



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:36 AM UTC

PDB ID : 5ZWM / pdb_00005zwm
EMDB ID : EMD-6972
Title : Cryo-EM structure of the yeast pre-B complex at an average resolution of 3.4 4.6 angstrom (tri-snRNP and U2 snRNP Part)
Authors : Bai, R.; Wan, R.; Yan, C.; Lei, J.; Shi, Y.
Deposited on : 2018-05-16
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

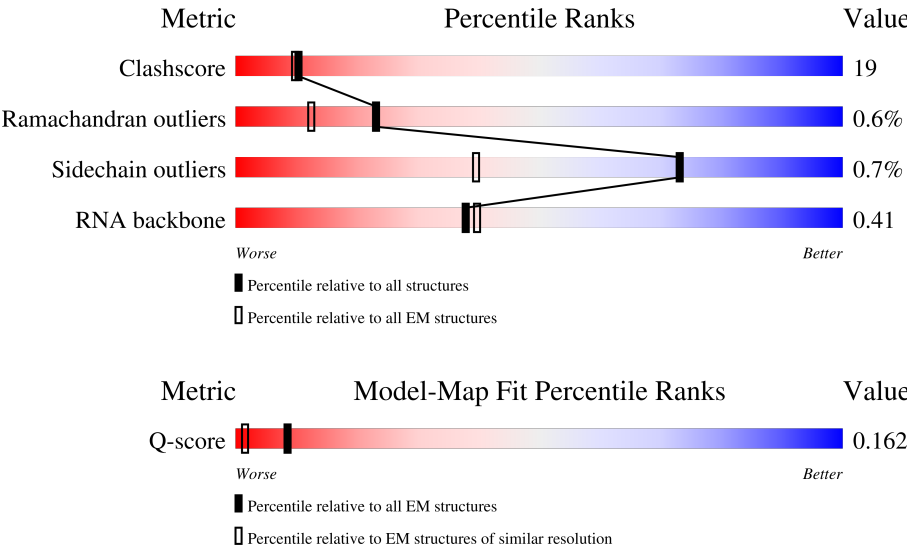
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2413	8% 60% 30% 10%
2	K	465	52% 38% 8%
3	L	494	57% 27% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	N	899	
5	J	469	
6	E	143	
7	M	126	
8	C	1008	
9	z	109	
10	q	95	
11	r	89	
12	x	86	
13	t	93	
14	y	115	
15	s	187	
16	F	112	
17	I	160	
18	B	214	
19	O	587	
20	S	101	
20	d	101	
20	l	101	
21	P	196	
21	a	196	
21	h	196	
22	Q	146	
22	b	146	
22	m	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	R	110	
23	c	110	
23	n	110	
24	T	94	
24	e	94	
24	i	94	
25	U	86	
25	f	86	
25	j	86	
26	V	77	
26	g	77	
26	k	77	
27	D	2163	
28	G	44	
29	H	1175	
30	o	238	
31	p	111	
32	1	971	
33	2	436	
34	3	1361	
35	4	213	
36	5	107	
37	6	85	
38	X	148	
39	Y	266	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	Z	204	11%5%5%•89%
41	u	530	86%53%33%•13%
42	w	280	45%26%17%•55%
43	v	266	59%42%23%•35%

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 111041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2177	Total	C	N	O	S	0	0
			17877	11496	3054	3263	64		

- Molecule 2 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	429	Total	C	N	O	S	0	0
			3375	2101	610	650	14		

- Molecule 3 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	416	Total	C	N	O	S	0	0
			3171	2001	573	585	12		

- Molecule 4 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	728	Total	C	N	O	S	0	0
			4897	3045	905	933	14		

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	304	Total	C	N	O	S	0	0
			2439	1545	445	435	14		

- Molecule 6 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	139	Total	C	N	O	S	0	0
			1146	725	199	211	11		

- Molecule 7 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	126	Total	C	N	O	S	0	0
			950	605	163	177	5		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	843	Total	C	N	O	S	0	0
			6732	4350	1119	1235	28		

- Molecule 9 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	z	65	Total	C	N	O	0	0
			260	130	65	65		

- Molecule 10 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	q	92	Total	C	N	O	0	0
			368	184	92	92		

- Molecule 11 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	r	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 12 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	x	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 13 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	t	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 14 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	y	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 15 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	s	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 16 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	99	Total	C	N	O	P	0	0
			2043	913	341	690	99		

- Molecule 17 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	110	Total	C	N	O	P	0	0
			2334	1044	399	781	110		

- Molecule 18 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	175	Total	C	N	O	P	0	0
			3715	1663	651	1227	174		

- Molecule 19 is a protein called 66 kDa U4/U6.U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	74	Total	C	N	O	S	0	0
			574	350	103	120	1		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	79	Total	C	N	O		0	0
			316	158	79	79			
20	S	82	Total	C	N	O	S	0	0
			632	402	109	119	2		
20	l	81	Total	C	N	O	S	0	0
			611	390	106	113	2		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	a	73	Total	C	N	O	0	0
			292	146	73	73		
21	P	70	Total	C	N	O	S	0
			563	360	98	102	3	0
21	h	78	Total	C	N	O	S	0
			610	389	110	108	3	0

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	b	77	Total	C	N	O	0	0
			308	154	77	77		
22	Q	99	Total	C	N	O	S	0
			751	475	137	137	2	0
22	m	82	Total	C	N	O	S	0
			644	409	110	123	2	0

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	c	90	Total	C	N	O	0	0
			360	180	90	90		
23	R	92	Total	C	N	O	S	0
			752	481	136	131	4	0
23	n	65	Total	C	N	O	S	0
			528	340	102	84	2	0

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	e	72	Total	C	N	O	0	0
			288	144	72	72		
24	T	77	Total	C	N	O	S	0
			602	396	95	108	3	0
24	i	75	Total	C	N	O	S	0
			575	379	92	101	3	0

- Molecule 25 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	f	70	Total	C	N	O	0	0
			280	140	70	70		
25	U	73	Total	C	N	O	S	0
			585	376	102	106	1	0
25	j	70	Total	C	N	O	S	0
			554	355	98	100	1	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	g	70	Total	C	N	O	0	0
			280	140	70	70		
26	V	75	Total	C	N	O	S	0
			577	363	100	112	2	0
26	k	69	Total	C	N	O	S	0
			529	337	93	97	2	0

- Molecule 27 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	D	1699	Total	C	N	O	S	1
			13601	8717	2266	2564	54	0

- Molecule 28 is a RNA chain called Pre-mRNA-BPS.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	G	44	Total	C	N	O	P	0
			928	419	161	304	44	0

- Molecule 29 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	H	206	Total	C	N	O	P	0
			4345	1940	722	1477	206	0

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	o	135	Total	C	N	O	0	0
			841	538	142	161		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	p	73	Total	C	N	O	0	0
			466	304	81	81		

- Molecule 32 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	816	Total	C	N	O	S	0	0
			6472	4165	1101	1166	40		

- Molecule 33 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	211	Total	C	N	O	S	0	0
			1726	1121	292	304	9		

- Molecule 34 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	1180	Total	C	N	O	S	0	0
			9380	5996	1580	1753	51		

- Molecule 35 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4	173	Total	C	N	O	S	0	0
			1429	930	239	258	2		

- Molecule 36 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5	103	Total	C	N	O	S	0	0
			814	503	154	143	14		

- Molecule 37 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	84	Total	C	N	O	S	0	0
			693	429	130	132	2		

- Molecule 38 is a protein called U2 snRNP component IST3.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	X	128	Total	C	N	O	0	0
			1051	662	181	208		

- Molecule 39 is a protein called Pre-mRNA-splicing factor CWC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Y	89	Total	C	N	O	S	0	0
			730	458	130	140	2		

- Molecule 40 is a protein called Pre-mRNA leakage protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Z	22	Total	C	N	O	S	0	0
			173	110	25	37	1		

- Molecule 41 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	u	461	Total	C	N	O	S	0	0
			3895	2475	675	730	15		

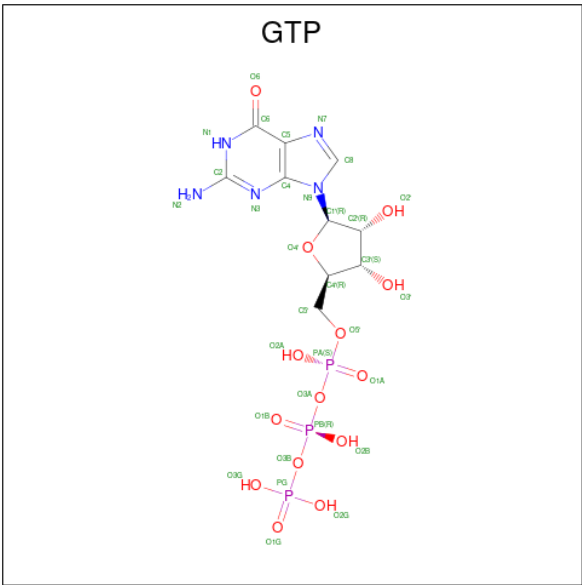
- Molecule 42 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	127	Total	C	N	O	S	0	0
			1084	689	193	196	6		

- Molecule 43 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	174	Total	C	N	O	S	0	0
			1372	862	235	269	6		

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

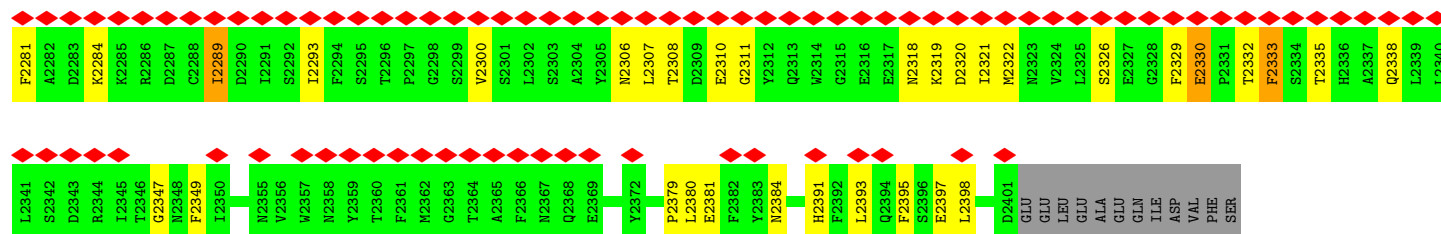
- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	C	1	Total	Mg	0
			1	1	

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

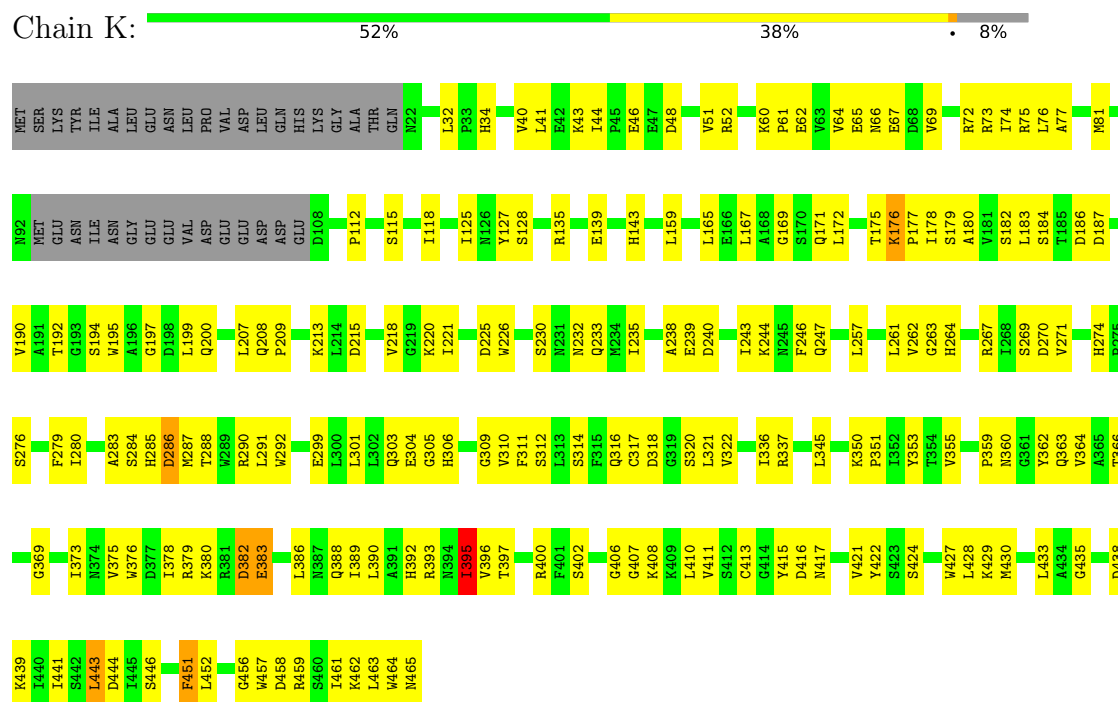
Mol	Chain	Residues	Atoms		AltConf
46	5	3	Total	Zn	0
			3	3	
46	u	2	Total	Zn	0
			2	2	
46	v	1	Total	Zn	0
			1	1	

