



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 10:51 AM JST

PDB ID : 5GM6
EMDB ID : EMD-9524
Title : Cryo-EM structure of the activated spliceosome (Bact complex) at 3.5 angstrom resolution
Authors : Yan, C.; Wan, R.; Bai, R.; Huang, G.; Shi, Y.
Deposited on : 2016-07-12
Resolution : 3.50 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:

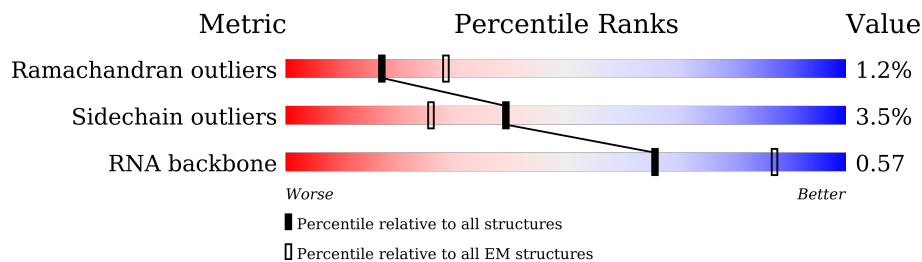
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.50 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2287	
2	B	2163	
3	C	1008	
4	D	214	
5	E	112	
6	F	1361	
7	H	436	
8	I	266	

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Mol	Chain	Length	Quality of chain
9	J	107	
10	K	85	
11	L	1175	
12	N	25	
13	M	61	
14	O	451	
15	P	379	
16	Q	364	
17	R	339	
18	S	175	
19	T	157	
20	U	207	
21	V	148	
22	W	266	
23	Y	876	
24	Z	577	
25	a	259	
26	b	301	
27	c	587	
28	G	971	
29	d	687	
30	X	135	
31	v	859	
32	e	213	
33	f	215	

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Mol	Chain	Length	Quality of chain
34	o	503	
34	p	503	
34	q	503	
34	r	503	
35	t	175	
36	n	455	
37	k	196	
38	i	94	
39	h	86	
40	j	77	
41	l	101	
42	m	146	
43	g	94	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 112064 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
			Total	C	N	O	S		
1	A	2200	18101	11636	3086	3315	64	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	-	expression tag	UNP P33334

- Molecule 2 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1809	14504	9283	2414	2750	57	0	0

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	878	7014	4526	1166	1293	29	0	0

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain CDRDR_sf_H chromosome VII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	117	2465	1104	414	830	117	0	0

- Molecule 5 is a RNA chain called Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	103	2192	982	391	716	103	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor RSE1.

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

- Molecule 7 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	151	1248	804	217	221	6	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	102	800	495	150	150	5	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor RDS3.

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

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

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

- Molecule 11 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	L	66	1388	622	228	472	66	0	0

- Molecule 12 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	N	25	521	234	77	185	25	0	0

- Molecule 13 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	M	50	1057	479	191	338	49	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	337	2646	1669	466	501	10	0	0

- Molecule 15 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	246	1978	1233	359	380	6	0	0

- Molecule 16 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	185	1472	930	256	271	15	0	0

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	261	2089	1320	369	388	12	0	0

- Molecule 18 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	71	578	361	117	99	1	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	157	1291	808	240	232	11	0	0

- Molecule 20 is a protein called Pre-mRNA leakage protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	176	1401	877	237	277	10	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	205	HIS	-	expression tag	UNP Q07930
U	206	HIS	-	expression tag	UNP Q07930
U	207	HIS	-	expression tag	UNP Q07930

- Molecule 21 is a protein called U2 snRNP component IST3.

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

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	104	842	528	145	167	2	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase-like protein PRP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Y	598	4047	2590	690	752	15	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	447	3651	2343	602	688	18	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	123	988	621	171	183	13	0	0

- Molecule 26 is a protein called Peptidyl-prolyl isomerase CWC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	150	Total	C	N	O	S	0	0
			1224	789	206	223	6		

- Molecule 27 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	415	Total	C	N	O	S	0	0
			2803	1741	518	537	7		

- Molecule 28 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	875	Total	C	N	O	S	0	0
			6970	4467	1196	1265	42		

- Molecule 29 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	545	Total	C	N	O	S	0	0
			3558	2212	671	667	8		

- Molecule 30 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	X	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 31 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	v	566	Total	C	N	O	S	0	0
			3047	1871	576	599	1		

- Molecule 32 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	149	Total	C	N	O	S	0	0
			947	617	154	174	2		

- Molecule 33 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	102	Total	C	N	O	S	0	0
			822	504	152	165	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	124	Total	C	N	O	S	0	0
			819	518	132	167	2		
34	p	128	Total	C	N	O	S	0	0
			843	533	136	172	2		
34	q	381	Total	C	N	O	S	0	0
			2315	1456	396	455	8		
34	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	155	Total	C	N	O	S	0	0
			921	582	159	179	1		

- Molecule 36 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	n	23	Total	C	N	O	0	0
			195	122	41	32		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	h	70	554	355	98	100	1	0	0

- Molecule 40 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	69	529	337	93	97	2	0	0

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	82	625	399	109	115	2	0	0

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	82	644	409	110	123	2	0	0

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	g	94	741	477	141	119	4	0	0

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

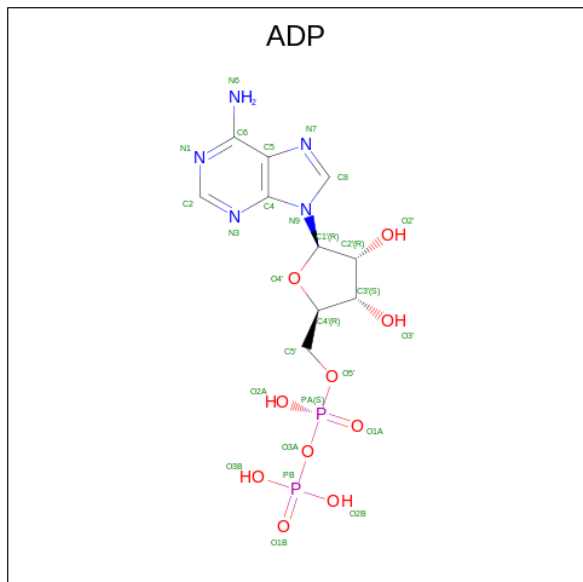
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	E	4	Total	Mg	0
			4	4	
45	Y	1	Total	Mg	0
			1	1	

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	I	1	Total	Zn	0
			1	1	
46	J	3	Total	Zn	0
			3	3	
46	Q	2	Total	Zn	0
			2	2	
46	R	1	Total	Zn	0
			1	1	
46	T	3	Total	Zn	0
			3	3	
46	a	3	Total	Zn	0
			3	3	

- Molecule 47 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	Y	1	27	10	5	10	2	0

3 Residue-property plots

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

• Molecule 1: Pre-mRNA-splicing factor 8

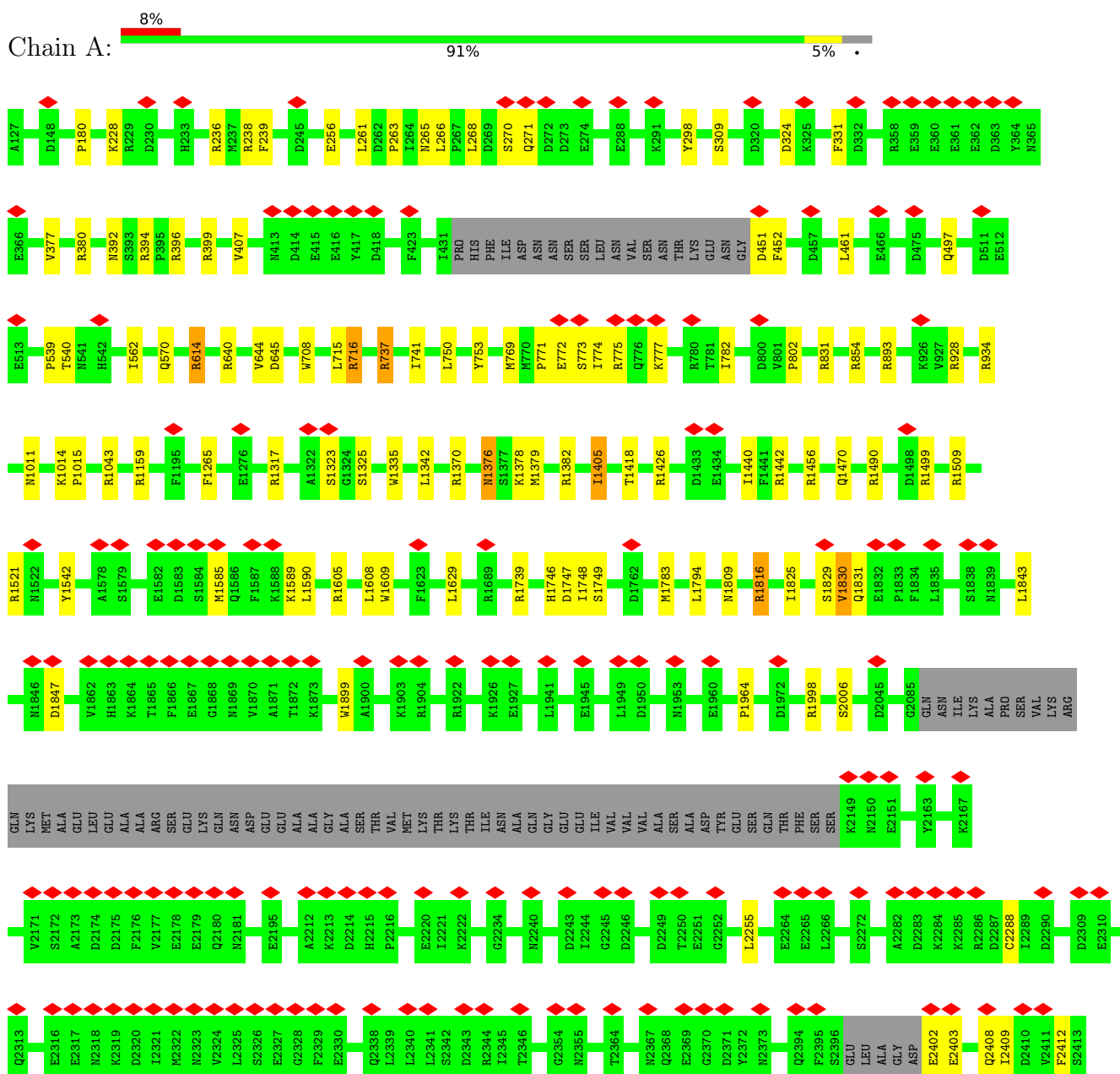
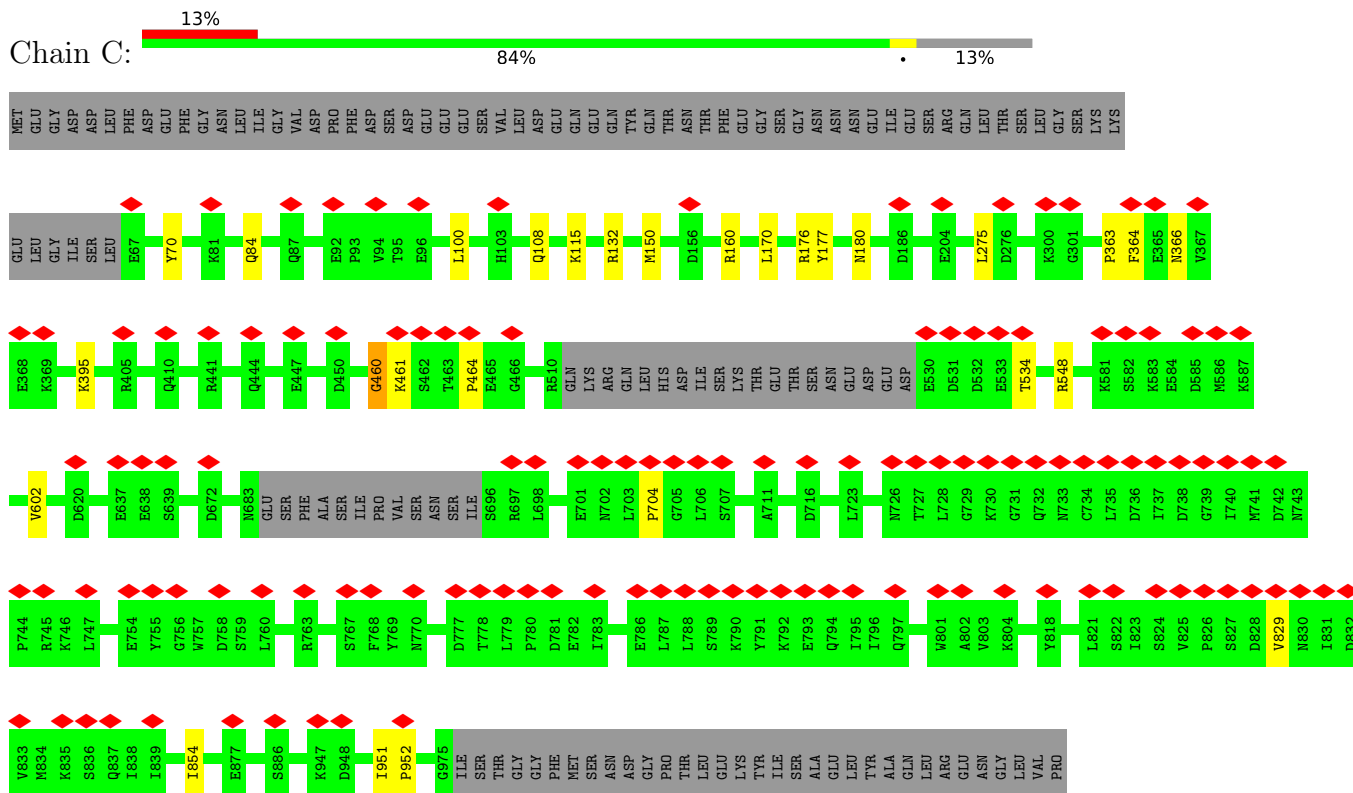


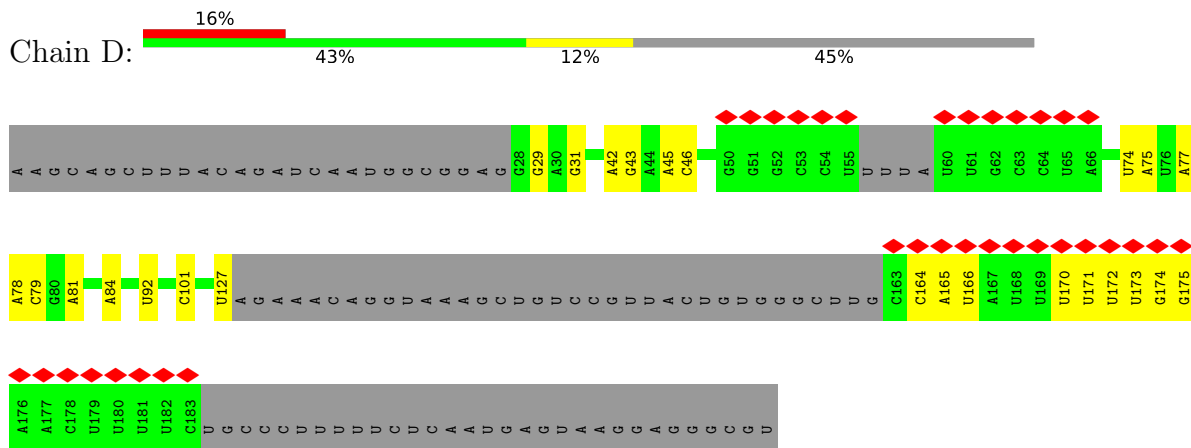
Table listing residue IDs and their corresponding validation status, organized into 12 columns. The table is visually represented as a grid of colored diamonds. The colors indicate the validation status: red for 'Good', yellow for 'Warning', and green for 'Bad'.

