Full wwPDB EM Validation 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 Full wwPDB EM Validation 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:

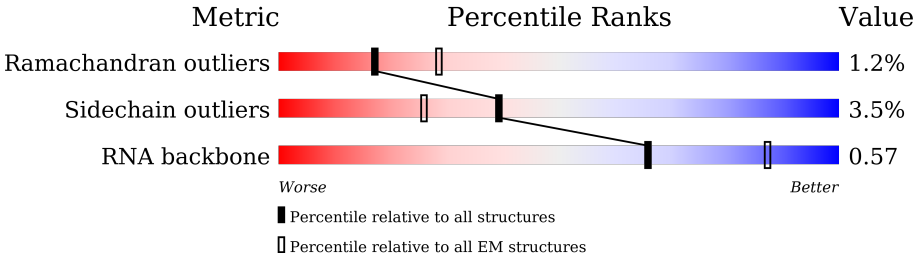
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

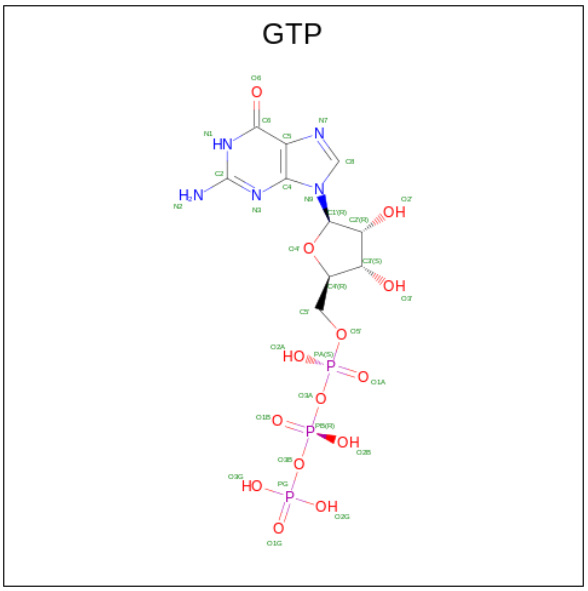
- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

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



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

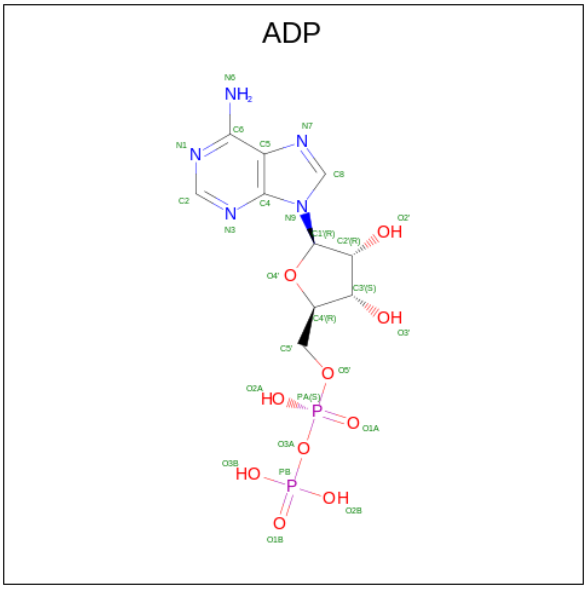
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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: $C_{10}H_{15}N_5O_{10}P_2$).



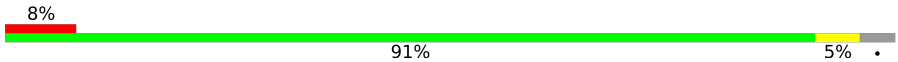
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	Y	1	27	10	5	10	2	0

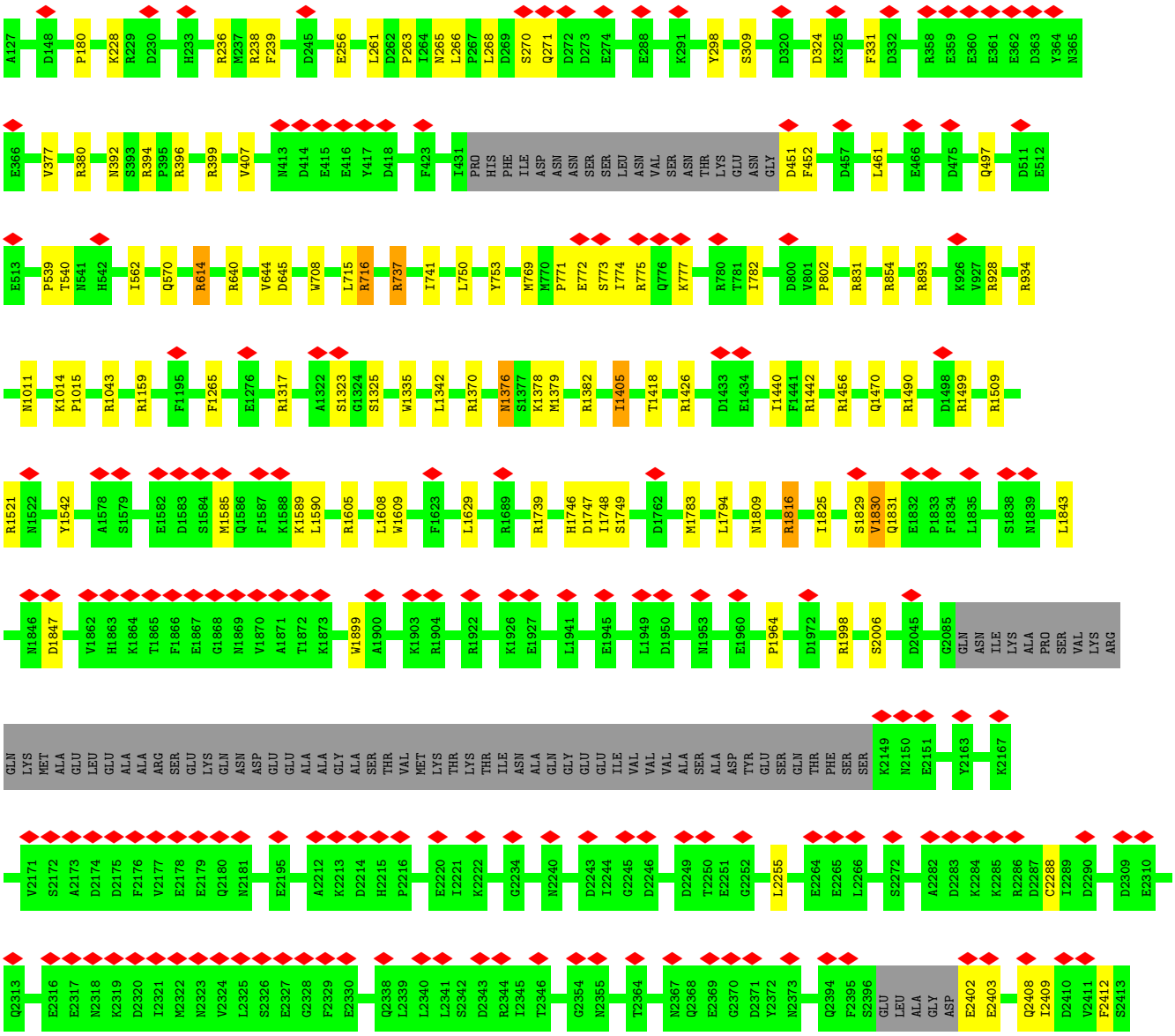
3 Residue-property plots (i)

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

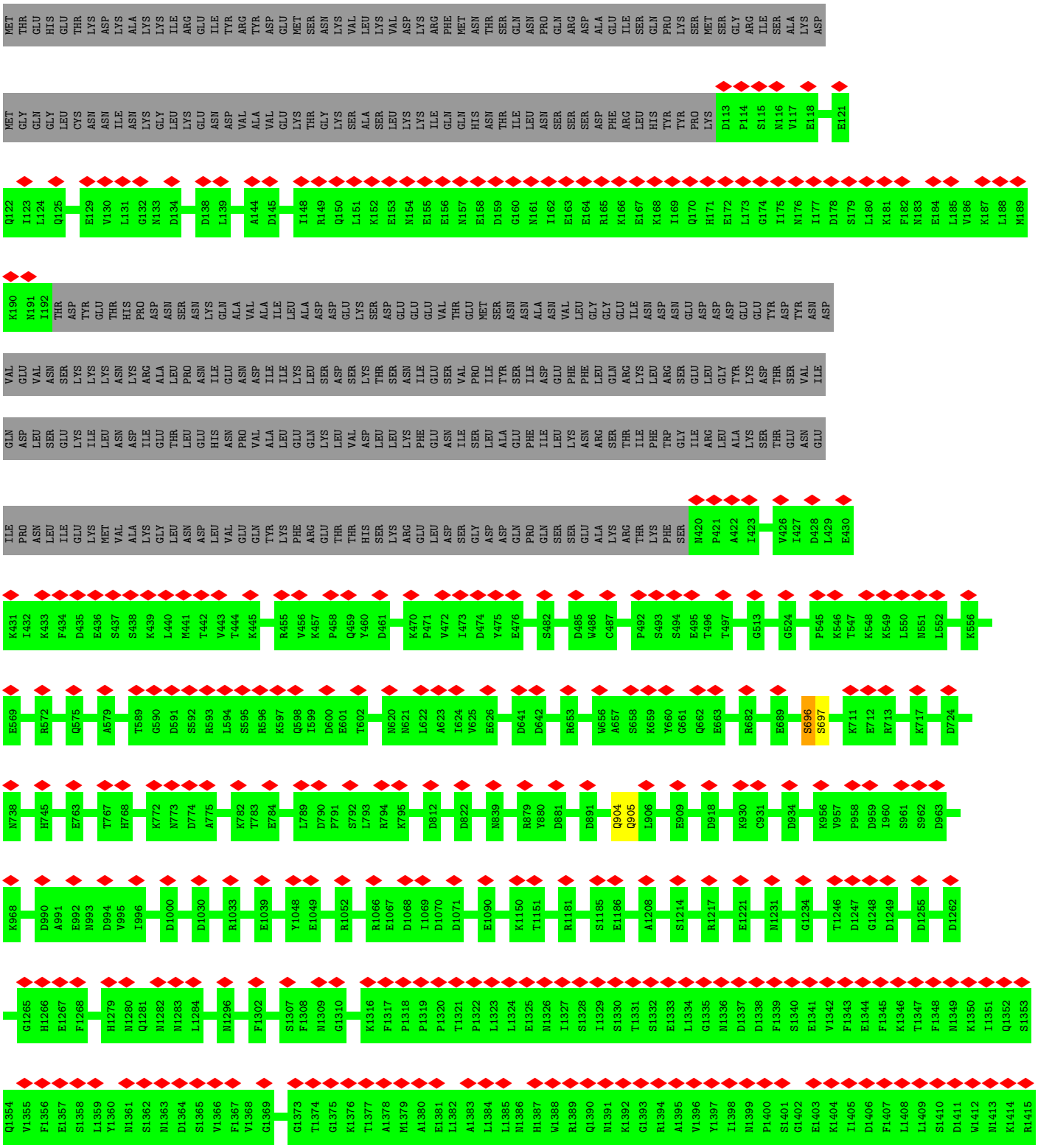
Chain A:





- Molecule 2: Pre-mRNA-splicing helicase BRR2

Chain B: 45% 83% 16%



F1416 S1417 H1418 L1419 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 A1973 L2033 T2034 D2035 S2036

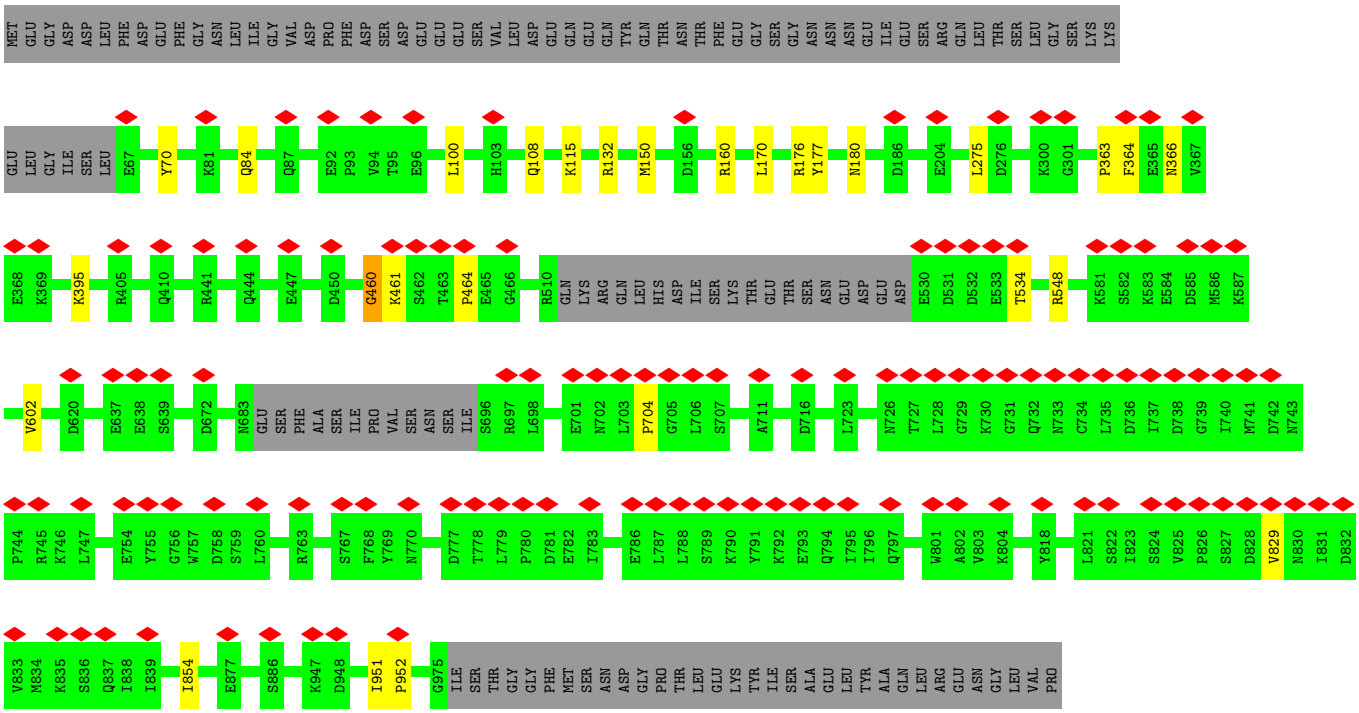
Q2037 L2038 A2039 Q2040 V2041 A2042 A2043 F2044 V2045 N2046 N2047 Y2048 P2049 N2050 V2051 E2052 L2053 T2054 Y2055 S2056 L2057 N2058 N2059 S2060 D2061 S2062 L2063 I2064 S2065 G2066 V2067 K2068 Q2069 K2070 I2071 T2072 I2073 Q2074 L2075 T2076 R2077 D2078 V2079 E2080 P2081 E2082 N2083 L2084 Q2085 V2086 D2147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

S2157 F2158 E2159 I2160 N2161 V2162 K2163

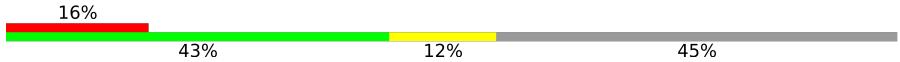
• Molecule 3: Pre-mRNA-splicing factor SNU114

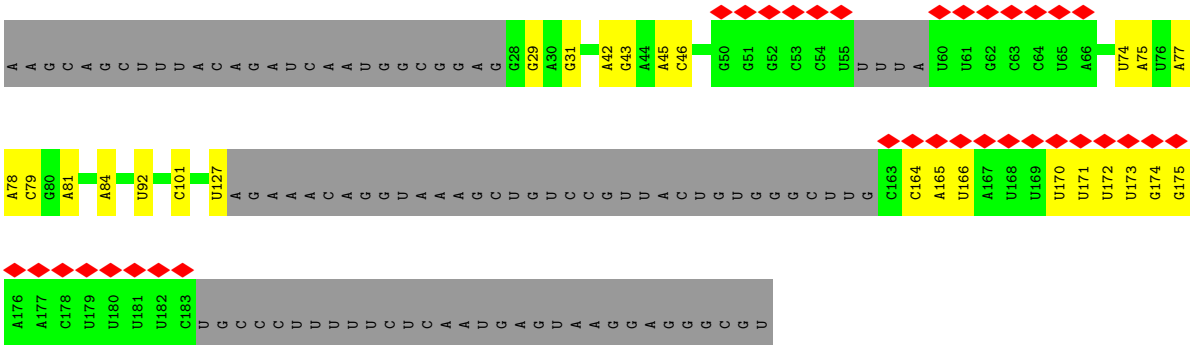
Chain C:



• Molecule 4: Saccharomyces cerevisiae strain CDRDR_sf_H chromosome VII sequence

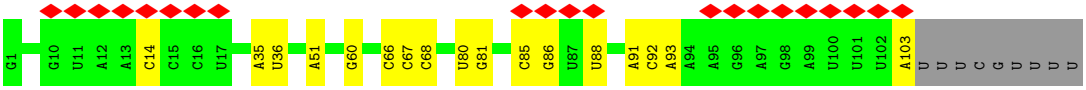
Chain D:





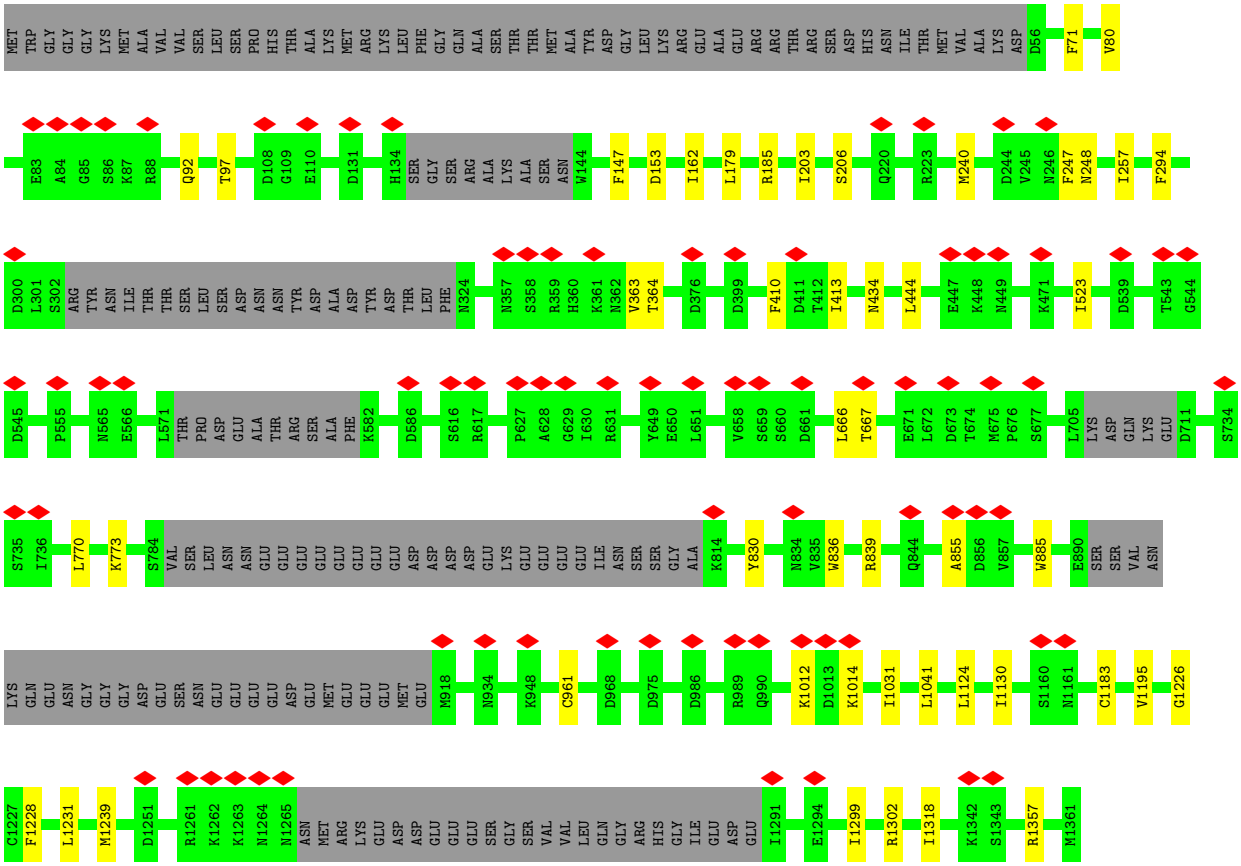
• Molecule 5: Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence

