



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:27 AM JST

PDB ID : 5Y88
EMDB ID : EMD-6817
Title : Cryo-EM structure of the intron-lariat spliceosome ready for disassembly from *S.cerevisiae* at 3.5 angstrom
Authors : Wan, R.; Yan, C.; Bai, R.; Lei, J.; Shi, Y.
Deposited on : 2017-08-20
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

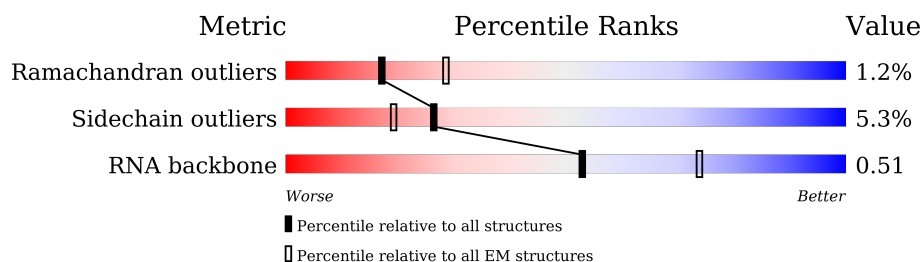
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2413	
2	B	214	
3	C	1008	
4	D	112	
5	E	38	
6	F	1175	
7	G	175	
8	H	859	

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Mol	Chain	Length	Quality of chain
9	I	687	
10	J	590	
11	K	215	
12	L	157	
13	M	364	
14	N	339	
15	O	451	
16	P	175	
17	Q	379	
18	R	278	
19	S	455	
20	T	283	
21	U	708	
22	V	322	
23	W	767	
24	a	196	
24	h	196	
25	b	94	
25	i	94	
26	c	86	
26	j	86	
27	d	77	
27	k	77	
28	e	101	
28	l	101	

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Mol	Chain	Length	Quality of chain
29	f	146	
29	m	146	
30	g	110	
30	n	110	
31	o	238	
32	p	111	
33	q	503	
33	r	503	
33	s	503	
33	t	503	
34	x	9	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 72347 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1903	Total	C	N	O	S	0	0
			15715	10107	2697	2854	57		

- Molecule 2 is a RNA chain called U5 snRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	913	Total	C	N	O	S	0	0
			7278	4696	1205	1347	30		

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	101	Total	C	N	O	P	0	0
			2150	963	384	702	101		

- Molecule 5 is a RNA chain called Intron lariat.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	28	Total	C	N	O	P	0	0
			587	264	95	200	28		

- Molecule 6 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	P	0	0
			1727	772	286	587	82		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNT309.

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

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	601	Total	C	N	O	S	0	0
			3204	1958	611	634	1		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	541	Total	C	N	O	S	0	0
			3542	2200	667	667	8		

- Molecule 10 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	431	Total	C	N	O	S	0	0
			2944	1824	544	568	8		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SYF2.

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

- Molecule 12 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	157	Total	C	N	O	S	0	0
			1290	808	240	231	11		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	182	Total	C	N	O	S	0	0
			1298	805	235	243	15		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC2.

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

- Molecule 15 is a protein called Pre-mRNA-splicing factor PRP46.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	68	Total	C	N	O	S	0	0
			554	348	111	94	1		

- Molecule 17 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	201	Total	C	N	O	S	0	0
			1583	988	290	298	7		

- Molecule 18 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	46	Total	C	N	O	S	0	0
			379	225	73	79	2		

- Molecule 19 is a protein called Pre-mRNA-processing factor 17.

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

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC23.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	107	Total	C	N	O	0	0
			816	523	144	149		

- Molecule 21 is a protein called Pre-mRNA-splicing factor SPP382.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	488	Total	C	N	O	S	0	0
			2690	1644	514	529	3		

- Molecule 22 is a protein called Pre-mRNA-splicing factor NTR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	91	Total	C	N	O	S	0	0
			619	381	112	124	2		

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	708	Total	C	N	O		0	0
			3505	2089	708	708			

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
24	h	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	70	Total	C	N	O	S	0	0
			554	355	98	100	1		
26	j	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	k	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	n	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

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

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

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	p	81	Total	C	N	O	0	0
			513	332	89	92		

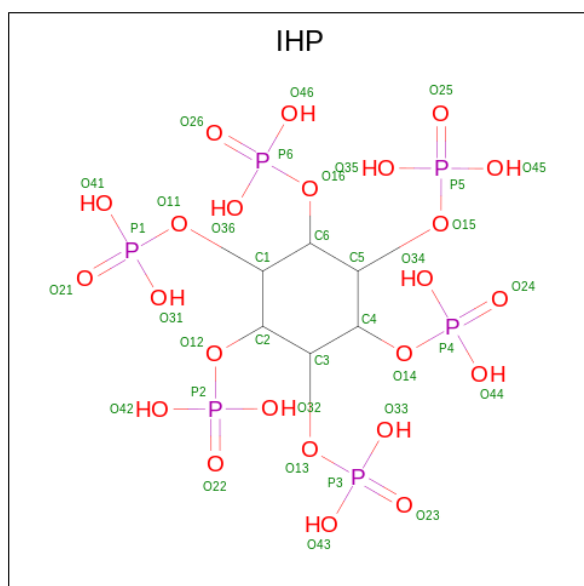
- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	q	126	Total	C	N	O	S	0	0
			831	526	134	169	2		
33	r	129	Total	C	N	O	S	0	0
			849	536	137	174	2		
33	s	129	Total	C	N	O	S	0	0
			850	537	137	174	2		
33	t	125	Total	C	N	O	S	0	0
			823	521	133	167	2		

- Molecule 34 is a RNA chain called RNA (intron or U6 snRNA).

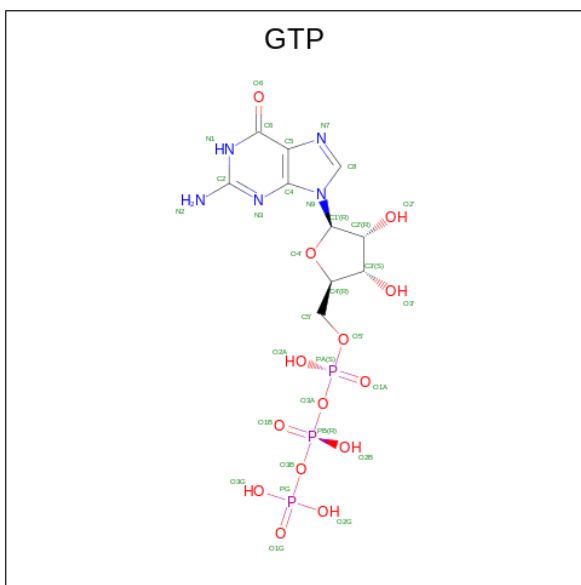
Mol	Chain	Residues	Atoms					AltConf	Trace
34	x	9	Total	C	N	O	P	0	0
			177	81	18	70	8		

- Molecule 35 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	C	1	Total	Mg	0
			1	1	
37	D	5	Total	Mg	0
			5	5	

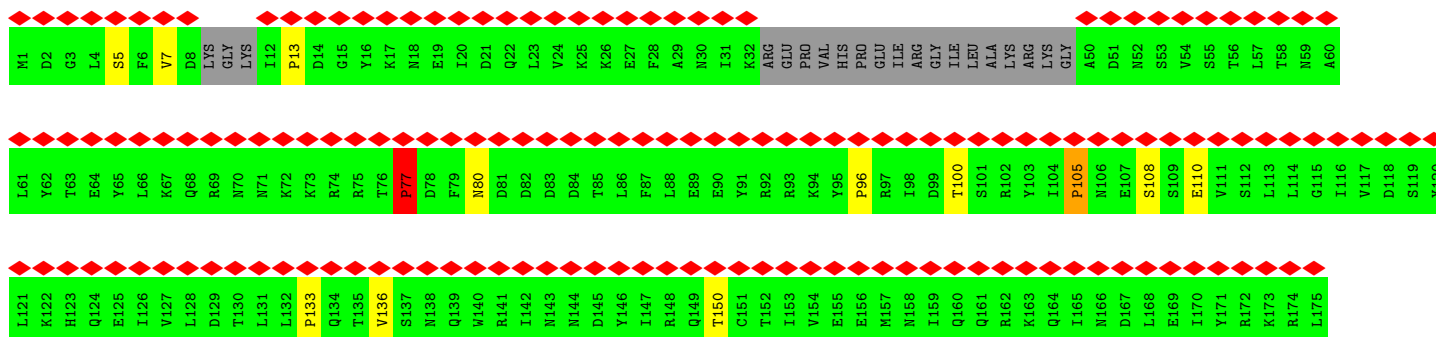
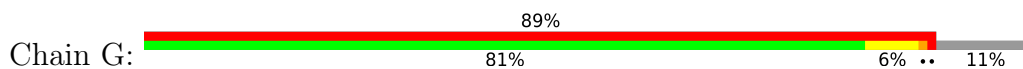
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	L	3	Total	Zn	0
			3	3	
38	M	2	Total	Zn	0
			2	2	
38	N	1	Total	Zn	0
			1	1	

