wwPDB EM Validation Summary Report (i)

Nov 7, 2026 – 10:02 am GMT

PDB ID	:	9TCR / pdb_00009tcr
EMDB ID	:	EMD-55797
Title	:	Structural characterization of hibernating ribosomes in the Gram-negative pathogen Klebsiella quasipneumoniae with bS21 and no E-site tRNA
Authors	:	Vasanthakrishnan, R.K.B.S.; Olivier, D.; Sophie, C.; Yann, L.C.; Sylvie, G.D.; Sassi, M.; Emmanuel, G.; Reynald, G.
Deposited on	:	2025-11-21
Resolution	:	2.70 Å(reported)
Based on initial model	:	8B0X

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

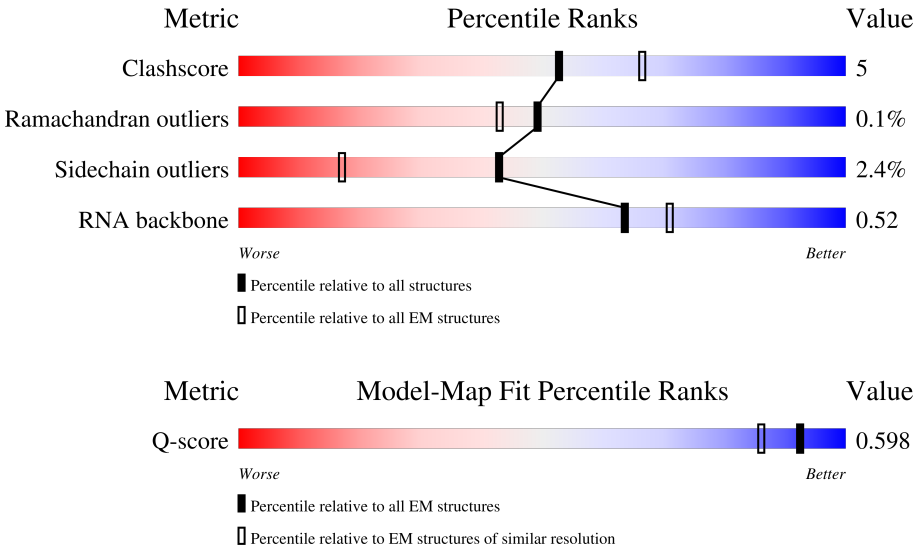
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.70 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.



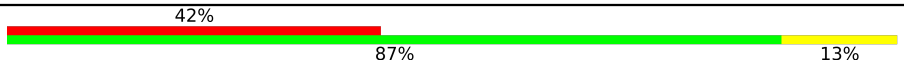
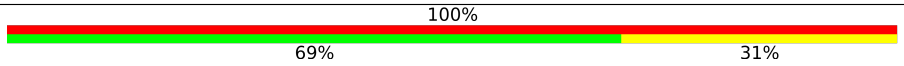
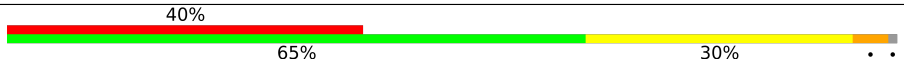
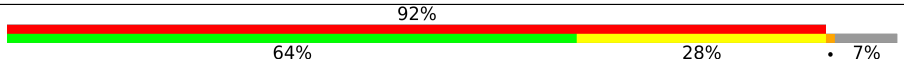
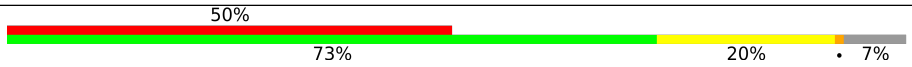
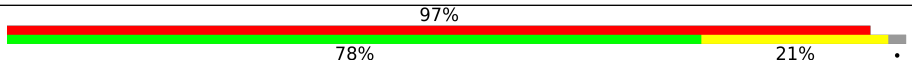
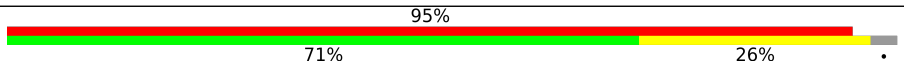
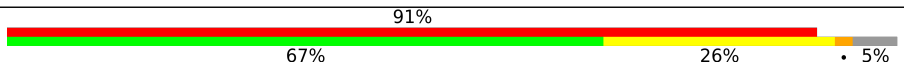
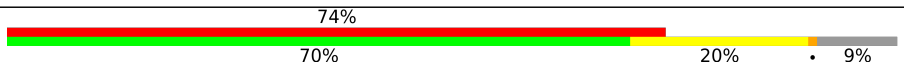
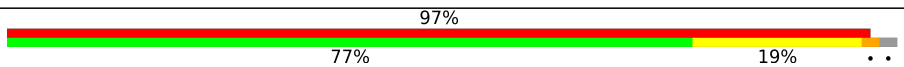
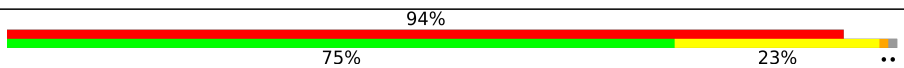
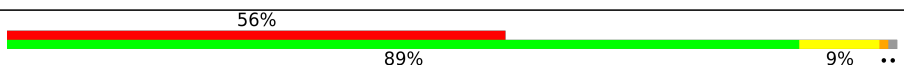
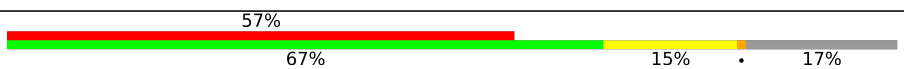
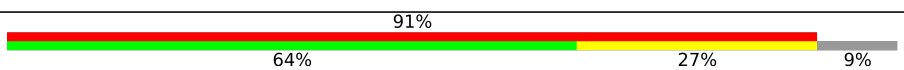
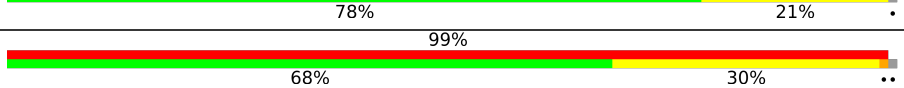
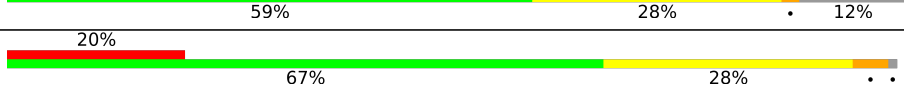
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	0	55	64% 85% 7% 7%
2	1	46	11% 93% 7%
3	2	65	12% 92% 6% •

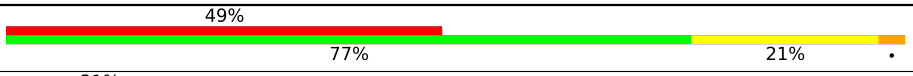
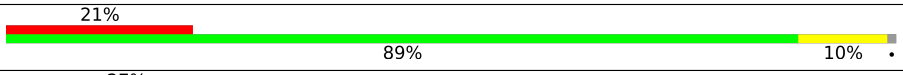
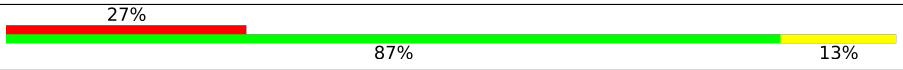
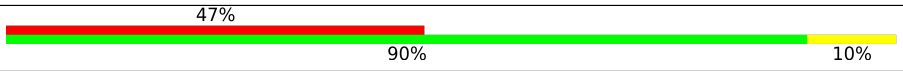
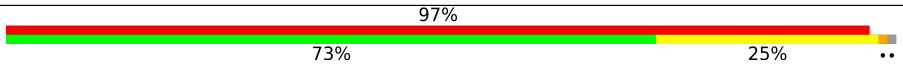
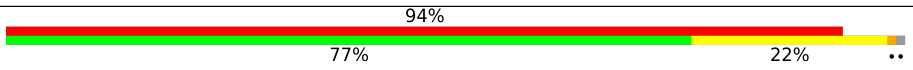
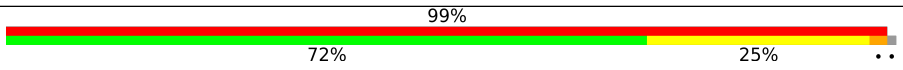
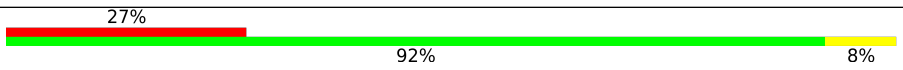
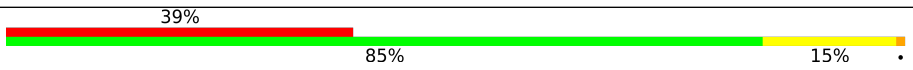
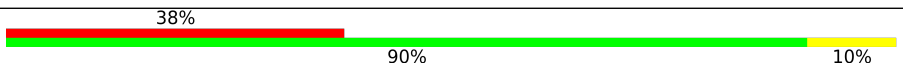
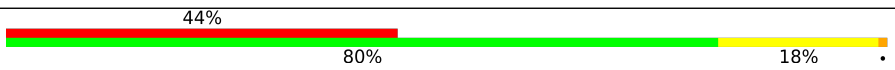
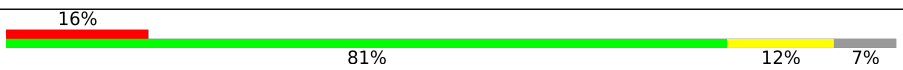
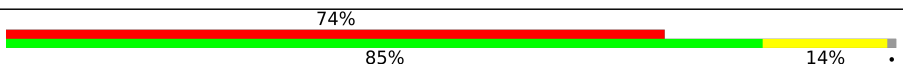
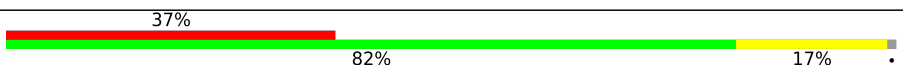
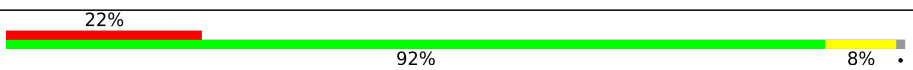
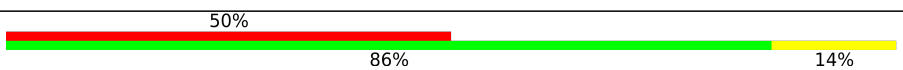
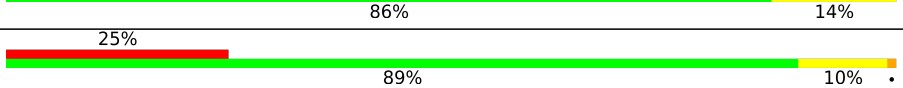
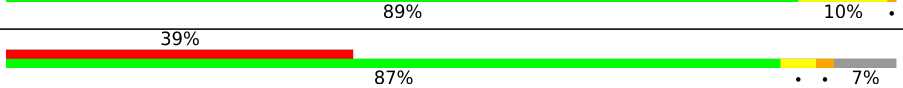
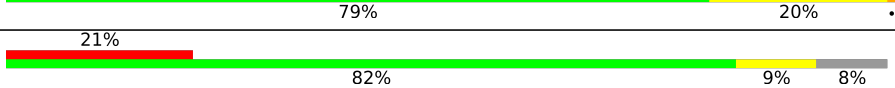
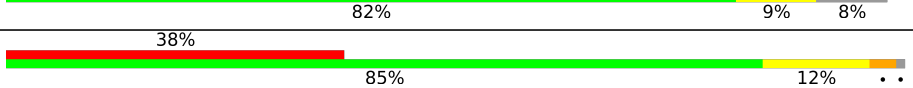
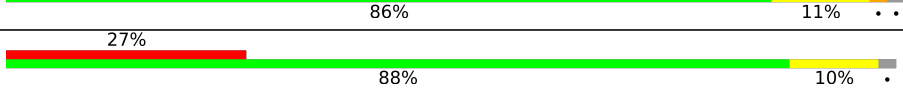
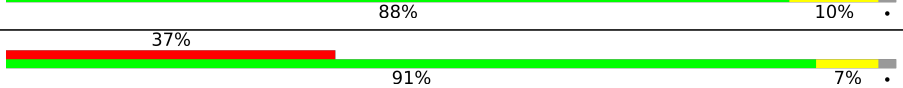
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1550	
7	B	241	
8	C	232	
9	D	206	
10	E	167	
11	F	131	
12	G	156	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	111	
28	a	2923	

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Mol	Chain	Length	Quality of chain
29	b	116	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	
35	h	149	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	128	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 143507 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			418	268	76	73	1		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	70	Total	C	N	O	S	0	0
			540	333	103	98	6		

- Molecule 6 is a RNA chain called 16s rRNA (1530-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1530	Total	C	N	O	P	0	0
			32847	14657	6028	10632	1530		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1749	1106	315	320	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	206	Total	C	N	O	S	0	0
			1623	1028	305	287	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1644	1025	316	298	5		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1155	719	219	211	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			832	524	151	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	62	MET	LEU	variant	UNP A0A2N4W582

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1204	751	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			977	616	171	184	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	126	Total	C	N	O	S	0	0
			1010	628	202	177	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			788	493	151	143	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			878	541	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP A0A1C1EGM1

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	123	Total	C	N	O	S	0	0
			958	592	196	165	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	116	Total	C	N	O	S	0	0
			907	564	181	158	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			805	500	164	138	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			710	438	144	127	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			636	397	127	111	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			639	402	121	112	4		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	62	Total	C	N	O	0	0
			507	321	94	92		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			667	426	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			669	413	138	115	3		

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 27 is a protein called Ribosomal subunit interface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	98	Total	C	N	O	S	0	0
			778	484	149	142	3		

- Molecule 28 is a RNA chain called 23S rRNA (2901-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2901	Total	C	N	O	P	0	0
			62284	27795	11452	20136	2901		

- Molecule 29 is a RNA chain called 5S rRNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	116	Total	C	N	O	P	0	0
			2483	1106	453	808	116		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	271	Total	C	N	O	S	0	0
			2080	1286	423	364	7		

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	209	Total	C	N	O	S	0	0
			1567	981	289	294	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	201	Total	C	N	O	S	0	0
			1554	975	284	290	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	176	Total	C	N	O	S	0	0
			1319	830	243	244	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	148	Total	C	N	O	S	0	0
			1099	693	197	208	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	142	Total	C	N	O	S	0	0
			1134	716	211	202	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	123	Total	C	N	O	S	0	0
			947	594	181	166	6		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	144	Total	C	N	O	S	0	0
			1063	658	211	191	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1074	685	204	179	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP A0A1C1EGZ5

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	119	Total 950	C 588	N 195	O 162	S 5	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	n	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	103	Total 816	C 517	N 153	O 144	S 2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	110	Total 855	C 530	N 166	O 156	S 3	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	93	Total 739	C 467	N 139	O 131	S 2	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	t	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	94	Total 749	C 477	N 136	O 134	S 2	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	78	Total 592	C 367	N 118	O 106	S 1	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	62	Total 499	C 308	N 98	O 92	S 1	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	58	Total 447	C 279	N 87	O 79	S 2	0	0

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	93	Total	Mg	0
			93	93	
55	K	1	Total	Mg	0
			1	1	
55	N	1	Total	Mg	0
			1	1	
55	Q	1	Total	Mg	0
			1	1	
55	a	252	Total	Mg	0
			252	252	
55	b	5	Total	Mg	0
			5	5	
55	c	1	Total	Mg	0
			1	1	
55	d	1	Total	Mg	0
			1	1	
55	p	1	Total	Mg	0
			1	1	
55	w	1	Total	Mg	0
			1	1	
55	z	2	Total	Mg	0
			2	2	

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	46	Total	K	0
			46	46	

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Mol	Chain	Residues	Atoms	AltConf
56	L	1	Total K 1 1	0
56	a	113	Total K 113 113	0
56	b	1	Total K 1 1	0
56	c	5	Total K 5 5	0
56	d	1	Total K 1 1	0
56	e	1	Total K 1 1	0
56	f	1	Total K 1 1	0

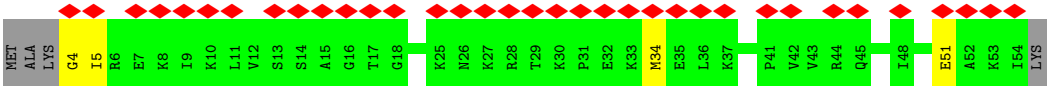
3 Residue-property plots (i)

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: Large ribosomal subunit protein bL33

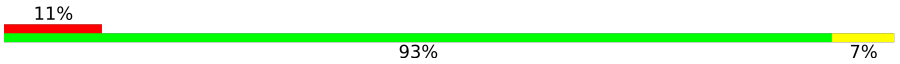
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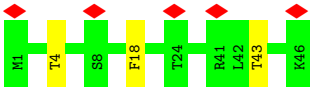




• Molecule 2: Large ribosomal subunit protein bL34

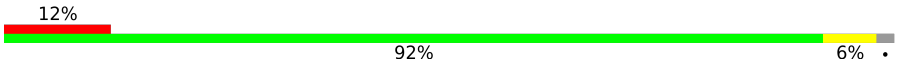
Chain 1:

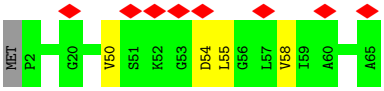




• Molecule 3: Large ribosomal subunit protein bL35

Chain 2:

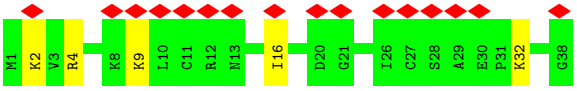




• Molecule 4: Large ribosomal subunit protein bL36

Chain 3:

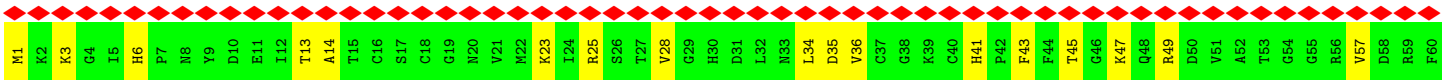




• Molecule 5: Large ribosomal subunit protein bL31

Chain 4:



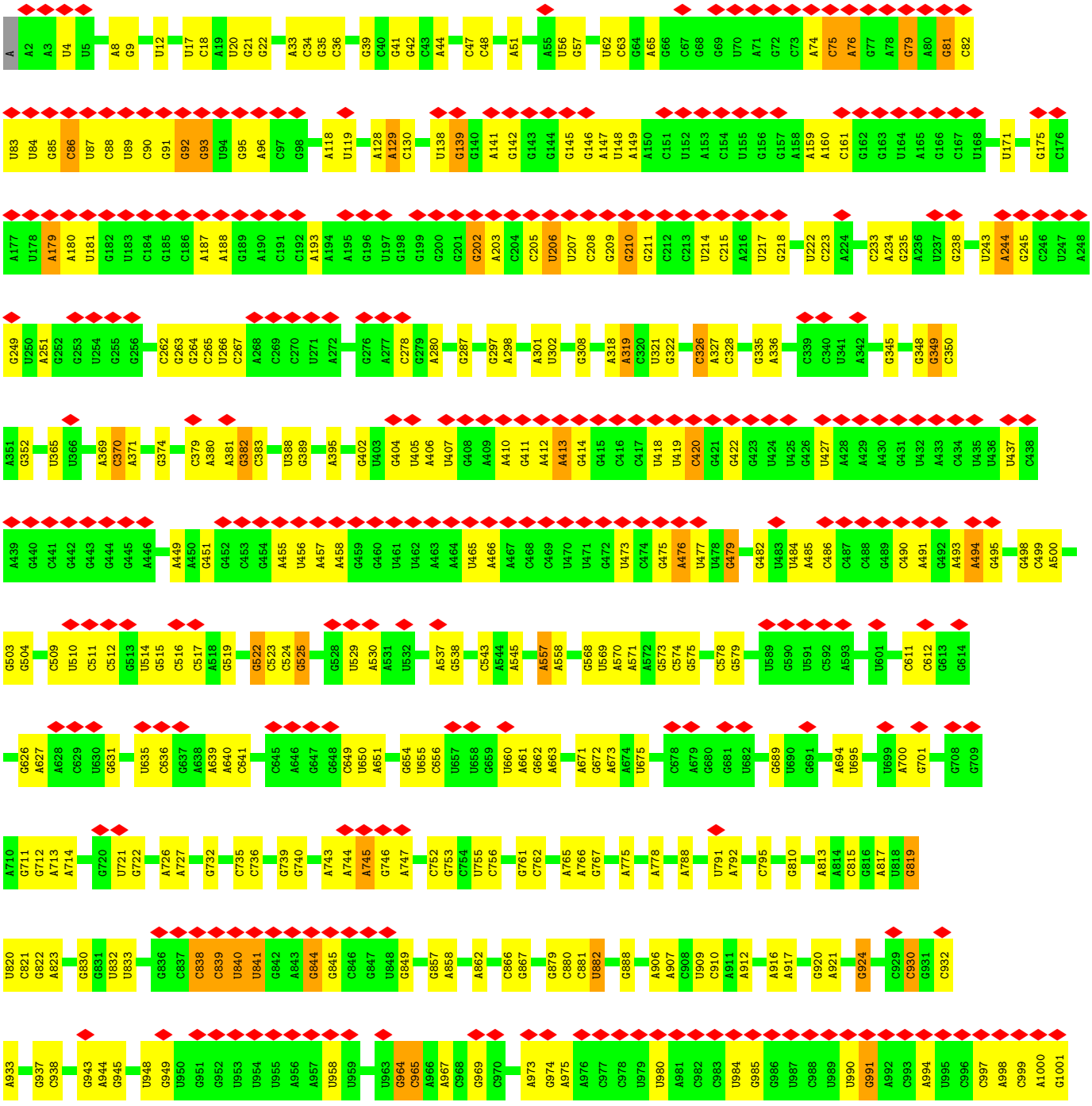


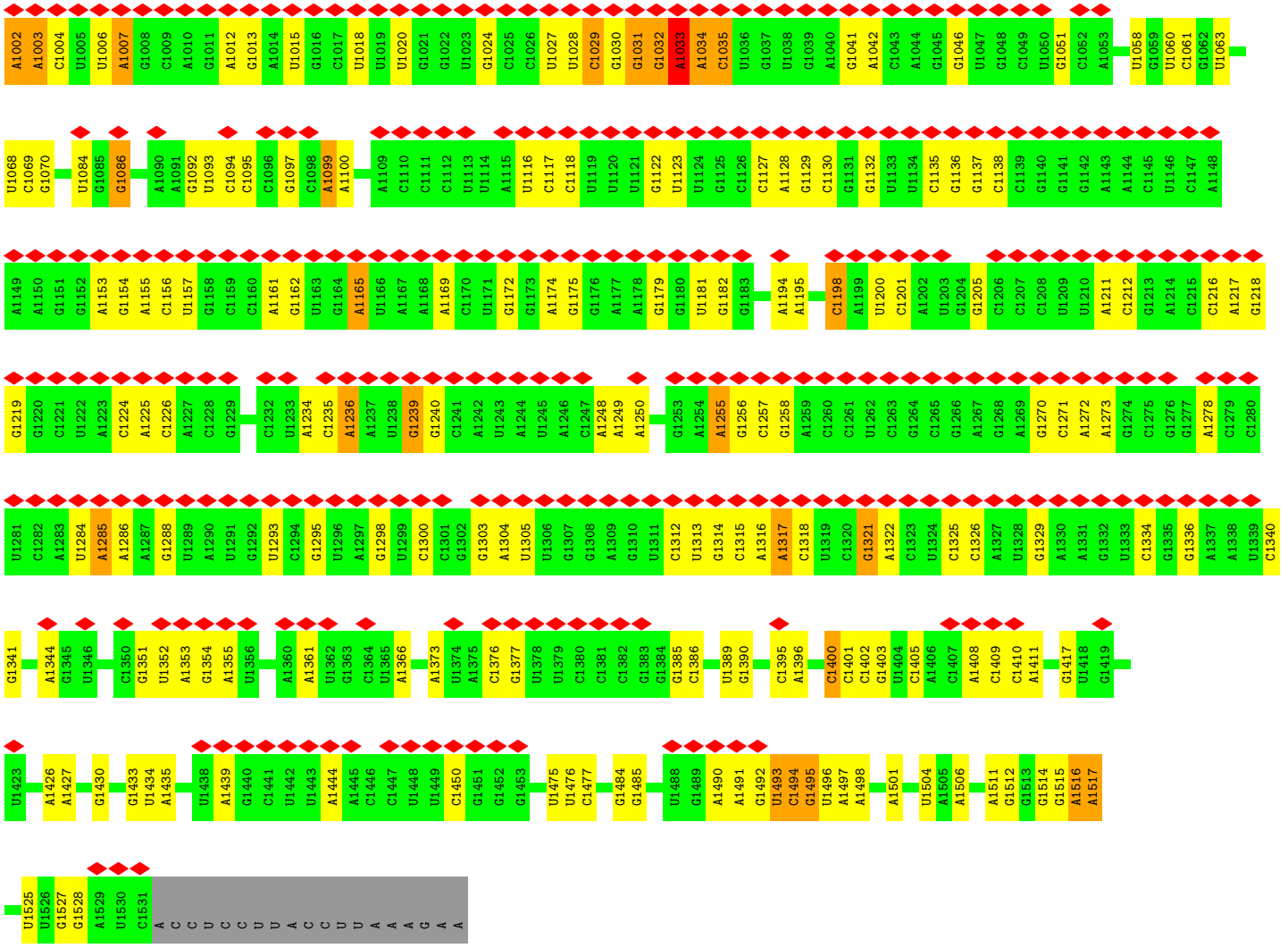


• Molecule 6: 16s rRNA (1530-MER)

Chain A:

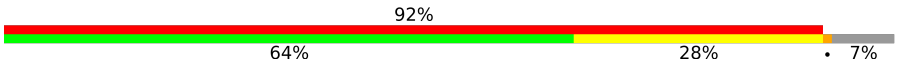


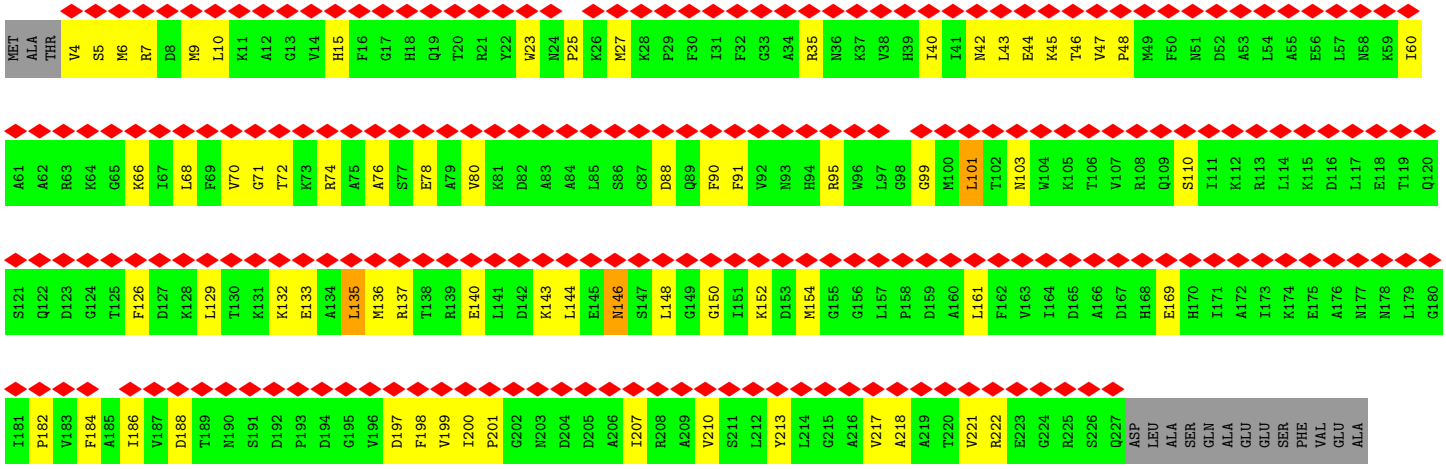




• Molecule 7: Small ribosomal subunit protein uS2

Chain B:



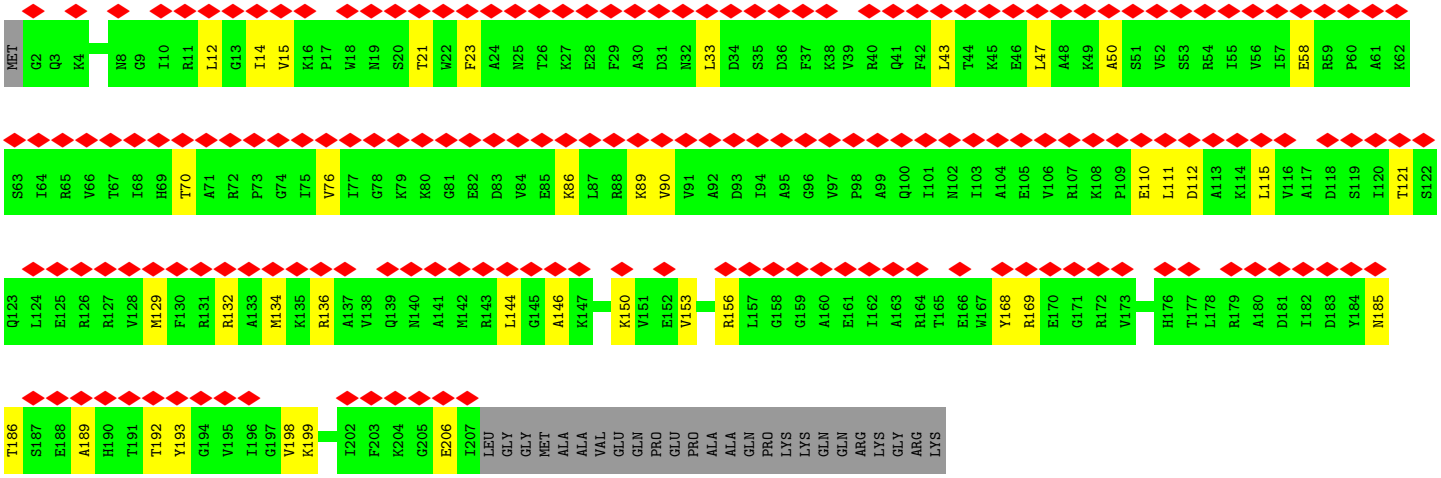




• Molecule 8: Small ribosomal subunit protein uS3

Chain C:





• Molecule 9: Small ribosomal subunit protein uS4

Chain D:

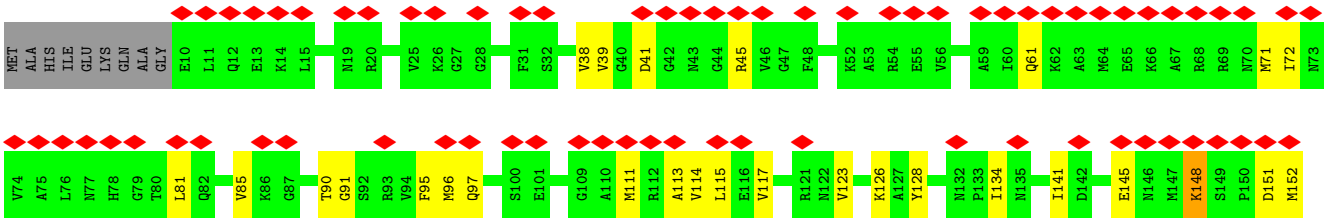


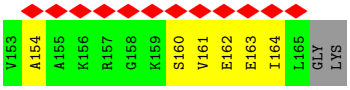


• Molecule 10: Small ribosomal subunit protein uS5

Chain E:



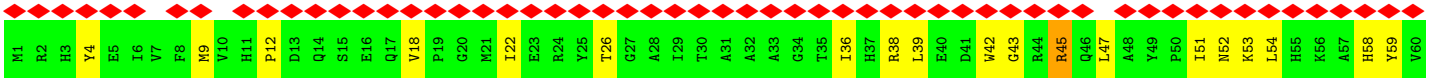


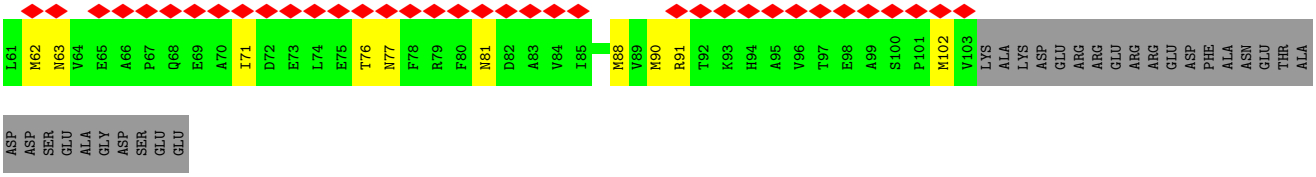


• Molecule 11: Small ribosomal subunit protein bS6

Chain F:

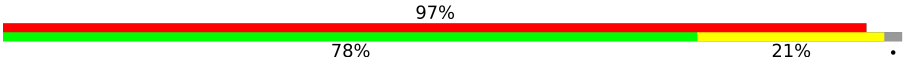


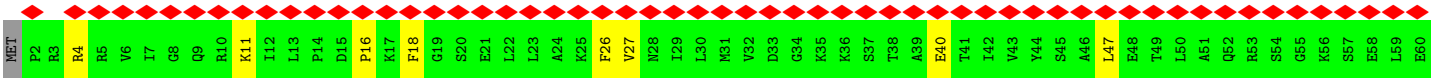


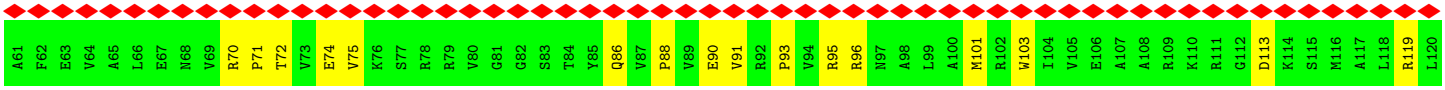


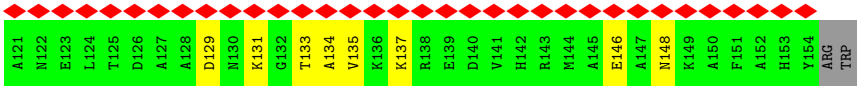
• Molecule 12: Small ribosomal subunit protein uS7

Chain G:





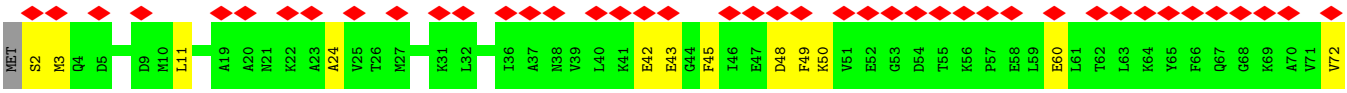


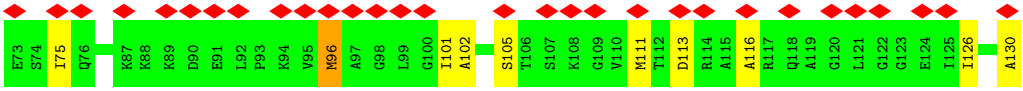


• Molecule 13: Small ribosomal subunit protein uS8

Chain H:

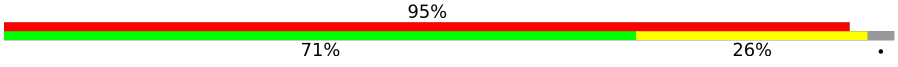


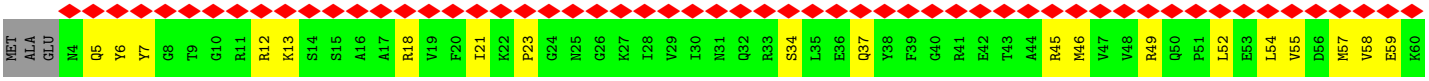


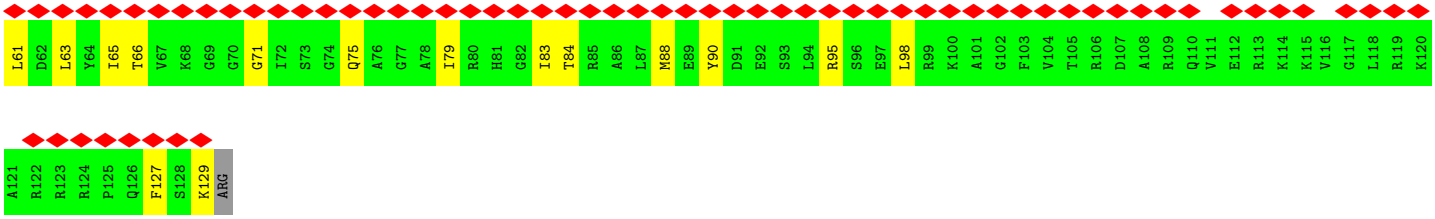


• Molecule 14: Small ribosomal subunit protein uS9

Chain I:

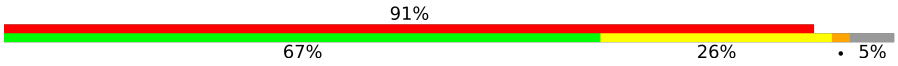


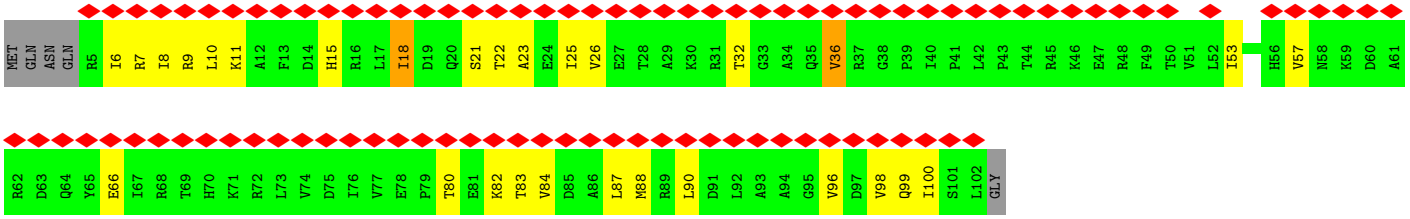




• Molecule 15: Small ribosomal subunit protein uS10

Chain J:

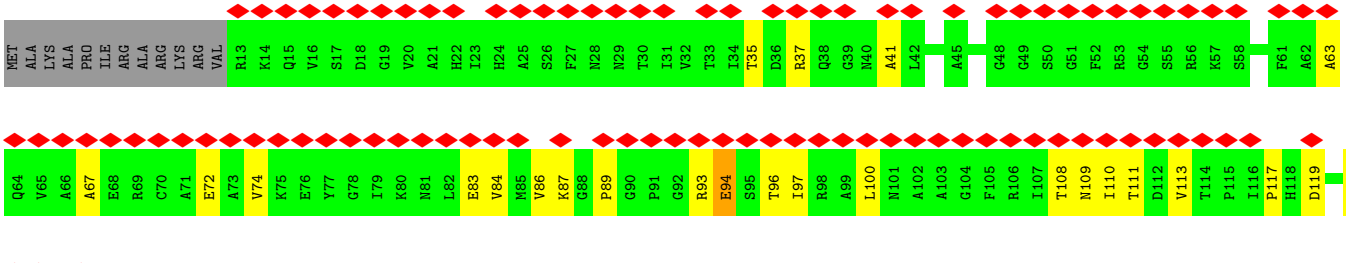




• Molecule 16: Small ribosomal subunit protein uS11

Chain K:

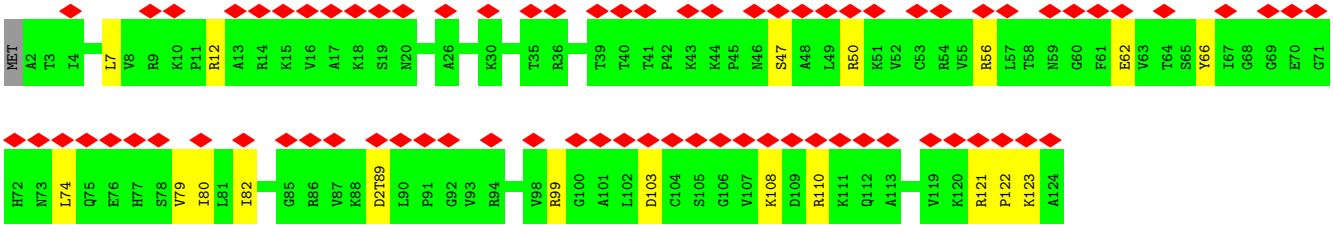




• Molecule 17: Small ribosomal subunit protein uS12

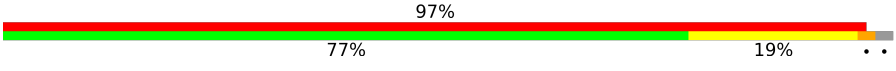
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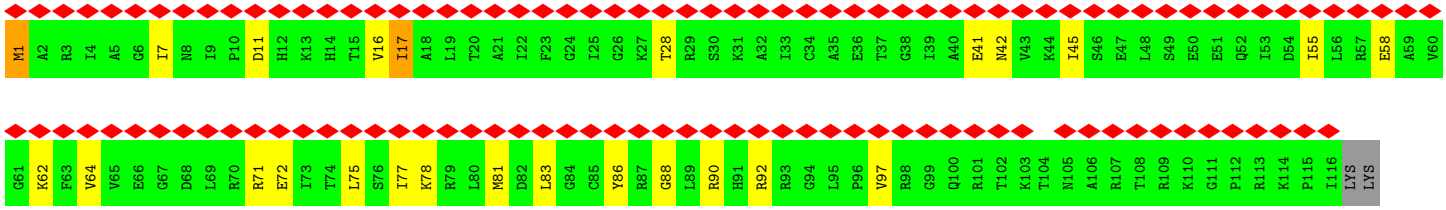




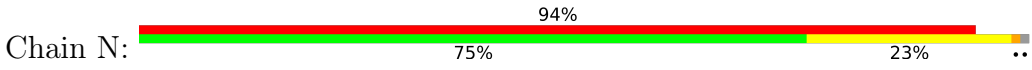
• Molecule 18: Small ribosomal subunit protein uS13

Chain M:

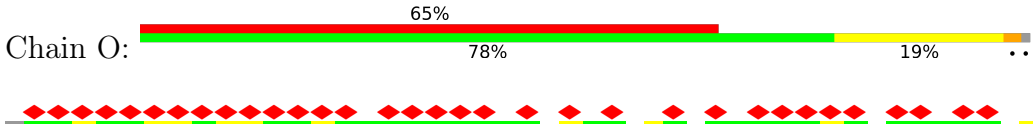




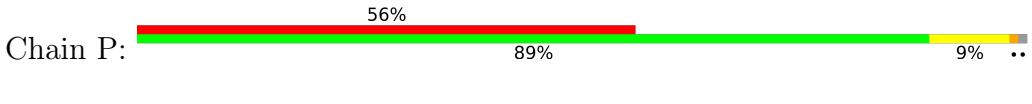
• Molecule 19: Small ribosomal subunit protein uS14



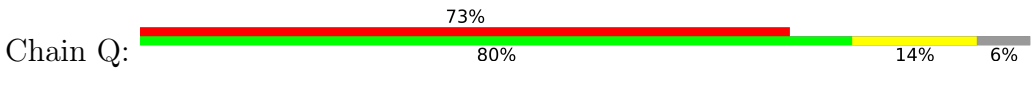
• Molecule 20: Small ribosomal subunit protein uS15



• Molecule 21: Small ribosomal subunit protein bS16



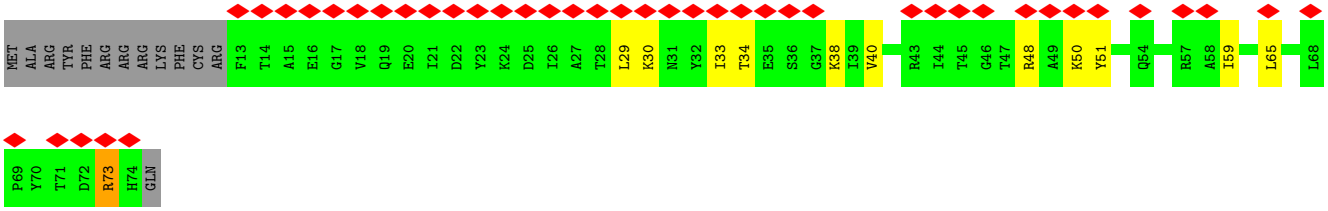
• Molecule 22: Small ribosomal subunit protein uS17



• Molecule 23: Small ribosomal subunit protein bS18

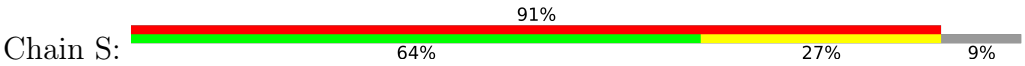
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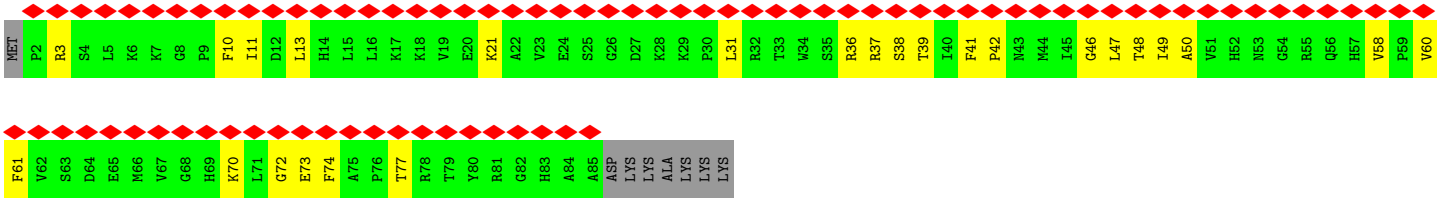




• Molecule 24: Small ribosomal subunit protein uS19

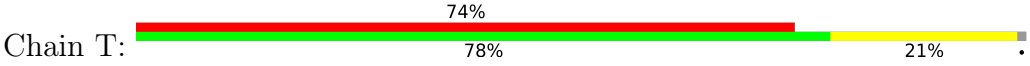
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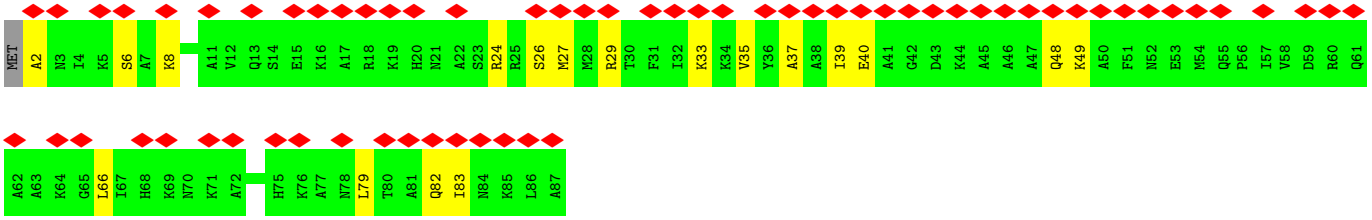




• Molecule 25: Small ribosomal subunit protein bS20

Chain T:

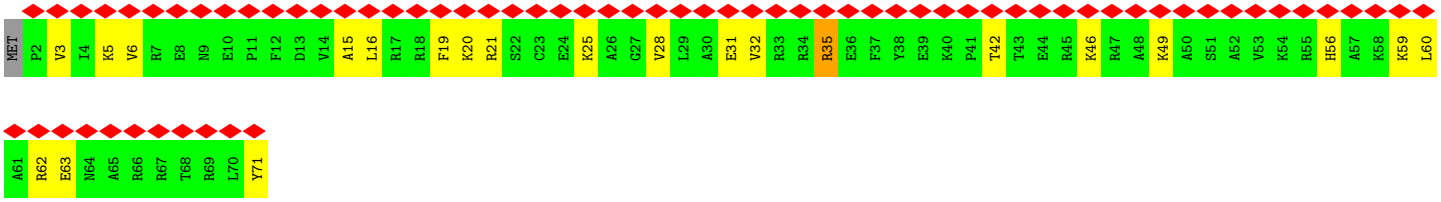




• Molecule 26: Small ribosomal subunit protein bS21

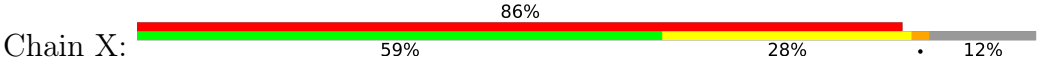
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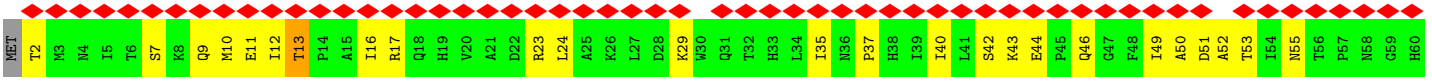


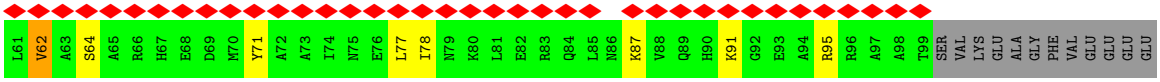


• Molecule 27: Ribosomal subunit interface protein

Chain X:



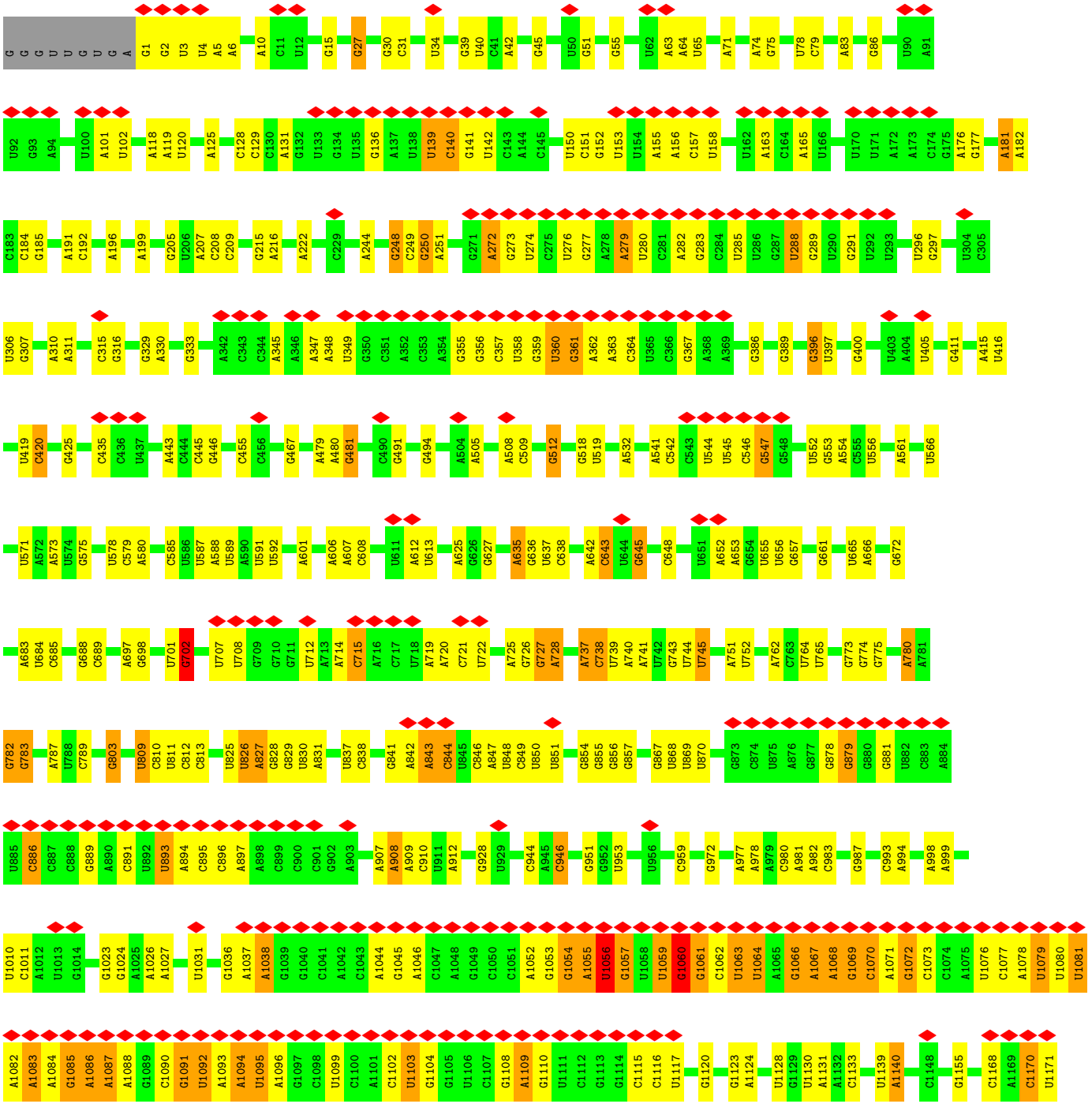


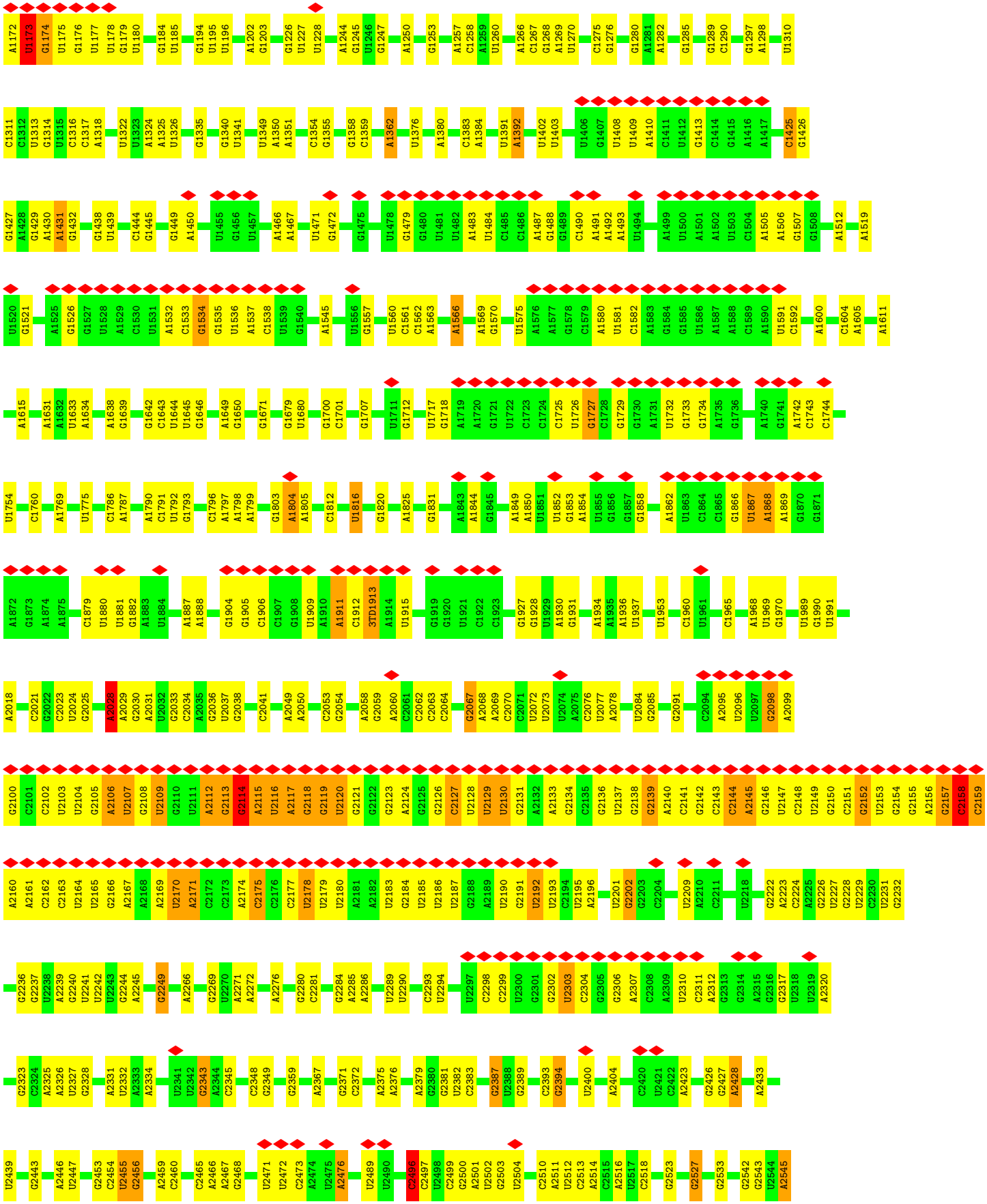


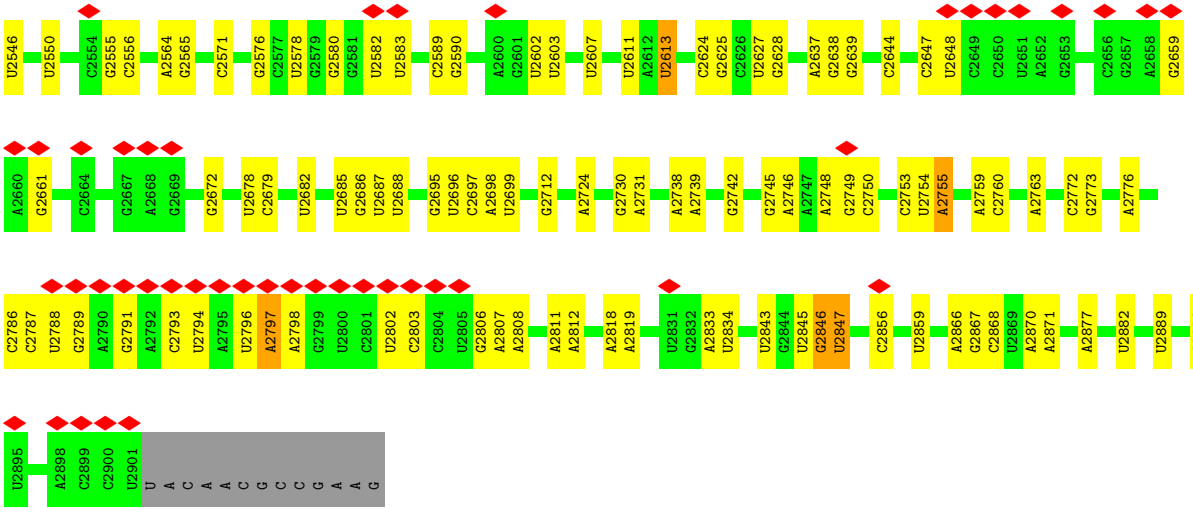
• Molecule 28: 23S rRNA (2901-MER)