E2220	T2160	GLU	L1891	M1802	T1702	Q1586	L1488	M1369	M1275	Y1161	L1054	T960
I2221	L2161	LEU	K1892	R1803	M1703	R1595	P1489	R1370	E1276	I1168	M1057	Y963
K2222	L2162	GLU	W1899	T1805	S1705	L1598	P1489	V1371	E1277	Y1169	A1058	
T2223	Y2163	ALA	L1905	M1809	W1709	L1598	L1494	L1375	V1279	M1170	K1060	P966
Y2224	L2164	ARG	K1910	P1810	V1711	T1601	L1376	S1377	V1285	L1171	I1061	Y967
V2225	R2165	SER	T1913	A1811	S1712	P1602	D1498	L1376	V1286	F1172	D1062	
L2226	L2166	GLU	L1913	W1814	K1713	M1603	R1499	F1383	D1287	H1173	F1063	N971
V2227	K2167	ASN	L1920	L1815	L1714	T1607	H1500	L1383	L1288	E1175	L1066	N972
P2228	R2168	GLN	L1920	R1816	L1716	R1616	T1501	F1383	L1288	N1197	L1070	E973
Q2229	S2169	ASP	S1923	E1817	L1717	A1617	R1509	Y1389	A1298	S1198	L1070	Y974
L2230	V2170	GLU	S1923	R1818	L1717	M1618	I1510	P1391	Y1301	I1199	L1070	Q976
G2231	V2171	GLU	P1925	I1819	L1717	N1618	R1511	E1392	L1302	G1200	I1073	N977
H2232	S2172	ALA	P1925	L1819	L1717	N1618	R1511	E1392	K1303	Y1201	V1074	Y978
V2233	A2173	ALA	Q1929	S1829	W1733	V1621	Y1517	L1394	E1306	N1202	I1078	Y981
G2234	D2174	ALA	Q1929	E1832	P1734	L1624	R1521	M1399	E1307	C1206	I1078	Y982
S2235	D2175	SER	V1935	P1833	D1735	L1624	R1521	M1399	E1308	W1207	K1085	S983
V2236	F2176	THR	T1936	P1833	D1735	L1624	R1521	M1399	E1308	P1207	N1086	Y984
Q2237	F2177	VAL	R1937	F1834	R1739	F1632	P1524	I1401	K1309	W1207	N1086	D985
L2238	V2177	MET	M1940	L1835	R1739	F1632	F1525	A1409	K1310	K1209	V1088	P986
I2239	E2178	LYS	L1941	L1835	S1745	H1635	W1526	A1409	K1311	D1210	V1088	P986
S2239	E2178	THR	L1941	M1836	S1745	H1635	W1526	A1409	K1311	S1211	V1089	L987
N2240	E2179	LYS	D1942	M1836	S1745	H1635	W1526	A1409	K1311	R1212	I1090	
I2241	T2180	THR	P1943	M1839	I1748	L1645	T1528	W1414	S1314	M1213		D992
P2242	N2181	ILE	P1943	M1839	I1748	L1645	T1528	W1414	S1314	M1213		D992
D2243	V2182	ASN	P1952	L1843	Y1751	I1647	M1529	Q1417	R1317	R1214	M1095	L995
Y2183	Y2183	ALA	P1952	L1843	Y1751	I1647	M1529	Q1417	R1317	R1214	M1095	L995
D2246	V2184	GLN	P1958	L1860	K1755	F1649	G1534	G1428	L1320	N1221	K1085	S983
L2247	L2185	GLY	P1958	F1851	F1756	R1650	G1534	G1428	L1320	N1221	N1086	Y984
L2248	F2186	GLY	P1958	F1851	F1756	R1650	G1534	G1428	L1320	N1221	N1086	Y984
D2249	K2187	VAL	P1965	T1857	Y1759	Q1655	Y1542	H1431	M1321	I1230	N1099	R1006
T2250	N2188	VAL	F1965	T1857	Y1759	Q1655	Y1542	H1431	M1321	I1230	N1099	R1006
E2251	E2188	ALA	Q1985	R1859	G1772	S1660	T1544	I1440	M1336	R1234	K1106	S1016
L2252	L2189	ALA	Q1985	R1859	G1772	S1660	T1544	I1440	M1336	R1234	K1106	S1016
E2253	L2190	SER	L1988	T1861	V1773	Q1667	Q1548	W1447	S1341	I1241	D1122	
E2254	K2191	ALA	F1989	V1862	M1774	I1668	Q1548	W1447	S1341	I1241	D1122	
L2255	K2192	ASP	D1993	H1863	I1775	I1668	T1555	E1448	F1343	F1343	L1125	L1023
L2256	F2193	TYR	D1993	H1863	I1775	I1668	T1555	E1448	F1343	F1343	L1125	L1023
G2257	I2194	GLU	D1993	H1863	I1775	I1668	T1555	E1448	F1343	F1343	L1125	L1023
W2258	E2195	SER	L1996	T1865	L1777	D1674	E1558	F1451	Y1345	F1247	L1126	Q1030
I2259	I2196	THR	L1996	T1865	L1777	D1674	E1558	F1451	Y1345	F1247	L1126	Q1030
H2260	S2197	THR	L1999	M1869	M1783	I1678	F1562	S1454	E1348	S1252	L1134	N1033
T2261	Q2262	GLN	I1999	M1869	M1783	I1678	F1562	S1454	E1348	S1252	L1134	N1033
Q2263	L2198	ASN	T2003	A1871	D1785	V1681	G1564	W1458	I1350	K1253	E1143	I1038
E2264	V2199	SER	T2003	A1871	A1786	T1682	G1566	W1458	I1350	K1253	E1143	I1038
E2265	K2200	SER	S2006	T1879	Y1787	P1688	G1566	W1458	I1350	K1253	E1143	I1038
E2266	K2201	LYS	S2006	T1879	Y1787	P1688	G1566	W1458	I1350	K1253	E1143	I1038
L2266	Q2202	VAL	T2009	F1880	G1788	R1689	W1570	Q1470	L1356	L1258	F1144	R1043
Q2267	V2203	VAL	T2009	F1880	G1788	R1689	W1570	Q1470	L1356	L1258	F1144	R1043
F2268	A2204	ARG	L2011	T1881	M1789	K1690	W1575	R1473	L1359	M1262	M1145	Q1046
M2269	A2205	GLN	L2011	T1881	M1789	K1690	W1575	R1473	L1359	M1262	M1145	Q1046
A2270	F2206	LYS	L2012	H1887	L1794	S1695	A1578	R1474	L1359	M1262	E1153	A1047
A2271	T2207	LYS	R2013	H1888	I1798	S1696	G1580	F1477	E1364	V1267	R1268	L1049
G2272	Y2208	MET	K2016	L1889	I1798	S1696	G1580	F1477	E1364	V1267	R1268	L1049
E2273	Q2209	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
V2274	M2210	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
A2275	A2212	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
L2276	D2214	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
H2277	H2215	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
S2278	F2216	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
K2279	K2217	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050
L2280	V2218	ALA	K2016	F1890	S1801	A1699	F1581	E1481	T1365	I1269	P1157	L1050



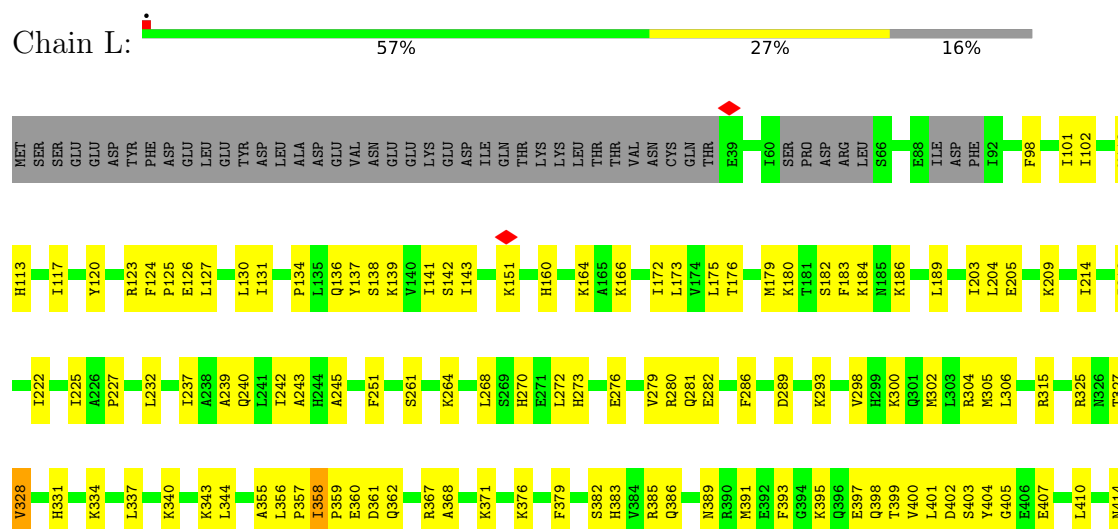
• Molecule 2: U4/U6 small nuclear ribonucleoprotein PRP4

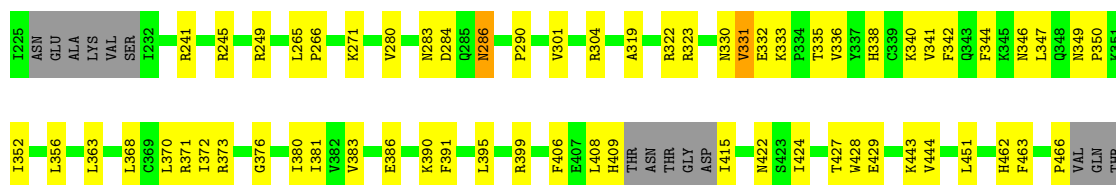
Chain K:



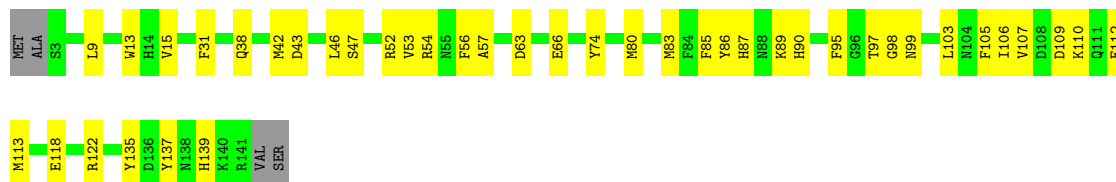
• Molecule 3: Pre-mRNA-processing factor 31

Chain L:

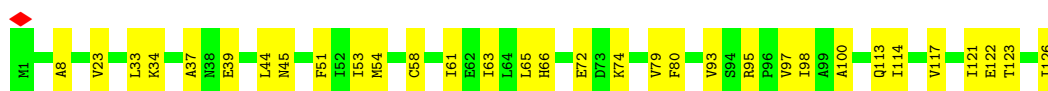




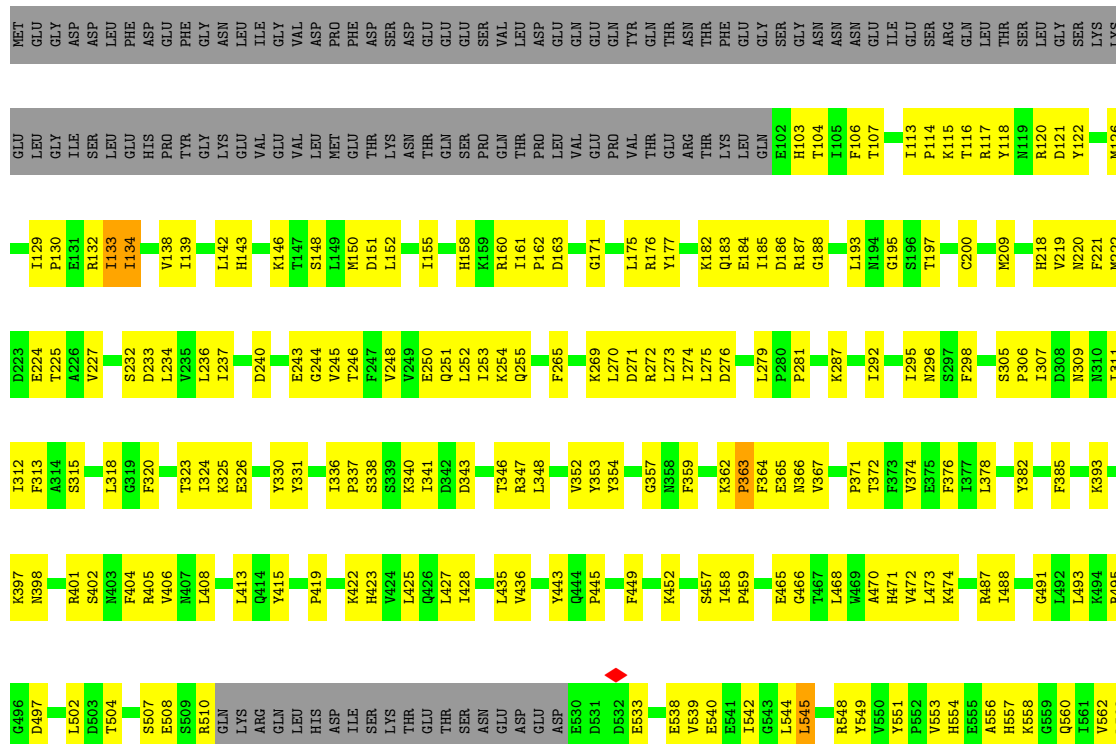
• Molecule 6: Spliceosomal protein DIB1

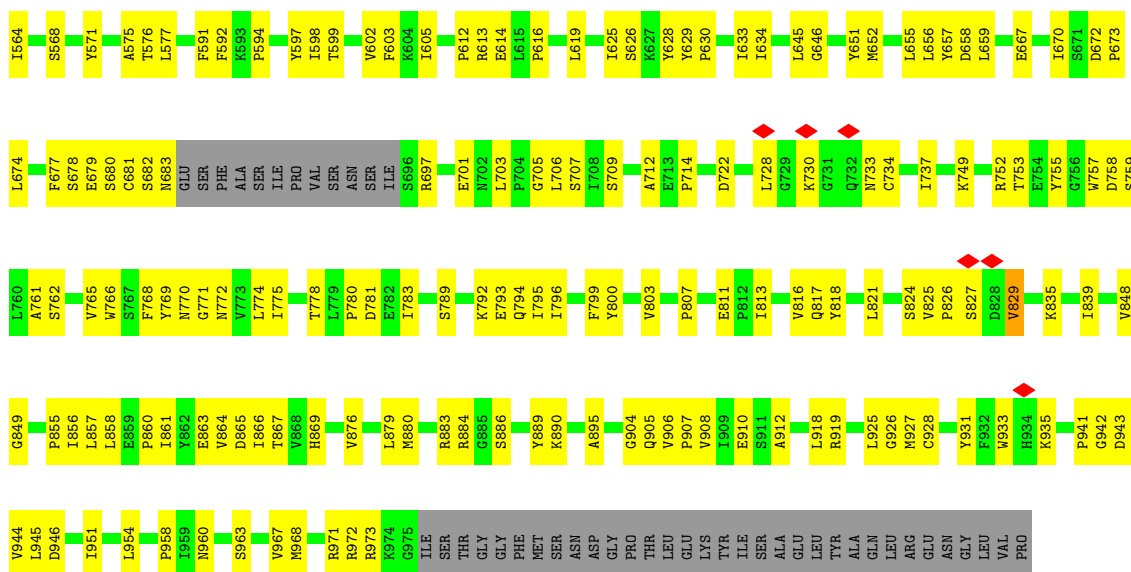


• Molecule 7: 13 kDa ribonucleoprotein-associated protein

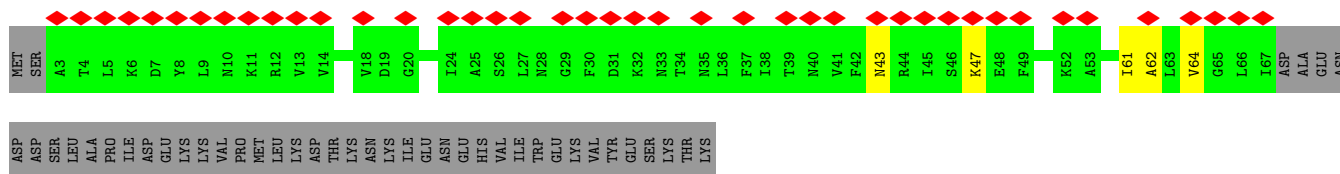
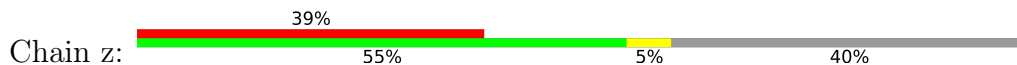


• Molecule 8: Pre-mRNA-splicing factor SNU114

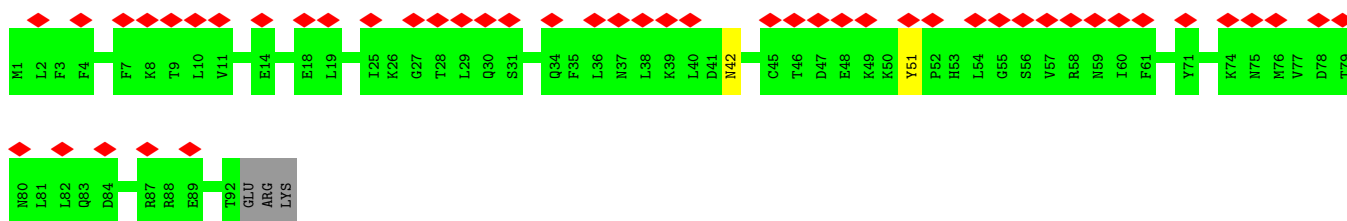




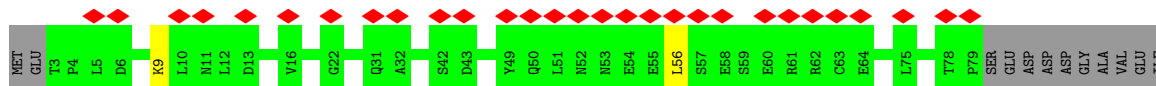
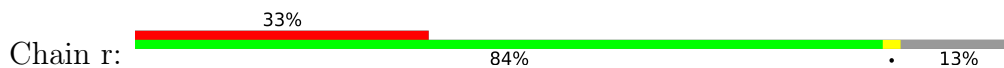
• Molecule 9: U6 snRNA-associated Sm-like protein LSm8



