wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 01:29 pm GMT

PDB ID	:	6SPG
EMDB ID	:	EMD-10285
Title	:	Pseudomonas aeruginosa 70s ribosome from a clinical isolate
Authors	:	Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen, H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin, S.; Yonath, A.
Deposited on	:	2019-09-01
Resolution	:	3.34 Å(reported)

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

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

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

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

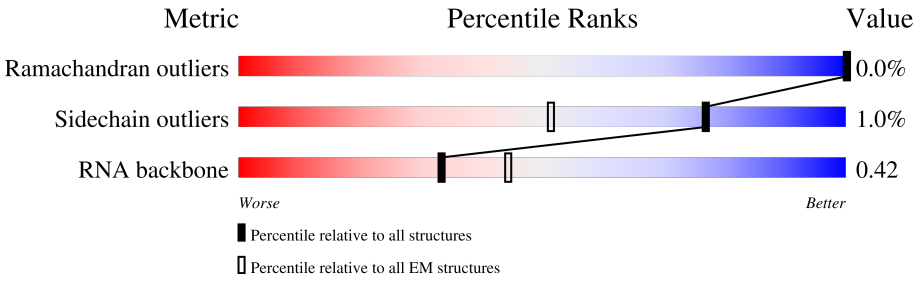
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1526	5% 74% 25%
2	b	239	94% 97%
3	c	205	45% 100%
4	d	205	22% 99%
5	e	156	13% 98%
6	f	105	32% 99%
7	g	154	80% 99%
8	h	129	11% 100%

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Mol	Chain	Length	Quality of chain
9	i	126	60% 98%
10	j	96	68% 96%
11	k	115	21% 100%
12	l	121	18% 98%
13	m	110	68% 96%
14	n	98	44% 100%
15	o	86	15% 100%
16	p	78	10% 100%
17	q	76	16% 96%
18	r	71	34% 97%
19	s	80	72% 99%
20	t	85	7% 99%
21	u	63	63% 97%
22	A	2888	6% 67% 30%
23	B	117	74% 24%
24	C	271	6% 100%
25	D	207	7% 98%
26	E	199	10% 100%
27	F	174	35% 99%
28	G	173	21% 99%
29	H	78	94% 100%
30	I	140	99% 99%
31	J	141	5% 99%
32	K	120	22% 99%
33	L	143	10% 99%

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Mol	Chain	Length	Quality of chain
34	M	135	10% 100%
35	N	118	100%
36	O	115	15% 100%
37	P	113	17% 100%
38	Q	117	100%
39	R	102	9% 98%
40	S	109	8% 100%
41	T	92	10% 100%
42	U	103	18% 99%
43	V	188	28% 99%
44	W	76	7% 97%
45	X	77	12% 97%
46	Y	60	10% 100%
47	Z	57	9% 100%
48	1	31	65% 100%
49	2	53	9% 100%
50	3	50	28% 100%
51	4	44	5% 98%
52	5	63	100%
53	6	38	5% 100%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 141963 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1526	32744	14606	6011	10602	1525	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	72	A	G	conflict	GB 1353913695

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	234	1822	1145	329	338	10	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	205	1627	1028	307	287	5	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1603	991	311	296	5	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	156	1145	720	209	210	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	105	Total	C	N	O	S	0	0
			853	531	158	159	5		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	154	Total	C	N	O	S	0	0
			1190	747	227	211	5		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	126	Total	C	N	O	S	0	0
			994	616	198	179	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	96	Total	C	N	O	S	0	0
			765	479	143	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total	C	N	O	S	0	0
			838	517	163	156	2		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			949	582	196	167	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	110	Total	C	N	O	S	0	0
			859	524	174	157	4		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	98	Total	C	N	O	S	0	0
			778	479	163	133	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	86	Total	C	N	O	S	0	0
			686	425	134	126	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	p	78	Total	C	N	O	0	0
			610	381	121	108		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	76	Total	C	N	O	S	0	0
			619	387	120	110	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	71	Total	C	N	O	S	0	0
			556	355	103	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	9	ARG	LYS	conflict	UNP A0A2V3DLV3