Chain a:



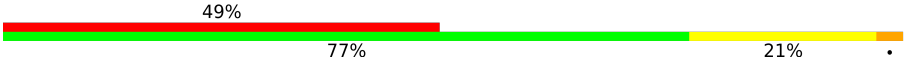


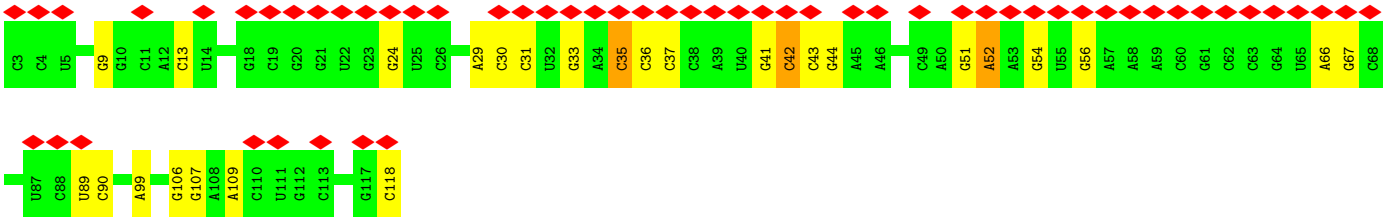

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A1615 A1631 A1632 U1633 A1634 A1638 G1639 G1642 C1643 U1644 U1645 G1646 A1649 G1650 G1671 G1679 U1680 G1700 C1701 G1707 U1711 G1712 U1717 G1718 A1719 A1720 G1721 U1722 C1723 C1724 C1725 U1726 G1727 C1728 G1729 G1730 A1731 U1732 G1733 G1734 A1735 G1736 A1740 G1741 A1742 C1743 C1744
U1754 C1760 A1769 U1775 C1786 A1787 A1790 C1791 U1792 G1793 C1796 A1797 A1798 A1799 G1803 A1804 A1805 C1812 U1816 G1820 A1825 G1831 A1843 A1844 G1845 A1849 A1850 U1851 U1852 G1853 A1854 U1855 G1856 G1857 G1858 A1862 U1863 C1864 C1865 G1866 U1867 A1868 A1869 G1870 G1871
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A2018 C2021 G2022 C2023 U2024 G2025 A2028 A2029 G2030 A2031 U2032 G2033 C2034 A2035 G2036 U2037 G2038 C2041 A2049 A2050 C2053 G2054 A2058 G2059 A2060 C2061 C2062 C2063 C2064 G2067 A2068 A2069 C2070 C2071 U2072 U2073 U2074 A2075 C2076 U2077 A2078 U2084 G2085 G2091 C2094 A2095 U2096 U2097 G2098 A2099
G2100 C2101 C2102 U2103 U2104 G2105 A2106 U2107 G2108 U2109 C2110 U2111 A2112 G2113 G2114 A2115 U2116 A2117 G2118 G2119 U2120 G2121 G2122 G2123 A2124 G2125 G2126 C2127 U2128 U2129 U2130 G2131 A2132 A2133 G2134 C2135 G2136 U2137 G2138 G2139 A2140 C2141 G2142 C2143 C2144 A2145 G2146 U2147 C2148 U2149 G2150 C2151 G2152 U2153 G2154 G2155 A2156 G2157 C2158 C2159
A2160 A2161 C2162 C2163 U2164 U2165 G2166 A2167 A2168 A2169 U2170 A2171 C2172 C2173 A2174 C2175 C2176 C2177 U2178 U2179 U2180 A2181 A2182 U2183 G2184 U2185 U2186 U2187 G2188 A2189 U2190 G2191 U2192 U2193 C2194 U2195 A2196 U2201 G2202 G2203 C2204 U2209 A2210 C2211 U2218 G2222 A2223 C2224 A2225 G2226 U2227 G2228 U2229 C2230 U2231 G2232
G2236 G2237 U2238 A2239 G2240 U2241 U2242 U2243 G2244 A2245 G2249 A2266 G2269 U2270 A2271 A2272 A2276 G2280 C2281 G2284 A2285 A2286 U2289 U2290 C2293 U2294 U2297 C2298 C2299 U2300 G2301 G2302 U2303 C2304 G2305 G2306 A2307 C2308 A2309 U2310 C2311 A2312 G2313 G2314 A2315 G2316 G2317 U2318 U2319 A2320
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• Molecule 29: 5S rRNA (119-MER)

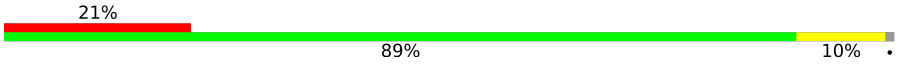
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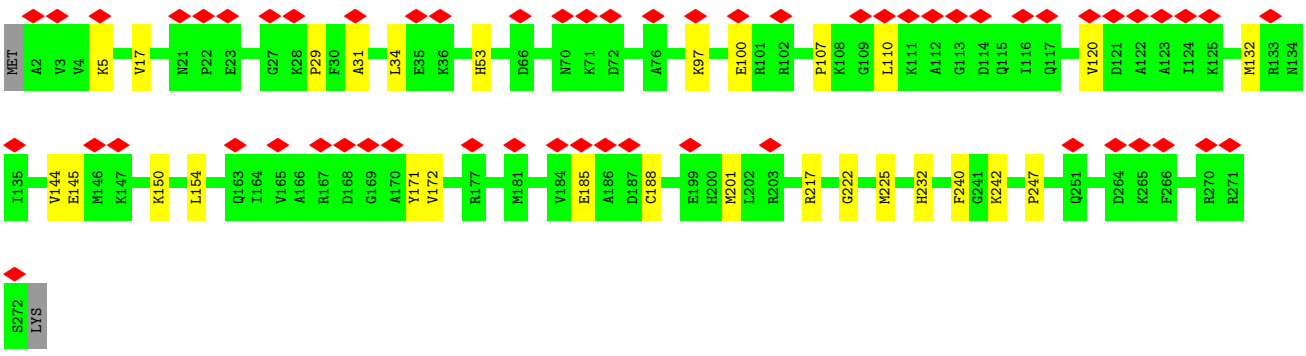




• Molecule 30: Large ribosomal subunit protein uL2

Chain c:

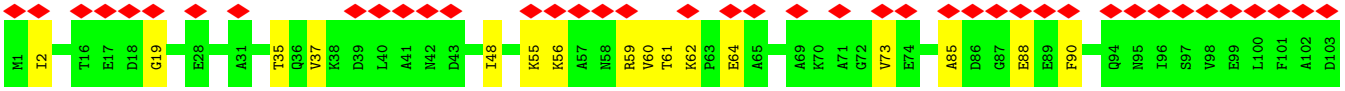


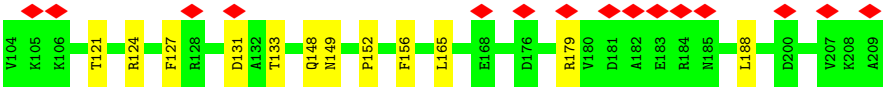


• Molecule 31: Large ribosomal subunit protein uL3

Chain d:

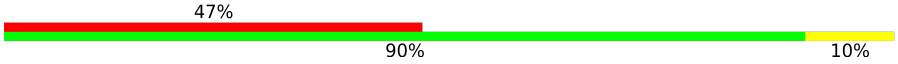


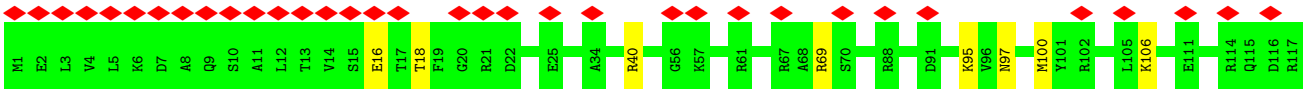


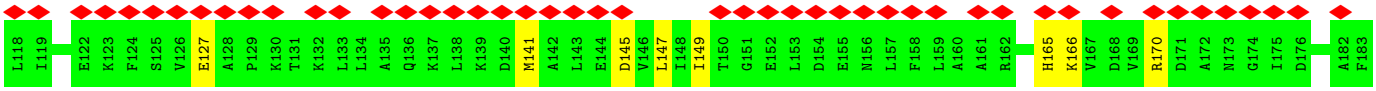


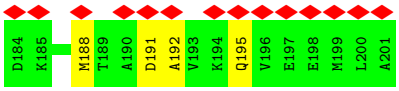
• Molecule 32: Large ribosomal subunit protein uL4

Chain e:



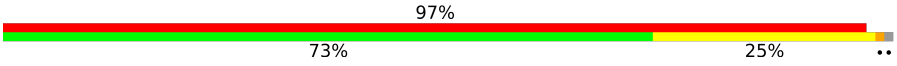


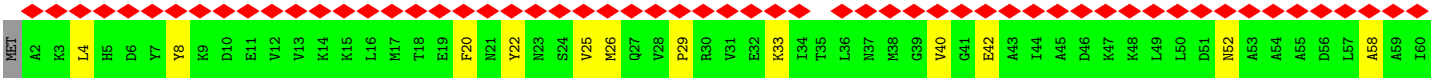


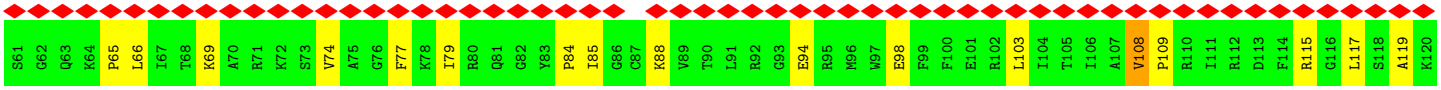


• Molecule 33: Large ribosomal subunit protein uL5

Chain f:



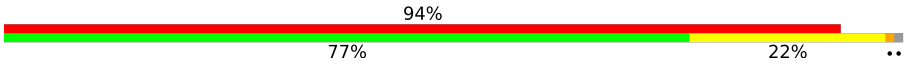


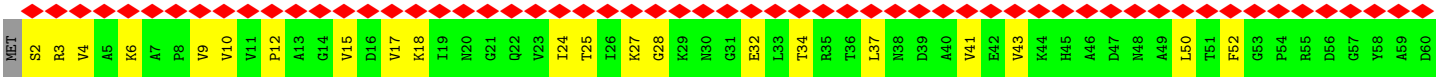


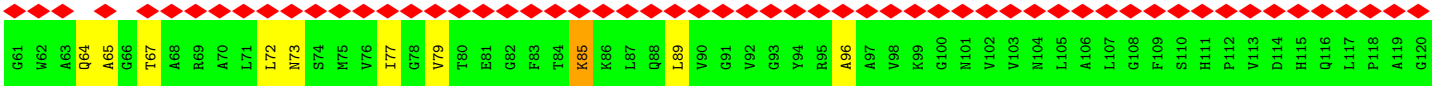


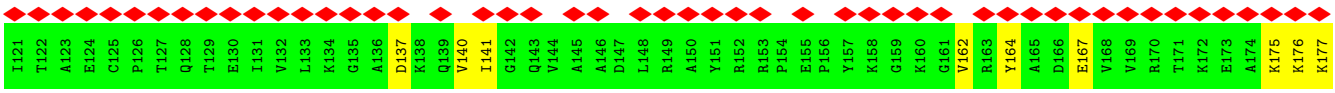
• Molecule 34: Large ribosomal subunit protein uL6

Chain g:



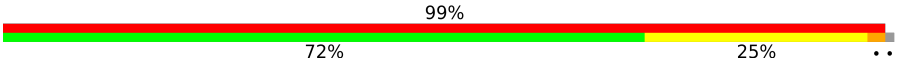


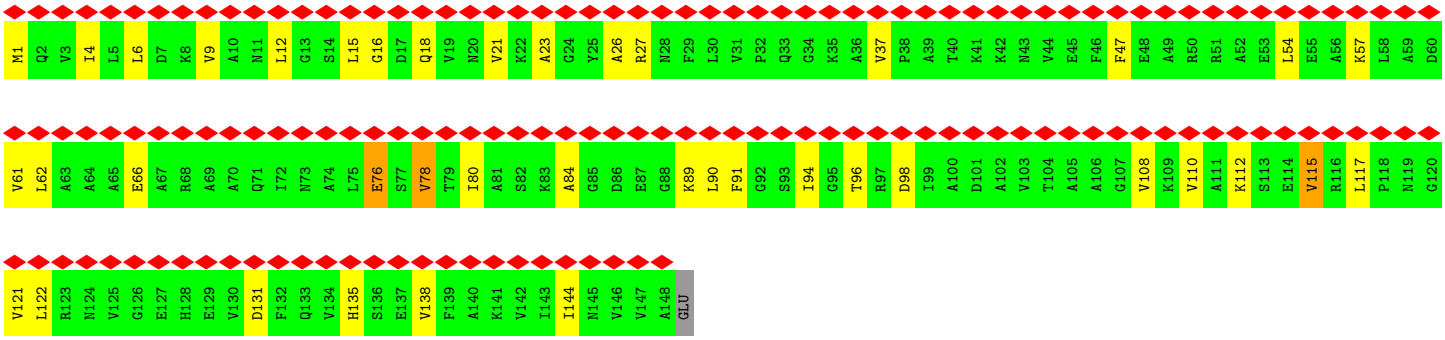




• Molecule 35: Large ribosomal subunit protein bL9

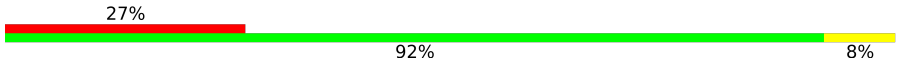
Chain h:

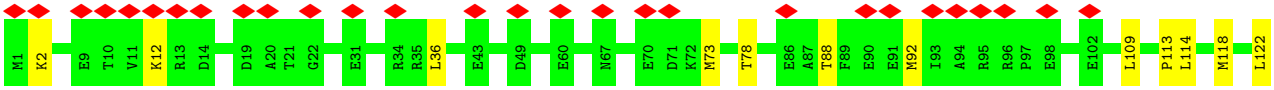


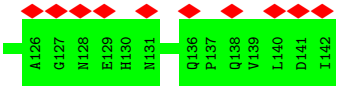


• Molecule 36: Large ribosomal subunit protein uL13

Chain i:



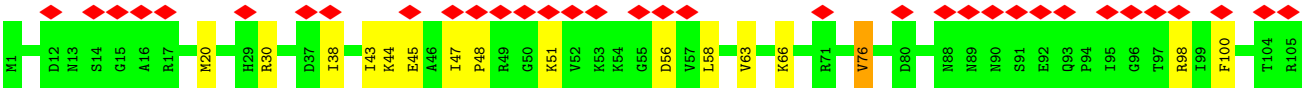


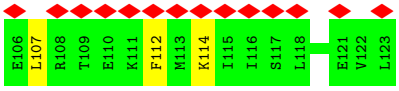


• Molecule 37: Large ribosomal subunit protein uL14

Chain j:



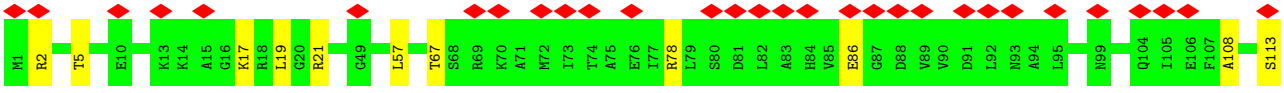


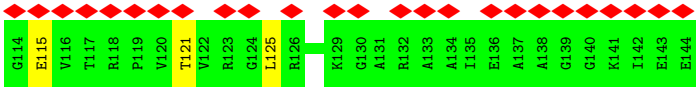


• Molecule 38: Large ribosomal subunit protein uL15

Chain k:



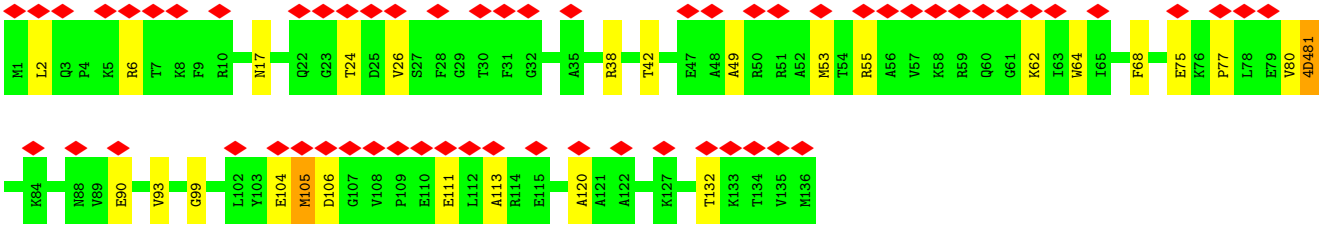




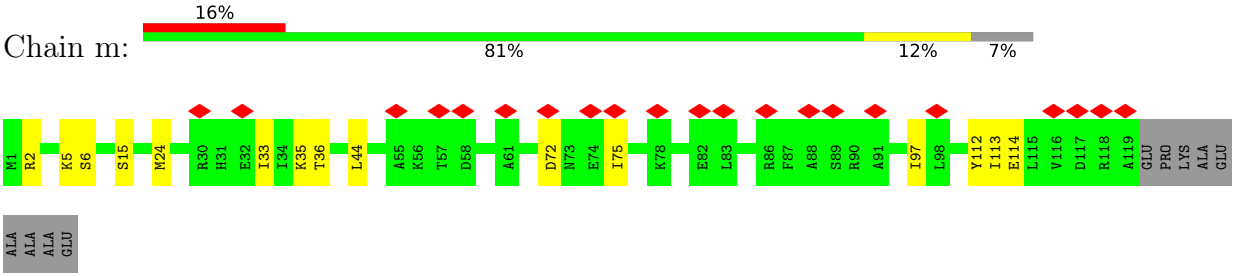
• Molecule 39: Large ribosomal subunit protein uL16

Chain l:

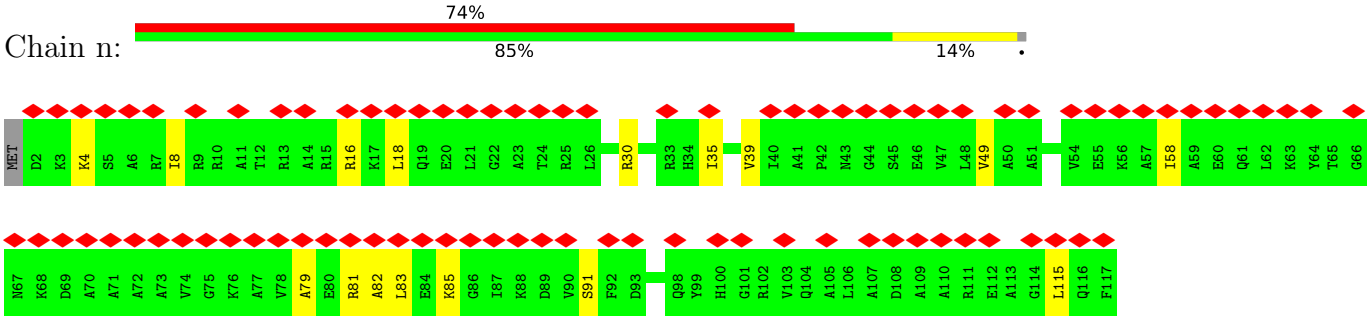




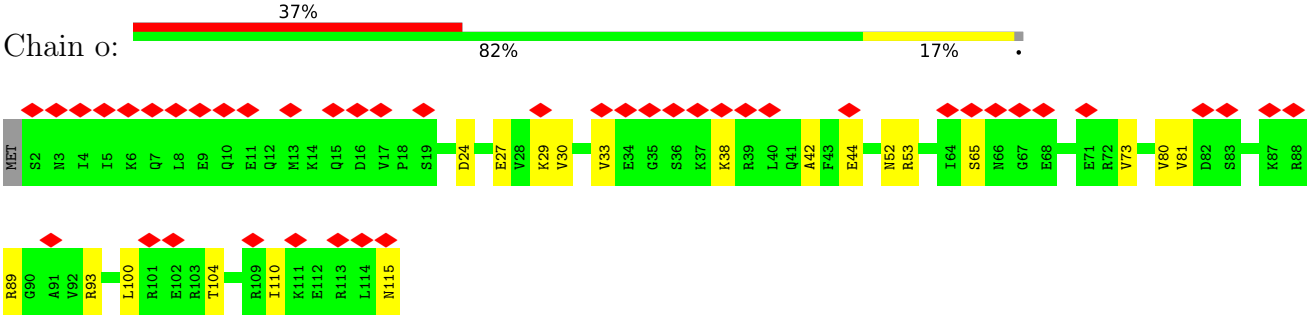
• Molecule 40: Large ribosomal subunit protein bL17



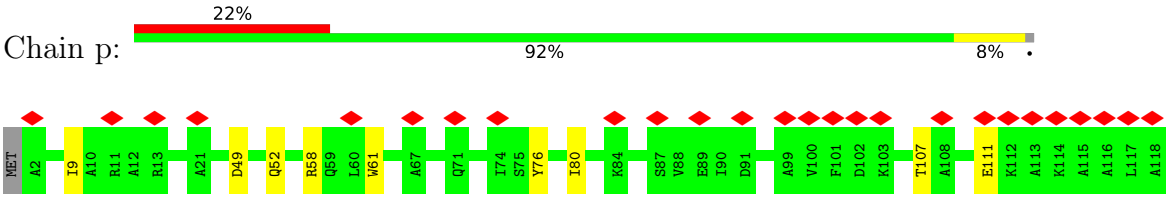
• Molecule 41: Large ribosomal subunit protein uL18



• Molecule 42: Large ribosomal subunit protein bL19

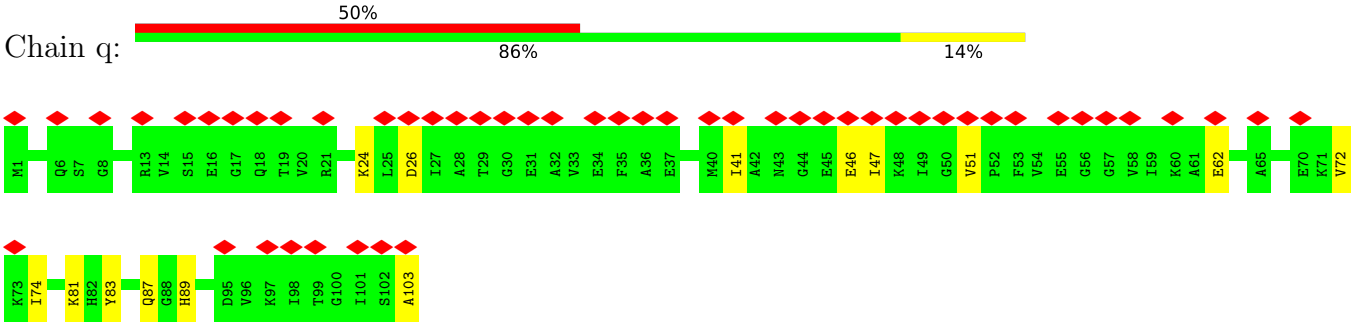


• Molecule 43: Large ribosomal subunit protein bL20



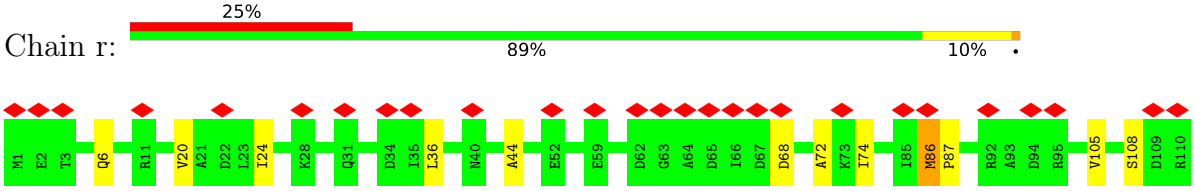
• Molecule 44: Large ribosomal subunit protein bL21

Chain q:



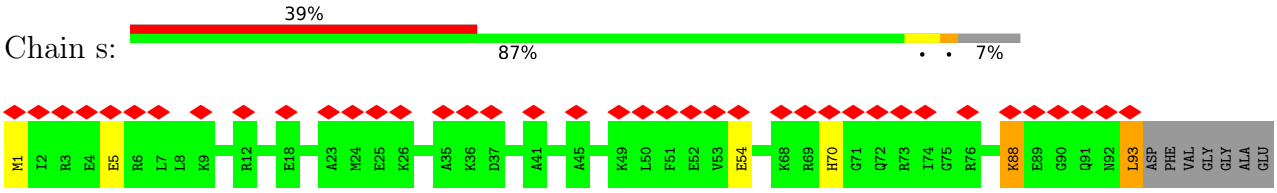
• Molecule 45: Large ribosomal subunit protein uL22

Chain r:



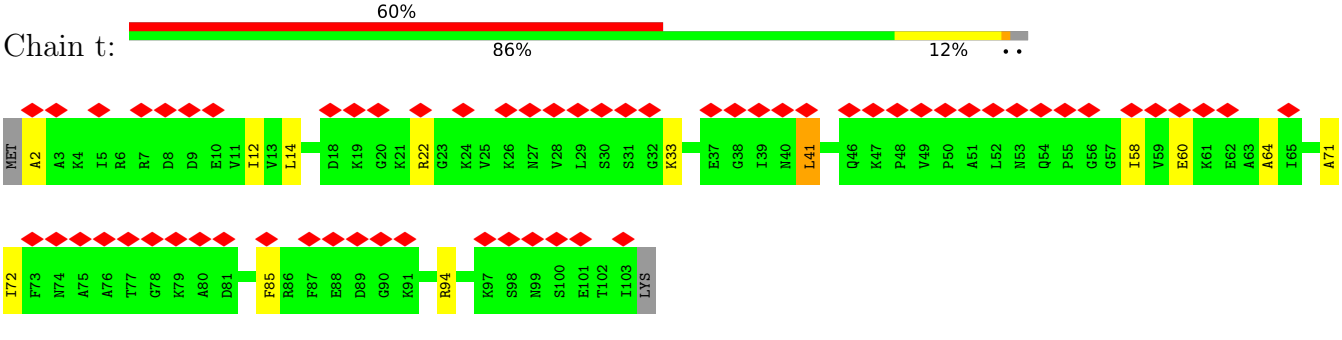
• Molecule 46: Large ribosomal subunit protein uL23

Chain s:



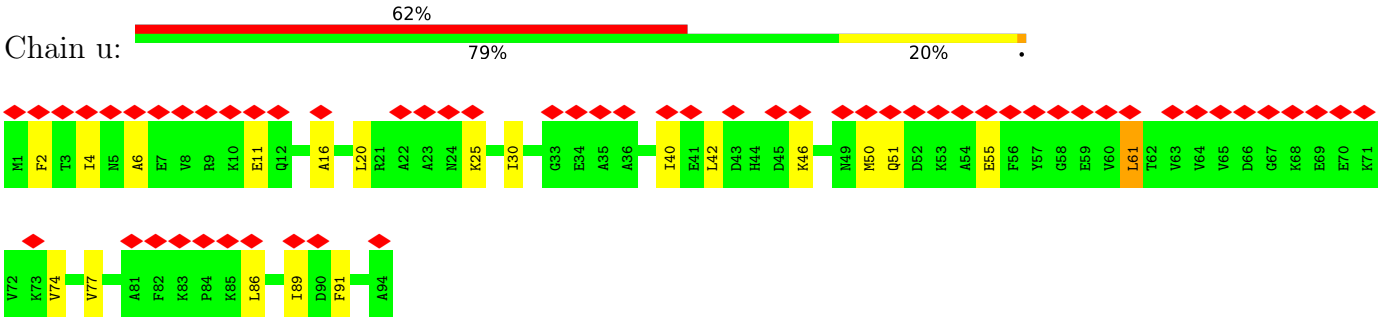
• Molecule 47: Large ribosomal subunit protein uL24

Chain t:



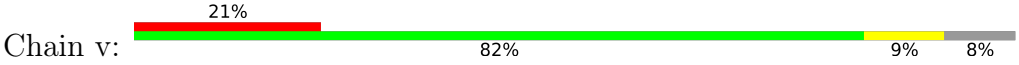
• Molecule 48: Large ribosomal subunit protein bL25

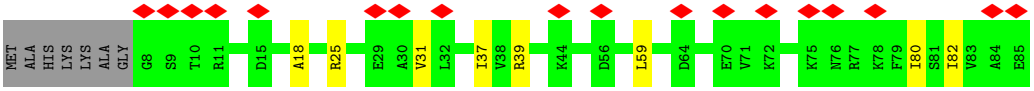
Chain u:



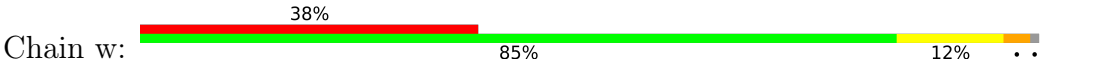
• Molecule 49: Large ribosomal subunit protein bL27

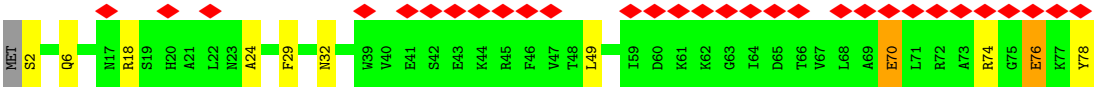
Chain v:



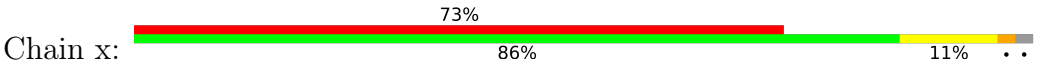


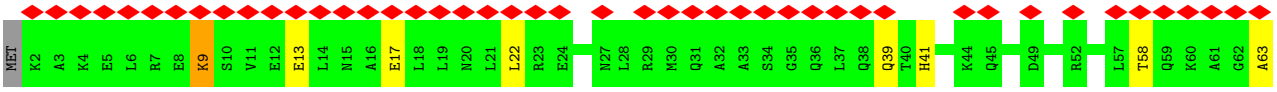
• Molecule 50: Large ribosomal subunit protein bL28



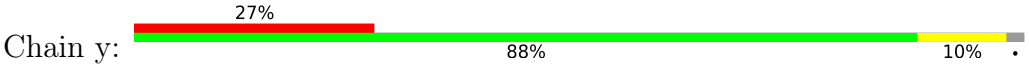


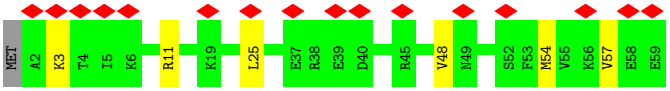
• Molecule 51: Large ribosomal subunit protein uL29



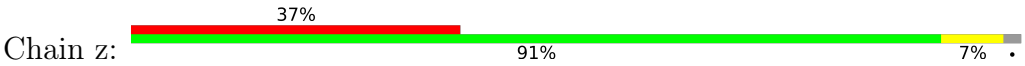


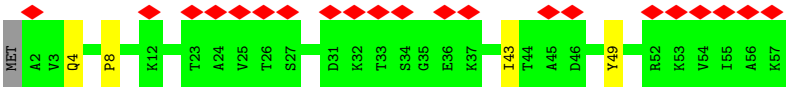
• Molecule 52: Large ribosomal subunit protein uL30





• Molecule 53: Large ribosomal subunit protein bL32





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.184	Depositor
Minimum map value	-0.911	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: K, MG, OMU, H2U, 6MZ, IAS, MA6, MS6, 2MG, ZN, UR3, 2MA, G7M, OMC, D2T, 4D4, PSU, 5MC, 1MG, 3TD, 5MU, 4OC, OMG, MEQ

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	0	0.33	0/425	0.38	0/566
2	1	0.47	0/380	0.39	0/498
3	2	0.41	0/513	0.33	0/676
4	3	0.39	0/303	0.38	0/397
5	4	0.23	0/550	0.45	0/734
6	A	0.83	0/36501	0.81	9/56938 (0.0%)
7	B	0.27	0/1780	0.51	0/2398
8	C	0.28	0/1650	0.38	0/2223
9	D	0.29	0/1665	0.30	0/2225
10	E	0.36	0/1168	0.39	0/1570
11	F	0.31	0/851	0.41	0/1152
12	G	0.24	0/1220	0.35	0/1638
13	H	0.35	0/987	0.40	0/1323
14	I	0.28	0/1022	0.37	0/1361
15	J	0.27	0/798	0.49	0/1078
16	K	0.31	0/885	0.38	0/1192
17	L	0.35	0/961	0.37	0/1287
18	M	0.24	0/916	0.41	0/1225
19	N	0.28	0/817	0.31	0/1088
20	O	0.33	0/718	0.36	0/955
21	P	0.36	0/646	0.40	0/870
22	Q	0.30	0/647	0.35	0/865
23	R	0.34	0/515	0.36	0/693
24	S	0.24	0/684	0.36	0/920
25	T	0.32	0/675	0.37	0/894
26	U	0.21	0/597	0.36	0/792
27	X	0.25	0/791	0.40	0/1069
28	a	1.03	0/69183	0.86	32/107924 (0.0%)
29	b	0.80	0/2776	0.78	0/4328
30	c	0.42	0/2118	0.37	0/2846
31	d	0.42	0/1577	0.38	0/2122

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.38	0/1573	0.38	0/2115
33	f	0.27	0/1434	0.38	0/1926
34	g	0.27	0/1339	0.36	0/1811
35	h	0.20	0/1110	0.41	0/1500
36	i	0.42	0/1157	0.37	0/1556
37	j	0.38	0/956	0.37	0/1281
38	k	0.39	0/1073	0.33	0/1427
39	l	0.39	0/1072	0.36	0/1434
40	m	0.42	0/963	0.41	0/1288
41	n	0.32	0/902	0.38	0/1209
42	o	0.40	0/929	0.34	0/1242
43	p	0.43	0/960	0.36	0/1278
44	q	0.39	0/829	0.37	0/1106
45	r	0.39	0/862	0.39	0/1154
46	s	0.34	0/745	0.38	0/996
47	t	0.34	0/787	0.34	0/1051
48	u	0.34	0/763	0.43	0/1024
49	v	0.42	0/599	0.35	0/795
50	w	0.40	0/635	0.36	0/848
51	x	0.32	0/500	0.31	0/665
52	y	0.35	0/451	0.37	0/603
53	z	0.40	0/449	0.38	0/597
All	All	0.83	0/154407	0.75	41/230753 (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
39	l	0	1