Chain E:



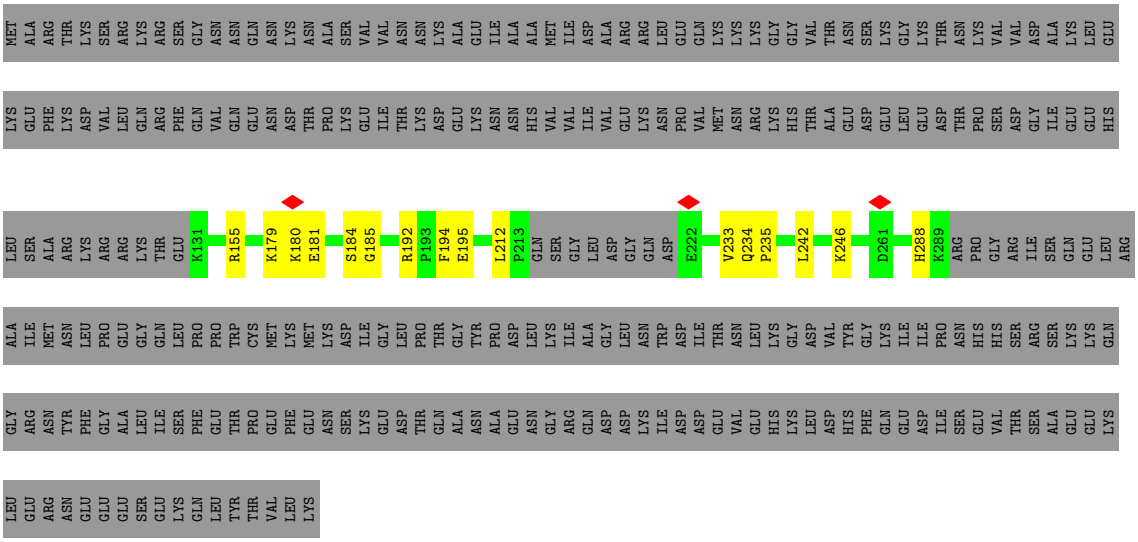
• Molecule 6: Pre-mRNA-splicing factor RSE1

Chain F:



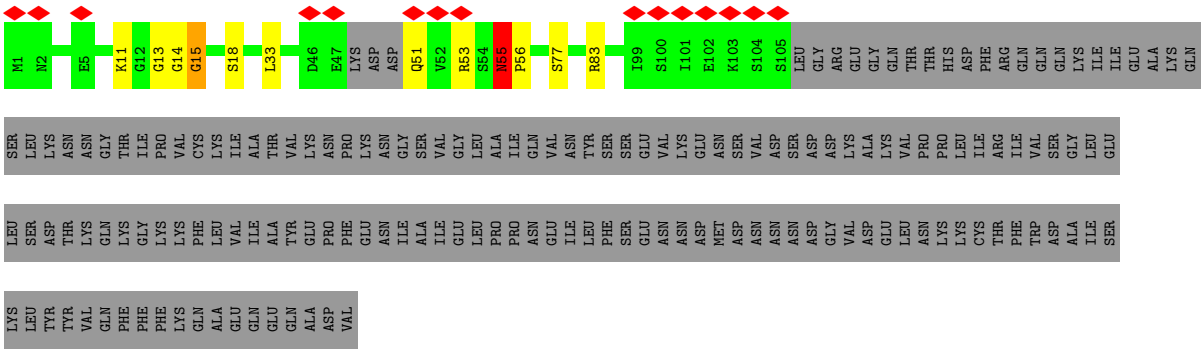
• Molecule 7: Cold sensitive U2 snRNA suppressor 1

Chain H:



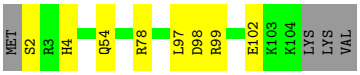
• Molecule 8: Pre-mRNA-splicing factor PRP11

Chain I:



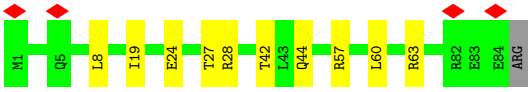
- Molecule 9: Pre-mRNA-splicing factor RDS3

Chain J:



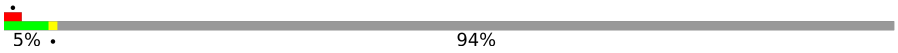
- Molecule 10: RDS3 complex subunit 10

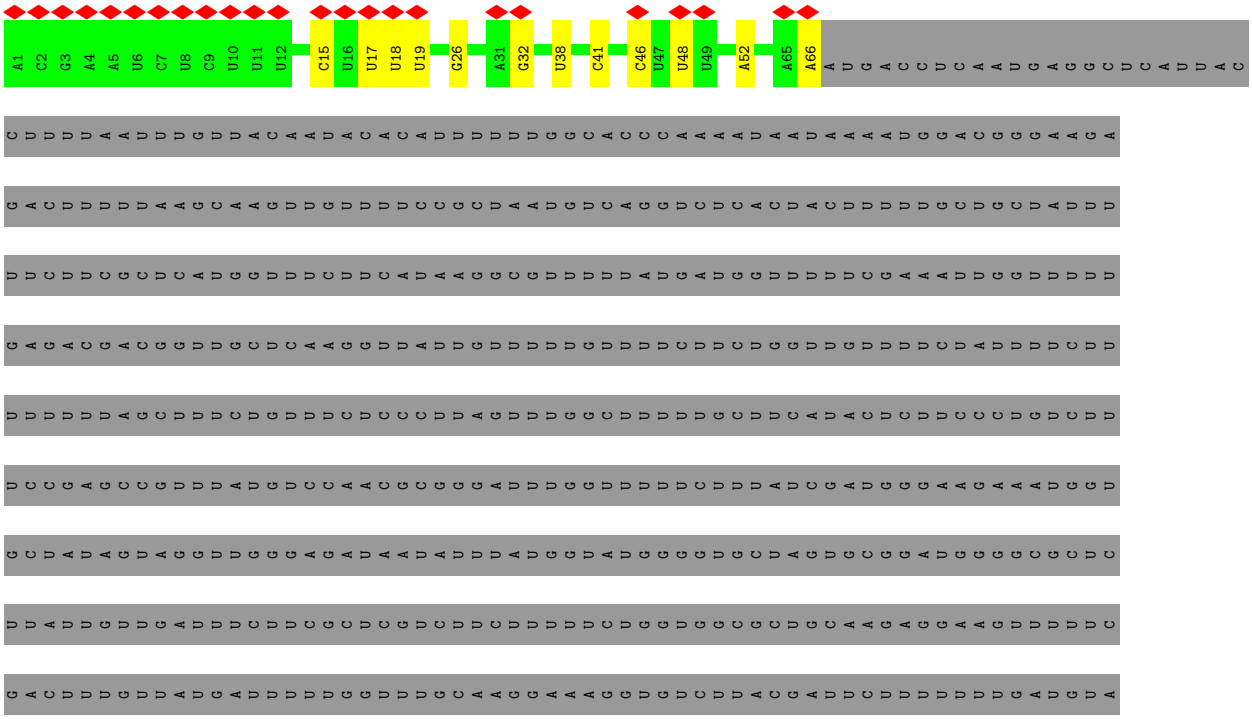
Chain K:

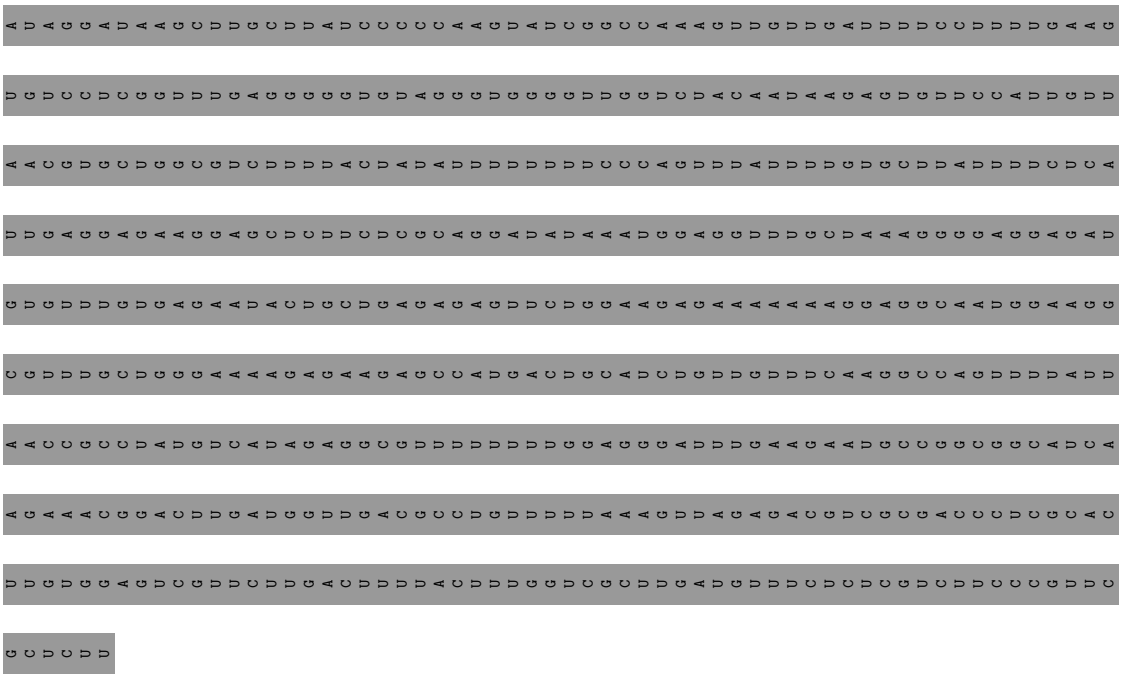


- Molecule 11: U2 snRNA

Chain L:

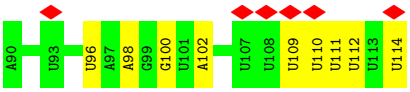






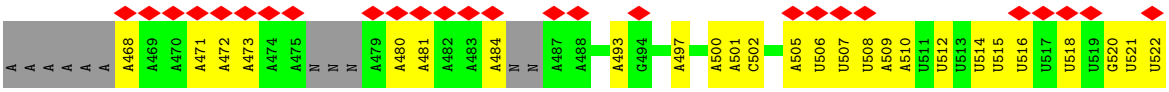
• Molecule 12: Pre-mRNA

Chain N:



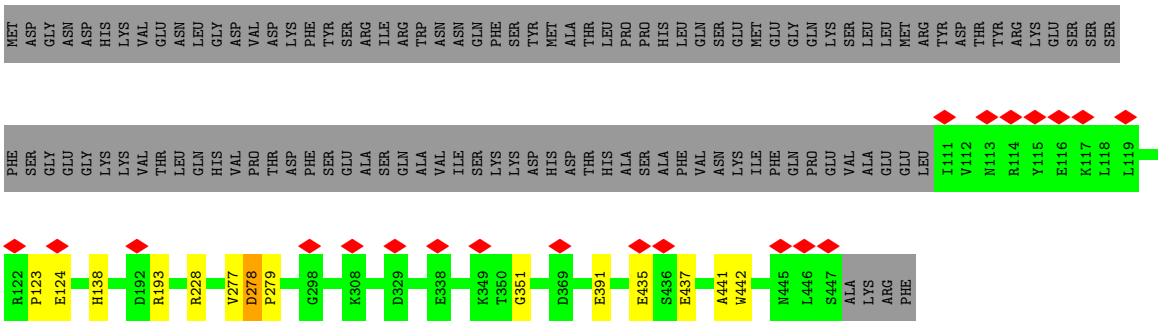
• Molecule 13: Pre-mRNA

Chain M:



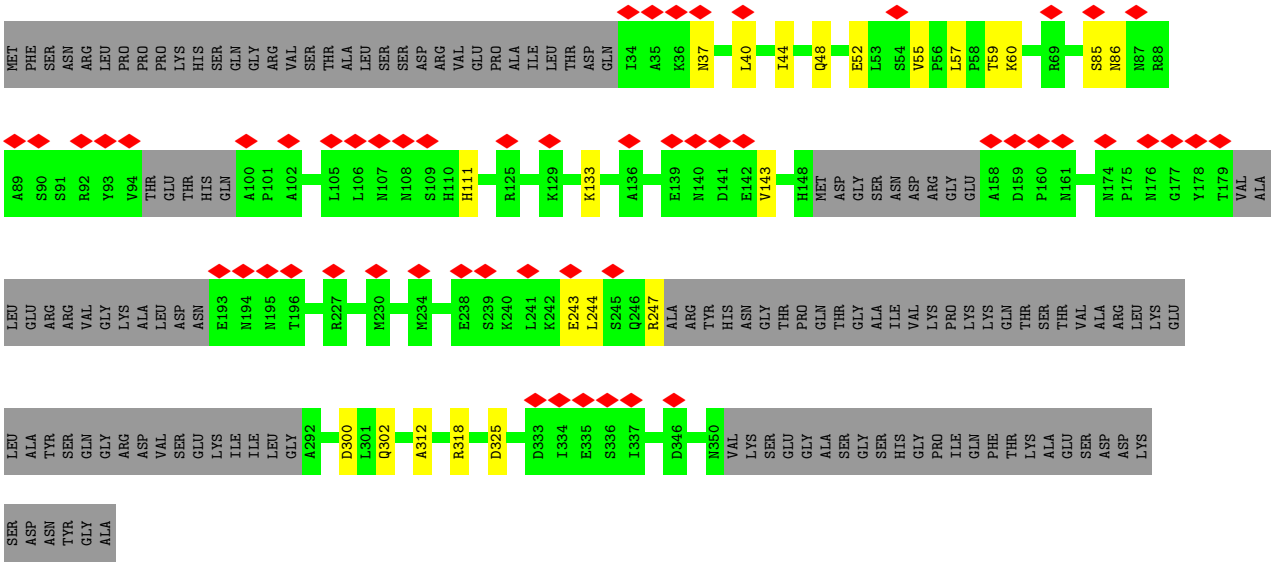
• Molecule 14: Pre-mRNA-splicing factor PRP46

Chain O:



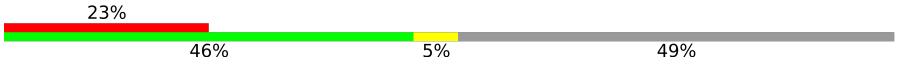
• Molecule 15: Pre-mRNA-processing protein 45

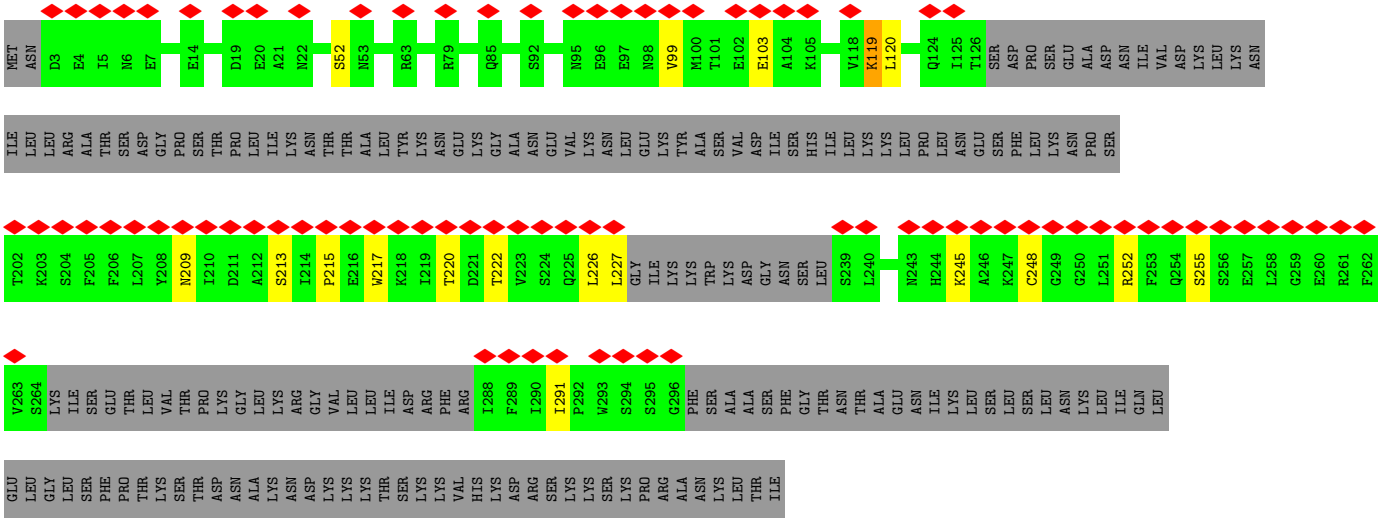
Chain P:



• Molecule 16: Pre-mRNA-splicing factor SLT11

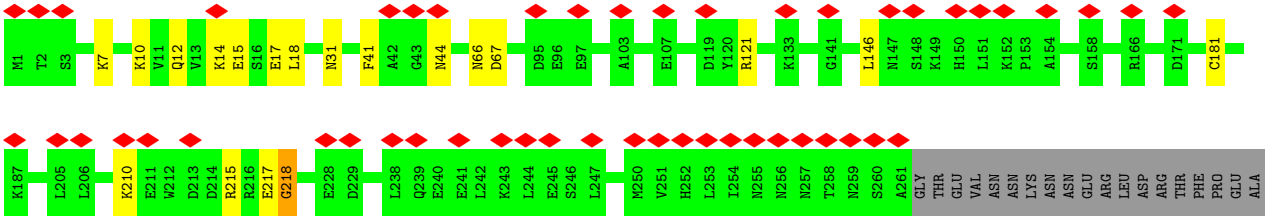
Chain Q:





• Molecule 17: Pre-mRNA-splicing factor CWC2

Chain R:



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

- Molecule 18: Pre-mRNA-splicing factor CWC15

Chain S: 25% 38% 59%

MET THR T3 S4 H5 R6 P7 Q8 L9 E10 A11 R12 S13 G14 A15 K16 A17 A18 A19 Y20 T21 P22 T23 R40 K41 PHE LYS GLU GLU GLU ASN LEU ARG ALA ASN CYS ALA GLN GLU ASP ARG SER ASN ASP LYS SER LEU GLU GLU ALA VAL MET ASN GLU GLU LYS GLN ASP VAL