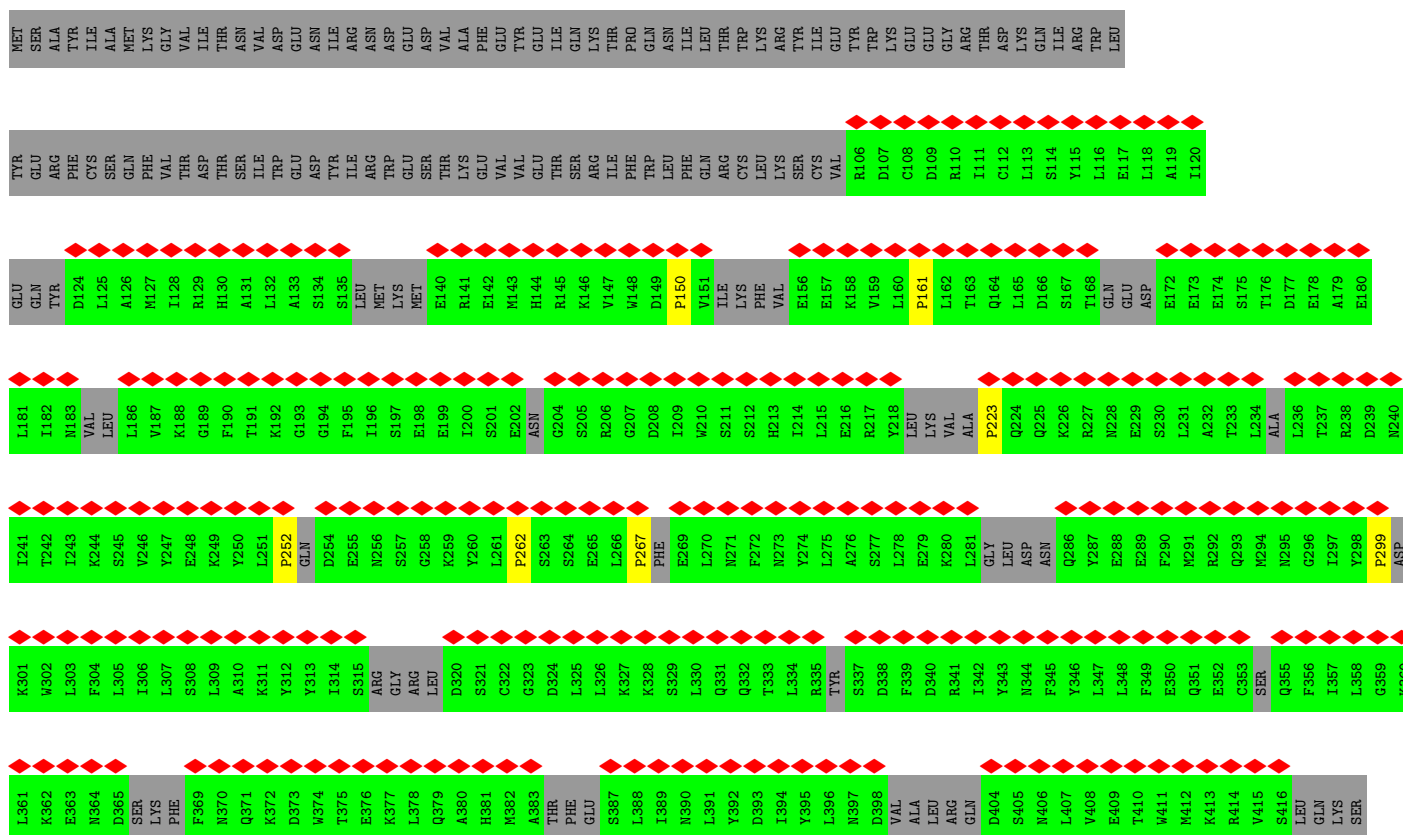
TRP	ASN	GLY	PRO	GLN	ILE	VAL	ALA	D2057	D1997	R1937	G1877	E1817	L1757	S1697	K1637	E1576	A1468
ASN	THR	THR	GLY	SER	THR	THR	SER	L2058	R1998	K1938	C1878	R1818	D1758	A1698	I1638	LYS	I1469
THR	THR	THR	VAL	SER	THR	THR	THR	I2059	I1999	A1939	I1879	I1819	Y1759	A1699	P1639	ALA	
PHE	THR	THR	VAL	ILE	THR	THR	THR	L2060	S2000	M1940	F1880	R1820	T1760	D1700	T1640	GLY	M1472
MET	THR	THR	VAL	ASN	THR	THR	THR	T2061	S2001	L1881	L1882	K1821	T1761	I1701	R1473	PHE	R1473
GLY	THR	THR	VAL	LYS	THR	THR	THR	E2062	Y2002	D1942	L1883	G1822	T1762	T1702	L1474	GLU	R1474
THR	ALA	ALA	VAL	LYS	THR	THR	THR	Y2063	T2003	P1943	N1883	G1823	N1763	M1703	L1475	ASP	
ALA	THR	THR	VAL	ILE	THR	THR	THR	G2064	A2004	L1944	P1884	Q1824	V1764	E1704	A1476	SER	A1476
PHE	ASN	ASN	PRO	LYS	ASN	ASN	ASN	E1945	T2005	E1945	K1885	I1825	S1765	S1705	F1477	MET	F1477
GLN	THR	THR	PRO	ASN	THR	THR	THR	K2066	S2006	V1946	T1886	Y1826	V1706	E1478	E1479	GLN	E1478
ASP	THR	THR	ASP	GLN	THR	THR	THR	Y2067	R2007	H1947	G1887	Q1827	Y1767	H1707	L1480	LYS	L1480
GLY	GLU	GLU	GLU	GLY	GLU	GLU	GLY	N2068	L2008	M1948	H1888	SER	P1768	E1708	E1481	THR	E1481
ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V2069	T2009	L1949	F1889	VAL	S1769	W1709	R1486	THR	R1486
ASN	THR	THR	THR	GLN	THR	THR	THR	N2070	L2010	D1950	F1890	GLN	P1770	E1710	A1497	ALA	A1497
PHE	THR	THR	THR	ILE	THR	THR	THR	M2071	L2011	F1951	L1891	GLU	T1771	V1711	H1500	ARG	H1500
LYS	THR	THR	THR	VAL	THR	THR	THR	I2072	L2012	P1952	K1892	PRO	Q1772	S1712	R1521	THR	R1521
THR	ALA	ALA	VAL	ALA	ALA	ALA	ALA	A2073	R2014	M1954	I1894	ASN	M1774	P1714	N1522	GLY	N1522
ASP	THR	THR	THR	LYS	ASP	ASP	ASP	L2074	A2014	I1954	I1894	SER	I1775	S1715	R1535	LEU	R1535
LEU	THR	THR	THR	LYS	THR	THR	THR	T2075	L2015	A1955	H1895	SER	I1776	L1716	L1536	GLN	L1536
PHE	THR	THR	THR	GLN	THR	THR	THR	Q2076	K2016	I1956	T1896	ASN	G1776	L1717	W1539	ILE	W1539
TYR	THR	THR	THR	SER	THR	THR	THR	E2077	T2017	R1957	S1897	Y1840	I1777	H1718	R1543	PRO	R1543
ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	T2078	N2018	P1958	W1898	A1841	D1778	H1719	F1606		F1606
GLU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	I2079	E2019	T1959	W1899	E1842	L1779	E1720	L1605		L1605
MET	THR	THR	THR	PHE	THR	THR	THR	L2080	E2020	E1960	A1900	L1843	A1780	T1720	F1607		F1607
ARG	THR	THR	THR	ILE	THR	THR	THR	S2021	S2021	L1961	G1901	F1844	Y1781	N1721	D1544		D1544
HIS	THR	THR	THR	SER	THR	THR	THR	I2082	A2022	R1962	K1903	N1845	N1782	S1723	W1545		W1545
PRO	ALA	ALA	ALA	GLY	ALA	ALA	ALA	L2083	K2023	L1963	K1903	M1846	M1783	S1723			
VAL	THR	THR	THR	SER	THR	THR	THR	I2084	M2024	P1964	R1904	D1847	Y1784	F1724			
PHE	THR	THR	THR	LYS	THR	THR	THR	G2085	I2025	F1965	L1905	T1848	D1785	K1725			
GLN	THR	THR	THR	ASP	THR	THR	THR	GLN	L2026	S1966	S1906	I1848	I1786	G1726			
THR	THR	THR	THR	LYS	THR	THR	THR	ASN	T2027	A1967	Q1907	K1849	Y1787	L1727			
THR	THR	THR	THR	ILE	THR	THR	THR	ILE	S2028	A1968	L1908	L1850	G1788	I1728			
GLU	ALA	ALA	ALA	LYS	THR	THR	THR	LYS	D2029	M1969	A1909	F1851	N1789	T1729			
ALA	THR	THR	THR	VAL	THR	THR	THR	ALA	P2030	S1970	K1910	V1852	W1790	M1730			
LEU	THR	THR	THR	ASN	THR	THR	THR	PRO	T2031	I1971	W1911	D1853	F1791	K1731			
GLY	THR	THR	THR	SER	THR	THR	THR	SER	I2032	D1972	K1912	L1854	N1792	M1732			
ASP	THR	THR	THR	LYS	THR	THR	THR	VAL	T2033	K1973	T1913	L1855	G1793	W1733			
LEU	THR	THR	THR	GLN	THR	THR	THR	GLN	I2034	L1974	A1914	N1856	L1794	F1734			
LEU	THR	THR	THR	LYS	THR	THR	THR	LYS	K2035	S1975	E1915	V1857	D1735	V1675			
ALA	THR	THR	THR	MET	THR	THR	THR	ALA	S2036	D1976	E1916	Y1858	V1736	I1676			
GLN	THR	THR	THR	ALA	THR	THR	THR	GLU	Y2037	V1977	W1917	R1859	Q1677	F1622			
ASP	THR	THR	THR	GLU	THR	THR	THR	LEU	H2038	V1978	S1918	L1861	L1738	F1623			
THR	THR	THR	THR	LEU	THR	THR	THR	GLU	L2039	M1979	A1919	V1862	R1739	L1624			
ALA	THR	THR	THR	ALA	THR	THR	THR	ALA	N2040	K1980	L1920	H1863	Y1740	V1625			
ASP	THR	THR	THR	ALA	THR	THR	THR	ARG	S2041	A1981	V1921	L1864	G1741	Q1626			
GLY	THR	THR	THR	ASP	THR	THR	THR	GLU	P2042	T1982	R1922	L1865	T1682	L1627			
ASP	THR	THR	THR	GLY	THR	THR	THR	GLY	F2043	E1983	S1923	T1866	Y1743	D1628			
THR	THR	THR	THR	VAL	THR	THR	THR	LYS	T2044	P1984	L1924	F1866	Y1744	K1683			
				ASN	THR	THR	THR	GLN	D2045	Q1985	P1925	E1867	T1684	E1684			
				ASN	THR	THR	THR	ASP	E2046	Q1986	K1926	G1868	S1745	T1685			
				GLU	THR	THR	THR	GLU	Q2047	V1987	E1927	M1869	H1746	V1686			
				ALA	THR	THR	THR	ALA	N2048	L1988	E1928	V1870	D1747	P1687			
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									I2051	I1991	K1931	A1811	Y1751	K1690			
									E2052	Y1992	Q1932	L1812	Y1752	R1693			
									Q2053	D1993	I1933	Y1813	R1753	M1694			
									Q2054	D1994	I1934	V1814	K1755	N1695			
									M2055	W1995	V1935	L1815	K1756	S1696			
									R2056	L1996	T1936	L1816	F1756				

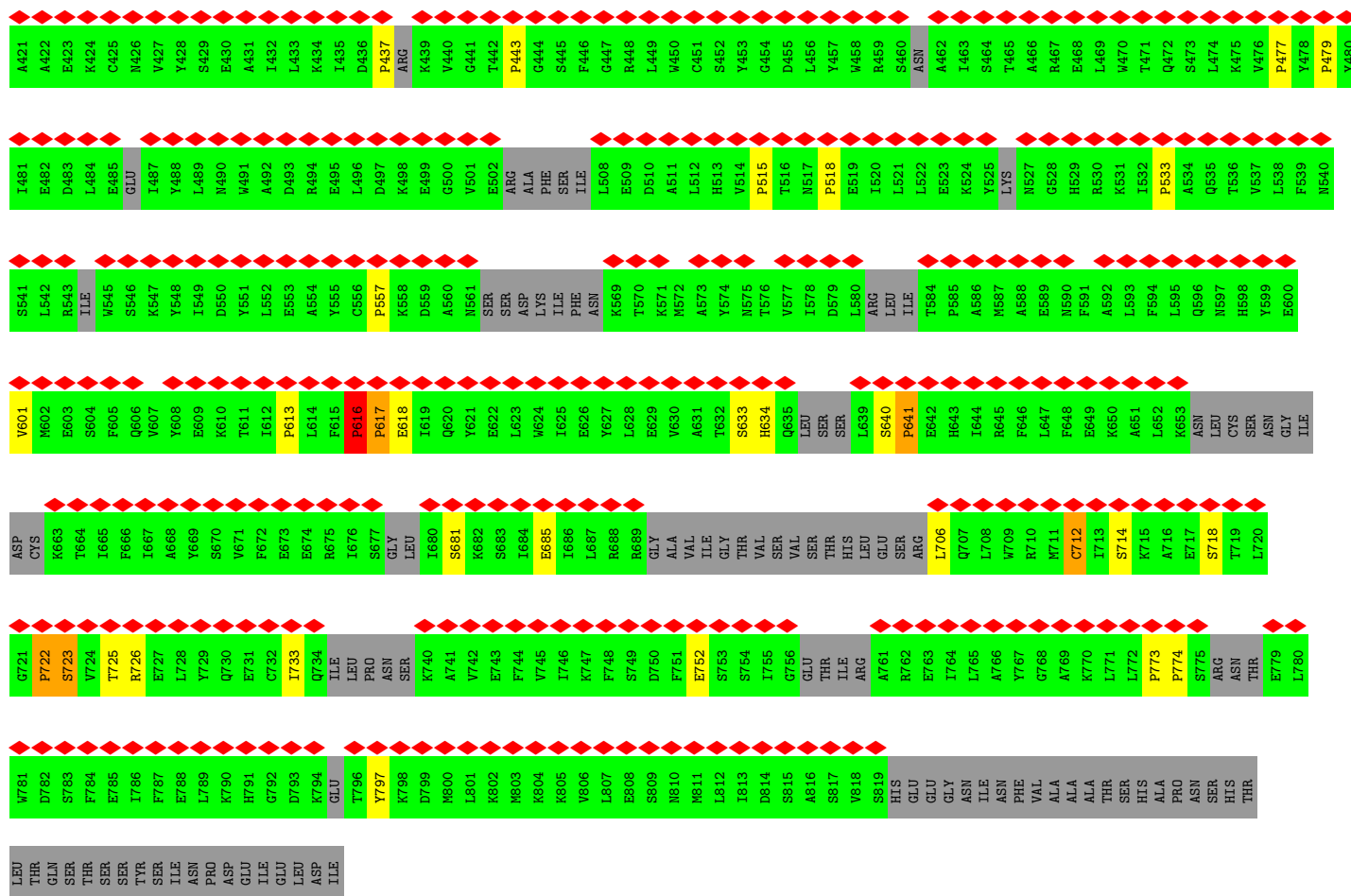


• Molecule 7: Pre-mRNA-splicing factor SNT309

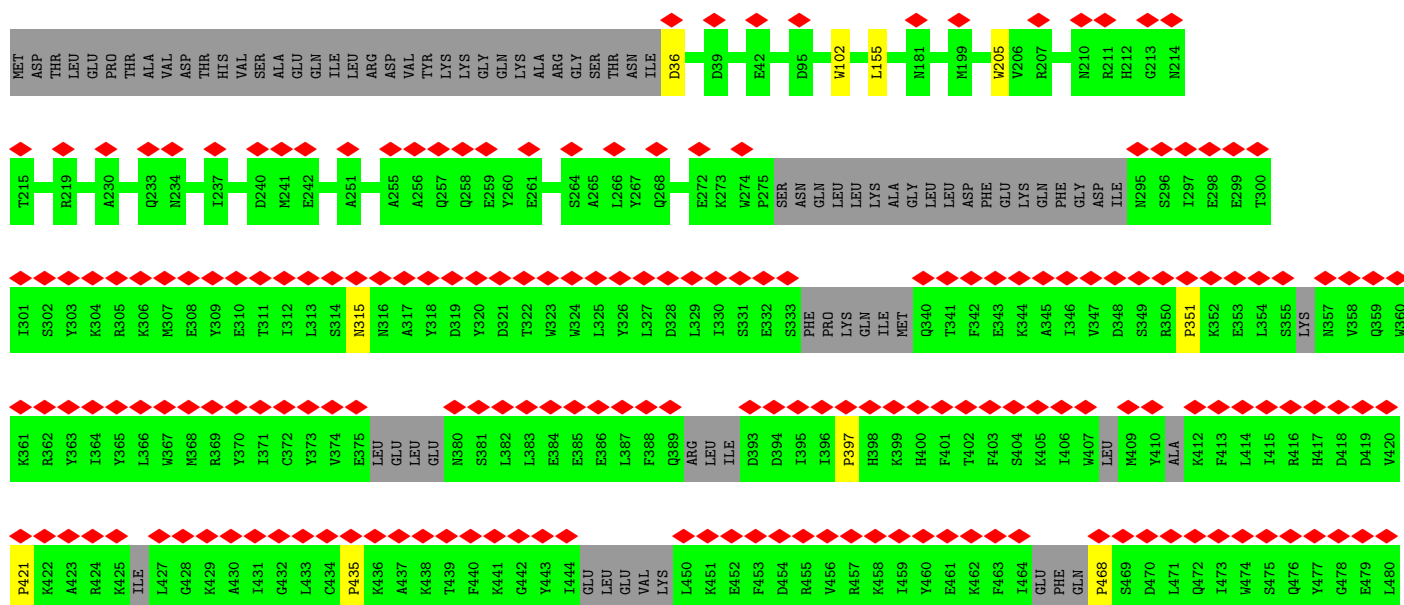
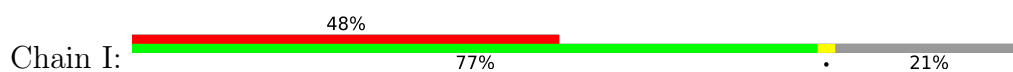


• Molecule 8: Pre-mRNA-splicing factor SYF1





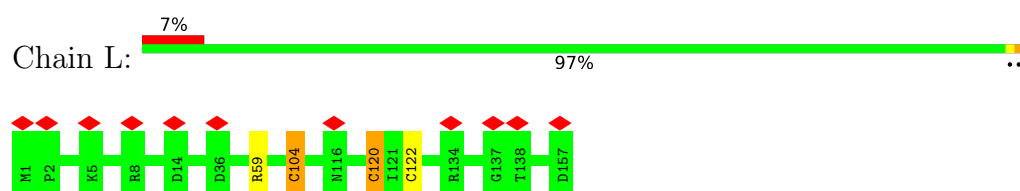
• Molecule 9: Pre-mRNA-splicing factor CLF1