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2098	G	OP1-P-O3'	-11.40	73.81	108.00
28	a	2098	G	OP2-P-O3'	-9.18	80.47	108.00
28	a	1310	U	C2-N1-C1'	7.62	126.85	117.70
28	a	1056	U	C2-N1-C1'	7.56	126.77	117.70
6	A	1033	A	O4'-C1'-N9	7.52	114.21	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	l	81	4D4	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	418	0	449	2	0
2	1	377	0	418	2	0
3	2	504	0	572	3	0
4	3	302	0	340	3	0
5	4	540	0	537	16	0
6	A	32847	0	16540	253	0
7	B	1749	0	1774	50	0
8	C	1623	0	1696	23	0
9	D	1644	0	1706	21	0
10	E	1155	0	1206	19	0
11	F	832	0	821	18	0
12	G	1204	0	1256	20	0
13	H	977	0	1031	13	0
14	I	1010	0	1057	23	0
15	J	788	0	830	16	0
16	K	878	0	884	19	0
17	L	958	0	1019	12	0
18	M	907	0	977	23	0
19	N	805	0	846	19	0
20	O	710	0	735	12	0
21	P	636	0	649	5	0
22	Q	639	0	684	5	0
23	R	507	0	525	8	0
24	S	667	0	691	19	0
25	T	669	0	717	12	0
26	U	589	0	629	18	0
27	X	778	0	793	25	0
28	a	62284	0	31328	445	0
29	b	2483	0	1258	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	2080	0	2152	19	0
31	d	1567	0	1619	16	0
32	e	1554	0	1620	12	0
33	f	1410	0	1444	33	0
34	g	1319	0	1367	24	0
35	h	1099	0	1139	18	0
36	i	1134	0	1161	8	0
37	j	947	0	1025	13	0
38	k	1063	0	1130	8	0
39	l	1074	0	1138	17	0
40	m	950	0	994	7	0
41	n	892	0	923	11	0
42	o	917	0	962	12	0
43	p	947	0	1019	4	0
44	q	816	0	841	7	0
45	r	855	0	915	7	0
46	s	739	0	809	5	0
47	t	779	0	831	8	0
48	u	749	0	763	11	0
49	v	592	0	612	4	0
50	w	625	0	652	7	0
51	x	499	0	534	5	0
52	y	447	0	484	4	0
53	z	443	0	458	3	0
54	3	1	0	0	0	0
54	4	1	0	0	0	0
55	A	93	0	0	0	0
55	K	1	0	0	0	0
55	N	1	0	0	0	0
55	Q	1	0	0	0	0
55	a	252	0	0	0	0
55	b	5	0	0	0	0
55	c	1	0	0	0	0
55	d	1	0	0	0	0
55	p	1	0	0	0	0
55	w	1	0	0	0	0
55	z	2	0	0	0	0
56	A	46	0	0	0	0
56	L	1	0	0	0	0
56	a	113	0	0	0	0
56	b	1	0	0	0	0
56	c	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	d	1	0	0	0	0
56	e	1	0	0	0	0
56	f	1	0	0	0	0
All	All	143507	0	96560	1269	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1269 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:76:A:N6	6:A:91:G:H1	1.24	1.30
28:a:2794:U:H3	28:a:2797:A:H61	1.12	0.97
28:a:544:U:O2	28:a:547:G:O6	1.87	0.90
28:a:1036:G:N2	28:a:1115:C:O2	2.07	0.88
28:a:2102:C:H42	28:a:2183:U:H3	1.13	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	68/70 (97%)	58 (85%)	10 (15%)	0	100	100
7	B	222/241 (92%)	204 (92%)	18 (8%)	0	100	100
8	C	204/232 (88%)	197 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
10	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
11	F	101/131 (77%)	97 (96%)	4 (4%)	0	100	100
12	G	151/156 (97%)	143 (95%)	8 (5%)	0	100	100
13	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
14	I	124/130 (95%)	118 (95%)	6 (5%)	0	100	100
15	J	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	12	32
16	K	113/129 (88%)	105 (93%)	8 (7%)	0	100	100
17	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
18	M	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
19	N	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
20	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
21	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
22	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
23	R	60/75 (80%)	58 (97%)	2 (3%)	0	100	100
24	S	82/92 (89%)	77 (94%)	5 (6%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
27	X	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
30	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
31	d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	24	48
32	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
33	f	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
34	g	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
35	h	146/149 (98%)	136 (93%)	8 (6%)	2 (1%)	9	23
36	i	140/142 (99%)	140 (100%)	0	0	100	100
37	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
38	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
39	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
40	m	117/128 (91%)	113 (97%)	4 (3%)	0	100	100
41	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
43	p	115/118 (98%)	115 (100%)	0	0	100	100
44	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
45	r	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
46	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
47	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
48	u	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
49	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
All	All	5693/5997 (95%)	5476 (96%)	213 (4%)	4 (0%)	49	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	d	149	ASN
15	J	57	VAL
35	h	76	GLU
35	h	115	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	45 (98%)	1 (2%)	45	74
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	60/60 (100%)	58 (97%)	2 (3%)	33	63
7	B	185/198 (93%)	176 (95%)	9 (5%)	22	49
8	C	170/189 (90%)	166 (98%)	4 (2%)	43	72
9	D	171/172 (99%)	170 (99%)	1 (1%)	78	91
10	E	119/126 (94%)	114 (96%)	5 (4%)	26	55
11	F	88/111 (79%)	85 (97%)	3 (3%)	32	62
12	G	126/129 (98%)	123 (98%)	3 (2%)	43	72
13	H	104/105 (99%)	103 (99%)	1 (1%)	68	86
14	I	104/107 (97%)	101 (97%)	3 (3%)	37	67
15	J	87/91 (96%)	80 (92%)	7 (8%)	11	28
16	K	89/98 (91%)	88 (99%)	1 (1%)	65	85
17	L	102/103 (99%)	102 (100%)	0	100	100
18	M	96/98 (98%)	92 (96%)	4 (4%)	26	55
19	N	83/84 (99%)	79 (95%)	4 (5%)	23	50
20	O	75/76 (99%)	72 (96%)	3 (4%)	28	56
21	P	63/63 (100%)	62 (98%)	1 (2%)	55	80
22	Q	73/78 (94%)	71 (97%)	2 (3%)	39	69
23	R	53/65 (82%)	52 (98%)	1 (2%)	50	77
24	S	72/79 (91%)	71 (99%)	1 (1%)	59	82
25	T	65/66 (98%)	63 (97%)	2 (3%)	35	65
26	U	60/61 (98%)	56 (93%)	4 (7%)	15	36
27	X	83/94 (88%)	81 (98%)	2 (2%)	43	72
30	c	215/217 (99%)	215 (100%)	0	100	100
31	d	163/163 (100%)	163 (100%)	0	100	100
32	e	165/165 (100%)	163 (99%)	2 (1%)	63	84
33	f	148/150 (99%)	141 (95%)	7 (5%)	23	51
34	g	135/136 (99%)	133 (98%)	2 (2%)	57	81
35	h	112/113 (99%)	103 (92%)	9 (8%)	11	28
36	i	116/116 (100%)	115 (99%)	1 (1%)	70	87
37	j	104/104 (100%)	101 (97%)	3 (3%)	37	67
38	k	105/105 (100%)	102 (97%)	3 (3%)	37	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	l	107/107 (100%)	105 (98%)	2 (2%)	50	77
40	m	98/103 (95%)	96 (98%)	2 (2%)	48	76
41	n	86/87 (99%)	86 (100%)	0	100	100
42	o	99/100 (99%)	97 (98%)	2 (2%)	48	76
43	p	89/90 (99%)	88 (99%)	1 (1%)	65	85
44	q	83/83 (100%)	80 (96%)	3 (4%)	31	60
45	r	92/92 (100%)	90 (98%)	2 (2%)	45	74
46	s	80/84 (95%)	78 (98%)	2 (2%)	42	71
47	t	83/85 (98%)	81 (98%)	2 (2%)	43	72
48	u	76/76 (100%)	75 (99%)	1 (1%)	61	83
49	v	60/64 (94%)	59 (98%)	1 (2%)	53	79
50	w	67/68 (98%)	65 (97%)	2 (3%)	36	66
51	x	53/54 (98%)	51 (96%)	2 (4%)	29	58
52	y	48/49 (98%)	48 (100%)	0	100	100
53	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4728/4885 (97%)	4615 (98%)	113 (2%)	43	72

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	T	26	SER
50	w	76	GLU
33	f	137	ILE
50	w	70	GLU
44	q	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
41	n	61	GLN
51	x	36	GLN
41	n	98	GLN
45	r	9	HIS
23	R	31	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2899/2923 (99%)	438 (15%)	0
29	b	115/116 (99%)	17 (14%)	0
6	A	1529/1550 (98%)	227 (14%)	2 (0%)
All	All	4543/4589 (98%)	682 (15%)	2 (0%)

5 of 682 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	9	G
6	A	22	G
6	A	39	G
6	A	44	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1033	A
6	A	1492	G

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

40 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
39	4D4	l	81	39	9,11,12	0.86	0	8,13,15	1.78	2 (25%)
28	2MG	a	1831	28	23,26,27	2.56	7 (30%)	32,38,41	2.16	10 (31%)
6	G7M	A	525	6,56	23,26,27	2.17	5 (21%)	35,39,42	1.91	7 (20%)
6	UR3	A	1496	6	19,22,23	2.57	6 (31%)	26,32,35	1.28	1 (3%)
28	5MU	a	1937	28,56	19,22,23	2.73	7 (36%)	28,32,35	3.84	10 (35%)
28	H2U	a	2447	28	18,21,22	3.92	5 (27%)	21,30,33	5.72	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	D2T	L	89	17	7,9,10	1.20	0	6,11,13	1.49	1 (16%)
28	6MZ	a	2028	28	22,25,26	2.52	4 (18%)	30,36,39	2.25	10 (33%)
28	PSU	a	2602	28	18,21,22	2.24	8 (44%)	22,30,33	1.95	4 (18%)
28	1MG	a	743	28	22,26,27	2.52	6 (27%)	33,39,42	2.02	7 (21%)
28	5MC	a	1960	28,56	18,22,23	2.00	5 (27%)	26,32,35	1.32	2 (7%)
28	OMG	a	2249	28,56	23,26,27	2.35	6 (26%)	33,38,41	1.86	10 (30%)
28	PSU	a	744	28,55	18,21,22	2.22	9 (50%)	22,30,33	1.79	3 (13%)
31	MEQ	d	150	31	8,9,10	0.86	0	5,10,12	0.54	0
6	5MC	A	1405	6	18,22,23	1.94	6 (33%)	26,32,35	1.33	1 (3%)
39	MS6	l	82	39	5,7,8	0.60	0	2,7,9	1.43	0
6	2MG	A	1205	6,56	23,26,27	2.57	6 (26%)	32,38,41	2.06	10 (31%)
28	PSU	a	1909	28	18,21,22	2.17	8 (44%)	22,30,33	1.86	4 (18%)
28	2MA	a	2501	28,55,56	22,25,26	1.39	4 (18%)	33,37,40	2.03	8 (24%)
6	5MC	A	965	6	18,22,23	2.01	6 (33%)	26,32,35	1.38	2 (7%)
6	PSU	A	514	6,55	18,21,22	2.16	7 (38%)	22,30,33	1.92	5 (22%)
6	2MG	A	1514	6	23,26,27	2.62	7 (30%)	32,38,41	2.10	9 (28%)
28	5MU	a	745	28	19,22,23	2.57	7 (36%)	28,32,35	4.01	12 (42%)
28	PSU	a	1915	28	18,21,22	2.10	8 (44%)	22,30,33	1.81	3 (13%)
6	4OC	A	1400	6	20,23,24	2.20	4 (20%)	26,32,35	1.13	4 (15%)
28	OMU	a	2550	28,55,56	19,22,23	2.80	7 (36%)	26,31,34	1.82	5 (19%)
6	2MG	A	964	6	23,26,27	2.59	6 (26%)	32,38,41	2.08	10 (31%)
28	PSU	a	2502	28,56	18,21,22	2.30	8 (44%)	22,30,33	1.93	5 (22%)
28	6MZ	a	1615	28	22,25,26	2.31	4 (18%)	30,36,39	2.62	11 (36%)
16	IAS	K	119	16	6,7,8	1.78	1 (16%)	6,8,10	2.58	2 (33%)
6	MA6	A	1516	6	23,26,27	1.34	3 (13%)	34,38,41	2.18	9 (26%)
28	PSU	a	2455	28	18,21,22	2.31	6 (33%)	22,30,33	2.02	4 (18%)
28	3TD	a	1913	-	18,22,23	2.71	7 (38%)	22,32,35	1.71	2 (9%)
28	PSU	a	2578	28	18,21,22	2.38	9 (50%)	22,30,33	2.04	5 (22%)
28	PSU	a	953	28	18,21,22	2.31	8 (44%)	22,30,33	1.92	3 (13%)
28	PSU	a	2603	28	18,21,22	2.33	8 (44%)	22,30,33	2.13	4 (18%)
28	2MG	a	2443	28	23,26,27	2.61	7 (30%)	32,38,41	2.10	10 (31%)
6	MA6	A	1517	6	23,26,27	1.31	3 (13%)	34,38,41	2.28	9 (26%)
28	G7M	a	2067	28,56	23,26,27	2.23	5 (21%)	35,39,42	1.88	7 (20%)
28	OMC	a	2496	28,55	19,22,23	1.86	5 (26%)	26,31,34	1.18	2 (7%)

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
39	4D4	l	81	39	-	2/11/12/14	-
28	2MG	a	1831	28	-	0/9/27/28	0/3/3/3
6	G7M	A	525	6,56	-	3/7/25/26	0/3/3/3
6	UR3	A	1496	6	-	0/7/25/26	0/2/2/2
28	5MU	a	1937	28,56	-	0/7/25/26	0/2/2/2
28	H2U	a	2447	28	-	0/7/38/39	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
28	6MZ	a	2028	28	-	2/9/27/28	0/3/3/3
28	PSU	a	2602	28	-	0/7/25/26	0/2/2/2
28	1MG	a	743	28	-	0/7/25/26	0/3/3/3
28	5MC	a	1960	28,56	-	0/7/25/26	0/2/2/2
28	OMG	a	2249	28,56	-	1/9/27/28	0/3/3/3
28	PSU	a	744	28,55	-	1/7/25/26	0/2/2/2
31	MEQ	d	150	31	-	3/8/9/11	-
6	5MC	A	1405	6	-	0/7/25/26	0/2/2/2
39	MS6	l	82	39	-	2/4/6/8	-
6	2MG	A	1205	6,56	-	0/9/27/28	0/3/3/3
28	PSU	a	1909	28	-	0/7/25/26	0/2/2/2
28	2MA	a	2501	28,55,56	-	2/7/25/26	0/3/3/3
6	5MC	A	965	6	-	0/7/25/26	0/2/2/2
6	PSU	A	514	6,55	-	0/7/25/26	0/2/2/2
6	2MG	A	1514	6	-	0/9/27/28	0/3/3/3
28	5MU	a	745	28	-	0/7/25/26	0/2/2/2
28	PSU	a	1915	28	-	0/7/25/26	0/2/2/2
6	4OC	A	1400	6	-	0/9/29/30	0/2/2/2
28	OMU	a	2550	28,55,56	-	0/9/27/28	0/2/2/2
6	2MG	A	964	6	-	0/9/27/28	0/3/3/3
28	PSU	a	2502	28,56	-	2/7/25/26	0/2/2/2
28	6MZ	a	1615	28	-	0/9/27/28	0/3/3/3
16	IAS	K	119	16	-	1/7/7/8	-
6	MA6	A	1516	6	-	0/11/29/30	0/3/3/3
28	PSU	a	2455	28	-	0/7/25/26	0/2/2/2
28	3TD	a	1913	-	-	0/7/25/26	0/2/2/2
28	PSU	a	2578	28	-	0/7/25/26	0/2/2/2
28	PSU	a	953	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2603	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2443	28	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MA6	A	1517	6	-	3/11/29/30	0/3/3/3
28	G7M	a	2067	28,56	-	3/7/25/26	0/3/3/3
28	OMC	a	2496	28,55	-	0/9/27/28	0/2/2/2

The worst 5 of 218 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2028	6MZ	C6-N6	9.95	1.45	1.34
28	a	2447	H2U	O4-C4	9.75	1.43	1.23
6	A	964	2MG	O6-C6	9.10	1.40	1.23
28	a	1615	6MZ	C6-N6	9.06	1.44	1.34
6	A	1205	2MG	O6-C6	8.90	1.40	1.23

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2447	H2U	C4-N3-C2	-19.08	109.96	125.79
28	a	2447	H2U	O2-C2-N1	-10.55	109.86	123.11
28	a	745	5MU	C5M-C5-C4	9.24	128.94	118.77
28	a	1937	5MU	C4-N3-C2	-8.90	115.83	127.35
28	a	745	5MU	C4-N3-C2	-8.69	116.09	127.35

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
31	d	150	MEQ	O-C-CA-CB
16	K	119	IAS	CA-CB-CG-OD1
28	a	2249	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2028	6MZ	2	0
28	a	2249	OMG	1	0
6	A	965	5MC	1	0
6	A	1400	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	964	2MG	2	0
6	A	1516	MA6	1	0
28	a	2455	PSU	1	0
28	a	2496	OMC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 530 ligands modelled in this entry, 530 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	a	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1913:3TD	O3'	1914:A	P	4.63
1	a	1912:C	O3'	1913:3TD	P	3.01

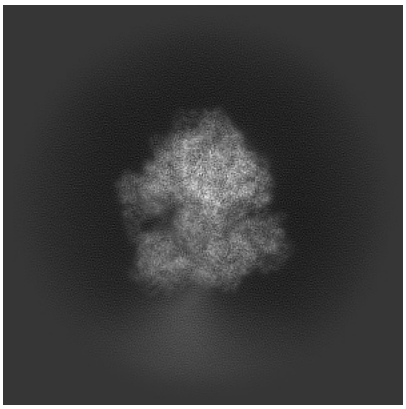
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55797. These allow visual inspection of the internal detail of the map and identification of artifacts.