VAL GLY SER GLY ASN LEU GLN GLU THR ARG SER GLU LYS ASP GLN LYS ASP SER LEU GLN GLU LEU LEU VAL THR GLN LYS ASN LYS VAL GLU ASP LYS ALA GLU LEU GLU GLY ASN GLU GLN LEU LYS GLY GLY ASN SER SER ARG R125 S126 G130 T131 A132 F133 G134 R135 HIS LYS

VAL THR LYS GLU THR ASN ILE LYS GLU HIS ALA THR LYS LYS SER ALA SER G155 Y156 I157 N158 D159 M160 T161 K162 S163 E164 Y165 H166 Q167 E168 F169 L170 H171 K172 H173 V174 R175

- Molecule 19: Pre-mRNA-splicing factor BUD31

Chain T: 7% 95%

M1 P2 K5 R8 D14 K37 Q54 D76 C104 T119 C122 R123 R126 K136 G137 T138 Q139 V140 C148 D157

- Molecule 20: Pre-mRNA leakage protein 1

Chain U: 46% 81% 15%

MET PHE HIS ARG ARG LYS ARG PRO TYR ASN THR ARG ASN TYR GLY HIS ASP ASP LYS LYS PHE K22 S23 Q24 Y25 I26 D27 I28 L38 E39 L40 E41 S42 N43 N44 K45 E46 G47 I48 A49 L50 K51 H52 V53 Q56 D57 N63 Y64 M65 D66 M67 L68 G69 L70 E71 A72 R73

D74 R75 T76 W77 Y78 E79 L80 Y83 R84 K85 N86 D87 K88 D89 K90 G91 P92 W93 K94 R95 Y96 D97 L98 L105 R108 E109 L110 G111 H112 SER LEU ASP THR ASP LEU ASP ASP ARG T122 E123 I124 V125 V126 A127 D128 I129 G130 I131 E134 S137 K138 R149 D158

L159 D160 S161 S162 N163 G164 T165 C166 L167 N168 N169 V170 V171 I172 P173 G174 I178 E179 L180 R181 S182 G183 D184 V185 L186 T187 L188 S189 E190 F191 E192 E193 D194 N195 D196 Y197 E198 F201 M202 N203 V204 H205 H206 HIS

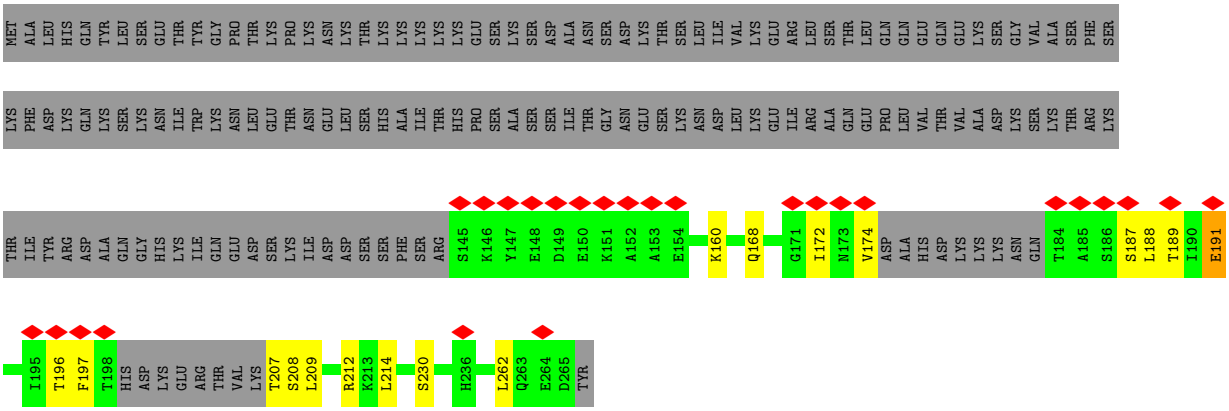
- Molecule 21: U2 snRNP component IST3

Chain V: 83% 14%

MET N2 K3 Q6 L17 S18 E66 L87 R110 E124 D127 R128 D129 ILE VAL SER LYS ASN ASN ALA GLU LYS LEU ILE LEU ALA LYS LYS ASP GLN PRO ASN

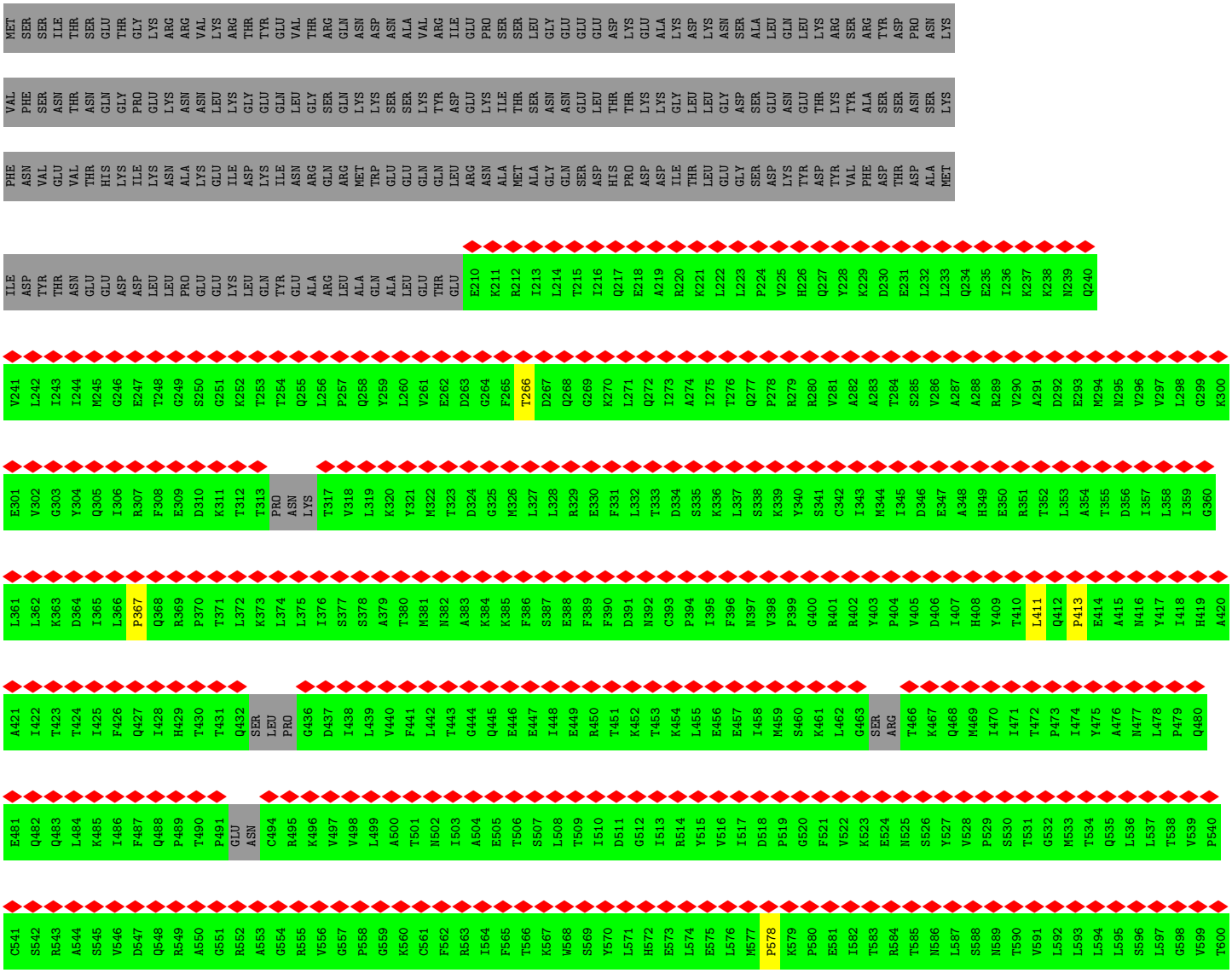
- Molecule 22: Pre-mRNA-splicing factor CWC26

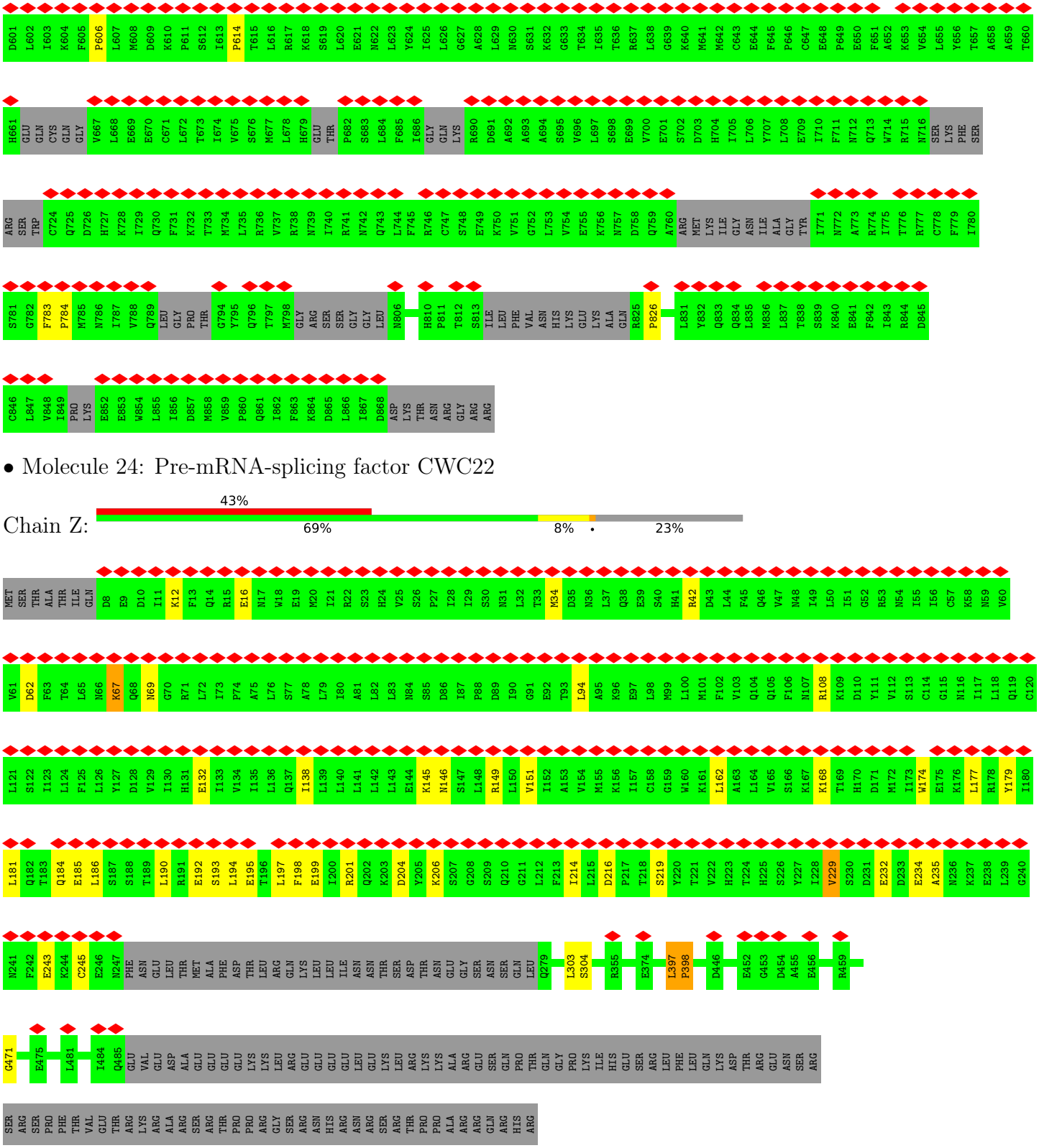
Chain W: 10% 33% 6% 61%



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

Chain Y:



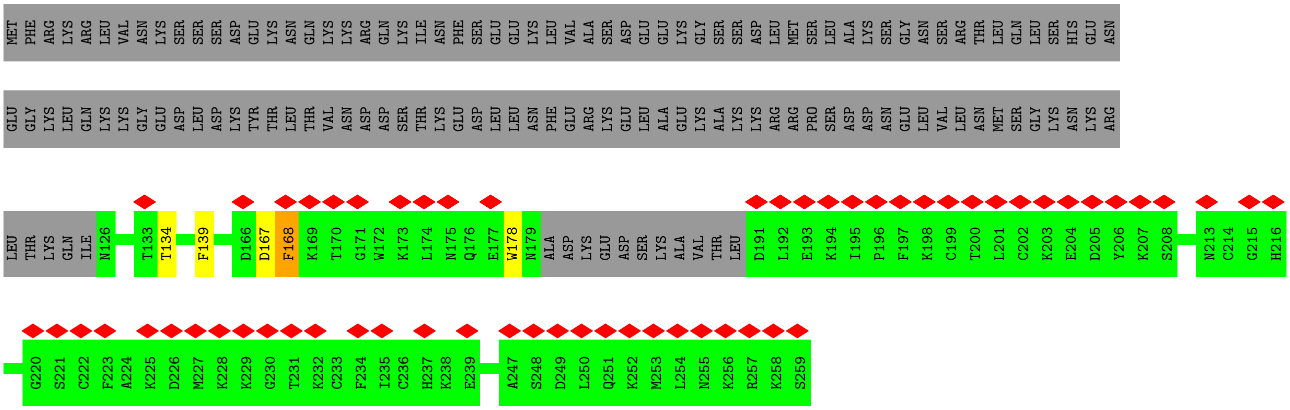


- Molecule 24: Pre-mRNA-splicing factor CWC22

Chain Z:

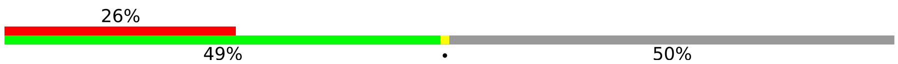
- Molecule 25: Pre-mRNA-splicing factor CWC24

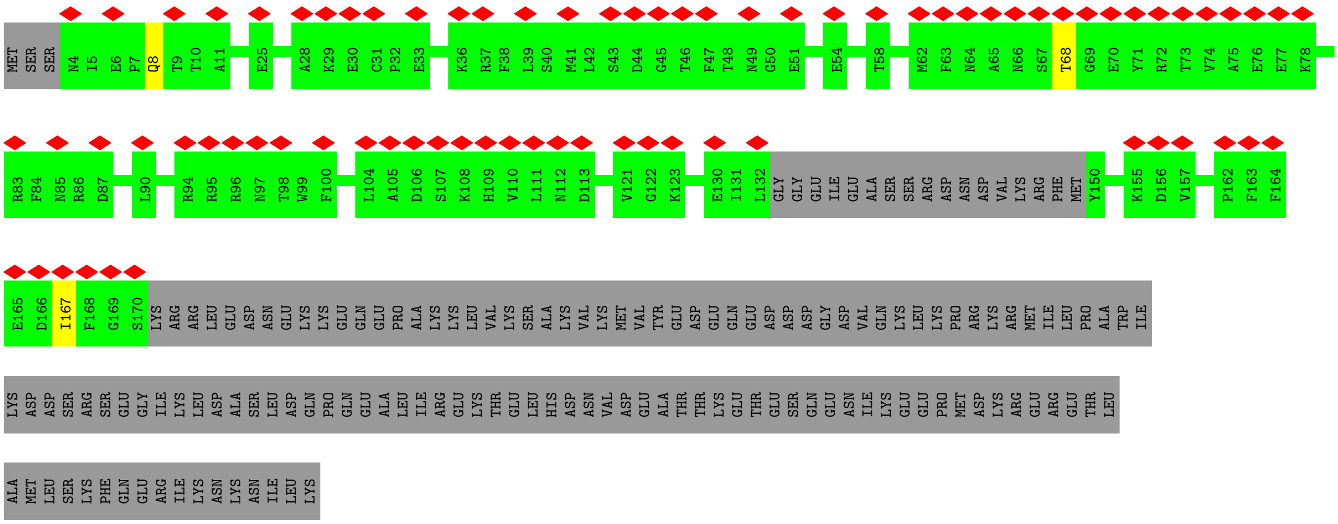
Chain a:



• Molecule 26: Peptidyl-prolyl isomerase CWC27

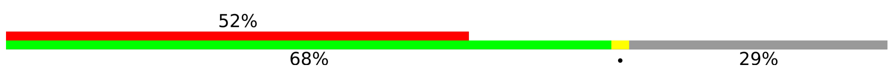
Chain b:

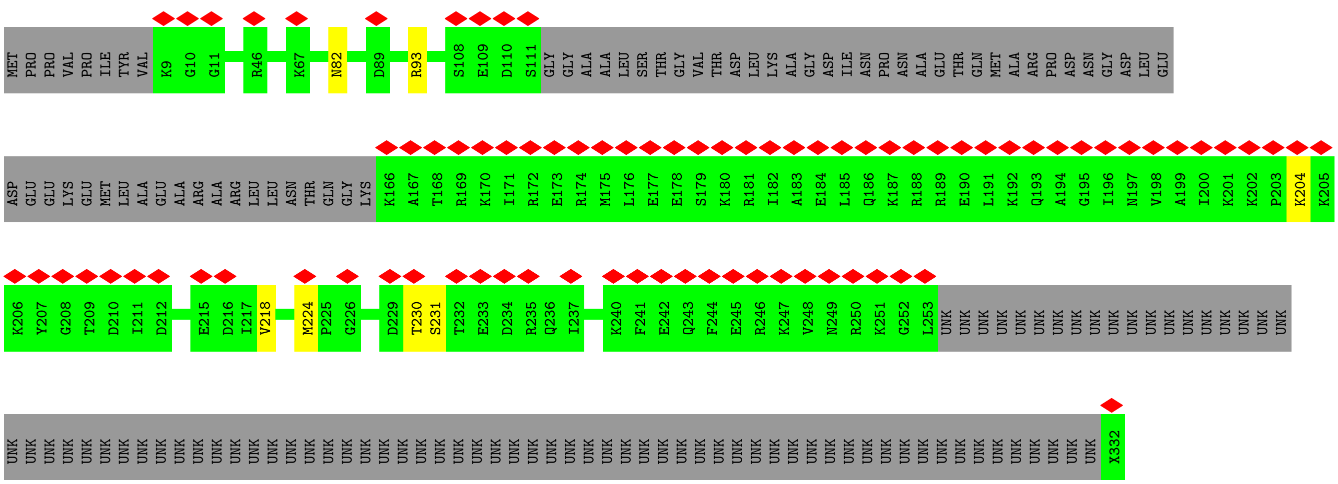


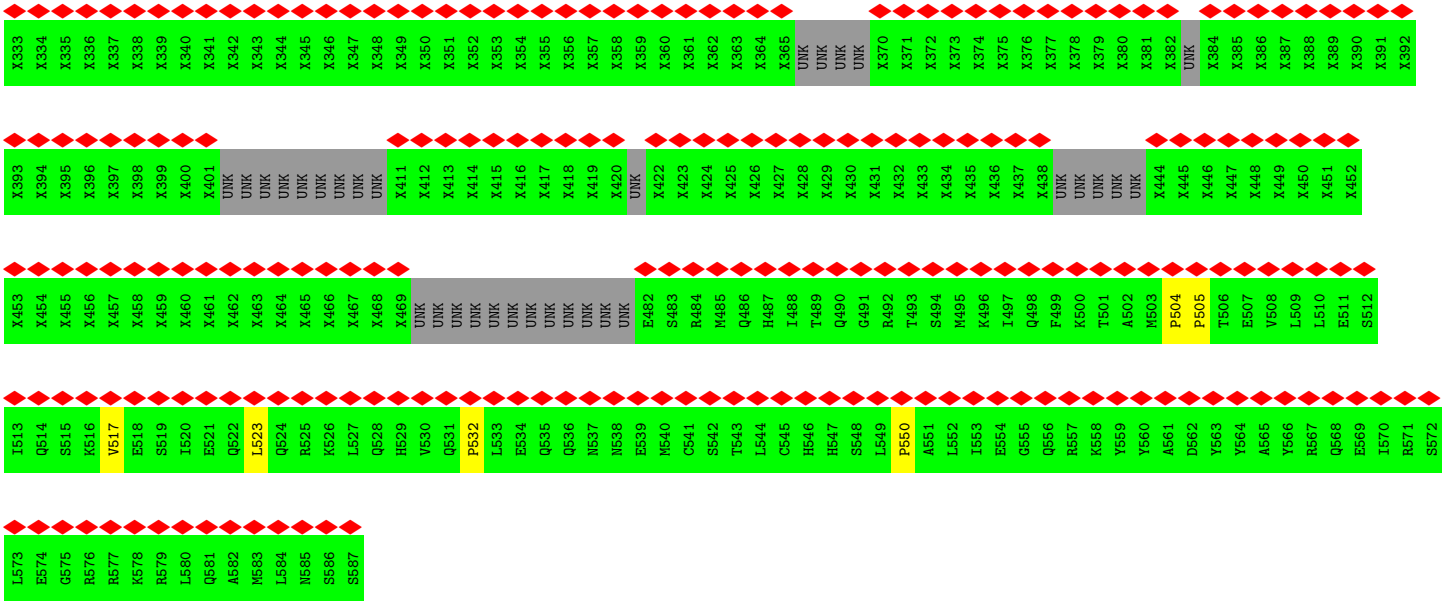


• Molecule 27: Pre-mRNA-splicing factor CEF1

Chain c:

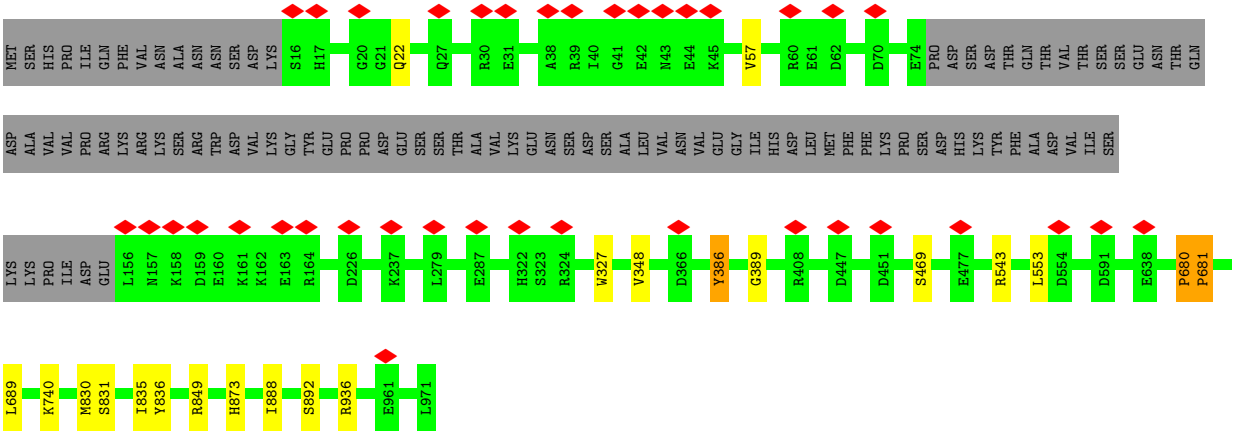






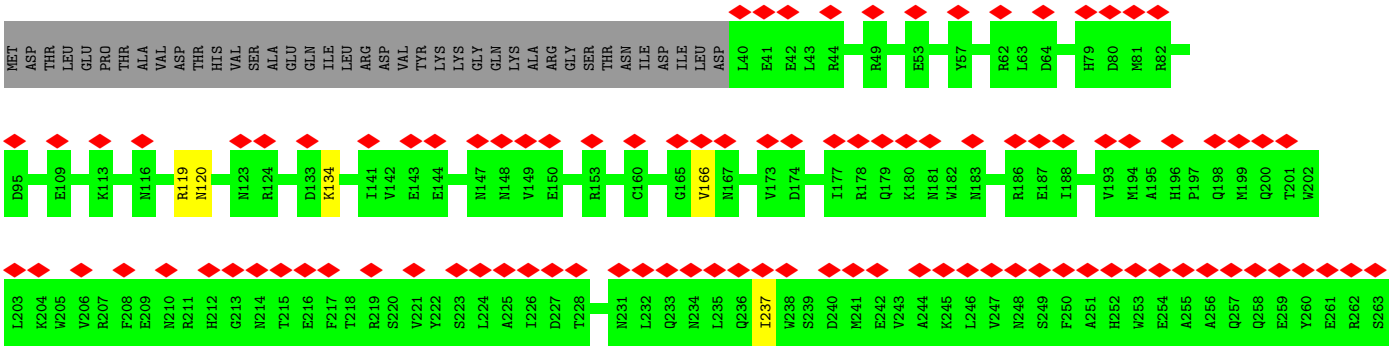
- Molecule 28: U2 snRNP component HSH155

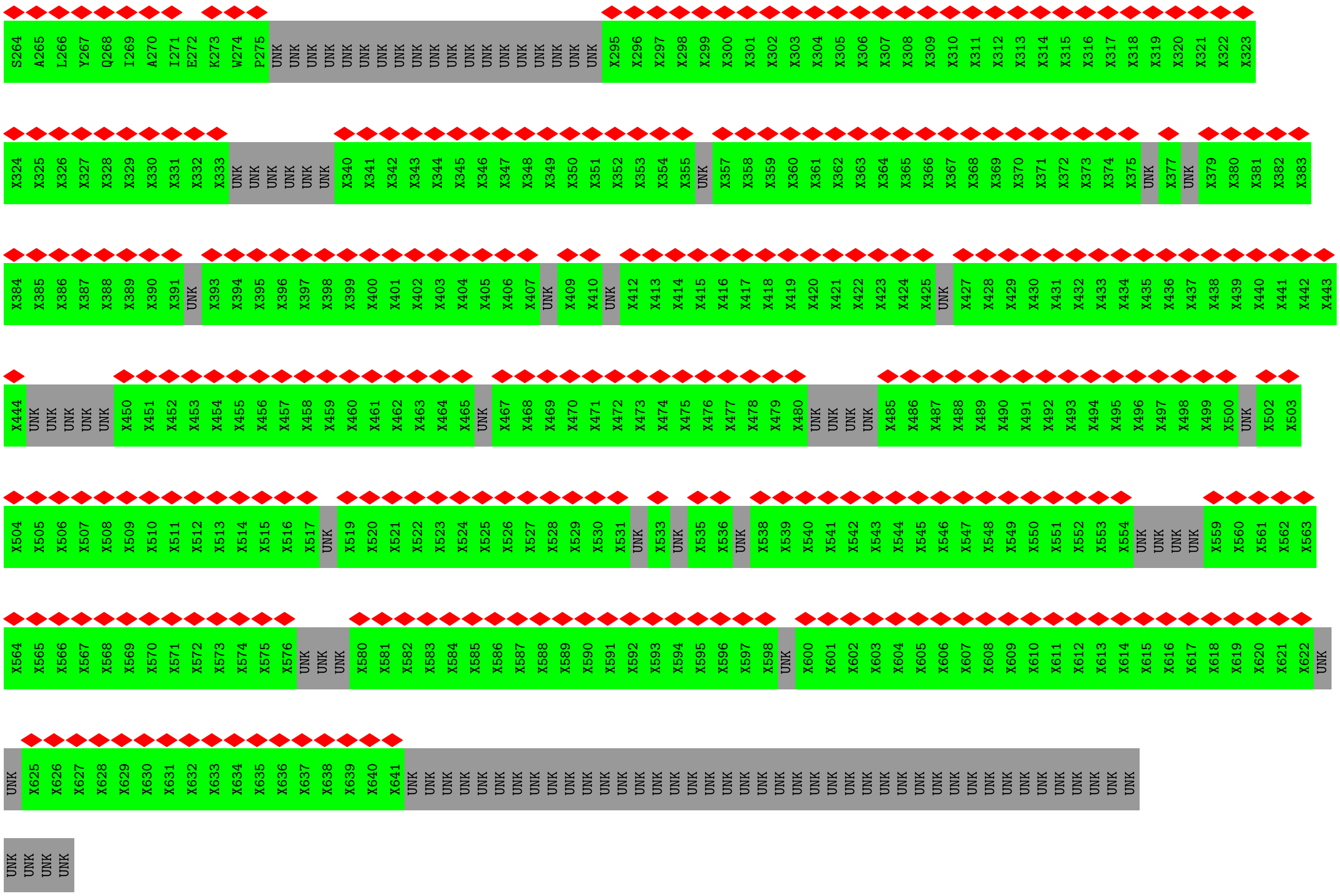
Chain G:



- Molecule 29: Pre-mRNA-splicing factor CLF1

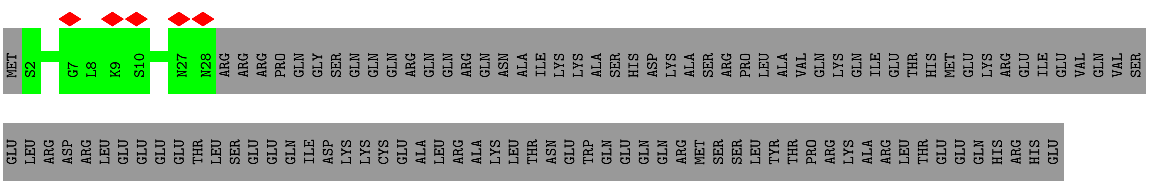
Chain d:





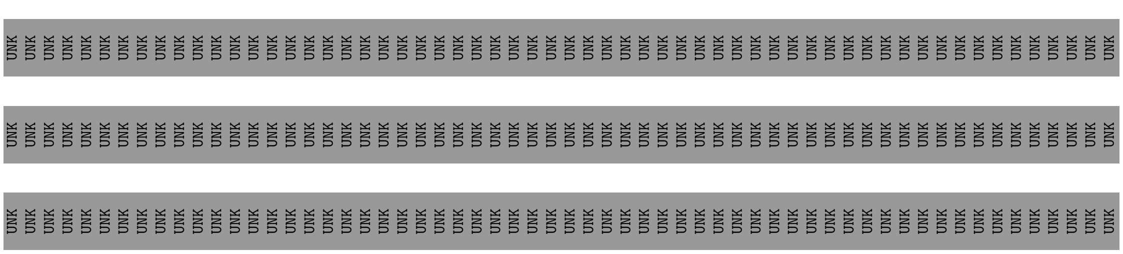
- Molecule 30: Pre-mRNA-splicing factor CWC21

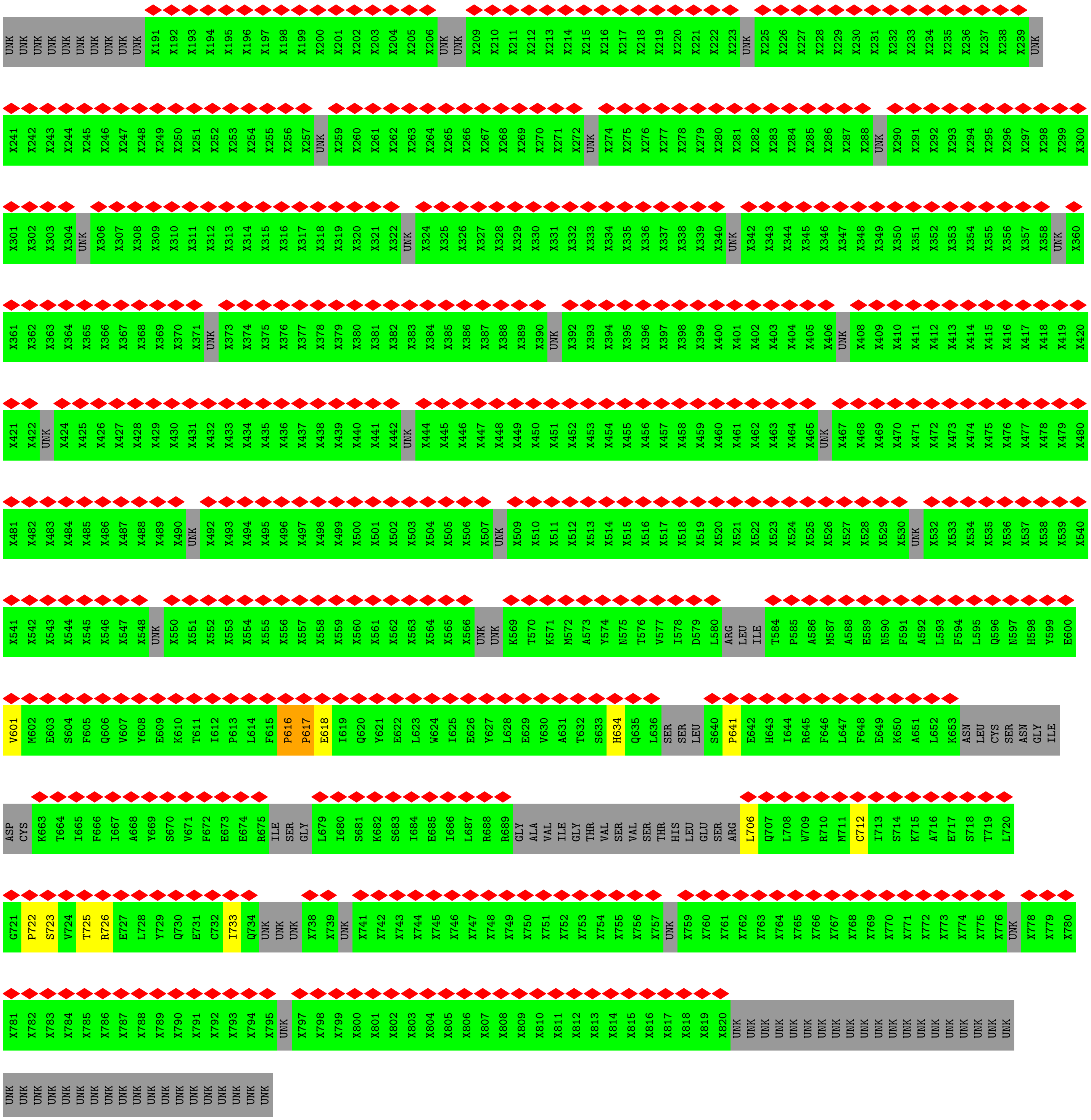
Chain X:



- Molecule 31: Pre-mRNA-splicing factor SYF1

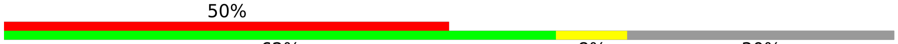
Chain v:

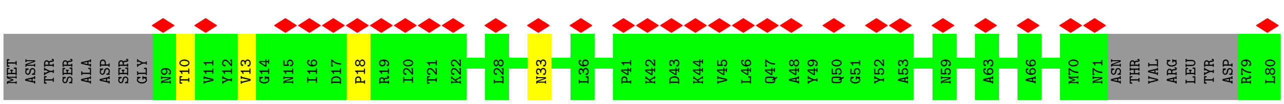




- Molecule 32: Protein HSH49

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

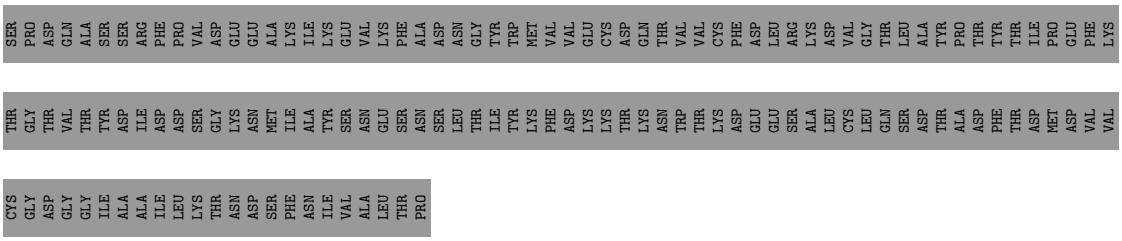
S61 L62 T63 E64 S65 THR ASN SER ALA THR LEU LYS ALA ASN TYR SER I77 P78 N79 L80 L81 T82 S83 L84 Q85 N86 E87 W88 D89 A90 I91 M92 L93 E94 N95 F96 K97 L98 R99 S100 T101 L102 D103 S104 L105 T106 K107 K108 L109 S110 T111 V112 M113 Y114 E115 R116 D117 A118 A119 K120

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

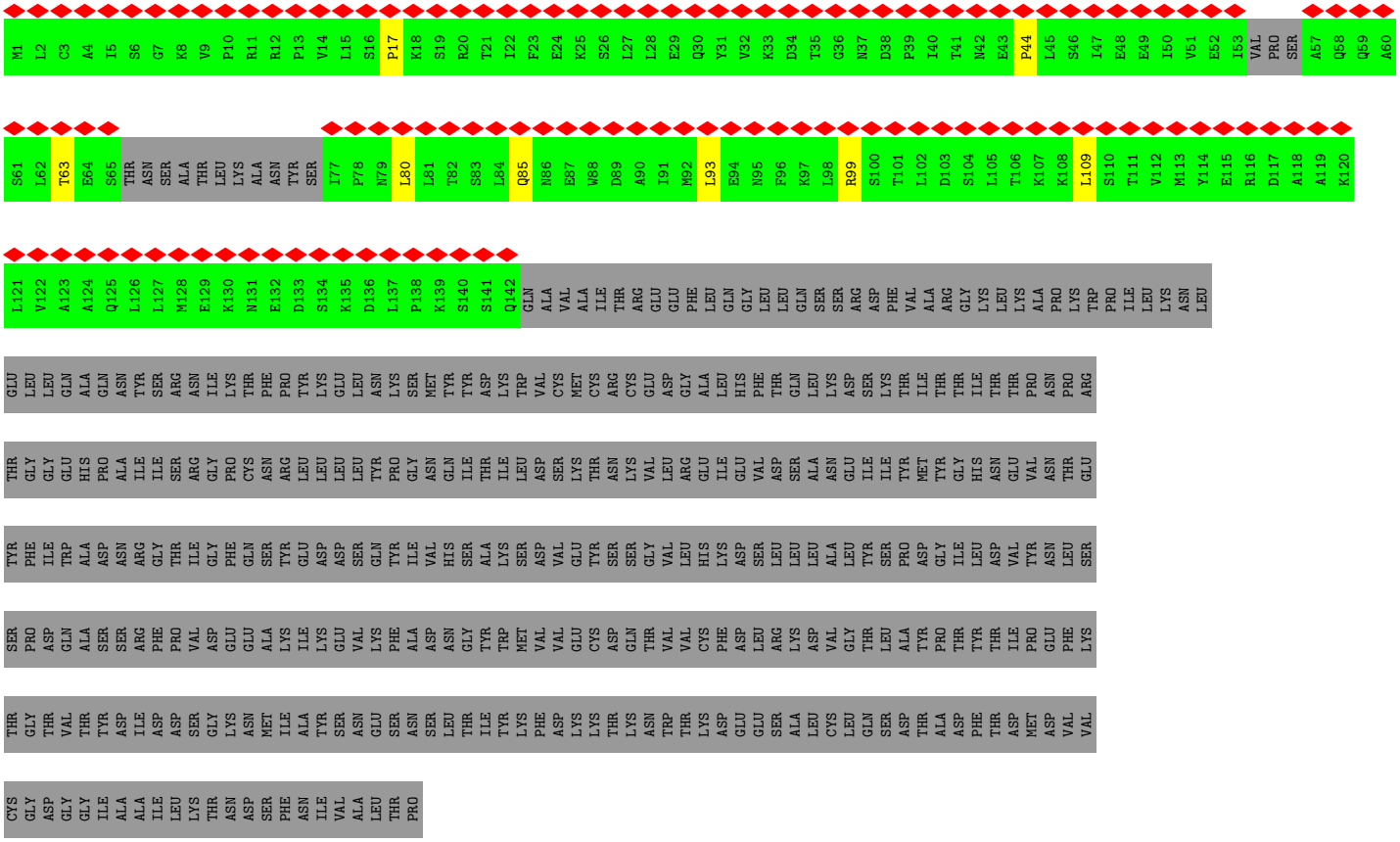
THR GLY GLY GLU HIS PRO ALA ILE ILE SER ARG GLY PRO CYS ASN ARG LEU LEU LEU LEU TYR PRO GLY ASN GLN ILE THR ILE LEU ASP SER LYS THR ASN LYS VAL LEU ARG GLU ILE GLU VAL ASP SER ALA ASN GLU ILE ILE TYR MET TYR GLY HIS ASN GLU VAL ASN THR GLU