F1416	S1417	H1418	L1419	A1420	G1421	G1422	K1423	L1424	I1425	M1426	K1427	L1428	A1429	M1430	D1431	P1432	S1433	L1434	N1435	L1436	K1437	L1438	L1439	A1440	K1441	S1442	H1443	L1444	L1445	L1446	L1447	F1508	V1509	P1449	V1450	Q1451	F1452	E1453	L1454	L1455	S1456	A1518	L1457	R1458	L1459	R1460	Q1461	R1462	K1463	M1464	I1465	Q1466	S1467	L1468	E1469	L1470	M1471	I1472	Y1473	D1474	D1475																																																
A1476	H1477	E1478	I1479	S1480	Q1481	G1482	V1483	Y1484	G1485	A1486	V1487	Y1488	E1489	T1490	L1491	I1492	S1493	R1494	M1495	I1496	F1497	I1498	A1499	T1500	Q1501	L1502	E1503	K1504	K1505	I1506	R1507	L1508	A1447	V1509	C1510	L1511	S1512	N1513	C1514	L1515	A1516	N1517	A1518	R1519	D1520	F1521	G1522	E1523	W1524	A1525	G1526	M1527	I1528	K1529	S1530	N1531	I1532	A1533	N1534	S1535	A1536	H1537	A1538	L1610	M1611	V1612	E1613	E1614	E1615	Q1616	I1617	V1618	P1619	Y1620	I1621	K1623	L1624	T1625	Q1626	G1627	H1628	L1629	R1630	A1631	P1632	L1633	G1636	V1637	G1638	I1639	L1640	Y1641	K1642	G1643	M1644	F1645	S1646	M1647	D1648	E1649	K1650	I1651	V1652	K1653	R1654	L1655	Y1656	E1657	Y1658
S1536	P1537	S1538	E1539	R1540	I1541	E1542	P1543	L1544	E1545	I1546	M1547	I1548	Q1549	S1550	F1551	K1552	D1553	V1554	E1555	H1556	F1559	M1560	F1561	T1562	M1563	Q1565	M1566	A1567	F1568	E1569	A1570	S1571	A1572	A1573	A1574	A1575	G1576	N1577	R1578	M1579	S1580	S1581	S1582	F1583	L1585	P1586	S1587	K1588	D1590	E1593	V1594	A1595	S1596	A1597																																																							
F1598	M1599	K1600	F1601	S1602	K1603	A1604	I1605	E1606	V1607	D1608	M1609	L1610	M1611	V1612	E1613	E1614	E1615	Q1616	I1617	V1618	P1619	Y1620	I1621	K1623	L1624	T1625	Q1626	G1627	H1628	L1629	R1630	A1631	P1632	L1633	G1636	V1637	G1638	I1639	L1640	Y1641	K1642	G1643	M1644	F1645	S1646	M1647	D1648	E1649	K1650	I1651	V1652	K1653	R1654	L1655	Y1656	E1657	Y1658																																																				
G1659	A1660	V1661	S1662	V1663	L1664	L1665	I1666	S1667	K1668	D1669	C1670	S1671	A1672	F1673	E1674	C1675	K1676	T1677	E1679	V1680	I1681	I1682	L1683	L1687	Y1688	D1689	G1690	A1691	E1692	H1693	K1694	Y1698	T1699	I1700	N1701	E1702	L1703	L1704	M1705	M1706	V1707	G1708	A1710	S1711	G1712	N1713	D1714	S1715	M1716	A1717	G1718	K1719	V1720	L1721	I1722																																																						
L1723	T1724	M1727	M1730	K1734	F1735	L1736	I1737	E1738	P1739	L1740	Y1745	L1746	Q1747	Y1748	I1749	I1750	H1751	D1752	L1753	I1754	N1755	M1756	E1757	I1758	I1759	M1760	S1761	I1762	L1763	Q1764	S1765	K1766	Q1767	D1768	C1769	V1770	D1771	W1772	F1773	T1774	I1775	S1776	Y1777	M1780	R1781	Y1784	G1790	V1791	R1792	D1793	T1794	S1795																																																									
P1796	H1797	G1798	I1799	F1802	L1803	S1804	M1805	L1806	L1807	E1808	T1809	L1810	L1811	M1812	D1813	L1814	L1815	E1816	S1817	L1818	F1819	I1820	E1821	I1822	D1824	L1825	GLU	ALA	GLU	VAL	THR	ALA	GLU	VAL	ASN	GLY	ASP	ASP	GLU	ALA	T1841	E1842	I1843	I1844	S1845	T1846	L1847	S1848	N1849	G1850	L1851	I1852	A1853	S1854	Y1856																																																						
G1857	V1858	S1859	F1860	F1861	I1862	I1863	Q1864	S1865	F1866	V1867	S1868	S1869	L1870	S1871	N1872	T1873	S1874	T1875	L1876	K1877	N1878	M1879	L1880	Y1881	V1882	L1883	S1884	T1885	A1886	V1887	E1888	F1889	E1890	S1891	V1892	P1893	L1894	R1895	K1896	G1897	D1898	R1899	A1900	L1901	L1902	V1903	K1904	L1905	S1906	K1907	R1908	L1909	P1910	L1911	F1912	P1913	E1915	H1916																																																			
T1917	S1918	S1919	G1920	S1921	V1922	S1923	F1924	K1925	V1926	F1927	L1928	L1929	L1930	Q1931	A1932	Y1933	F1934	S1935	R1936	L1937	E1938	L1939	P1940	V1941	D1942	F1943	Q1944	N1945	D1946	L1947	K1948	L1949	I1950	L1951	E1952	K1953	V1954	V1955	P1956	L1957	I1958	N1959	V1960	V1961	V1962	D1963	Q1964	L1965	S1966	A1967	N1968	G1969	Y1970	L1971	N1972	A1973	T1974	T1975	A1976																																																		
M1977	D1978	L1979	A1980	Q1981	M1982	L1983	I1984	Q1985	G1986	V1987	D1988	D1989	V1990	D1991	N1992	P1993	L1994	R1995	Q1996	I1997	P1998	H1999	F2000	M2001	M2002	K2003	I2004	L2005	E2006	K2007	C2008	K2009	E2010	I2011	M2012	V2013	E2014	T2015	V2016	Y2017	D2018	I2019	M2020	A2021	L2022	E2023	D2024	E2025	E2026	R2027	D2028	E2029	I2030	L2031	T2032	L2033	F2034	D2035	S2036																																																		
Q2037	L2038	A2039	Q2040	V2041	A2042	A2043	F2044	V2045	M2046	M2047	Y2048	P2049	N2050	V2051	E2052	L2053	T2054	Y2055	S2056	L2057	N2058	M2059	S2060	D2061	S2062	L2063	L2064	S2065	E2066	V2067	K2068	Q2069	E2070	I2071	T2072	Q2073	E2074	Q2075	L2076	T2077	R2078	D2079	V2079	E2080	P2081	E2082	M2083	L2084	Q2085	V2086	D2087	S2088	E2089	L2090	Y2091	P2092	F2093	K2094	E2095	L2096																																																	
E2097	S2098	W2099	W2100	L2101	V2102	L2103	G2104	E2105	V2106	S2107	K2108	K2109	E2110	L2111	Y2112	A2113	I2114	K2115	K2116	T2117	L2118	L2119	N2120	K2121	E2122	T2123	Q2124	Q2125	Y2126	E2127	L2128	E2129	F2130	D2131	T2132	P2133	L2134	S2135	G2136	K2137	H2138	N2139	L2140	T2141	I2142	W2143	C2144	T2145	C2146	D2147	S2148	Y2149	L2150	D2151	A2152	D2153	K2154	E2155	L2156																																																		
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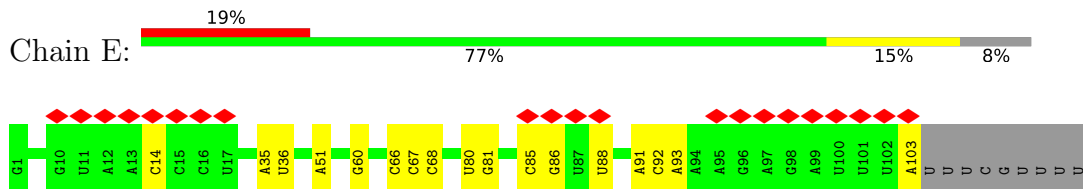
● Molecule 3: Pre-mRNA-splicing factor SNU114



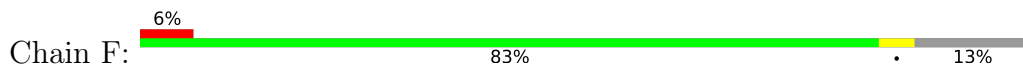
● Molecule 4: Saccharomyces cerevisiae strain CDRDR_sf_H chromosome VII sequence

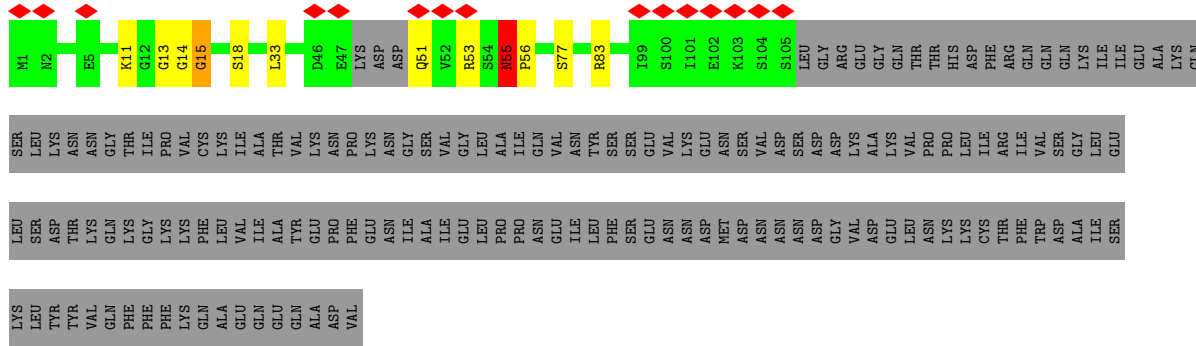


● Molecule 5: Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence

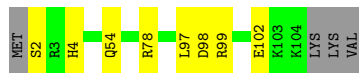
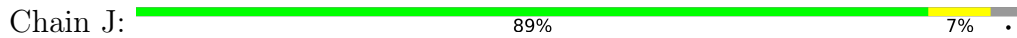


● Molecule 6: Pre-mRNA-splicing factor RSE1

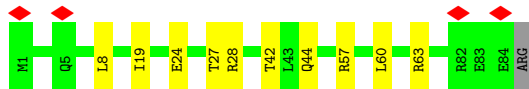
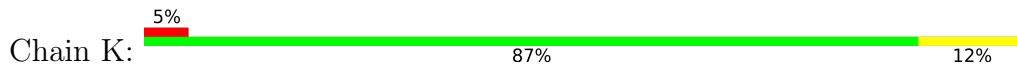




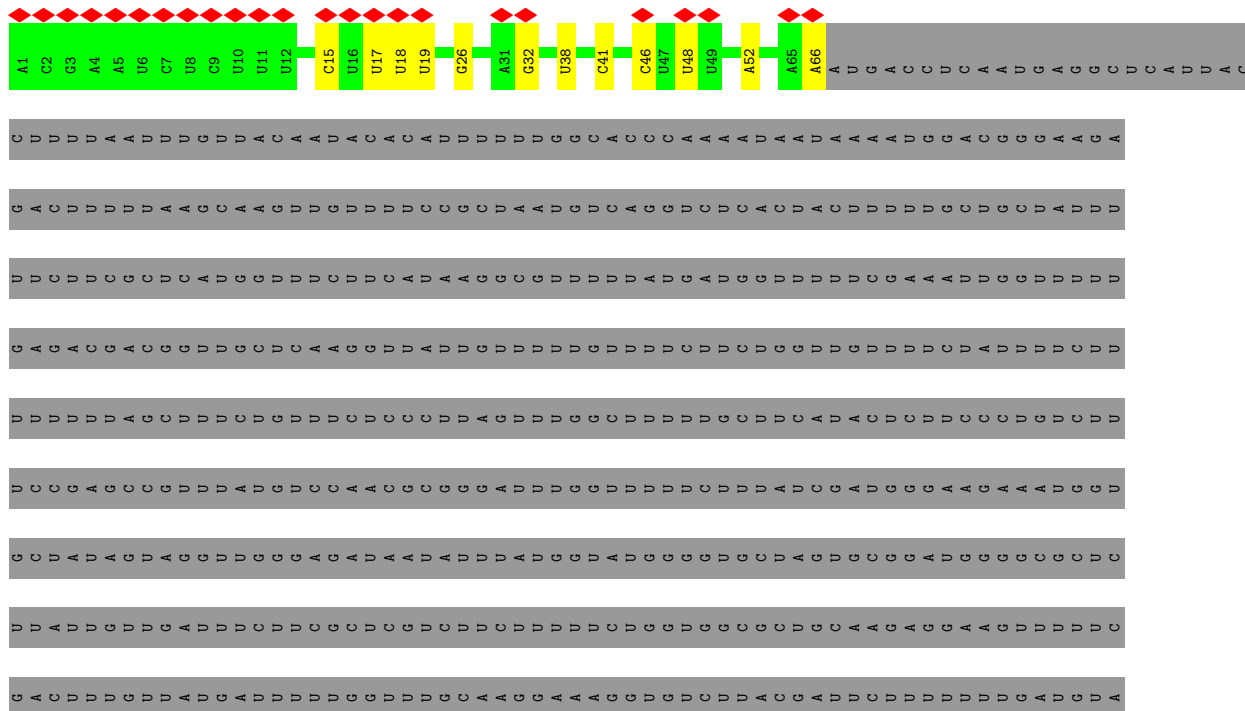
• Molecule 9: Pre-mRNA-splicing factor RDS3



• Molecule 10: RDS3 complex subunit 10

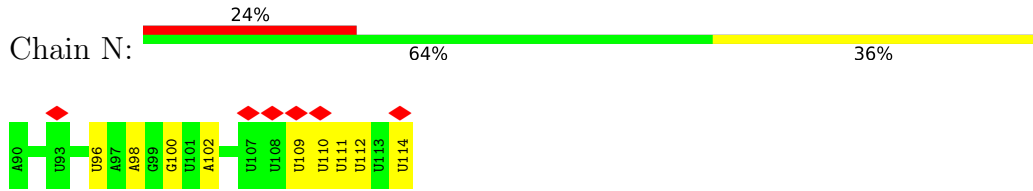


• Molecule 11: U2 snRNA

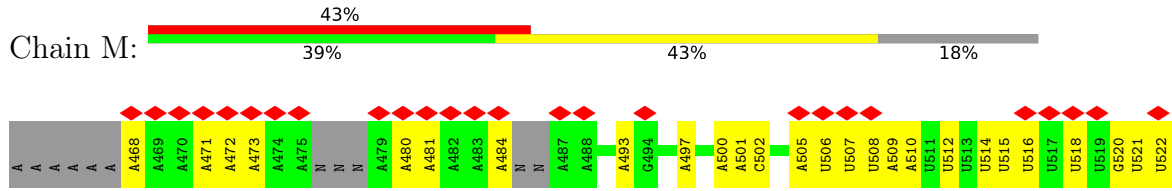


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A A C G C G C C U G U G C C U U U A C U U U A C C A A U U U A C C A G U U U U G U U C C A
U U G A A G G A G A G A G A G A G C U U C U U C U U C U U C U U C U U C U U C U U C U U
G U G U U U G G A G A A U A C C U G A G C C G G A G A G U U U A A A A G A G A A G G
C G U U U U G C U U G G A G A A A A G A G A G A G A G A G A G A G A G A G A G A G A G
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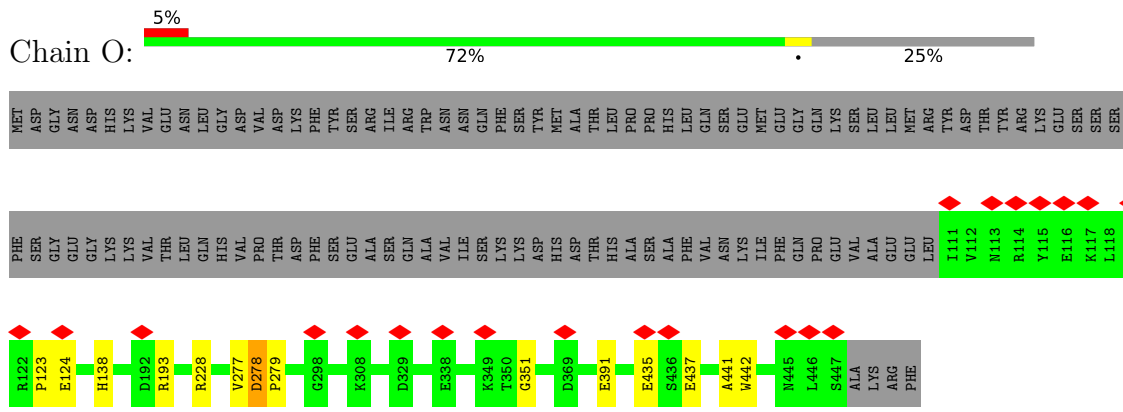
• Molecule 12: Pre-mRNA