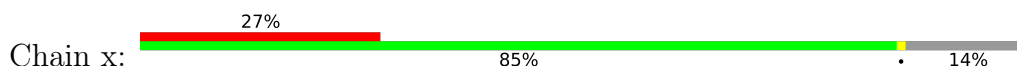
• Molecule 10: U6 snRNA-associated Sm-like protein LSm2

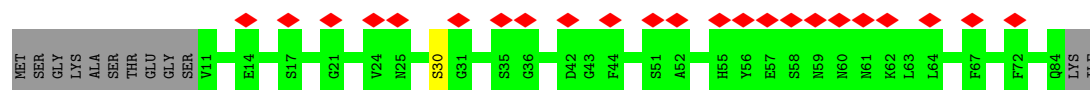


• Molecule 11: U6 snRNA-associated Sm-like protein LSm3

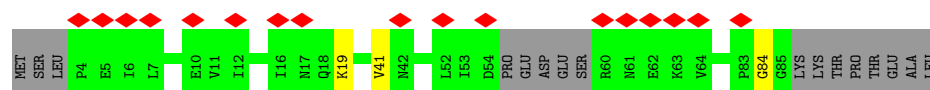
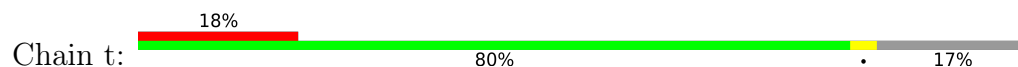


• Molecule 12: U6 snRNA-associated Sm-like protein LSm6

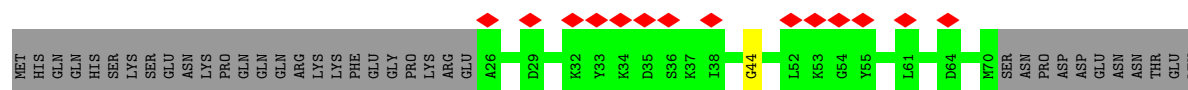




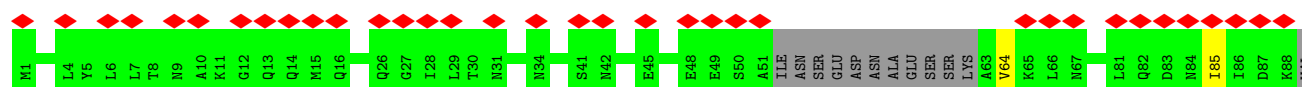
• Molecule 13: U6 snRNA-associated Sm-like protein LSm5



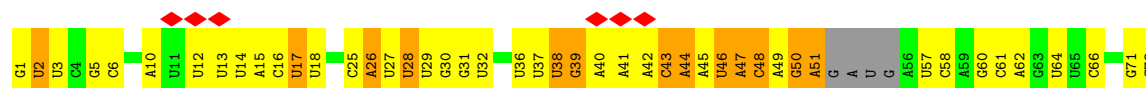
• Molecule 14: U6 snRNA-associated Sm-like protein LSm7



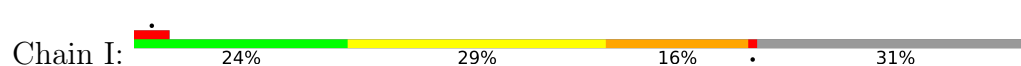
• Molecule 15: U6 snRNA-associated Sm-like protein LSm4

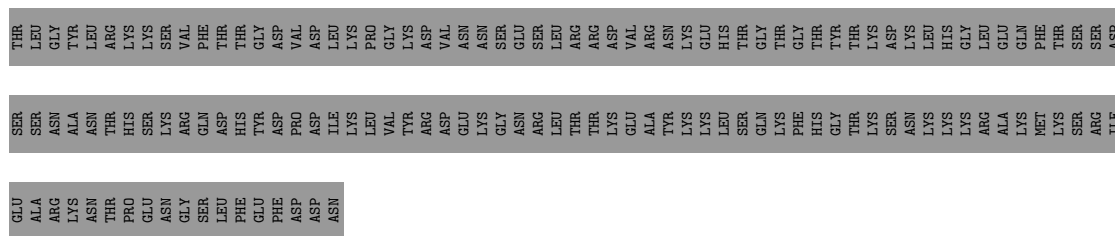


• Molecule 16: U6 snRNA

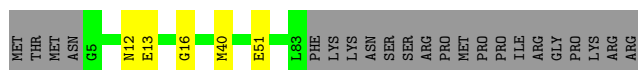


• Molecule 17: U4 snRNA

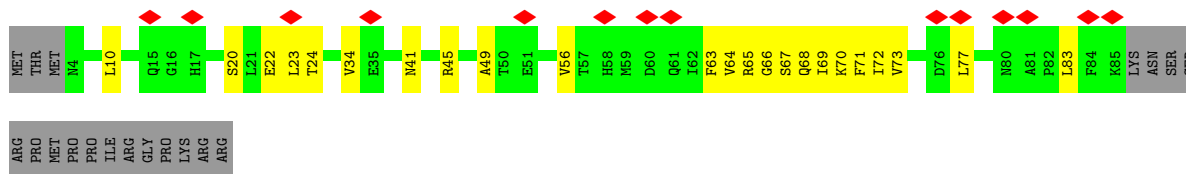




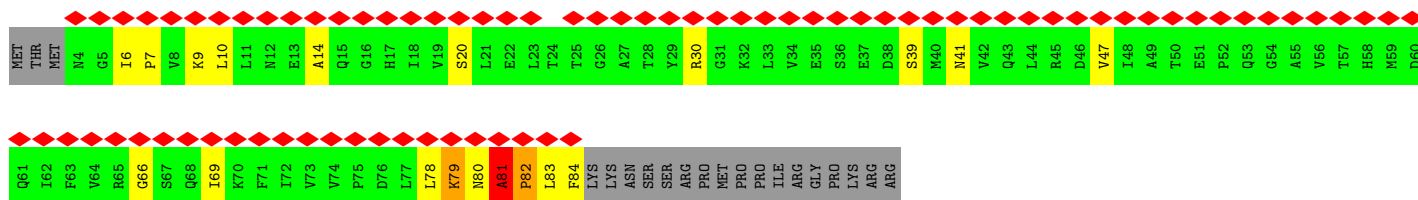
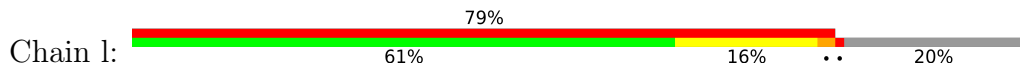
- Molecule 20: Small nuclear ribonucleoprotein Sm D3



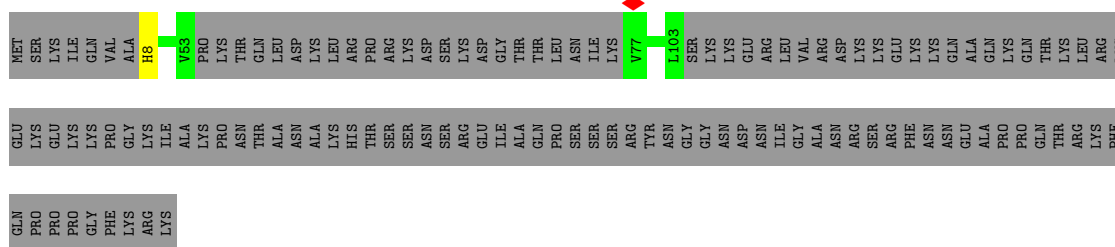
- Molecule 20: Small nuclear ribonucleoprotein Sm D3



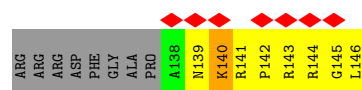
- Molecule 20: Small nuclear ribonucleoprotein Sm D3



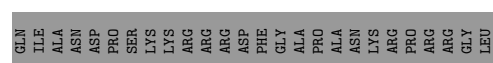
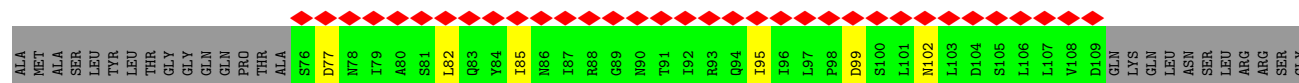
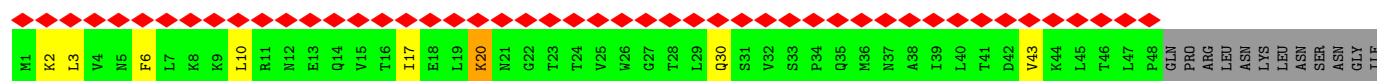
- Molecule 21: Small nuclear ribonucleoprotein-associated protein B



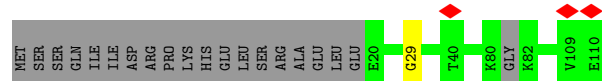
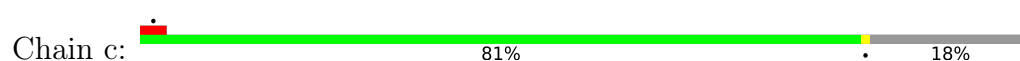
- Molecule 21: Small nuclear ribonucleoprotein-associated protein B



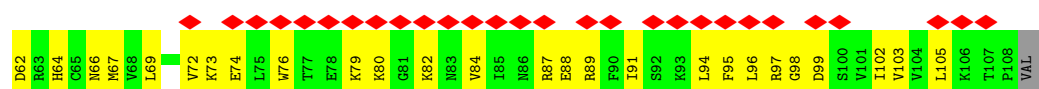
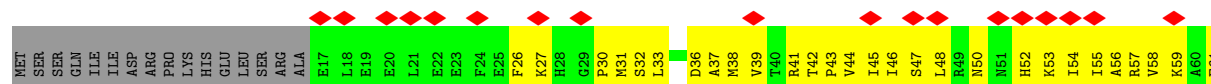
• Molecule 22: Small nuclear ribonucleoprotein Sm D1



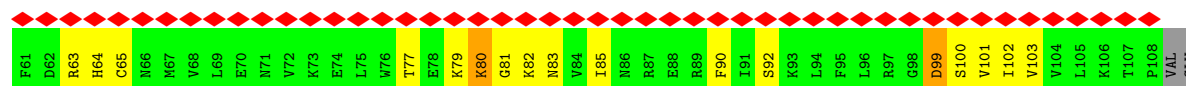
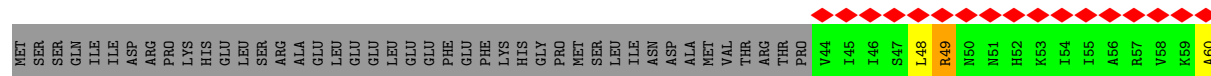
• Molecule 23: Small nuclear ribonucleoprotein Sm D2



• Molecule 23: Small nuclear ribonucleoprotein Sm D2

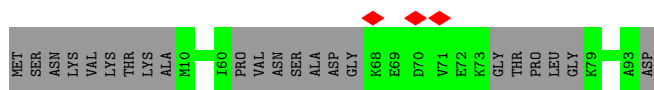


• Molecule 23: Small nuclear ribonucleoprotein Sm D2

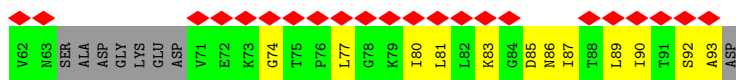
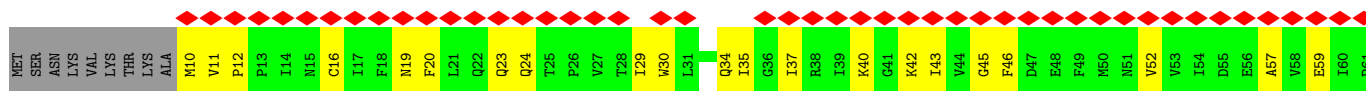
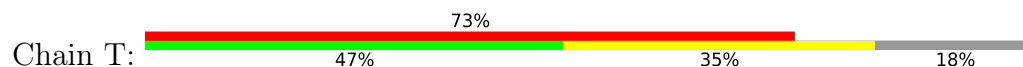


• Molecule 24: Small nuclear ribonucleoprotein E

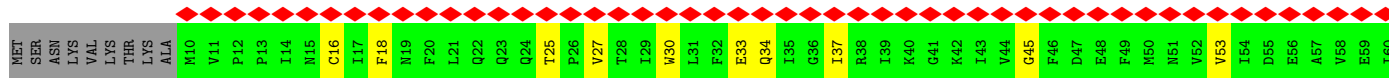
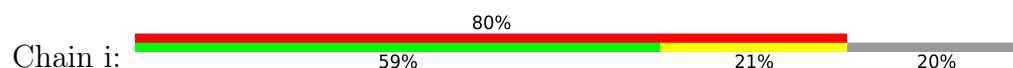




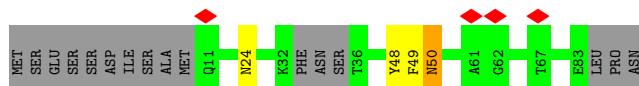
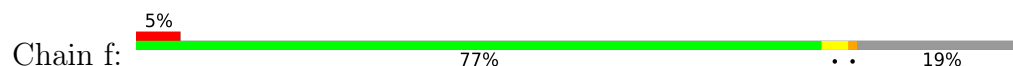
- Molecule 24: Small nuclear ribonucleoprotein E



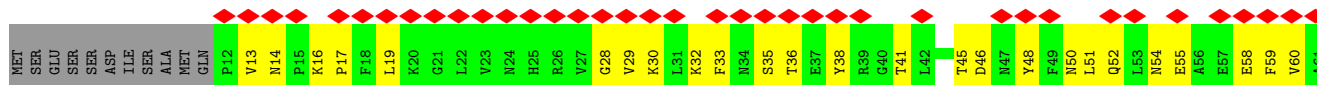
- Molecule 24: Small nuclear ribonucleoprotein E



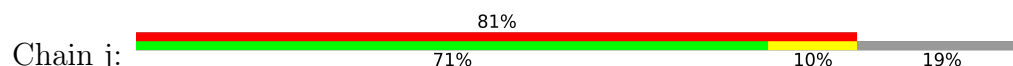
- Molecule 25: Small nuclear ribonucleoprotein F