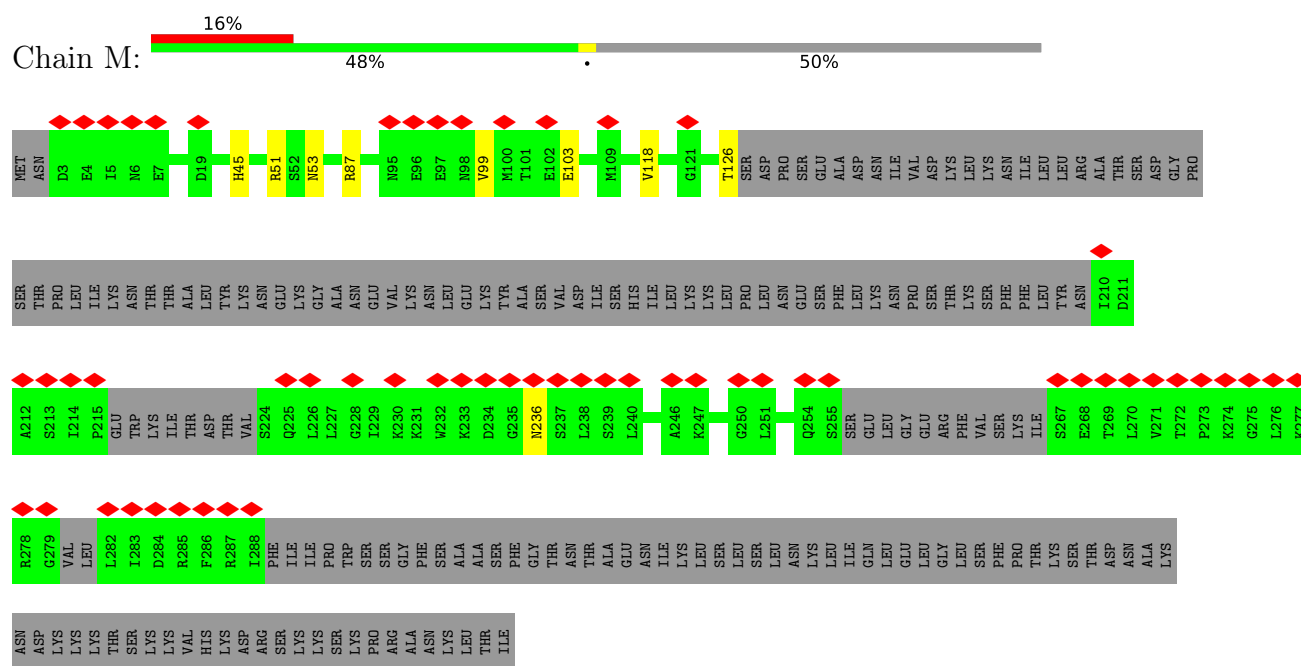
- Molecule 11: Pre-mRNA-splicing factor SYF2



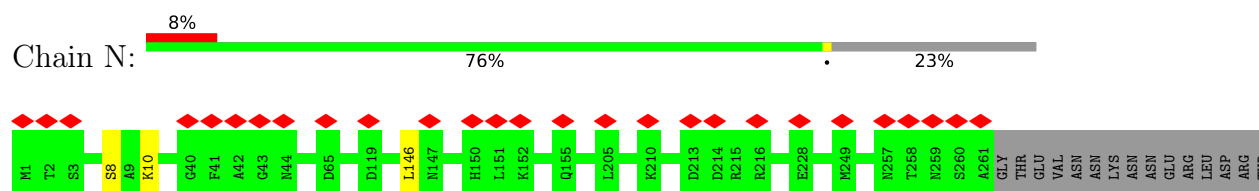
- Molecule 12: Pre-mRNA-splicing factor BUD31



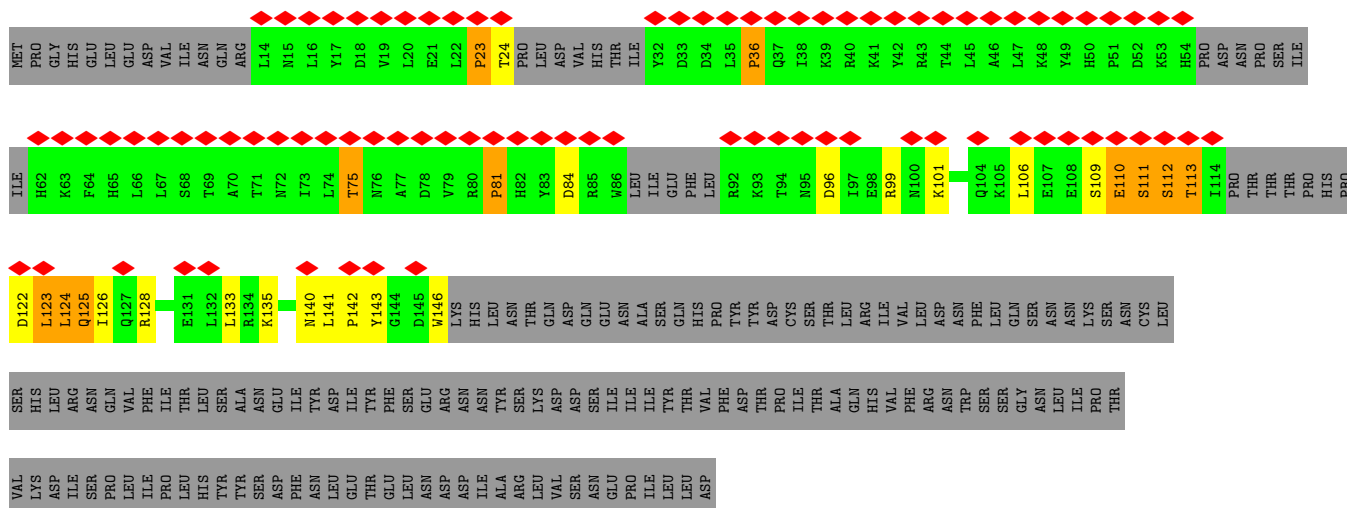
- Molecule 13: Pre-mRNA-splicing factor SLT11



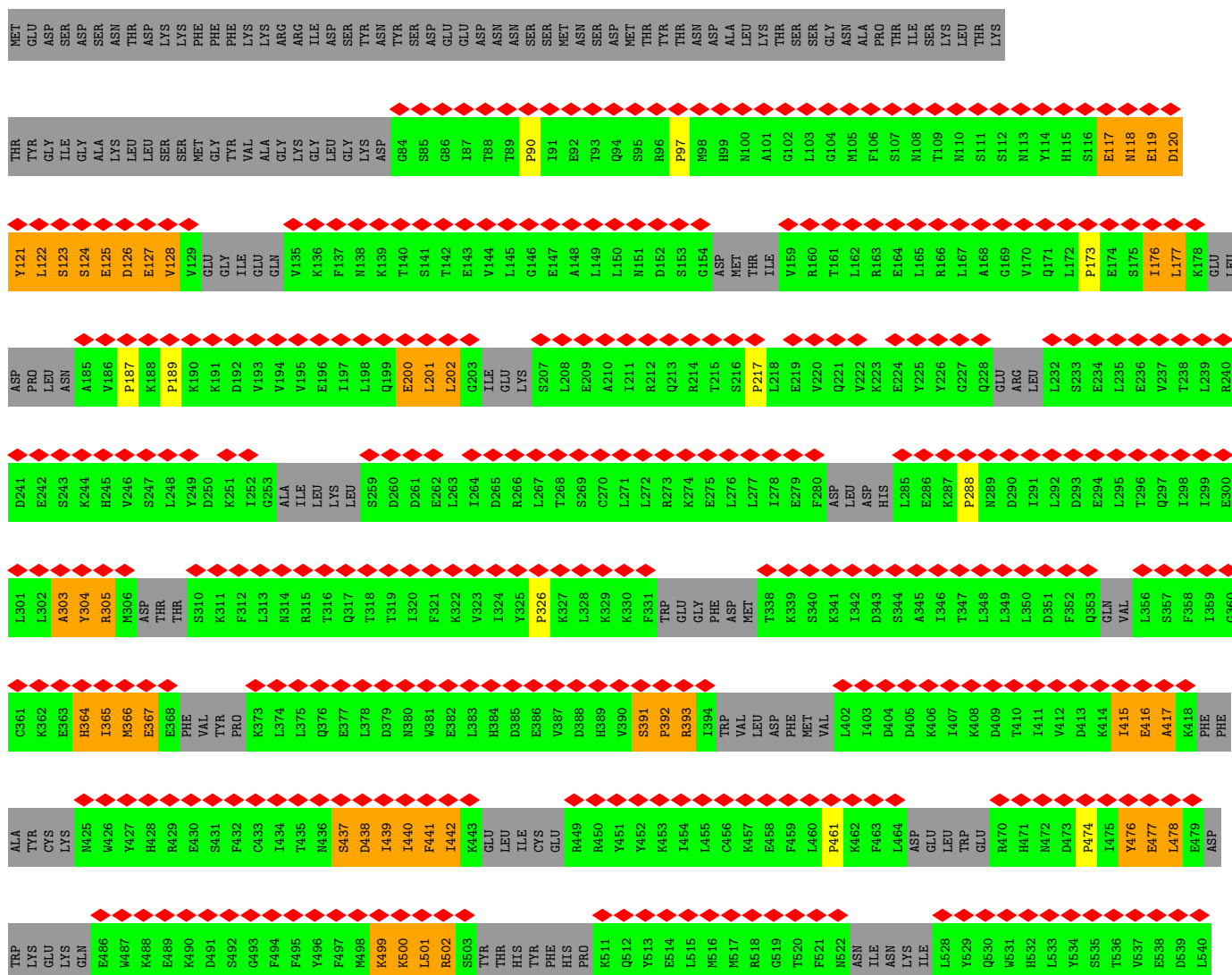
- Molecule 14: Pre-mRNA-splicing factor CWC2

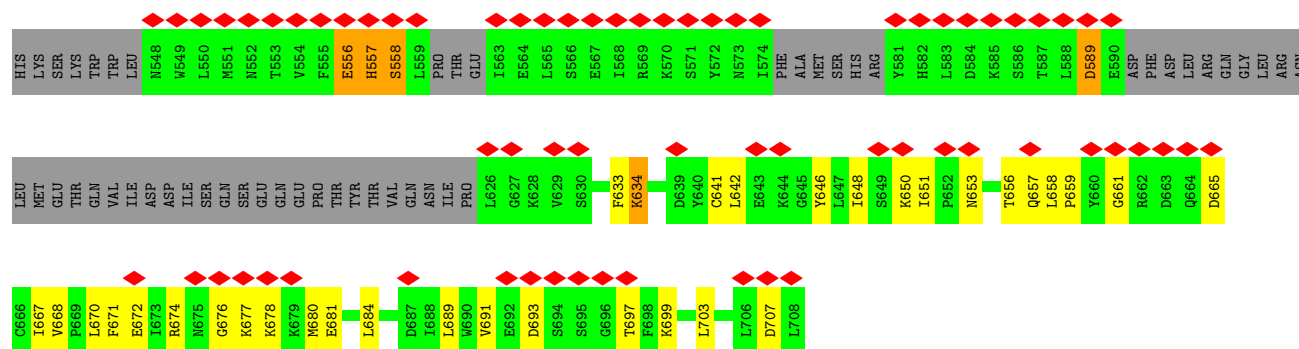




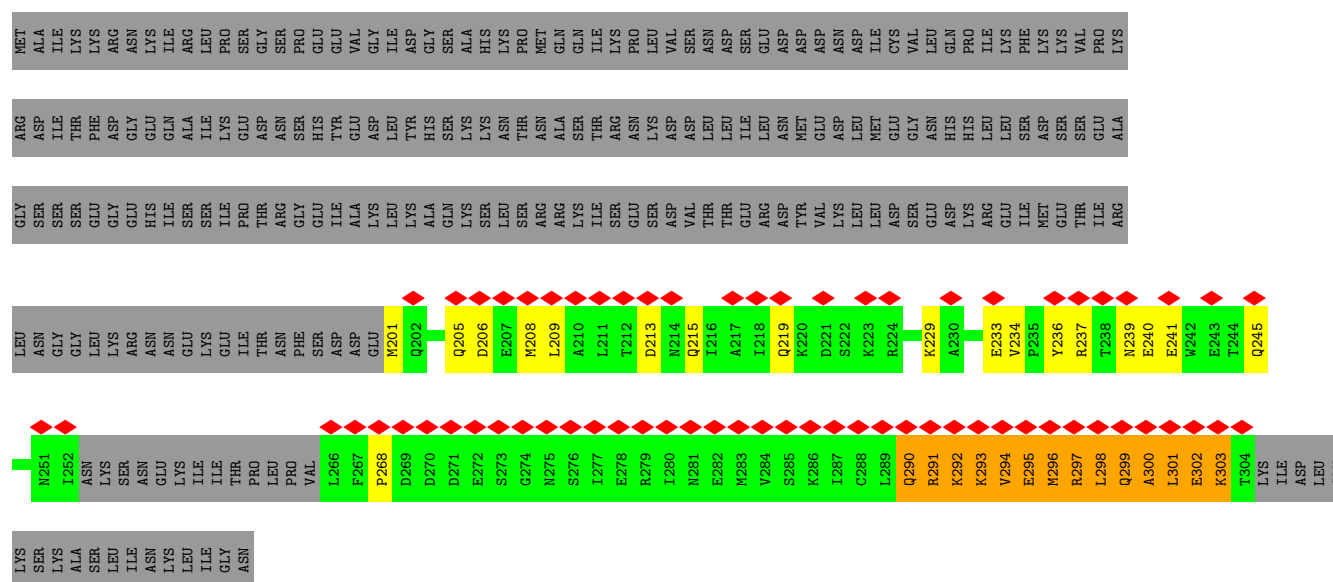


• Molecule 21: Pre-mRNA-splicing factor SPP382

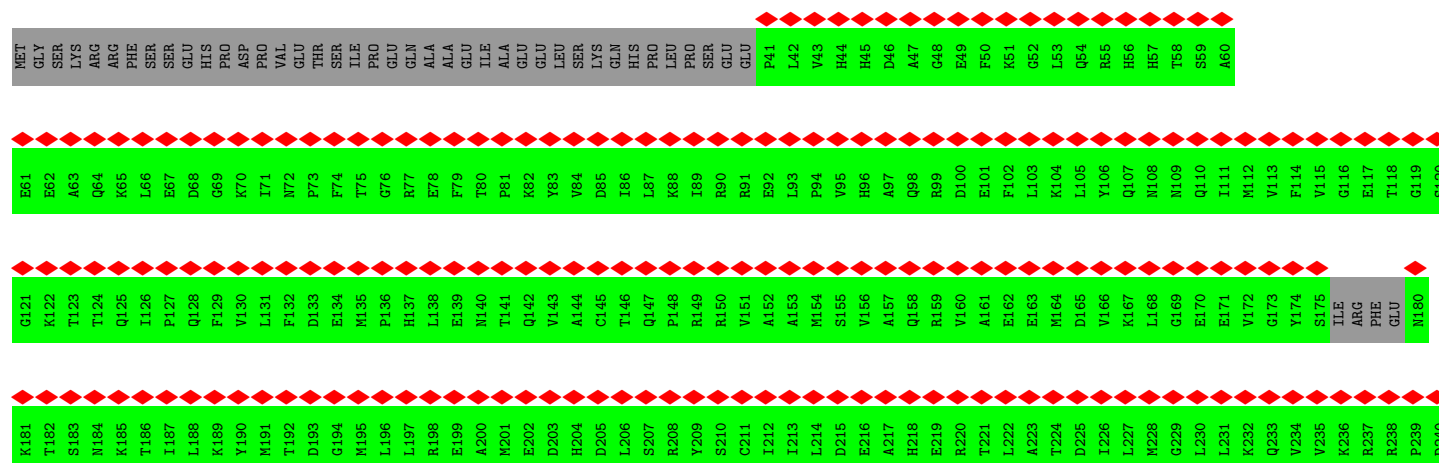
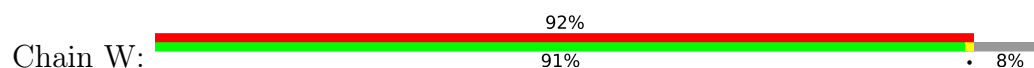