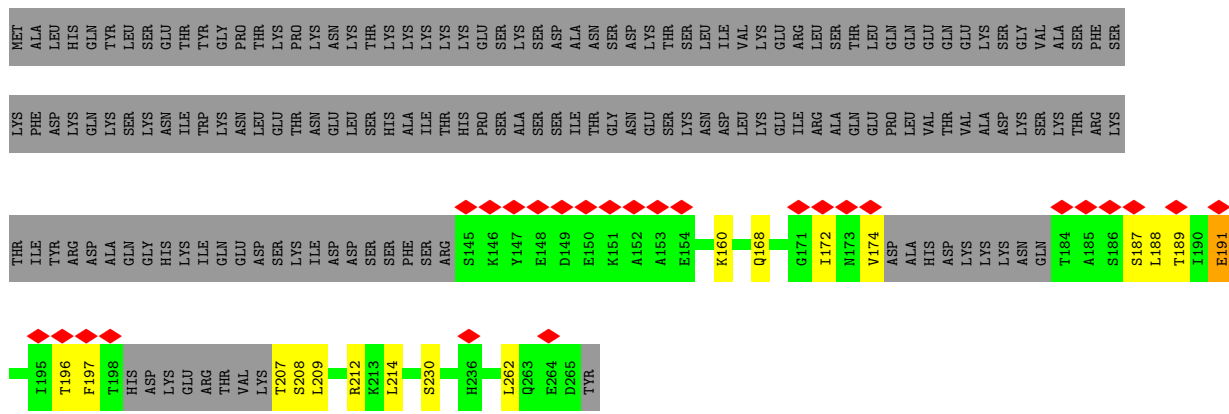
• Molecule 13: Pre-mRNA



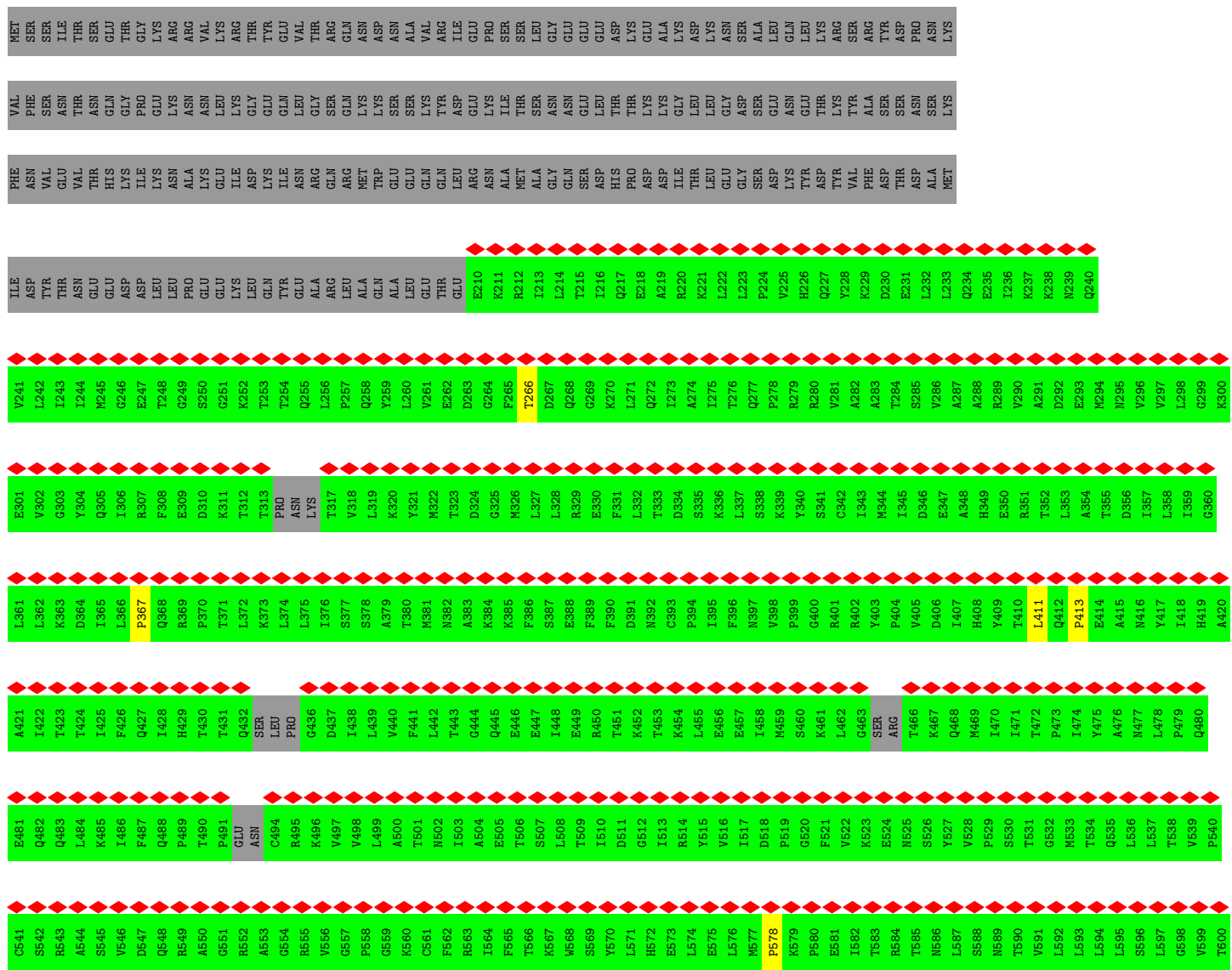
• Molecule 14: Pre-mRNA-splicing factor PRP46

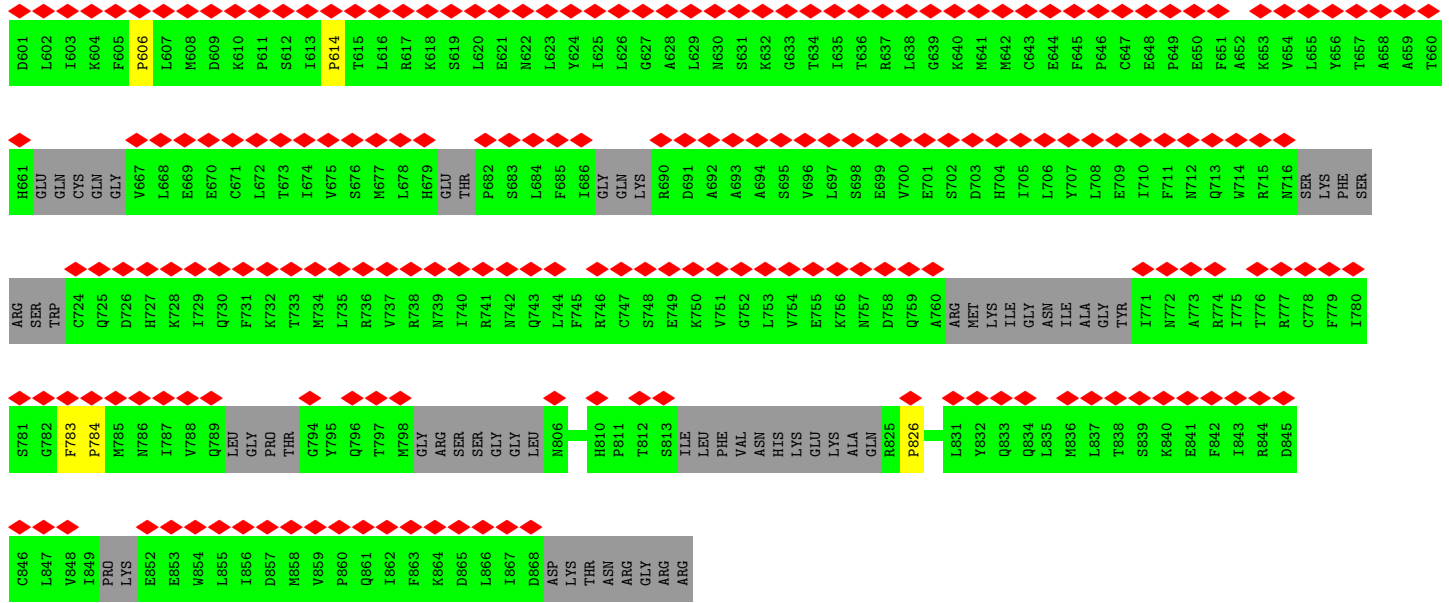


• Molecule 15: Pre-mRNA-processing protein 45

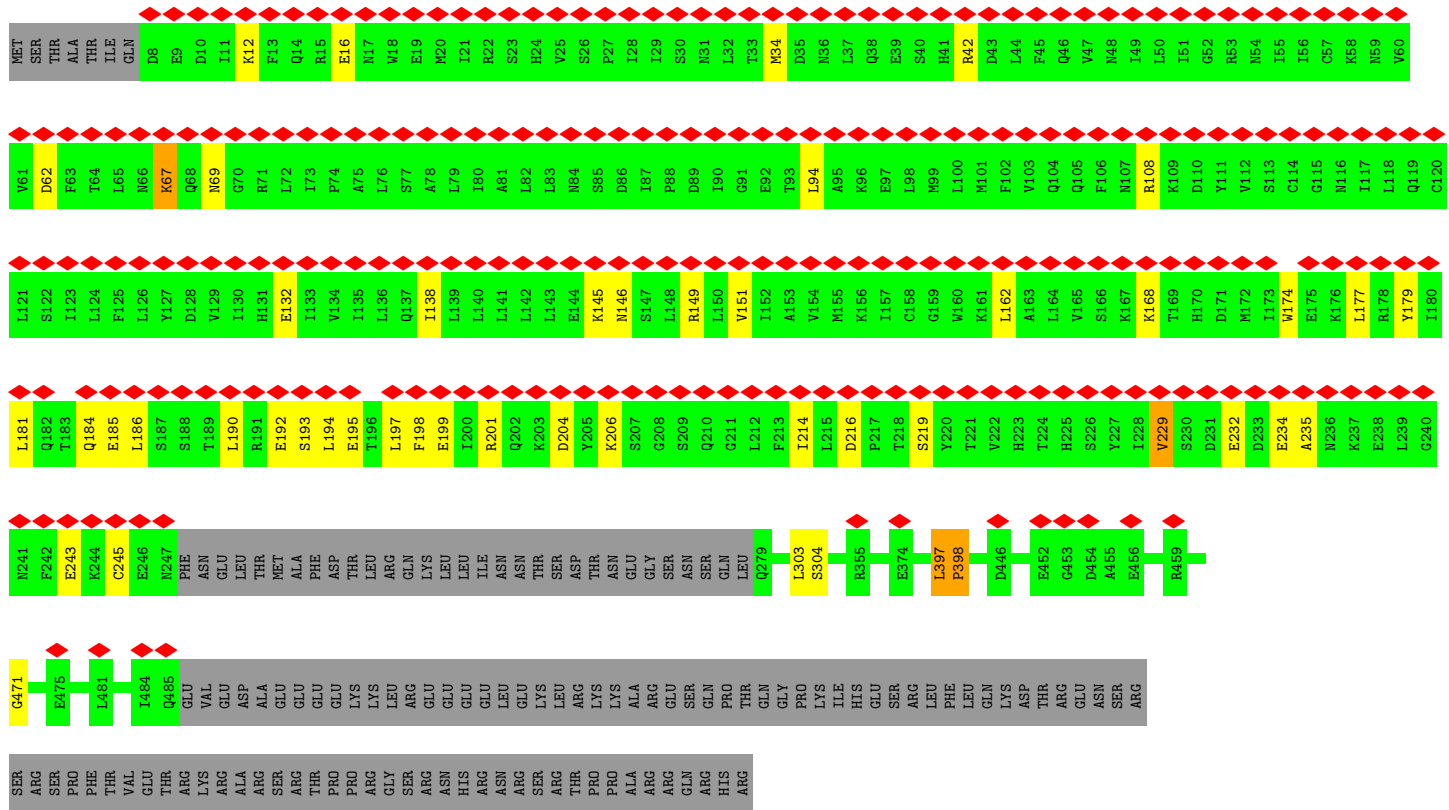
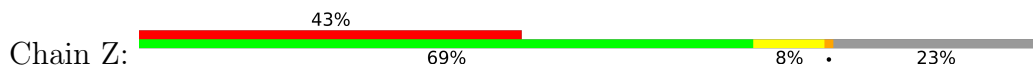


• Molecule 23: Pre-mRNA-splicing factor ATP-dependent RNA helicase-like protein PRP2