- Molecule 25: Small nuclear ribonucleoprotein F



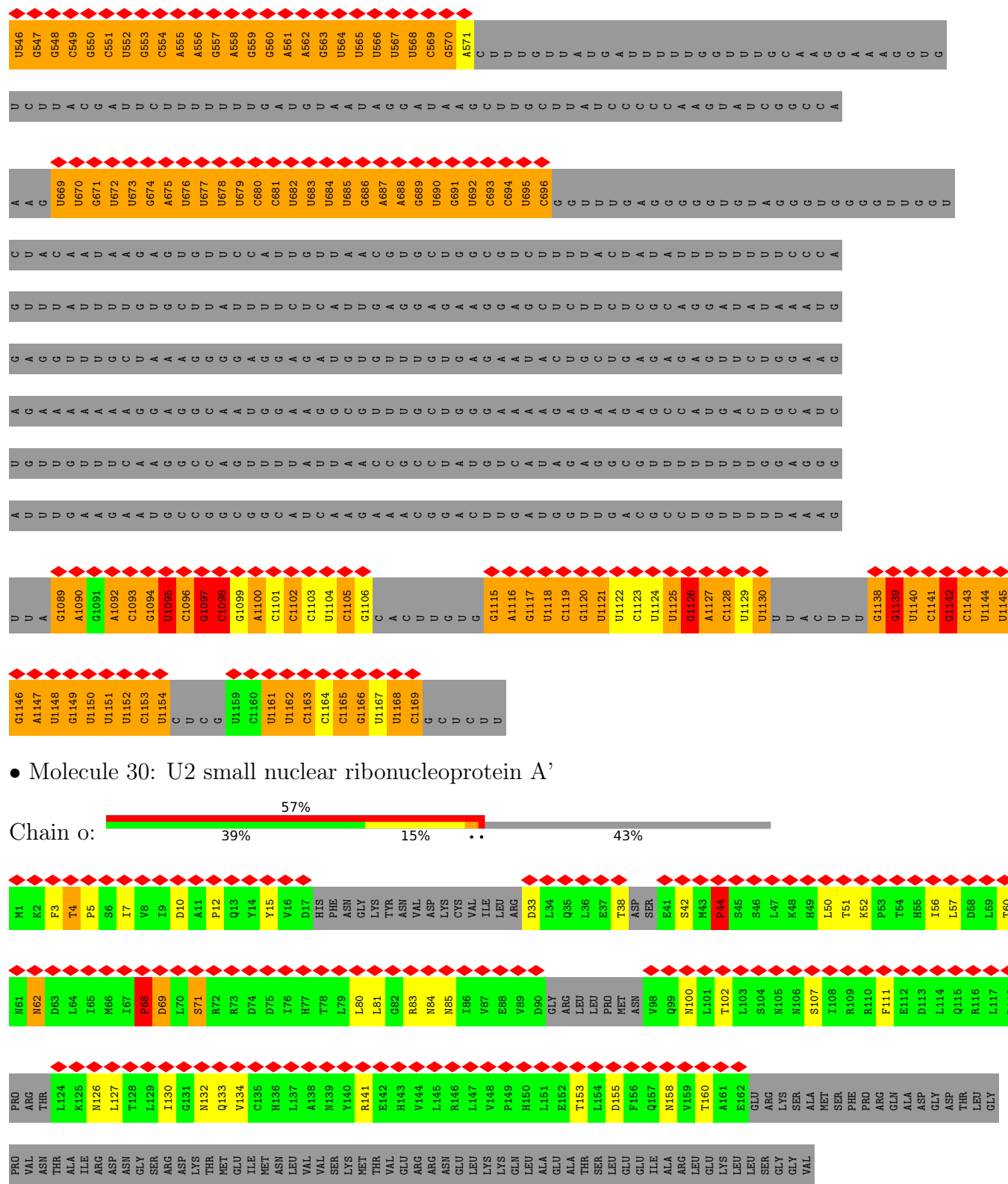
- Molecule 25: Small nuclear ribonucleoprotein F





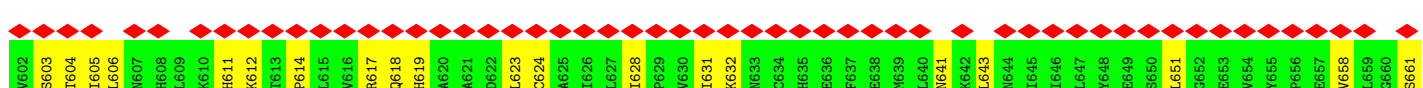
R1895	K1896	G1897	D1898	R1899	A1900	L1901	L1902	L1905	S1906	R1912	R1913	R1903	L1909	P1910	L1911	S1907	K1906	R1908	L1905	L1902	L1905	H1916	L1917	S1918	S1919	G1920	S1921	F1924	K1925	V1926	F1927	L1928	L1929	R1930	F1931	R1932	R1933	F1934	S1935	R1936	L1937	E1938	L1939	P1940	V1941	F1942	F1943	Q1944	M1945	D1946	T1950	L1951	E1952	K1953	V1954	V1960	V1961	V1962	
VAL	ASN	GLY	GLY	ASP	ASP	GLU	ALA	T1841	E1842	I1843	I1844	S1845	T1846	L1847	S1848	N1849	G1850	L1851	L1852	A1853	S1854	H1855	I1856	G1857	V1858	S1859	F1860	F1861	T1862	I1863	Q1864	S1865	F1866	V1867	S1868	S1869	L1870	S1871	N1872	T1873	S1874	T1875	L1876	K1877	M1878	M1879	L1880	V1881	L1882	S1883	T1884	T1885	A1886	V1887	E1888	F1889	E1890	L1894	
F1773	T1774	Y1775	S1776	Y1777	F1778	Y1779	R1780	R1781	I1782	H1783	V1784	L1785	P1786	S1787	Y1788	Y1789	G1790	V1791	R1792	T1793	T1794	S1795	P1796	H1797	F1798	I1799	S1800	V1801	F1802	L1803	N1804	L1805	L1806	V1807	E1808	C1809	L1811	N1812	D1813	L1814	V1815	E1816	S1817	S1818	F1819	I1820	E1821	I1822	D1823	T1824	GLU	ALA	GLU	VAL	THR	ALA	GLU		
V1652	K1653	R1654	L1655	Y1656	E1657	Y1658	G1659	V1660	V1661	S1662	V1663	L1664	L1665	I1666	S1667	K1668	S1671	A1672	F1673	A1674	C1675	K1676	T1677	D1678	E1679	V1680	I1681	I1682	L1683	G1684	T1685	N1686	L1687	D1688	G1689	A1691	E1692	H1693	K1694	Y1695	M1696	P1697	Y1698	T1699	I1700	N1701	E1702	L1703	L1704	E1705	M1706	V1707	G1708	L1709	A1710	S1711	G1712		
M1592	E1593	V1594	A1595	S1596	A1597	F1598	M1599	K1600	F1601	S1602	K1603	A1604	I1605	E1606	W1607	D1608	M1609	L1610	N1611	V1612	E1613	E1614	E1615	Q1616	I1617	V1618	P1619	Y1620	I1621	E1622	K1623	L1624	T1625	D1626	G1627	H1628	L1629	R1630	A1631	P1632	L1633	K1634	H1635	G1636	V1637	G1638	I1639	L1640	Y1641	K1642	G1643	M1644	A1645	N1647	D1648	E1649	R1650	I1651	
I1532	Y1533	M1534	F1535	S1536	P1537	S1538	E1539	R1540	I1541	E1542	P1543	L1544	G1545	I1546	N1547	I1548	Q1549	S1550	F1551	K1552	D1553	V1554	E1555	H1556	I1557	S1558	F1559	M1560	F1561	S1562	M1563	L1564	Q1565	M1566	A1567	F1568	E1569	A1570	S1571	A1572	A1573	A1574	A1575	G1576	M1577	R1578	N1579	Y1580	S1581	S1582	V1583	F1584	L1585	P1586	S1587	K1588	K1589	C1591	
L1472	Y1473	D1474	D1475	A1476	H1477	E1478	I1479	S1480	Q1481	G1482	V1483	L1484	G1485	A1486	V1487	Y1488	E1489	T1490	L1491	I1492	S1493	R1494	M1495	F1496	F1497	I1498	A1499	T1500	Q1501	L1502	E1503	K1504	I1505	I1506	R1507	F1508	V1509	C1510	L1511	S1512	N1513	C1514	L1515	A1516	M1517	A1518	R1519	D1520	F1521	G1522	E1523	W1524	I1525	G1526	M1527	T1528	S1530	N1531	
W1412	N1413	K1414	R1415	F1416	H1417	H1418	L1419	A1420	G1421	G1422	K1423	L1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	F1432	K1433	L1434	N1435	L1436	K1437	L1438	A1439	A1440	K1441	S1442	H1443	V1444	L1445	L1446	A1447	T1448	P1449	V1450	Q1451	F1452	E1453	L1454	L1455	S1456	R1457	R1458	W1459	R1460	Q1461	R1462	K1463	N1464	I1465	Q1466	S1467	L1468	E1469	L1470	M1471
Q1352	S1353	Q1354	V1355	F1356	E1357	S1358	L1359	Y1360	N1361	S1362	N1363	D1364	S1365	V1366	F1367	V1368	G1369	S1370	G1371	K1372	K1373	T1374	G1375	K1376	T1377	A1378	M1379	A1380	E1381	L1382	A1383	L1384	L1385	N1386	H1387	W1388	R1389	Q1390	N1391	K1392	G1393	R1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411
F1288	F1289	L1292	E1295	N1296	W1297	W1298	H1299	S1300	E1301	I1304	S1307	F1308	N1309	G1310	F1311	K1312	L1313	P1314	K1315	K1316	F1317	P1318	P1319	P1320	T1321	P1322	L1323	L1324	E1325	N1326	I1327	S1328	I1329	S1330	T1331	S1332	V1333	L1334	G1335	M1336	D1337	D1338	F1339	S1340	E1341	V1342	F1343	E1344	F1345	K1346	T1347	F1348	N1349	K1350	I1351				
Q1209	P1210	I1211	T1212	R1213	S1214	V1215	M1216	R1217	F1218	N1219	I1220	E1221	I1222	I1223	A1224	D1225	W1226	I1227	W1228	L1240	L1241	M1242	L1243	E1244	D1245	T1246	D1247	G1248	W1249	S1250	L1251	L1252	Y1253	E1254	D1255	V1256	L1257	F1258	P1261	D1262	I1263	V1264	G1265	H1266	F1272	E1275	L1276	K1277	Q1278	H1279	N1280	Q1281	N1282	N1283					
K1138	M1139	W1140	P1141	T1142	N1143	C1144	Q1148	F1149	K1150	T1151	C1152	P1153	V1154	E1155	V1156	I1157	K1158	R1159	L1160	A1161	A1162	S1163	T1164	V1165	P1166	W1167	G1168	D1169	Y1170	L1171	Q1172	L1173	E1174	T1175	P1176	A1177	E1178	V1179	G1180	R1181	A1182	I1183	R1184	S1185	E1186	K1187	D1194	R1198	M1202	S1203	V1204	T1205	C1206	N1207	A1208				



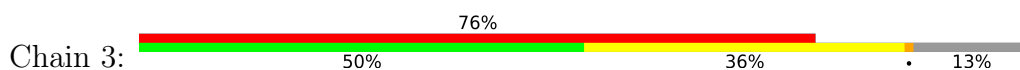


• Molecule 31: U2 small nuclear ribonucleoprotein B''

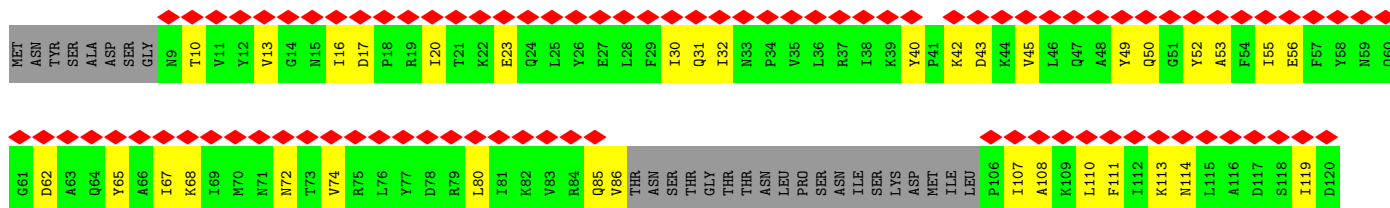


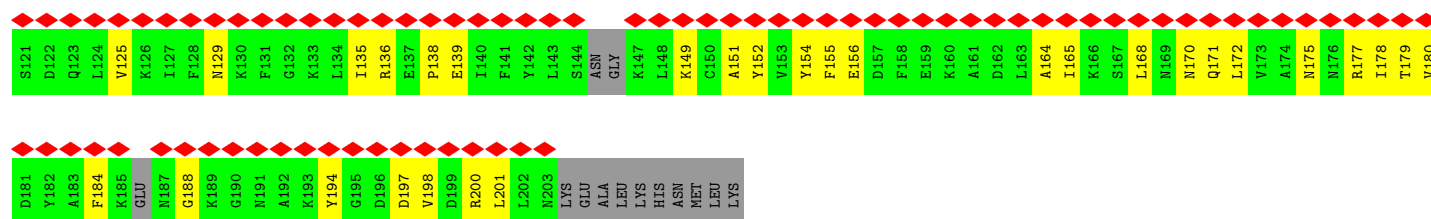




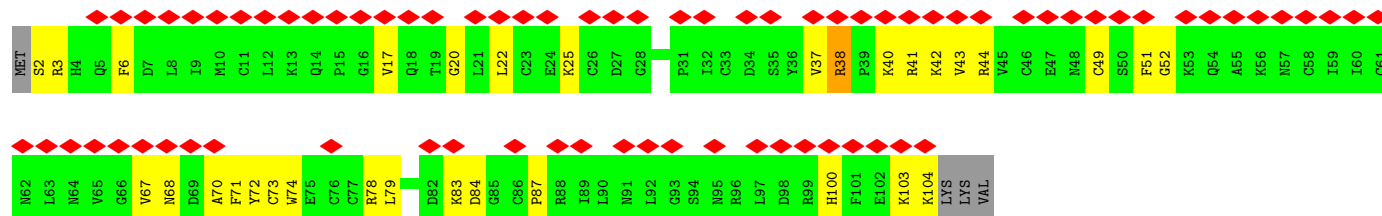


MET	TRP	GLY	GLY	LYS	MET	ALA	VAL	ALA	SER	LEU	SER	SER	PRO	HIS	THR	ALA	LYS	ASP	GLY	LEU	LYS	ARG	GLU	ALA	GLU	ARG	THR	ARG	SER	ASP	HIS	ASN	ILE	THR	MET	VAL	ALA	LYS	ASP	D56	E57	L58	Y59	L60																	
Y61	H62	L63	T64	L65	K66	K67	Q68	T69	N70	F71	V72	H73	S74	C75	I76	G77	H78	F79	V80	D81	L82	E83	A84	G85	S86	K87	R88	E89	Q90	S91	G92	N93	C94	V95	A96	T97	E98	T99	H100	L101	E102	L103	Y104	D105	T106	A107	D108	G109	E110	L111	K112	L113	I114	A115	K116	F117	Q118	N119	L120		
F121	I124	T125	S126	M127	K128	S129	L130	D131	L132	P133	H134	SER	GLY	SER	ARG	ALA	LYS	ALA	ASN	W144	P145	T146	F147	L148	A149	L150	T151	S152	D153	S154	G155	N156	L157	S158	I159	V160	Q161	I162	I163	M164	H165	A166	G167	A168	L169	R170	E171	K172	T173	L174	V175	N176	Q177	P178	L179	T180	R181				
T182	T183	L184	R185	R186	V187	P188	S189	S191	Y192	M193	E194	I195	D196	P197	N198	G199	R200	C201	L202	I203	L204	S205	S206	V207	E208	Q209	N210	K211	L212	C213	F214	L215	V216	D217	Y218	A219	Q220	K221	L222	R223	I224	S225	S226	P227	L228	E229	I230	L231	R232	P233	H234	M235	V236	T237	L238	D239	M240	A241			
V242	V243	D244	V245	M246	F247	M248	N249	P250	C251	F252	V253	T254	L255	E256	I257	D258	N259	A260	A261	T262	Q263	L264	S265	V266	H267	L268	I269	F270	Y271	V272	L273	E274	L275	Q276	L277	N278	H279	K280	L281	K282	K283	A284	D285	V286	L287	V288	N289	P290	S291	A292	F293	V294	V295	L296	L297	L298	P299	D300	L301		
S302	ARG	TYR	ASN	ILE	THR	SER	LEU	SER	ASP	ASN	ASN	TYR	ASP	ALA	ASP	TYR	LEU	PHE	N324	P325	F326	V327	V328	I329	G330	F331	E332	N333	H334	I335	L336	K338	D339	K340	N341	G342	F343	F344	S345	L346	K347	V348	E349	I350	P351	K352	R353	S354	I355	T356	N357	S358	R359	H360	K361						
N362	V363	T364	I365	I366	G368	V369	V370	Q371	K372	L373	K374	N375	D376	F377	F378	V379	L380	L381	Q382	S383	N384	H385	G386	D387	L388	F389	K390	L391	T392	V393	S394	P395	D396	T397	N398	D399	R400	N401	R402	P403	L404	V405	Q406	E407	P408	S409	I410	D411	T412	T413	Q414	N415	S416	H417	Q418	L419	H420	I421			
F422	K423	N424	G425	Y426	L427	F428	A429	L430	S431	E432	N433	N434	N435	N436	F437	L438	F439	Q440	F441	E442	K443	L444	C445	V446	E447	K448	N449	D450	F451	N452	N453	V454	L455	T456	S457	K458	D459	P460	N461	K462	S463	L464	V465	P466	E467	P468	S469	I470	K471	L472	Q473	N474	L475	S476	I477	L478	S479	Q480	Q481		
L482	N483	L484	N485	P486	S487	L488	K489	L492	V493	S494	D495	S496	L498	S499	I500	A501	T502	K503	H504	F505	T506	N507	N508	K509	I510	I511	T512	L513	T514	N515	A516	V517	N518	Y519	S520	N521	L522	S523	S524	T525	S526	L527	P528	P529	N530	A531	T532	K533	L534	W535	L536	I537	P538	D539	A541	T542					
T543	G544	D545	N546	N547	L548	L549	L550	F551	I552	T553	F554	P555	K556	K557	T558	M559	I560	L561	Q562	I563	D564	M565	E566	S567	M568	E569	E570	L571	THR	PRO	ASP	GLU	ALA	THR	ARG	SER	ALA	PHE	K582	L583	S584	Q585	D586	T587	T588	I589	H590	T591	C592	L593	M594	G595	L596	H597	S598	I599	I600	Q601	V602		
G603	T604	A605	E606	L607	H608	H609	I610	V611	P612	T613	G614	K615	S616	R617	Y618	S619	N620	K621	L622	T623	W624	V625	P626	P627	A628	G629	I630	R631	L632	V633	G634	A635	T636	S637	S638	K639	T640	Q641	L642	I643	S644	S645	L646	L647	S648	N649	E650	L651	V652	Y653	S654	K655	I656	D657	V658	S659	S660	D661	S662		
L663	I664	E665	L666	T667	T668	H669	P670	E671	L672	D673	T674	M675	P676	S677	K678	V679	A680	I681	V682	Q683	D684	T685	Q686	H687	A688	D689	L690	L691	A692	I693	A694	D695	N696	E697	G698	M699	I700	K701	I702	M703	D586	S704	L705	L706	LYS	ASP	GLN	LYS	GLU	D711	F712	L713	T714	K715	P716	T717	L718	S719	Q720	V721	S722
E723	K724	I725	S726	D727	T728	H729	M730	V731	R732	D733	S734	S735	I736	G737	Q738	L739	N740	L741	H742	V743	G744	L745	E746	N747	G748	V749	Y750	M751	K752	F753	H754	I755	G756	D757	V758	D759	G760	S761	F762	T763	S764	I765	K766	R767	N768	F769	L770	G771	L772	K773	P774	V775	S776	L777	Y778	L779	V780	R781	E782		