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



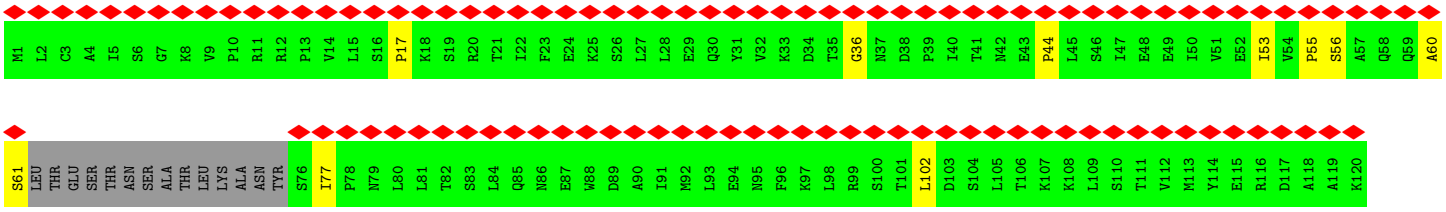
• Molecule 34: Pre-mRNA-processing factor 19

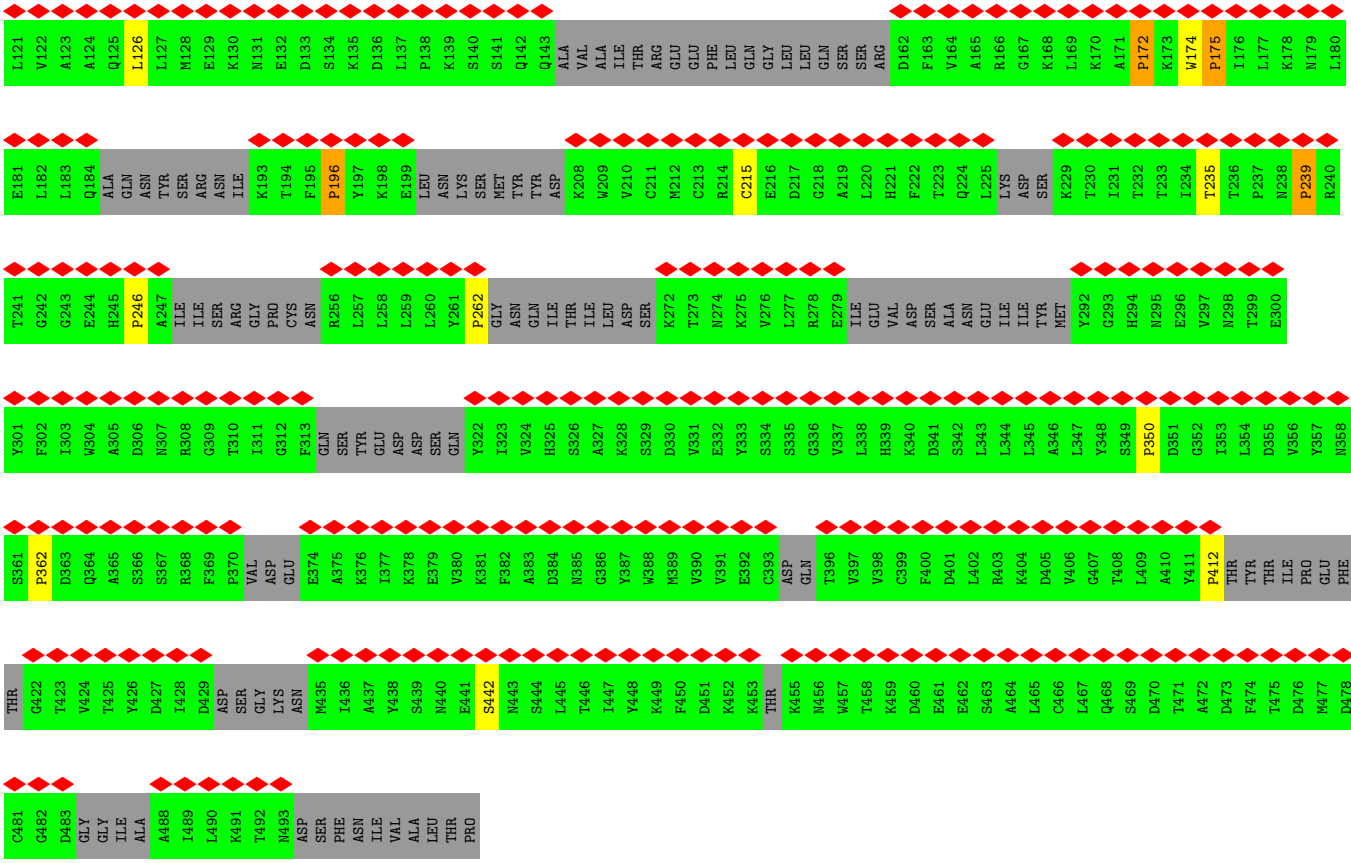
Chain p:



• Molecule 34: Pre-mRNA-processing factor 19

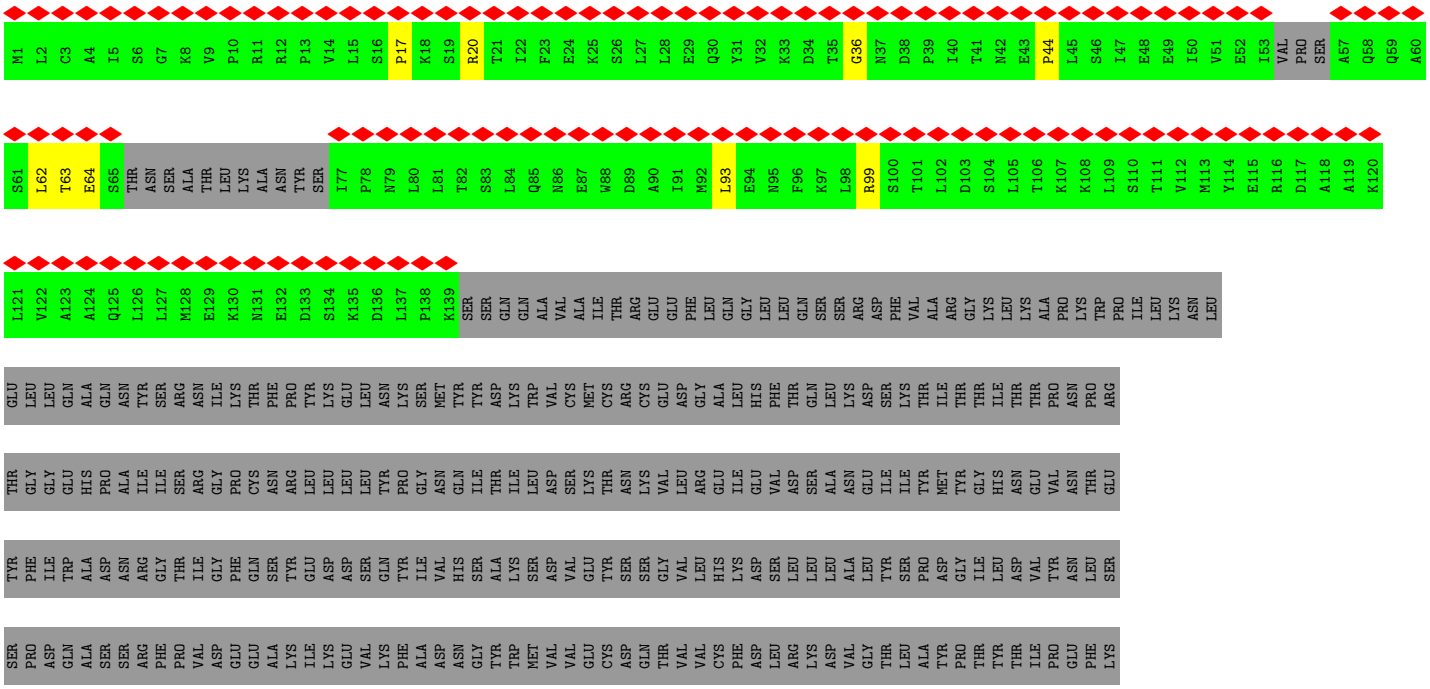
Chain q:





- 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:

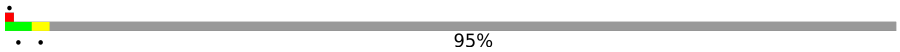
M1 D2 G3 L4 S5 F6 V7 D8 K9 GLY LYS ILE P13 D14 G15 Y16 K17 N18 E19 I20 D21 Q22 L23 V24 K25 K26 E27 F28 A29 N30 I31 K32 ARG GLU PRO VAL HIS PRO GLU ILE ARG GLY ILE LEU ALA LYS ARG LYS GLY A50 D51 N52 S53 V54 S55 T56 L57 T58 N59 A60

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

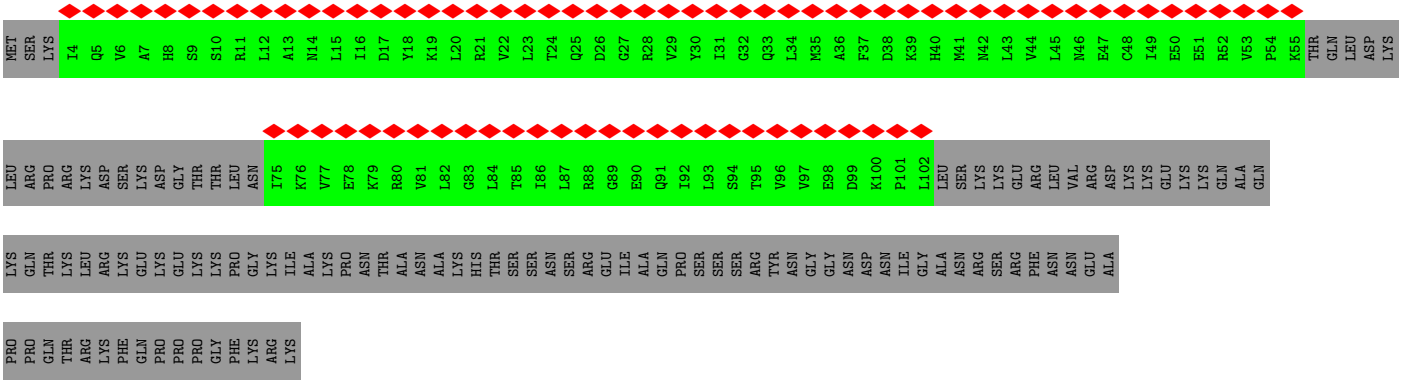
LYS PHE ILE SER SER SER GLU ASP LYS THR VAL ARG ILE TRP GLU ASN GLN ILE ASN VAL PRO ILE LYS GLN ILE SER ASP THR ALA GLN HIS SER MET PRO PHE LEU ASN VAL HIS PRO SER GLN ASN TYR PHE CYS ALA GLN SER MET ASP ASN ARG ILE TYR SER PHE SER LEU LYS

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

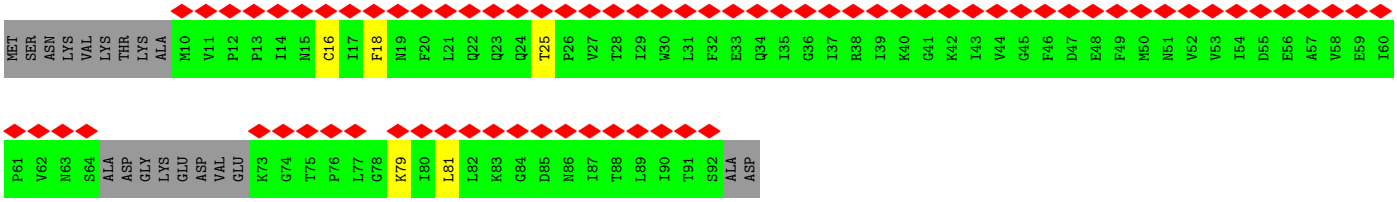
- Molecule 37: Small nuclear ribonucleoprotein-associated protein B

Chain k:



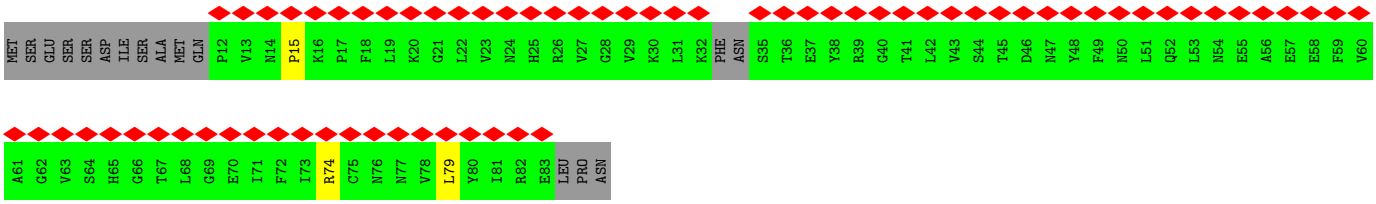
- Molecule 38: Small nuclear ribonucleoprotein E

Chain i:



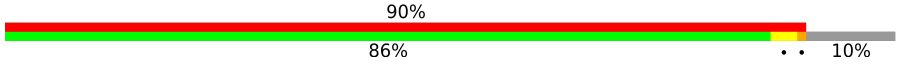
- Molecule 39: Small nuclear ribonucleoprotein F

Chain h:



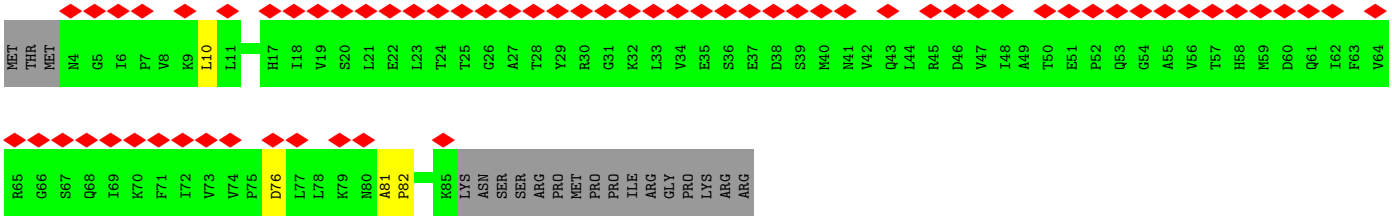
- Molecule 40: Small nuclear ribonucleoprotein G

Chain j:



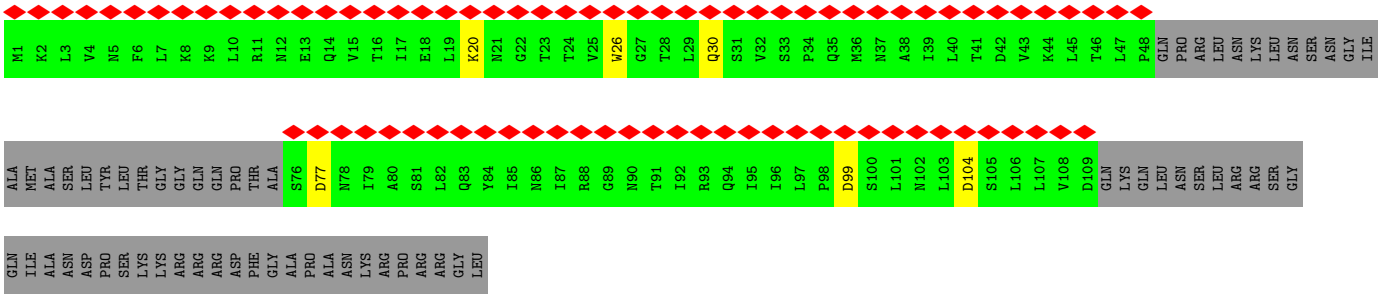
- Molecule 41: Small nuclear ribonucleoprotein Sm D3

Chain l:



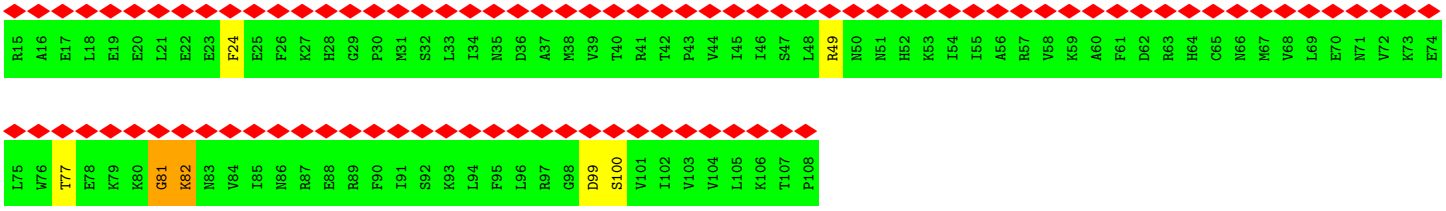
• Molecule 42: Small nuclear ribonucleoprotein Sm D1

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

All (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
1	A	1335	TRP	CG-CD1	5.94	1.45	1.36
6	F	71	PHE	CG-CD1	-5.93	1.29	1.38
19	T	148	CYS	CB-SG	-5.92	1.72	1.81
1	A	1609	TRP	CB-CG	-5.78	1.39	1.50
6	F	836	TRP	CB-CG	-5.65	1.40	1.50
1	A	298	TYR	CG-CD2	-5.48	1.32	1.39
6	F	1226	GLY	CA-C	-5.46	1.43	1.51
16	Q	215	PRO	N-CD	5.35	1.55	1.47
1	A	708	TRP	CG-CD1	-5.07	1.29	1.36
1	A	1542	TYR	CG-CD2	-5.06	1.32	1.39
6	F	1228	PHE	CG-CD1	-5.05	1.31	1.38

