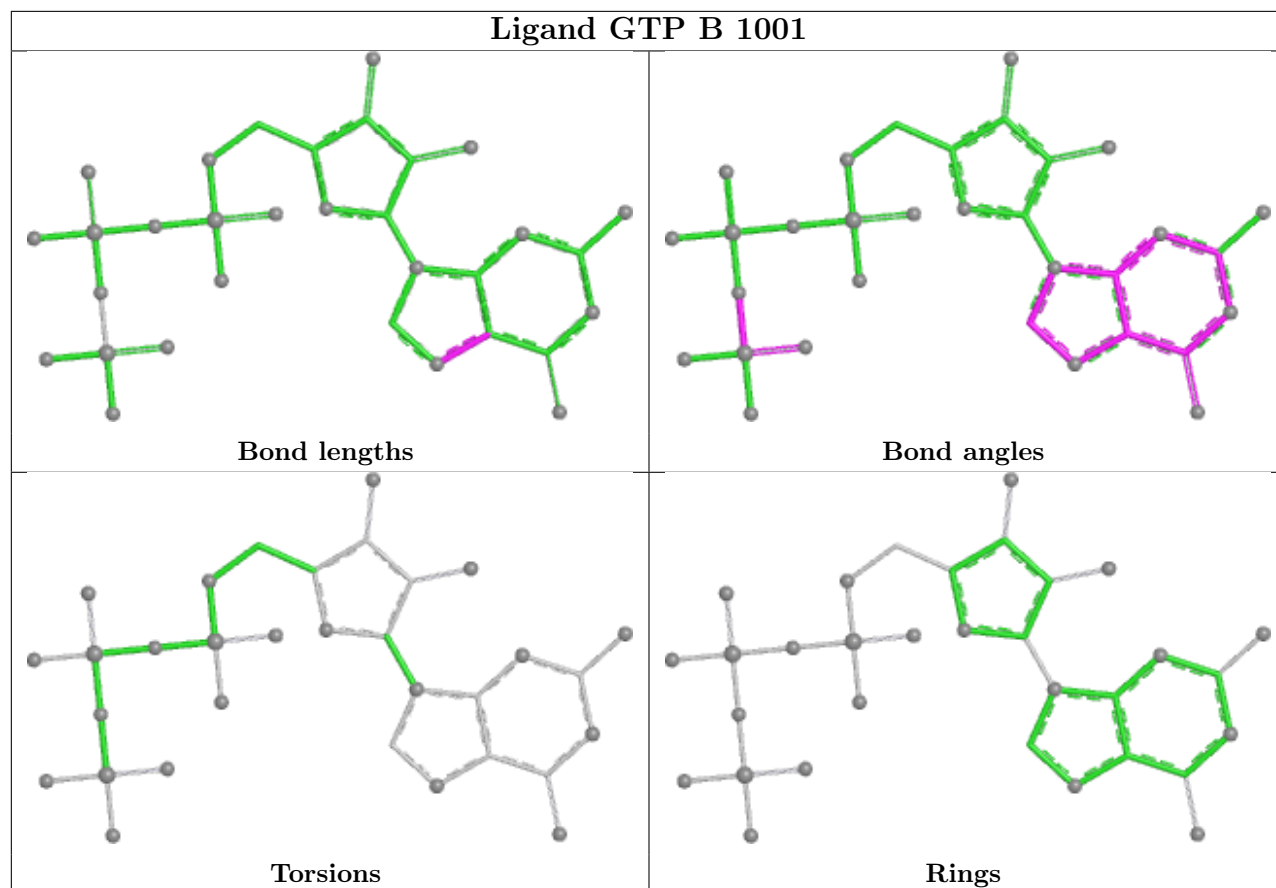
Mol	Chain	Res	Type	Atoms
41	A	2401	IHP	C1-O11-P1-O41
41	A	2401	IHP	C5-O15-P5-O35
41	A	2401	IHP	C6-O16-P6-O26

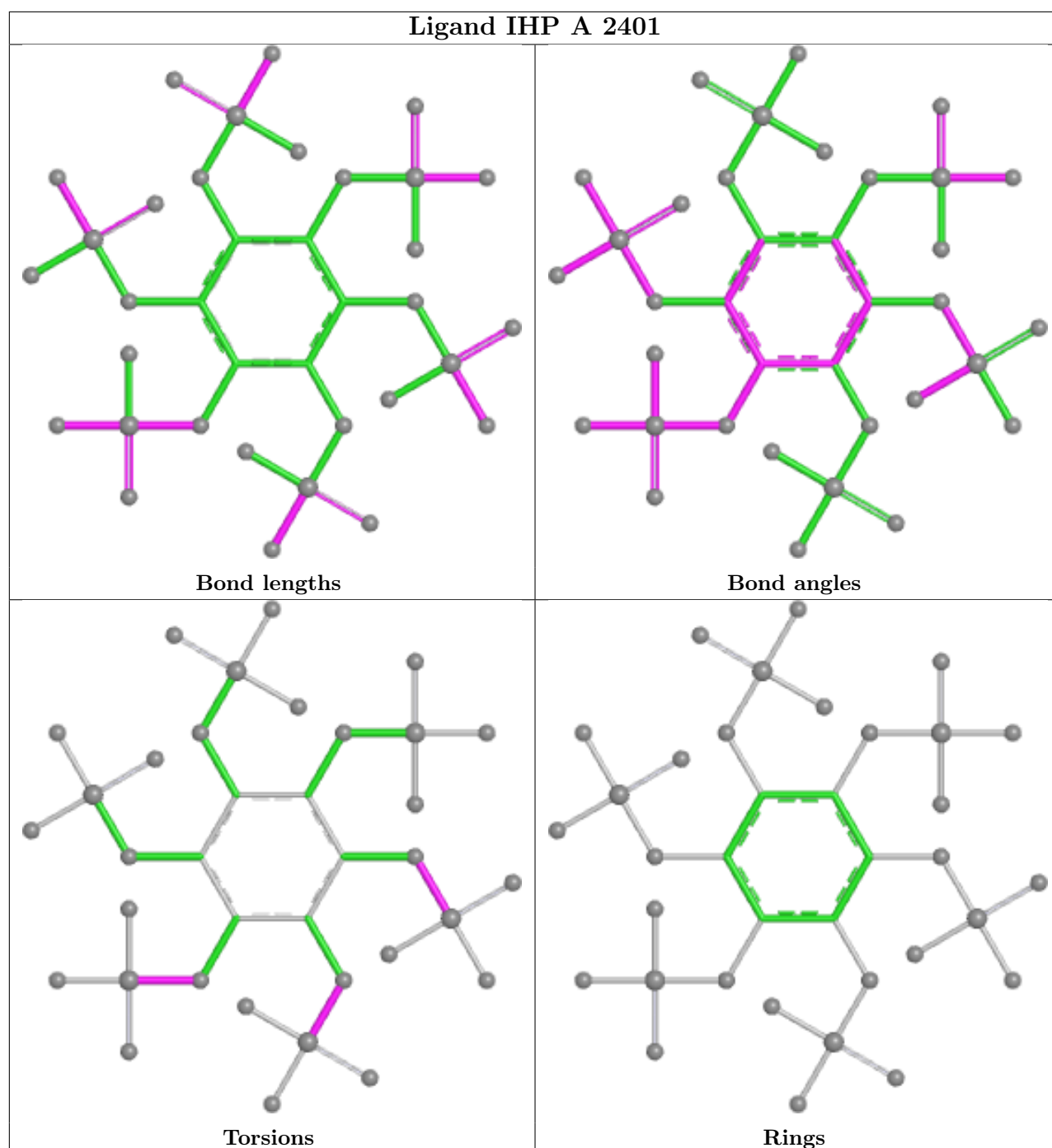
There are no ring outliers.