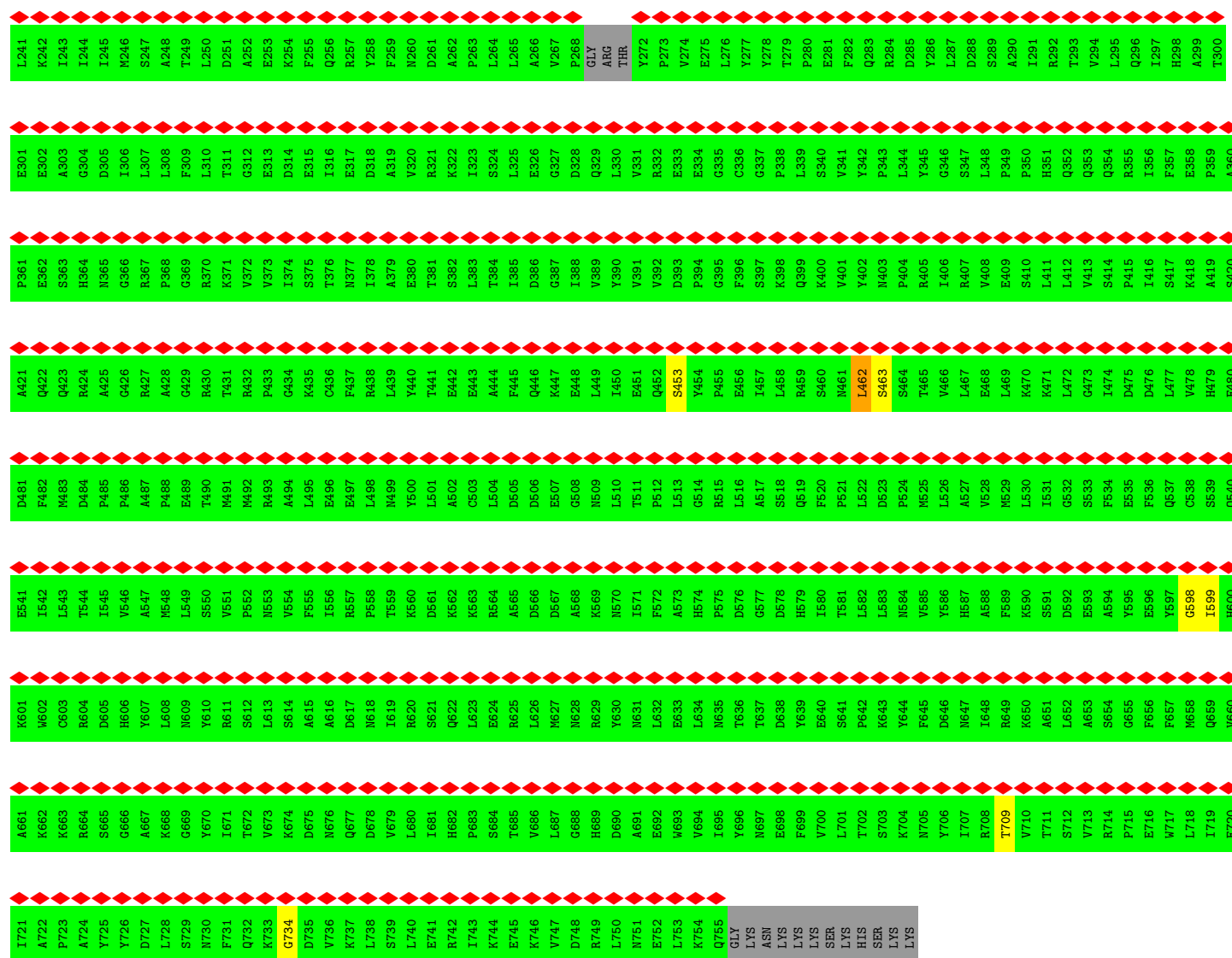


• Molecule 22: Pre-mRNA-splicing factor NTR2

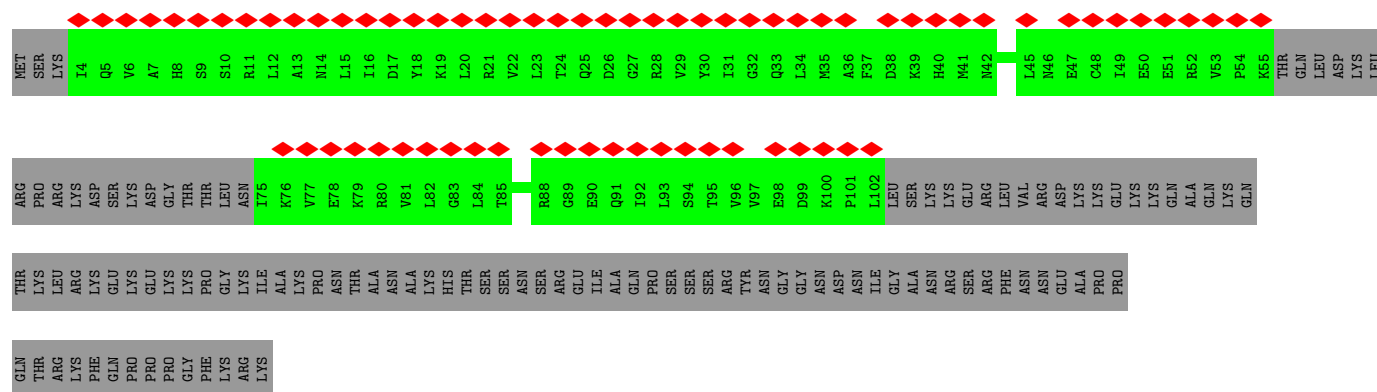


• Molecule 23: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43

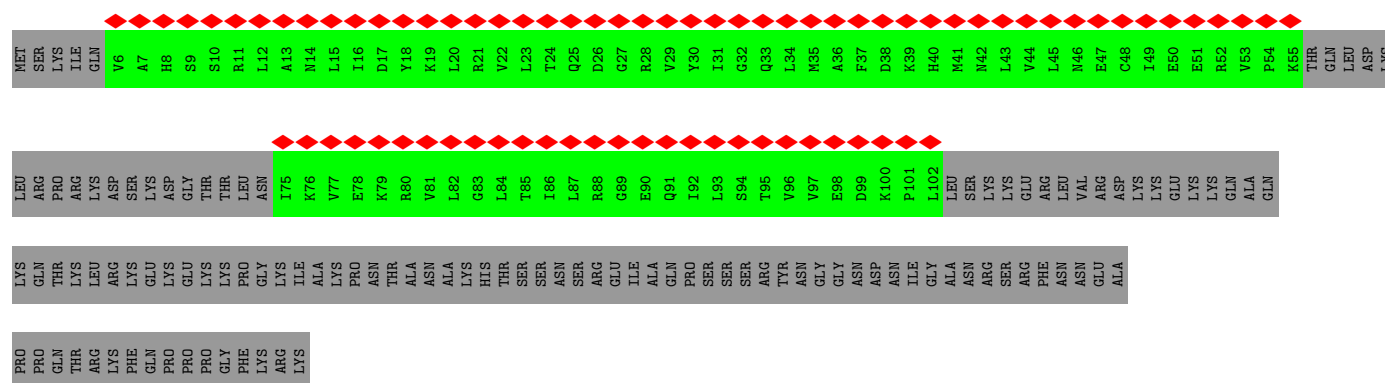




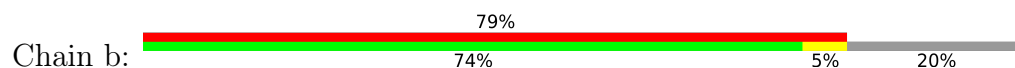
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B



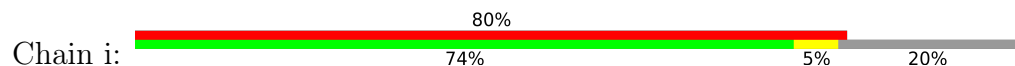
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B



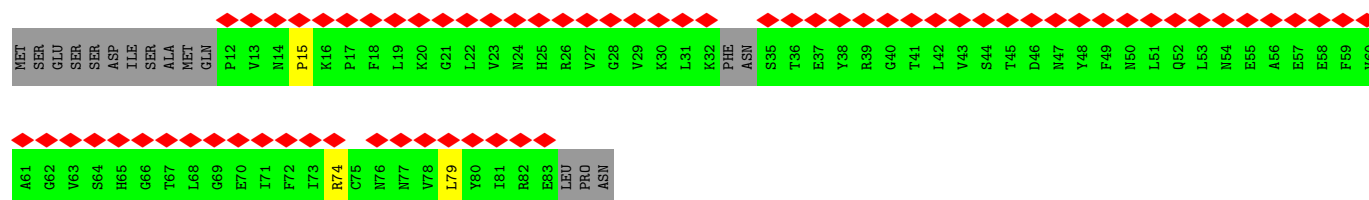
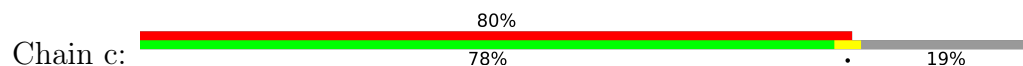
• Molecule 25: Small nuclear ribonucleoprotein E



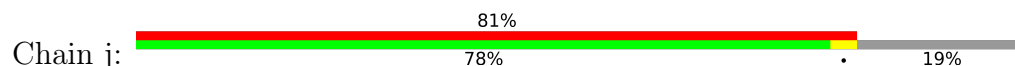
• Molecule 25: Small nuclear ribonucleoprotein E

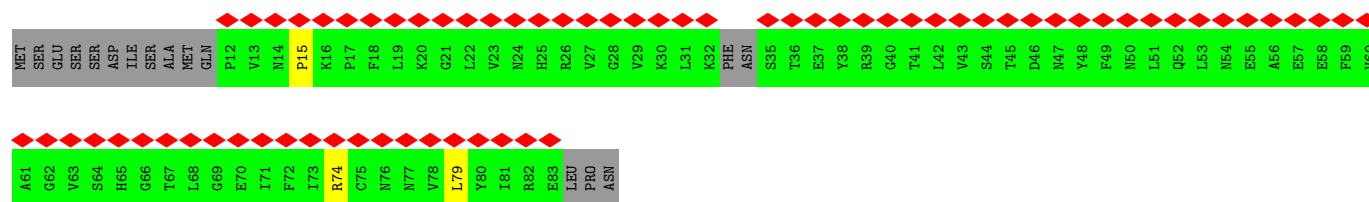


• Molecule 26: Small nuclear ribonucleoprotein F

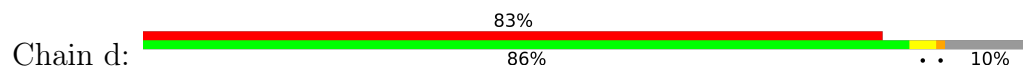


• Molecule 26: Small nuclear ribonucleoprotein F

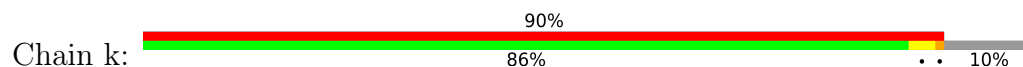




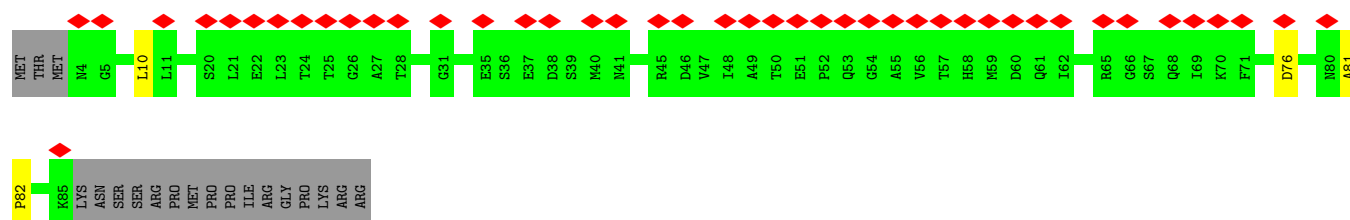
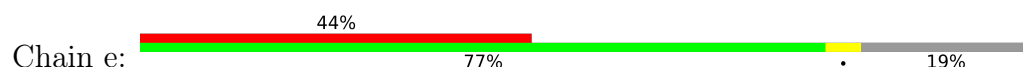
• Molecule 27: Small nuclear ribonucleoprotein G



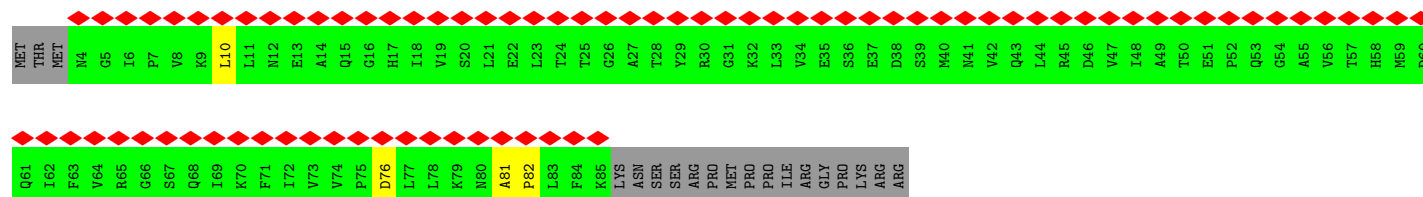
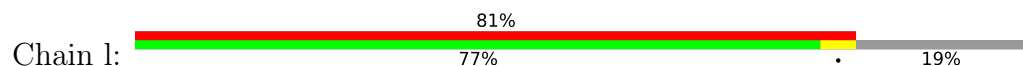
• Molecule 27: Small nuclear ribonucleoprotein G