All (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
1	A	1405	ILE	CG1-CB-CG2	-6.74	96.58	111.40
6	F	1124	LEU	CB-CG-CD1	6.63	122.27	111.00
17	R	218	GLY	N-CA-C	6.41	129.12	113.10
28	G	680	PRO	C-N-CD	-6.34	106.64	120.60
24	Z	42	ARG	NE-CZ-NH2	6.09	123.34	120.30
28	G	689	LEU	CB-CG-CD2	-6.08	100.66	111.00
27	c	93	ARG	NE-CZ-NH2	-6.04	117.28	120.30
6	F	179	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	399	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	1317	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	1159	ARG	NE-CZ-NH2	-5.77	117.41	120.30
35	t	105	PRO	CA-CB-CG	5.76	115.75	104.80
3	C	461	LYS	N-CA-CB	5.76	120.96	110.60
6	F	839	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	A	1440	ILE	CG1-CB-CG2	-5.71	98.84	111.40
14	O	193	ARG	NE-CZ-NH2	-5.63	117.49	120.30
6	F	1130	ILE	CG1-CB-CG2	-5.59	99.11	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	888	ILE	CG1-CB-CG2	-5.57	99.15	111.40
43	g	81	GLY	CA-C-N	-5.55	104.98	117.20
15	P	318	ARG	NE-CZ-NH1	5.55	123.07	120.30
22	W	197	PHE	CB-CG-CD1	-5.54	116.93	120.80
1	A	1816	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	1816	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	C	464	PRO	N-CA-CB	5.49	109.89	103.30
1	A	716	ARG	NE-CZ-NH1	5.48	123.04	120.30
21	V	87	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	A	614	ARG	NE-CZ-NH1	5.46	123.03	120.30
19	T	123	ARG	NE-CZ-NH2	-5.41	117.60	120.30
35	t	77	PRO	CA-CB-CG	5.34	114.94	104.80
24	Z	62	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	716	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	831	ARG	NE-CZ-NH1	5.26	122.93	120.30
34	r	62	LEU	CA-CB-CG	-5.23	103.26	115.30
1	A	1825	ILE	CG1-CB-CG2	-5.19	99.97	111.40
6	F	1357	ARG	NE-CZ-NH1	-5.19	117.70	120.30
23	Y	411	LEU	CA-CB-CG	-5.16	103.44	115.30
8	I	15	GLY	N-CA-C	5.15	125.98	113.10
6	F	1041	LEU	CB-CG-CD1	-5.13	102.27	111.00
39	h	74	ARG	NE-CZ-NH1	5.13	122.86	120.30
6	F	240	MET	CA-CB-CG	5.12	122.00	113.30
24	Z	108	ARG	NE-CZ-NH2	5.12	122.86	120.30
17	R	217	GLU	N-CA-C	5.11	124.79	111.00
1	A	1342	LEU	CB-CG-CD2	-5.09	102.35	111.00
43	g	82	LYS	N-CA-C	5.08	124.71	111.00
8	I	33	LEU	CB-CG-CD1	-5.04	102.44	111.00
33	f	109	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	A	1382	ARG	NE-CZ-NH2	-5.01	117.80	120.30
29	d	119	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	1426	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Group
2	B	696	SER	Peptide
2	B	904	GLN	Peptide
3	C	460	GLY	Mainchain,Peptide
3	C	534	THR	Peptide
3	C	70	TYR	Peptide
3	C	951	ILE	Peptide
6	F	1012	LYS	Mainchain,Peptide
6	F	1014	LYS	Mainchain,Peptide
6	F	1183	CYS	Mainchain,Peptide
6	F	185	ARG	Peptide
6	F	206	SER	Peptide
6	F	666	LEU	Peptide
6	F	667	THR	Mainchain,Peptide
6	F	855	ALA	Mainchain,Peptide
28	G	389	GLY	Peptide
28	G	680	PRO	Mainchain,Peptide
7	H	184	SER	Peptide
7	H	185	GLY	Peptide
7	H	212	LEU	Mainchain,Peptide
7	H	234	GLN	Mainchain,Peptide
8	I	13	GLY	Peptide
8	I	14	GLY	Peptide
8	I	15	GLY	Peptide
14	O	123	PRO	Peptide
14	O	278	ASP	Peptide
14	O	351	GLY	Mainchain,Peptide
14	O	437	GLU	Peptide
14	O	441	ALA	Peptide
15	P	85	SER	Peptide
16	Q	103	GLU	Peptide
16	Q	291	ILE	Peptide
19	T	104	CYS	Peptide
19	T	140	VAL	Peptide
20	U	44	ASN	Peptide
20	U	71	GLU	Peptide
24	Z	219	SER	Peptide
24	Z	232	GLU	Peptide
24	Z	397	LEU	Mainchain,Peptide
29	d	237	ILE	Peptide
33	f	92	ARG	Peptide
43	g	81	GLY	Mainchain,Peptide
40	j	41	ASP	Peptide

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Mol	Chain	Res	Type	Group
41	l	81	ALA	Mainchain,Peptide
36	n	67	GLY	Mainchain,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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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

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Mol	Chain	Res	Type
1	A	1847	ASP
1	A	2288	CYS
2	B	696	SER
2	B	697	SER
2	B	905	GLN
3	C	364	PHE
3	C	602	VAL
6	F	363	VAL
6	F	413	ILE
6	F	1299	ILE
8	I	55	ASN
8	I	56	PRO
16	Q	99	VAL
18	S	7	PRO
19	T	140	VAL
21	V	17	LEU
22	W	172	ILE
22	W	191	GLU
25	a	139	PHE
26	b	167	ILE
27	c	204	LYS
28	G	57	VAL
28	G	386	TYR
28	G	681	PRO
28	G	830	MET
28	G	831	SER
28	G	835	ILE
28	G	836	TYR
31	v	616	PRO
32	e	83	VAL
32	e	117	ASP
32	e	144	SER
32	e	148	LEU
32	e	170	ASN
34	q	53	ILE
34	q	77	ILE
34	q	172	PRO
34	q	174	TRP
34	q	239	PRO
34	q	246	PRO
34	q	362	PRO
34	q	442	SER

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Mol	Chain	Res	Type
34	r	64	GLU
35	t	77	PRO
1	A	1323	SER
1	A	1746	HIS
3	C	460	GLY
6	F	961	CYS
16	Q	255	SER
17	R	44	ASN
17	R	146	LEU
17	R	218	GLY
20	U	52	HIS
22	W	230	SER
24	Z	69	ASN
24	Z	206	LYS
24	Z	234	GLU
24	Z	235	ALA
24	Z	398	PRO
25	a	168	PHE
27	c	230	THR
31	v	601	VAL
31	v	618	GLU
31	v	634	HIS
32	e	147	LYS
32	e	149	LYS
32	e	171	GLN
34	q	196	PRO
35	t	110	GLU
36	n	61	LYS
1	A	645	ASP
1	A	1585	MET
3	C	952	PRO
6	F	364	THR
10	K	19	ILE
14	O	124	GLU
14	O	391	GLU
14	O	442	TRP
15	P	59	THR
18	S	131	THR
24	Z	67	LYS
24	Z	204	ASP
26	b	68	THR
27	c	82	ASN

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Mol	Chain	Res	Type
32	e	82	LYS
34	o	17	PRO
34	r	20	ARG
35	t	80	ASN
1	A	540	THR
1	A	562	ILE
2	B	1609	MET
3	C	84	GLN
14	O	278	ASP
14	O	279	PRO
14	O	435	GLU
15	P	86	ASN
19	T	119	THR
24	Z	304	SER
26	b	8	GLN
27	c	224	MET
27	c	231	SER
32	e	33	ASN
41	l	82	PRO
43	g	82	LYS
1	A	1015	PRO
1	A	1490	ARG
3	C	366	ASN
3	C	854	ILE
6	F	92	GLN
6	F	247	PHE
6	F	248	ASN
6	F	434	ASN
6	F	773	LYS
7	H	194	PHE
7	H	235	PRO
15	P	312	ALA
16	Q	52	SER
16	Q	119	LYS
21	V	18	SER
24	Z	229	VAL
28	G	873	HIS
34	q	60	ALA
3	C	363	PRO
18	S	22	PRO
19	T	104	CYS
23	Y	783	PHE

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Mol	Chain	Res	Type
24	Z	146	ASN
28	G	348	VAL
28	G	892	SER
1	A	1964	PRO
29	d	166	VAL
34	q	36	GLY
39	h	15	PRO
1	A	407	VAL
1	A	741	ILE
1	A	802	PRO
3	C	704	PRO
3	C	829	VAL
24	Z	471	GLY
31	v	617	PRO
34	q	175	PRO
6	F	523	ILE
24	Z	214	ILE
32	e	18	PRO
1	A	644	VAL
1	A	771	PRO
6	F	1031	ILE
14	O	277	VAL
15	P	143	VAL
27	c	218	VAL
34	r	36	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	89/236 (38%)	82 (92%)	7 (8%)	12	41
9	J	93/97 (96%)	85 (91%)	8 (9%)	10	38
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	h	61/77 (79%)	60 (98%)	1 (2%)	62	83
40	j	58/66 (88%)	55 (95%)	3 (5%)	23	56
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

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	PRO
1	A	228	LYS
1	A	236	ARG
1	A	238	ARG
1	A	256	GLU
1	A	261	LEU
1	A	263	PRO
1	A	266	LEU
1	A	268	LEU
1	A	270	SER
1	A	271	GLN
1	A	309	SER
1	A	324	ASP
1	A	331	PHE
1	A	377	VAL
1	A	380	ARG
1	A	392	ASN
1	A	394	ARG
1	A	396	ARG
1	A	451	ASP
1	A	452	PHE
1	A	461	LEU
1	A	497	GLN
1	A	570	GLN
1	A	614	ARG
1	A	640	ARG
1	A	715	LEU
1	A	716	ARG
1	A	737	ARG
1	A	750	LEU

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Mol	Chain	Res	Type
1	A	769	MET
1	A	773	SER
1	A	774	ILE
1	A	775	ARG
1	A	777	LYS
1	A	782	ILE
1	A	854	ARG
1	A	893	ARG
1	A	928	ARG
1	A	934	ARG
1	A	1011	ASN
1	A	1043	ARG
1	A	1325	SER
1	A	1370	ARG
1	A	1376	ASN
1	A	1378	LYS
1	A	1379	MET
1	A	1442	ARG
1	A	1456	ARG
1	A	1470	GLN
1	A	1499	ARG
1	A	1509	ARG
1	A	1521	ARG
1	A	1589	LYS
1	A	1590	LEU
1	A	1605	ARG
1	A	1608	LEU
1	A	1629	LEU
1	A	1739	ARG
1	A	1747	ASP
1	A	1748	ILE
1	A	1749	SER
1	A	1783	MET
1	A	1794	LEU
1	A	1809	ASN
1	A	1816	ARG
1	A	1830	VAL
1	A	1831	GLN
1	A	1843	LEU
1	A	1899	TRP
1	A	1998	ARG
1	A	2006	SER

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Mol	Chain	Res	Type
1	A	2255	LEU
1	A	2402	GLU
1	A	2403	GLU
1	A	2408	GLN
1	A	2409	ILE
1	A	2412	PHE
3	C	100	LEU
3	C	108	GLN
3	C	115	LYS
3	C	132	ARG
3	C	150	MET
3	C	160	ARG
3	C	170	LEU
3	C	176	ARG
3	C	177	TYR
3	C	180	ASN
3	C	275	LEU
3	C	395	LYS
3	C	548	ARG
6	F	80	VAL
6	F	97	THR
6	F	147	PHE
6	F	153	ASP
6	F	162	ILE
6	F	203	ILE
6	F	257	ILE
6	F	294	PHE
6	F	410	PHE
6	F	444	LEU
6	F	770	LEU
6	F	885	TRP
6	F	1195	VAL
6	F	1231	LEU
6	F	1239	MET
6	F	1302	ARG
6	F	1318	ILE
7	H	155	ARG
7	H	179	LYS
7	H	180	LYS
7	H	181	GLU
7	H	192	ARG
7	H	195	GLU

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Mol	Chain	Res	Type
7	H	233	VAL
7	H	242	LEU
7	H	246	LYS
7	H	288	HIS
8	I	11	LYS
8	I	18	SER
8	I	51	GLN
8	I	53	ARG
8	I	55	ASN
8	I	77	SER
8	I	83	ARG
9	J	2	SER
9	J	4	HIS
9	J	54	GLN
9	J	78	ARG
9	J	97	LEU
9	J	98	ASP
9	J	99	ARG
9	J	102	GLU
10	K	8	LEU
10	K	24	GLU
10	K	27	THR
10	K	28	ARG
10	K	42	THR
10	K	44	GLN
10	K	57	ARG
10	K	60	LEU
10	K	63	ARG
14	O	138	HIS
14	O	228	ARG
15	P	37	ASN
15	P	40	LEU
15	P	44	ILE
15	P	48	GLN
15	P	52	GLU
15	P	55	VAL
15	P	57	LEU
15	P	60	LYS
15	P	111	HIS
15	P	133	LYS
15	P	243	GLU
15	P	244	LEU

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Mol	Chain	Res	Type
15	P	247	ARG
15	P	300	ASP
15	P	302	GLN
15	P	325	ASP
16	Q	119	LYS
16	Q	120	LEU
16	Q	209	ASN
16	Q	213	SER
16	Q	217	TRP
16	Q	220	THR
16	Q	222	THR
16	Q	226	LEU
16	Q	227	LEU
16	Q	245	LYS
16	Q	248	CYS
16	Q	252	ARG
17	R	7	LYS
17	R	10	LYS
17	R	12	GLN
17	R	14	LYS
17	R	15	GLU
17	R	17	GLU
17	R	18	LEU
17	R	31	ASN
17	R	41	PHE
17	R	66	ASN
17	R	67	ASP
17	R	121	ARG
17	R	181	CYS
17	R	210	LYS
17	R	215	ARG
18	S	10	GLU
18	S	40	ARG
19	T	54	GLN
19	T	122	CYS
19	T	126	ARG
20	U	38	LEU
20	U	40	LEU
20	U	42	SER
20	U	44	ASN
20	U	45	LYS
20	U	46	GLU

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Mol	Chain	Res	Type
20	U	50	LEU
21	V	6	GLN
21	V	110	ARG
22	W	160	LYS
22	W	168	GLN
22	W	174	VAL
22	W	187	SER
22	W	188	LEU
22	W	189	THR
22	W	191	GLU
22	W	196	THR
22	W	207	THR
22	W	208	SER
22	W	209	LEU
22	W	212	ARG
22	W	214	LEU
22	W	262	LEU
23	Y	266	THR
23	Y	367	PRO
23	Y	413	PRO
23	Y	578	PRO
23	Y	606	PRO
23	Y	614	PRO
23	Y	784	PRO
23	Y	826	PRO
24	Z	12	LYS
24	Z	16	GLU
24	Z	34	MET
24	Z	67	LYS
24	Z	94	LEU
24	Z	132	GLU
24	Z	138	ILE
24	Z	145	LYS
24	Z	149	ARG
24	Z	151	VAL
24	Z	162	LEU
24	Z	168	LYS
24	Z	174	TRP
24	Z	177	LEU
24	Z	179	TYR
24	Z	181	LEU
24	Z	184	GLN

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Mol	Chain	Res	Type
24	Z	185	GLU
24	Z	186	LEU
24	Z	190	LEU
24	Z	192	GLU
24	Z	193	SER
24	Z	194	LEU
24	Z	195	GLU
24	Z	197	LEU
24	Z	198	PHE
24	Z	199	GLU
24	Z	201	ARG
24	Z	216	ASP
24	Z	229	VAL
24	Z	243	GLU
24	Z	245	CYS
24	Z	303	LEU
24	Z	398	PRO
25	a	134	THR
25	a	167	ASP
25	a	168	PHE
25	a	178	TRP
27	c	504	PRO
27	c	505	PRO
27	c	517	VAL
27	c	523	LEU
27	c	532	PRO
27	c	550	PRO
28	G	22	GLN
28	G	327	TRP
28	G	386	TYR
28	G	469	SER
28	G	543	ARG
28	G	553	LEU
28	G	681	PRO
28	G	740	LYS
28	G	849	ARG
28	G	936	ARG
29	d	120	ASN
29	d	134	LYS
31	v	616	PRO
31	v	617	PRO
31	v	641	PRO

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Mol	Chain	Res	Type
31	v	706	LEU
31	v	712	CYS
31	v	722	PRO
31	v	723	SER
31	v	725	THR
31	v	726	ARG
31	v	733	ILE
32	e	10	THR
32	e	13	VAL
32	e	87	THR
32	e	153	VAL
32	e	179	THR
34	o	17	PRO
34	o	26	SER
34	o	44	PRO
34	o	63	THR
34	o	96	PHE
34	o	109	LEU
34	o	134	SER
34	p	17	PRO
34	p	44	PRO
34	p	63	THR
34	p	80	LEU
34	p	85	GLN
34	p	93	LEU
34	p	99	ARG
34	p	109	LEU
34	q	17	PRO
34	q	44	PRO
34	q	55	PRO
34	q	56	SER
34	q	61	SER
34	q	102	LEU
34	q	126	LEU
34	q	172	PRO
34	q	175	PRO
34	q	196	PRO
34	q	215	CYS
34	q	235	THR
34	q	239	PRO
34	q	262	PRO
34	q	350	PRO

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Mol	Chain	Res	Type
34	q	412	PRO
34	r	17	PRO
34	r	44	PRO
34	r	63	THR
34	r	93	LEU
34	r	99	ARG
35	t	5	SER
35	t	7	VAL
35	t	13	PRO
35	t	77	PRO
35	t	96	PRO
35	t	100	THR
35	t	105	PRO
35	t	108	SER
35	t	133	PRO
35	t	136	VAL
35	t	150	THR
36	n	51	PHE
36	n	55	GLU
36	n	57	LYS
36	n	58	ARG
36	n	59	ARG
36	n	61	LYS
36	n	62	THR
36	n	66	ASP
38	i	16	CYS
38	i	18	PHE
38	i	25	THR
38	i	79	LYS
38	i	81	LEU
39	h	79	LEU
40	j	18	ASN
40	j	41	ASP
40	j	71	LEU
41	l	10	LEU
41	l	76	ASP
42	m	20	LYS
42	m	26	TRP
42	m	30	GLN
42	m	77	ASP
42	m	99	ASP
42	m	104	ASP

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Mol	Chain	Res	Type
43	g	24	PHE
43	g	49	ARG
43	g	77	THR
43	g	99	ASP
43	g	100	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (173) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	392	ASN
1	A	429	ASN
1	A	541	ASN
1	A	574	GLN
1	A	785	HIS
1	A	848	ASN
1	A	868	GLN
1	A	997	GLN
1	A	1034	ASN
1	A	1045	GLN
1	A	1115	GLN
1	A	1156	HIS
1	A	1231	GLN
1	A	1295	GLN
1	A	1368	GLN
1	A	1376	ASN
1	A	1789	ASN
1	A	1836	ASN
1	A	1845	ASN
1	A	1895	HIS
1	A	2229	GLN
1	A	2355	ASN
1	A	2394	GLN
1	A	2408	GLN
2	B	116	ASN
2	B	122	GLN
2	B	170	GLN
2	B	191	ASN
2	B	529	ASN
2	B	706	GLN
2	B	739	GLN
2	B	773	ASN

