wwPDB EM Validation Summary Report (i)

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 (i) 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 (1)) were used in the production of this report:

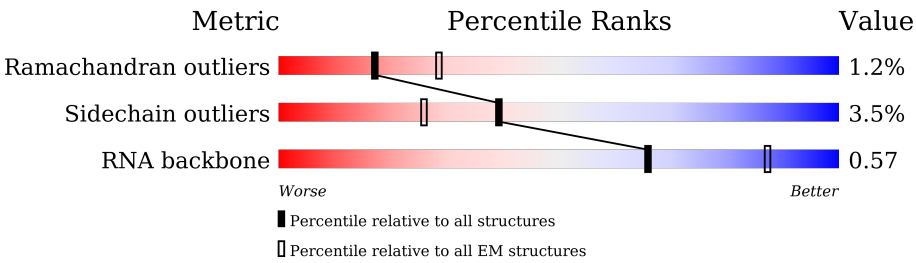
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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 <=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	8%, 91%, 5%, •
2	B	2163	45%, 83%, 16%
3	C	1008	13%, 84%, •, 13%
4	D	214	16%, 43%, 12%, 45%
5	E	112	19%, 77%, 15%, 8%
6	F	1361	6%, 83%, •, 13%
7	H	436	•, 31%, •, 65%
8	I	266	6%, 34%, •, 62%

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Mol	Chain	Length	Quality of chain
9	J	107	89% 7%
10	K	85	5% 87% 12%
11	L	1175	5% 94%
12	N	25	24% 64% 36%
13	M	61	43% 39% 43% 18%
14	O	451	5% 72% 25%
15	P	379	15% 59% 6% 35%
16	Q	364	23% 46% 5% 49%
17	R	339	15% 71% 5% 23%
18	S	175	25% 38% 59%
19	T	157	7% 95%
20	U	207	46% 81% 15%
21	V	148	83% 14%
22	W	266	10% 33% 6% 61%
23	Y	876	67% 67% 32%
24	Z	577	43% 69% 8% 23%
25	a	259	23% 46% 53%
26	b	301	26% 49% 50%
27	c	587	52% 68% 29%
28	G	971	88% 10%
29	d	687	61% 79% 21%
30	X	135	20% 80%
31	v	859	66% 64% 34%
32	e	213	50% 62% 8% 30%
33	f	215	36% 47% 53%

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Mol	Chain	Length	Quality of chain
34	o	503	25% 23% 75%
34	p	503	25% 24% 75%
34	q	503	76% 71% 24%
34	r	503	25% 23% 75%
35	t	175	89% 81% 6% 11%
36	n	455	95%
37	k	196	41% 41% 59%
38	i	94	79% 74% 5% 20%
39	h	86	81% 78% 19%
40	j	77	90% 86% 10%
41	l	101	64% 77% 19%
42	m	146	56% 52% 44%
43	g	94	100% 93% 5%

2 Entry composition (i)

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
			Total	C	N	O	S		
26	b	150	1224	789	206	223	6	0	0

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

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

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

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

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

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

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

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

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

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

- Molecule 32 is a protein called Protein HSH49.

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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.

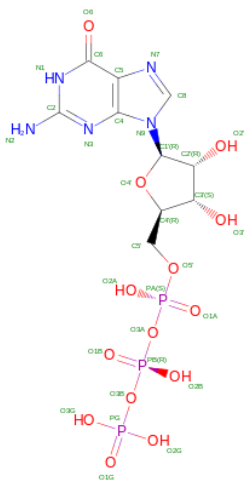
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	82	644	409	110	123	2	0	0

- 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: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



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

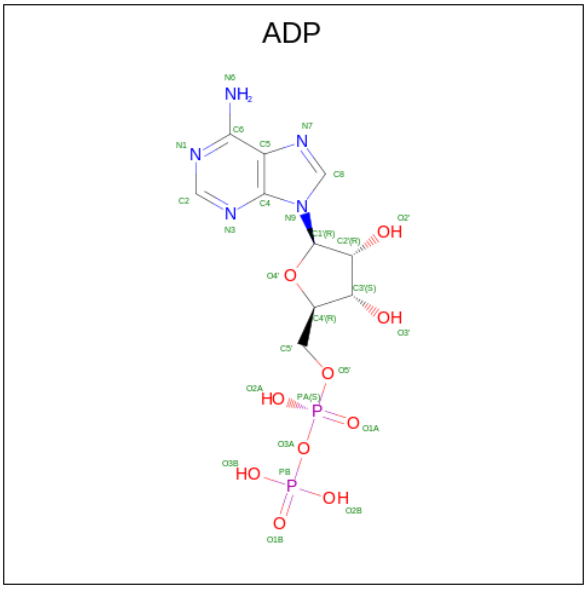
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



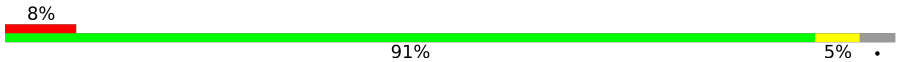
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	Y	1	27	10	5	10	2	0

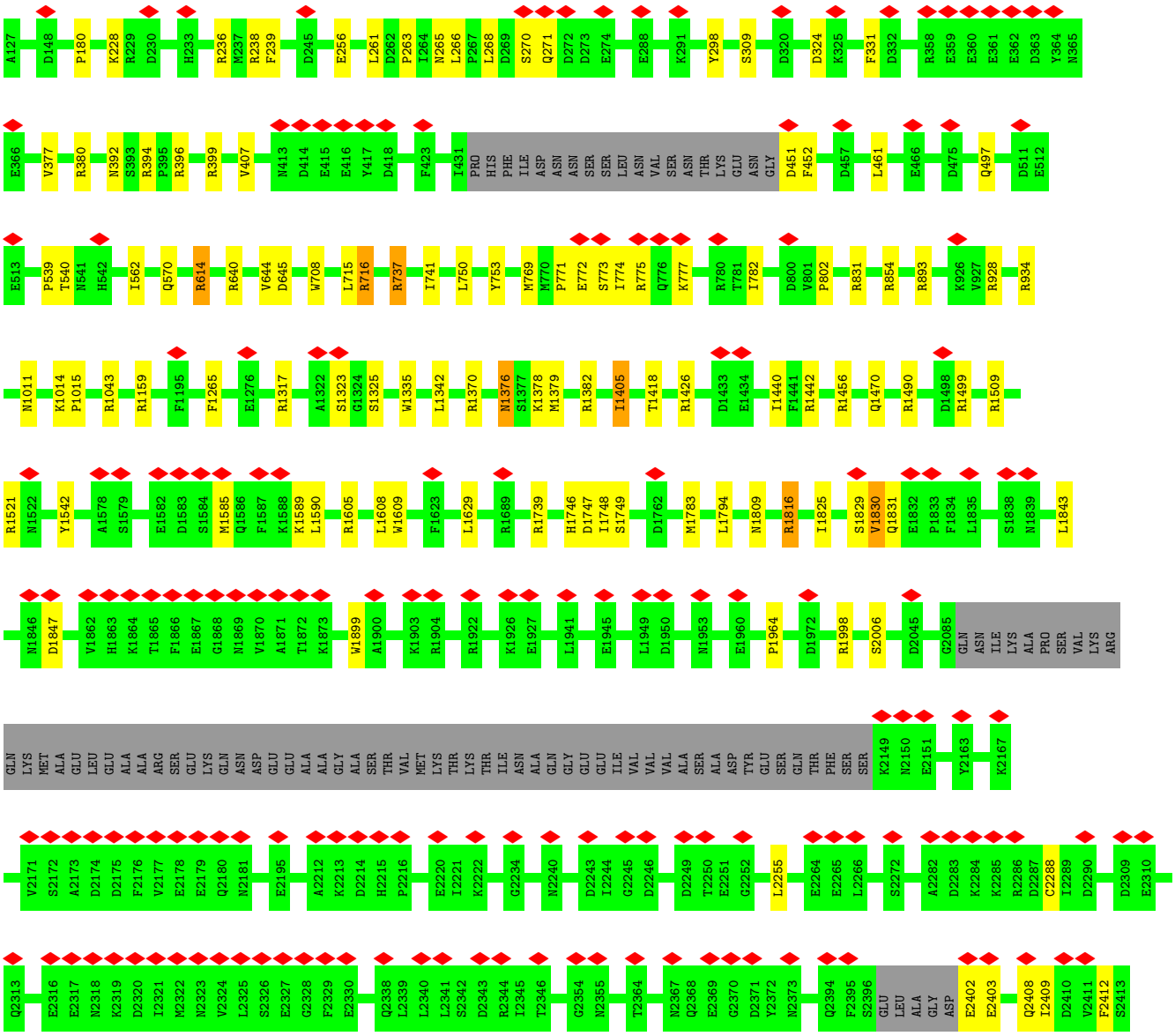
3 Residue-property plots (i)

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

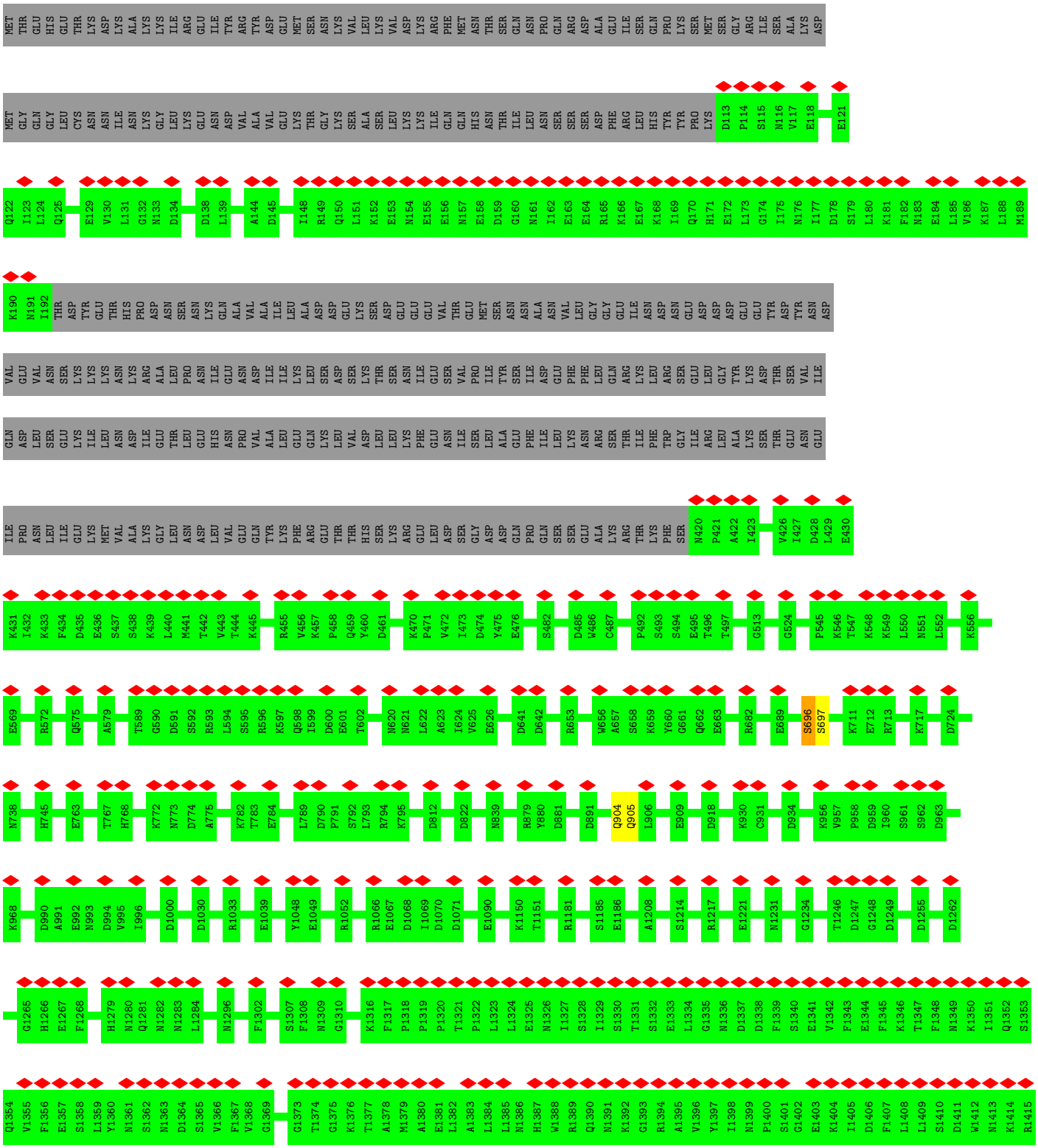
Chain A:





- Molecule 2: Pre-mRNA-splicing helicase BRR2

Chain B: 45% 83% 16%



F1416 S1417 H1418 I1419 A1420 G1421 G1422 K1423 I1424 I1425 N1426 K1427 L1428 G1429 N1430 D1431 P1432 S1433 L1434 N1435 L1436 K1437 L1438 L1439 A1440 K1441 S1442 H1443 V1444 L1445 L1446 A1447 T1448 P1449 V1450 Q1451 F1452 E1453 L1454 L1455 S1456 R1457 R1458 W1459 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 F1508 V1509 C1510 L1511 S1512 N1513 C1514 L1515 A1516 N1517 A1518 R1519 D1520 F1521 G1522 E1523 W1524 A1525 G1526 M1527 T1528 K1529 S1530 N1531 I1532 Y1533 N1534 F1535

S1536 P1537 S1538 E1539 R1540 I1541 E1542 P1543 L1544 E1545 I1546 N1547 I1548 Q1549 S1550 F1551 K1552 D1553 V1554 E1555 H1556 F1559 N1560 F1561 S1562 M1563 L1564 Q1565 M1566 A1567 F1568 E1569 A1570 S1571 A1572 A1573 A1574 A1575 G1576 N1577 R1578 N1579 S1580 S1581 S1582 V1583 F1584 L1585 P1586 S1587 R1588 K1589 D1590 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 G1636 V1637 G1638 I1639 L1640 Y1641 K1642 G1643 M1644 A1645 S1646 N1647 D1648 E1649 R1650 I1651 V1652 K1653 R1654 L1655 Y1656 E1657 Y1658

G1659 A1660 V1661 S1662 V1663 L1664 L1665 I1666 S1667 K1668 D1669 C1670 S1671 A1672 F1673 A1674 C1675 K1676 T1677 D1678 E1679 V1680 I1681 I1682 L1683 L1687 Y1688 D1689 G1690 A1691 E1692 H1693 K1694 Y1698 T1699 I1700 N1701 E1702 L1703 L1704 E1705 M1706 V1707 G1708 L1709 A1710 S1711 G1712 N1713 D1714 S1715 M1716 A1717 G1718 K1719 V1720 L1721 I1722

L1723 T1724 N1727 A1730 K1734 F1735 L1736 I1737 E1738 P1739 L1740 Y1745 L1746 Q1747 Y1748 I1749 I1750 H1751 D1752 T1753 L1754 N1755 N1756 E1757 I1758 A1759 N1760 S1761 I1762 I1763 Q1764 S1765 K1766 Q1767 D1768 C1769 V1770 D1771 W1772 F1773 T1774 Y1775 S1776 Y1777 R1780 R1781 V1784 G1790 V1791 R1792 D1793 T1794 S1795

P1796 H1797 G1798 I1799 F1802 L1803 S1804 N1805 L1806 V1807 E1808 T1809 C1810 L1811 N1812 D1813 L1814 V1815 E1816 S1817 S1818 F1819 I1820 E1821 I1822 D1823 D1824 T1825 GLU ALA GLU VAL THR ALA GLU VAL ASN GLY GLY ASP ASP GLU ALA T1841 E1842 I1843 I1844 S1845 T1846 L1847 S1848 N1849 G1850 L1851 I1852 A1853 S1854 H1855 Y1856

G1857 V1858 S1859 F1860 F1861 T1862 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 R1912 F1913 P1914 E1915 H1916

T1917 S1918 S1919 G1920 S1921 V1922 S1923 F1924 K1925 V1926 F1927 Y1928 L1929 L1930 Q1931 A1932 Y1933 F1934 S1935 R1936 L1937 E1938 L1939 P1940 V1941 D1942 F1943 Q1944 N1945 D1946 L1947 K1948 D1949 I1950 L1951 E1952 K1953 V1954 V1955 P1956 L1957 I1958 N1959 V1960 V1961 V1962 D1963 I1964 L1965 S1966 A1967 N1968 G1969 Y1970 L1971 N1972 A1973 T1974 T1975 A1976

M1977 D1978 L1979 A1980 Q1981 M1982 L1983 I1984 Q1985 G1986 V1987 W1988 D1989 V1990 D1991 N1992 P1993 L1994 R1995 Q1996 I1997 P1998 H1999 F2000 N2001 N2002 K2003 I2004 L2005 E2006 K2007 C2008 K2009 E2010 I2011 N2012 V2013 E2014 T2015 V2016 Y2017 D2018 N1959 I2019 M2020 A2021 L2022 E2023 D2024 E2025 E2026 R2027 D2028 E2029 I2030 L2031 T2032 L2033 T2034 D2035 S2036

Q2037 L2038 A2039 Q2040 V2041 A2042 A2043 F2044 V2045 N2046 N2047 Y2048 P2049 N2050 V2051 E2052 L2053 T2054 Y2055 S2056 L2057 N2058 N2059 S2060 D2061 S2062 L2063 I2064 S2065 G2066 V2067 K2068 Q2069 K2070 I2071 T2072 I2073 Q2074 L2075 T2076 R2077 D2078 V2079 E2080 P2081 E2082 N2083 L2084 Q2085 V2086 D2147 T2087 S2088 E2089 K2090 Y2091 P2092 F2093 D2094 K2095 L2096