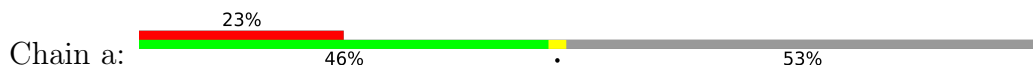


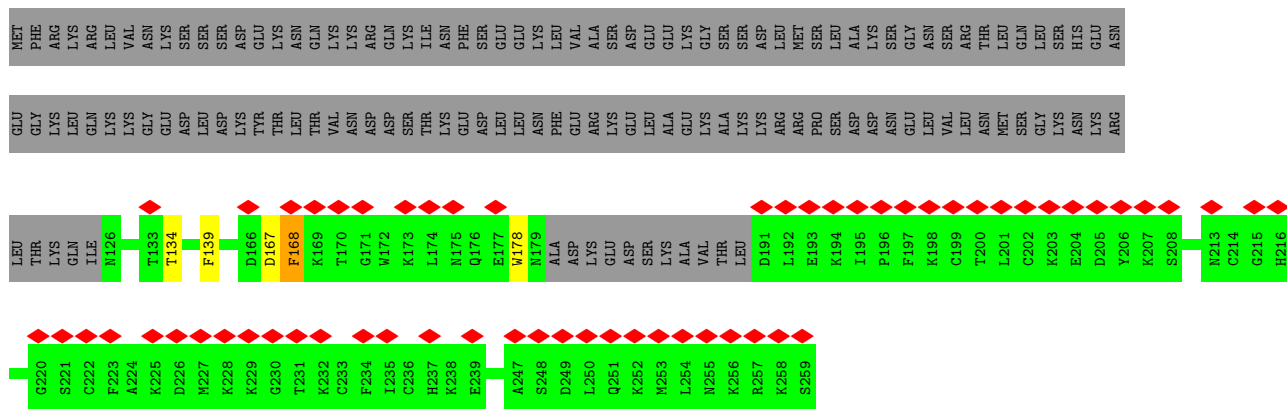


• Molecule 24: Pre-mRNA-splicing factor CWC22

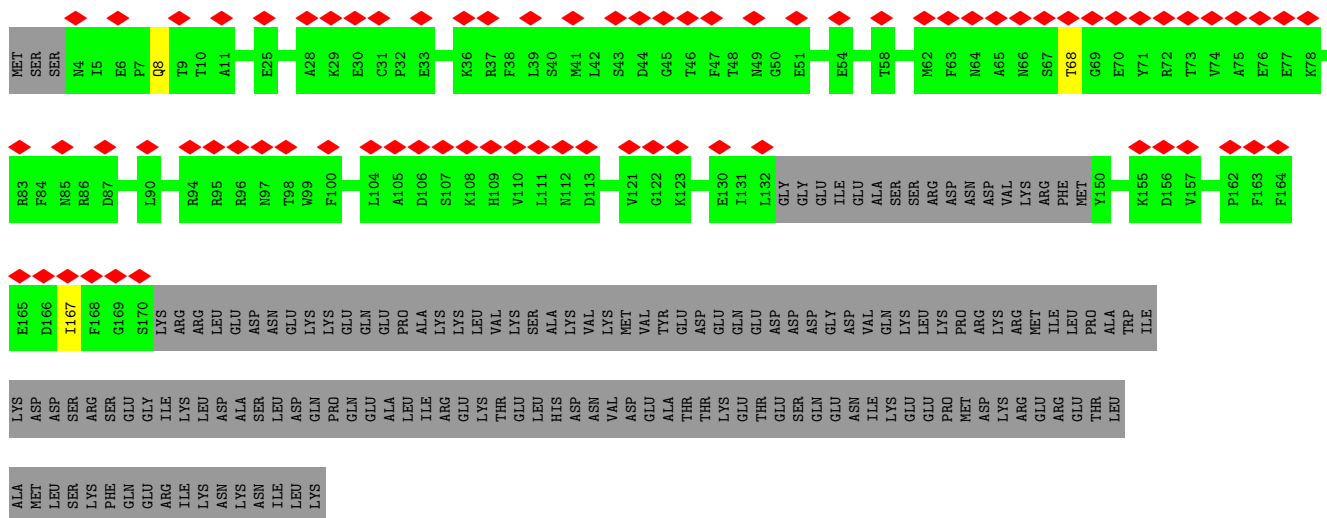


• Molecule 25: Pre-mRNA-splicing factor CWC24

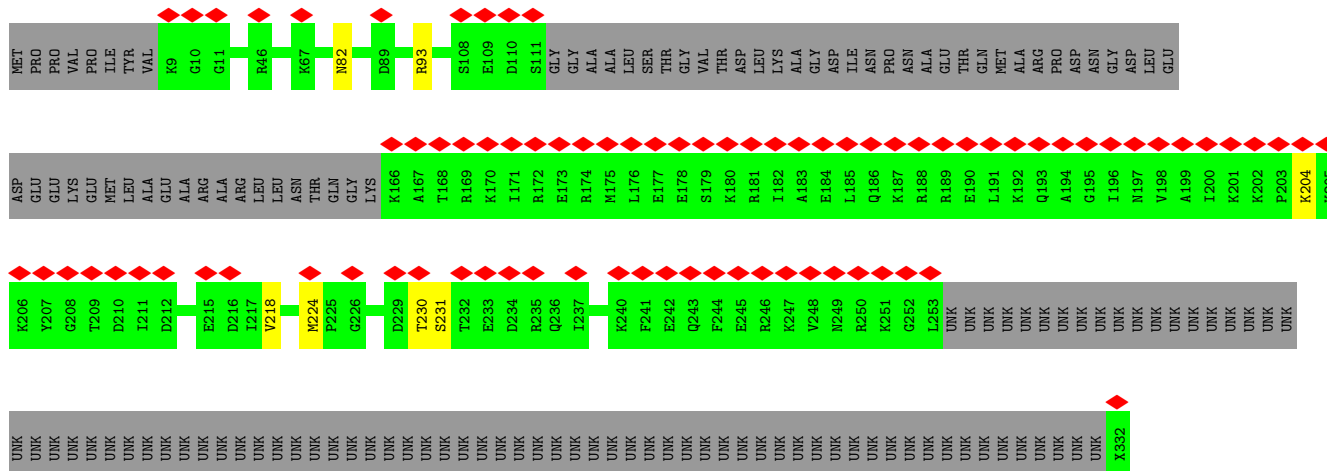


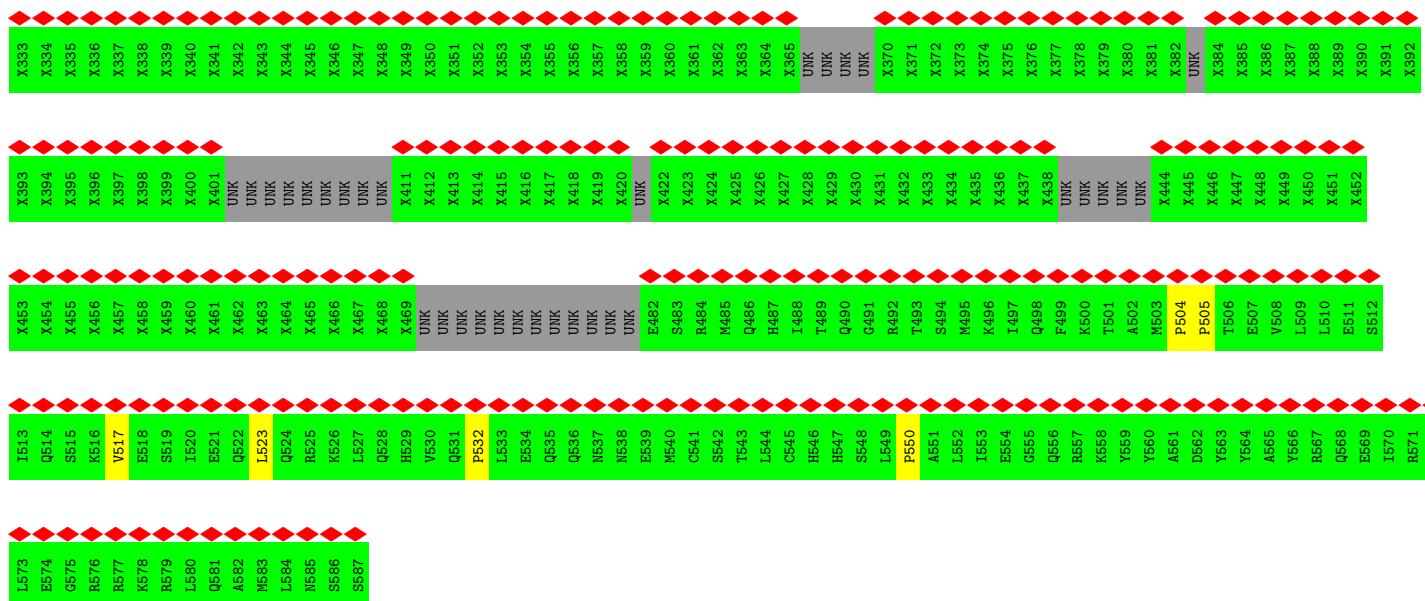


• Molecule 26: Peptidyl-prolyl isomerase CWC27



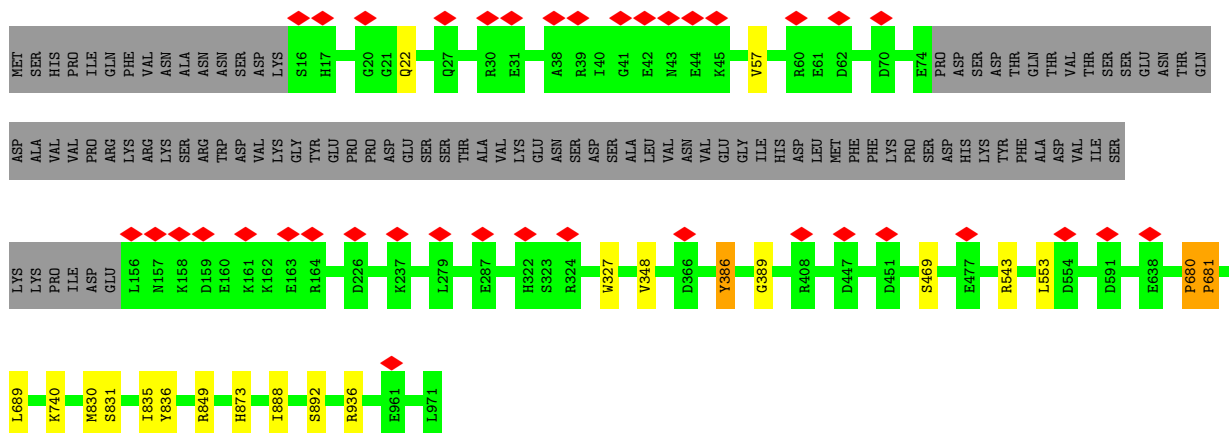
• Molecule 27: Pre-mRNA-splicing factor CEF1





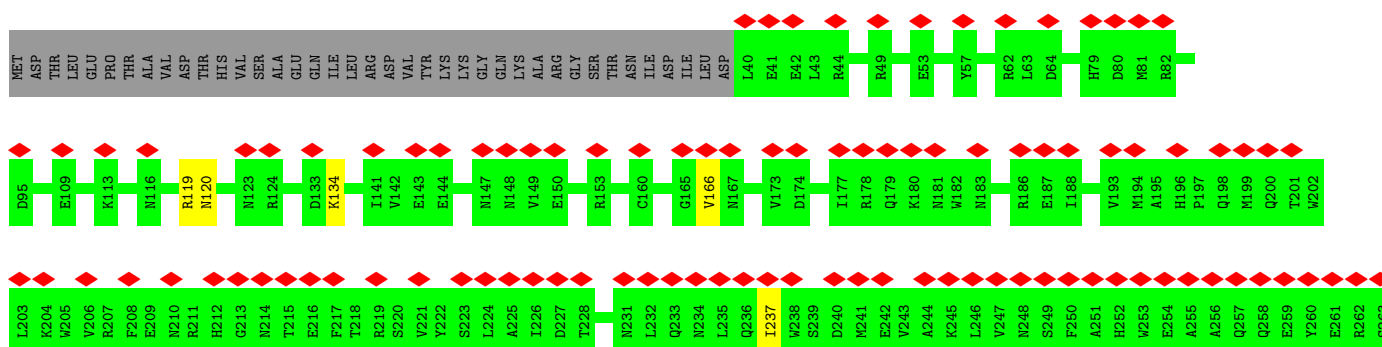
• Molecule 28: U2 snRNP component HSH155

Chain G: 88% 10%



• Molecule 29: Pre-mRNA-splicing factor CLF1

Chain d: 61% 79% 21%

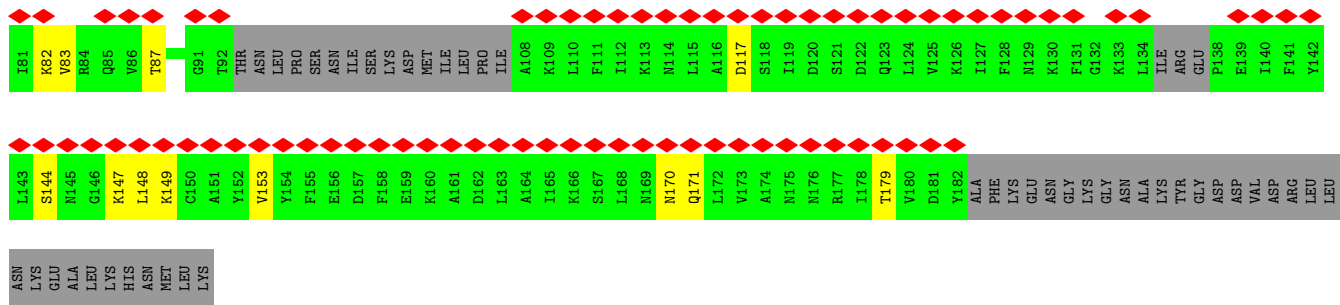


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UNK	X243	X303	X363	UNK	X483	X543	E603	K663	S723	X783	UNK
UNK	X244	X304	X364	X424	X484	X544	S604	T664	W724	X784	UNK
UNK	X245	UNK	X365	X425	X485	X545	F605	F665	T725	X785	UNK
UNK	X246	X306	X366	X426	X486	X546	Q606	L667	R726	X786	UNK
UNK	X247	X307	X367	X427	X487	X547	V607	A668	E727	X787	UNK
UNK	X248	X308	X368	X428	X488	X548	Y608	S670	L728	X788	UNK
X191	X249	X309	X369	X429	X489	X550	E609	S671	Y729	X789	UNK
X192	X250	X310	X370	X430	X490	X551	K610	V671	Q730	X790	UNK
X193	X251	X311	UNK	X431	UNK	X552	T611	F672	E731	X791	UNK
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X196	X254	X314	X375	X434	X494	X555	L615	E675	O734	X794	UNK
X197	X255	X315	X376	X435	X495	X556	F616	I675	UNK	X795	UNK
X198	X256	X316	X377	X436	X496	X557	P617	S677	UNK	UNK	UNK
X199	X257	X317	X378	X437	X497	X558	E618	L679	X738	X797	UNK
X200	UNK	X318	X379	X438	X498	X559	L619	L680	X739	X798	UNK
X201	X259	X319	X380	X439	X499	X560	Q620	S681	W741	X800	UNK
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X203	X261	X321	X382	X441	X501	X562	E622	L683	X743	X802	UNK
X204	X262	X322	X383	UNK	X502	X563	L623	L684	X744	X803	UNK
X205	X263	X324	X384	X444	X503	X564	W624	E685	X745	X804	UNK
X206	X264	X325	X385	X445	X504	X565	I625	L686	X746	X805	UNK
UNK	X265	X326	X386	X446	X505	X566	E626	L687	X747	X806	UNK
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X210	X268	X329	X389	X449	X509	K669	E629	G750	X750	X809	UNK
X211	X269	X330	X390	X450	X510	T570	V630	ALA	X751	X810	UNK
X212	X270	X331	X391	X451	X511	K571	A631	VAL	X752	X811	UNK
X213	X271	X332	X392	X452	X512	M572	T632	ILE	X753	X812	UNK
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X217	X275	X336	X396	X456	X516	T576	L636	VAL	X757	X816	UNK
X218	X276	X337	X397	X457	X517	V577	SER	THR	UNK	X817	UNK
X219	X277	X338	X398	X458	X518	I578	SER	HIS	X759	X818	UNK
X220	X278	X339	X399	X459	X519	D579	LEU	LEU	X760	X819	UNK
X221	X279	X340	X400	X460	X520	D580	S640	GLU	X761	X820	UNK
X222	X280	UNK	X401	X461	X521	ARG	P641	SER	X762	UNK	UNK
X223	X281	X342	X402	X462	X522	LEU	E642	ARG	L706	UNK	UNK
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X225	X283	X344	X404	X464	X524	T584	I644	L708	X763	UNK	UNK
X226	X284	X345	X405	X465	X525	P685	F645	W709	X764	UNK	UNK
X227	X285	X346	X406	UNK	X526	A586	R646	R710	X765	UNK	UNK
X228	X286	X347	UNK	UNK	X527	M587	F646	R711	X766	UNK	UNK
X229	X287	X348	X408	X468	X528	A588	L647	M711	X767	UNK	UNK
X230	X288	X349	X409	X469	X529	E589	F648	C712	X768	UNK	UNK
X231	UNK	X350	X410	X470	X530	E590	E649	I713	X769	UNK	UNK
X232	X290	X351	X411	X471	UNK	N591	K650	S714	X770	UNK	UNK
X233	X291	X352	X412	X472	X532	F591	A651	A651	X771	UNK	UNK
X234	X292	X353	X413	X473	X533	A592	L652	L652	X772	UNK	UNK
X235	X293	X354	X414	X474	X534	L593	A653	A653	X773	UNK	UNK
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X237	X295	X356	X416	X476	X536	L595	LEU	LEU	X775	UNK	UNK
X238	X296	X357	X417	X477	X537	Q596	CYS	CYS	X776	UNK	UNK
X239	X297	X358	X418	X478	X538	M597	SER	SER	X777	UNK	UNK
UNK	X298	UNK	X419	X479	X539	H598	ASN	ASN	X778	UNK	UNK
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											X780