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Mol	Chain	Res	Type
2	B	862	GLN
2	B	904	GLN
2	B	1003	ASN
2	B	1148	GLN
2	B	1219	ASN
2	B	1281	GLN
2	B	1352	GLN
2	B	1386	ASN
2	B	1390	GLN
2	B	1430	ASN
2	B	1435	ASN
2	B	1531	ASN
2	B	1701	ASN
2	B	1959	ASN
2	B	2046	ASN
2	B	2050	ASN
2	B	2139	ASN
2	B	2161	ASN
3	C	82	ASN
3	C	112	ASN
3	C	183	GLN
3	C	251	GLN
3	C	289	ASN
3	C	309	ASN
3	C	432	GLN
3	C	772	ASN
3	C	776	ASN
3	C	794	GLN
6	F	62	HIS
6	F	119	ASN
6	F	248	ASN
6	F	382	GLN
6	F	384	ASN
6	F	420	HIS
6	F	481	GLN
6	F	547	ASN
6	F	590	HIS
6	F	609	HIS
6	F	641	GLN
6	F	686	GLN
6	F	687	HIS
6	F	738	GLN

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Mol	Chain	Res	Type
6	F	754	HIS
6	F	944	ASN
6	F	950	GLN
6	F	1011	ASN
6	F	1091	HIS
6	F	1117	HIS
6	F	1192	HIS
6	F	1222	GLN
6	F	1304	HIS
6	F	1359	ASN
7	H	145	GLN
7	H	175	HIS
7	H	262	HIS
8	I	2	ASN
8	I	25	GLN
8	I	55	ASN
8	I	72	ASN
9	J	95	ASN
9	J	100	HIS
10	K	32	GLN
10	K	37	ASN
10	K	41	ASN
10	K	44	GLN
10	K	46	HIS
14	O	138	HIS
14	O	382	HIS
15	P	50	ASN
15	P	86	ASN
15	P	302	GLN
15	P	313	ASN
15	P	319	HIS
15	P	322	GLN
16	Q	67	GLN
16	Q	69	ASN
16	Q	106	ASN
16	Q	209	ASN
16	Q	225	GLN
17	R	31	ASN
17	R	58	HIS
17	R	69	GLN
17	R	91	HIS
17	R	201	ASN

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Mol	Chain	Res	Type
17	R	248	ASN
17	R	259	ASN
18	S	173	HIS
19	T	54	GLN
19	T	57	HIS
19	T	116	ASN
19	T	143	HIS
20	U	44	ASN
20	U	52	HIS
20	U	99	ASN
20	U	139	GLN
21	V	5	GLN
22	W	168	GLN
22	W	173	ASN
22	W	236	HIS
22	W	239	ASN
23	Y	272	GLN
23	Y	349	HIS
23	Y	429	HIS
24	Z	170	HIS
24	Z	184	GLN
24	Z	354	HIS
24	Z	362	ASN
24	Z	457	HIS
24	Z	463	ASN
25	a	140	GLN
25	a	175	ASN
25	a	176	GLN
27	c	82	ASN
27	c	214	ASN
28	G	17	HIS
28	G	58	GLN
28	G	59	ASN
28	G	65	HIS
28	G	216	GLN
28	G	219	HIS
28	G	295	ASN
28	G	311	ASN
28	G	407	HIS
28	G	572	GLN
28	G	618	GLN
28	G	695	ASN

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Mol	Chain	Res	Type
28	G	697	HIS
28	G	760	HIS
28	G	853	HIS
29	d	79	HIS
29	d	120	ASN
29	d	147	ASN
29	d	179	GLN
29	d	258	GLN
33	f	200	ASN
38	i	34	GLN
38	i	86	ASN
40	j	66	ASN
41	l	41	ASN
42	m	30	GLN

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%)

All (83) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	29	G
4	D	31	G
4	D	42	A
4	D	43	G
4	D	45	A
4	D	46	C
4	D	74	U
4	D	75	A
4	D	77	A
4	D	79	C
4	D	81	A
4	D	84	A
4	D	92	U

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Mol	Chain	Res	Type
4	D	101	C
4	D	127	U
4	D	164	C
4	D	165	A
4	D	166	U
4	D	170	U
4	D	171	U
4	D	172	U
4	D	173	U
4	D	174	G
4	D	175	G
5	E	14	C
5	E	35	A
5	E	36	U
5	E	51	A
5	E	60	G
5	E	66	C
5	E	67	C
5	E	68	C
5	E	80	U
5	E	81	G
5	E	85	C
5	E	86	G
5	E	88	U
5	E	91	A
5	E	92	C
5	E	93	A
5	E	103	A
11	L	15	C
11	L	17	U
11	L	18	U
11	L	19	U
11	L	26	G
11	L	32	G
11	L	38	U
11	L	41	C
11	L	46	C
11	L	48	U
11	L	52	A
11	L	66	A
12	N	96	U
12	N	98	A

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Mol	Chain	Res	Type
12	N	100	G
12	N	102	A
12	N	109	U
12	N	110	U
12	N	111	U
12	N	112	U
12	N	114	U
13	M	471	A
13	M	473	A
13	M	481	A
13	M	484	A
13	M	493	A
13	M	497	A
13	M	501	A
13	M	502	C
13	M	505	A
13	M	506	U
13	M	507	U
13	M	508	U
13	M	509	A
13	M	510	A
13	M	512	U
13	M	515	U
13	M	516	U
13	M	518	U
13	M	520	G
13	M	521	U
13	M	522	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	78	A
4	D	172	U
13	M	472	A
13	M	480	A
13	M	500	A
13	M	514	U
13	M	515	U

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

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

5.5 Carbohydrates (i)

There are no 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

All (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
47	Y	902	ADP	N3-C2-N1	-3.48	123.24	128.68
47	Y	902	ADP	C3'-C2'-C1'	3.14	105.70	100.98
47	Y	902	ADP	C4-C5-N7	-2.88	106.40	109.40
44	C	1500	GTP	C2-N1-C6	-2.36	120.75	125.10
44	C	1500	GTP	C8-N7-C5	2.24	107.25	102.99

There are no chirality outliers.

All (10) torsion outliers are listed below:

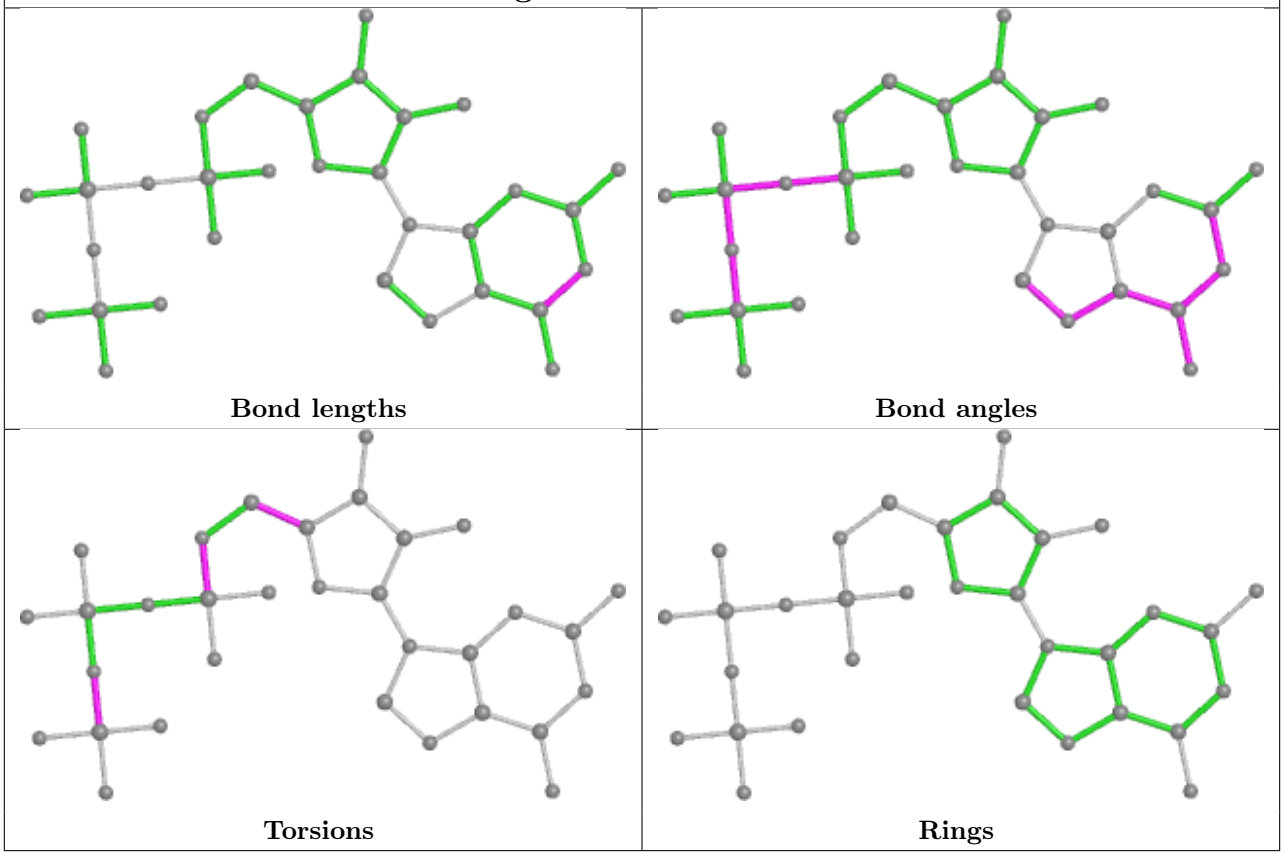
Mol	Chain	Res	Type	Atoms
44	C	1500	GTP	C5'-O5'-PA-O3A
44	C	1500	GTP	C5'-O5'-PA-O1A
44	C	1500	GTP	C5'-O5'-PA-O2A
44	C	1500	GTP	O4'-C4'-C5'-O5'
44	C	1500	GTP	C3'-C4'-C5'-O5'
47	Y	902	ADP	O4'-C4'-C5'-O5'
47	Y	902	ADP	C3'-C4'-C5'-O5'
44	C	1500	GTP	PB-O3B-PG-O1G
44	C	1500	GTP	PB-O3B-PG-O2G
44	C	1500	GTP	PB-O3B-PG-O3G

There are no ring outliers.

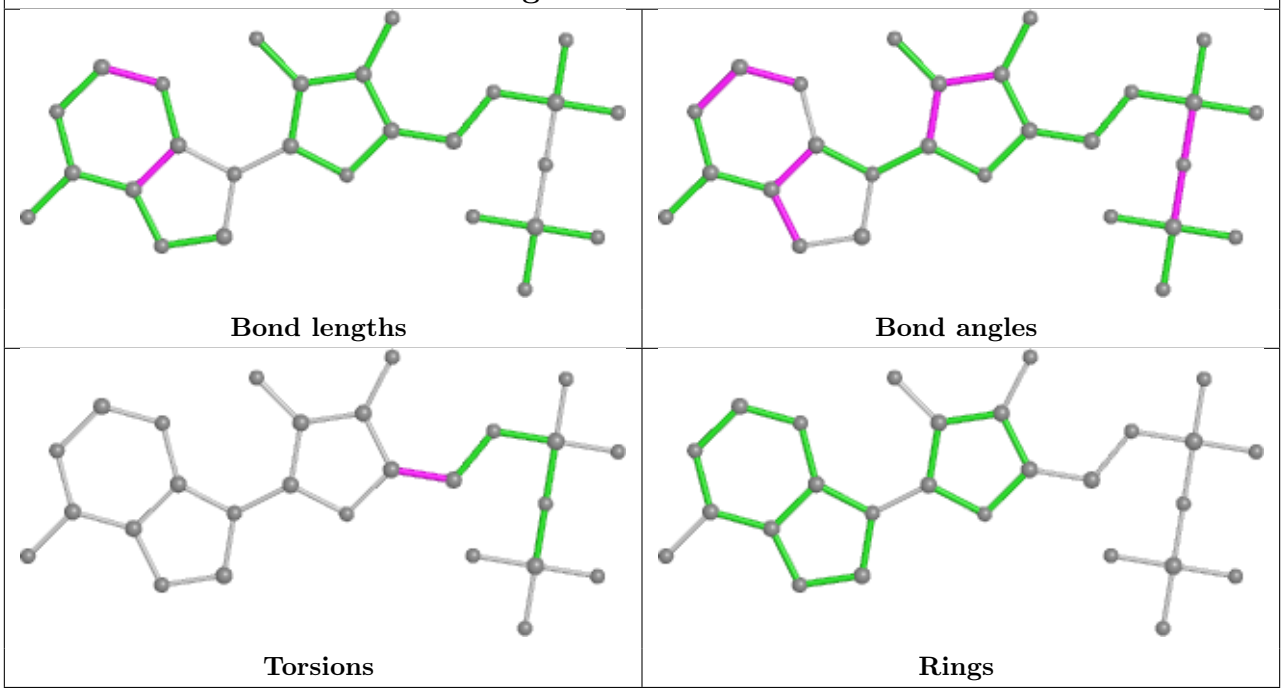
No monomer is involved in short contacts.

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.

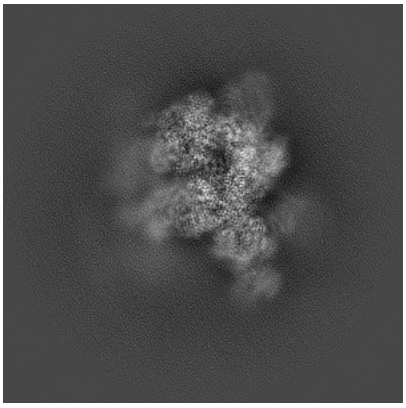
6 Map visualisation (i)

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.

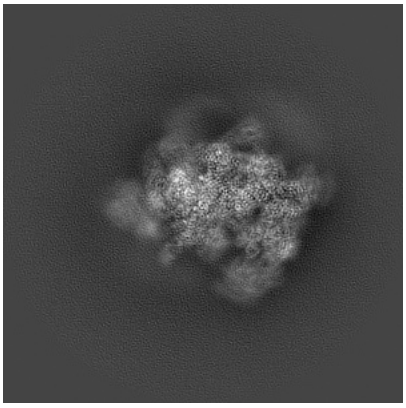
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

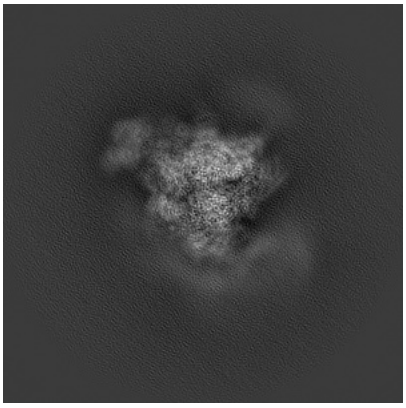
6.1.1 Primary map



X



Y

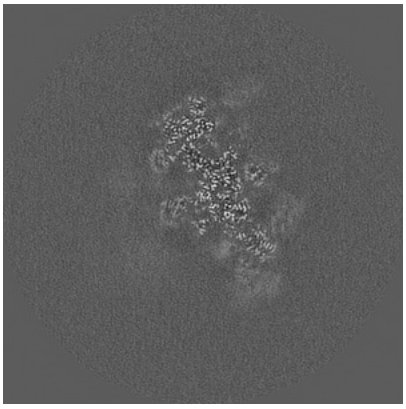


Z

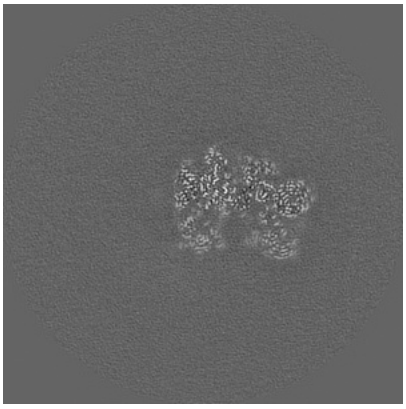
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

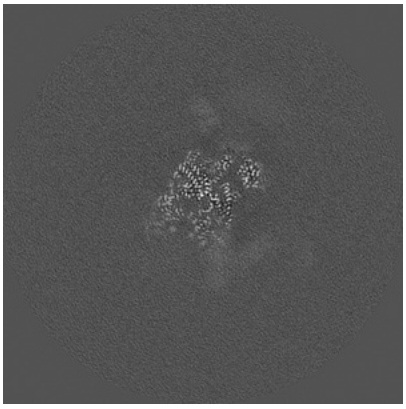
6.2.1 Primary map



X Index: 200



Y Index: 200

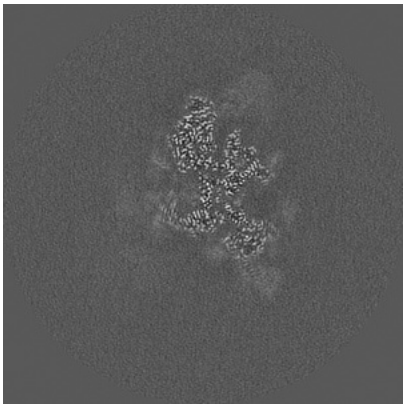


Z Index: 200

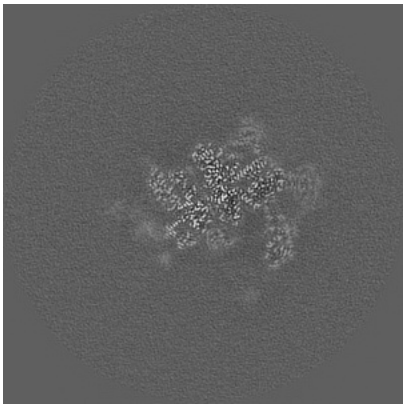
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

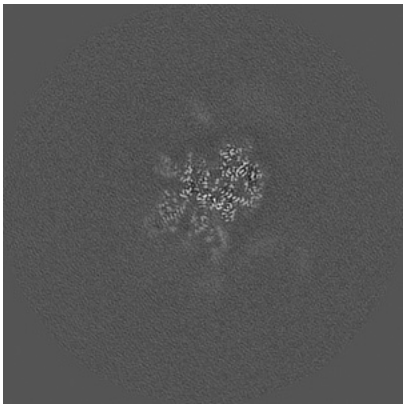
6.3.1 Primary map



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.