E2097 S2098 W2099 W2100 L2101 V2102 L2103 G2104 E2105 V2106 S2107 K2108 K2109 E2110 L2111 Y2112 A2113 I2114 K2115 K2116 V2117 T2118 L2119 N2120 K2121 E2122 T2123 Q2124 Q2125 Y2126 E2127 L2128 E2129 F2130 D2131 T2132 P2133 T2134 S2135 G2136 K2137 H2138 N2139 L2140 T2141 I2142 W2143 C2144 V2145 C2146 S2148 Y2149 L2150 D2151 A2152 D2153 K2154 E2155 L2156

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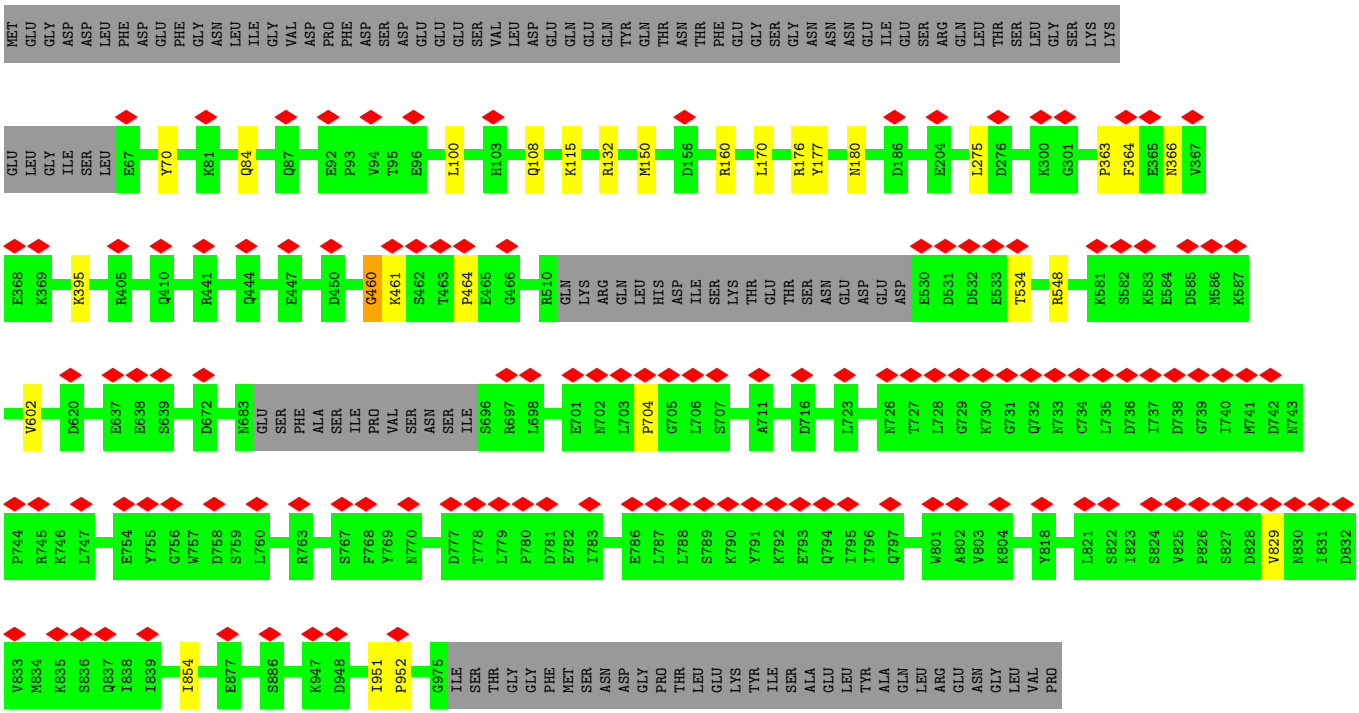
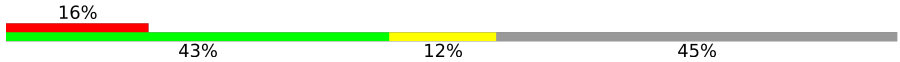
• Molecule 3: Pre-mRNA-splicing factor SNU114

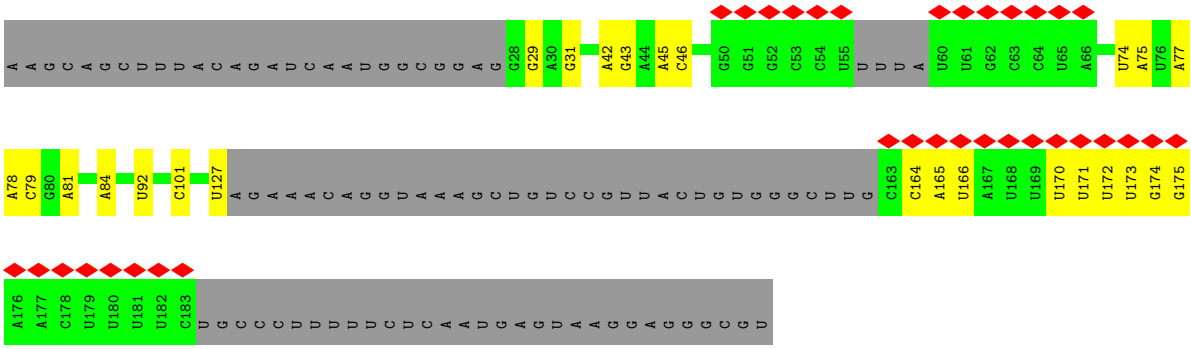
Chain C:



• Molecule 4: Saccharomyces cerevisiae strain CDRDR_sf_H chromosome VII sequence

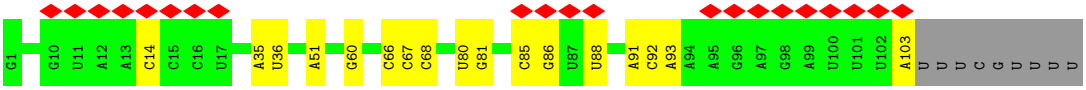
Chain D:





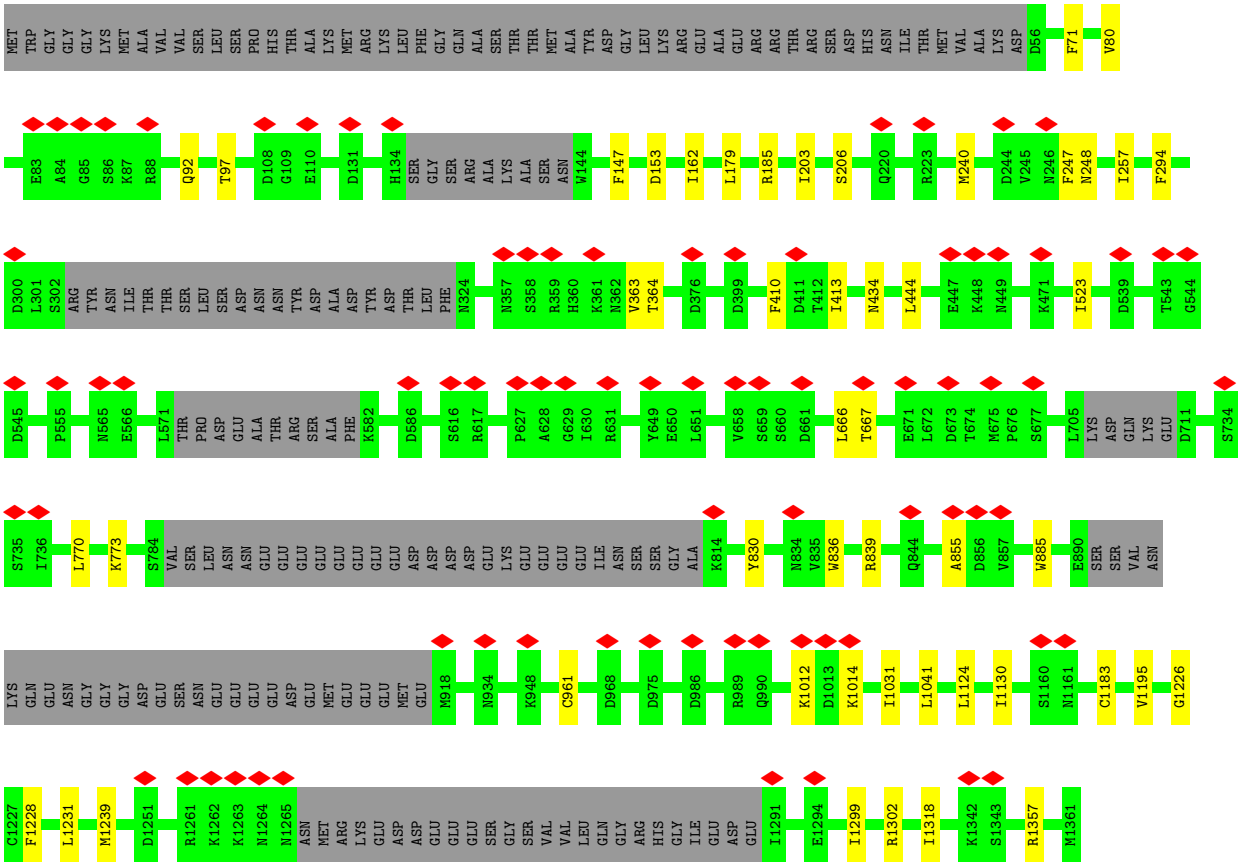
• Molecule 5: Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence

Chain E:



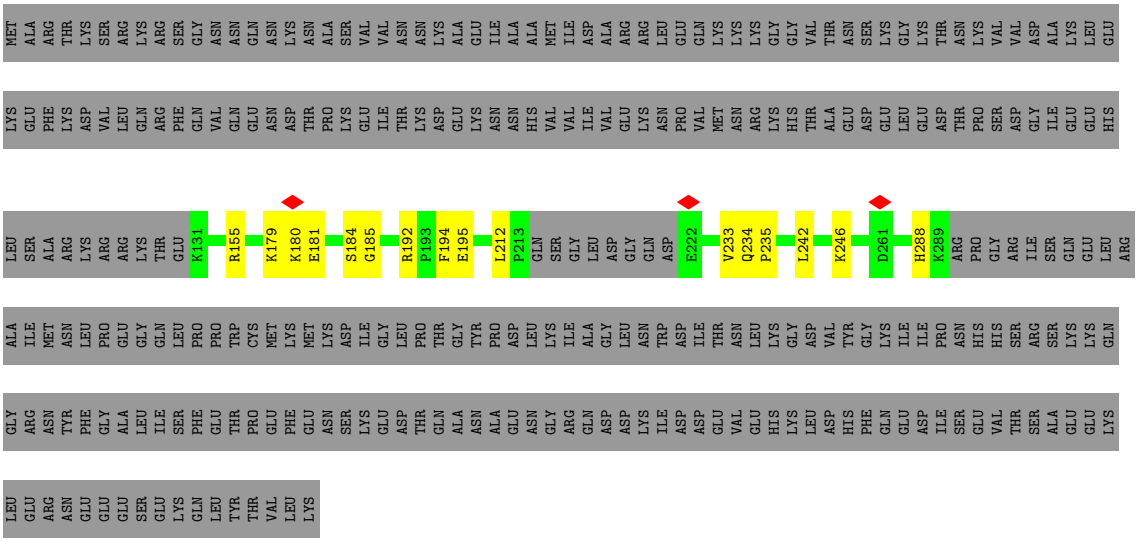
• Molecule 6: Pre-mRNA-splicing factor RSE1

Chain F:



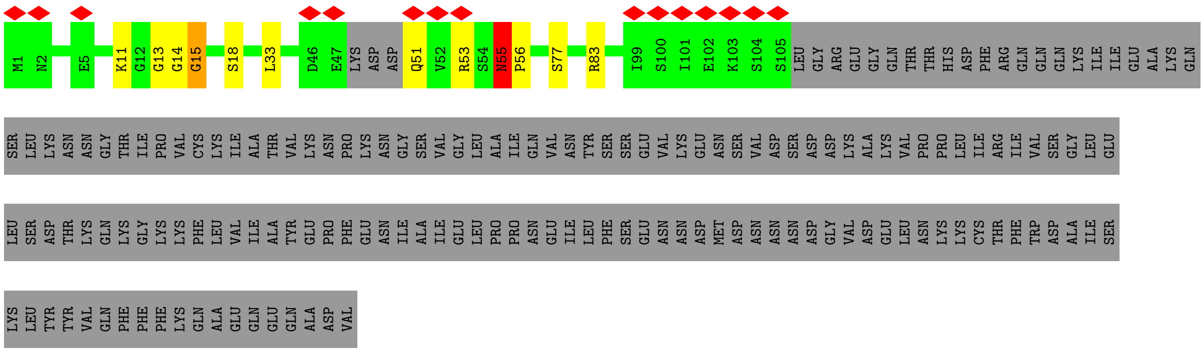
• Molecule 7: Cold sensitive U2 snRNA suppressor 1

Chain H:



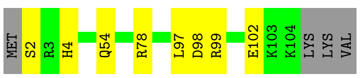
• Molecule 8: Pre-mRNA-splicing factor PRP11

Chain I:



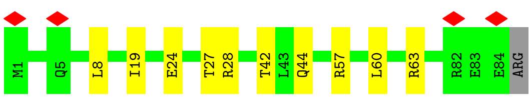
• Molecule 9: Pre-mRNA-splicing factor RDS3

Chain J:



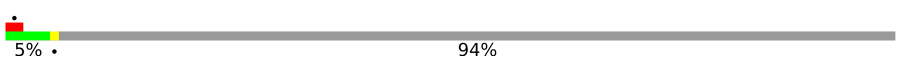
• Molecule 10: RDS3 complex subunit 10

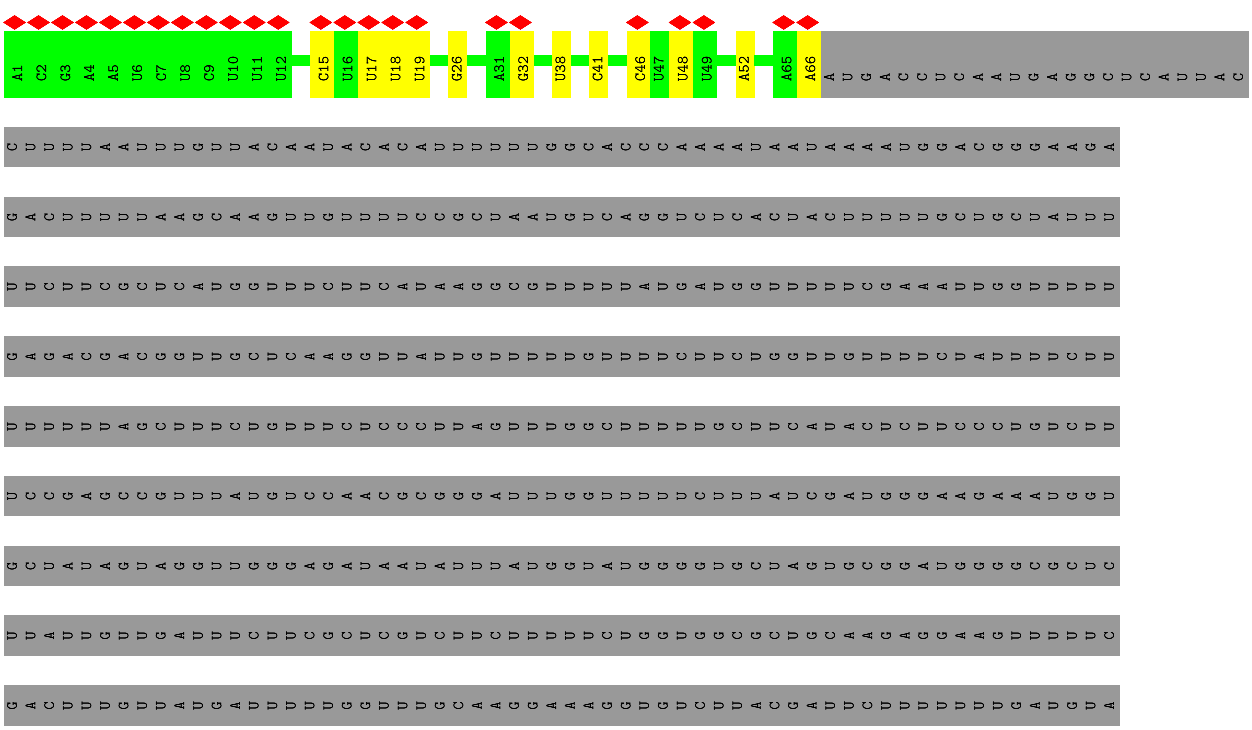
Chain K:

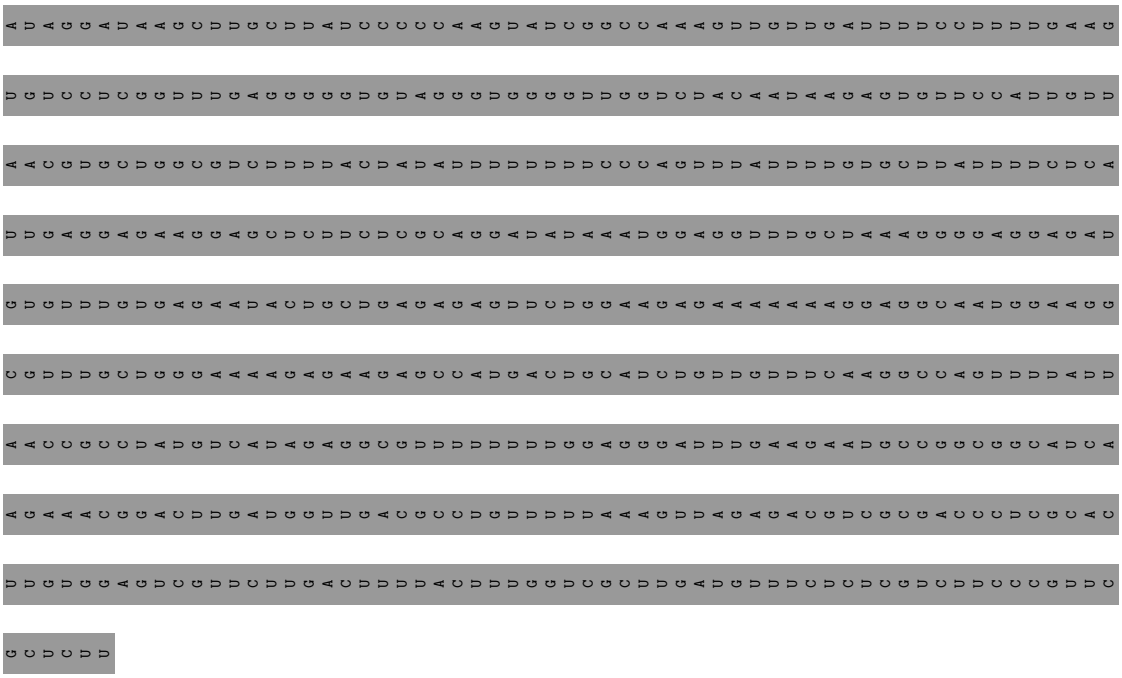


• Molecule 11: U2 snRNA

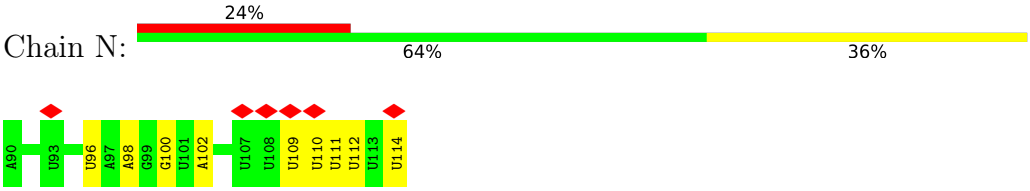
Chain L:



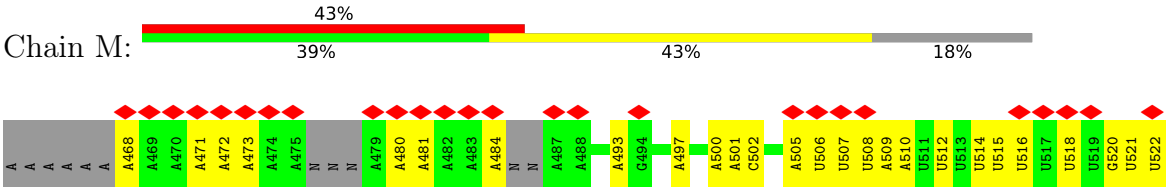




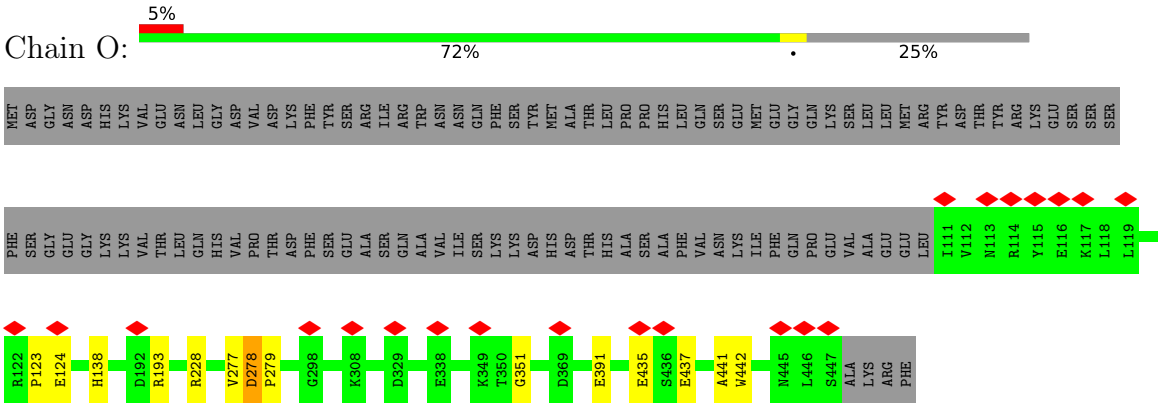
• Molecule 12: Pre-mRNA



• Molecule 13: Pre-mRNA

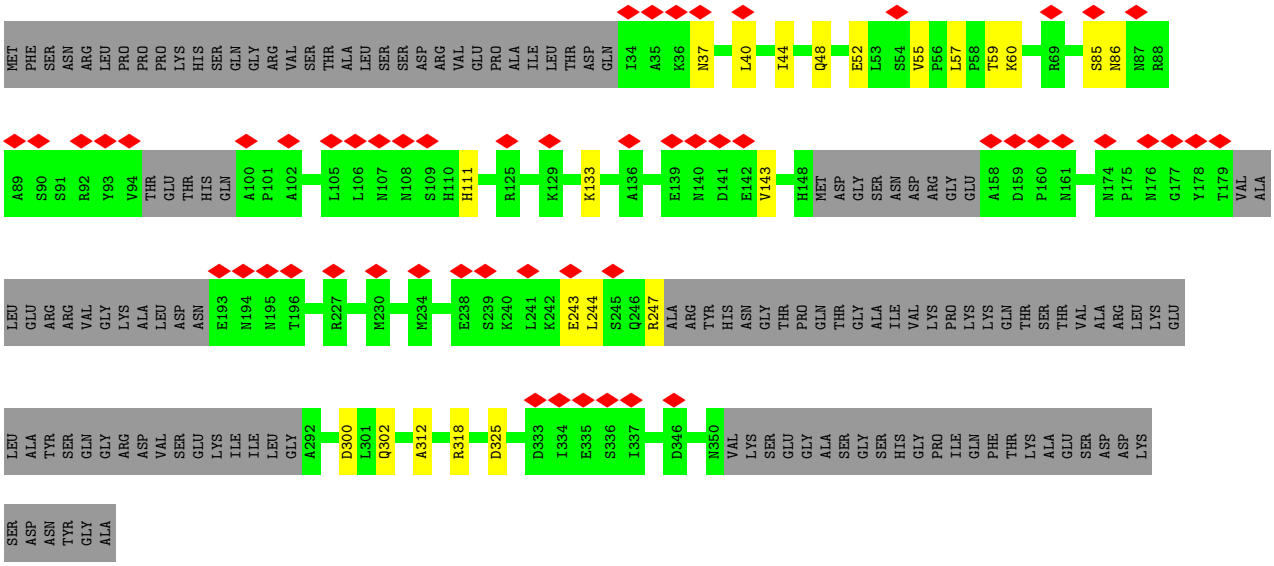


• Molecule 14: Pre-mRNA-splicing factor PRP46



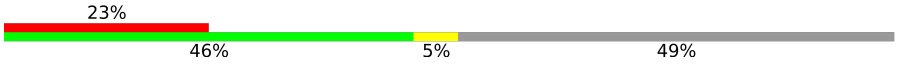
• Molecule 15: Pre-mRNA-processing protein 45

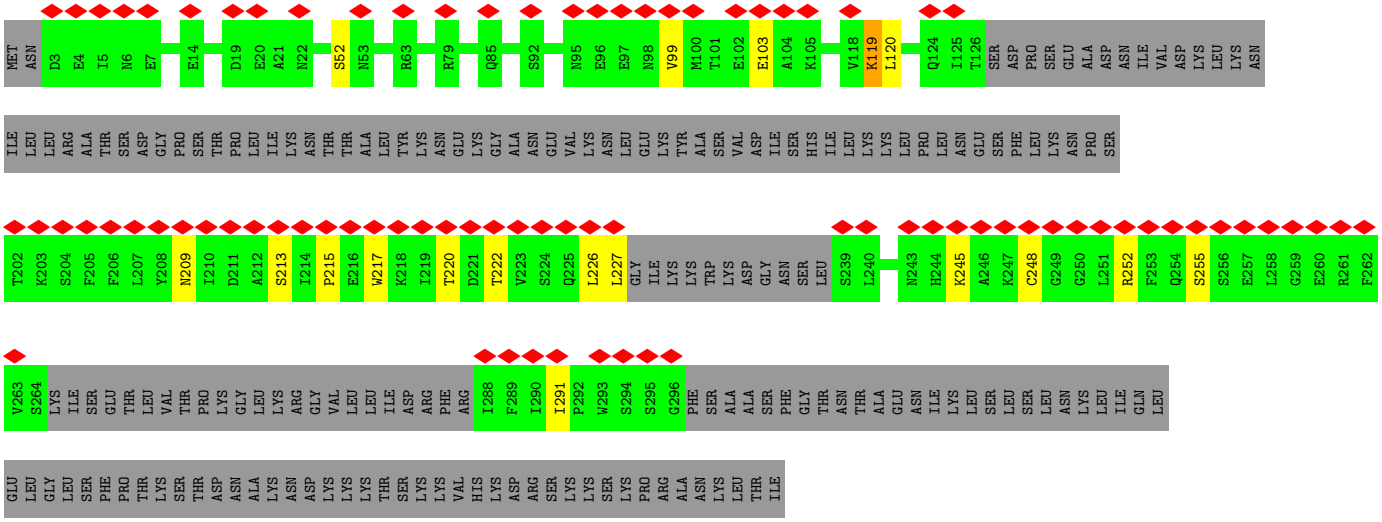
Chain P:



• Molecule 16: Pre-mRNA-splicing factor SLT11

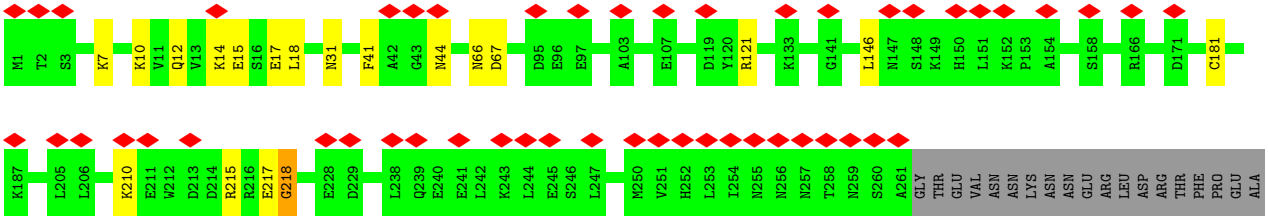
Chain Q:

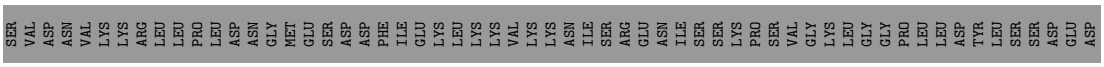




• Molecule 17: Pre-mRNA-splicing factor CWC2

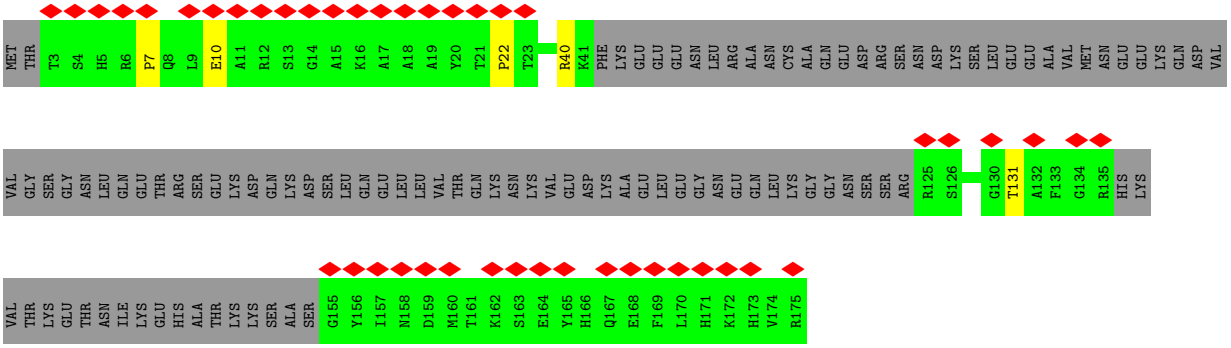
Chain R:





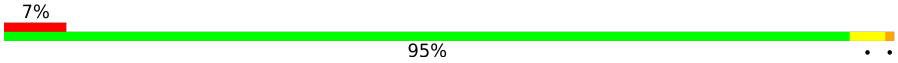
• Molecule 18: Pre-mRNA-splicing factor CWC15

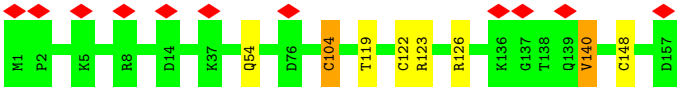
Chain S:



• Molecule 19: Pre-mRNA-splicing factor BUD31

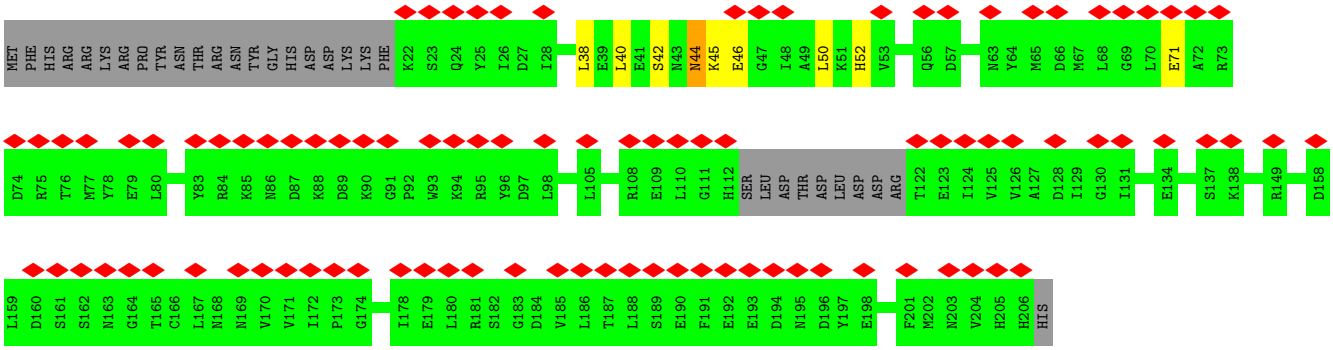
Chain T:





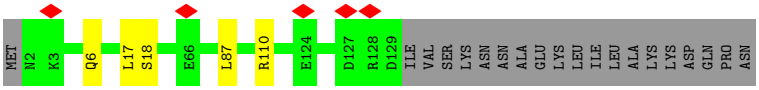
• Molecule 20: Pre-mRNA leakage protein 1

Chain U:



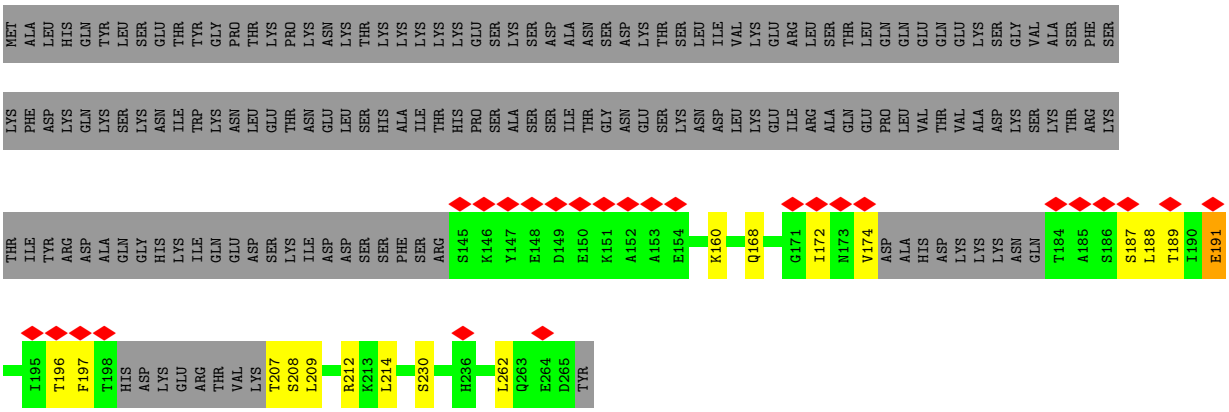
• Molecule 21: U2 snRNP component IST3

Chain V:



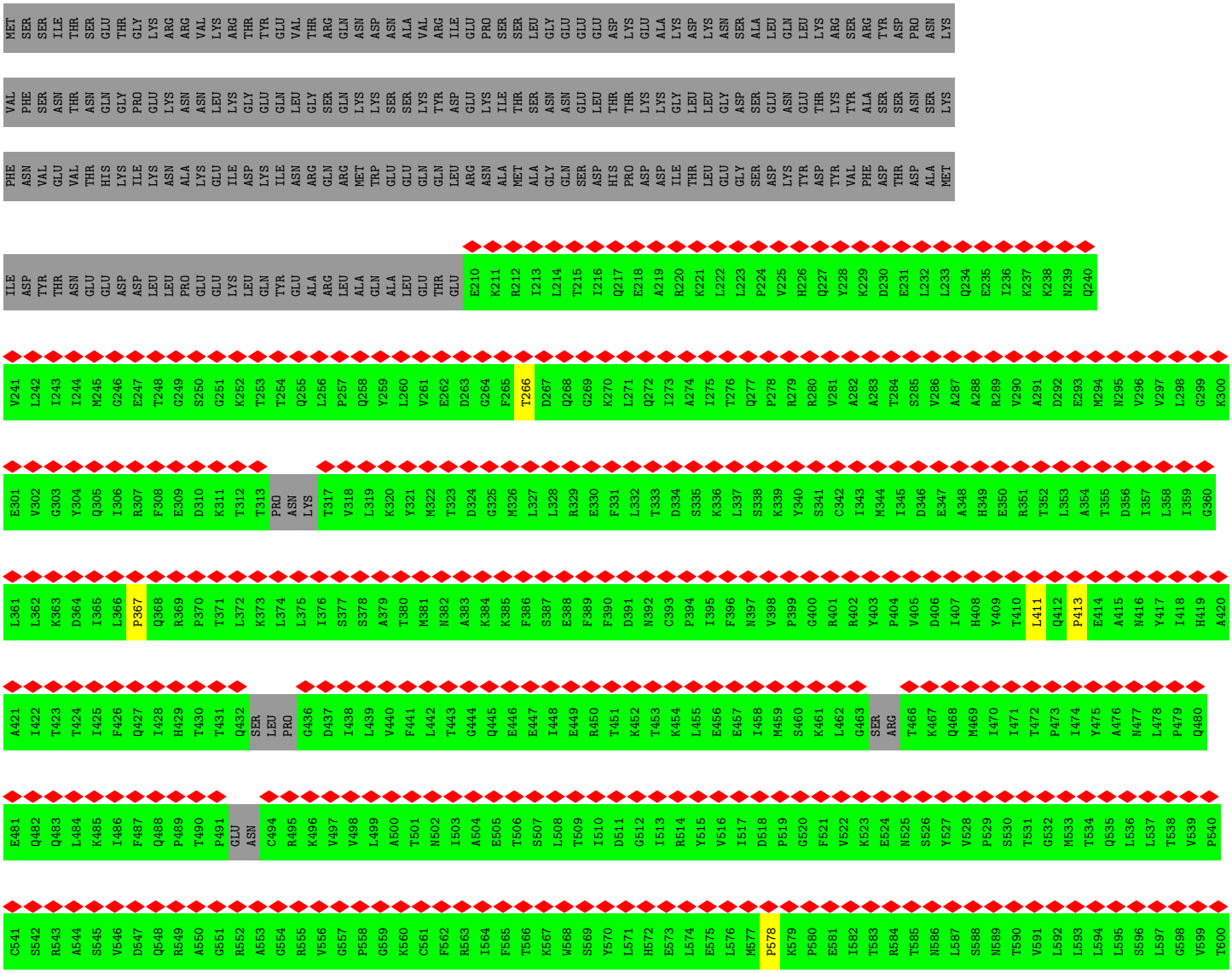
• Molecule 22: Pre-mRNA-splicing factor CWC26

Chain W:



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

Chain Y:



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H661 GLU GLN CYS GLN GLY V667 L668 E669 E670 C671 L672 T673 I674 V675 S676 M677 L678 H679 GLU THR P682 S683 L684 F685 I686 GLY GLN LYS R690 D691 A692 A693 A694 S695 V696 L697 S698 E699 V700 E701 S702 D703 H704 I705 L706 Y707 L708 E709 I710 F711 N712 Q713 W714 R715 N716 SER LYS PHE SER

ARG SER TRP C724 Q725 D726 H727 K728 I729 Q730 F731 K732 T733 M734 L735 R736 V737 R738 N739 I740 R741 N742 Q743 L744 F745 R746 C747 S748 E749 K750 V751 G752 L753 V754 E755 K756 N757 D758 Q759 A760 ARG MET LYS ILE GLY ASN ILE ALA GLY TYR I771 N772 A773 R774 I775 T776 R777 C778 F779 I780

S781 G782 F783 P784 M785 N786 I787 V788 Q789 LEU GLY PRO THR G794 Y795 Q796 T797 M798 GLY ARG SER SER GLY GLY LEU N806 H810 P811 T812 S813 ILE LEU PHE VAL ASN HIS LYS GLU LYS ALA GLN R825 P826 L831 Y832 Q833 Q834 L835 M836 L837 T838 S839 K840 E841 F842 I843 R844 D845

C846 L847 V848 I849 PRO LYS E852 E853 W854 L855 I856 D857 M858 V859 P860 Q861 I862 F863 K864 D865 L866 I867 D868 ASP LYS THR ASN ARG GLY ARG ARG

- Molecule 24: Pre-mRNA-splicing factor CWC22

Chain Z:

MET SER THR ALA THR ILE GLN D8 E9 D10 I11 K12 F13 Q14 R15 E16 N17 W18 E19 M20 I21 R22 S23 H24 V25 S26 P27 I28 I29 S30 N31 L32 T33 M34 D35 N36 L37 Q38 E39 S40 H41 R42 D43 L44 F45 Q46 V47 N48 I49 L50 I51 G52 R53 N54 I55 I56 C57 K58 N59 V60

V61 D62 F63 T64 L65 N66 K67 Q68 N69 G70 R71 L72 I73 P74 A75 L76 S77 A78 L79 I80 A81 L82 L83 N84 S85 D86 I87 P88 D89 I90 N91 E92 T93 L94 A95 K96 E97 L98 M99 L100 M101 F102 V103 Q104 Q105 F106 N107 R108 K109 D110 Y111 V112 S113 C114 G115 N116 I117 L118 Q119 C120

L121 S122 I123 L124 F125 L126 Y127 D128 V129 I130 H131 E132 I133 V134 I135 L136 Q137 I138 L139 L140 L141 L142 L143 E144 K145 N146 S147 L148 R149 L150 V151 I152 A153 V154 M155 K156 I157 C158 G159 W160 K161 L162 A163 L164 V165 S166 K167 K168 T169 H170 D171 M172 I173 W174 E175 K176 L177 R178 Y179 I180

L181 Q182 T183 Q184 E185 L186 S187 S188 T189 L190 R191 E192 S193 L194 E195 T196 L197 F198 E199 I200 R201 Q202 K203 D204 Y205 K206 S207 G208 S209 Q210 G211 L212 F213 I214 L215 D216 P217 T218 S219 Y220 T221 V222 H223 T224 H225 S226 Y227 I228 V229 S230 D231 E232 D233 E234 A235 N236 K237 E238 L239 G240

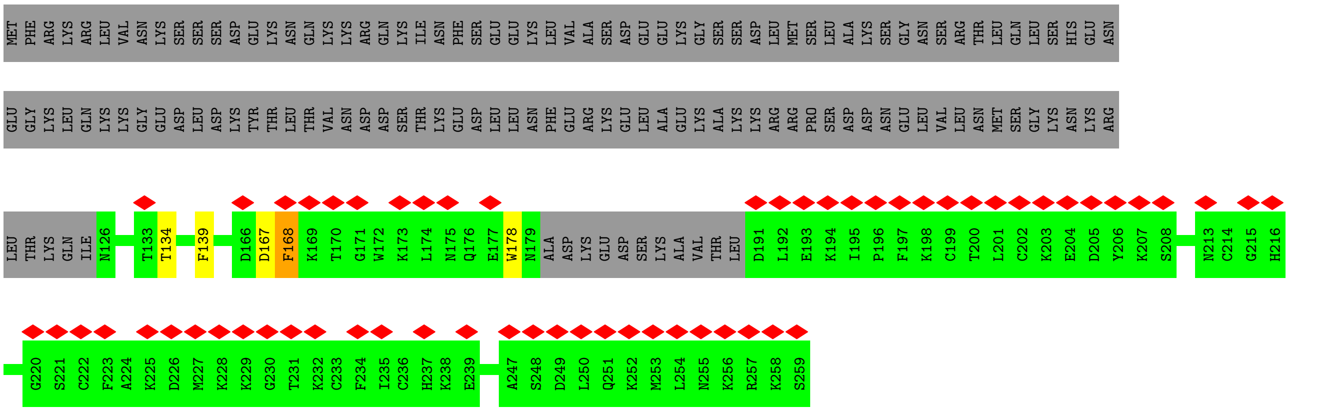
N241 F242 E243 K244 C245 E246 N247 PHE ASN GLU LEU THR MET ALA PHE ASP THR LEU ARG GLN LYS LEU LEU ILE ASN ASN THR SER ASP THR ASN GLU GLY SER ASN SER GLN LEU Q279 L303 S304 R355 E374 L397 P398 D446 E452 G453 D454 A455 E456 R459

G471 E475 L481 I484 Q485 GLU VAL GLU ASP ALA GLU GLU GLU GLU LYS LYS LEU ARG GLU GLU GLU LEU GLU LYS LEU ARG LYS LYS ALA ARG GLU SER GLN PRO THR GLN GLY PRO LYS ILE HIS GLU SER ARG LEU PHE LEU GLN LYS ASP THR ARG GLU ASN SER ARG

SER ARG SER PRO PHE THR VAL GLU THR ARG LYS ARG ALA ARG SER ARG THR PRO PRO ARG GLY SER ARG ASN HIS ARG ASN ARG SER ARG THR PRO PRO ALA ARG ARG GLN ARG HIS ARG

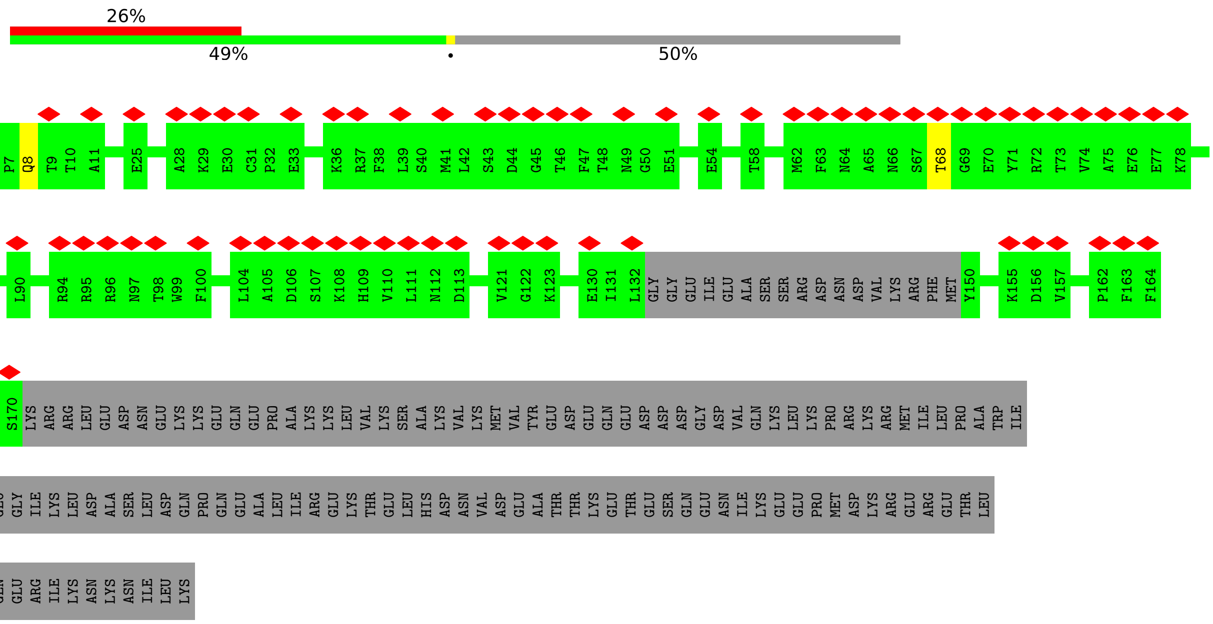
- Molecule 25: Pre-mRNA-splicing factor CWC24

Chain a:



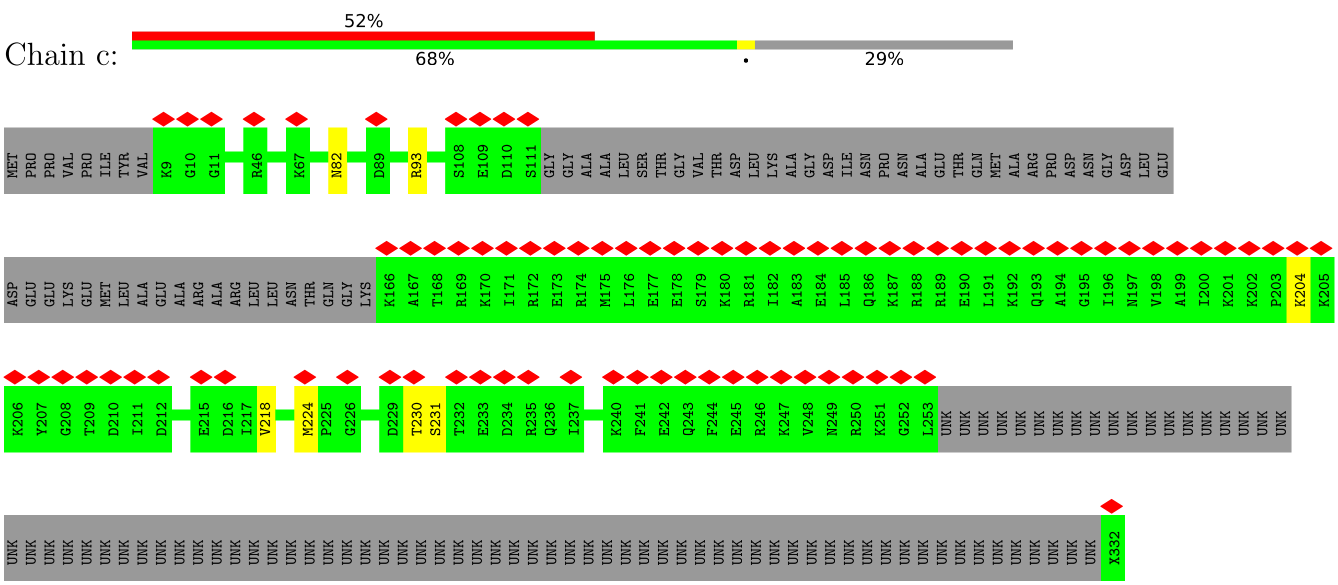
- Molecule 26: Peptidyl-prolyl isomerase CWC27

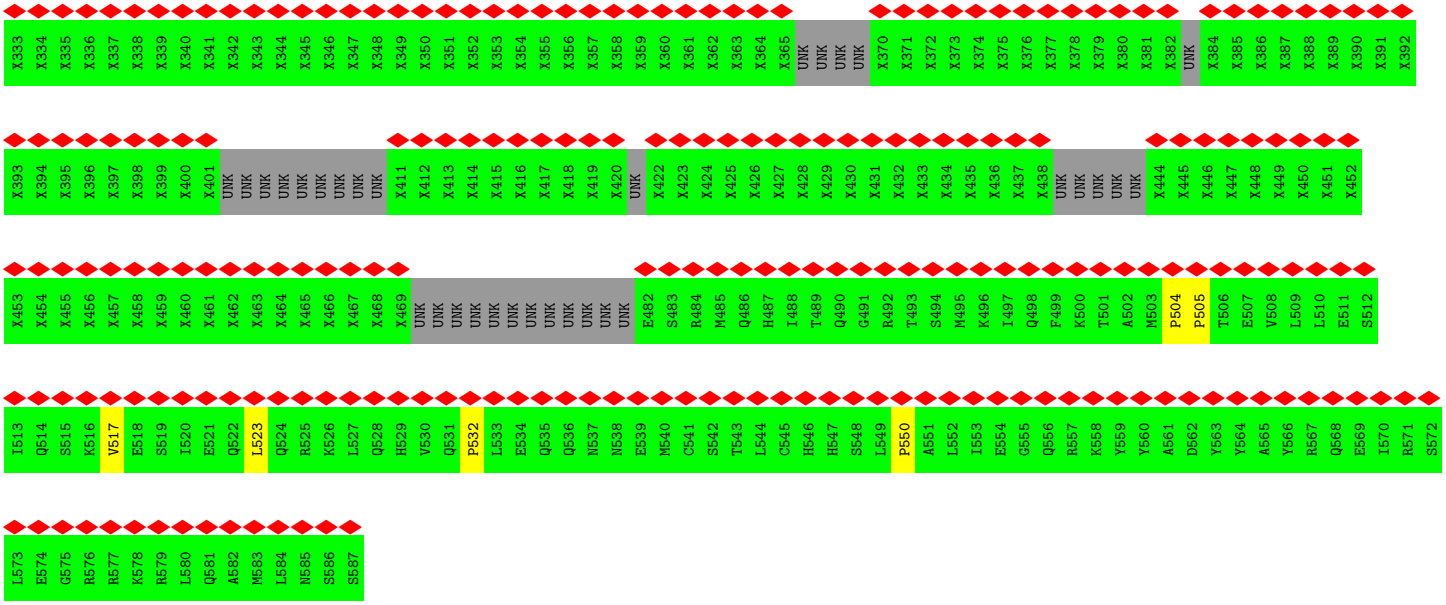
Chain b:



- Molecule 27: Pre-mRNA-splicing factor CEF1

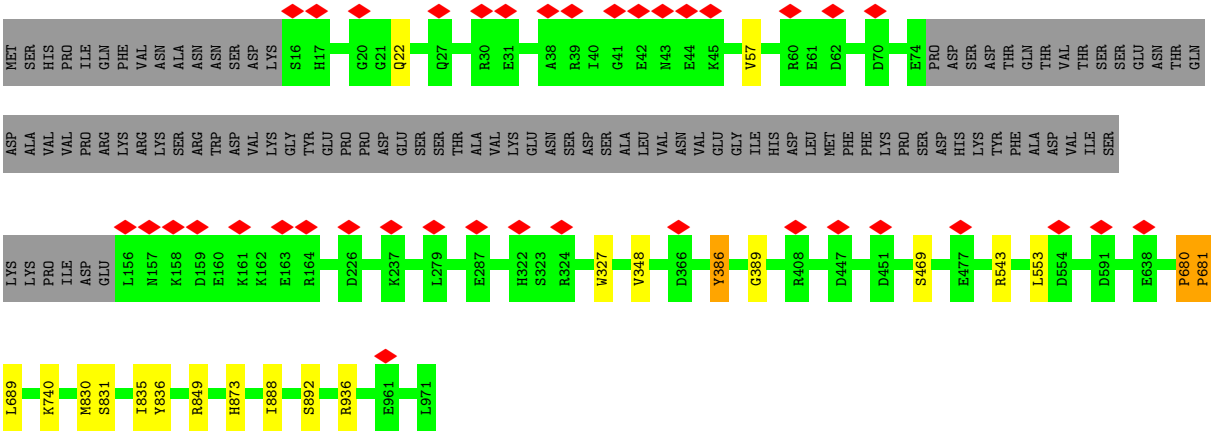
Chain c:





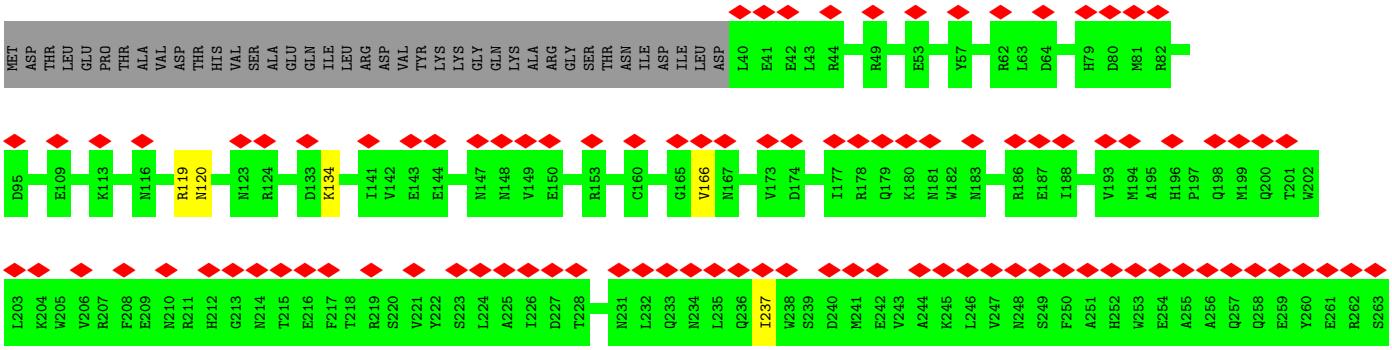
- Molecule 28: U2 snRNP component HSH155

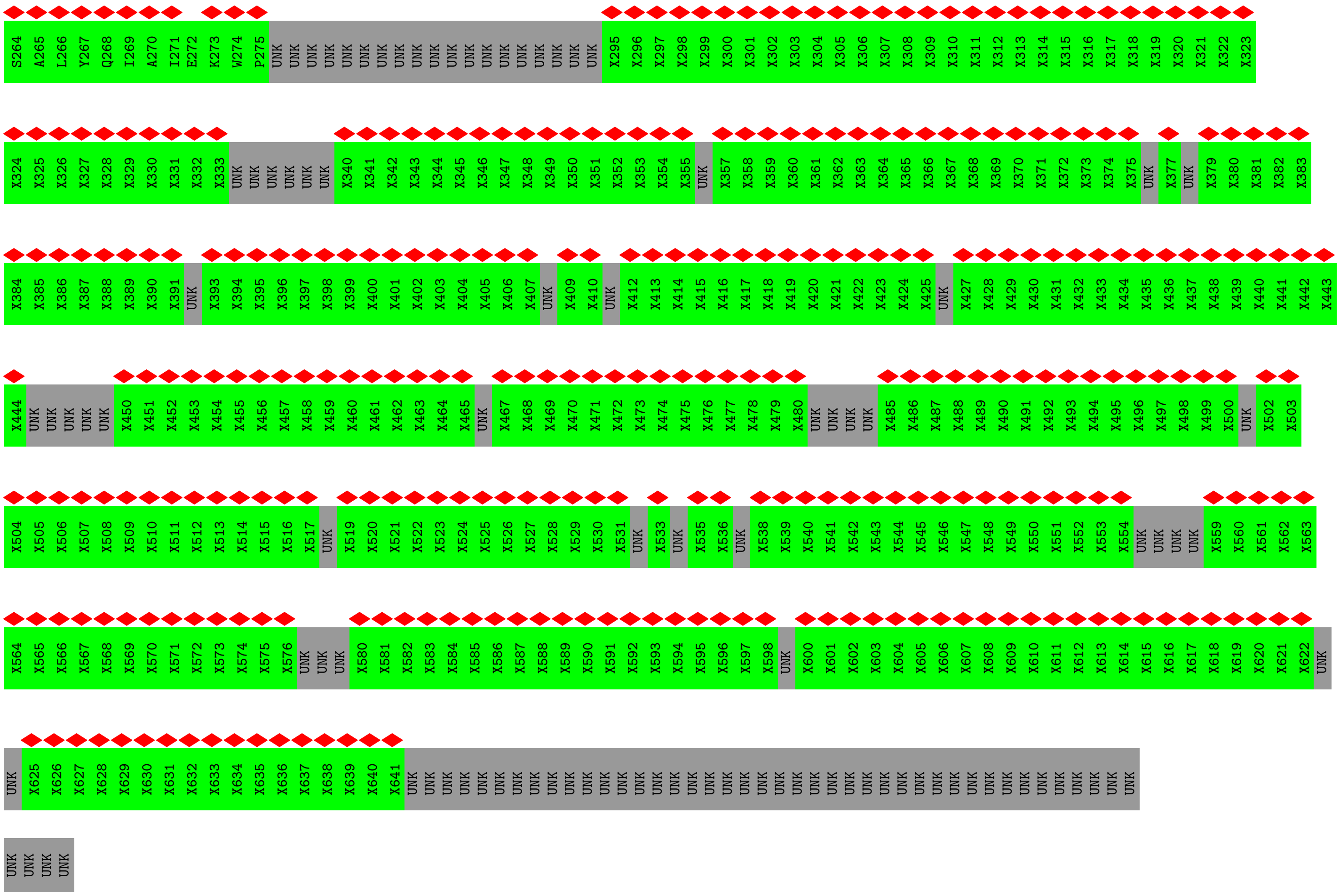
Chain G:



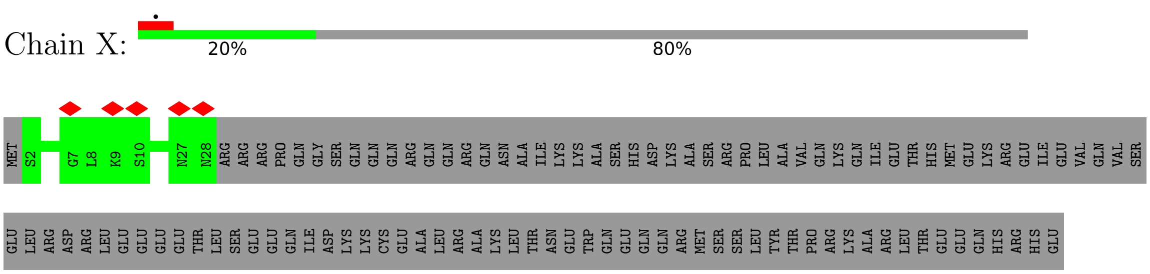
- Molecule 29: Pre-mRNA-splicing factor CLF1

Chain d:

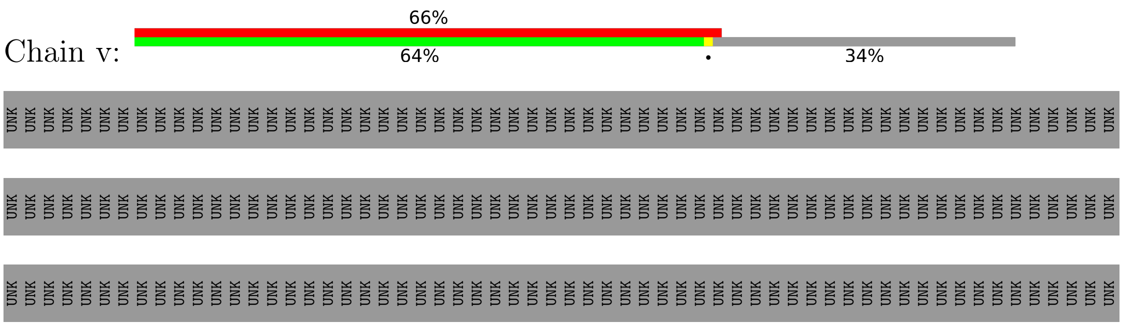


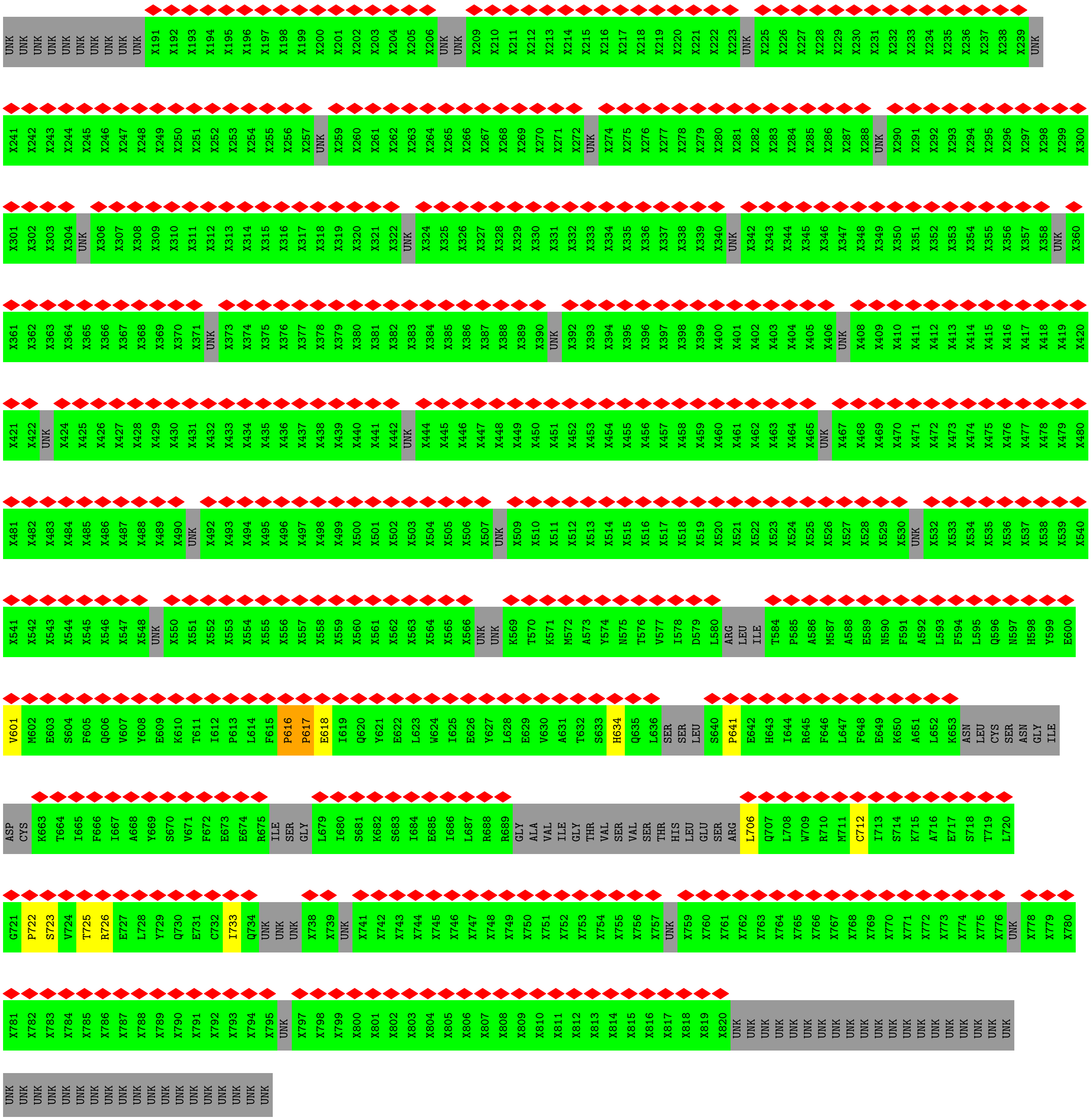


• Molecule 30: Pre-mRNA-splicing factor CWC21



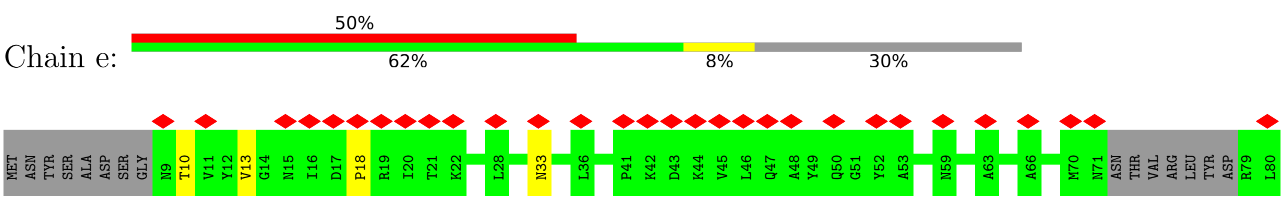
• Molecule 31: Pre-mRNA-splicing factor SYF1





• Molecule 32: Protein HSH49

Chain e:



I81 K82 V83 R84 Q85 V86 T87 G91 T92 THR ASN LEU PRO SER ASN ILE SER LYS ASP MET ILE LEU PRO ILE A108 K109 L110 F111 I112 K113 N114 L115 A116 D117 S118 I119 D120 S121 D122 Q123 L124 V125 K126 I127 F128 N129 K130 F131 G132 K133 L134 ILE ARG GLU P138 E139 I140 F141 Y142

L143 S144 N145 G146 K147 L148 K149 C150 A151 Y152 V153 Y154 F155 E156 D157 F158 E159 K160 A161 D162 L163 A164 I165 K166 S167 L168 N169 N170 Q171 L172 V173 A174 N175 N176 R177 I178 T179 V180 D181 Y182 ALA PHE LYS GLU ASN GLY LYS GLY ASN ALA LYS TYR GLY ASP ASP VAL ASP ARG LEU LEU

ASN LYS GLU ALA LEU LYS HIS ASN MET LEU LYS

- Molecule 33: Pre-mRNA-splicing factor SYF2

Chain f: 36% 47% 53%

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

SER PRO GLU LYS GLU LYS ALA PHE HIS TYR THR VAL GLN GLU TYR ASP ALA TRP GLU ARG ARG HIS PRO GLN GLY LYS THR GLY GLN SER GLN R92 G93 G94 I95 D98 Q99 L103 E106 L109 R110 N111 L112 A113 T114 Q115 T116 Q117 N118 S119 S120 K121 Q122 D123 SER SER

ALA ASP GLU GLU ASP ASN LYS ASN VAL PRO LYS LYS GLY ARG ILE GLY K142 V143 Q144 K145 D146 T147 K148 T149 G150 K151 I154 A155 D156 D157 D158 K159 L160 V161 N162 K163 V166 S167 L168 Q169 S170 E171 S172 K173 K174 A178 R179 K180 R181 Q182 M183 Q184 N185 A186 K187 T188 L189

Y190 G191 V192 E193 S194 F195 I196 N197 D198 K199 N200 K201 Q202 F203 N204 E205 K206 L207 S208 R209 E210 S211 LYS GLY SER GLU

- Molecule 34: Pre-mRNA-processing factor 19

Chain o: 25% 23% 75%

M1 L2 C3 A4 I5 S6 G7 K8 V9 P10 R11 R12 P13 V14 L15 S16 P17 K18 S19 R20 T21 I22 F23 E24 K25 S26 L27 L28 E29 Q30 Y31 V32 K33 D34 T35 G36 N37 D38 P39 I40 T41 N42 E43 P44 L45 S46 I47 E48 E49 I50 V51 GLU ILE VAL PRO SER A57 Q58 Q59 A60

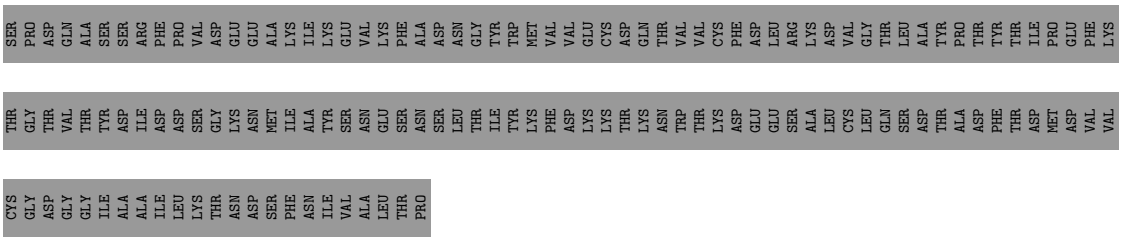
S61 L62 T63 E64 S65 THR ASN SER ALA THR LEU LYS ALA ASN TYR SER I77 P78 N79 L80 L81 T82 S83 L84 Q85 N86 E87 W88 D89 A90 I91 M92 L93 E94 N95 F96 K97 L98 R99 S100 T101 L102 D103 S104 L105 T106 K107 K108 L109 S110 T111 V112 M113 Y114 E115 R116 D117 A118 A119 K120

L121 V122 A123 A124 Q125 L126 L127 M128 E129 K130 N131 E132 D133 S134 K135 D136 L137 P138 K139 S140 SER GLN GLN ALA VAL ALA ILE THR ARG GLU GLU PHE LEU GLN GLY LEU LEU GLN SER SER ARG ASP PHE VAL ALA ARG GLY LYS LEU LYS ALA PRO LYS TRP PRO ILE LEU LYS ASN LEU