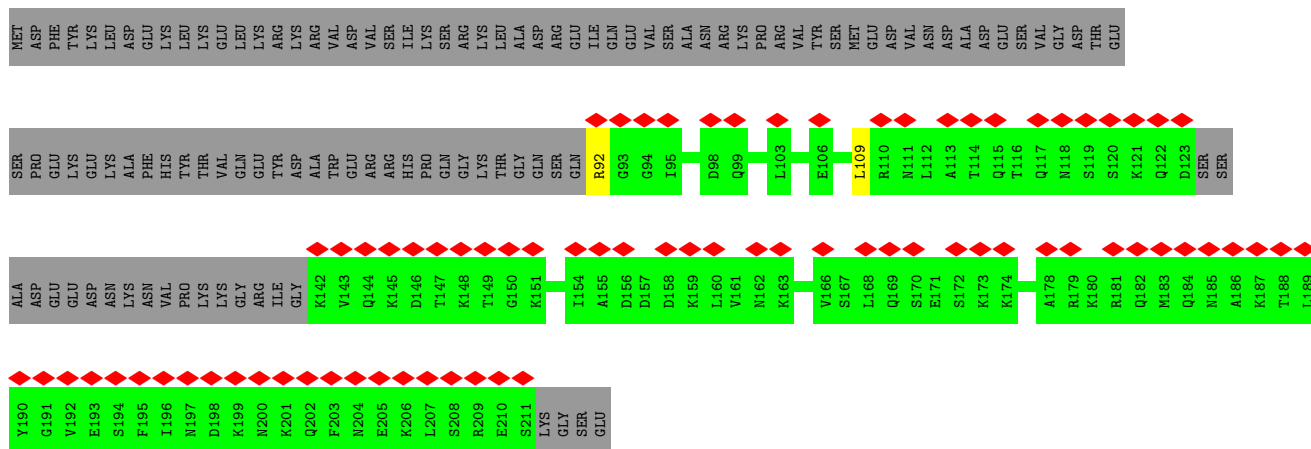
• Molecule 32: Protein HSH49



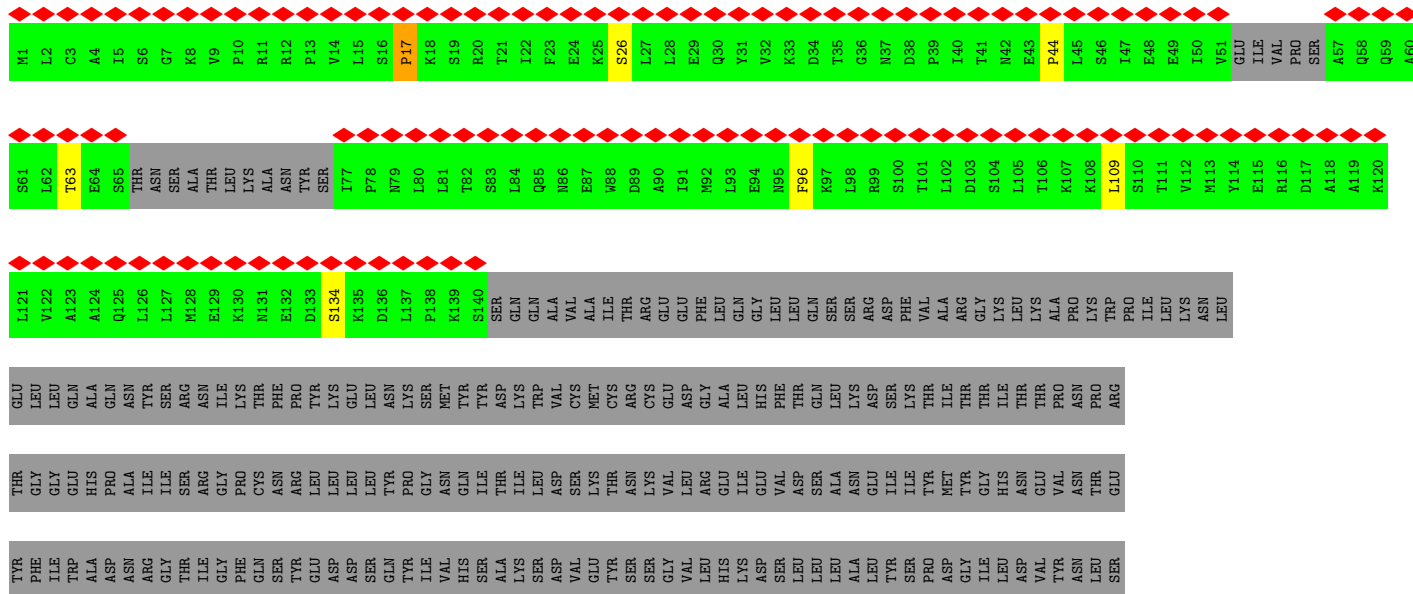
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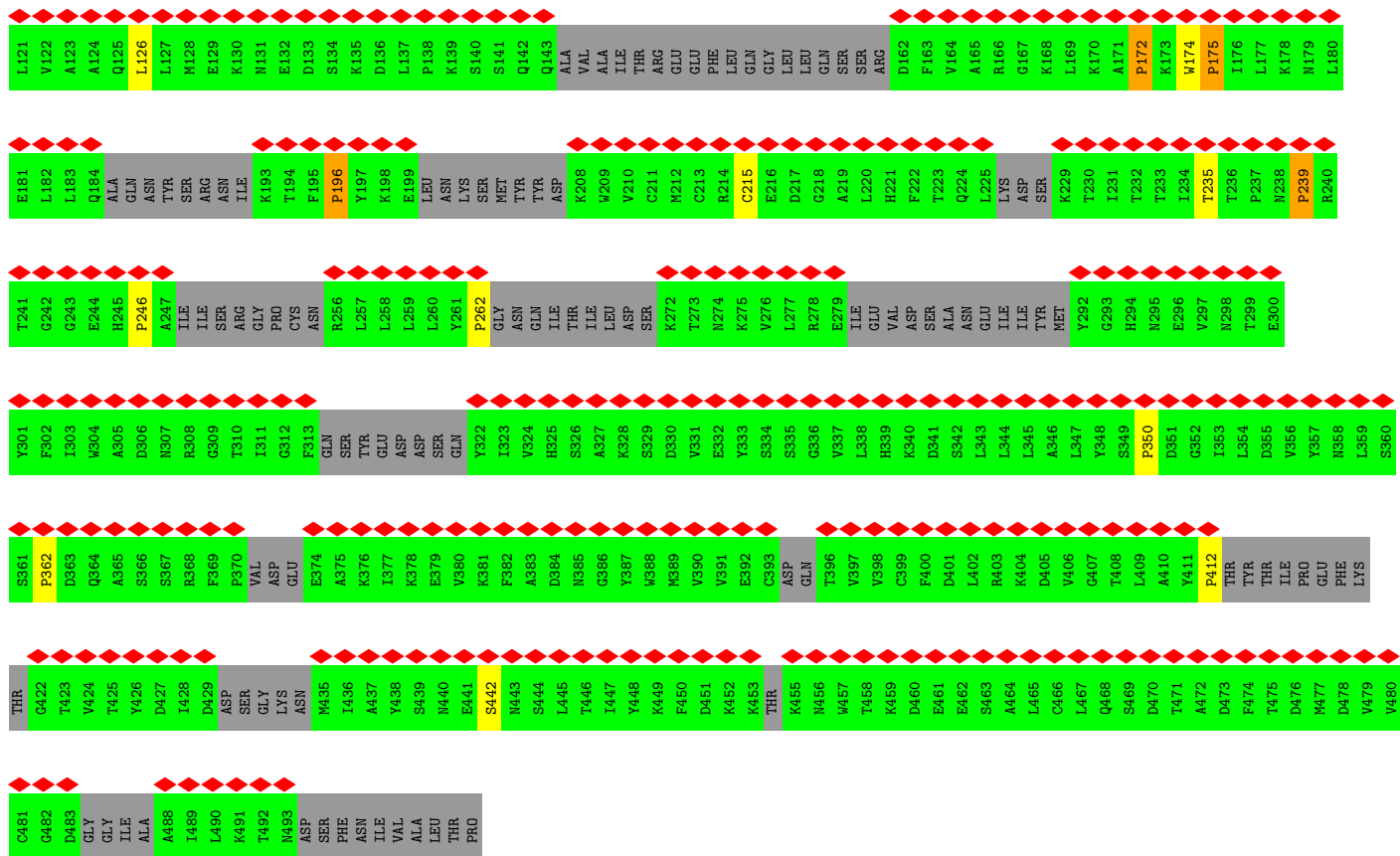


• Molecule 33: Pre-mRNA-splicing factor SYF2

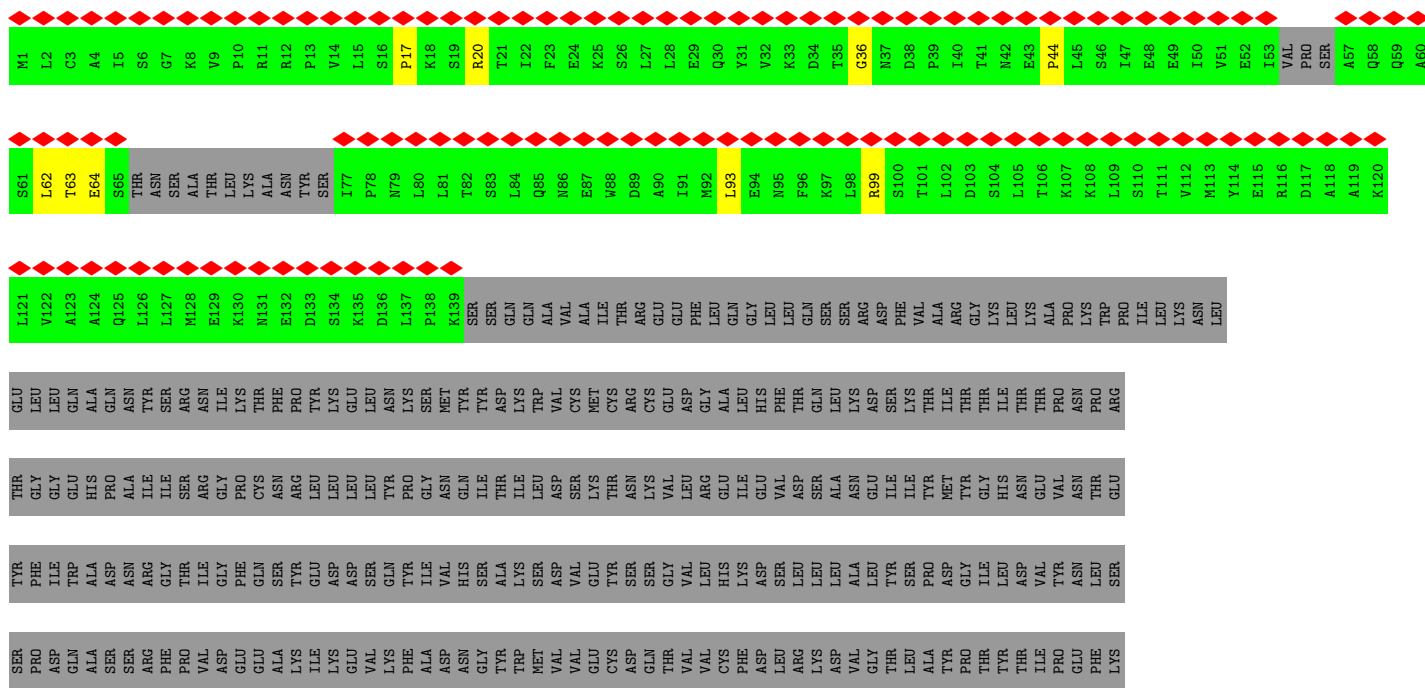


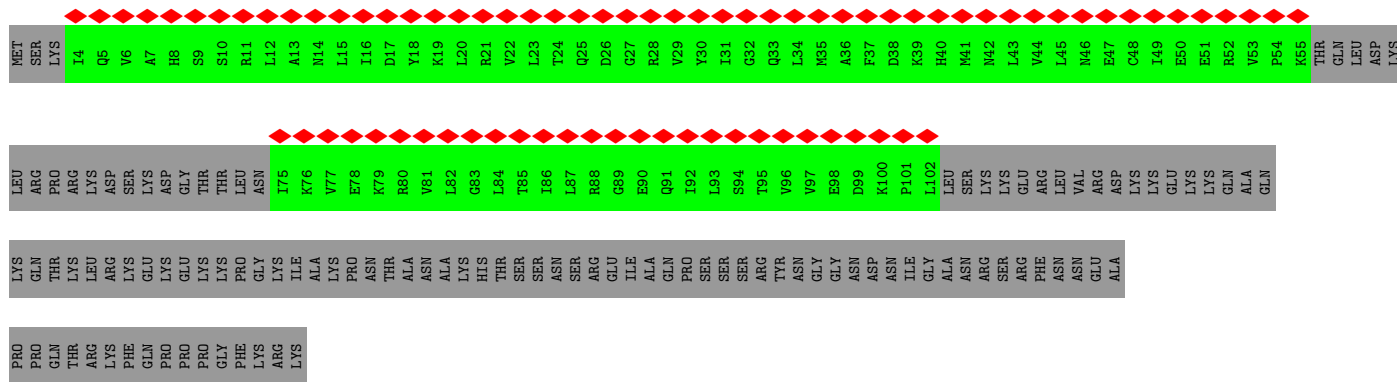
• Molecule 34: Pre-mRNA-processing factor 19



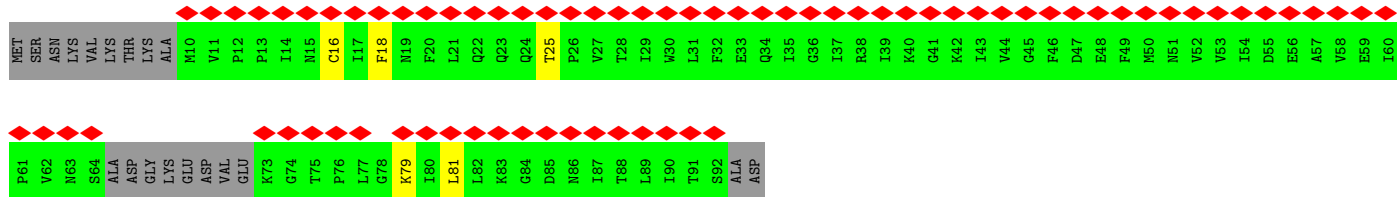
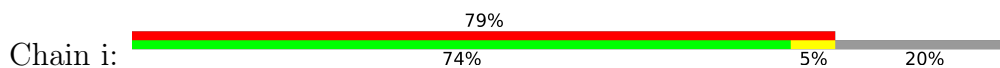


• Molecule 34: Pre-mRNA-processing factor 19

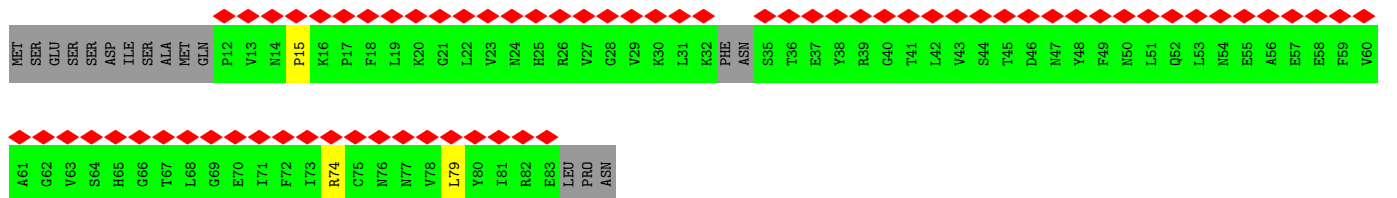
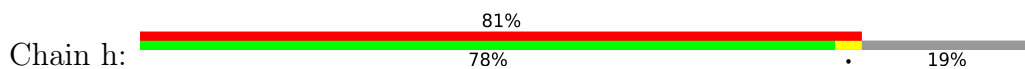