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.

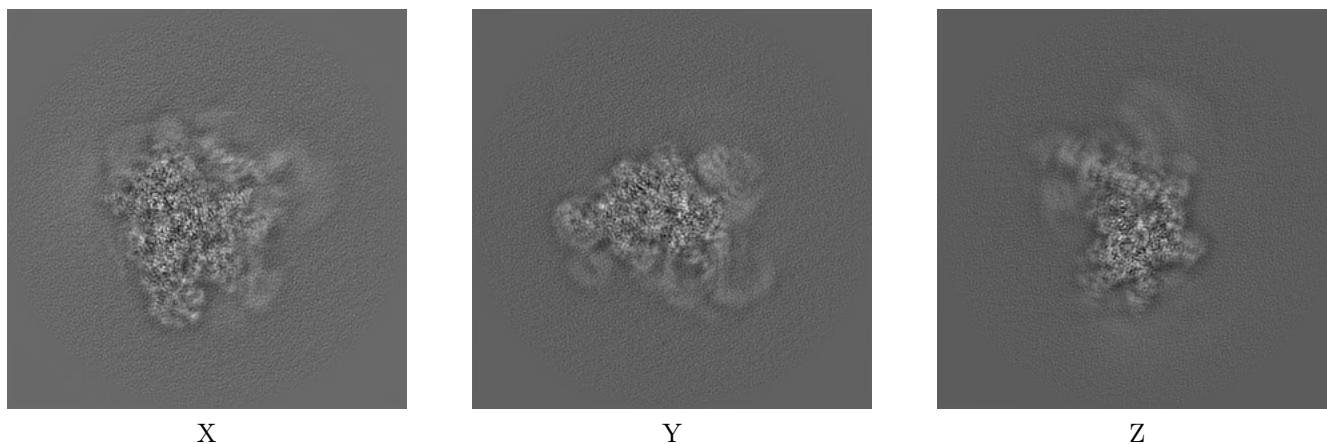
## 6 Map visualisation [i](#)

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.

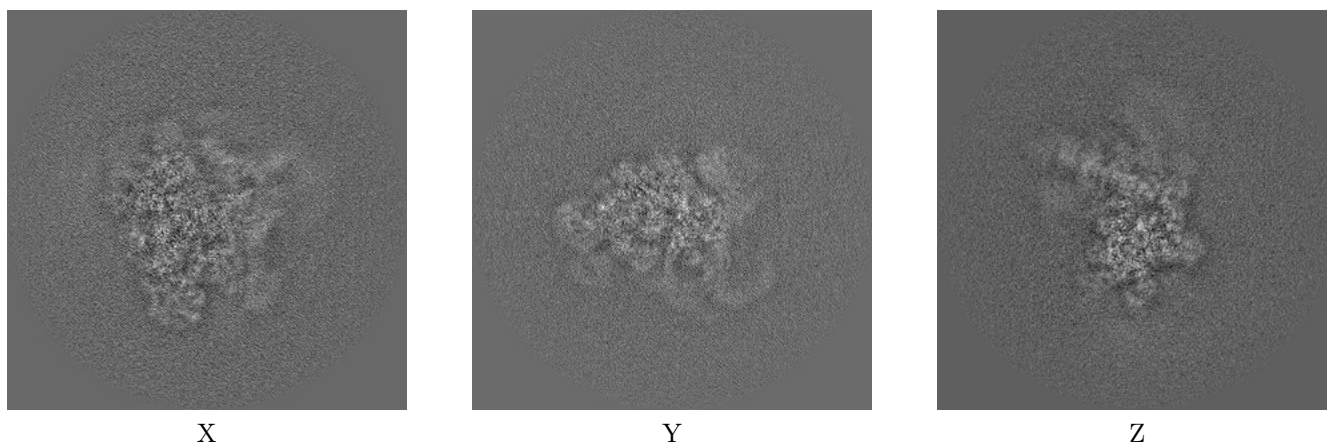
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



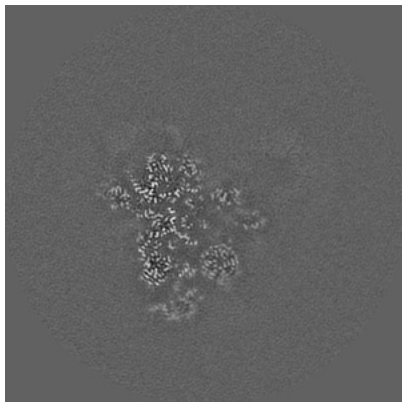
#### 6.1.2 Raw map



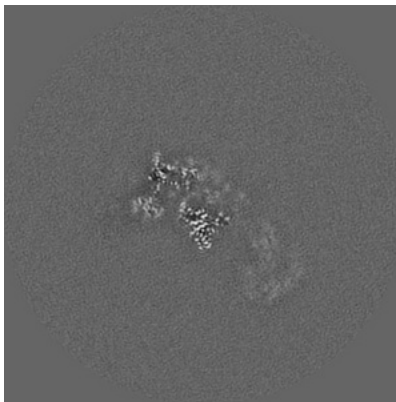
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