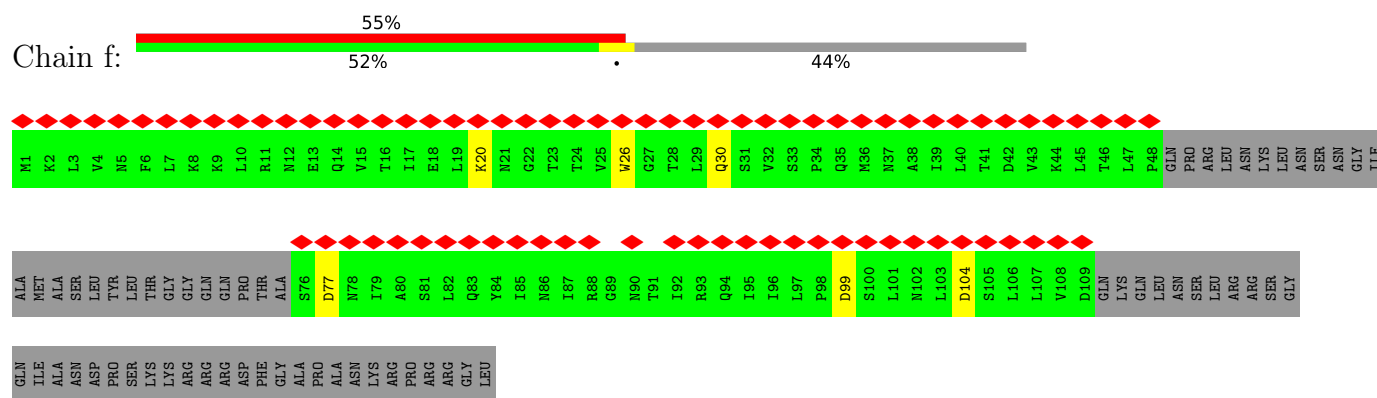
• Molecule 28: Small nuclear ribonucleoprotein Sm D3



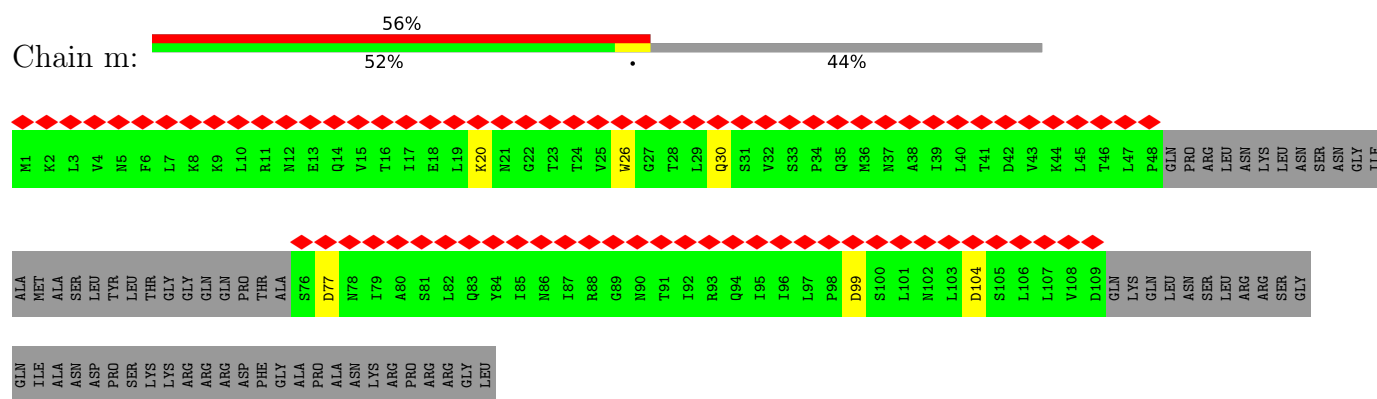
• Molecule 28: Small nuclear ribonucleoprotein Sm D3



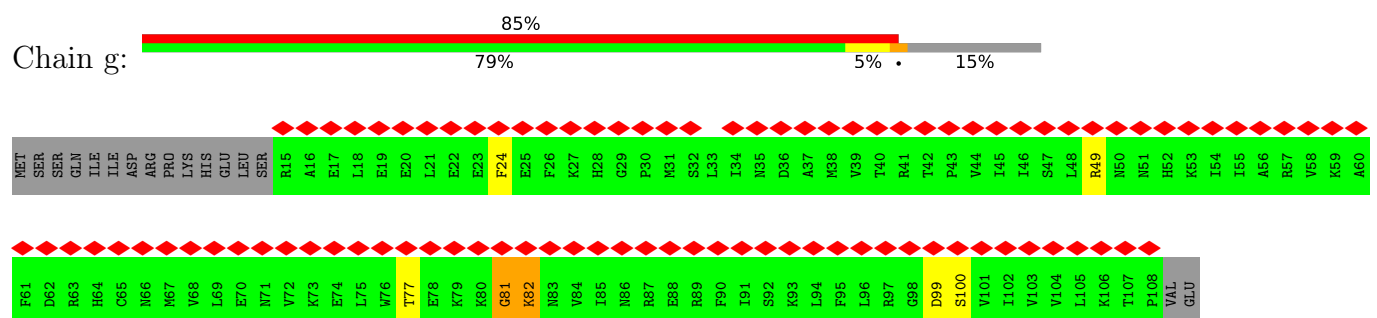
- Molecule 29: Small nuclear ribonucleoprotein Sm D1



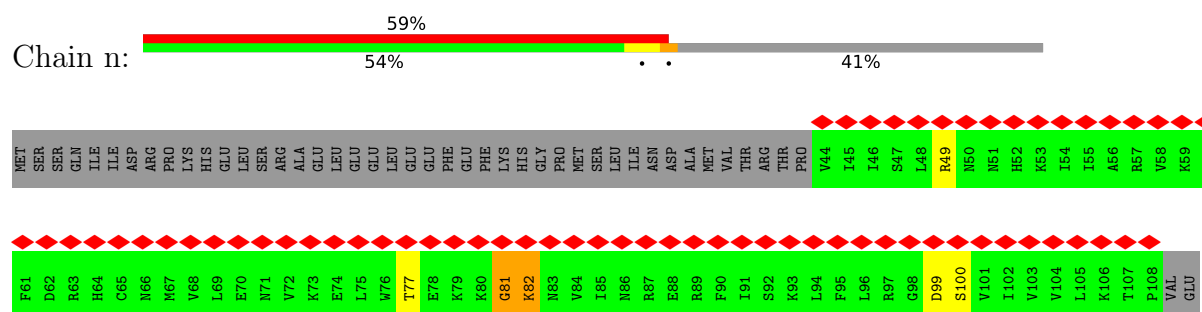
- Molecule 29: Small nuclear ribonucleoprotein Sm D1



- Molecule 30: Small nuclear ribonucleoprotein Sm D2



- Molecule 30: Small nuclear ribonucleoprotein Sm D2



- Molecule 31: U2 small nuclear ribonucleoprotein A'



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

- Molecule 33: Pre-mRNA-processing factor 19



M1	L2	C3	A4	I5	S6	G7	K8	V9	P10	R11	A12	P13	V14	L15	S16	P17	K18	S19	R20	T21	I22	F23	E24	K25	S26	L27	I28	E29	Q30	Y31	V32	K33	D34	T35	G36	N37	D38	P39	I40	T41	N42	E43	P44	L45	S46	I47	E48	A49	I50	V51	E52	I53	VAL	PRO	S56	A57	Q58	O59	A60
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S61	L62	T63	E64	S65	THR	ASN	SER	ALA	THR	LEU	LYS	ALA	ASN	TYR	SER	L77	F78	M79	L80	L81	T82	S83	L84	Q85	M86	E87	W88	D89	A90	I91	M92	L93	E94	N95	F96	K97	L98	R99	S100	T101	L102	D103	S104	L105	T106	K107	L108	L109	S110	T111	V112	M113	Y114	E115	R116	D117	A118	A119	K120
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L121	V122	A123	A124	Q125	L126	L127	L128	E129	K130	M131	E132	D133	S134	K135	D136	L137	P138	K139	S140	S141	Q142	G1N	A1A	V1A	A1A	I1E	T1R	A1G	A1R	G1U	G1U	P1E	L1U	L1U	G1N	S1R	S1R	A1R	A1S	P1E	V1A	A1A	A1R	G1Y	L1S	L1U	L1U	L1S	A1A	P1O	L1S	T1P	P1O	I1E	L1U	L1S	A1S
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GLU LEU LEU GLN ALA GLN ASN TYR SER ARG ASN ILE LYS THR PHE PRO LYS GLU LEU ASN LYS SER MET TYR TYR ASP LYS TRP VAL CYS CYC ASP GLY GLY ALA LEU HIS PHE THR GLN LEU LYS ASP SER LYS THR ILE THR THR THR THR THR THR THR

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

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

- Molecule 33: Pre-mRNA-processing factor 19



M1	L2	C3	A4	I5	S6	G7	K8	V9	P10	R11	I12	P13	V14	L15	S16	P17	K18	S19	R20	T21	I22	F23	F24	K25	S26	L27	L28	E29	Q30	Y31	V32	K33	D34	T35	C36	N37	D38	P39	I40	T41	M42	E43	P44	L45	S46	I47	E48	E49	I50	V51	E52	I53	V54	P55	S56	A57	Q58	O59	A60
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S61	LEU	THR	GLU	SER	THR	ASN	SER	ALA	THR	LEU	LYS	ALA	ASN	TYR	S76	S77	P78	M79	L80	L81	T82	S83	L84	Q85	R86	E87	W88	D89	A90	I91	M92	L93	E94	N95	P96	K97	L98	R99	S100	T101	L102	D103	S104	L105	T106	K107	L108	L109	S110	T111	M112	M113	Y114	E115	R116	D117	A118	A119	K120
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L121	V122	A123	A124	Q125	L126	L127	M128	E129	K130	M131	E132	D133	S134	K135	D136	L137	P138	K139	S140	S141	Q142	Q143	ALA	VAL	ALA	ALA	ILE	THR	ARG	GLU	GLU	PHE	LEU	LEU	GLN	GLY	LEU	LEU	GLN	SER	SER	ARG	ASP	PHE	VAL	ALA	ALA	GLY	GLY	LYS	PRO	PRO	ILE	LEU	LYS	ASN
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[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.6	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	0.282	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, IHP, MG, 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	0.63	9/16117 (0.1%)	0.71	12/21848 (0.1%)
2	B	0.54	1/2747 (0.0%)	0.72	0/4267
3	C	0.70	7/7434 (0.1%)	0.78	12/10070 (0.1%)
4	D	0.53	1/2405 (0.0%)	0.72	0/3744
5	E	0.29	0/653	0.66	0/1010
6	F	0.77	11/1922 (0.6%)	1.13	18/2984 (0.6%)
7	G	0.42	0/919	0.56	2/1237 (0.2%)
8	H	0.65	8/3180 (0.3%)	0.62	23/4331 (0.5%)
9	I	0.55	1/3574 (0.0%)	0.61	8/4863 (0.2%)
10	J	0.45	1/2962 (0.0%)	0.59	9/3987 (0.2%)
11	K	0.51	0/826	0.64	0/1097
12	L	0.71	0/1314	0.78	1/1759 (0.1%)
13	M	0.59	0/1308	0.71	0/1758
14	N	0.61	0/2135	0.67	0/2871
15	O	0.79	0/2704	0.82	1/3676 (0.0%)
16	P	0.54	0/568	0.94	3/758 (0.4%)
17	Q	0.49	0/1604	0.63	0/2160
18	R	0.25	0/378	0.54	2/498 (0.4%)
19	S	0.57	0/200	0.85	0/264
20	T	0.64	1/825 (0.1%)	0.99	14/1100 (1.3%)
21	U	0.67	0/2684	1.23	58/3680 (1.6%)
22	V	0.51	0/622	1.36	18/843 (2.1%)
23	W	0.21	0/3502	0.47	2/4877 (0.0%)
24	a	0.37	0/636	0.62	0/856
24	h	0.37	0/615	0.61	0/829
25	b	0.42	0/585	0.62	0/795
25	i	0.42	0/585	0.62	0/795
26	c	0.44	0/564	0.65	1/761 (0.1%)
26	j	0.44	0/564	0.66	1/761 (0.1%)
27	d	0.37	0/532	0.60	0/715
27	k	0.37	0/532	0.60	0/715
28	e	0.40	0/634	0.70	0/859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	l	0.40	0/634	0.70	0/859
29	f	0.41	0/649	0.61	0/880
29	m	0.41	0/649	0.61	0/880
30	g	0.46	0/753	0.69	2/1013 (0.2%)
30	n	0.43	0/535	0.66	2/717 (0.3%)
31	o	1.03	9/839 (1.1%)	1.65	11/1127 (1.0%)
32	p	0.82	4/514 (0.8%)	1.32	2/686 (0.3%)
33	q	0.40	0/837	0.52	0/1129
33	r	0.40	0/854	0.56	0/1151
33	s	0.40	0/856	0.54	0/1155
33	t	0.39	0/828	0.54	1/1117 (0.1%)
34	x	0.18	0/194	0.64	0/298
All	All	0.59	53/73972 (0.1%)	0.76	203/101780 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
3	C	0	2
11	K	0	1
13	M	0	2
15	O	0	6
16	P	0	2
17	Q	0	1
19	S	0	2
20	T	0	9
21	U	0	47
22	V	0	14
23	W	0	1
27	d	0	1
27	k	0	1
28	e	0	2
28	l	0	2
30	g	0	2
30	n	0	2
All	All	0	104

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	712	CYS	CB-SG	-17.12	1.53	1.82
6	F	1096	C	O3'-P	-10.09	1.49	1.61
8	H	718	SER	CB-OG	8.66	1.53	1.42
8	H	723	SER	CB-OG	8.49	1.53	1.42
8	H	714	SER	CB-OG	7.89	1.52	1.42