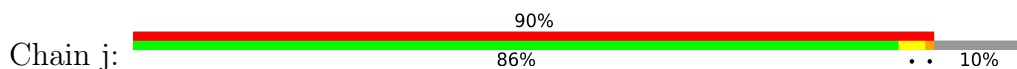
• Molecule 38: Small nuclear ribonucleoprotein E



• Molecule 39: Small nuclear ribonucleoprotein F

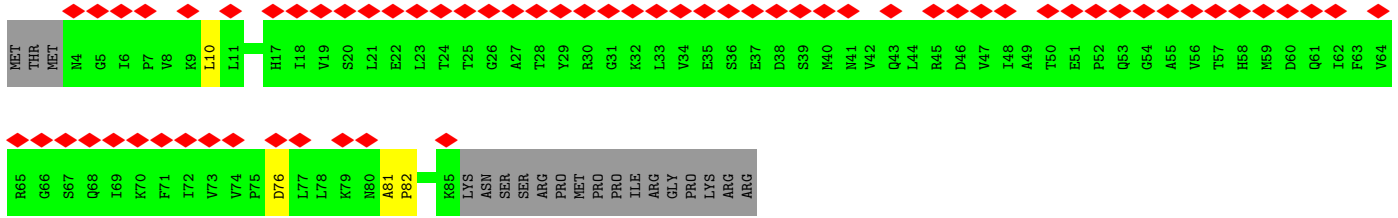


• Molecule 40: Small nuclear ribonucleoprotein G

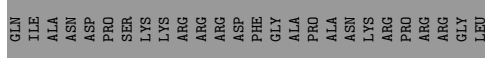
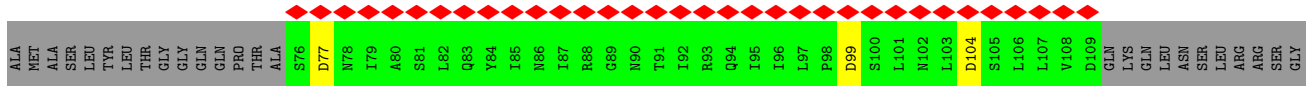
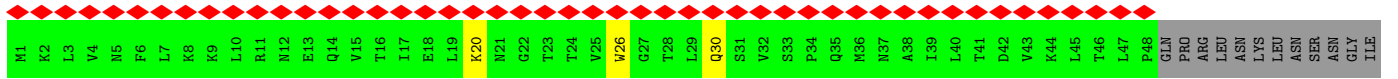


• Molecule 41: Small nuclear ribonucleoprotein Sm D3

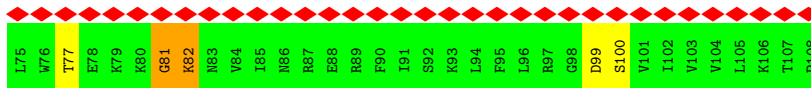
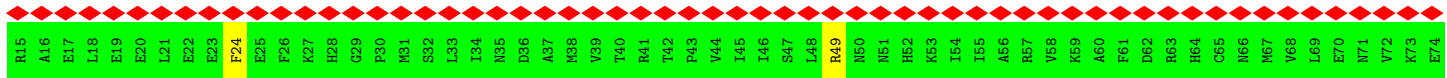




• Molecule 42: Small nuclear ribonucleoprotein Sm D1



• Molecule 43: Small nuclear ribonucleoprotein Sm D2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77312	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 ($e^-/\text{\AA}^2$)	4.7	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	0.285	Depositor
Minimum map value	-0.174	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0405	Depositor
Map size (Å)	522.4, 522.4, 522.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3060001, 1.3060001, 1.3060001	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: MG, GTP, ADP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	7/18560 (0.0%)	0.79	16/25158 (0.1%)
2	B	0.35	0/14812	0.48	0/20077
3	C	0.51	0/7162	0.65	2/9698 (0.0%)
4	D	0.63	0/2747	0.76	0/4267
5	E	0.63	0/2452	0.78	0/3817
6	F	0.76	5/9564 (0.1%)	0.84	7/12963 (0.1%)
7	H	0.72	0/1281	0.84	0/1727
8	I	0.77	0/812	0.92	3/1081 (0.3%)
9	J	0.81	0/827	0.85	0/1105
10	K	0.81	0/702	0.85	0/939
11	L	0.59	0/1547	0.78	0/2404
12	N	0.55	0/579	0.82	0/897
13	M	0.62	2/1183 (0.2%)	0.93	2/1833 (0.1%)
14	O	0.72	0/2704	0.77	1/3676 (0.0%)
15	P	0.52	0/2008	0.66	1/2703 (0.0%)
16	Q	0.45	1/1496 (0.1%)	0.63	0/2014
17	R	0.50	0/2135	0.63	2/2871 (0.1%)
18	S	0.42	0/592	0.60	0/790
19	T	0.63	1/1315 (0.1%)	0.73	1/1759 (0.1%)
20	U	0.32	0/1424	0.52	0/1922
21	V	0.66	0/1071	0.73	1/1445 (0.1%)
22	W	0.61	0/856	0.73	1/1149 (0.1%)
23	Y	0.34	0/4085	0.50	1/5499 (0.0%)
24	Z	0.59	0/3712	0.76	4/5004 (0.1%)
25	a	0.60	0/1010	0.68	0/1351
26	b	0.38	0/1252	0.54	0/1692
27	c	0.54	0/2237	0.63	1/2995 (0.0%)
28	G	0.72	0/7104	0.81	3/9632 (0.0%)
29	d	0.42	0/2075	0.55	1/2808 (0.0%)
30	X	0.57	0/191	0.75	0/254
31	v	0.41	0/899	0.54	0/1206
32	e	0.47	0/954	0.74	0/1285

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.43	0/826	0.59	1/1097 (0.1%)
34	o	0.40	0/824	0.52	0/1111
34	p	0.40	0/848	0.55	0/1143
34	q	0.44	0/2312	0.65	0/3097
34	r	0.39	0/828	0.54	1/1117 (0.1%)
35	t	0.42	0/919	0.56	2/1237 (0.2%)
36	n	0.48	0/200	0.71	0/264
37	k	0.37	0/636	0.61	0/856
38	i	0.42	0/585	0.62	0/795
39	h	0.44	0/564	0.65	1/761 (0.1%)
40	j	0.37	0/532	0.60	0/715
41	l	0.40	0/634	0.70	0/859
42	m	0.41	0/649	0.61	0/880
43	g	0.45	0/753	0.69	2/1013 (0.2%)
All	All	0.60	16/110458 (0.0%)	0.70	54/150966 (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
1	A	0	6
2	B	0	2
3	C	0	5
6	F	0	13
7	H	0	6
8	I	0	3
14	O	0	6
15	P	0	1
16	Q	0	2
19	T	0	2
20	U	0	2
24	Z	0	4
28	G	0	3
29	d	0	1
33	f	0	1
36	n	0	2
40	j	0	1
41	l	0	2
43	g	0	2
All	All	0	64

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	468	A	N9-C4	-7.77	1.33	1.37
13	M	468	A	C3'-O3'	6.84	1.51	1.42
1	A	1265	PHE	CG-CD1	-6.29	1.29	1.38
6	F	830	TYR	CG-CD2	-6.15	1.31	1.39
1	A	753	TYR	CE1-CZ	-6.00	1.30	1.38

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	55	ASN	C-N-CD	-15.28	86.99	120.60
13	M	468	A	C2'-C3'-O3'	9.32	130.00	109.50
13	M	468	A	C4'-C3'-O3'	-9.29	89.89	109.40
1	A	737	ARG	NE-CZ-NH2	-7.86	116.37	120.30
24	Z	397	LEU	C-N-CD	-7.43	104.25	120.60

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1418	THR	Peptide
1	A	239	PHE	Mainchain,Peptide
1	A	539	PRO	Peptide
1	A	772	GLU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	2192/2287 (96%)	2037 (93%)	134 (6%)	21 (1%)	15	54
2	B	1803/2163 (83%)	1687 (94%)	112 (6%)	4 (0%)	47	81
3	C	872/1008 (86%)	800 (92%)	62 (7%)	10 (1%)	14	52
6	F	1164/1361 (86%)	1042 (90%)	110 (10%)	12 (1%)	15	54
7	H	147/436 (34%)	139 (95%)	6 (4%)	2 (1%)	11	46
8	I	98/266 (37%)	87 (89%)	9 (9%)	2 (2%)	7	39
9	J	101/107 (94%)	87 (86%)	14 (14%)	0	100	100
10	K	82/85 (96%)	78 (95%)	3 (4%)	1 (1%)	13	50
14	O	335/451 (74%)	302 (90%)	26 (8%)	7 (2%)	7	38
15	P	236/379 (62%)	209 (89%)	23 (10%)	4 (2%)	9	42
16	Q	177/364 (49%)	157 (89%)	16 (9%)	4 (2%)	6	36
17	R	259/339 (76%)	238 (92%)	18 (7%)	3 (1%)	13	50
18	S	65/175 (37%)	53 (82%)	9 (14%)	3 (5%)	2	21
19	T	155/157 (99%)	139 (90%)	13 (8%)	3 (2%)	8	40
20	U	172/207 (83%)	162 (94%)	9 (5%)	1 (1%)	25	64
21	V	126/148 (85%)	118 (94%)	6 (5%)	2 (2%)	9	43
22	W	98/266 (37%)	89 (91%)	6 (6%)	3 (3%)	4	30
23	Y	570/876 (65%)	548 (96%)	21 (4%)	1 (0%)	47	81
24	Z	443/577 (77%)	399 (90%)	32 (7%)	12 (3%)	5	33
25	a	119/259 (46%)	104 (87%)	13 (11%)	2 (2%)	9	42
26	b	146/301 (48%)	134 (92%)	9 (6%)	3 (2%)	7	38
27	c	291/587 (50%)	276 (95%)	9 (3%)	6 (2%)	7	38
28	G	871/971 (90%)	820 (94%)	41 (5%)	10 (1%)	14	52
29	d	234/687 (34%)	214 (92%)	19 (8%)	1 (0%)	34	72
30	X	25/135 (18%)	20 (80%)	5 (20%)	0	100	100
31	v	120/859 (14%)	110 (92%)	5 (4%)	5 (4%)	3	23
32	e	141/213 (66%)	114 (81%)	16 (11%)	11 (8%)	1	10
33	f	98/215 (46%)	95 (97%)	3 (3%)	0	100	100
34	o	118/503 (24%)	113 (96%)	4 (3%)	1 (1%)	19	58
34	p	122/503 (24%)	116 (95%)	6 (5%)	0	100	100
34	q	349/503 (69%)	321 (92%)	16 (5%)	12 (3%)	3	28
34	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	t	149/175 (85%)	133 (89%)	13 (9%)	3 (2%)	7	39
36	n	21/455 (5%)	19 (90%)	1 (5%)	1 (5%)	2	20
37	k	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
38	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
39	h	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	45
40	j	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
41	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	48
42	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
43	g	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	14	52
All	All	12546/19315 (65%)	11559 (92%)	831 (7%)	156 (1%)	17	50

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	1376	ASN
1	A	1405	ILE
1	A	1829	SER
1	A	1830	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1994/2066 (96%)	1916 (96%)	78 (4%)	32	64
2	B	1632/1955 (84%)	1632 (100%)	0	100	100
3	C	791/910 (87%)	778 (98%)	13 (2%)	62	83
6	F	1088/1244 (88%)	1071 (98%)	17 (2%)	62	83
7	H	139/392 (36%)	129 (93%)	10 (7%)	14	45
8	I	89/236 (38%)	82 (92%)	7 (8%)	12	41
9	J	93/97 (96%)	85 (91%)	8 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	76/77 (99%)	67 (88%)	9 (12%)	5	25
14	O	295/397 (74%)	293 (99%)	2 (1%)	84	93
15	P	218/328 (66%)	202 (93%)	16 (7%)	14	45
16	Q	171/332 (52%)	159 (93%)	12 (7%)	15	46
17	R	224/296 (76%)	209 (93%)	15 (7%)	16	48
18	S	58/151 (38%)	56 (97%)	2 (3%)	37	68
19	T	141/141 (100%)	138 (98%)	3 (2%)	53	79
20	U	157/189 (83%)	150 (96%)	7 (4%)	27	61
21	V	114/132 (86%)	112 (98%)	2 (2%)	59	81
22	W	91/240 (38%)	77 (85%)	14 (15%)	2	16
23	Y	299/789 (38%)	291 (97%)	8 (3%)	44	73
24	Z	417/538 (78%)	383 (92%)	34 (8%)	11	40
25	a	112/237 (47%)	108 (96%)	4 (4%)	35	66
26	b	134/273 (49%)	134 (100%)	0	100	100
27	c	196/316 (62%)	190 (97%)	6 (3%)	40	70
28	G	778/867 (90%)	768 (99%)	10 (1%)	69	86
29	d	215/249 (86%)	213 (99%)	2 (1%)	78	90
30	X	21/121 (17%)	21 (100%)	0	100	100
31	v	59/152 (39%)	49 (83%)	10 (17%)	2	12
32	e	48/189 (25%)	43 (90%)	5 (10%)	7	31
33	f	92/193 (48%)	92 (100%)	0	100	100
34	o	61/451 (14%)	54 (88%)	7 (12%)	5	26
34	p	62/451 (14%)	54 (87%)	8 (13%)	4	22
34	q	121/451 (27%)	105 (87%)	16 (13%)	4	21
34	r	59/451 (13%)	54 (92%)	5 (8%)	10	39
35	t	39/165 (24%)	28 (72%)	11 (28%)	0	3
36	n	20/413 (5%)	12 (60%)	8 (40%)	0	1
37	k	70/176 (40%)	70 (100%)	0	100	100
38	i	65/83 (78%)	60 (92%)	5 (8%)	13	42
39	h	61/77 (79%)	60 (98%)	1 (2%)	62	83
40	j	58/66 (88%)	55 (95%)	3 (5%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	l	69/89 (78%)	67 (97%)	2 (3%)	42	71
42	m	77/129 (60%)	71 (92%)	6 (8%)	12	42
43	g	79/87 (91%)	74 (94%)	5 (6%)	18	51
All	All	10583/16196 (65%)	10212 (96%)	371 (4%)	39	67

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	Z	149	ARG
31	v	725	THR
24	Z	181	LEU
25	a	178	TRP
34	o	134	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such sidechains are listed below:

Mol	Chain	Res	Type
17	R	91	HIS
25	a	175	ASN
18	S	173	HIS
22	W	173	ASN
28	G	65	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	L	65/1175 (5%)	12 (18%)	0
12	N	24/25 (96%)	9 (37%)	0
13	M	47/61 (77%)	21 (44%)	5 (10%)
4	D	114/214 (53%)	24 (21%)	2 (1%)
5	E	102/112 (91%)	17 (16%)	0
All	All	352/1587 (22%)	83 (23%)	7 (1%)

5 of 83 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	29	G
4	D	31	G
4	D	42	A

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Mol	Chain	Res	Type
4	D	43	G
4	D	45	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	M	480	A
13	M	500	A
13	M	515	U
13	M	514	U
13	M	472	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 18 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
44	GTP	C	1500	-	26,34,34	1.00	1 (3%)	32,54,54	1.81	6 (18%)
47	ADP	Y	902	45	24,29,29	1.04	2 (8%)	29,45,45	1.48	4 (13%)

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	-	-	8/18/38/38	0/3/3/3
47	ADP	Y	902	45	-	2/12/32/32	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	C6-N1	-3.21	1.33	1.37
47	Y	902	ADP	C5-C4	2.59	1.47	1.40
47	Y	902	ADP	C2-N3	2.17	1.35	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	C	1500	GTP	PB-O3B-PG	-4.28	118.15	132.83
44	C	1500	GTP	PA-O3A-PB	-4.20	118.42	132.83
44	C	1500	GTP	O6-C6-C5	-3.92	116.71	124.37
44	C	1500	GTP	C5-C6-N1	3.85	120.74	113.95
47	Y	902	ADP	PA-O3A-PB	-3.77	119.89	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