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

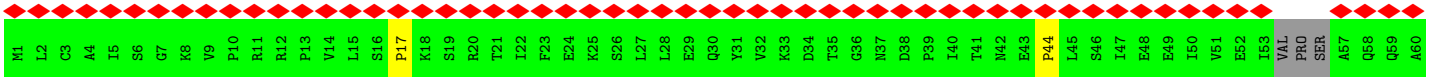
THR GLY GLY GLU HIS PRO ALA ILE ILE SER ARG GLY PRO CYS ASN ARG LEU LEU LEU LEU TYR PRO GLY ASN GLN ILE THR ILE LEU ASP SER LYS THR ASN LYS VAL LEU ARG GLU ILE GLU VAL ASP SER ALA ASN GLU ILE ILE TYR MET TYR GLY HIS ASN GLU VAL ASN THR GLU

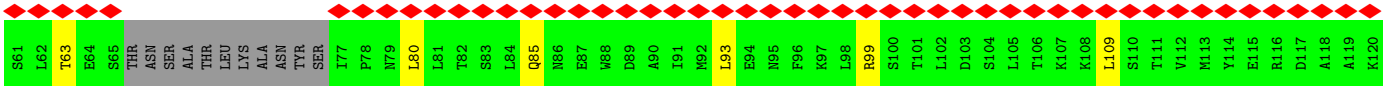
TYR PHE ILE TRP ALA ASP ASN ARG GLY THR ILE GLY PHE GLN SER TYR GLU ASP ASP SER GLN TYR ILE VAL HIS SER ALA LYS SER ASP VAL GLU TYR SER SER GLY VAL LEU HIS LYS ASP SER LEU LEU LEU ALA LEU TYR SER PRO ASP GLY ILE LEU ASP VAL TYR ASN LEU SER

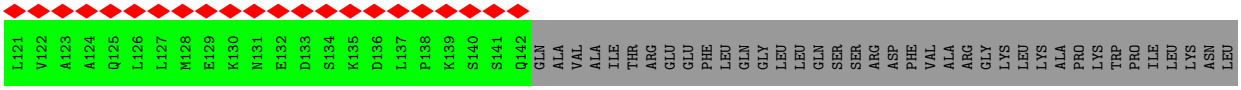


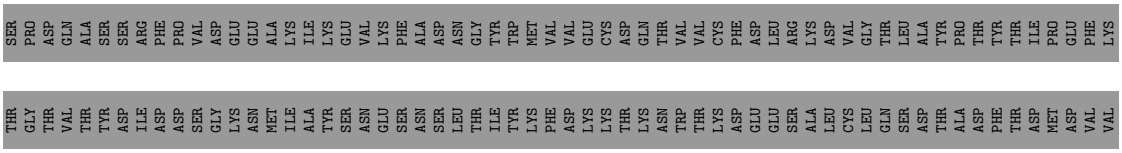
• Molecule 34: Pre-mRNA-processing factor 19

Chain p:



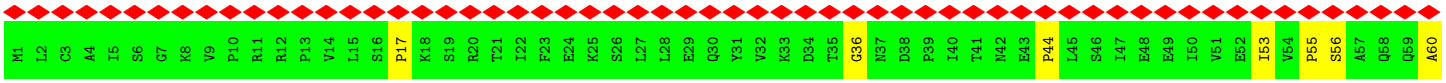


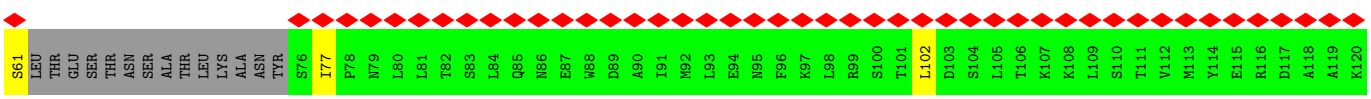


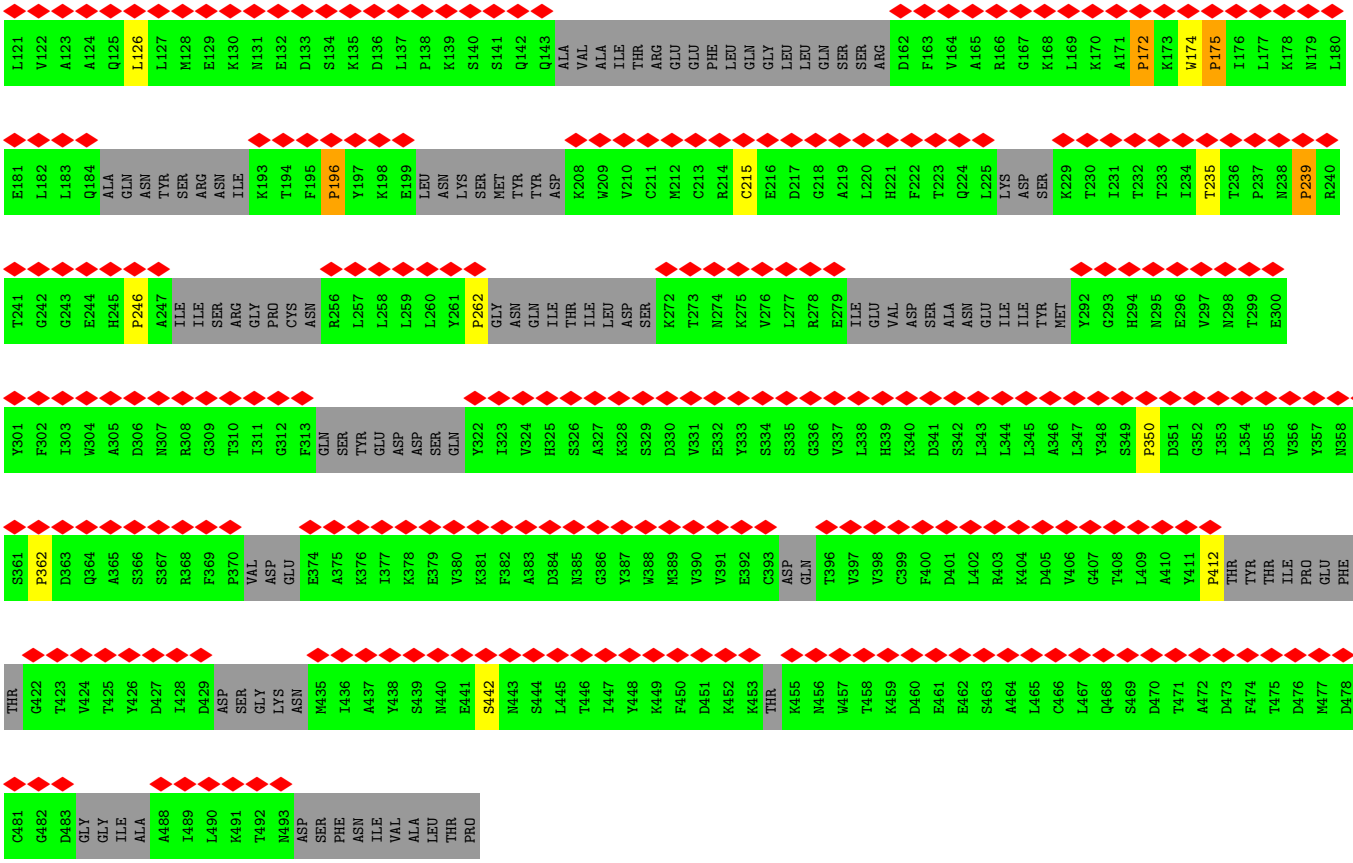


• Molecule 34: Pre-mRNA-processing factor 19

Chain q:

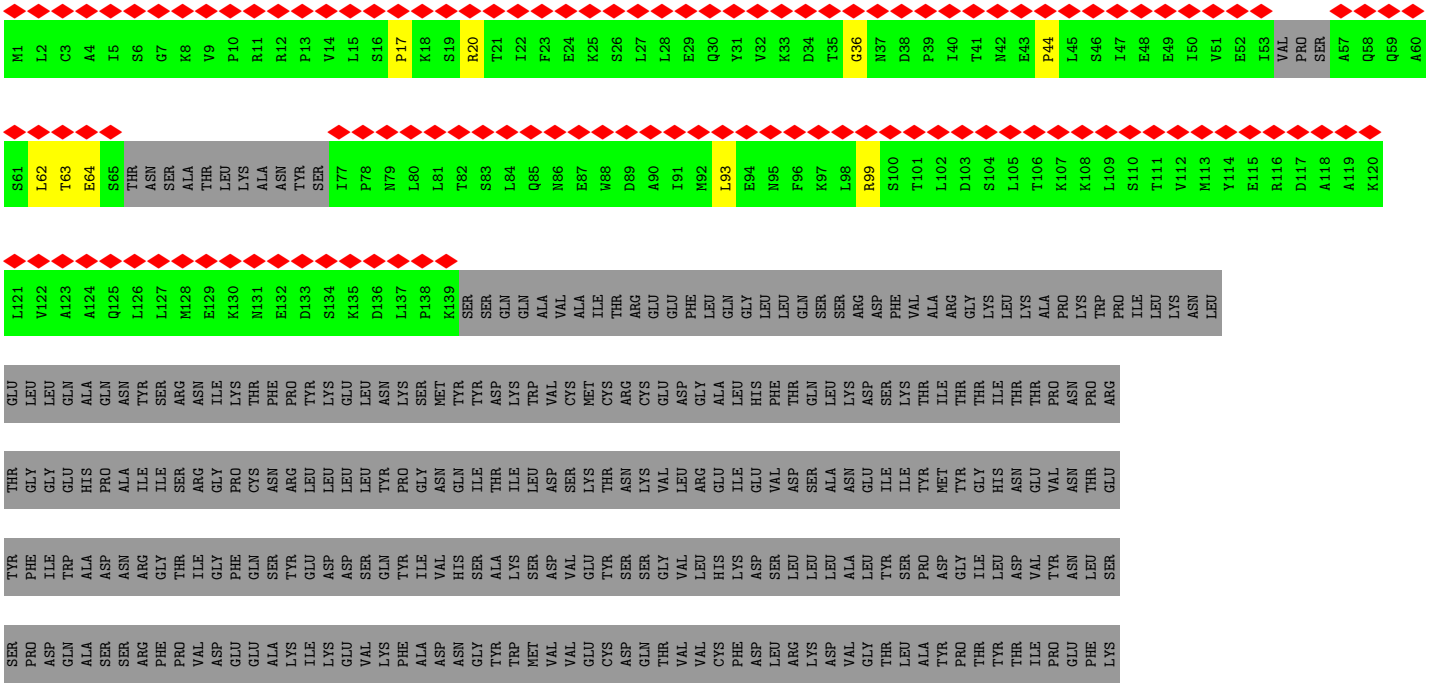






- Molecule 34: Pre-mRNA-processing factor 19

Chain r:



THR GLY THR VAL THR TYR ASP ILE ASP ASP SER GLY LYS ASN MET ILE ALA TYR SER ASN GLU SER ASN SER LEU THR ILE TYR LYS PHE ASP LYS LYS THR LYS ASN TRP THR LYS ASP GLU GLU SER ALA LEU CYS LEU GLN SER ASP THR ALA ASP PHE THR ASP MET ASP VAL VAL

CYS GLY ASP GLY GLY ILE ALA ALA ILE LEU LYS THR ASN ASP SER PHE ASN ILE VAL ALA LEU THR PRO

- Molecule 35: Pre-mRNA-splicing factor SNT309

Chain t:

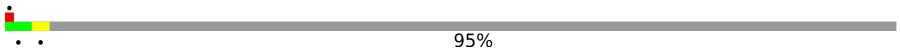
M1 D2 G3 L4 S5 F6 V7 D8 K9 GLY LYS ILE P13 D14 G15 Y16 K17 N18 E19 I20 D21 Q22 L23 V24 K25 K26 E27 F28 A29 N30 I31 K32 ARG GLU PRO VAL HIS PRO GLU ILE ARG GLY ILE LEU ALA LYS ARG LYS GLY A50 D51 N52 S53 V54 S55 T56 L57 T58 N59 A60

L61 Y62 T63 E64 Y65 L66 K67 Q68 R69 N70 N71 K72 K73 R74 R75 T76 P77 D78 F79 N80 D81 D82 D83 D84 T85 L86 F87 L88 E89 E90 Y91 R92 R93 K94 Y95 P96 R97 I98 D99 T100 S101 R102 Y103 I104 P105 N106 E107 S108 S109 E110 V111 S112 L113 L114 G115 I116 V117 D118 S119 Y120

L121 K122 H123 Q124 E125 I126 V127 L128 D129 T130 L131 L132 P133 Q134 T135 V136 S137 N138 Q139 W140 R141 I142 N143 N144 D145 Y146 I147 R148 Q149 T150 C151 T152 I153 V154 E155 E156 M157 N158 I159 Q160 Q161 R162 K163 Q164 I165 N166 D167 L168 E169 I170 Y171 R172 K173 R174 L175

- Molecule 36: Pre-mRNA-processing factor 17

Chain n:



MET GLY LEU VAL ASP GLY TYR ASP THR SER SER ASP SER ASP LEU ASN PHE ASP GLU GLY LYS SER VAL HIS GLU LYS LYS ASN GLY ASN LEU HIS GLU ASP THR SER TYR GLU PRO SER SER ASN ASN ILE HIS LYS ARG LYS SER HIS F51 E55 L56 K57 R58 R59 R60 K61 T62

R63 K64 G65 D66 G67 S73 SER SER ASP ASP GLU THR SER GLN ALA SER GLU THR GLN LYS GLU ASP GLN ASP ILE PHE VAL HIS ALA LEU ALA GLU ASP ASN LEU ASP SER GLU GLN ILE GLU VAL GLU GLU VAL SER HIS PHE TYR GLY LYS SER GLU LYS ASP TYR GLN GLY ARG

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

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

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

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

PRO LYS TYR LYS ARG HIS PRO LYS LYS ILE PHE LYS GLY HIS SER SER ALA GLY TYR GLY ILE SER LEU ALA PHE SER GLY ASP GLY ARG TYR ILE CYS SER GLY ASP SER LYS SER ARG LEU PHE THR TRP ASP TRP ASN THR SER ARG LEU LEU ASN ASN ILE ILE LYS ILE PRO GLY ASN

LYS PRO ILE THR GLN VAL ASP TRP HIS PRO GLN GLU THR SER LYS VAL ILE CYS SER GLY ALA ALA GLY LYS ILE TYR VAL CYS ASP

- Molecule 37: Small nuclear ribonucleoprotein-associated protein B

Chain k:

MET SER LYS I4 Q5 V6 A7 H8 S9 S10 R11 L12 A13 N14 L15 I16 D17 Y18 K19 L20 R21 V22 L23 T24 Q25 D26 G27 R28 V29 Y30 I31 G32 Q33 L34 M35 A36 F37 D38 K39 H40 M41 N42 L43 V44 L45 N46 E47 C48 I49 E50 E51 R52 V53 P54 K55 THR GLN LEU ASP LYS

LEU ARG PRO ARG LYS ASP SER LYS ASP GLY THR THR LEU ASN I75 K76 V77 E78 K79 R80 V81 L82 G83 L84 T85 I86 L87 R88 G89 E90 Q91 I92 L93 S94 T95 V96 V97 E98 D99 K100 P101 L102 LEU SER LYS LYS GLU ARG LEU VAL ARG ASP LYS LYS GLU LYS LYS GLN ALA GLN

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

PRO PRO GLN THR ARG LYS PHE GLN PRO PRO PRO GLY PHE LYS ARG LYS

- Molecule 38: Small nuclear ribonucleoprotein E

Chain i: 79% 74% 5% 20%

MET SER ASN LYS VAL LYS THR LYS ALA M10 V11 P12 P13 I14 N15 C16 I17 F18 N19 F20 L21 Q22 Q23 Q24 T25 P26 V27 T28 I29 W30 L31 F32 E33 Q34 I35 G36 I37 R38 I39 K40 G41 K42 I43 V44 G45 F46 D47 E48 F49 M50 N51 V52 V53 I54 D55 E56 A57 V58 E59 I60

P61 V62 N63 S64 ALA ASP GLY LYS GLU ASP VAL GLU K73 G74 T75 P76 L77 G78 K79 I80 L81 L82 K83 G84 D85 N86 I87 T88 L89 I90 T91 S92 ALA ASP

- Molecule 39: Small nuclear ribonucleoprotein F

Chain h: 81% 78% • 19%

MET SER GLU SER SER ASP ILE SER ALA MET GLN P12 V13 N14 P15 K16 P17 F18 L19 K20 G21 L22 V23 N24 H25 R26 V27 G28 V29 K30 L31 K32 PHE ASN S35 T36 E37 Y38 R39 G40 T41 L42 V43 S44 T45 D46 N47 Y48 F49 N50 L51 Q52 L53 N54 E55 A56 E57 E58 F59 V60