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	80	Total	C	N	O	S	0	0
			635	405	121	106	3		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			655	404	135	114	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	62	Total	C	N	O	S	0	0
			519	320	112	86	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	28	ALA	VAL	conflict	UNP A0A069QC99

- Molecule 22 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2883	Total	C	N	O	P	0	0
			61859	27600	11347	20030	2882		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	A	G	conflict	REF 470469287
A	2872	G	U	conflict	REF 470469287

- Molecule 23 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	117	Total	C	N	O	P	0	0
			2495	1114	448	816	117		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	271	Total	C	N	O	S	0	0
			2048	1258	422	362	6		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	207	Total	C	N	O	S	0	0
			1549	960	297	287	5		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	199	Total	C	N	O	S	0	0
			1509	948	281	278	2		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	174	Total	C	N	O	S	0	0
			1288	811	228	246	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	7	LEU	ILE	conflict	UNP A0A072ZMU2

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	173	Total	C	N	O	S	0	0
			1294	815	238	239	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	H	78	Total	C	N	O	0	0
			577	363	104	110		

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	140	Total	C	N	O	S	0	0
			1026	642	183	198	3		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J	141	Total	C	N	O	S	0	0
			1122	713	205	201	3		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	120	Total	C	N	O	S	0	0
			922	576	178	162	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	143	Total	C	N	O	S	0	0
			1055	648	213	192	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	135	Total	C	N	O	S	0	0
			1069	679	209	178	3		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	118	Total	C	N	O	S	0	0
			945	590	190	160	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	113	Total	C	N	O	S	0	0
			891	563	168	159	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Q	117	Total	C	N	O	0	0
			936	592	196	148		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	102	Total	C	N	O	S	0	0
			801	509	154	136	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S	109	Total	C	N	O	S	0	0
			825	510	160	152	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	T	92	Total	C	N	O	0	0
			701	449	124	128		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U	103	Total	C	N	O	S	0	0
			801	503	152	144	2		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V	188	Total	C	N	O	S	0	0
			1397	888	254	253	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	6	VAL	LEU	conflict	UNP A0A072ZBM5
V	71	VAL	ALA	conflict	UNP A0A072ZBM5

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	W	76	Total	C	N	O	0	0
			574	365	110	99		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	40	LEU	GLN	conflict	UNP A0A071LFT4

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	77	Total	C	N	O	S	0	0
			626	389	134	101	2		

- Molecule 46 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	60	Total	C	N	O	S	0	0
			468	286	96	85	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	31	Total	C	N	O	S	0	0
			232	144	40	45	3		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	53	Total	C	N	O	S	0	0
			423	254	90	78	1		

- Molecule 50 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	3	50	Total	C	N	O	0	0
			418	267	77	74		

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	44	Total	C	N	O	S	1	0
			376	228	91	55	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	5	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	38	Total	C	N	O	S	0	0
			303	184	69	46	4		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