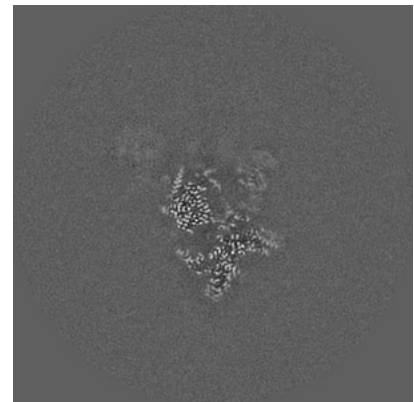
### 6.2.1 Primary map



X Index: 280

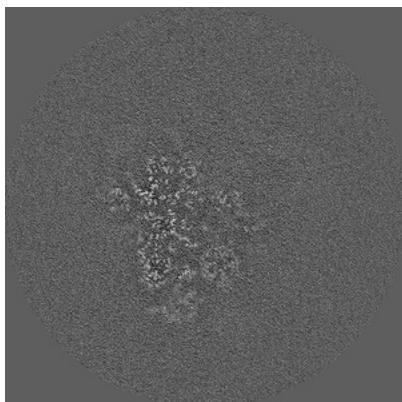


Y Index: 280

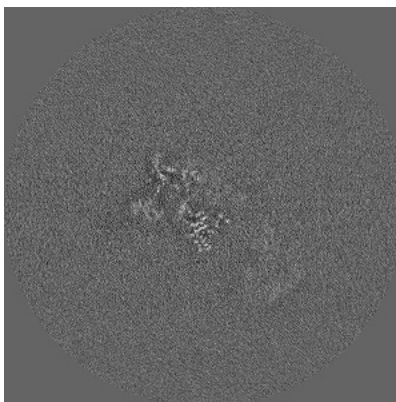


Z Index: 280

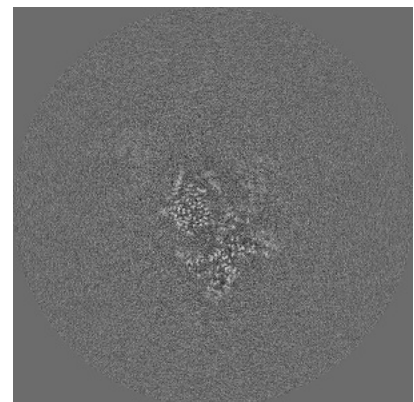
### 6.2.2 Raw map



X Index: 280



Y Index: 280

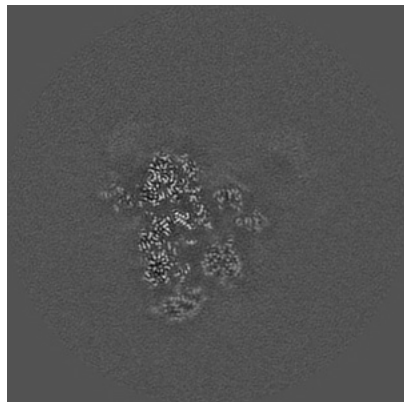


Z Index: 280

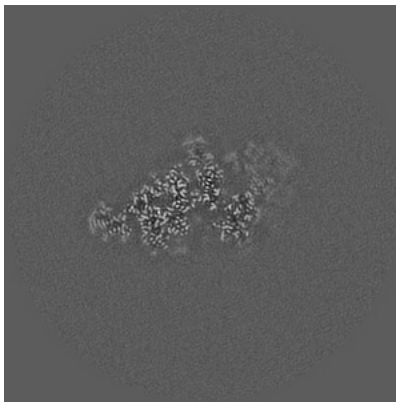
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