A61 G62 V63 S64 H65 G66 T67 L68 G69 E70 I71 F72 I73 R74 C75 N76 N77 V78 L79 Y80 I81 R82 E83 LEU PRO ASN

- Molecule 40: Small nuclear ribonucleoprotein G

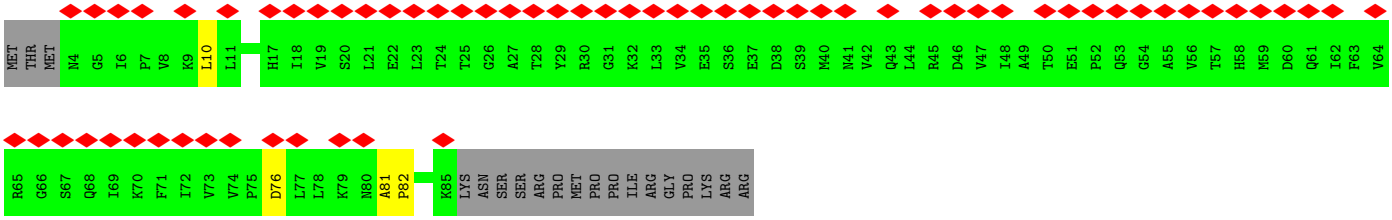
Chain j: 90% 86% • • 10%

MET V2 S3 T4 P5 E6 L7 K8 K9 Y10 M11 D12 K13 K14 I15 L16 L17 N18 I19 N20 G21 S22 R23 K24 V25 A26 G27 I28 L29 R30 G31 Y32 D33 I34 F35 L36 N37 V38 V39 L40 D41 D42 A43 N44 E45 I46 ASN GLY GLU ASP PRO ALA N53 N54 H55 Q56 L57 G58 L59 Q60

T61 V62 I63 R64 G65 N66 S67 I68 I69 S70 L71 E72 A73 L74 D75 A76 ILE

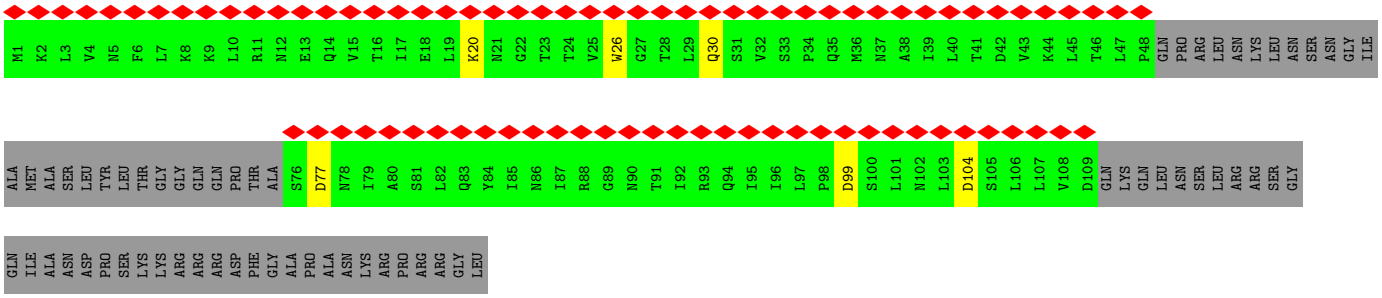
- Molecule 41: Small nuclear ribonucleoprotein Sm D3

Chain l: 64% 77% • 19%



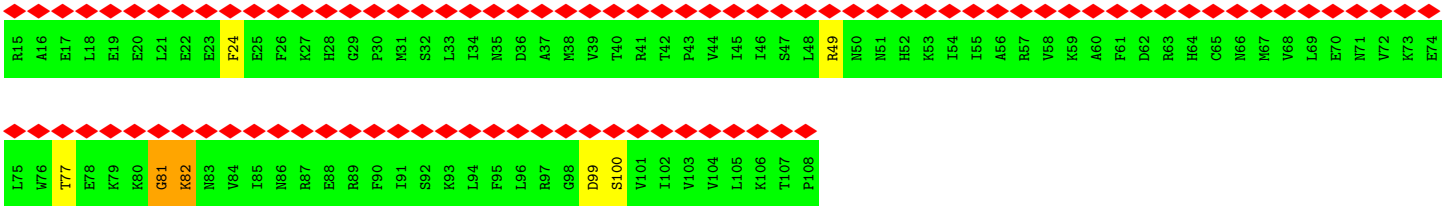
• Molecule 42: Small nuclear ribonucleoprotein Sm D1

Chain m:



• Molecule 43: Small nuclear ribonucleoprotein Sm D2

Chain g:



4 Experimental information (i)

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 ($e^-/Å^2$)	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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'

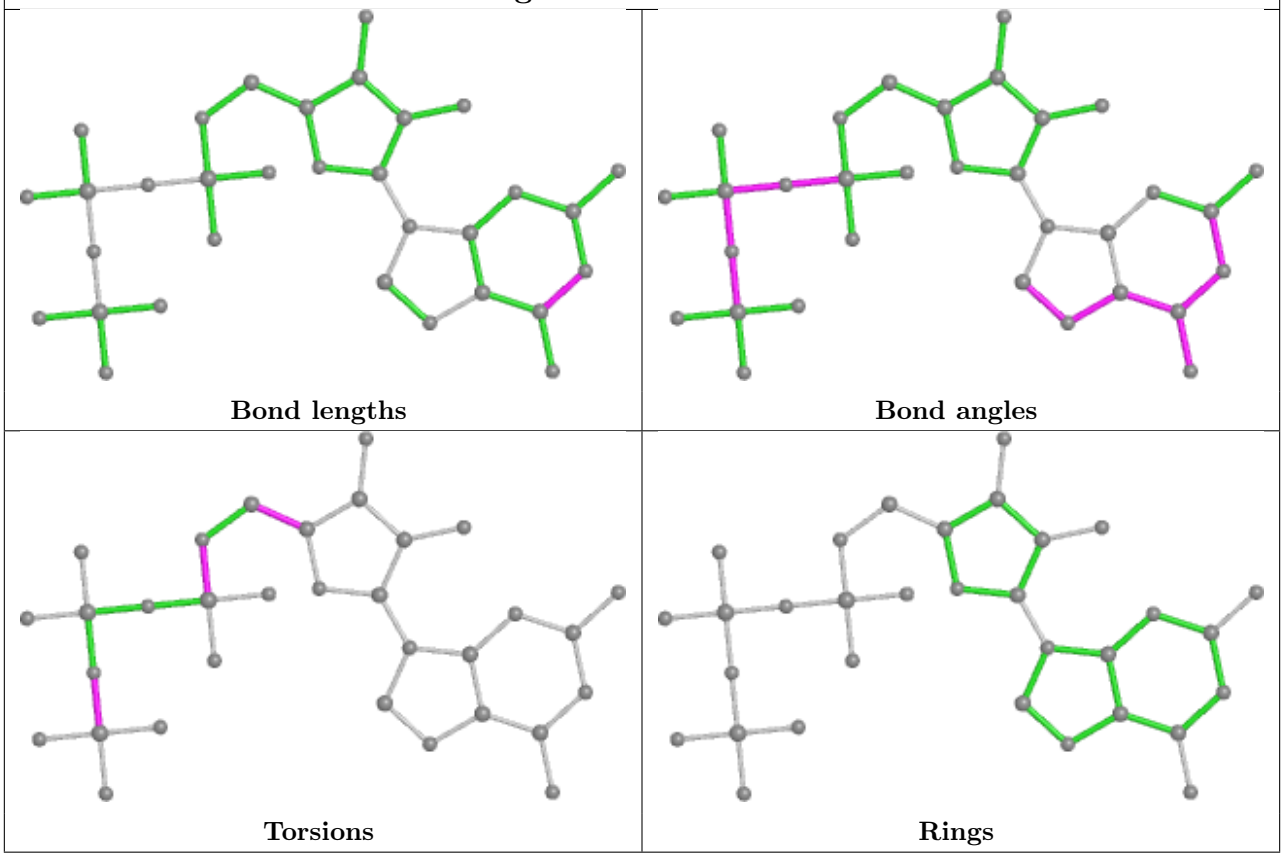
There are no ring outliers.

No monomer is involved in short contacts.

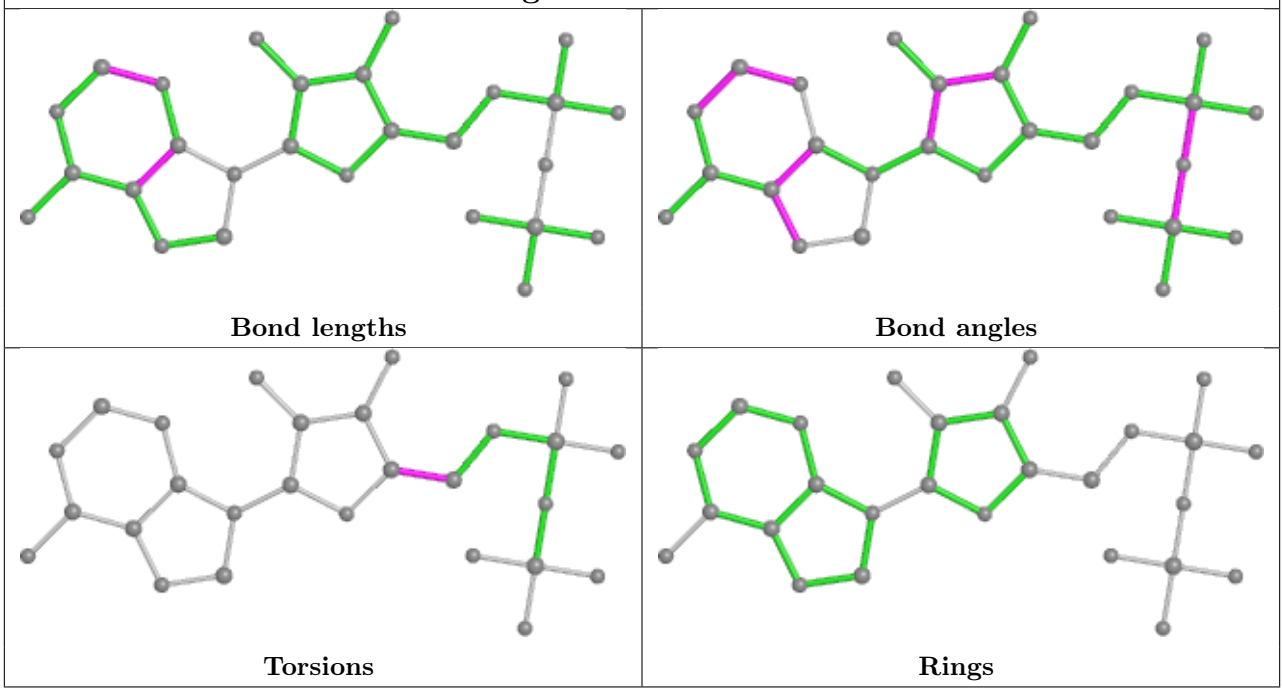
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand GTP C 1500



Ligand ADP Y 902



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.

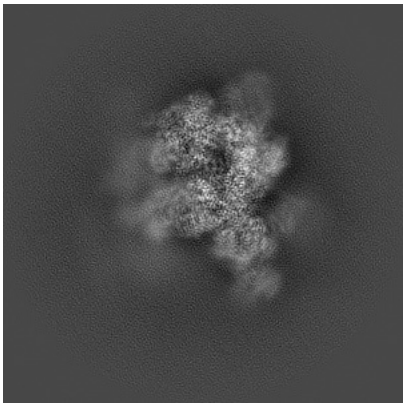
6 Map visualisation (i)

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.

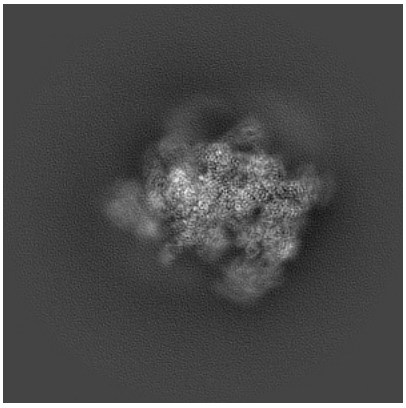
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

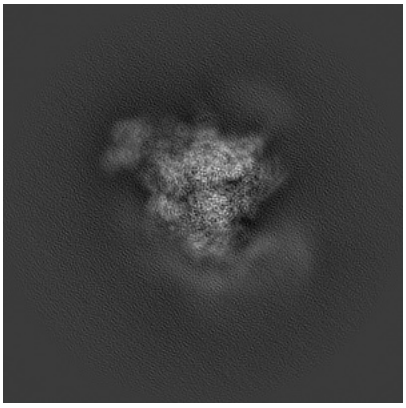
6.1.1 Primary map



X



Y

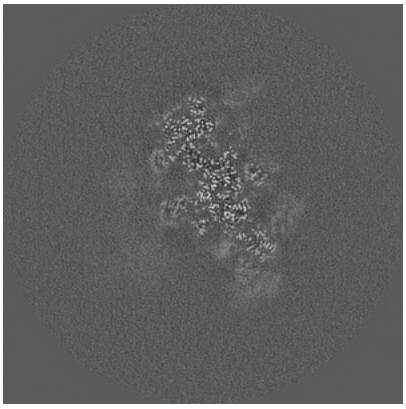


Z

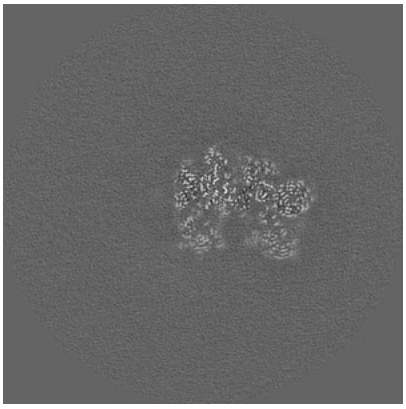
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

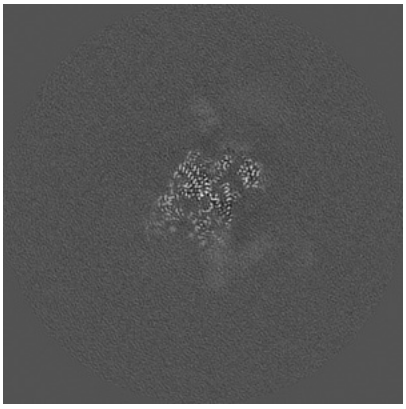
6.2.1 Primary map



X Index: 200



Y Index: 200

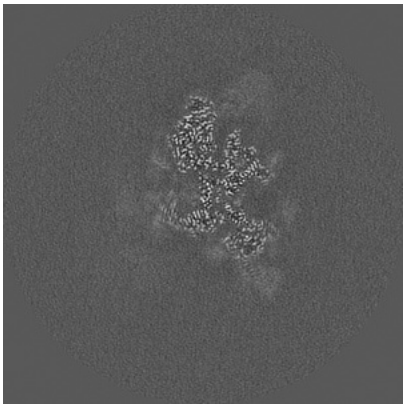


Z Index: 200

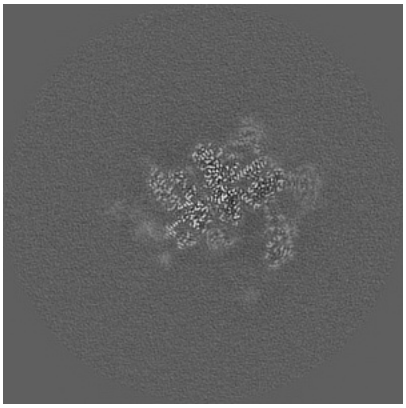
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

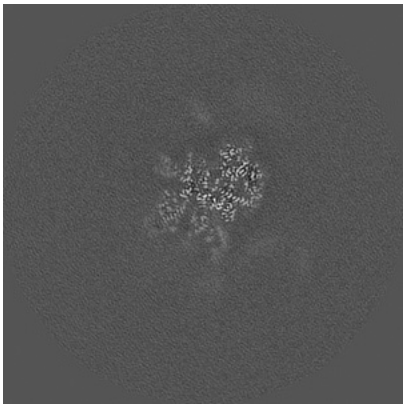
6.3.1 Primary map



X Index: 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.