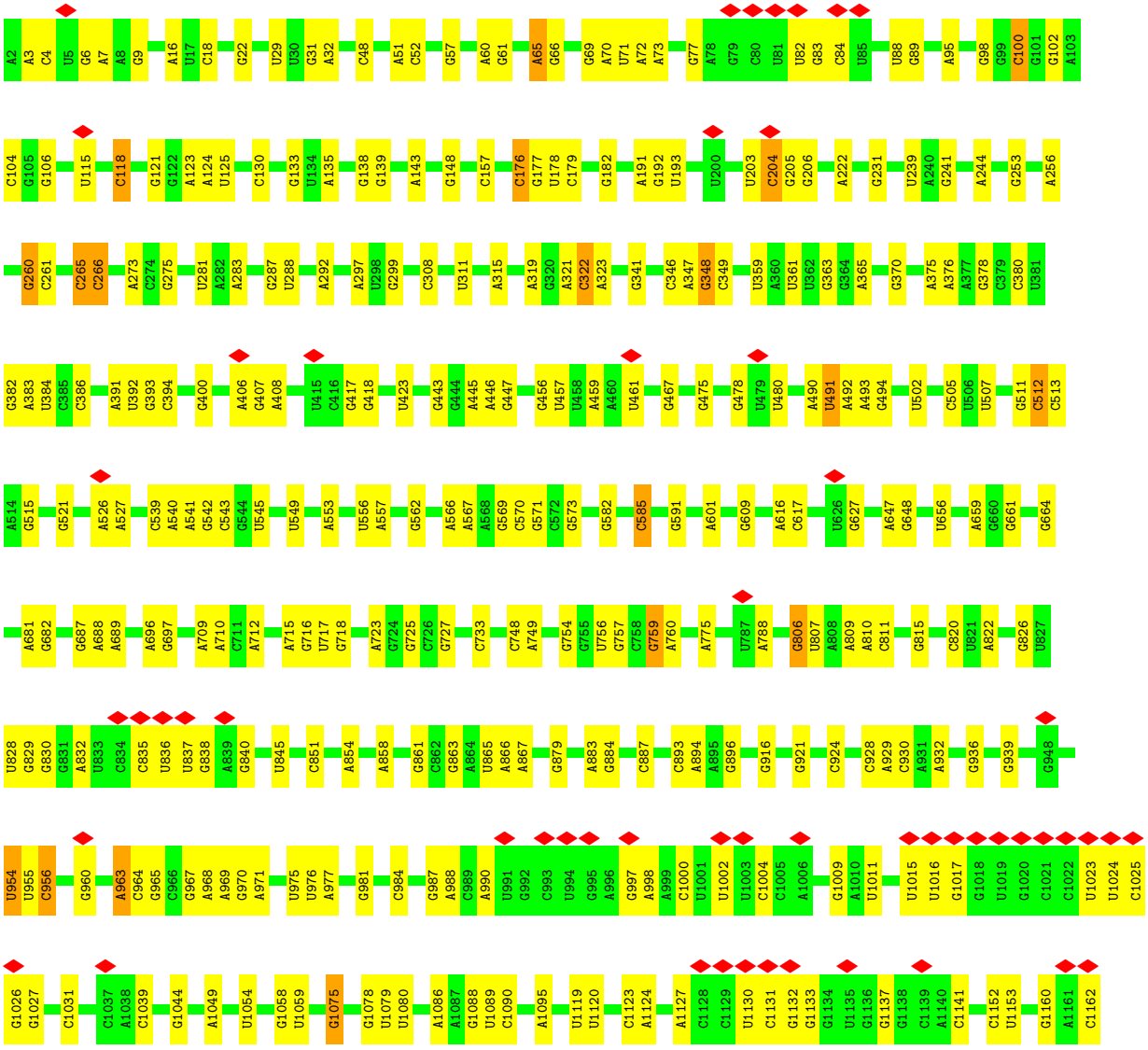
Mol	Chain	Residues	Atoms		AltConf
54	a	17	Total	Mg	0
			17	17	
54	A	152	Total	Mg	0
			152	152	
54	B	1	Total	Mg	0
			1	1	
54	D	1	Total	Mg	0
			1	1	
54	P	1	Total	Mg	0
			1	1	