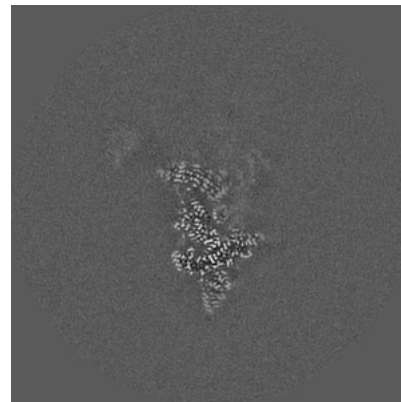
### 6.3.1 Primary map



X Index: 276

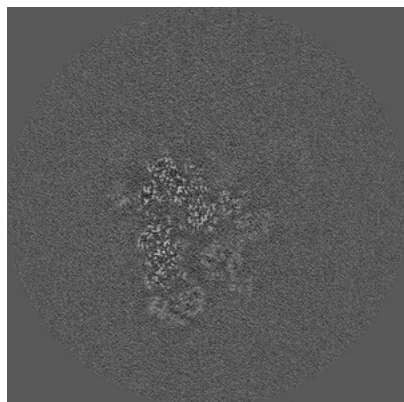


Y Index: 219

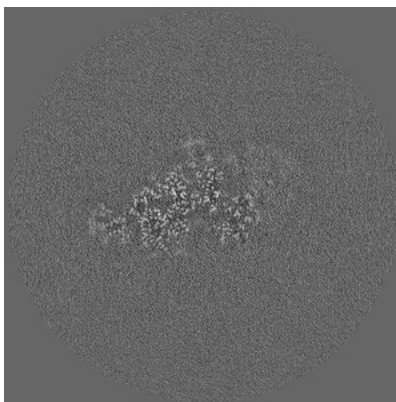


Z Index: 295

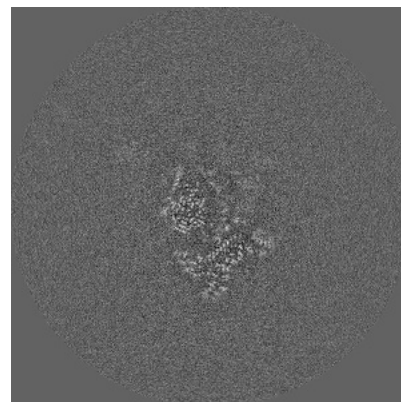
### 6.3.2 Raw map



X Index: 269



Y Index: 219

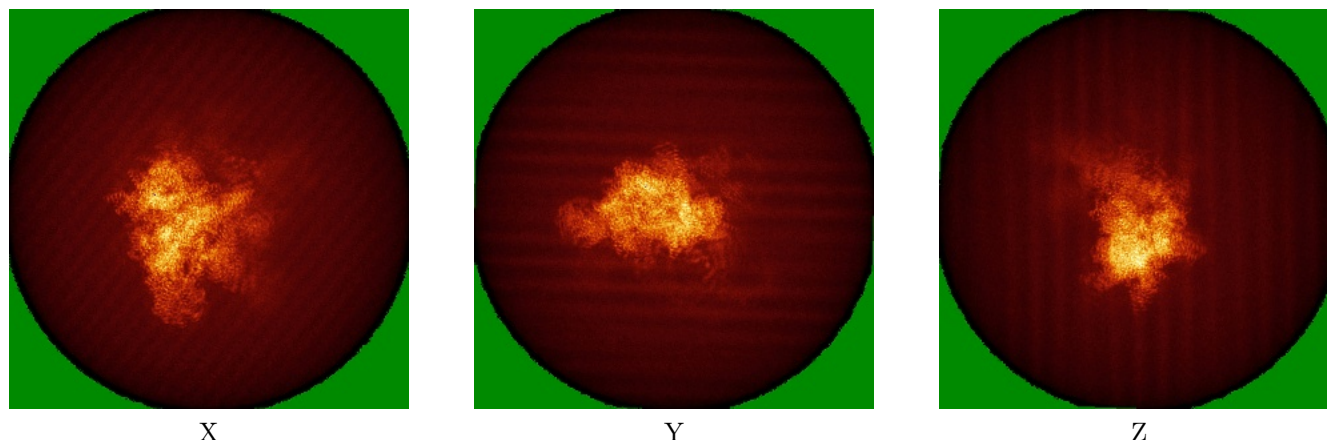


Z Index: 282

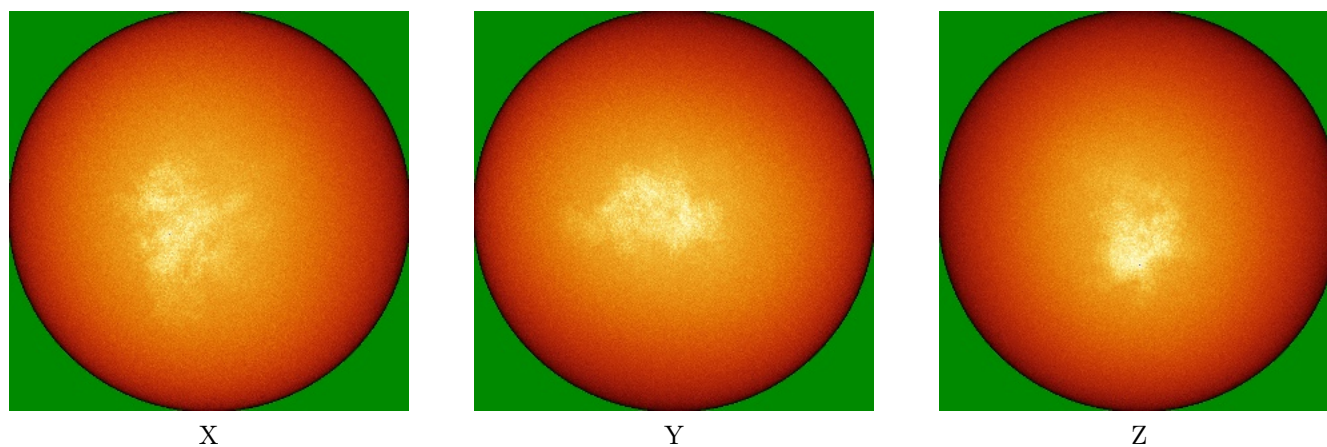
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



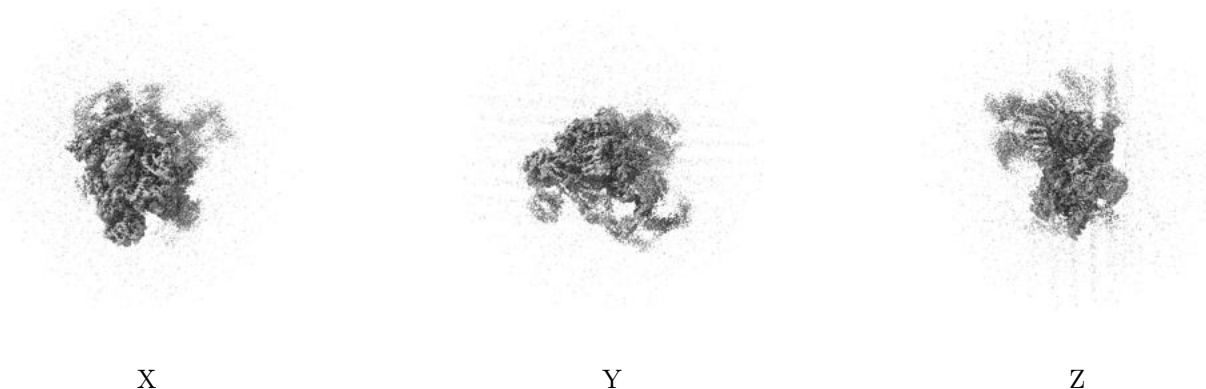
### 6.4.2 Raw map



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.

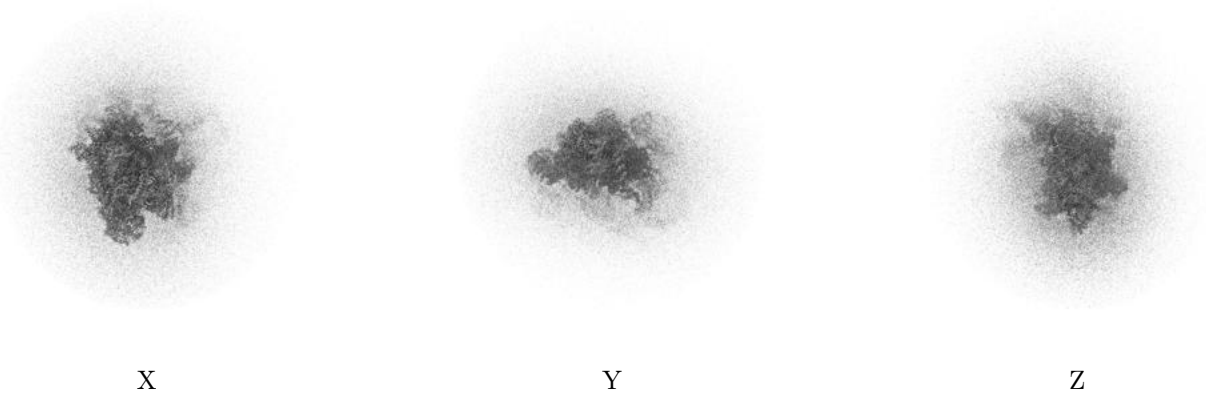
## 6.5 Orthogonal surface views [i](#)

### 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.

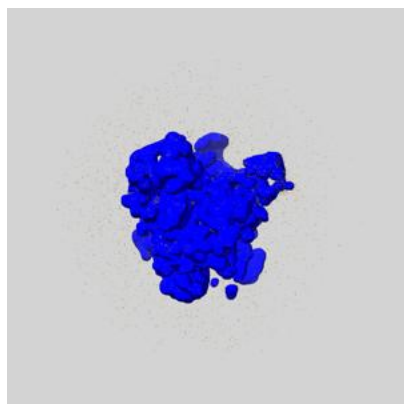
## 6.6 Mask visualisation [i](#)