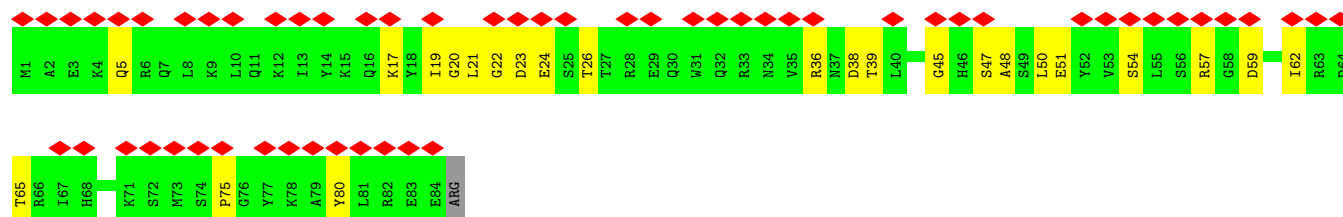




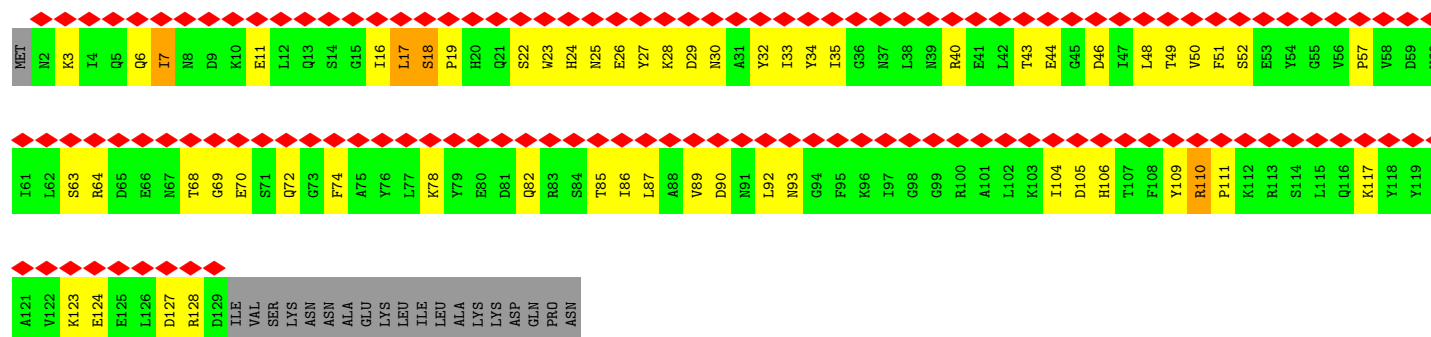
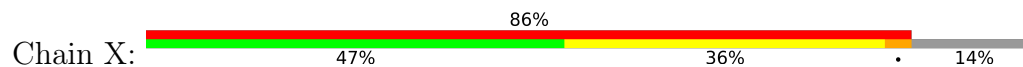
• Molecule 36: Pre-mRNA-splicing factor RDS3



• Molecule 37: RDS3 complex subunit 10

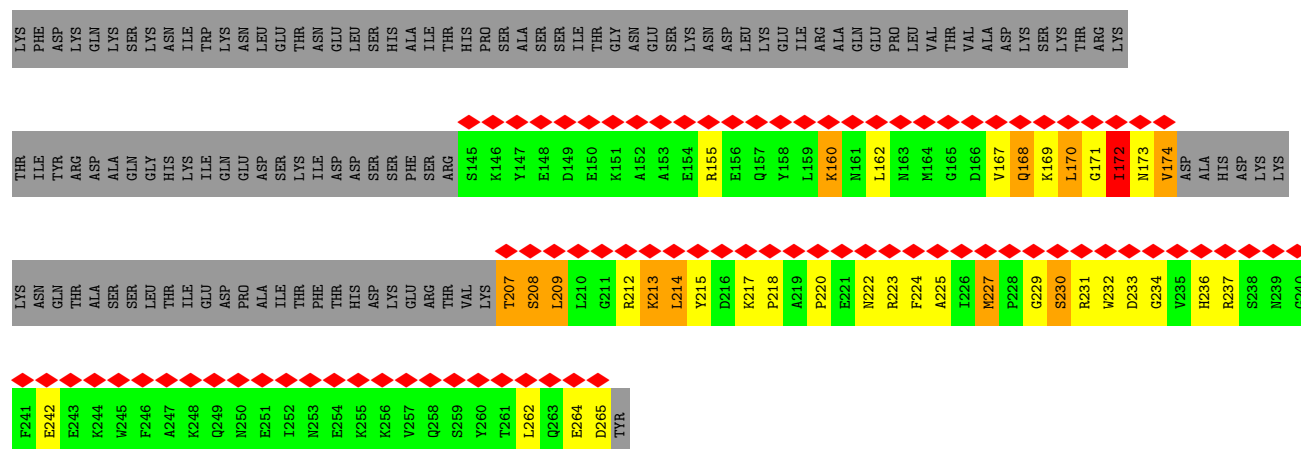


• Molecule 38: U2 snRNP component IST3

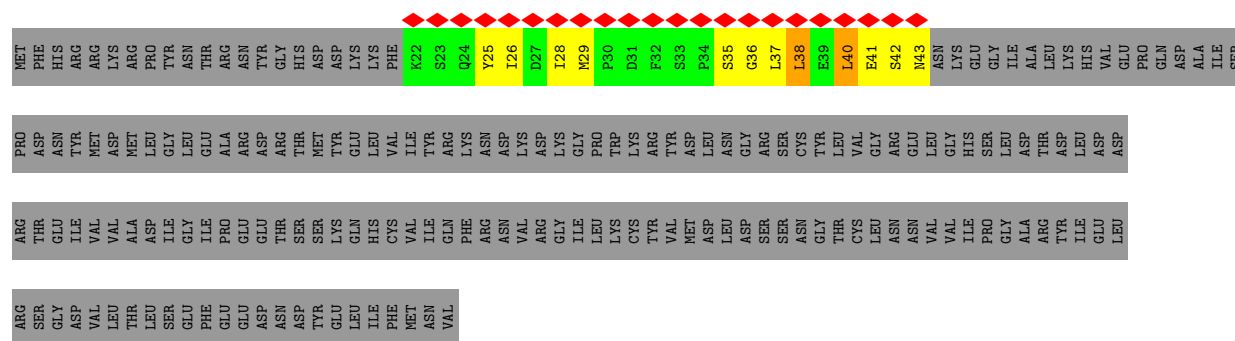


• Molecule 39: Pre-mRNA-splicing factor CWC26

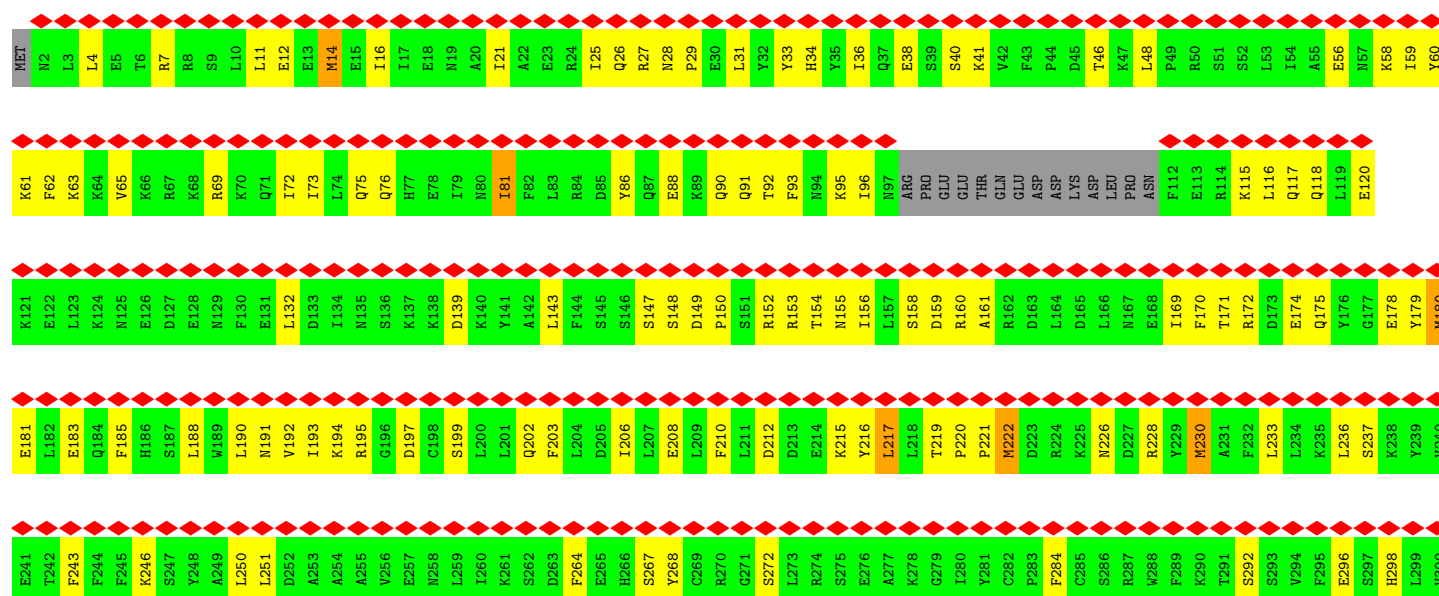
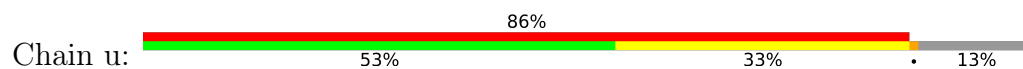


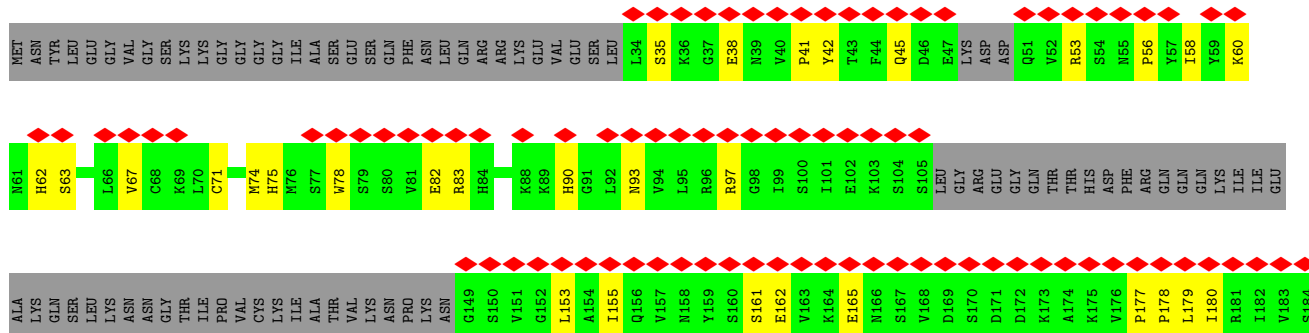


• Molecule 40: Pre-mRNA leakage protein 1



• Molecule 41: Pre-mRNA-splicing factor PRP9







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	500657	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.386	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.023	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	1/18332 (0.0%)	0.54	7/24851 (0.0%)
2	K	0.30	0/3431	0.65	4/4631 (0.1%)
3	L	0.24	0/3219	0.53	0/4332
4	N	0.21	0/4937	0.54	2/6704 (0.0%)
5	J	0.22	0/2485	0.52	2/3333 (0.1%)
6	E	0.25	0/1167	0.52	0/1571
7	M	0.27	0/963	0.55	0/1310
8	C	0.24	0/6874	0.55	0/9305
9	z	0.78	0/259	1.35	4/322 (1.2%)
10	q	0.83	0/367	1.31	2/457 (0.4%)
11	r	0.99	0/307	1.47	2/382 (0.5%)
12	x	0.83	0/295	1.41	2/367 (0.5%)
13	t	0.81	0/306	1.26	0/379
14	y	0.83	0/262	1.22	2/324 (0.6%)
15	s	0.79	0/306	1.39	2/379 (0.5%)
16	F	0.20	0/2277	0.39	0/3534
17	I	0.32	3/2604 (0.1%)	0.43	0/4046
18	B	0.25	1/4151 (0.0%)	0.47	1/6462 (0.0%)
19	O	0.19	0/573	0.53	0/763
20	S	0.33	0/641	0.56	0/868
20	d	0.47	0/315	0.92	0/392
20	l	0.59	1/620 (0.2%)	0.95	1/841 (0.1%)
21	P	0.33	0/567	0.56	0/762
21	a	0.51	0/290	0.87	0/359
21	h	0.55	0/615	0.77	0/829
22	Q	0.35	0/756	0.72	1/1023 (0.1%)
22	b	0.51	0/305	0.89	0/376
22	m	0.59	0/649	0.81	0/880
23	R	0.29	0/764	0.55	0/1026
23	c	0.49	0/358	0.94	2/444 (0.5%)
23	n	0.60	0/535	0.80	0/717
24	T	0.46	1/612 (0.2%)	0.65	1/830 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
24	e	0.53	0/285	0.85	0/351
24	i	0.64	0/585	0.86	0/795
25	U	0.28	0/597	0.62	0/807
25	f	0.53	0/278	0.80	0/344
25	j	0.61	0/564	0.88	0/761
26	V	0.43	2/582 (0.3%)	0.80	2/785 (0.3%)
26	g	0.44	0/277	0.83	0/341
26	k	0.52	0/532	0.82	0/715
27	D	0.32	0/13899	0.67	10/18845 (0.1%)
28	G	0.14	0/1038	0.36	0/1611
29	H	0.99	57/4835 (1.2%)	1.63	141/7502 (1.9%)
30	o	1.24	6/839 (0.7%)	2.35	44/1127 (3.9%)
31	p	0.98	1/467 (0.2%)	1.88	7/623 (1.1%)
32	1	0.19	0/6600	0.49	2/8962 (0.0%)
33	2	0.16	0/1775	0.41	0/2402
34	3	0.22	0/9564	0.56	0/12963
35	4	0.13	0/1453	0.35	0/1954
36	5	0.21	0/827	0.47	0/1105
37	6	0.20	0/702	0.45	0/939
38	X	0.64	0/1071	0.81	0/1445
39	Y	0.67	0/743	1.01	2/994 (0.2%)
40	Z	0.60	0/176	0.72	0/237
41	u	0.41	10/3972 (0.3%)	0.65	2/5322 (0.0%)
42	w	0.58	8/1105 (0.7%)	0.64	0/1475
43	v	0.33	2/1396 (0.1%)	0.63	1/1881 (0.1%)
All	All	0.40	93/114304 (0.1%)	0.73	246/157085 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	K	0	2
3	L	0	1
4	N	0	2
8	C	0	2
27	D	0	4
32	1	0	4
34	3	0	1
41	u	0	2
All	All	0	19