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	462	LEU	CA-C-N	-14.21	85.94	117.20
6	F	1110	U	C5-C4-O4	11.98	133.09	125.90
1	A	831	ARG	NE-CZ-NH2	-11.67	114.47	120.30
23	W	462	LEU	C-N-CA	-10.96	94.29	121.70
22	V	240	GLU	N-CA-CB	10.82	130.08	110.60

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1375	LEU	Peptide
1	A	239	PHE	Peptide,Mainchain
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	1895/2413 (78%)	1750 (92%)	125 (7%)	20 (1%)	14	50
3	C	907/1008 (90%)	820 (90%)	70 (8%)	17 (2%)	8	40
7	G	149/175 (85%)	134 (90%)	12 (8%)	3 (2%)	7	39
8	H	529/859 (62%)	505 (96%)	18 (3%)	6 (1%)	14	50
9	I	500/687 (73%)	468 (94%)	30 (6%)	2 (0%)	34	69
10	J	413/590 (70%)	384 (93%)	22 (5%)	7 (2%)	9	42
11	K	98/215 (46%)	96 (98%)	2 (2%)	0	100	100
12	L	155/157 (99%)	136 (88%)	17 (11%)	2 (1%)	12	47
13	M	172/364 (47%)	151 (88%)	19 (11%)	2 (1%)	13	48
14	N	259/339 (76%)	241 (93%)	18 (7%)	0	100	100
15	O	335/451 (74%)	295 (88%)	34 (10%)	6 (2%)	8	41
16	P	62/175 (35%)	56 (90%)	4 (6%)	2 (3%)	4	31
17	Q	193/379 (51%)	175 (91%)	13 (7%)	5 (3%)	5	34
18	R	44/278 (16%)	44 (100%)	0	0	100	100
19	S	21/455 (5%)	19 (90%)	1 (5%)	1 (5%)	2	22
20	T	97/283 (34%)	93 (96%)	4 (4%)	0	100	100
21	U	442/708 (62%)	430 (97%)	5 (1%)	7 (2%)	9	43
22	V	87/322 (27%)	82 (94%)	4 (5%)	1 (1%)	14	50
23	W	702/767 (92%)	657 (94%)	39 (6%)	6 (1%)	17	54
24	a	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
24	h	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
25	b	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
25	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
26	c	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	44
26	j	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	10	44
27	d	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
28	e	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	47
28	l	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	12	47
29	f	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
29	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
30	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	n	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	9	43
31	o	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	9	43
32	p	77/111 (69%)	75 (97%)	2 (3%)	0	100	100
33	q	120/503 (24%)	114 (95%)	4 (3%)	2 (2%)	9	42
33	r	123/503 (24%)	117 (95%)	6 (5%)	0	100	100
33	s	125/503 (25%)	115 (92%)	6 (5%)	4 (3%)	4	31
33	t	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	5	35
All	All	8774/14606 (60%)	8126 (93%)	544 (6%)	104 (1%)	17	48

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1347	ARG
1	A	1359	ILE
1	A	1385	PRO
1	A	1403	SER
3	C	363	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1727/2182 (79%)	1661 (96%)	66 (4%)	33	61
3	C	822/910 (90%)	785 (96%)	37 (4%)	27	57
7	G	40/165 (24%)	29 (72%)	11 (28%)	0	3
8	H	59/786 (8%)	49 (83%)	10 (17%)	2	13
9	I	219/633 (35%)	217 (99%)	2 (1%)	78	88
10	J	213/525 (41%)	204 (96%)	9 (4%)	30	59
11	K	92/193 (48%)	92 (100%)	0	100	100
12	L	141/141 (100%)	138 (98%)	3 (2%)	53	74
13	M	121/332 (36%)	116 (96%)	5 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	224/296 (76%)	221 (99%)	3 (1%)	69	83
15	O	295/397 (74%)	295 (100%)	0	100	100
16	P	55/151 (36%)	54 (98%)	1 (2%)	59	77
17	Q	173/328 (53%)	163 (94%)	10 (6%)	20	52
18	R	40/256 (16%)	31 (78%)	9 (22%)	1	6
19	S	20/413 (5%)	13 (65%)	7 (35%)	0	0
20	T	75/272 (28%)	59 (79%)	16 (21%)	1	7
21	U	76/663 (12%)	48 (63%)	28 (37%)	0	0
22	V	47/296 (16%)	34 (72%)	13 (28%)	0	2
24	a	70/176 (40%)	70 (100%)	0	100	100
24	h	67/176 (38%)	67 (100%)	0	100	100
25	b	65/83 (78%)	60 (92%)	5 (8%)	13	43
25	i	65/83 (78%)	60 (92%)	5 (8%)	13	43
26	c	61/77 (79%)	60 (98%)	1 (2%)	62	80
26	j	61/77 (79%)	60 (98%)	1 (2%)	62	80
27	d	58/66 (88%)	55 (95%)	3 (5%)	23	55
27	k	58/66 (88%)	55 (95%)	3 (5%)	23	55
28	e	69/89 (78%)	67 (97%)	2 (3%)	42	66
28	l	69/89 (78%)	67 (97%)	2 (3%)	42	66
29	f	77/129 (60%)	71 (92%)	6 (8%)	12	42
29	m	77/129 (60%)	71 (92%)	6 (8%)	12	42
30	g	79/103 (77%)	74 (94%)	5 (6%)	18	49
30	n	59/103 (57%)	55 (93%)	4 (7%)	16	47
31	o	47/219 (22%)	44 (94%)	3 (6%)	17	48
32	p	25/100 (25%)	24 (96%)	1 (4%)	31	60
33	q	62/451 (14%)	55 (89%)	7 (11%)	6	28
33	r	62/451 (14%)	54 (87%)	8 (13%)	4	22
33	s	63/451 (14%)	56 (89%)	7 (11%)	6	28
33	t	60/451 (13%)	55 (92%)	5 (8%)	11	40
All	All	5693/12508 (46%)	5389 (95%)	304 (5%)	26	54

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	b	18	PHE
33	r	63	THR
27	d	71	LEU
25	i	81	LEU
33	t	44	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	191	ASN
21	U	664	GLN
14	N	248	ASN
16	P	173	HIS
27	d	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	114/214 (53%)	30 (26%)	3 (2%)
34	x	8/9 (88%)	5 (62%)	0
4	D	100/112 (89%)	35 (35%)	8 (8%)
5	E	27/38 (71%)	15 (55%)	7 (25%)
6	F	79/1175 (6%)	30 (37%)	11 (13%)
All	All	328/1548 (21%)	115 (35%)	29 (8%)

5 of 115 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	29	G
2	B	31	G
2	B	32	G
2	B	33	U
2	B	42	A

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	E	9	U
6	F	1107	C
5	E	500	A
6	F	40	U

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Mol	Chain	Res	Type
5	E	499	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 14 ligands modelled in this entry, 12 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	$\# Z > 2$
36	GTP	C	1500	37	26,34,34	1.11	1 (3%)	32,54,54	2.03	7 (21%)
35	IHP	A	3000	-	36,36,36	0.69	0	54,60,60	0.93	0

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
36	GTP	C	1500	37	-	5/18/38/38	0/3/3/3
35	IHP	A	3000	-	-	11/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	1500	GTP	C6-N1	-3.01	1.33	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	1500	GTP	PB-O3B-PG	-5.75	113.11	132.83
36	C	1500	GTP	O6-C6-C5	-4.28	116.02	124.37
36	C	1500	GTP	PA-O3A-PB	-3.61	120.45	132.83
36	C	1500	GTP	C5-C6-N1	3.25	119.69	113.95
36	C	1500	GTP	O6-C6-N1	3.08	124.29	120.65

There are no chirality outliers.

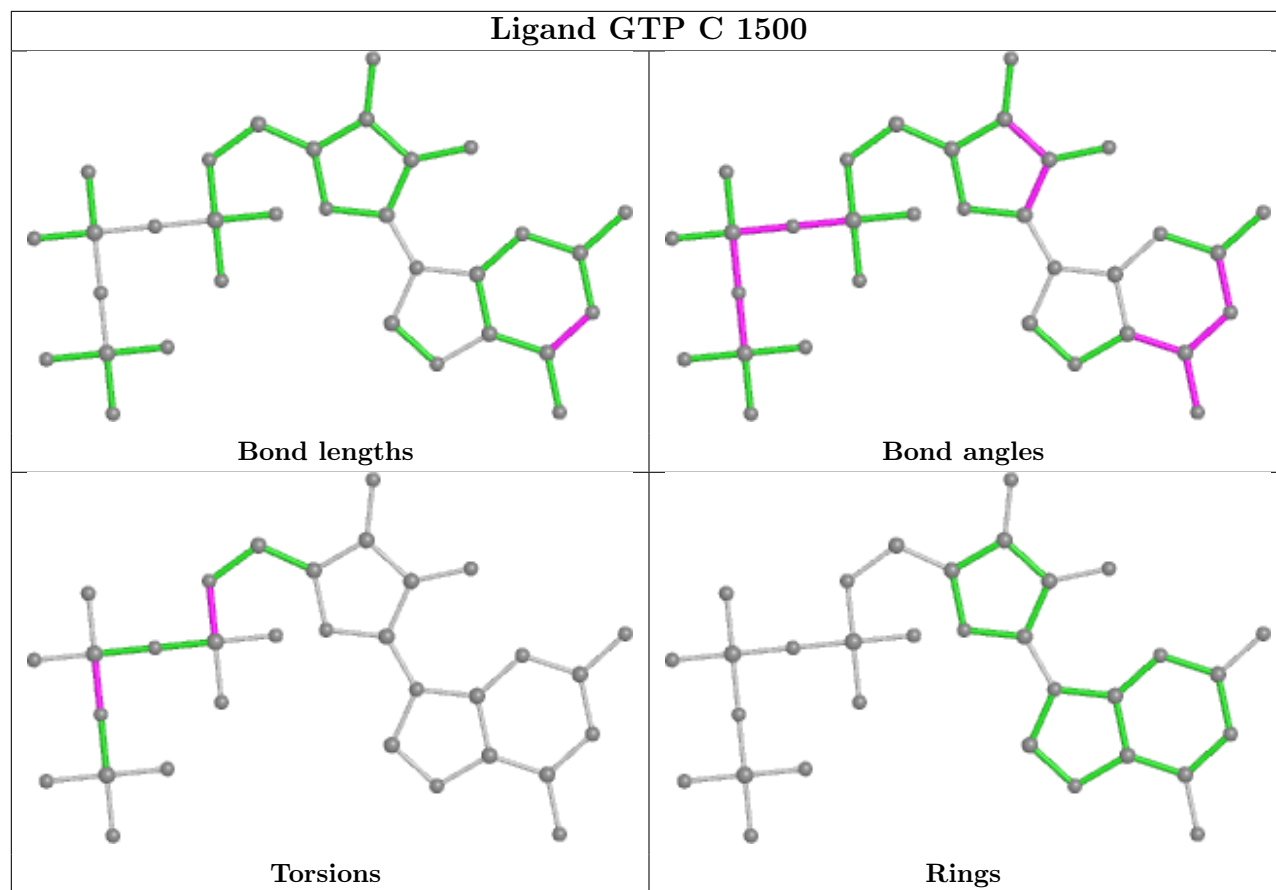
5 of 16 torsion outliers are listed below:

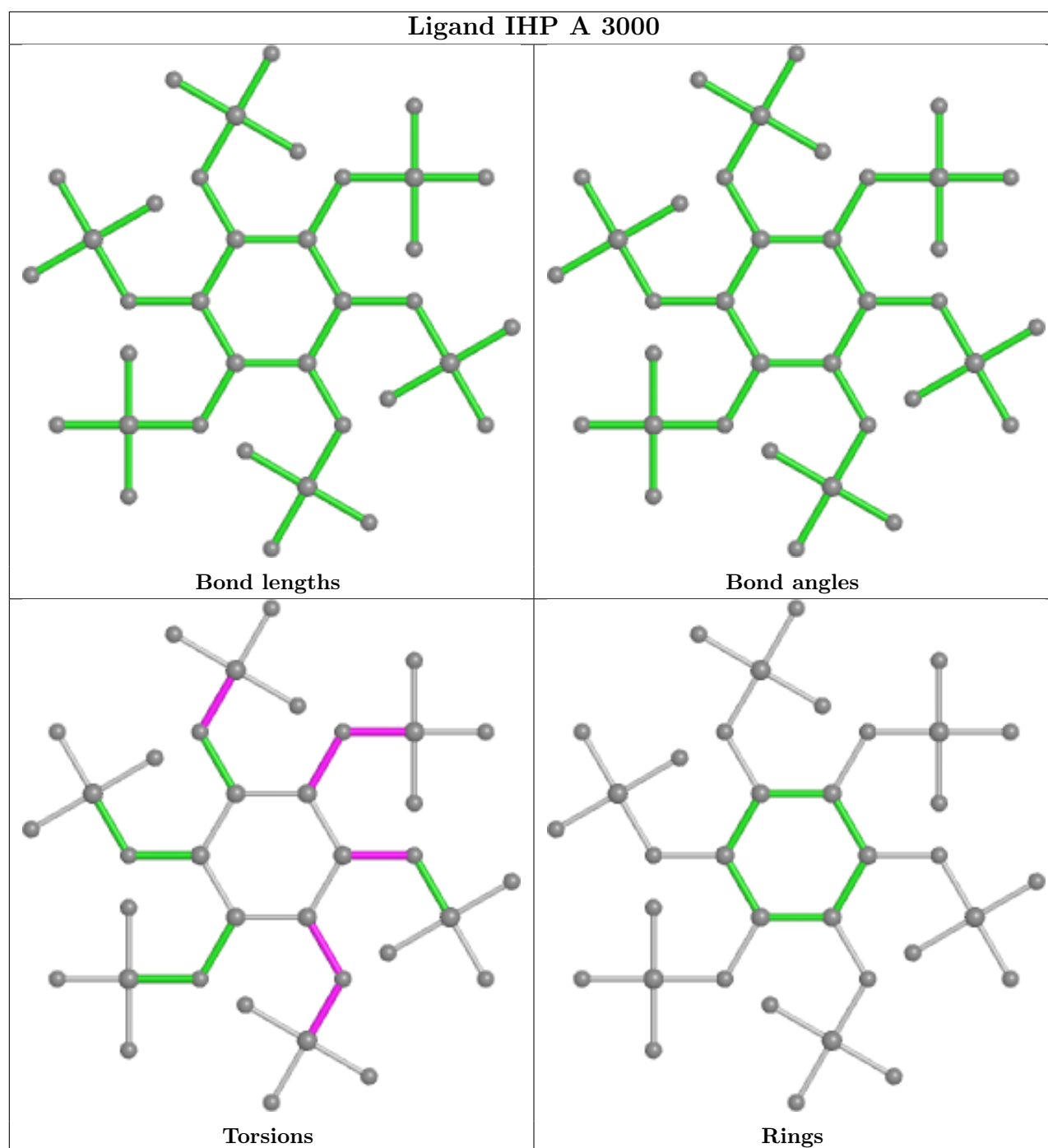
Mol	Chain	Res	Type	Atoms
35	A	3000	IHP	C1-C6-O16-P6
35	A	3000	IHP	C5-C6-O16-P6
35	A	3000	IHP	C4-O14-P4-O24
36	C	1500	GTP	C5'-O5'-PA-O3A
36	C	1500	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

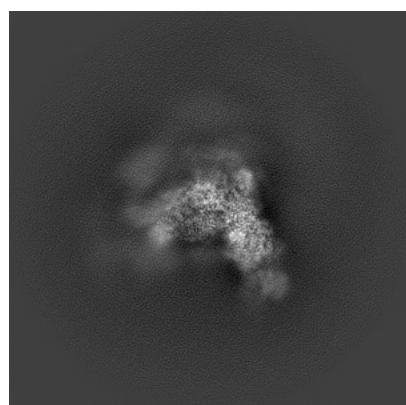
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6817. These allow visual inspection of the internal detail of the map and identification of artifacts.