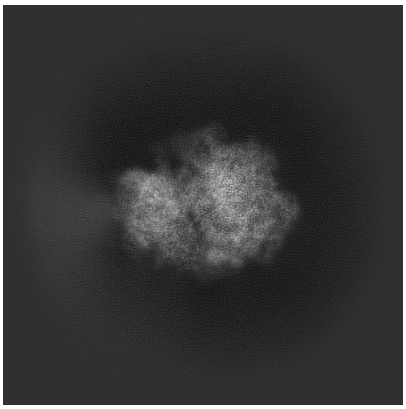
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

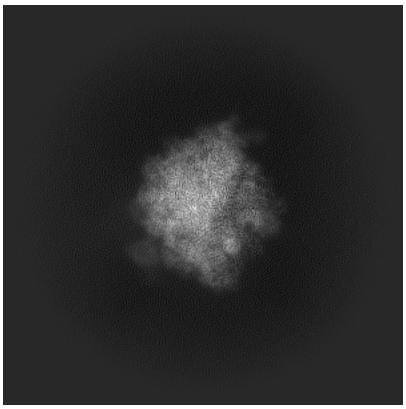
6.1.1 Primary map



X

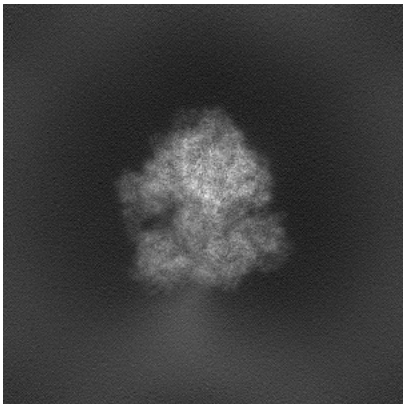


Y

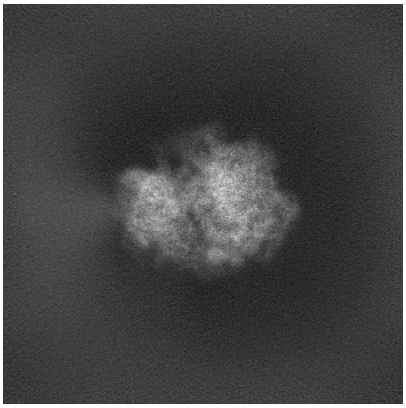


Z

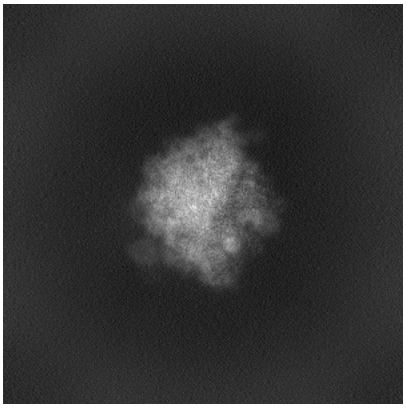
6.1.2 Raw map



X



Y

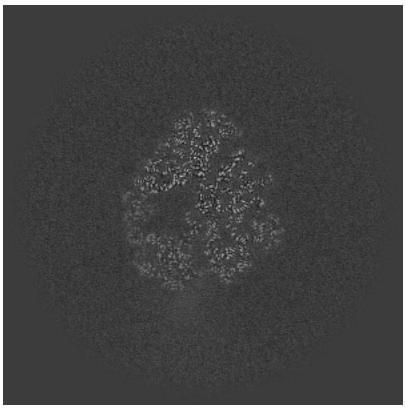


Z

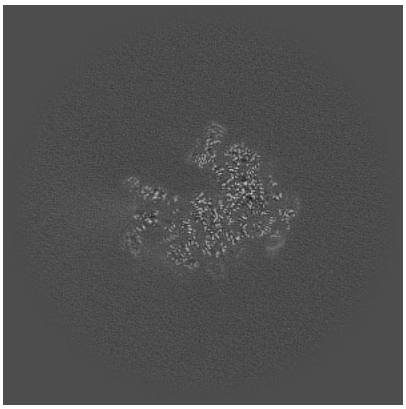
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

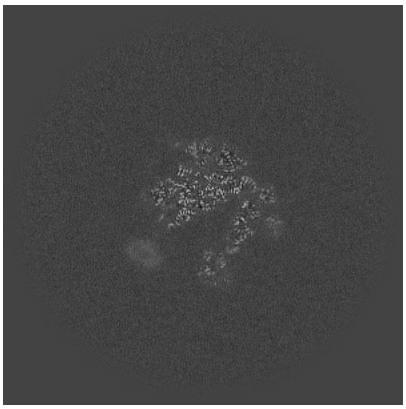
6.2.1 Primary map



X Index: 256

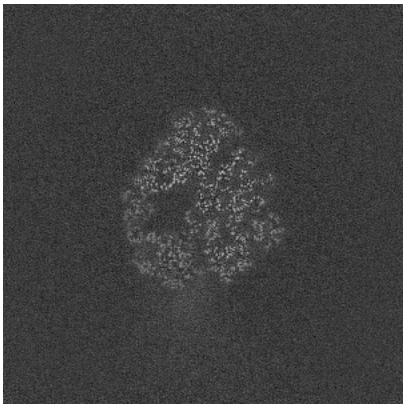


Y Index: 256

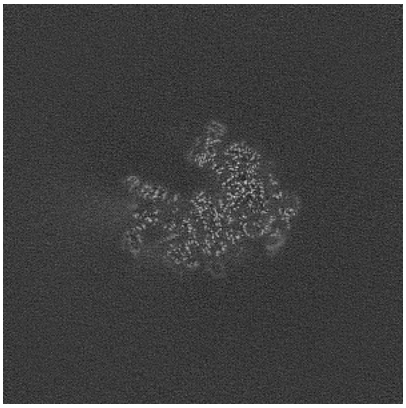


Z Index: 256

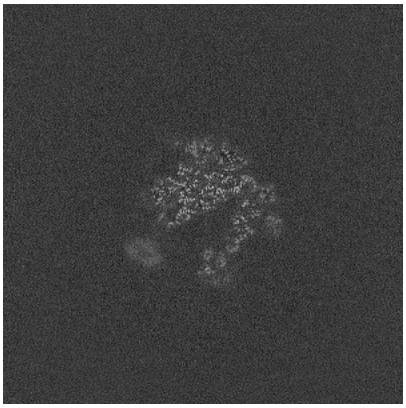
6.2.2 Raw map



X Index: 256



Y Index: 256

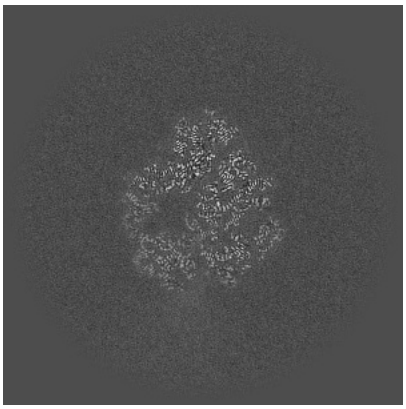


Z Index: 256

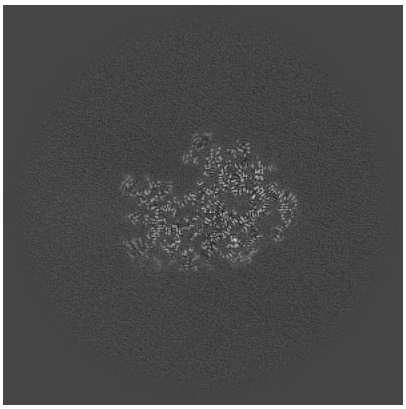
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

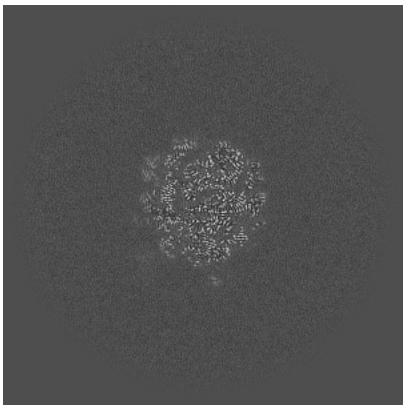
6.3.1 Primary map



X Index: 260

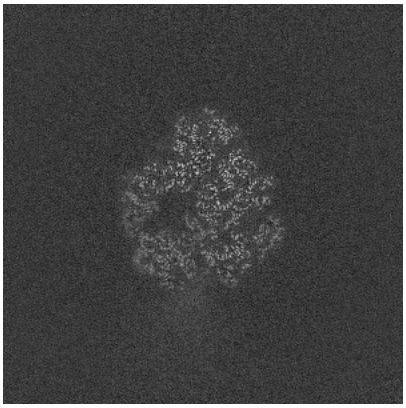


Y Index: 268

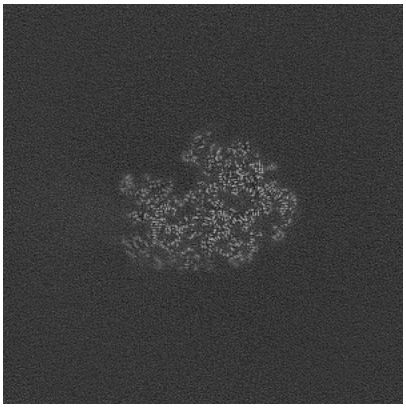


Z Index: 298

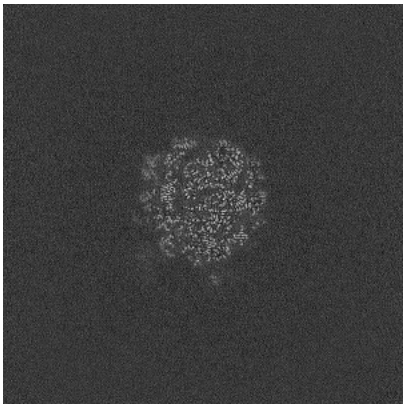
6.3.2 Raw map



X Index: 260



Y Index: 267

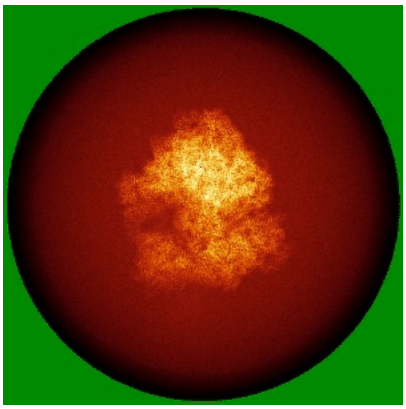


Z Index: 298

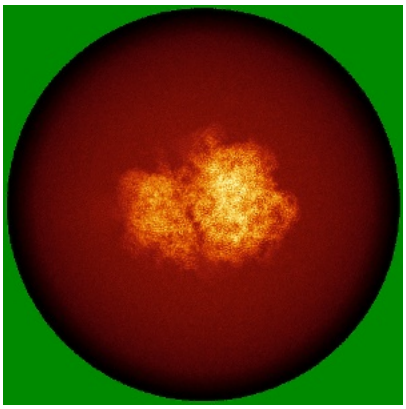
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

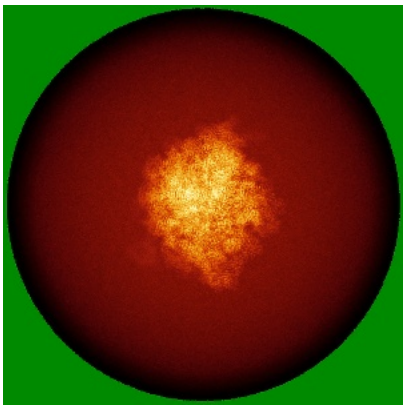
6.4.1 Primary map



X

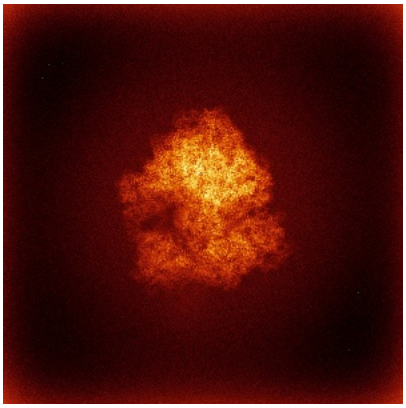


Y

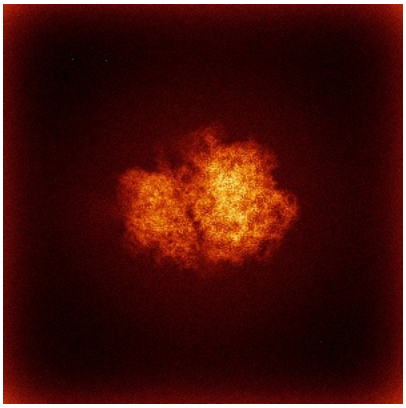


Z

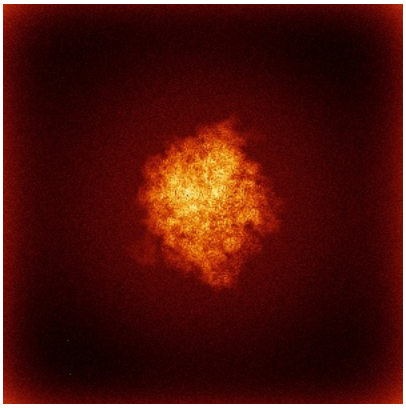
6.4.2 Raw map



X



Y

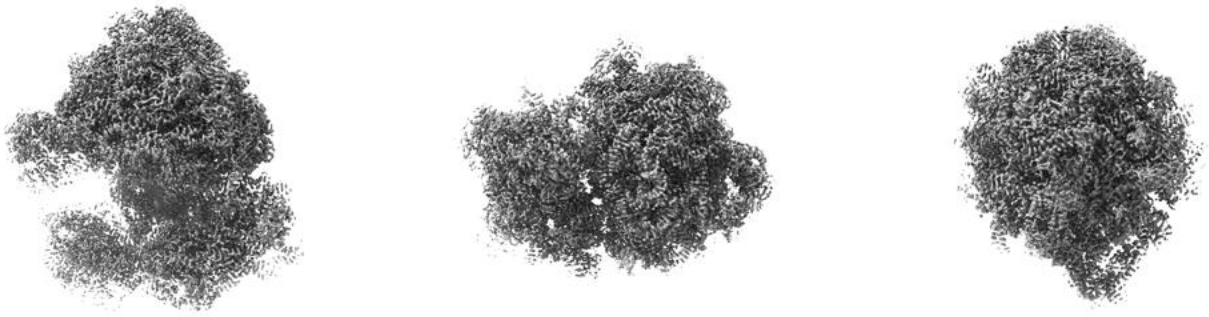


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

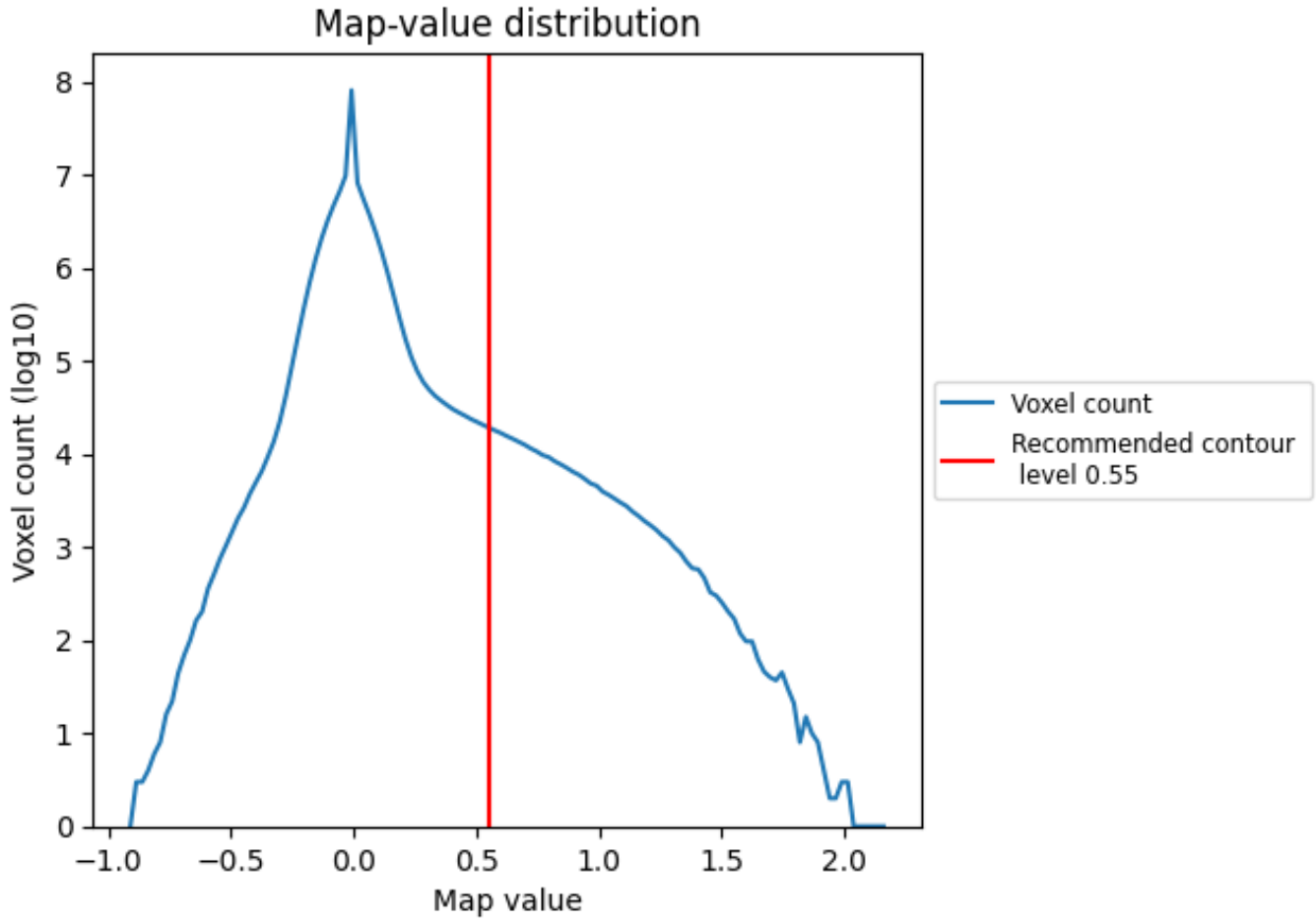
6.6 Mask visualisation (i)

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

7 Map analysis

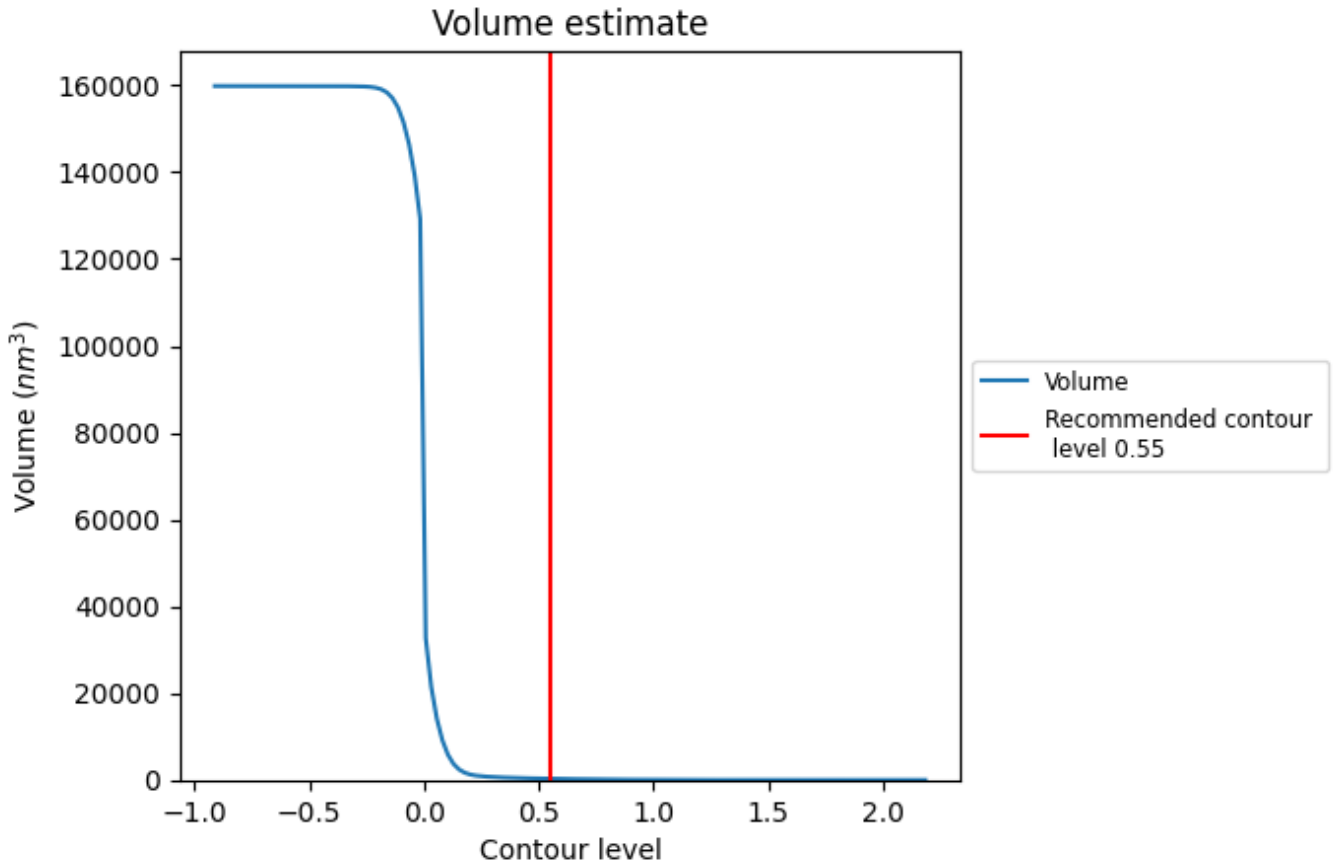
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