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	1161	U	O3'-P	-12.47	1.42	1.61
29	H	1092	A	O3'-P	-11.86	1.43	1.61
29	H	1163	C	O5'-C5'	11.04	1.59	1.42
30	o	69	ASP	CA-CB	-10.73	1.38	1.53
29	H	1116	A	O3'-P	-9.22	1.47	1.61

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	1151	U	C4'-C3'-O3'	-19.99	83.02	113.00
29	H	1092	A	C2'-C3'-O3'	17.86	140.49	113.70
29	H	1097	G	C3'-C2'-O2'	16.45	135.38	110.70
30	o	44	PRO	N-CA-CB	15.88	113.87	103.23
29	H	1093	C	P-O5'-C5'	15.75	144.53	120.90

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	PHE	Peptide
2	K	208	GLN	Peptide
2	K	383	GLU	Peptide
3	L	397	GLU	Peptide
4	N	11	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17877	0	17800	653	0
2	K	3375	0	3343	181	0
3	L	3171	0	3140	130	0
4	N	4897	0	3994	121	0
5	J	2439	0	2341	65	0
6	E	1146	0	1133	34	0
7	M	950	0	1004	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	6732	0	6904	298	0
9	z	260	0	72	1	0
10	q	368	0	99	2	0
11	r	308	0	80	0	0
12	x	296	0	83	0	0
13	t	308	0	85	3	0
14	y	264	0	76	0	0
15	s	308	0	85	0	0
16	F	2043	0	1033	49	0
17	I	2334	0	1173	108	0
18	B	3715	0	1878	153	0
19	O	574	0	552	32	0
20	S	632	0	653	26	0
20	d	316	0	86	14	0
20	l	611	0	627	34	0
21	P	563	0	600	40	0
21	a	292	0	78	5	0
21	h	610	0	640	8	0
22	Q	751	0	776	64	0
22	b	308	0	78	0	0
22	m	644	0	686	22	0
23	R	752	0	786	52	0
23	c	360	0	89	0	0
23	n	528	0	573	45	0
24	T	602	0	631	38	0
24	e	288	0	74	0	0
24	i	575	0	597	21	0
25	U	585	0	587	41	0
25	f	280	0	77	1	0
25	j	554	0	556	18	0
26	V	577	0	595	37	0
26	g	280	0	79	0	0
26	k	529	0	557	7	0
27	D	13601	0	13596	650	0
28	G	928	0	468	51	0
29	H	4345	0	2199	277	0
30	o	841	0	614	5	0
31	p	466	0	373	2	0
32	1	6472	0	6702	260	0
33	2	1726	0	1734	67	0
34	3	9380	0	9482	412	0
35	4	1429	0	1458	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	814	0	811	30	0
37	6	693	0	705	25	0
38	X	1051	0	1015	105	0
39	Y	730	0	710	55	0
40	Z	173	0	165	8	0
41	u	3895	0	3824	191	0
42	w	1084	0	1081	53	0
43	v	1372	0	1345	58	0
44	C	32	0	12	6	0
45	C	1	0	0	0	0
46	5	3	0	0	2	0
46	u	2	0	0	0	0
46	v	1	0	0	0	0
All	All	111041	0	100594	4006	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 19.

The worst 5 of 4006 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)
1:A:2310:GLU:CB	1:A:2333:PHE:CZ	1.85	1.52
1:A:2398:LEU:HD13	27:D:1060:LYS:CD	1.36	1.51
1:A:2310:GLU:CB	1:A:2333:PHE:HZ	1.19	1.44
1:A:2398:LEU:HD13	27:D:1060:LYS:CE	1.48	1.42
1:A:2310:GLU:HB2	1:A:2333:PHE:CZ	0.89	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2169/2413 (90%)	2040 (94%)	115 (5%)	14 (1%)	21	50
2	K	425/465 (91%)	388 (91%)	34 (8%)	3 (1%)	18	47
3	L	410/494 (83%)	392 (96%)	15 (4%)	3 (1%)	18	47
4	N	678/899 (75%)	626 (92%)	51 (8%)	1 (0%)	48	78
5	J	294/469 (63%)	281 (96%)	10 (3%)	3 (1%)	12	40
6	E	137/143 (96%)	128 (93%)	9 (7%)	0	100	100
7	M	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
8	C	837/1008 (83%)	779 (93%)	53 (6%)	5 (1%)	21	50
9	z	63/109 (58%)	61 (97%)	2 (3%)	0	100	100
10	q	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
11	r	75/89 (84%)	70 (93%)	5 (7%)	0	100	100
12	x	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
13	t	73/93 (78%)	69 (94%)	3 (4%)	1 (1%)	9	31
14	y	62/115 (54%)	62 (100%)	0	0	100	100
15	s	73/187 (39%)	72 (99%)	1 (1%)	0	100	100
19	O	68/587 (12%)	64 (94%)	3 (4%)	1 (2%)	8	30
20	S	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
20	d	77/101 (76%)	69 (90%)	6 (8%)	2 (3%)	4	21
20	l	79/101 (78%)	70 (89%)	8 (10%)	1 (1%)	9	33
21	P	66/196 (34%)	62 (94%)	4 (6%)	0	100	100
21	a	69/196 (35%)	63 (91%)	6 (9%)	0	100	100
21	h	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
22	Q	93/146 (64%)	89 (96%)	3 (3%)	1 (1%)	11	38
22	b	71/146 (49%)	66 (93%)	4 (6%)	1 (1%)	9	31
22	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
23	R	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
23	c	86/110 (78%)	83 (96%)	3 (4%)	0	100	100
23	n	63/110 (57%)	60 (95%)	3 (5%)	0	100	100
24	T	73/94 (78%)	72 (99%)	1 (1%)	0	100	100
24	e	66/94 (70%)	62 (94%)	4 (6%)	0	100	100
24	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
25	U	71/86 (83%)	68 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	f	66/86 (77%)	59 (89%)	4 (6%)	3 (4%)	2	12
25	j	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	8	30
26	V	73/77 (95%)	66 (90%)	6 (8%)	1 (1%)	9	31
26	g	64/77 (83%)	58 (91%)	6 (9%)	0	100	100
26	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	D	1694/2163 (78%)	1631 (96%)	60 (4%)	3 (0%)	43	71
30	o	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	7	29
31	p	69/111 (62%)	67 (97%)	2 (3%)	0	100	100
32	1	814/971 (84%)	762 (94%)	46 (6%)	6 (1%)	18	47
33	2	205/436 (47%)	192 (94%)	11 (5%)	2 (1%)	12	40
34	3	1164/1361 (86%)	1046 (90%)	109 (9%)	9 (1%)	16	44
35	4	165/213 (78%)	164 (99%)	1 (1%)	0	100	100
36	5	101/107 (94%)	87 (86%)	13 (13%)	1 (1%)	12	40
37	6	82/85 (96%)	78 (95%)	3 (4%)	1 (1%)	10	35
38	X	126/148 (85%)	117 (93%)	7 (6%)	2 (2%)	7	29
39	Y	85/266 (32%)	80 (94%)	3 (4%)	2 (2%)	4	22
40	Z	20/204 (10%)	14 (70%)	6 (30%)	0	100	100
41	u	453/530 (86%)	415 (92%)	38 (8%)	0	100	100
42	w	123/280 (44%)	112 (91%)	11 (9%)	0	100	100
43	v	168/266 (63%)	142 (84%)	25 (15%)	1 (1%)	21	50
All	All	12585/17187 (73%)	11769 (94%)	746 (6%)	70 (1%)	23	50

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	PRO
2	K	395	ILE
3	L	328	VAL
8	C	364	PHE
8	C	602	VAL

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1964/2182 (90%)	1959 (100%)	5 (0%)	86	84
2	K	373/410 (91%)	371 (100%)	2 (0%)	81	81
3	L	327/445 (74%)	327 (100%)	0	100	100
4	N	361/813 (44%)	361 (100%)	0	100	100
5	J	248/436 (57%)	248 (100%)	0	100	100
6	E	129/132 (98%)	129 (100%)	0	100	100
7	M	104/104 (100%)	104 (100%)	0	100	100
8	C	757/910 (83%)	756 (100%)	1 (0%)	88	89
19	O	60/534 (11%)	59 (98%)	1 (2%)	53	67
20	S	71/89 (80%)	71 (100%)	0	100	100
20	l	67/89 (75%)	65 (97%)	2 (3%)	36	59
21	P	64/176 (36%)	64 (100%)	0	100	100
21	h	67/176 (38%)	66 (98%)	1 (2%)	57	69
22	Q	81/129 (63%)	80 (99%)	1 (1%)	63	72
22	m	77/129 (60%)	74 (96%)	3 (4%)	28	53
23	R	85/103 (82%)	85 (100%)	0	100	100
23	n	59/103 (57%)	51 (86%)	8 (14%)	3	15
24	T	69/83 (83%)	69 (100%)	0	100	100
24	i	65/83 (78%)	60 (92%)	5 (8%)	12	37
25	U	65/77 (84%)	65 (100%)	0	100	100
25	j	61/77 (79%)	60 (98%)	1 (2%)	55	68
26	V	64/66 (97%)	64 (100%)	0	100	100
26	k	58/66 (88%)	55 (95%)	3 (5%)	21	48
27	D	1524/1955 (78%)	1520 (100%)	4 (0%)	86	84
30	o	46/219 (21%)	43 (94%)	3 (6%)	15	42
31	p	23/100 (23%)	23 (100%)	0	100	100
32	1	724/867 (84%)	723 (100%)	1 (0%)	88	89
33	2	190/392 (48%)	190 (100%)	0	100	100
34	3	1088/1244 (88%)	1086 (100%)	2 (0%)	87	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	4	154/189 (82%)	154 (100%)	0	100	100
36	5	93/97 (96%)	93 (100%)	0	100	100
37	6	76/77 (99%)	76 (100%)	0	100	100
38	X	114/132 (86%)	111 (97%)	3 (3%)	40	61
39	Y	77/240 (32%)	65 (84%)	12 (16%)	2	10
40	Z	21/186 (11%)	18 (86%)	3 (14%)	3	13
41	u	425/492 (86%)	417 (98%)	8 (2%)	50	66
42	w	118/259 (46%)	115 (98%)	3 (2%)	42	62
43	v	156/236 (66%)	154 (99%)	2 (1%)	61	71
All	All	10105/14097 (72%)	10031 (99%)	74 (1%)	73	78

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	Y	262	LEU
42	w	158	ARG
40	Z	40	LEU
41	u	298	HIS
20	l	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 203 such sidechains are listed below:

Mol	Chain	Res	Type
21	h	91	GLN
33	2	145	GLN
41	u	202	GLN
25	j	52	GLN
32	1	376	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	F	95/112 (84%)	38 (40%)	1 (1%)
17	I	106/160 (66%)	31 (29%)	6 (5%)
18	B	173/214 (80%)	64 (36%)	13 (7%)
28	G	43/44 (97%)	22 (51%)	2 (4%)
29	H	196/1175 (16%)	53 (27%)	23 (11%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	613/1705 (35%)	208 (33%)	45 (7%)

5 of 208 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	F	2	U
16	F	12	U
16	F	13	U
16	F	14	U
16	F	17	U

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	H	1100	A
29	H	1122	U
29	H	1101	C
29	H	1119	C
29	H	1124	U

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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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
44	GTP	C	1500	45	33,34,34	1.09	3 (9%)	50,54,54	1.71	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	GTP	C	1500	45	-	4/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	1500	GTP	C5-C4	3.15	1.47	1.38
44	C	1500	GTP	C6-N1	-2.45	1.34	1.38
44	C	1500	GTP	C5-N7	-2.14	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C	1500	GTP	C5-C4-N3	-6.09	118.70	128.39
44	C	1500	GTP	C2-N3-C4	4.84	120.63	112.30
44	C	1500	GTP	N9-C4-N3	4.33	134.60	125.95
44	C	1500	GTP	C6-C5-N7	3.27	136.24	130.29
44	C	1500	GTP	C4-C5-N7	-2.83	106.19	110.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

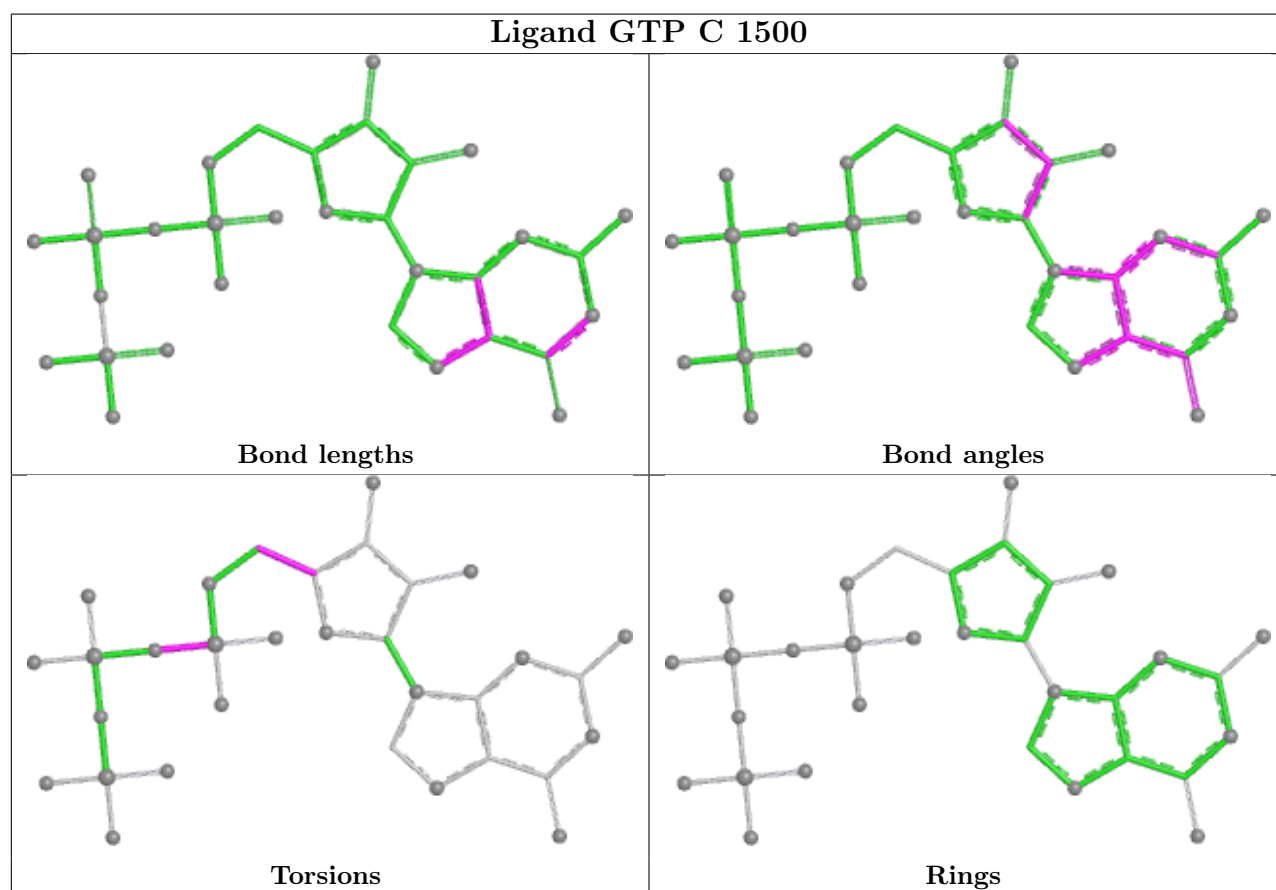
Mol	Chain	Res	Type	Atoms
44	C	1500	GTP	O4'-C4'-C5'-O5'
44	C	1500	GTP	C3'-C4'-C5'-O5'
44	C	1500	GTP	PB-O3A-PA-O2A
44	C	1500	GTP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	C	1500	GTP	6	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.