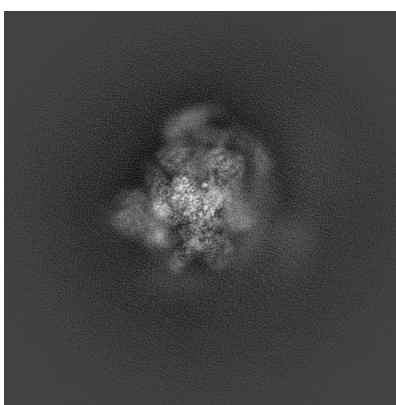
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

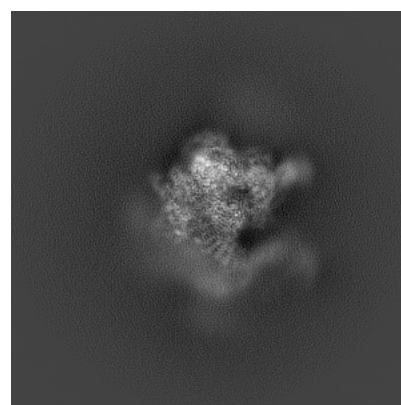
6.1.1 Primary map



X



Y

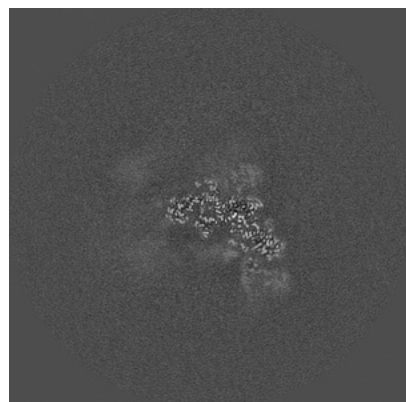


Z

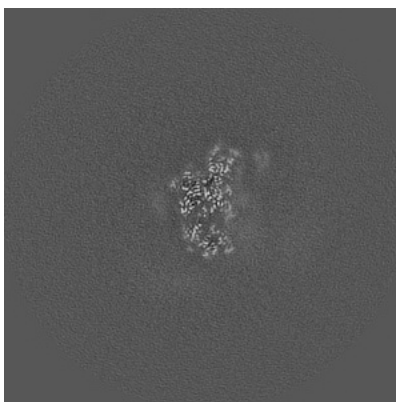
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

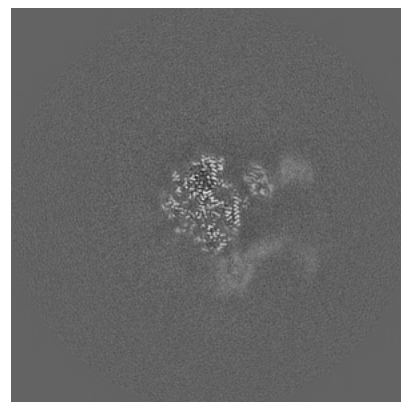
6.2.1 Primary map



X Index: 200



Y Index: 200

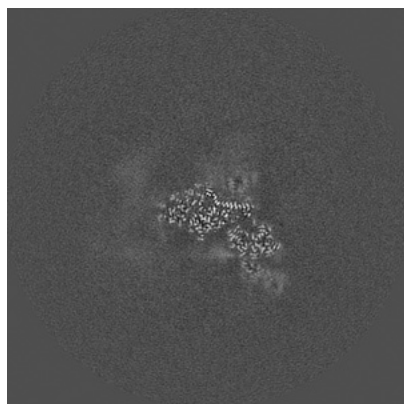


Z Index: 200

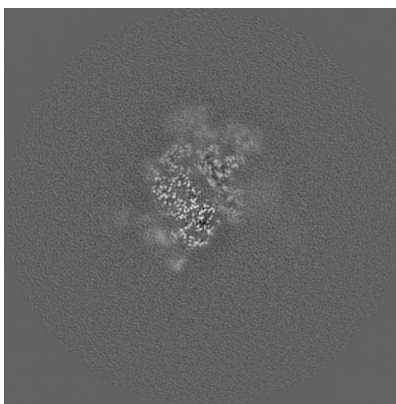
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

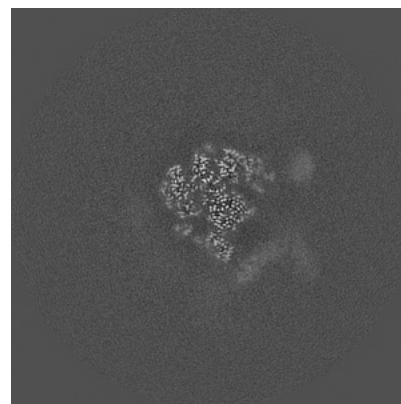
6.3.1 Primary map



X Index: 204



Y Index: 230



Z Index: 186

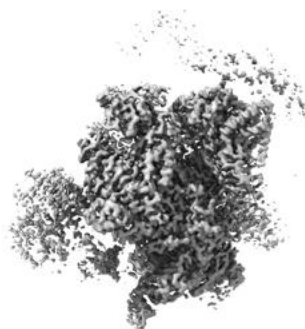
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

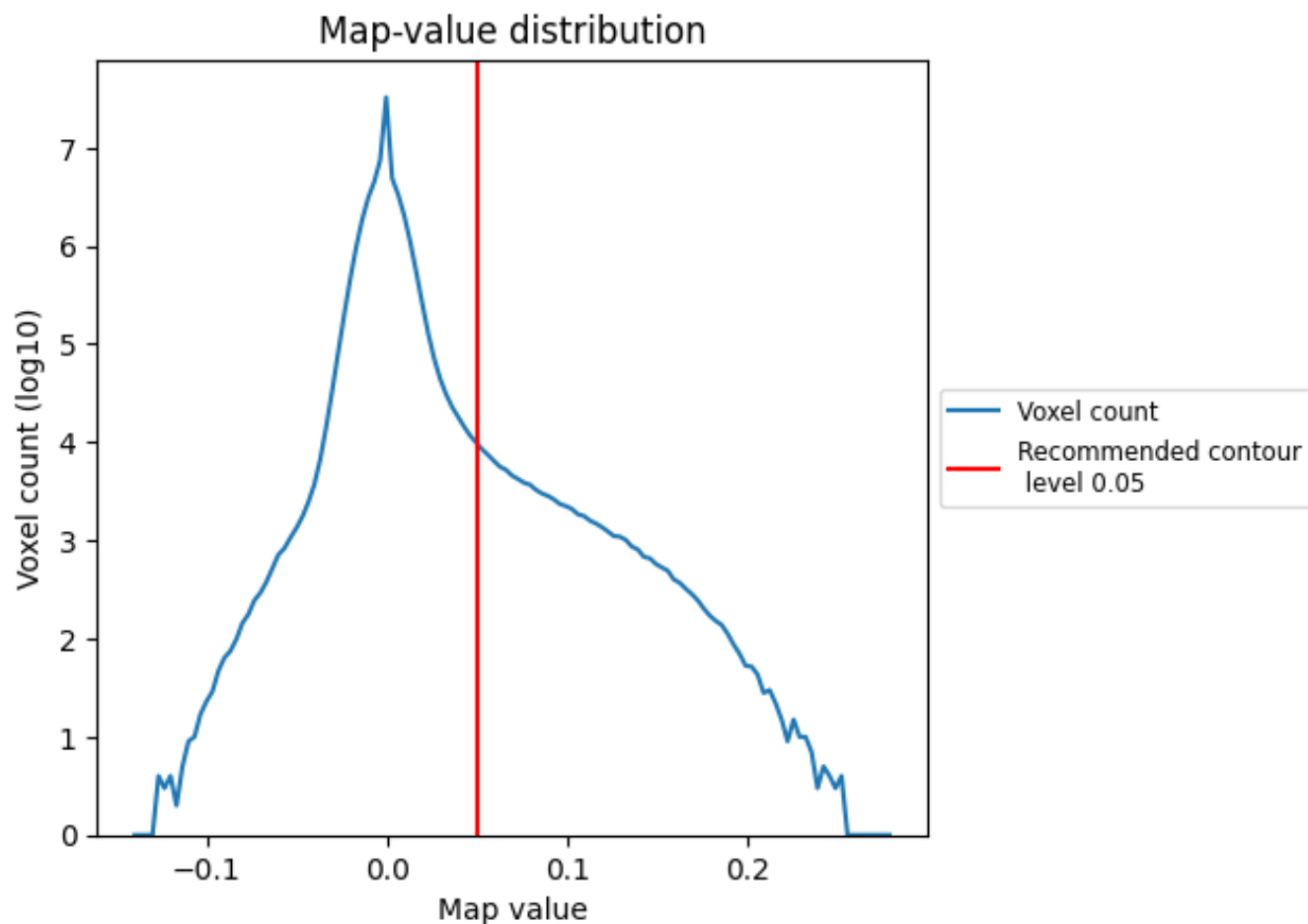
6.5 Mask visualisation

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

7 Map analysis [i](#)

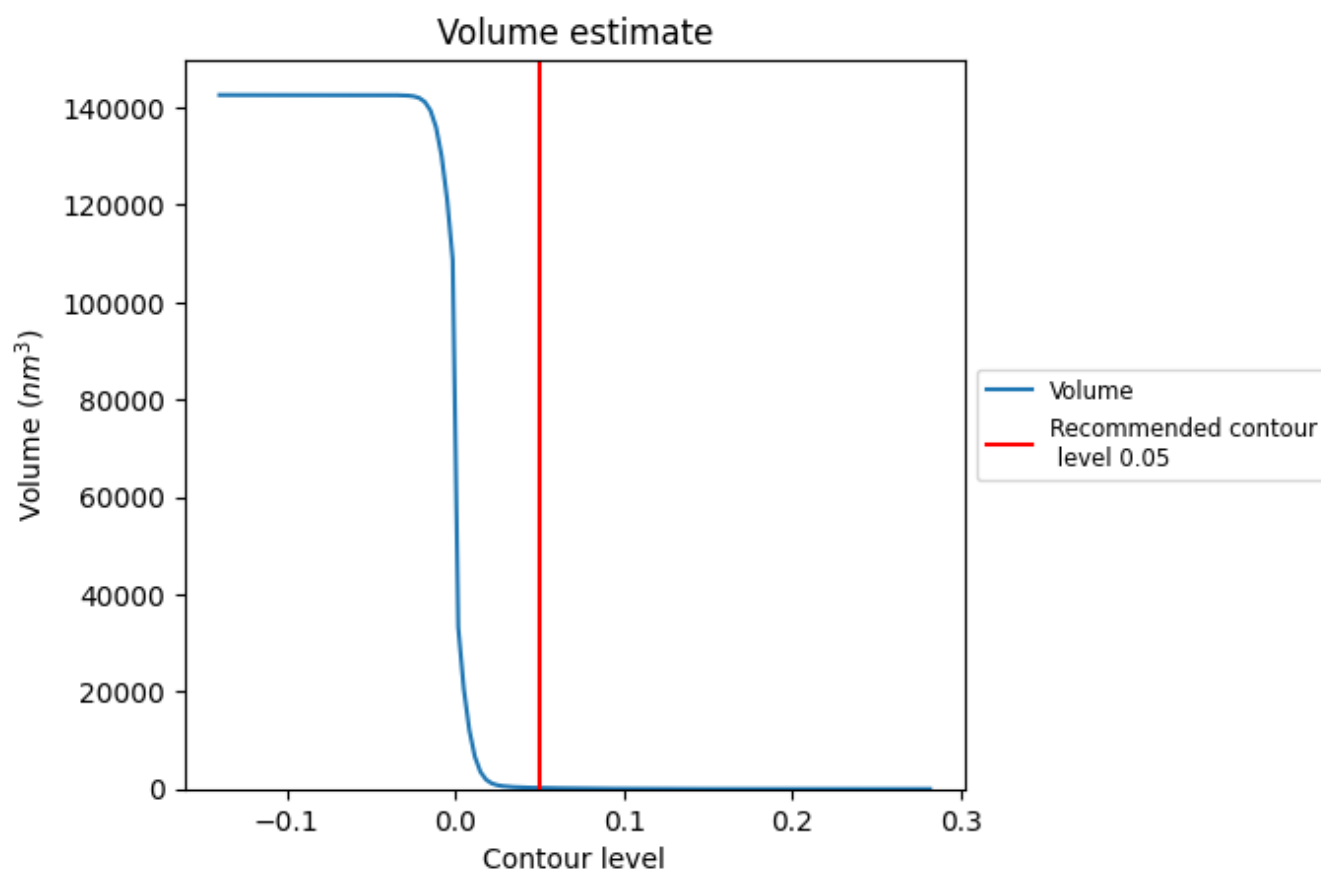
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