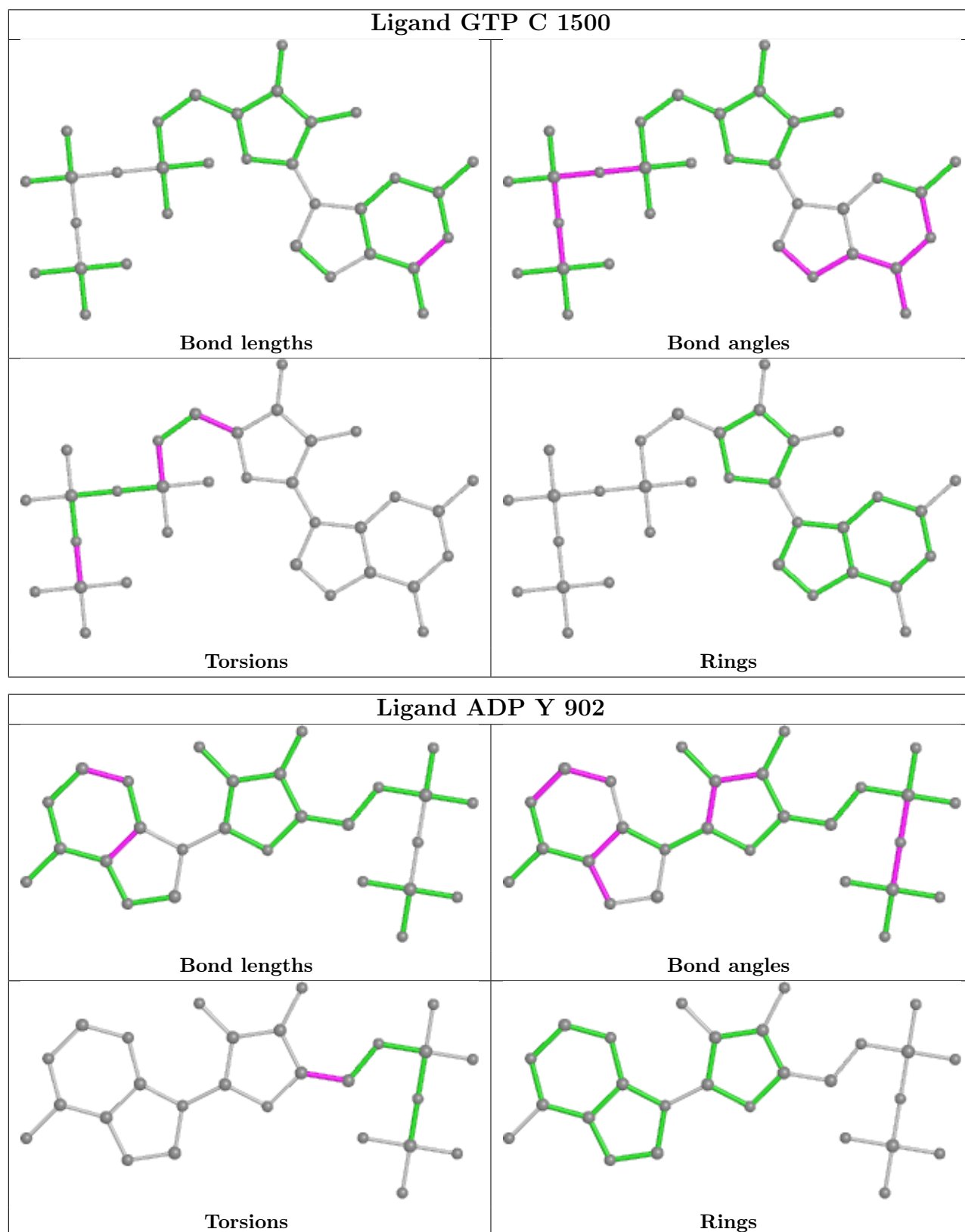
Mol	Chain	Res	Type	Atoms
44	C	1500	GTP	C5'-O5'-PA-O3A
44	C	1500	GTP	C5'-O5'-PA-O1A
44	C	1500	GTP	C5'-O5'-PA-O2A
44	C	1500	GTP	O4'-C4'-C5'-O5'
44	C	1500	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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.

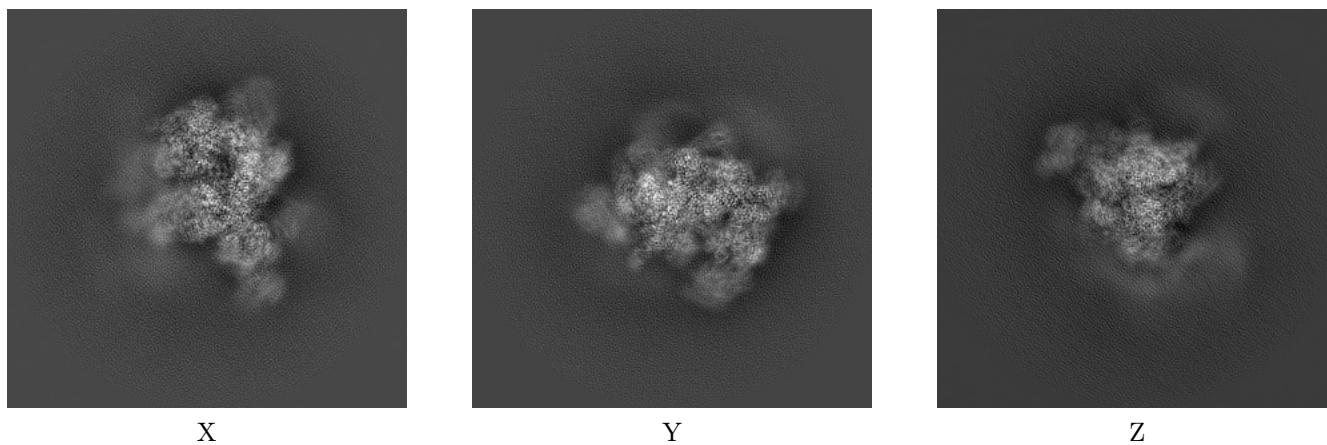
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9524. 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](#)

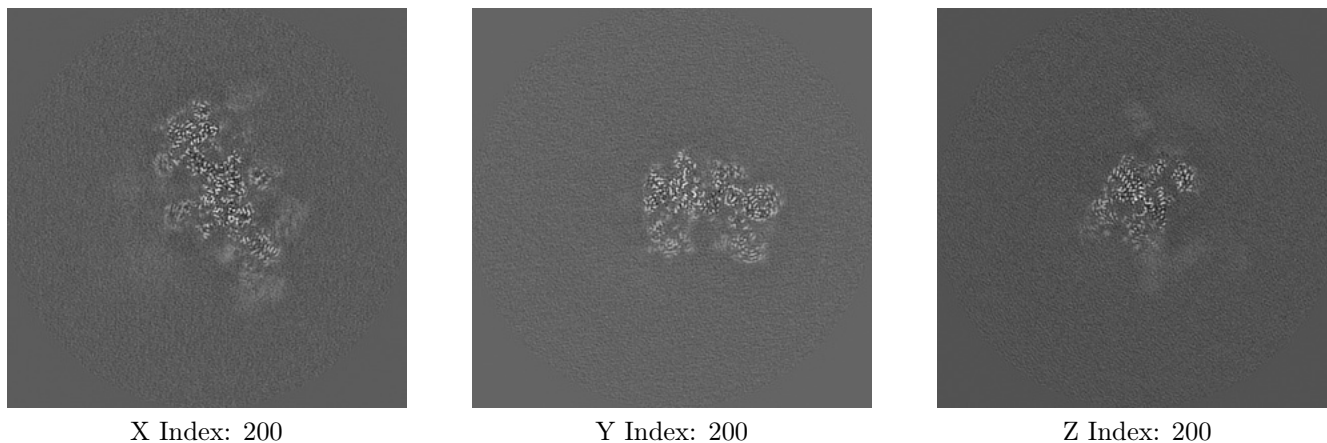
6.1.1 Primary map



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

6.2 Central slices [i](#)

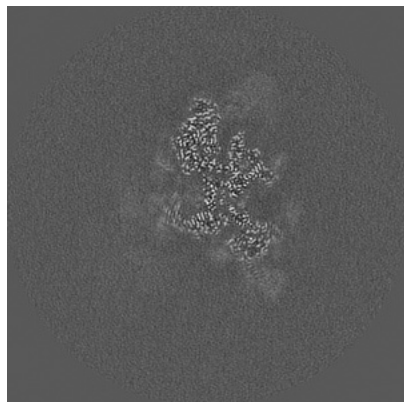
6.2.1 Primary map



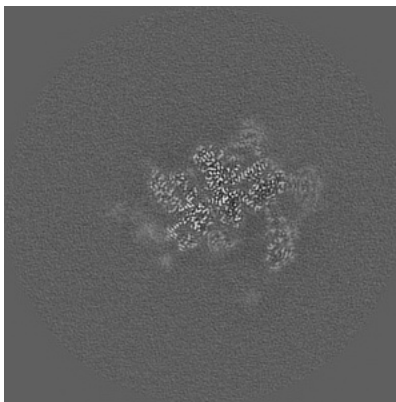
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

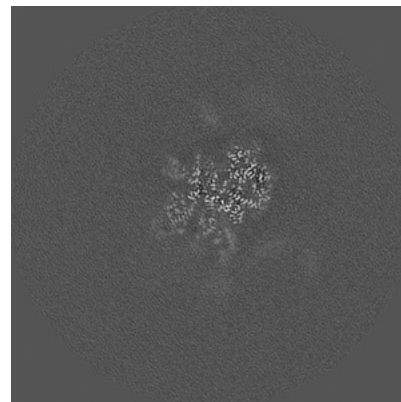
6.3.1 Primary map



X Index: 210



Y Index: 230



Z Index: 205

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0405. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

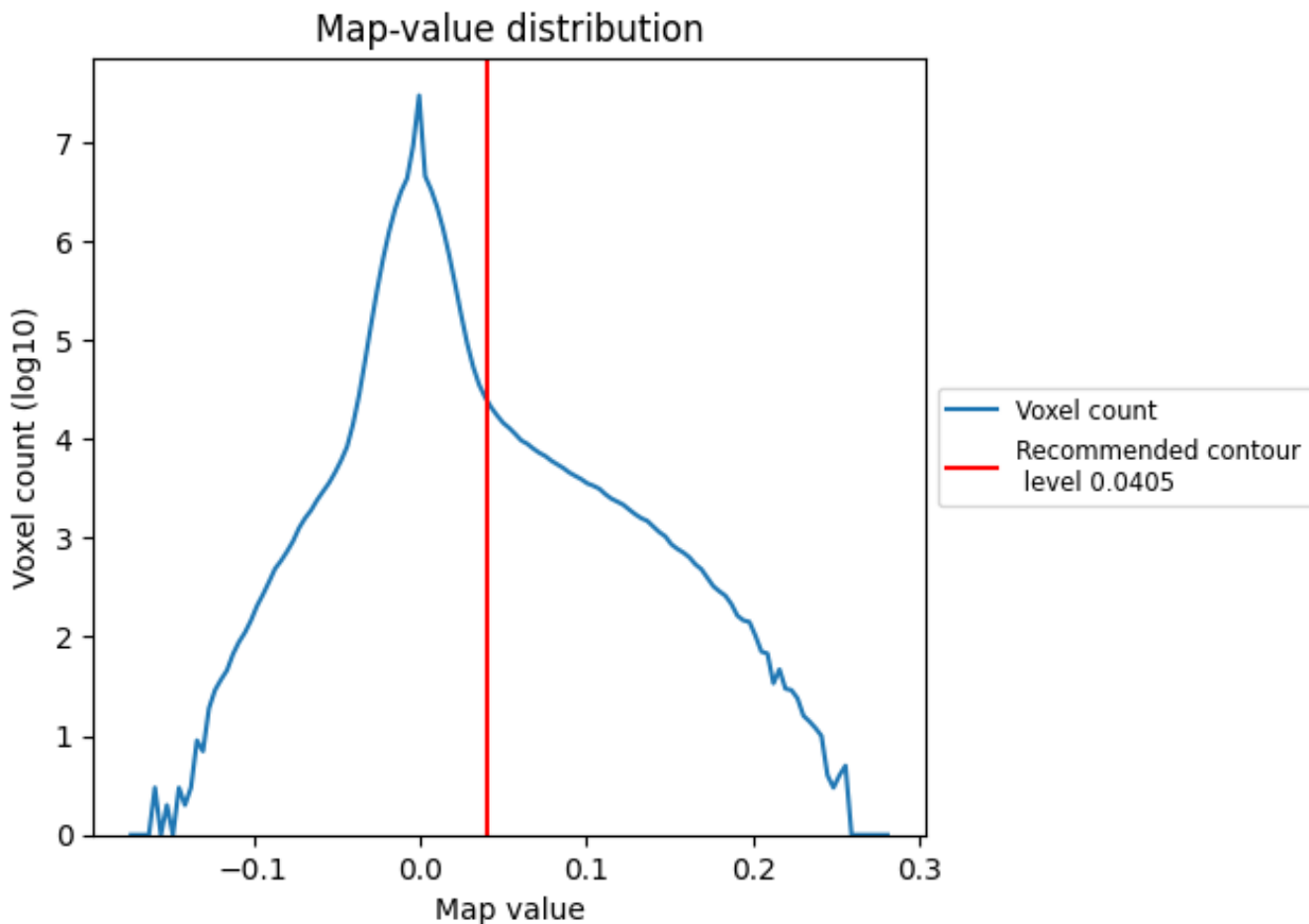
6.5 Mask visualisation

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

7 Map analysis [i](#)

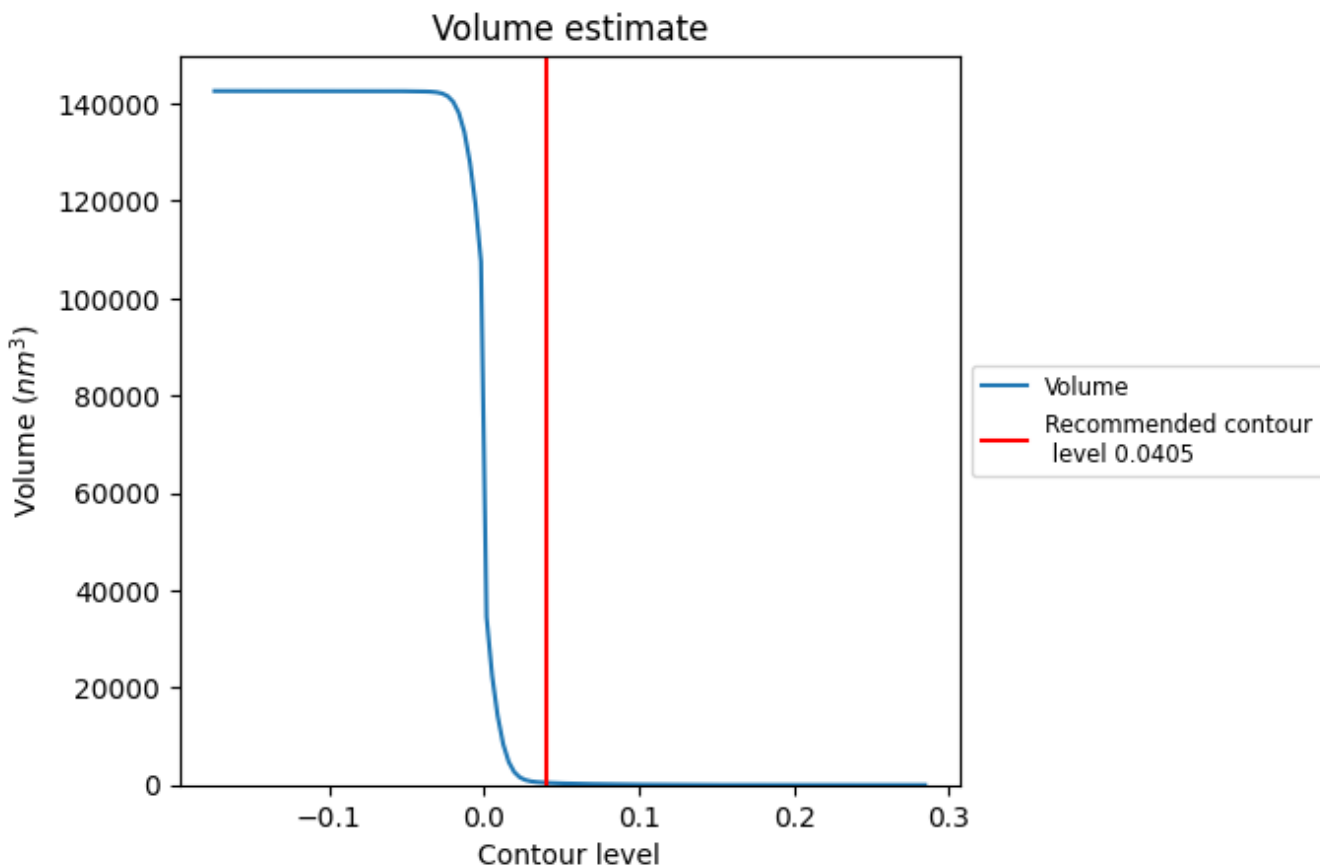
This section contains the results of statistical analysis of the map.