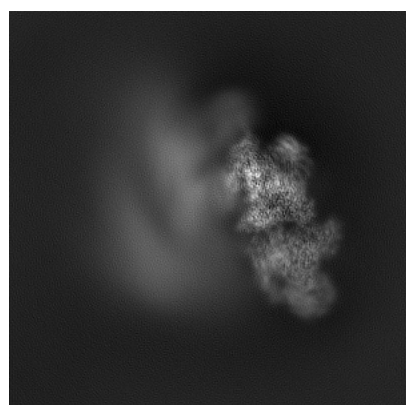
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6972. These allow visual inspection of the internal detail of the map and identification of artifacts.

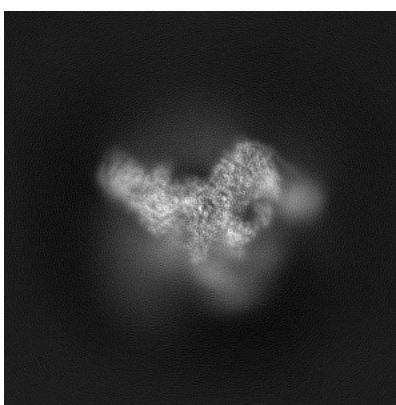
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

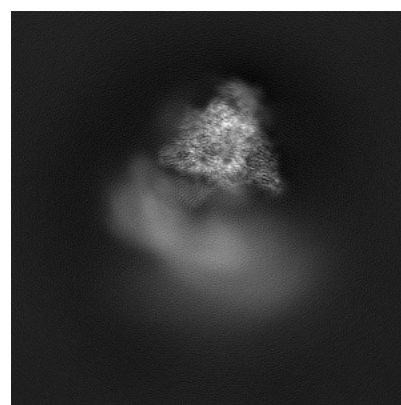
6.1.1 Primary map



X



Y

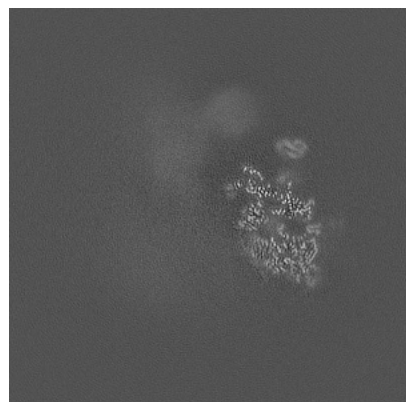


Z

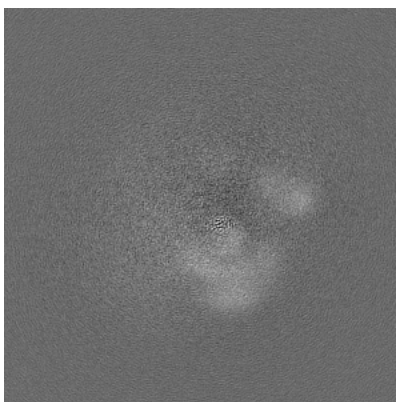
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

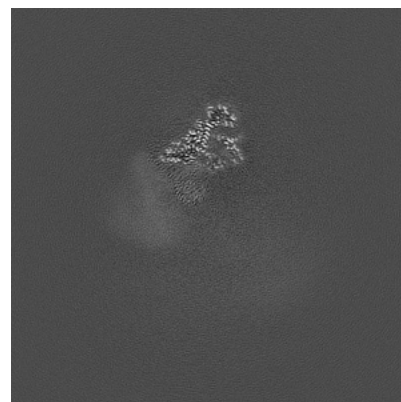
6.2.1 Primary map



X Index: 200



Y Index: 200

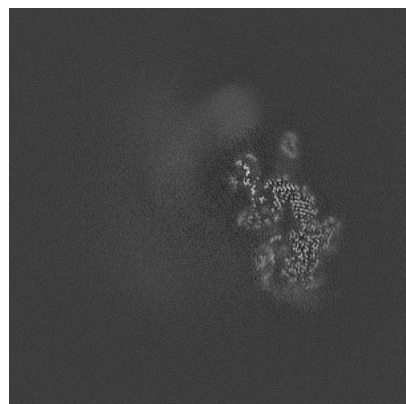


Z Index: 200

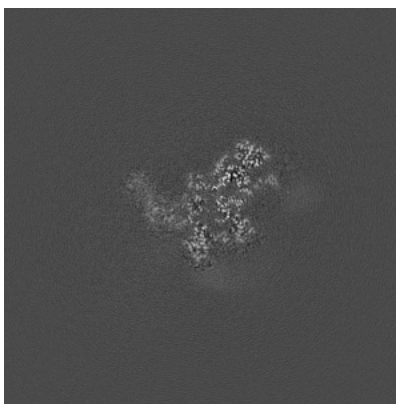
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

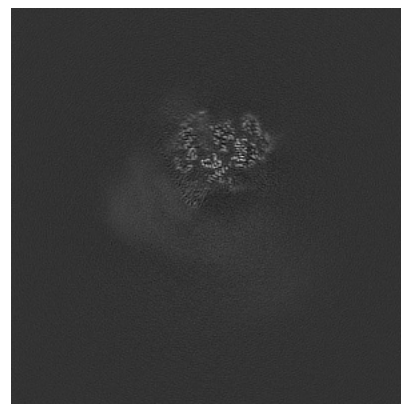
6.3.1 Primary map



X Index: 212



Y Index: 247

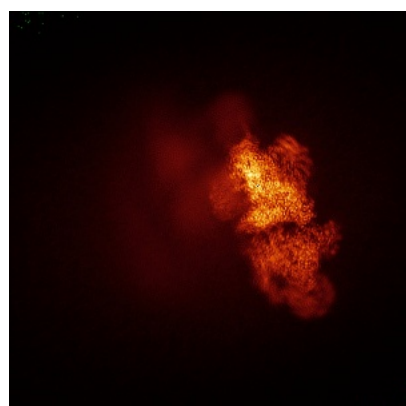


Z Index: 224

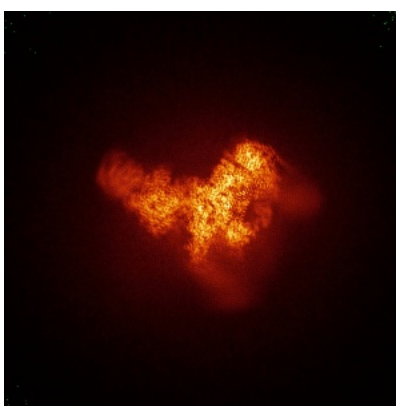
The images above show the largest variance slices of the map in three orthogonal directions.

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

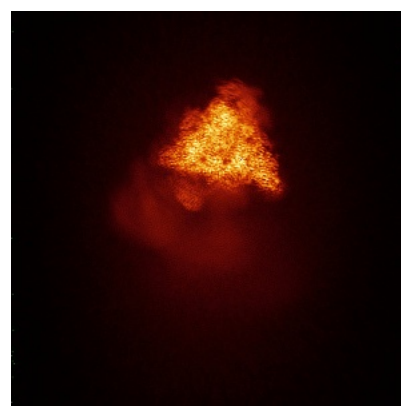
6.4.1 Primary map



X



Y



Z

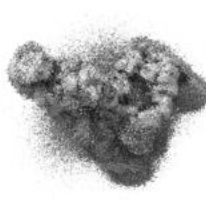
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

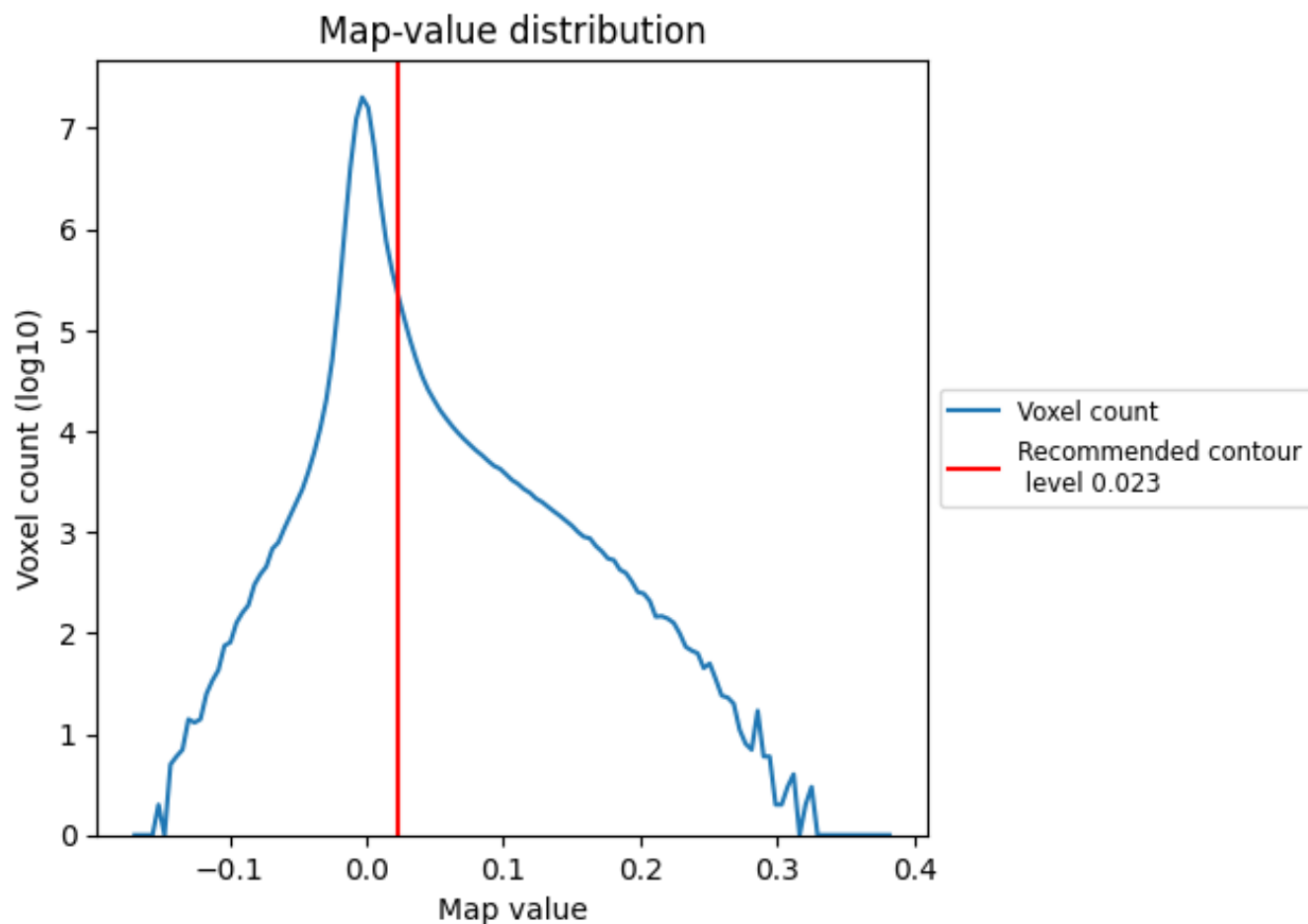
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

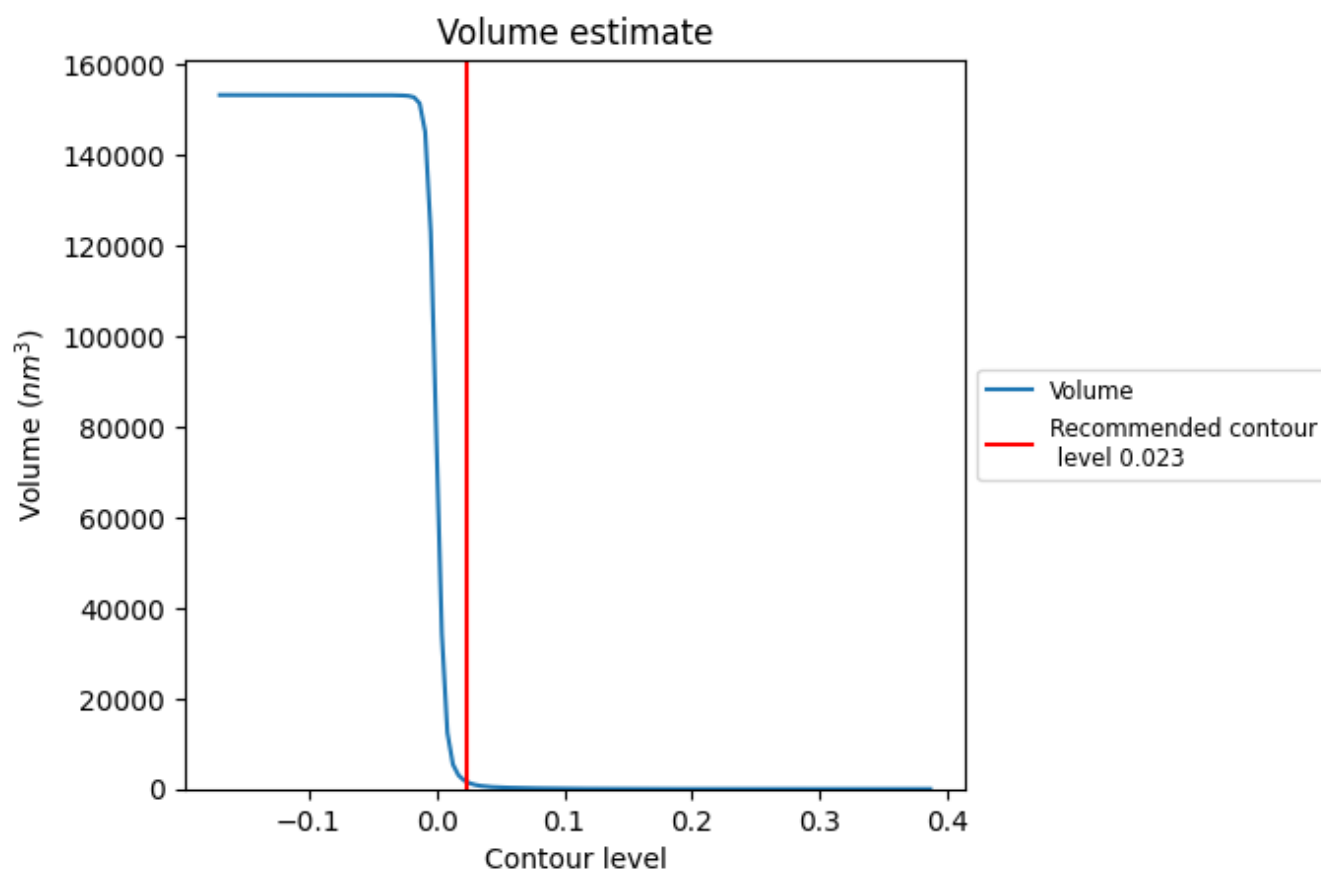
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