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

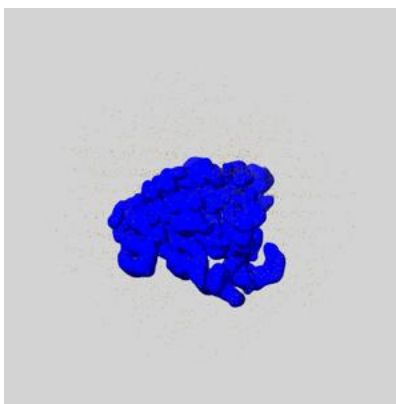
A mask typically either:

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

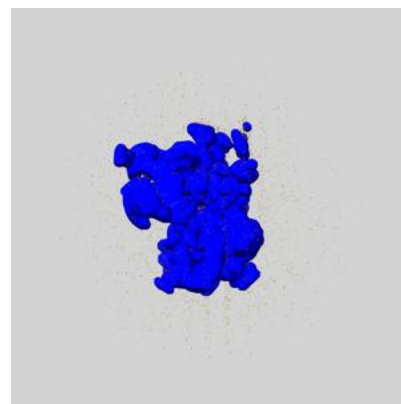
### 6.6.1 emd\_19942\_msk\_1.map [i](#)



X



Y

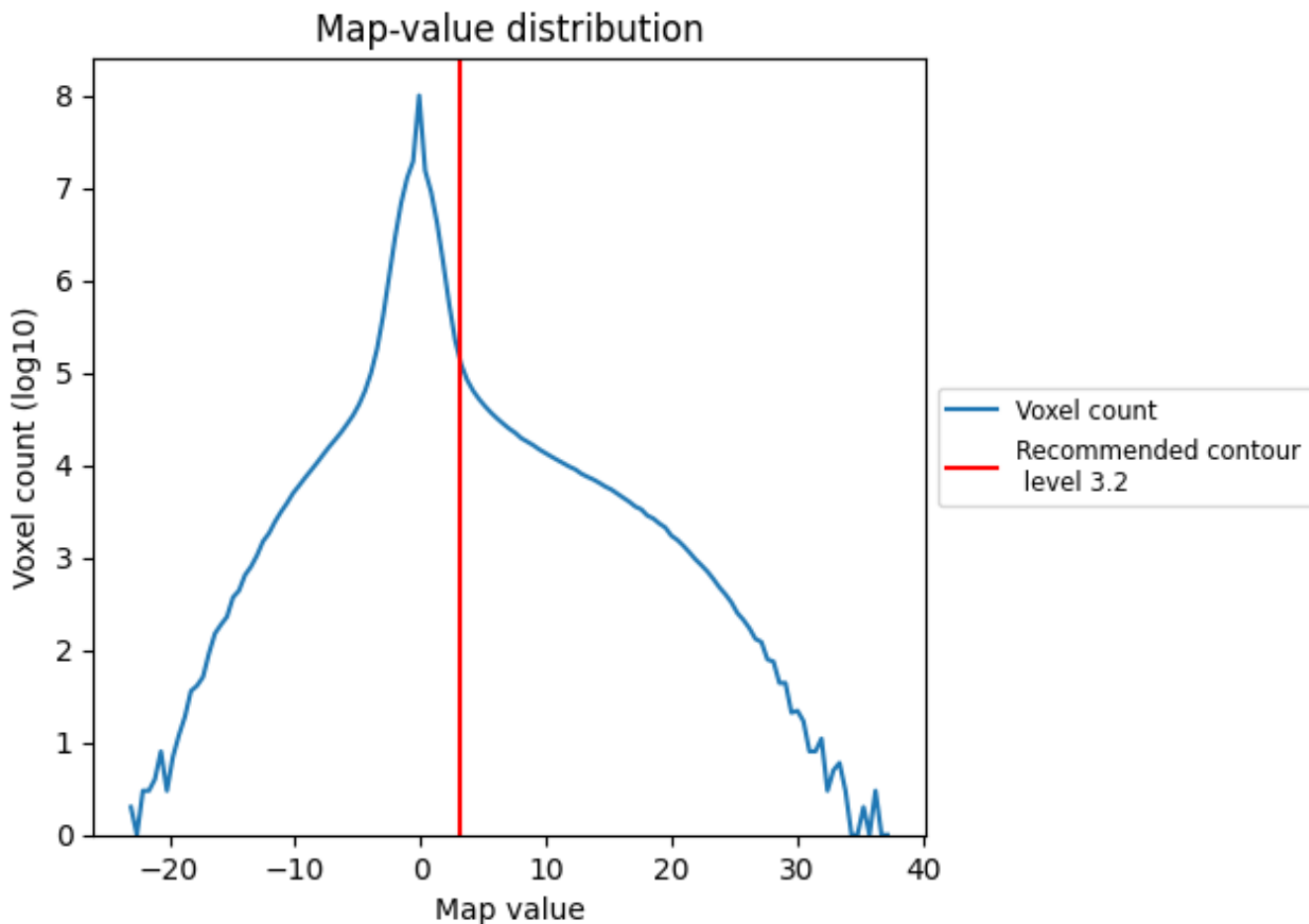


Z