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.

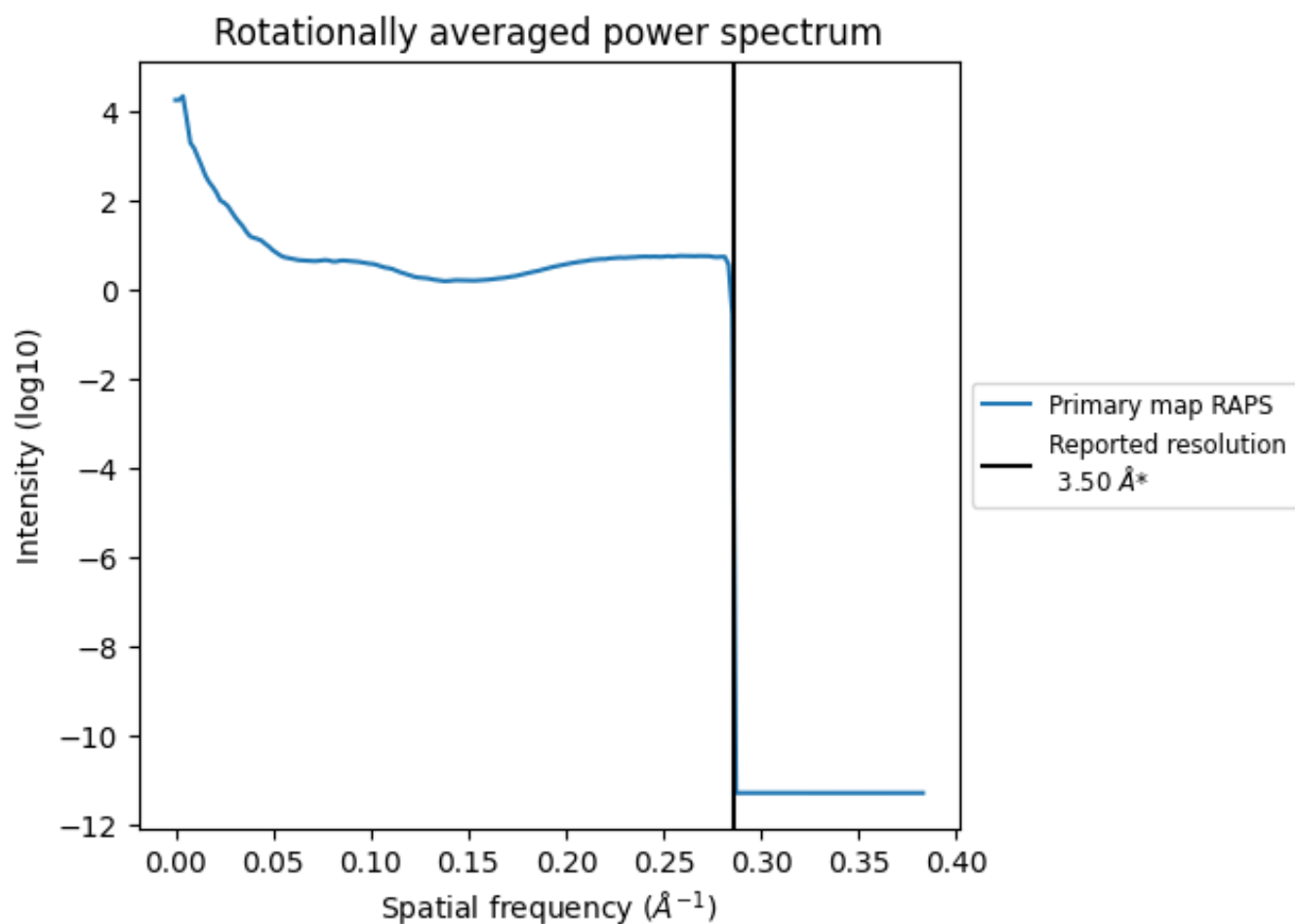
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 444 nm³; this corresponds to an approximate mass of 401 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 0.286\AA^{-1}

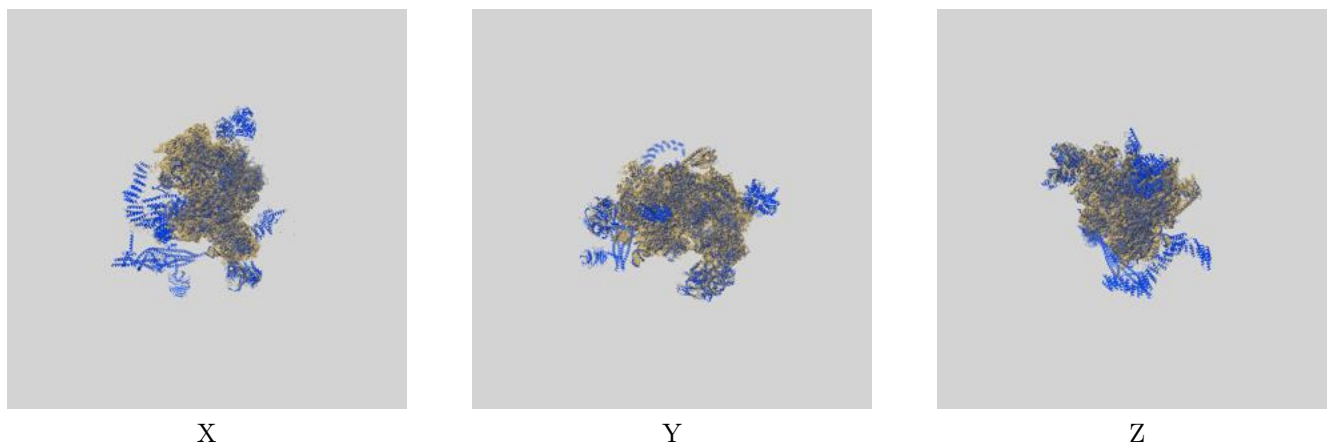
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

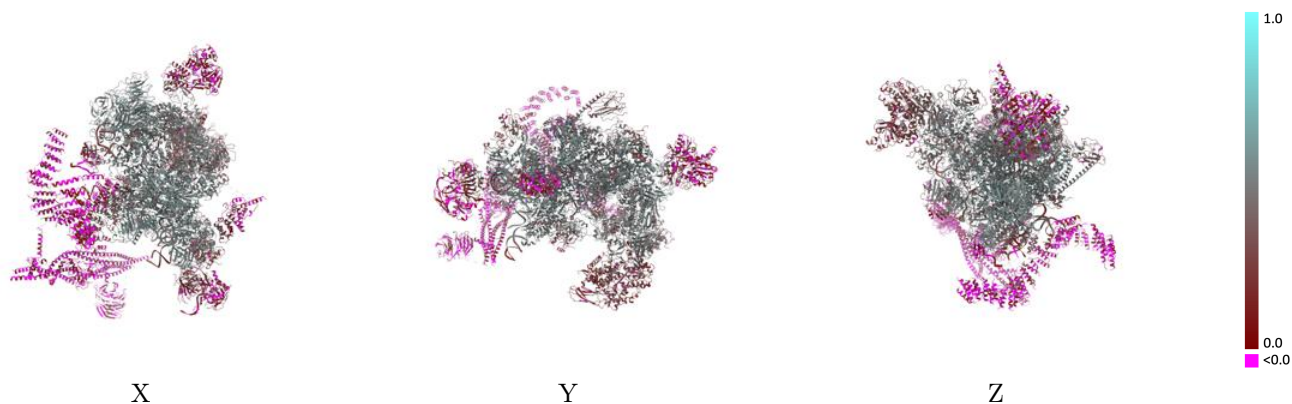
This section contains information regarding the fit between EMDB map EMD-9524 and PDB model 5GM6. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



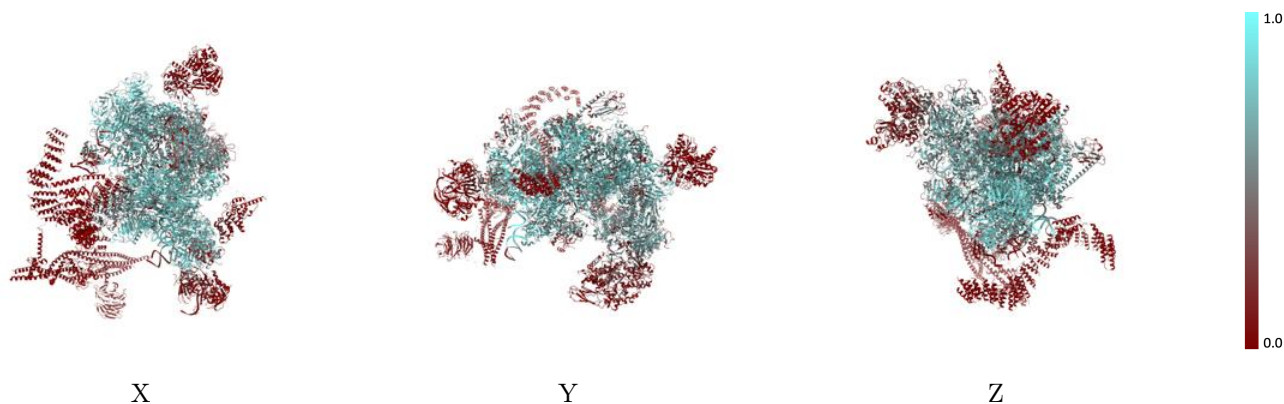
The images above show the 3D surface view of the map at the recommended contour level 0.0405 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



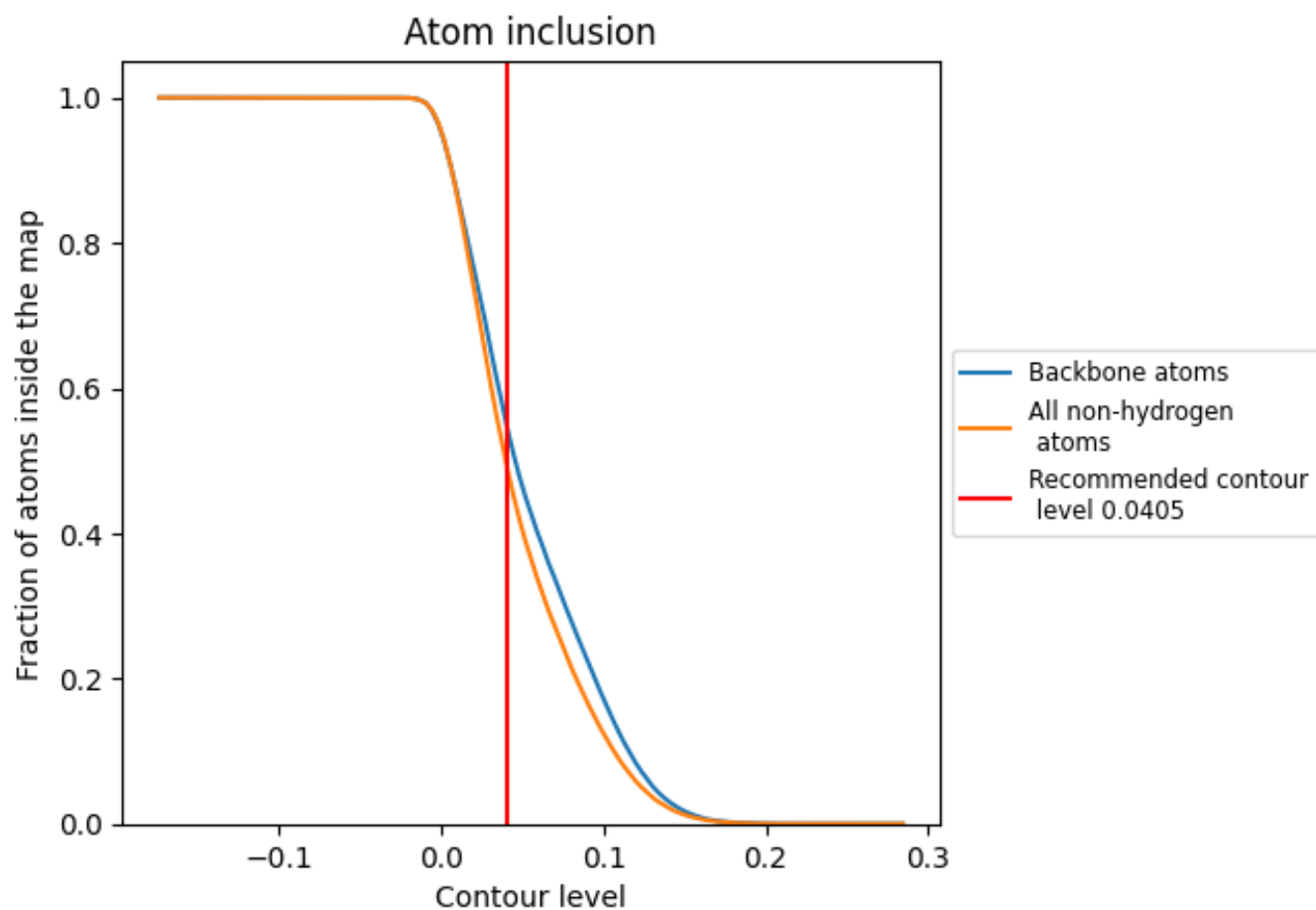
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0405).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 49% 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 (0.0405) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4904	 0.3770
A	 0.7176	 0.5060
B	 0.3691	 0.3670
C	 0.6528	 0.4590
D	 0.6507	 0.4110
E	 0.7099	 0.4250
F	 0.7261	 0.4990
G	 0.7372	 0.5160
H	 0.7322	 0.5150
I	 0.7079	 0.5150
J	 0.7820	 0.5380
K	 0.7556	 0.5180
L	 0.5519	 0.3720
M	 0.4314	 0.2930
N	 0.6833	 0.4730
O	 0.7485	 0.5090
P	 0.5776	 0.4550
Q	 0.4369	 0.3720
R	 0.6047	 0.4360
S	 0.3680	 0.4690
T	 0.7273	 0.5000
U	 0.3669	 0.3550
V	 0.7040	 0.4770
W	 0.5714	 0.4320
X	 0.6150	 0.5320
Y	 0.0382	 0.1520
Z	 0.3501	 0.2870
a	 0.4192	 0.4020
b	 0.3773	 0.4070
c	 0.2533	 0.2320
d	 0.2476	 0.2260
e	 0.2341	 0.1550
f	 0.2134	 0.1990
g	 0.0373	 0.0960
h	 0.0313	 0.0760



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Chain	Atom inclusion	Q-score
i	 0.0227	 0.1060
j	 0.0537	 0.1780
k	 0.0875	 0.2060
l	 0.2217	 0.3230
m	 0.0283	 0.1040
n	 0.6811	 0.4770
o	 0.0000	 0.0280
p	 0.0000	 0.0060
q	 0.0000	 0.0160
r	 0.0000	 0.0140
t	 0.0000	 0.0420
v	 0.0003	 0.0180