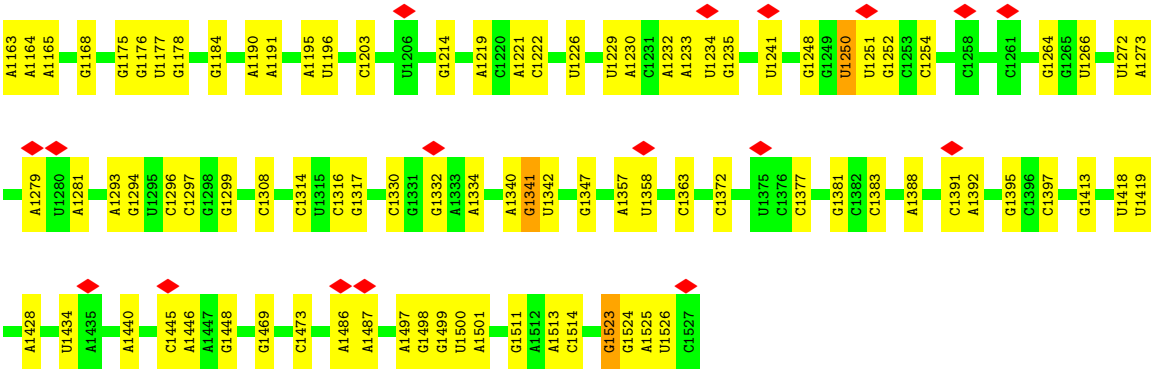
3 Residue-property plots (i)

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: 16S ribosomal RNA

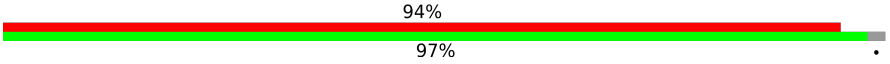
Chain a:

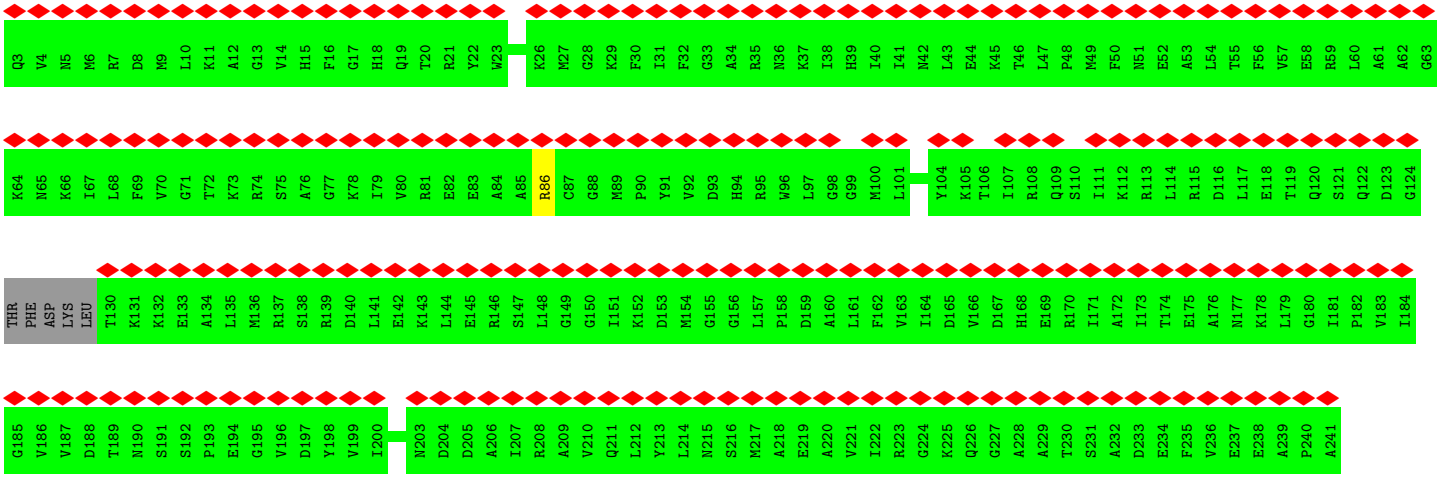




• Molecule 2: 30S ribosomal protein S2

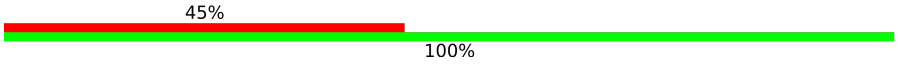
Chain b:

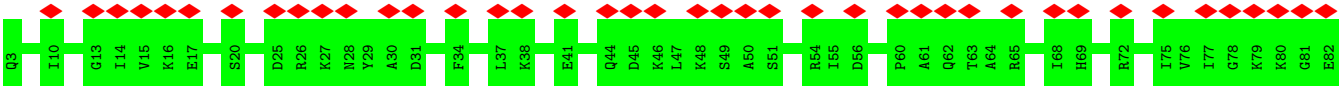


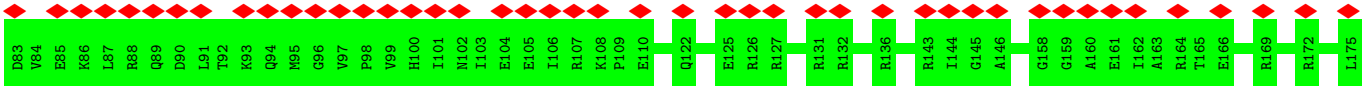


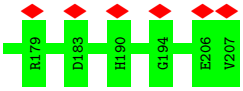
• Molecule 3: 30S ribosomal protein S3

Chain c:



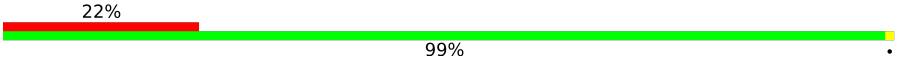


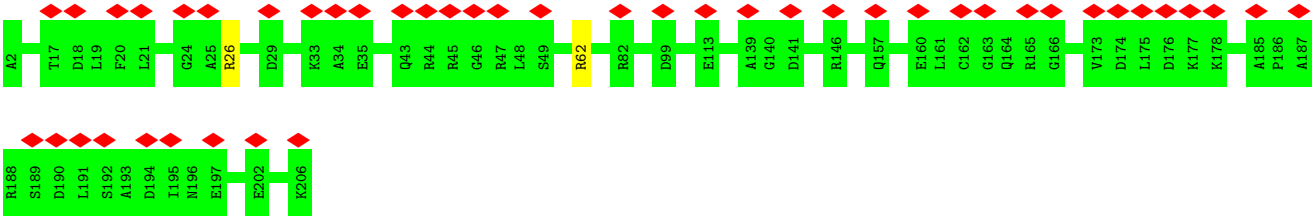




• Molecule 4: 30S ribosomal protein S4

Chain d:

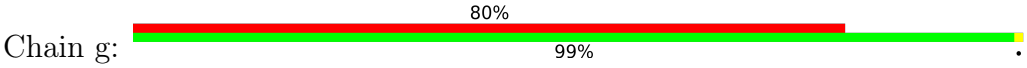




• Molecule 5: 30S ribosomal protein S5

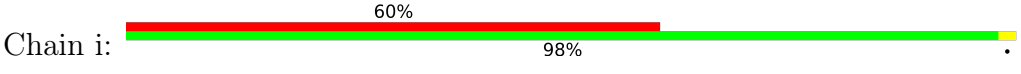
• Molecule 6: 30S ribosomal protein S6

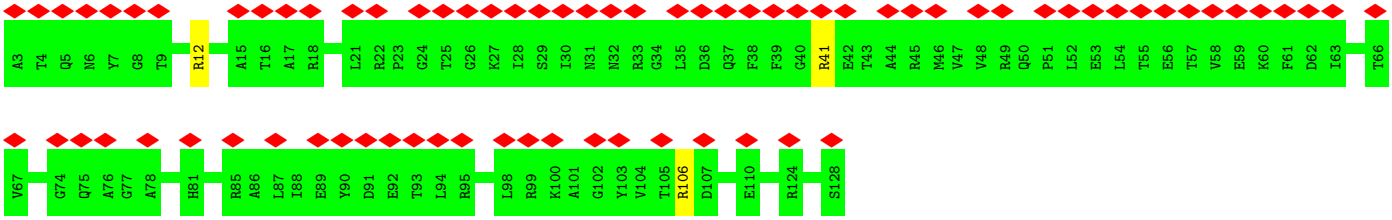
• Molecule 7: 30S ribosomal protein S7



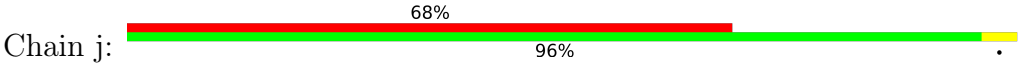
• Molecule 8: 30S ribosomal protein S8

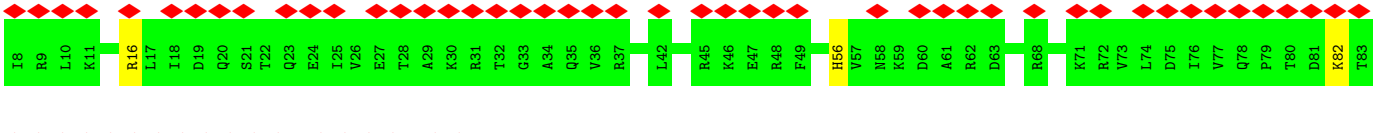
• Molecule 9: 30S ribosomal protein S9



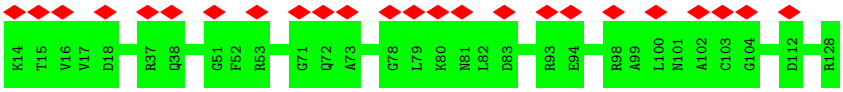


• Molecule 10: 30S ribosomal protein S10

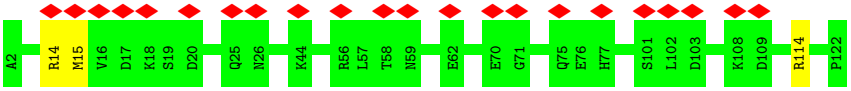




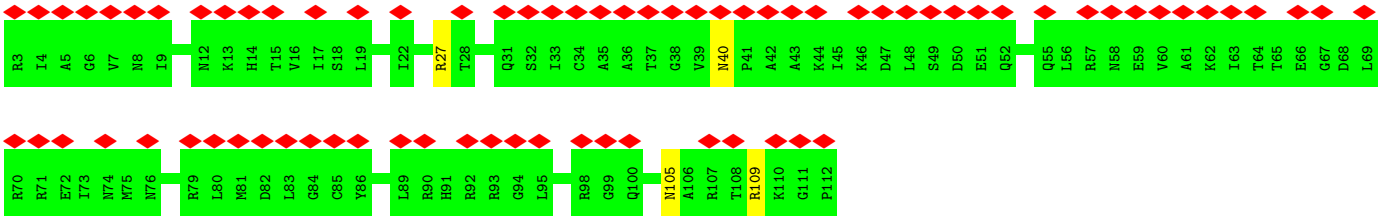
• Molecule 11: 30S ribosomal protein S11



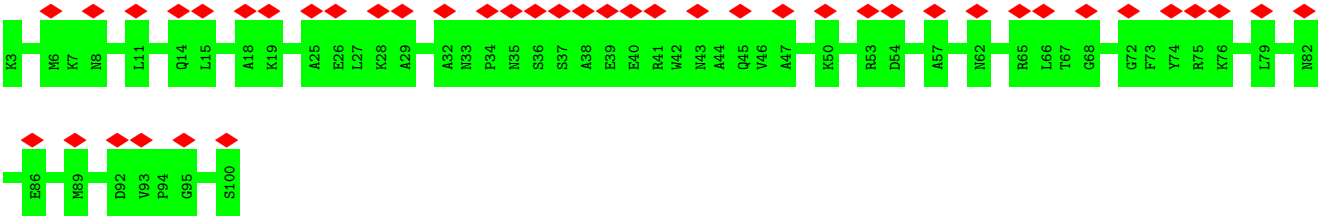
• Molecule 12: 30S ribosomal protein S12