## 7 Map analysis [i](#)

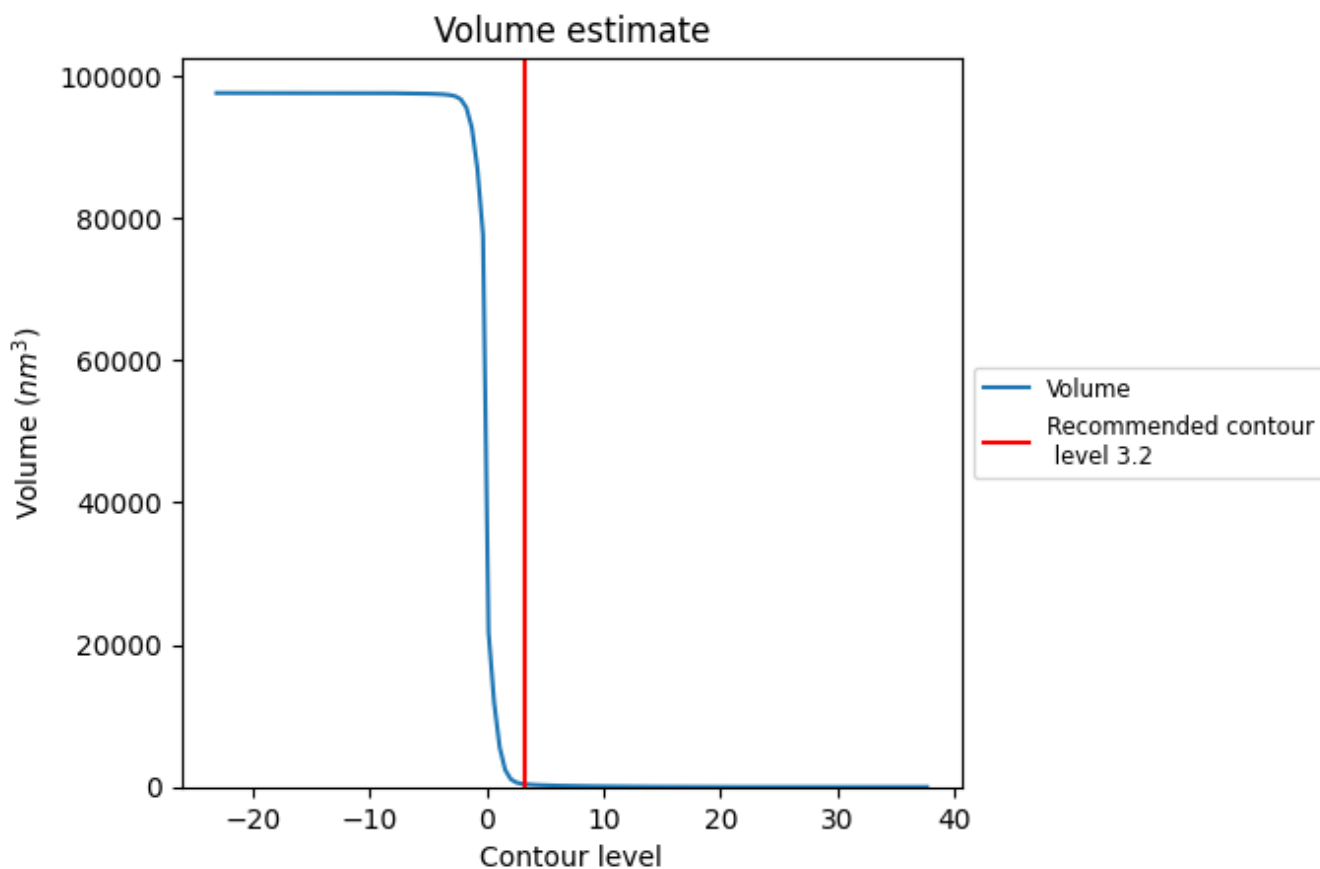
This section contains the results of statistical analysis of the map.

### 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.

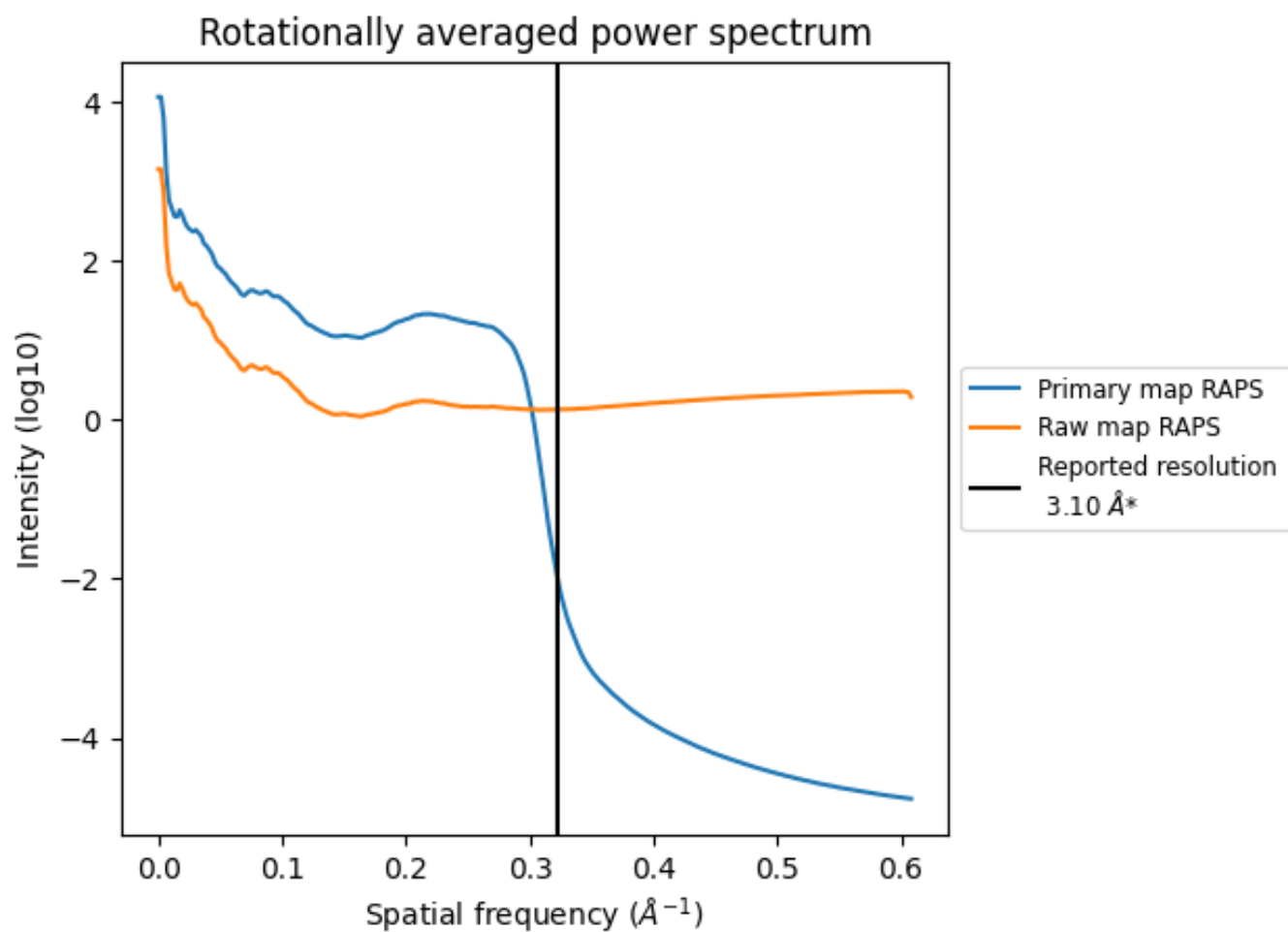
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 415 nm<sup>3</sup>; 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 [i](#)