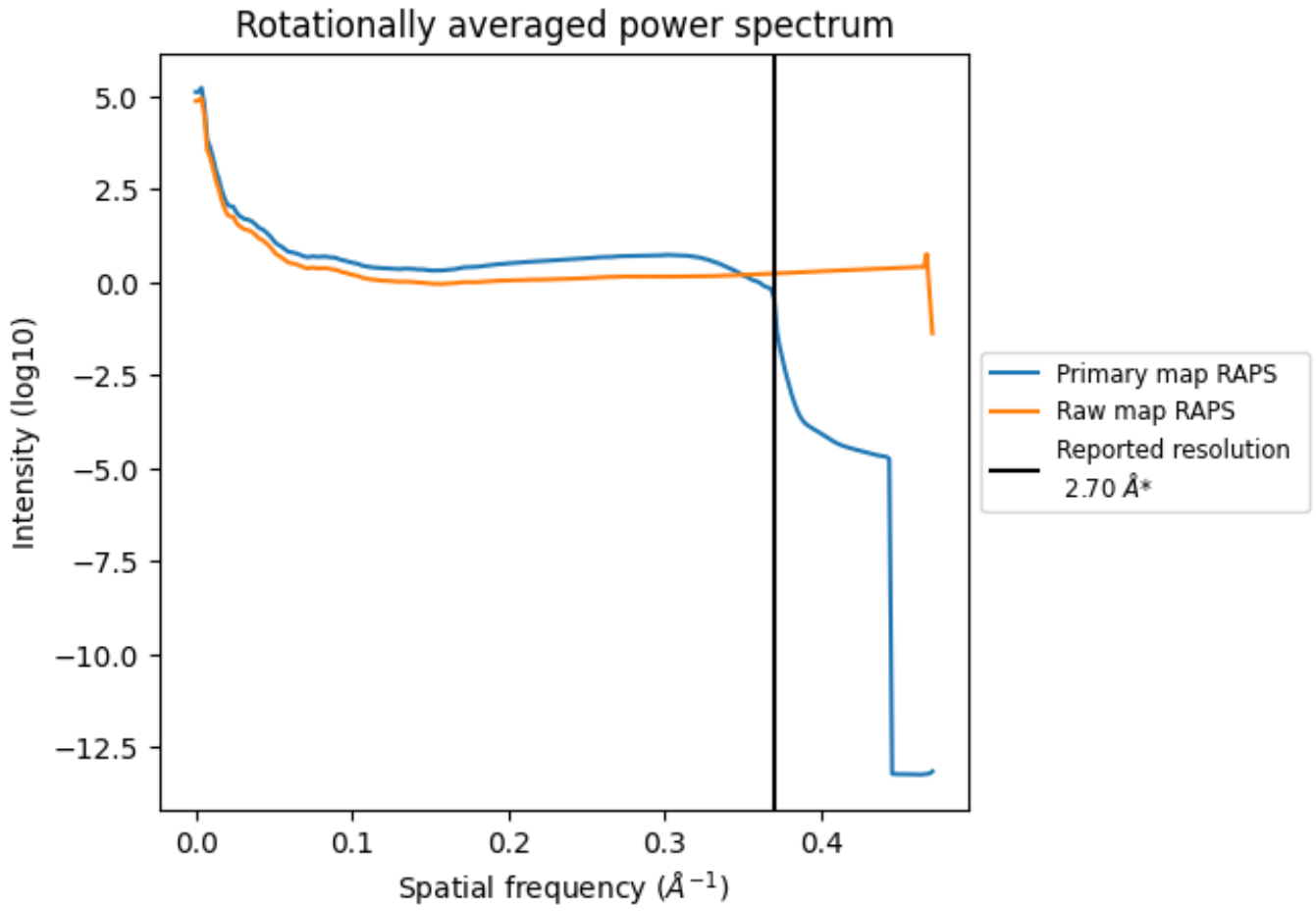
7.2 Volume estimate (i)



The volume at the recommended contour level is 283 nm^3; this corresponds to an approximate mass of 256 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)

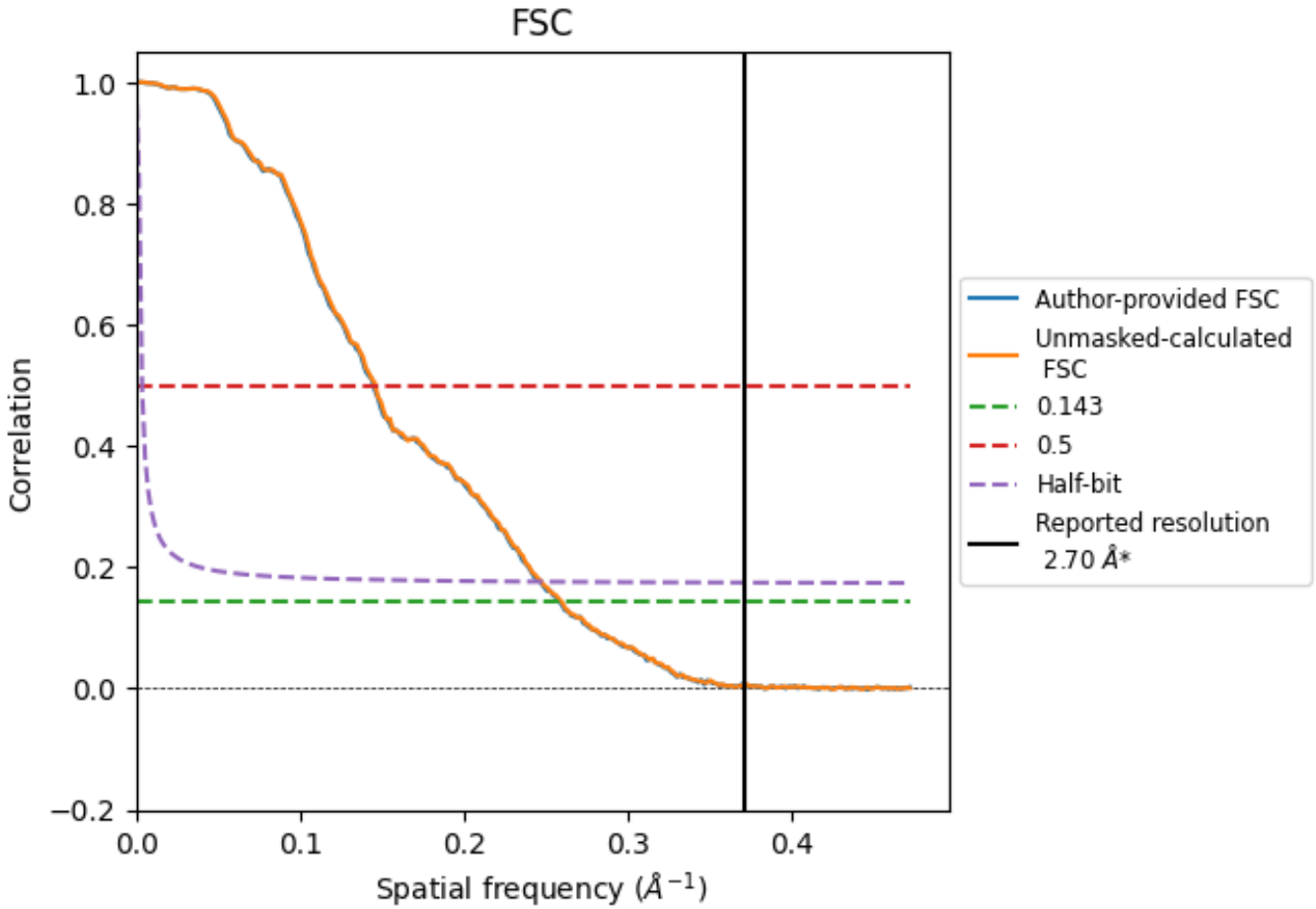


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	3.87	6.91	4.06
Unmasked-calculated*	3.86	6.85	4.05

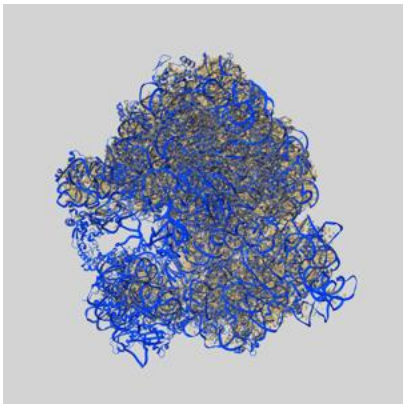
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.7 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 2.7 by more than 10 %

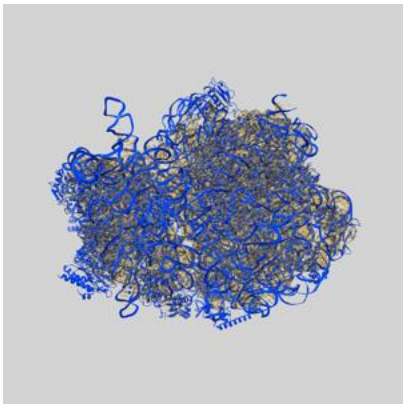
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55797 and PDB model 9TCR. Per-residue inclusion information can be found in section 3 on page 15.

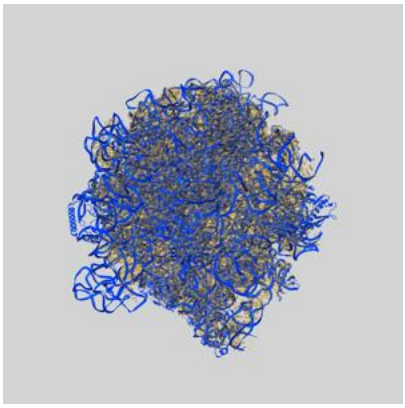
9.1 Map-model overlay



X



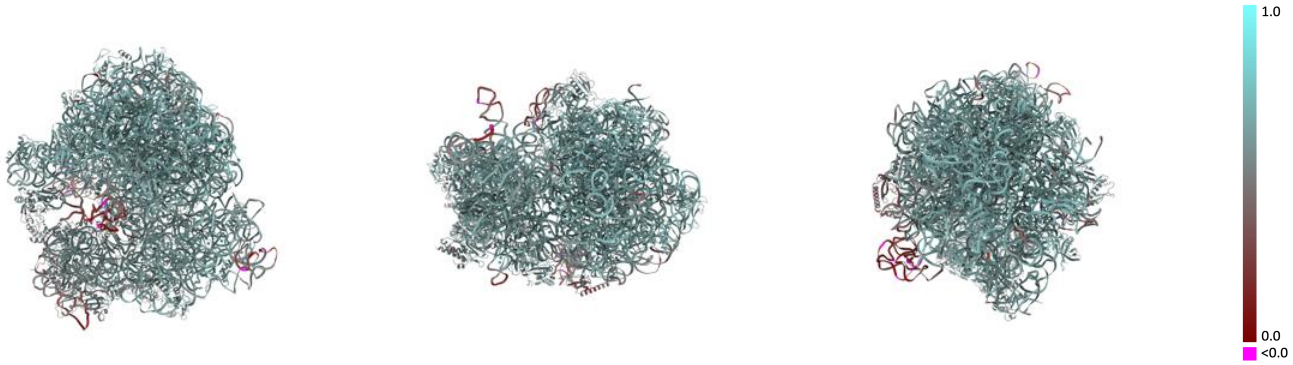
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

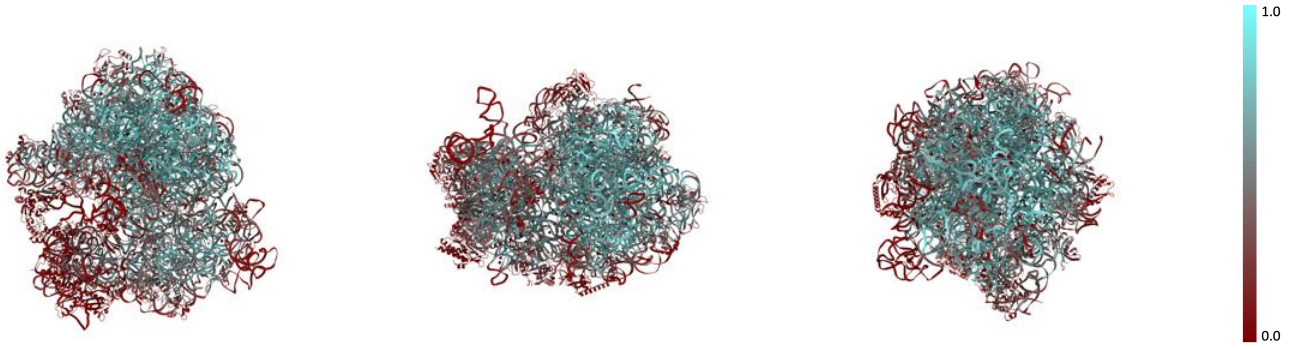
9.2 Q-score mapped to coordinate model (i)



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.

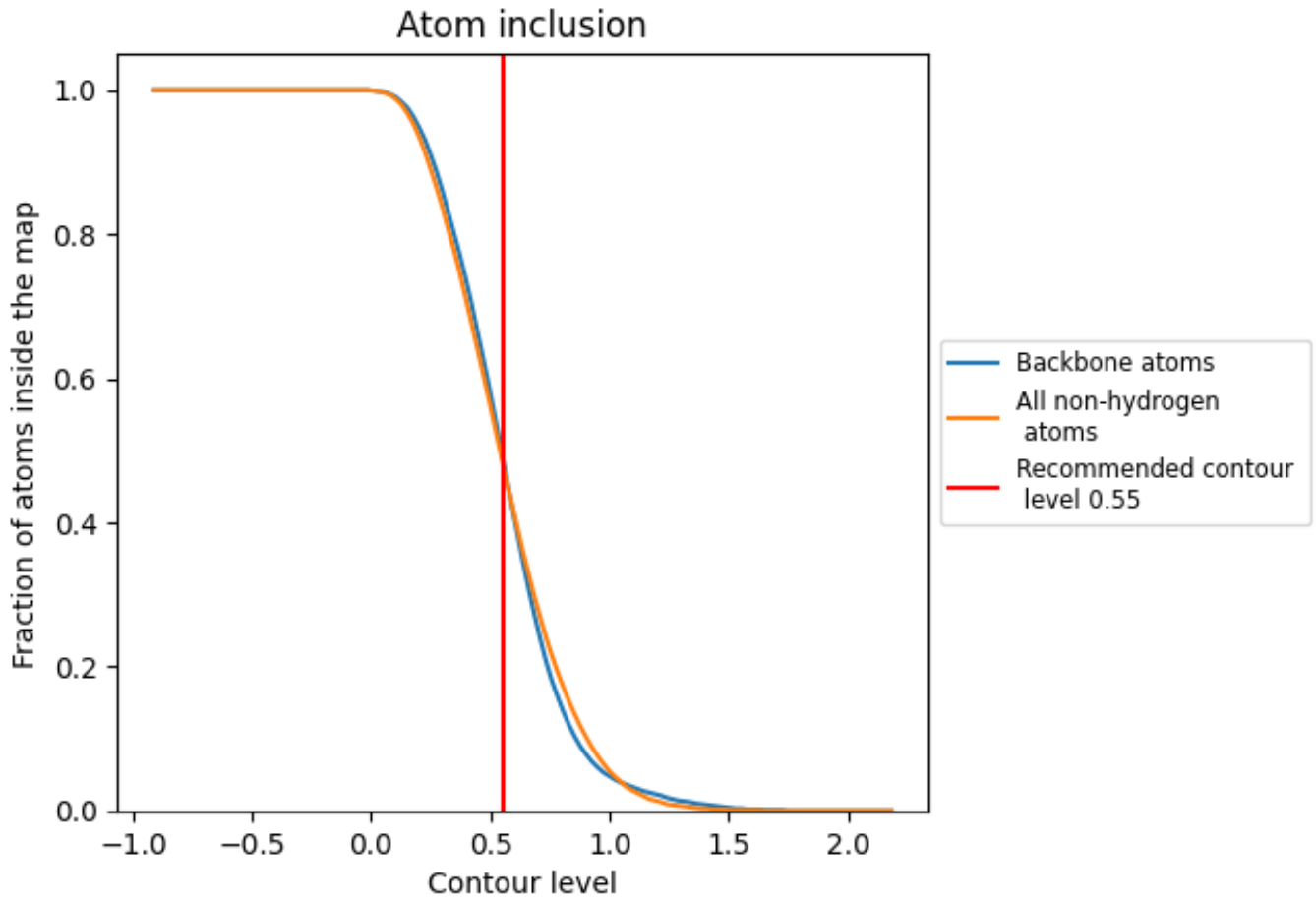
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 48% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.5980
0	0.2980	0.6200
1	0.6700	0.6580
2	0.6520	0.6550
3	0.4330	0.6380
4	0.0060	0.4420
A	0.4450	0.5890
B	0.0490	0.5240
C	0.1540	0.5710
D	0.1950	0.5940
E	0.3890	0.6160
F	0.1820	0.5800
G	0.0420	0.5450
H	0.3840	0.6240
I	0.0760	0.5420
J	0.0860	0.5170
K	0.2210	0.5900
L	0.3290	0.6170
M	0.0300	0.5340
N	0.1100	0.5620
O	0.3350	0.6090
P	0.3860	0.6160
Q	0.2770	0.5970
R	0.2950	0.5630
S	0.0210	0.5300
T	0.2970	0.5990
U	0.0250	0.4730
X	0.0770	0.5610
a	0.6280	0.6060
b	0.4280	0.5980
c	0.5860	0.6500
d	0.5510	0.6400
e	0.4100	0.6210
f	0.0670	0.5390
g	0.1210	0.5600



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Chain	Atom inclusion	Q-score
h	0.0100	0.4370
i	0.5620	0.6410
j	0.4720	0.6390
k	0.4970	0.6390
l	0.4430	0.6360
m	0.6260	0.6490
n	0.2800	0.5990
o	0.4800	0.6350
p	0.6170	0.6450
q	0.4530	0.6260
r	0.5370	0.6340
s	0.4160	0.6220
t	0.3310	0.6070
u	0.3270	0.6120
v	0.5730	0.6470
w	0.4750	0.6350
x	0.2890	0.6010
y	0.4800	0.6330
z	0.5330	0.6330