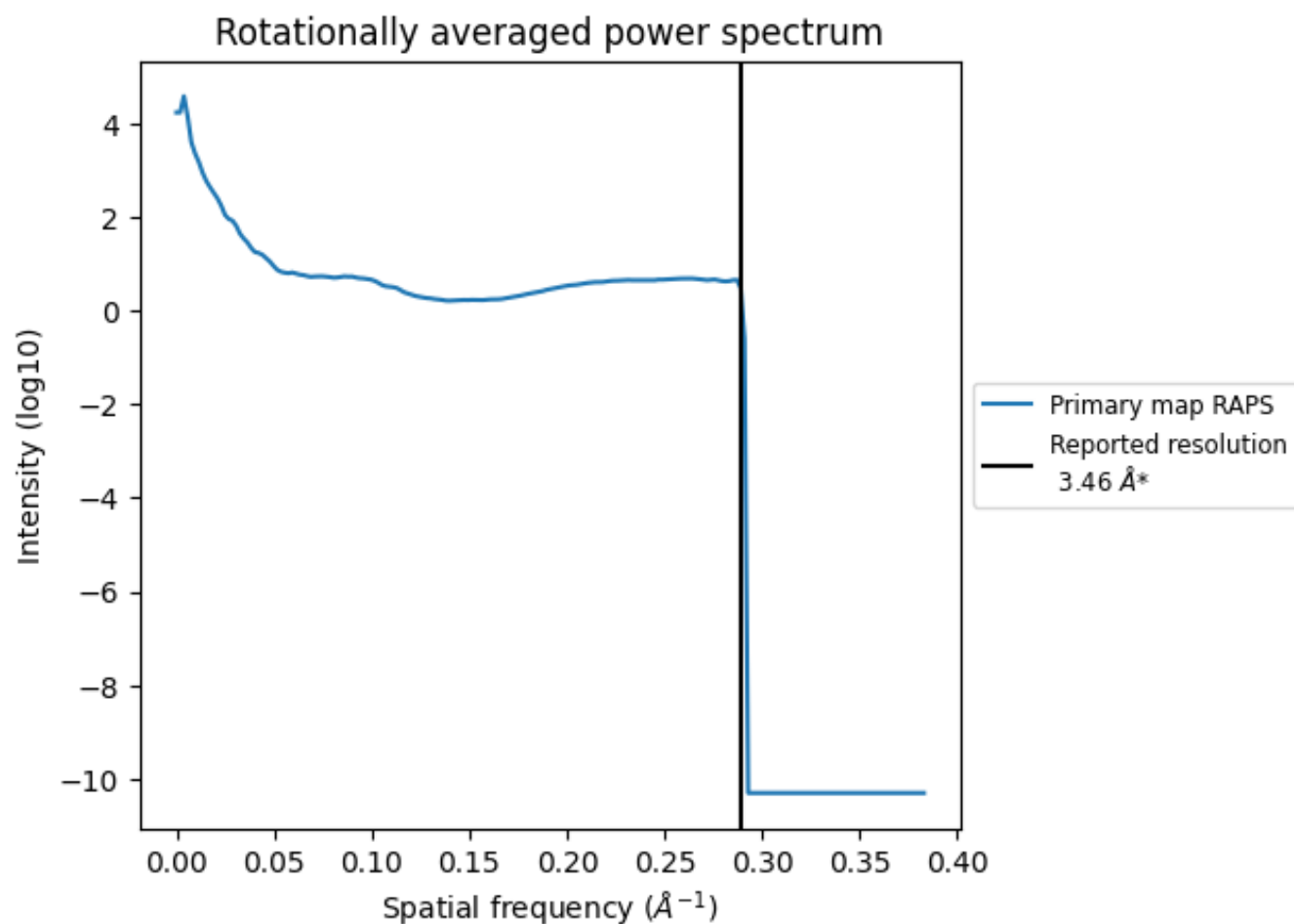
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214 nm³; this corresponds to an approximate mass of 193 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.289 \AA^{-1}

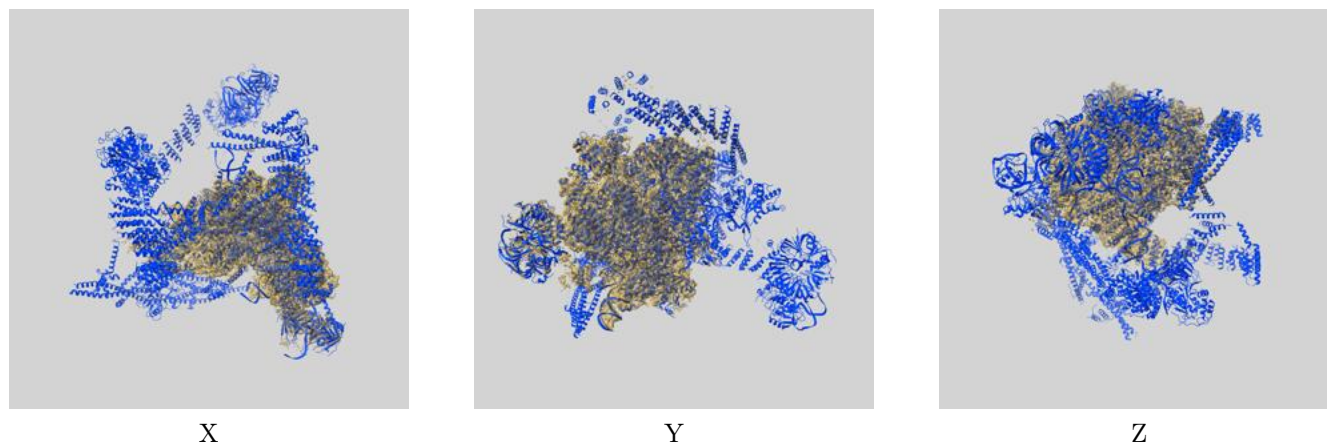
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

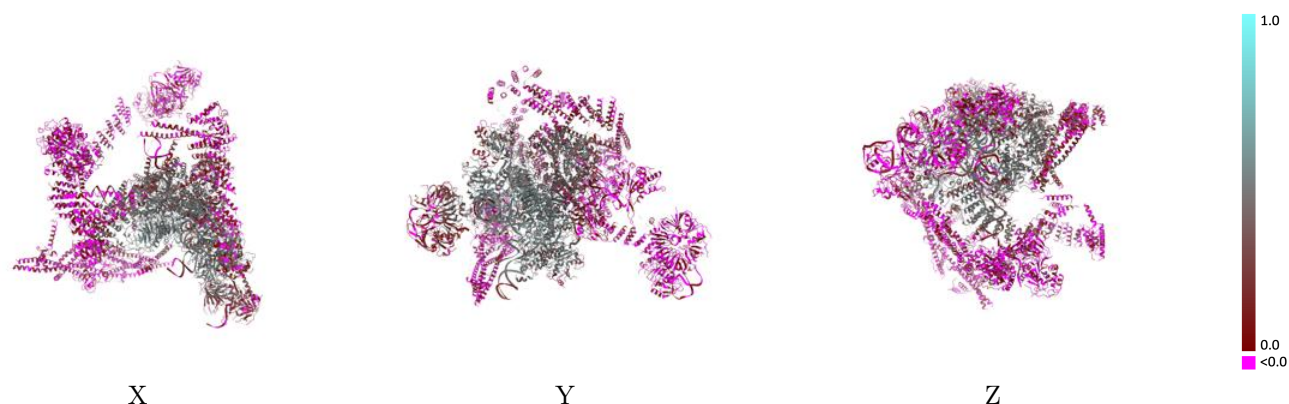
This section contains information regarding the fit between EMDB map EMD-6817 and PDB model 5Y88. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



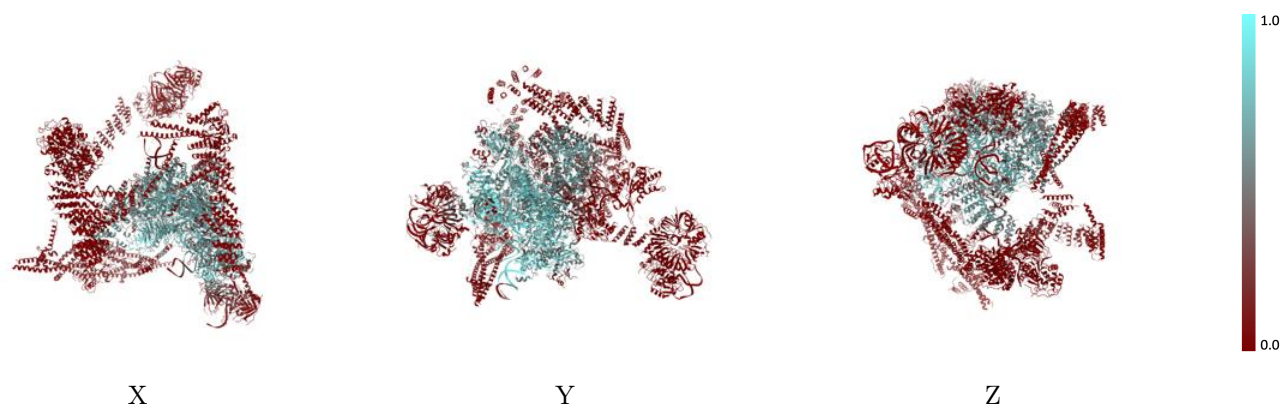
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



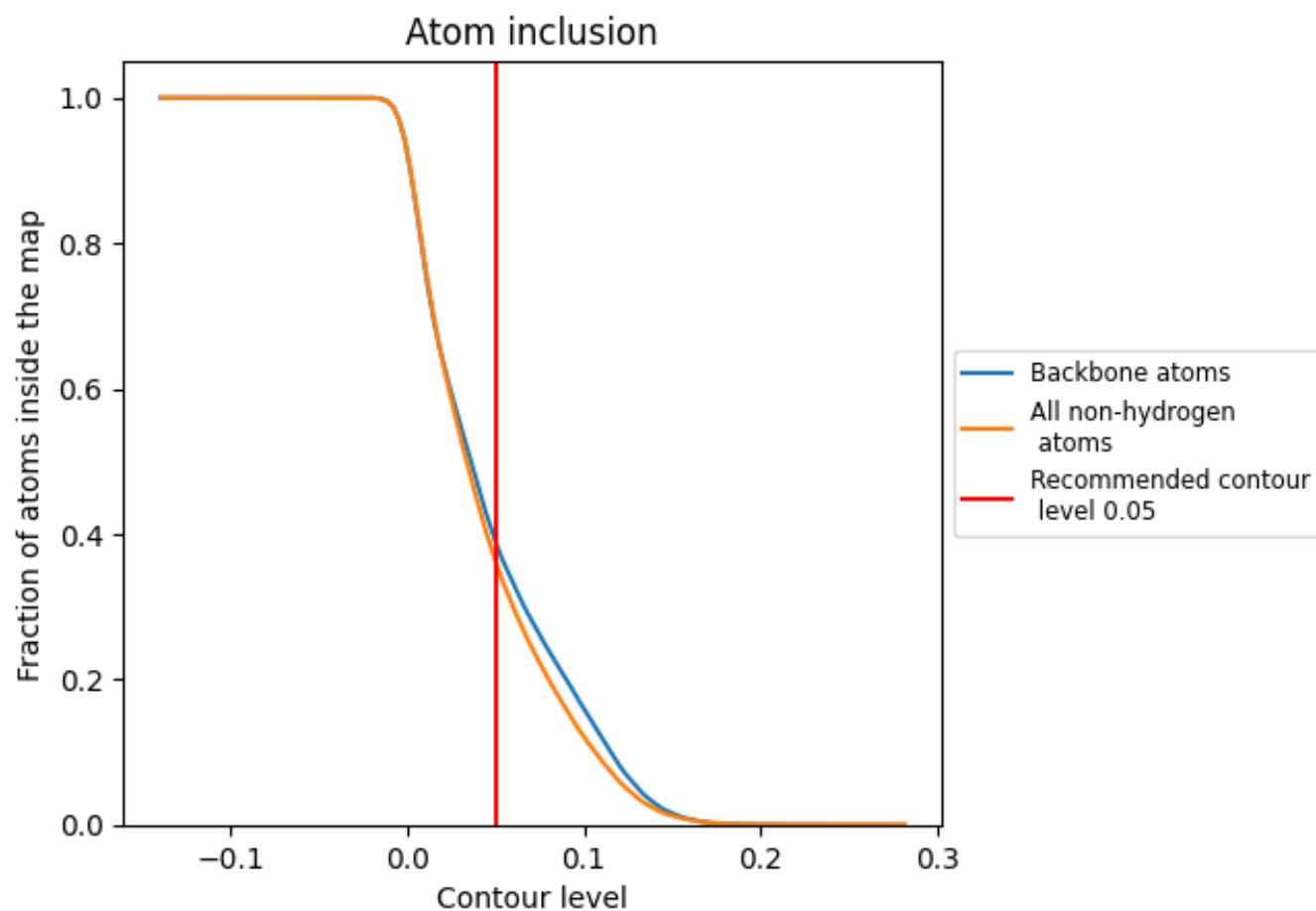
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3619	 0.2640
A	 0.4924	 0.3410
B	 0.6357	 0.3930
C	 0.6659	 0.4500
D	 0.7369	 0.4380
E	 0.2589	 0.1780
F	 0.1934	 0.1400
G	 0.0000	 0.0050
H	 0.0113	 0.0250
I	 0.3751	 0.2640
J	 0.2986	 0.2320
K	 0.3896	 0.3570
L	 0.7303	 0.4710
M	 0.5537	 0.4190
N	 0.6642	 0.4310
O	 0.7481	 0.5060
P	 0.4467	 0.4480
Q	 0.4961	 0.4030
R	 0.0916	 0.2520
S	 0.6432	 0.4470
T	 0.1837	 0.1710
U	 0.1330	 0.1710
V	 0.2626	 0.2790
W	 0.0000	 0.0080
a	 0.1669	 0.3050
b	 0.0385	 0.1550
c	 0.0368	 0.0920
d	 0.1574	 0.2530
e	 0.3560	 0.3730
f	 0.0770	 0.1570
g	 0.0497	 0.1510
h	 0.0000	 -0.0100
i	 0.0000	 -0.0110
j	 0.0000	 0.0030
k	 0.0000	 0.0180



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Chain	Atom inclusion	Q-score
l	0.0000	0.0080
m	0.0000	0.0270
n	0.0000	0.0050
o	0.0000	-0.0210
p	0.0000	0.0010
q	0.0000	0.0350
r	0.0000	-0.0090
s	0.0000	0.0000
t	0.0000	-0.0040
x	0.0000	-0.0440