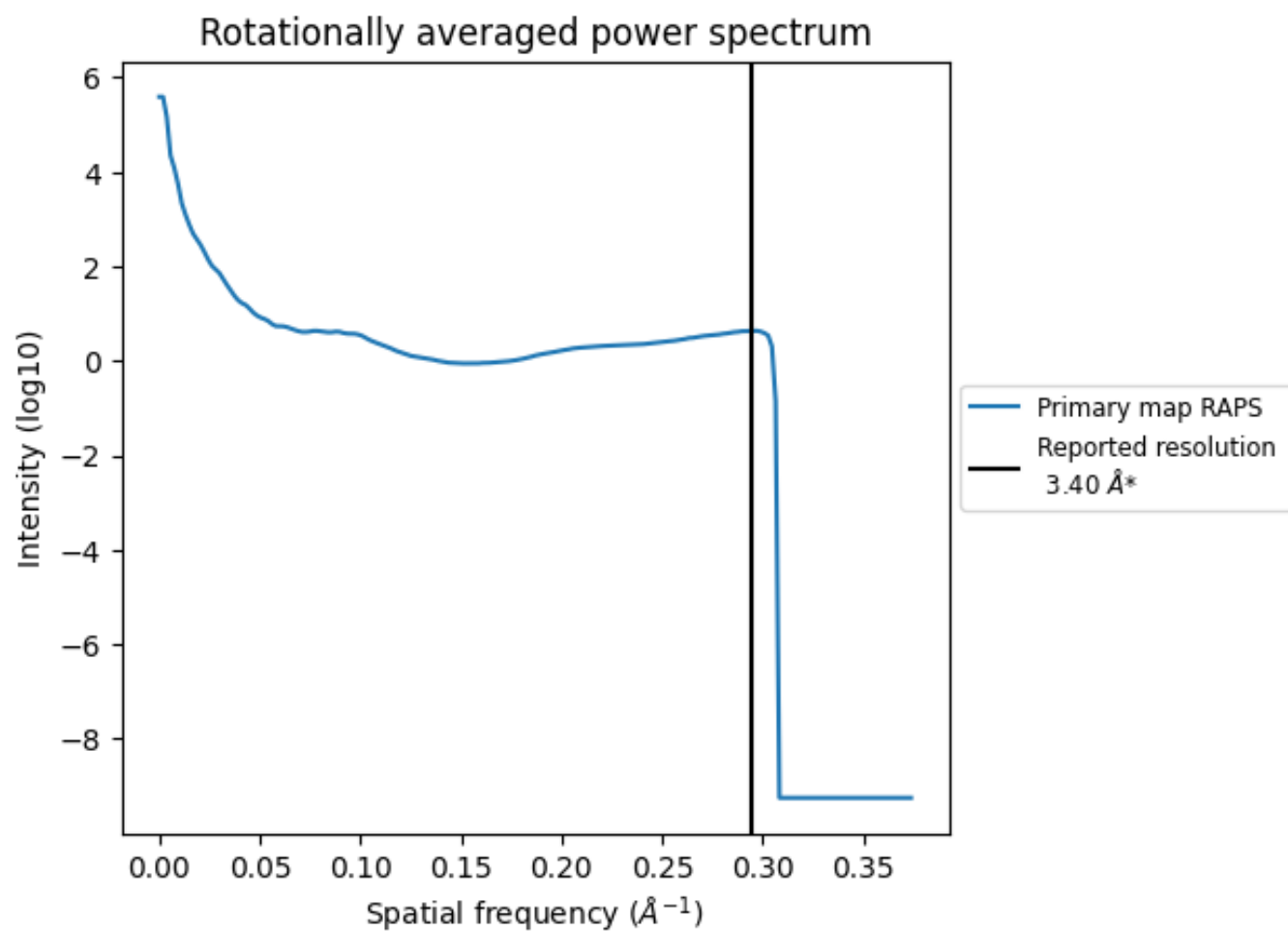
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1701 nm³; this corresponds to an approximate mass of 1536 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 0.294 Å⁻¹

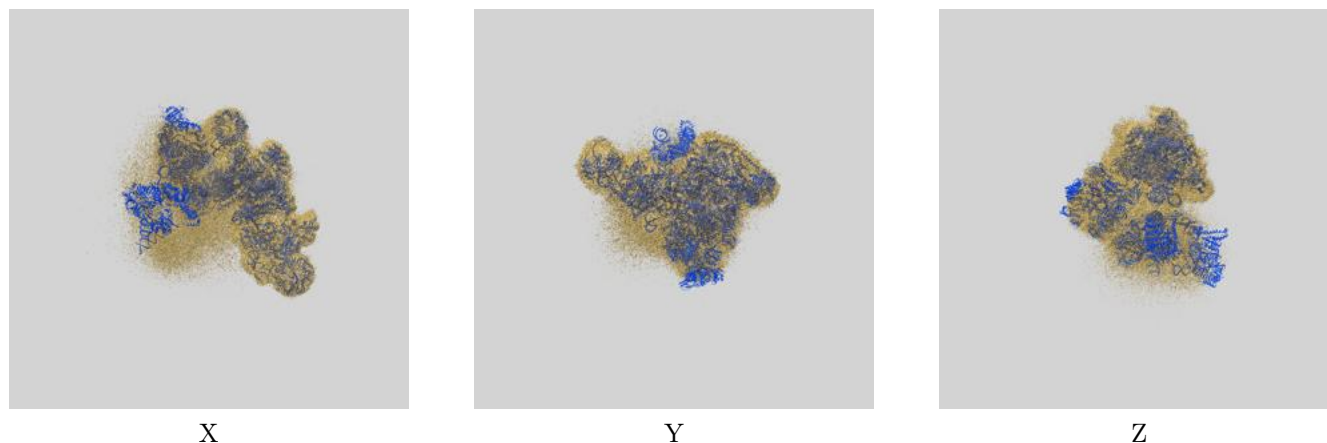
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

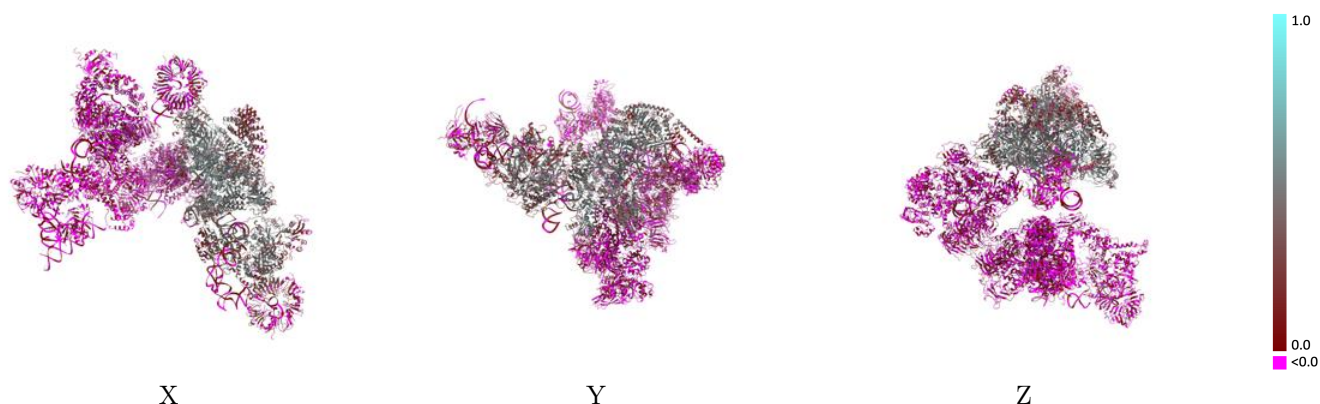
This section contains information regarding the fit between EMDB map EMD-6972 and PDB model 5ZWM. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



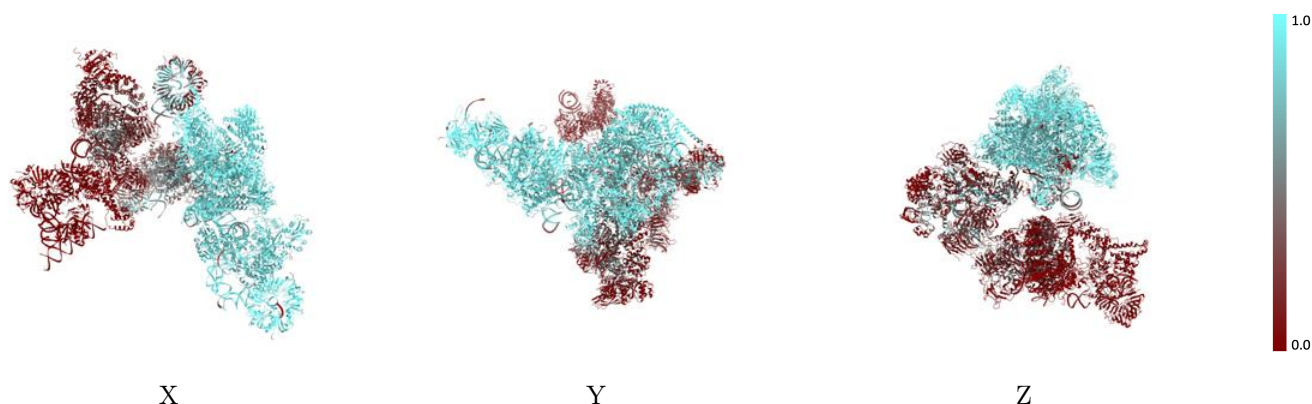
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



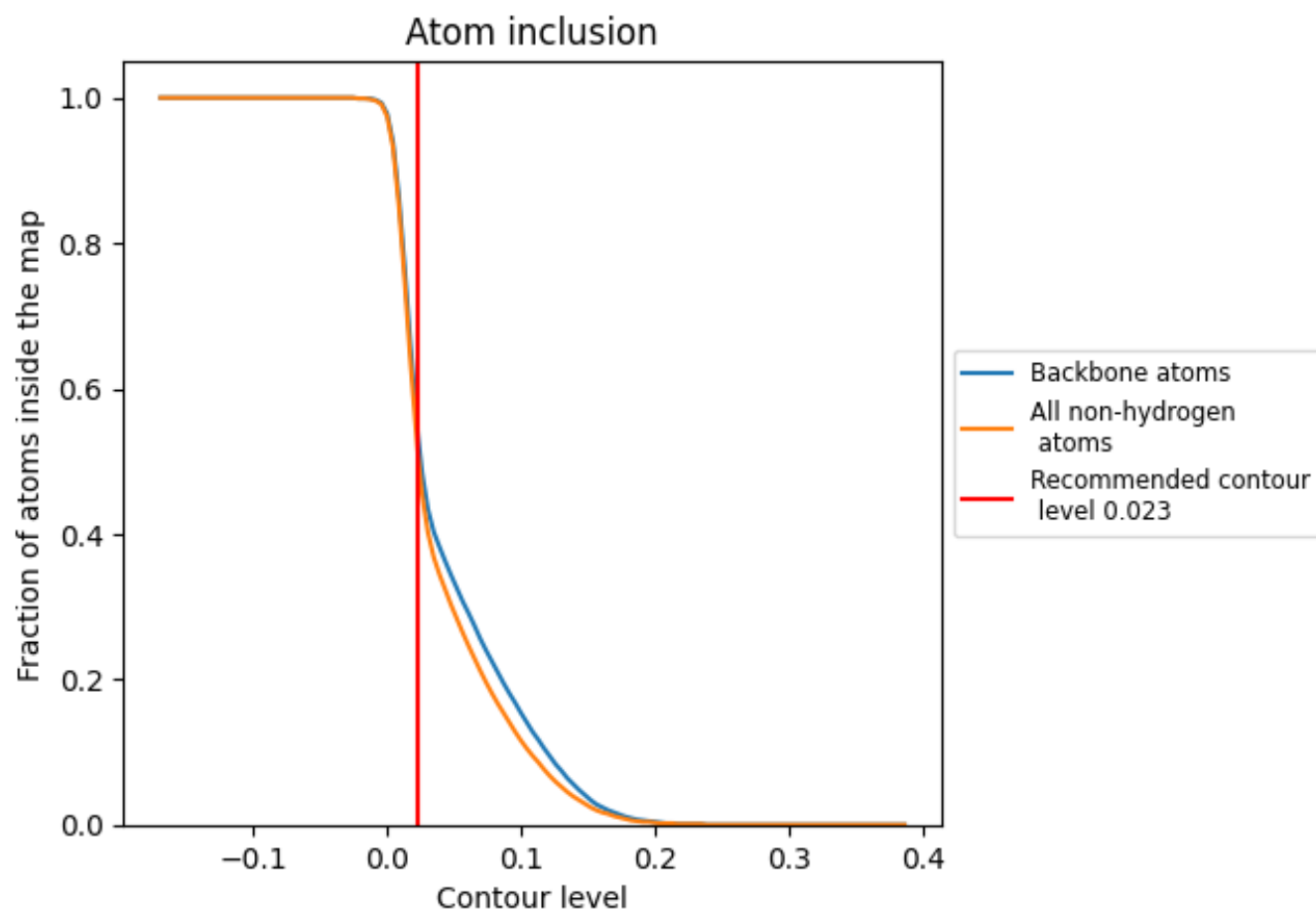
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.1620
1	 0.1700	 0.0010
2	 0.1600	 0.0170
3	 0.1710	 0.0070
4	 0.0560	 -0.0180
5	 0.2770	 0.0070
6	 0.3170	 -0.0020
A	 0.8430	 0.3780
B	 0.8820	 0.1520
C	 0.9060	 0.3540
D	 0.2770	 -0.0020
E	 0.9180	 0.4420
F	 0.8230	 0.2670
G	 0.2000	 -0.0050
H	 0.0740	 0.0020
I	 0.8240	 0.3140
J	 0.9240	 0.4150
K	 0.9220	 0.4350
L	 0.9290	 0.4290
M	 0.9550	 0.5200
N	 0.9200	 0.3230
O	 0.7580	 0.2720
P	 0.5390	 -0.0080
Q	 0.3850	 -0.0020
R	 0.4290	 -0.0110
S	 0.5940	 0.0110
T	 0.1550	 -0.0060
U	 0.2720	 -0.0290
V	 0.2620	 0.0160
X	 0.0050	 0.0070
Y	 0.0010	 -0.0100
Z	 0.0060	 -0.0350
a	 0.9490	 0.2050
b	 0.9380	 0.1490
c	 0.9310	 0.0690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.9810	 0.2910
e	 0.9510	 0.0850
f	 0.9210	 0.1000
g	 0.8570	 0.0540
h	 0.0070	 0.0250
i	 0.0020	 0.0280
j	 0.0040	 -0.0190
k	 0.0040	 -0.0070
l	 0.0150	 0.0050
m	 0.0080	 0.0080
n	 0.0020	 0.0010
o	 0.0080	 0.0140
p	 0.0060	 0.0150
q	 0.4430	 0.0150
r	 0.5030	 0.0150
s	 0.4160	 0.0280
t	 0.6400	 0.0210
u	 0.0320	 -0.0030
v	 0.0980	 -0.0010
w	 0.0060	 -0.0230
x	 0.5510	 0.0480
y	 0.6170	 0.0200
z	 0.2920	 -0.0110