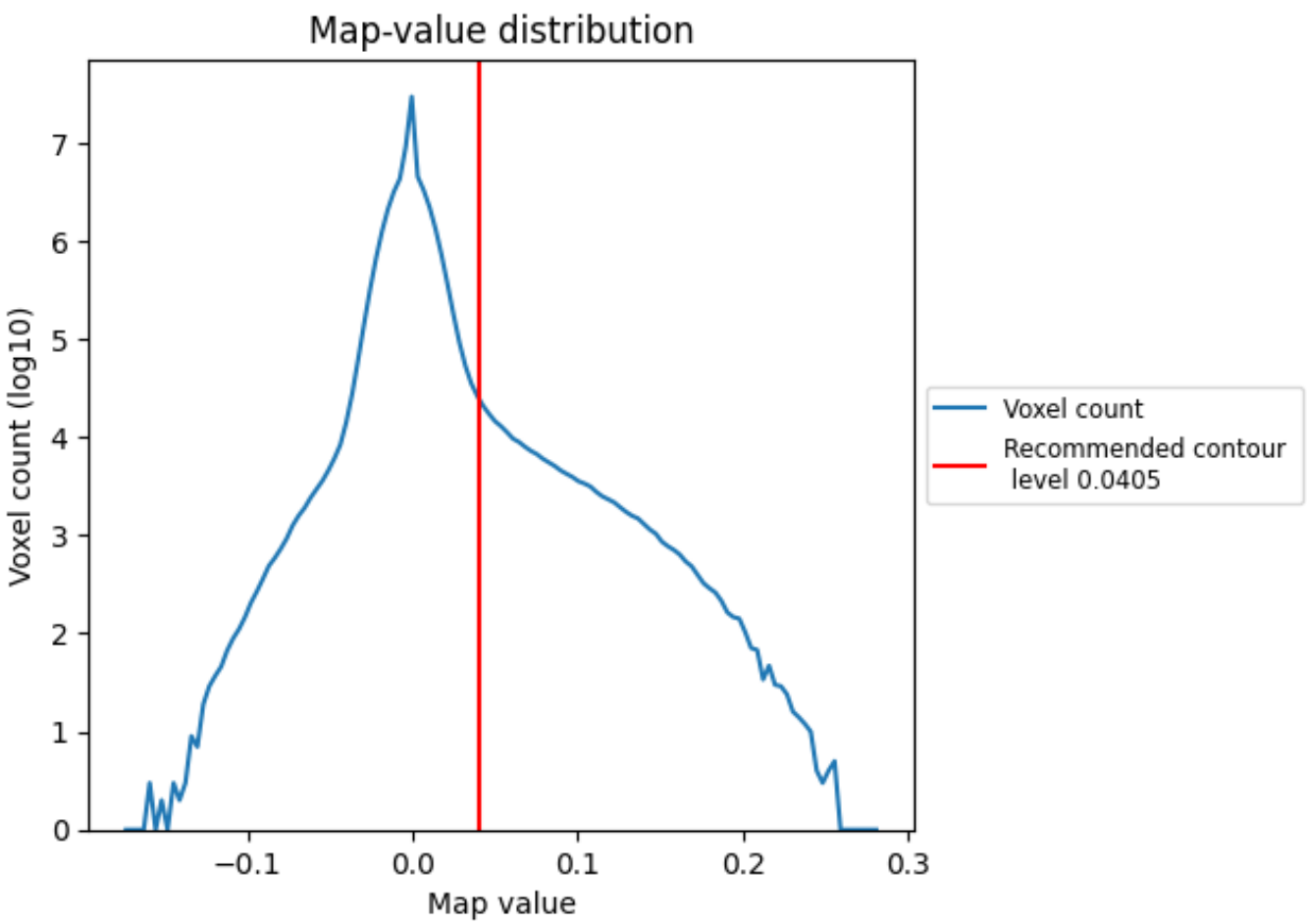
6.5 Mask visualisation (i)

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

7 Map analysis (i)

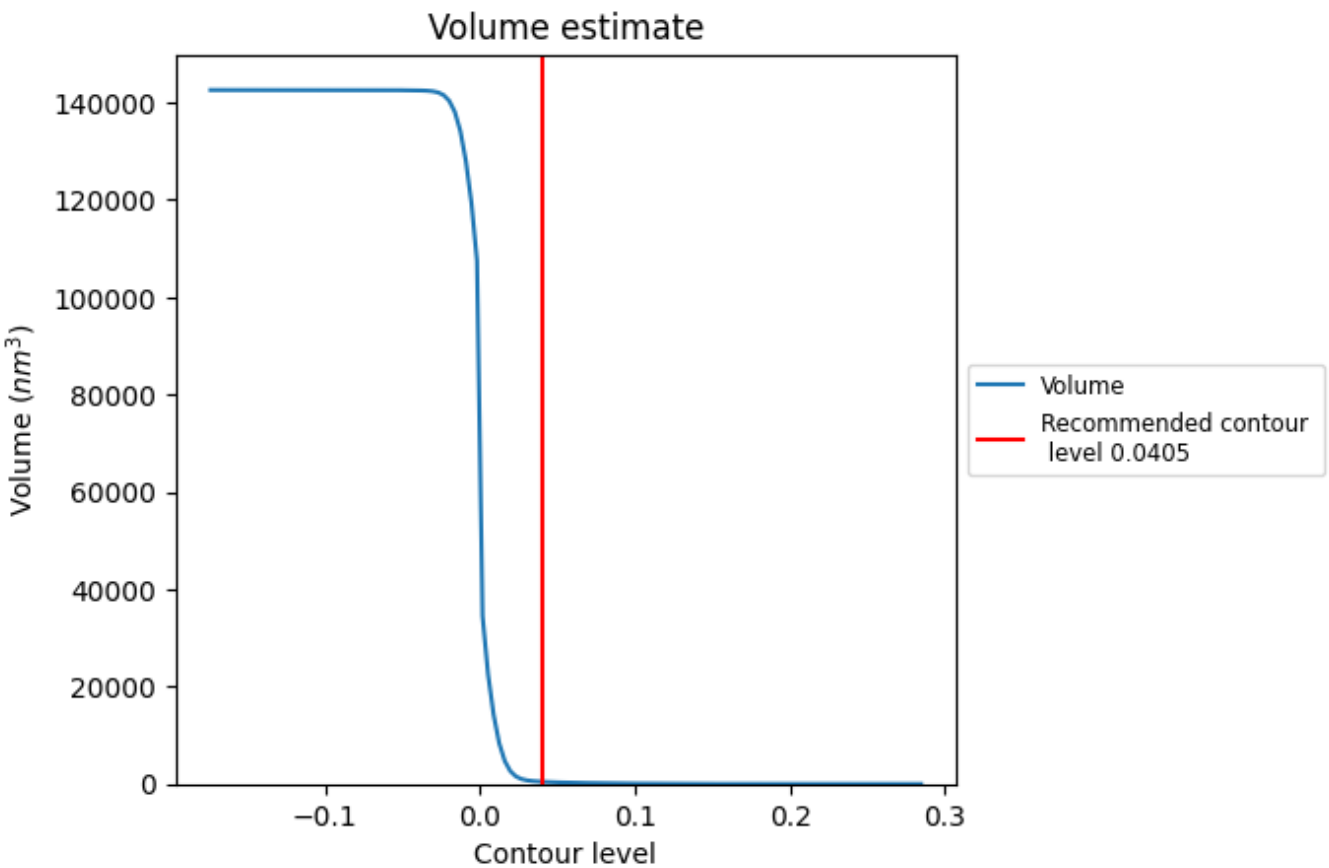
This section contains the results of statistical analysis of the map.

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.

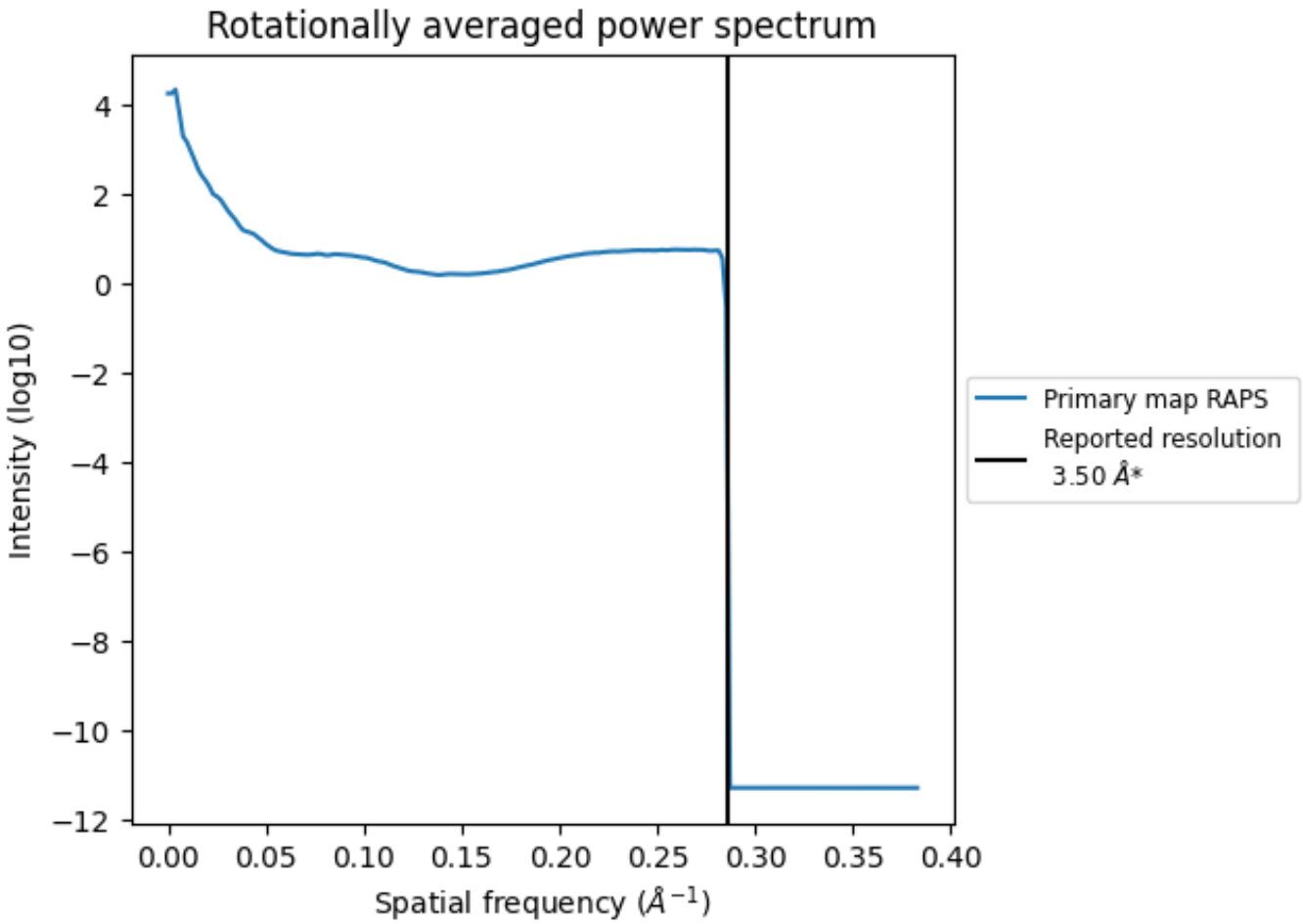
7.2 Volume estimate (i)



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}

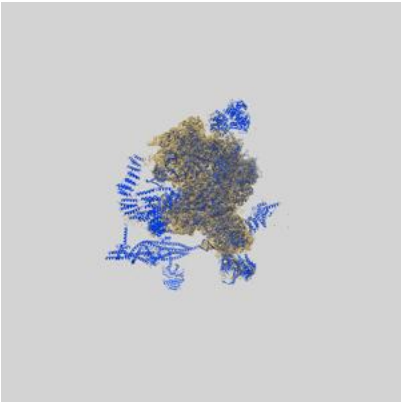
8 Fourier-Shell correlation (i)

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

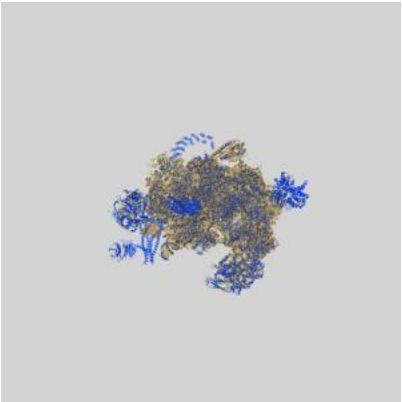
9 Map-model fit (i)

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.

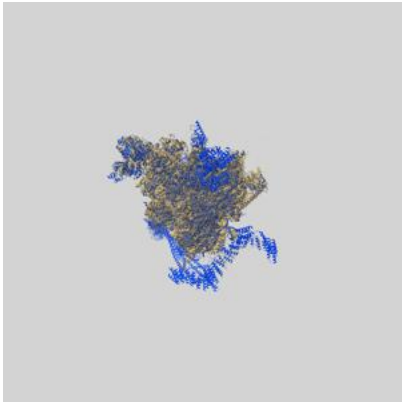
9.1 Map-model overlay (i)



X



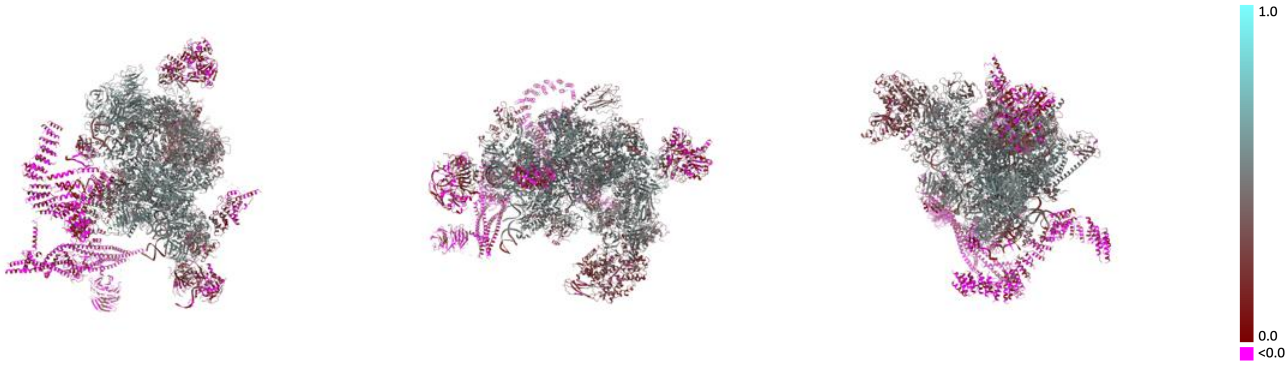
Y



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.

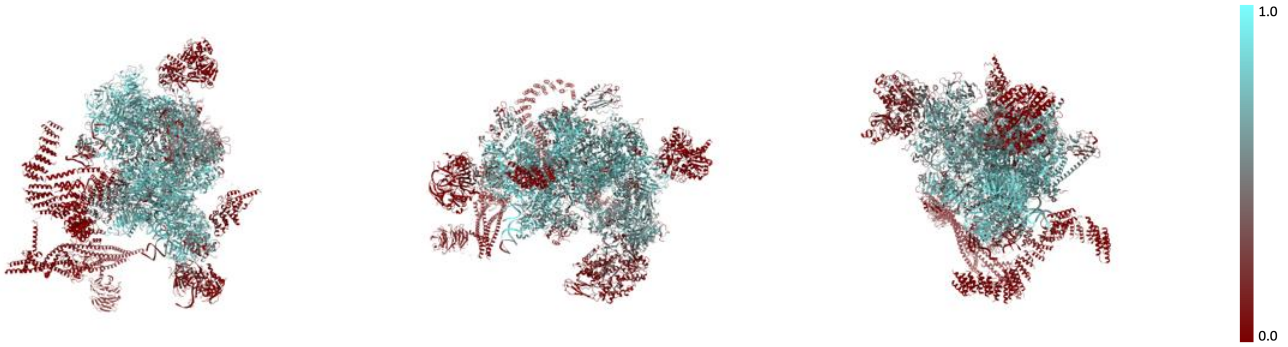
9.2 Q-score mapped to coordinate model (i)



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.

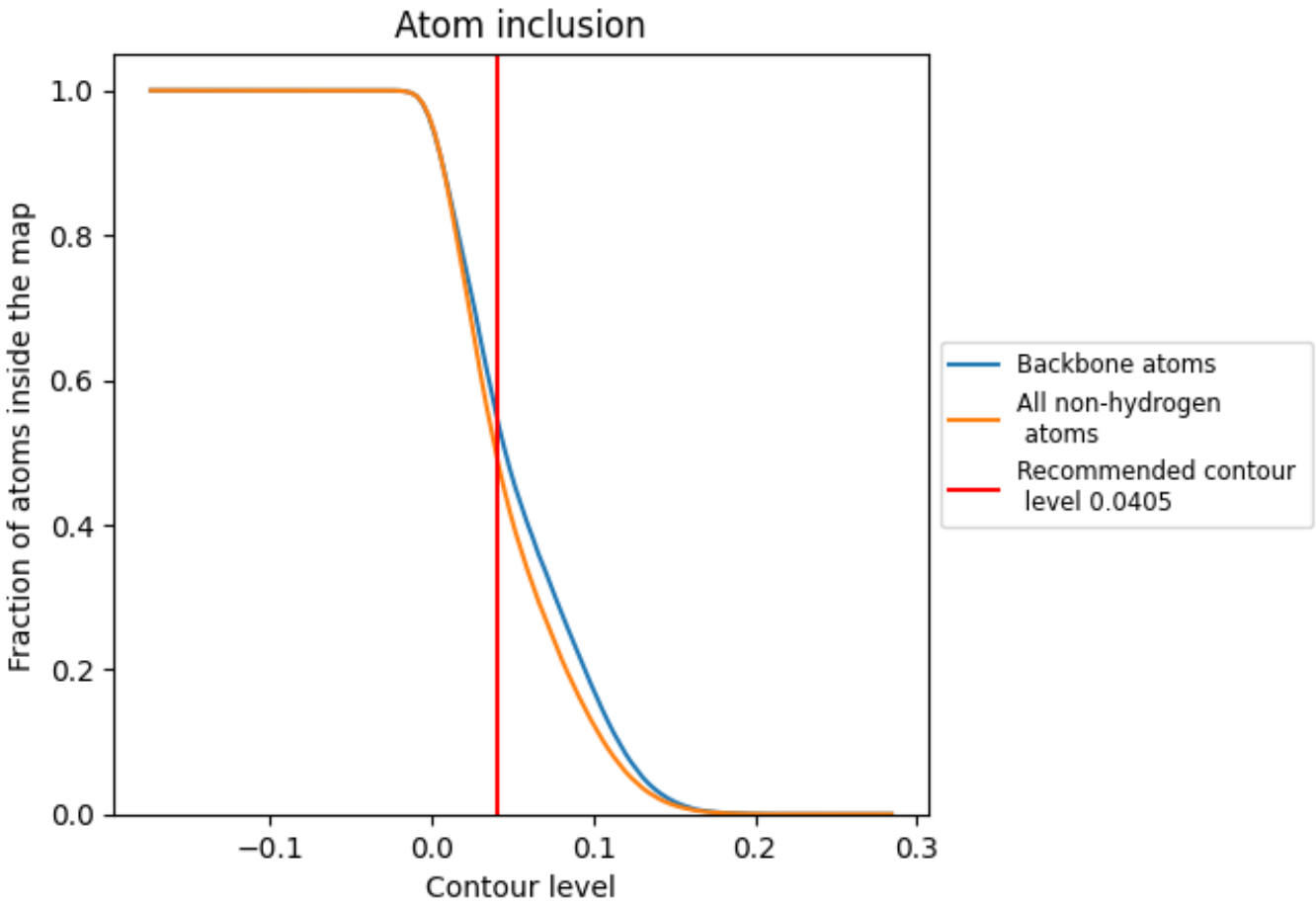
9.3 Atom inclusion mapped to coordinate model (i)



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