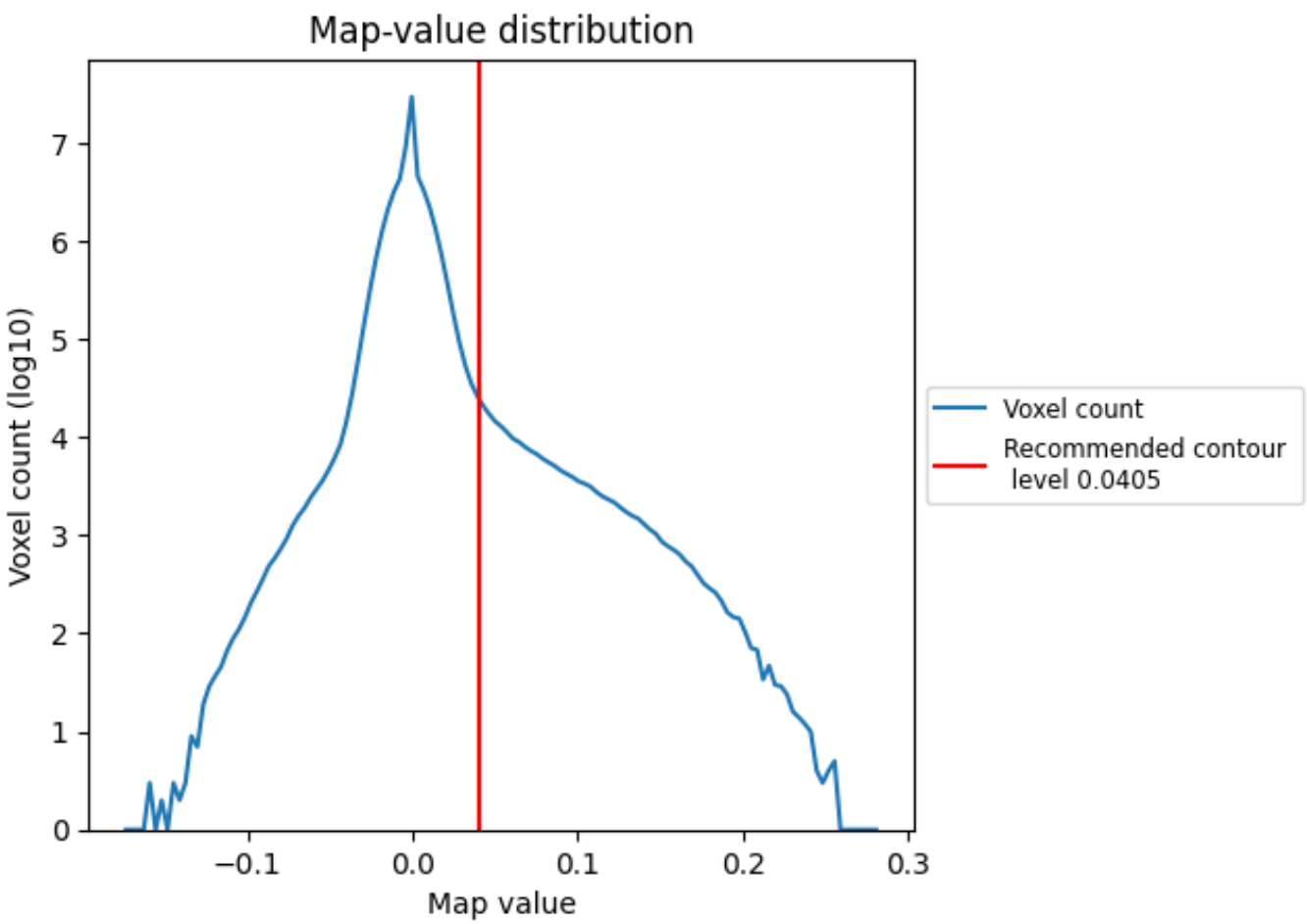
6.5 Mask visualisation (i)

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

7 Map analysis (i)

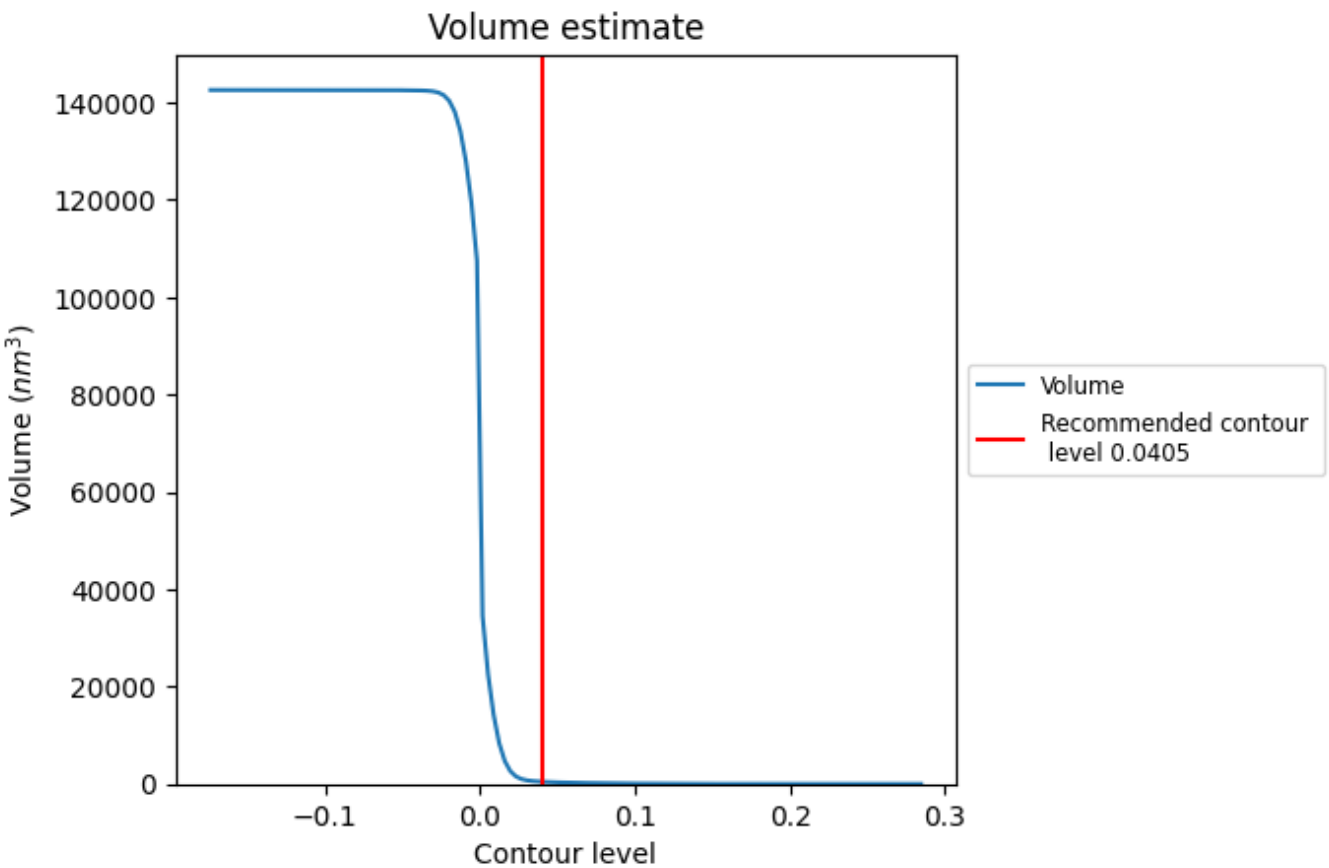
This section contains the results of statistical analysis of the map.

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.

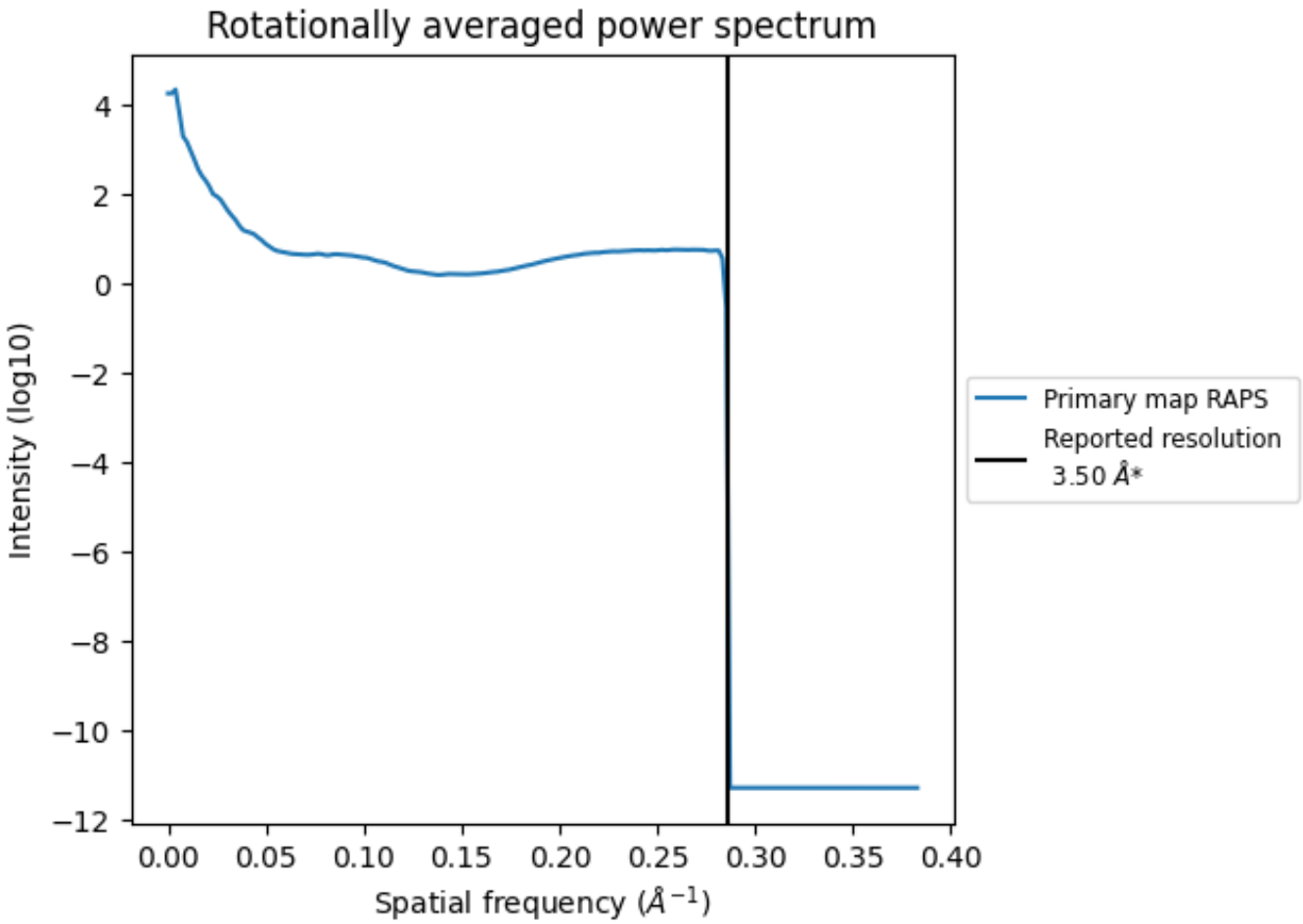
7.2 Volume estimate (i)



The volume at the recommended contour level is 444 nm^3; 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 Å^{-1}

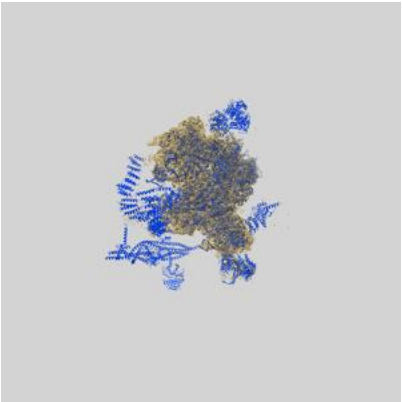
8 Fourier-Shell correlation (i)

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

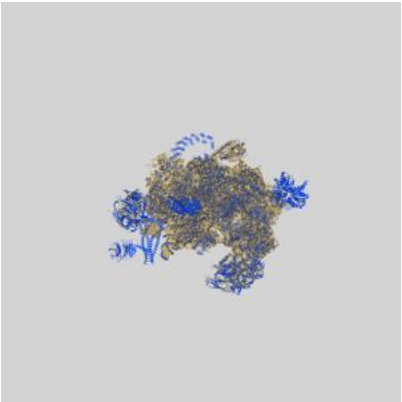
9 Map-model fit (i)

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.

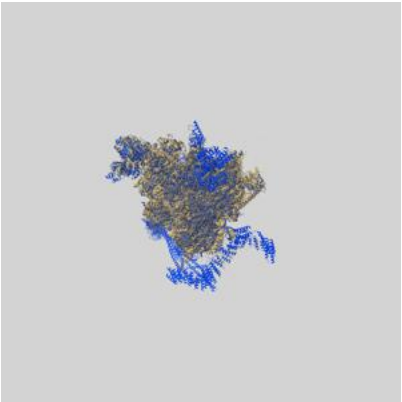
9.1 Map-model overlay (i)



X



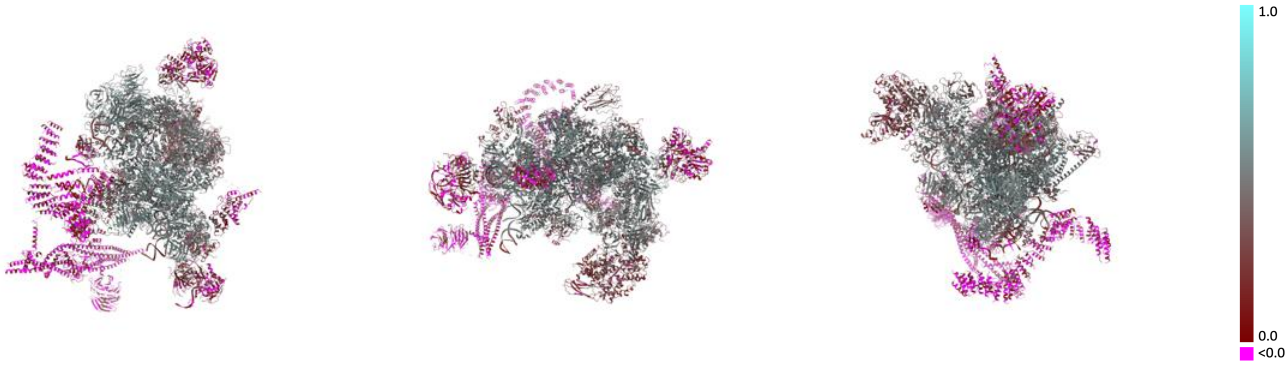
Y



Z

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.

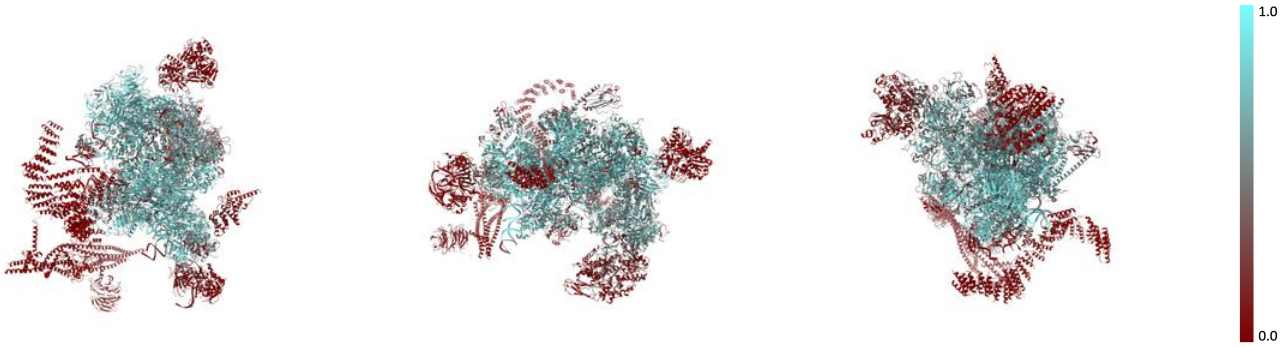
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

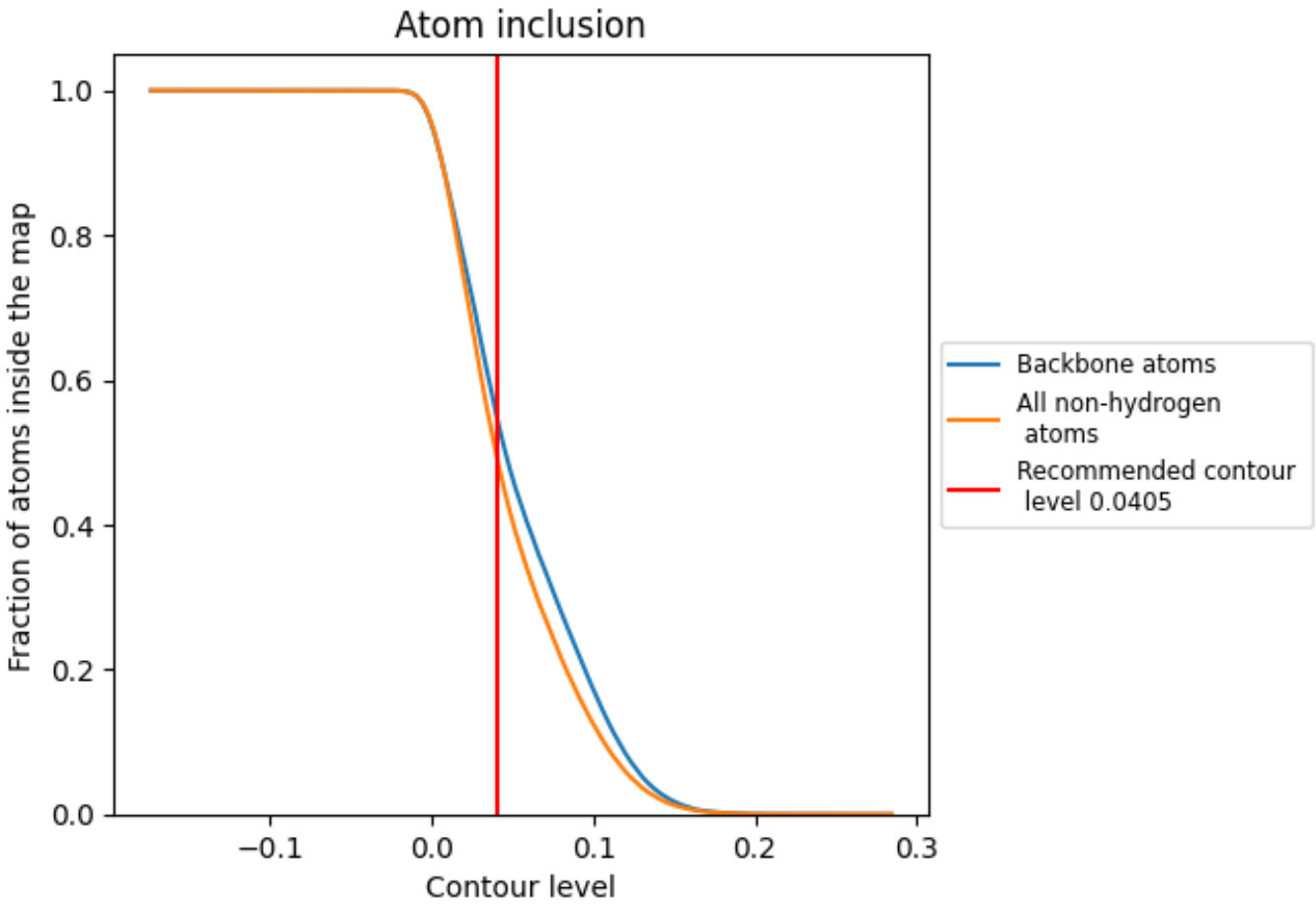
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)

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