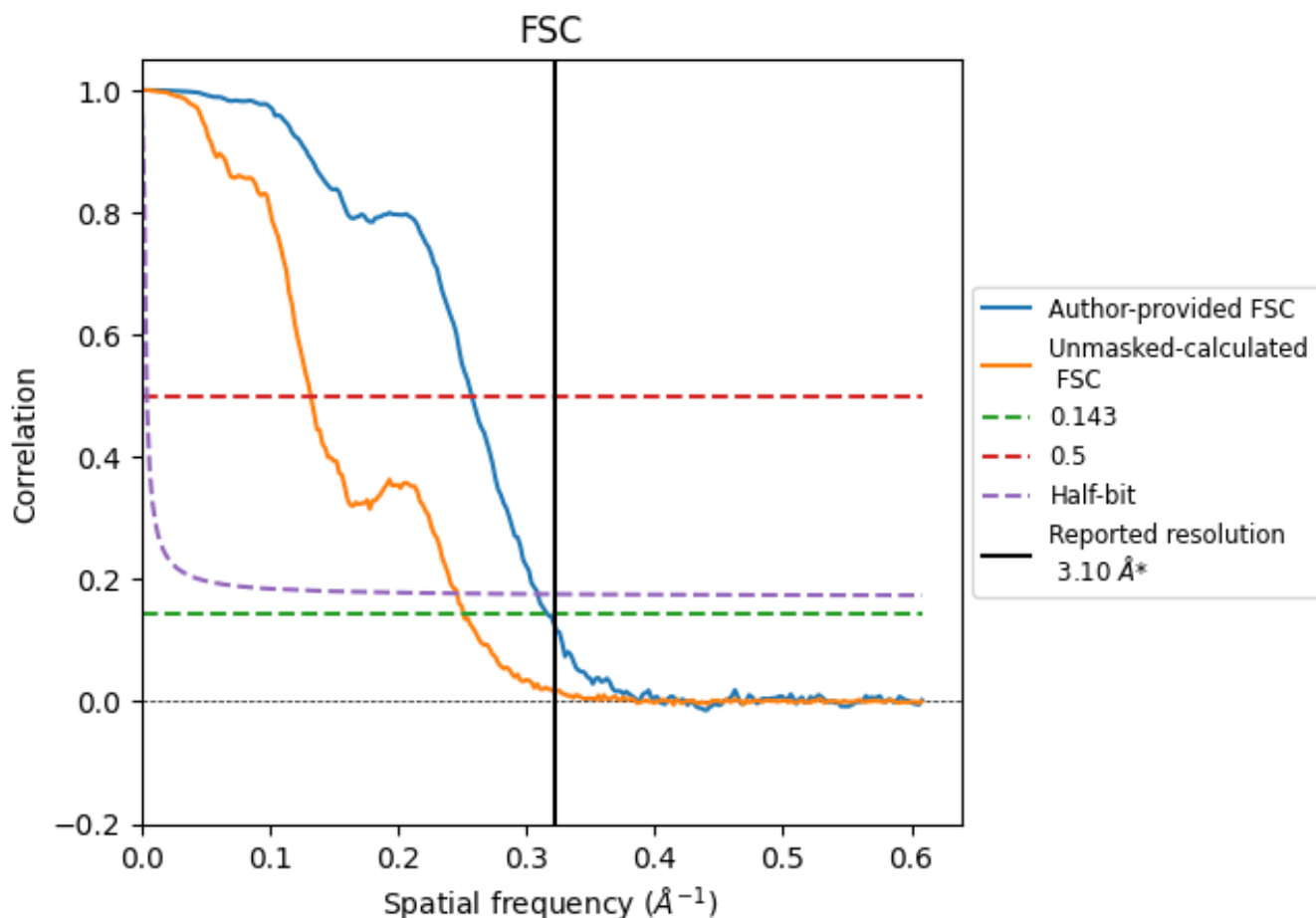


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

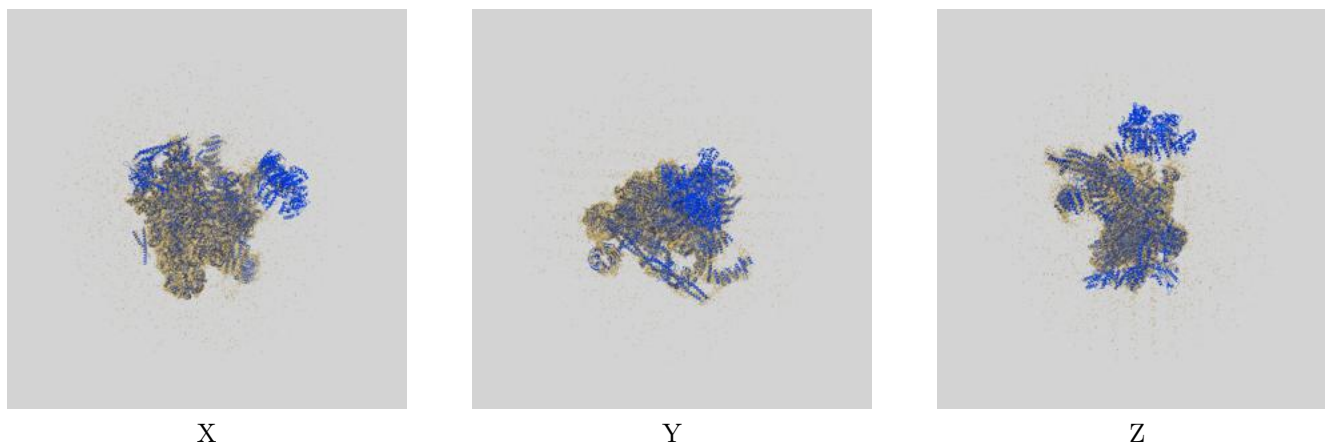
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.88	3.24
Unmasked-calculated*	3.98	7.58	4.06

\*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](#)

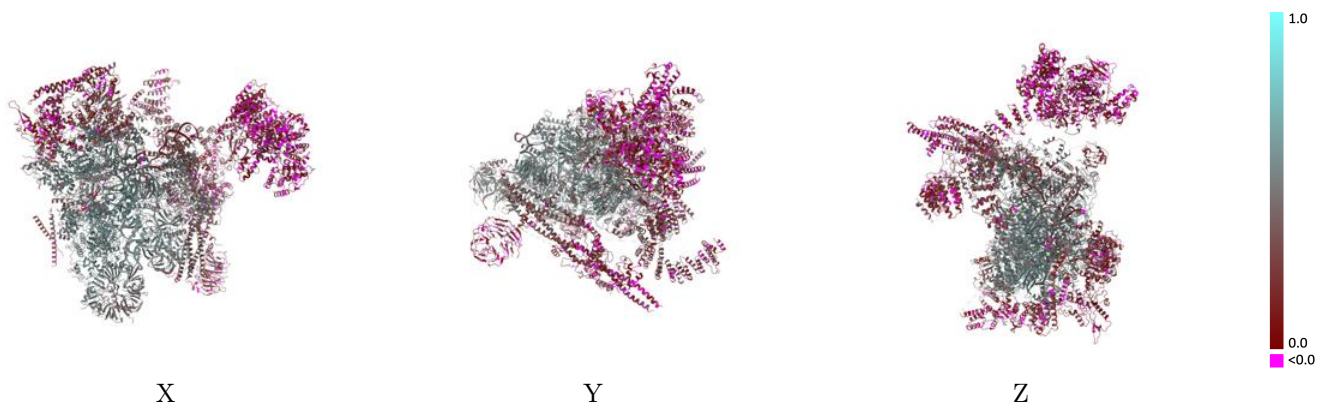
This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9ESI. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



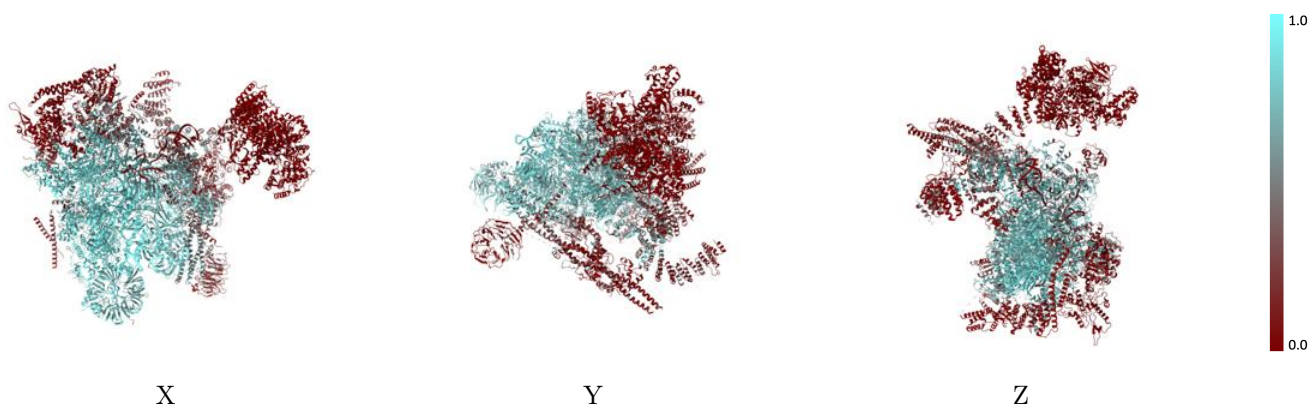
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



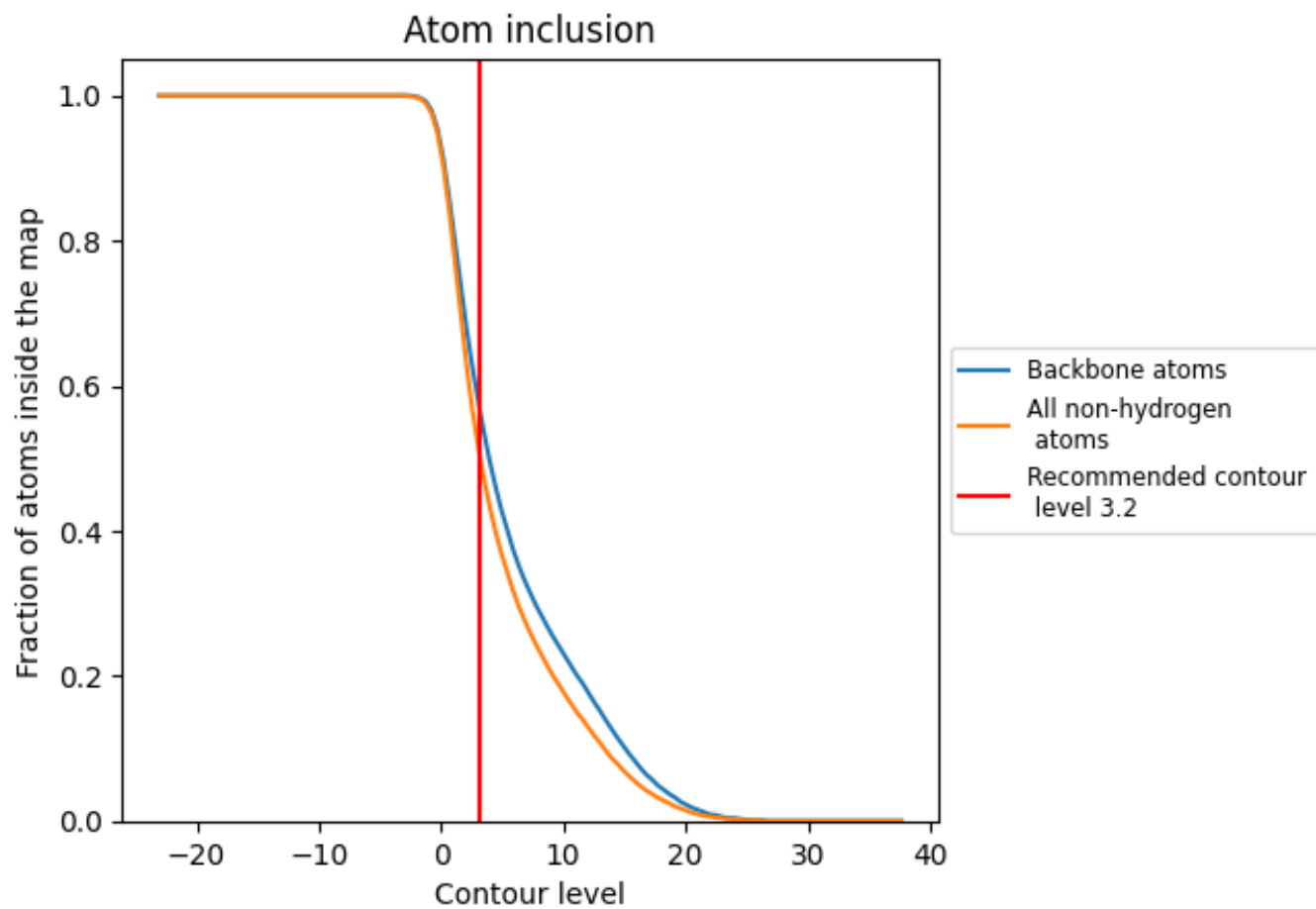
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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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