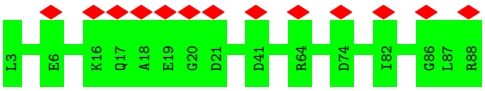
• Molecule 13: 30S ribosomal protein S13



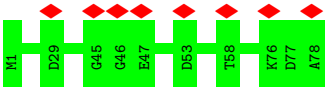
• Molecule 14: 30S ribosomal protein S14



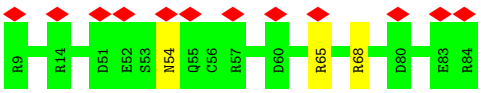
• Molecule 15: 30S ribosomal protein S15



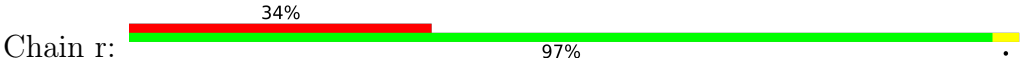
• Molecule 16: 30S ribosomal protein S16

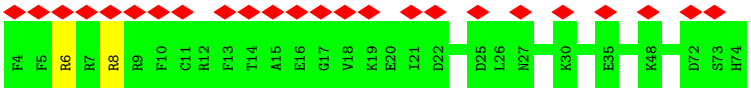


• Molecule 17: 30S ribosomal protein S17

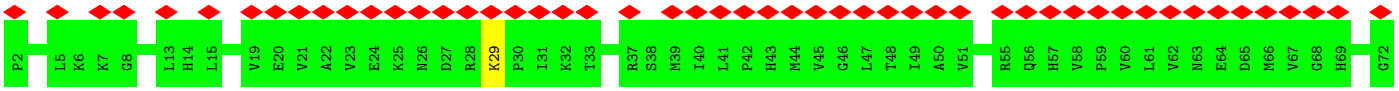


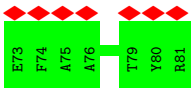
• Molecule 18: 30S ribosomal protein S18





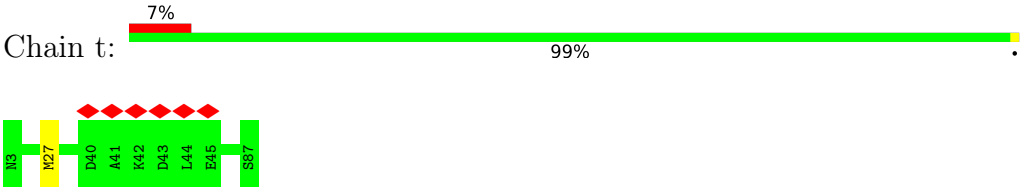
• Molecule 19: 30S ribosomal protein S19





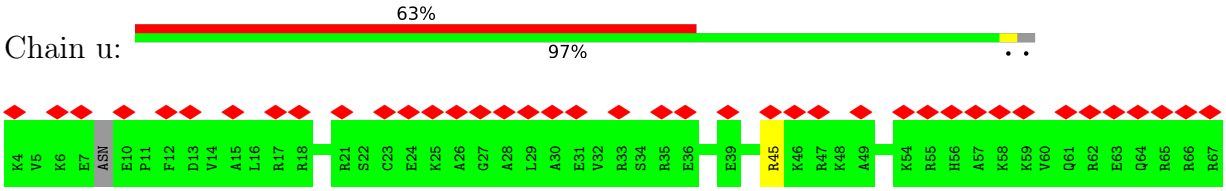
• Molecule 20: 30S ribosomal protein S20

Chain t:



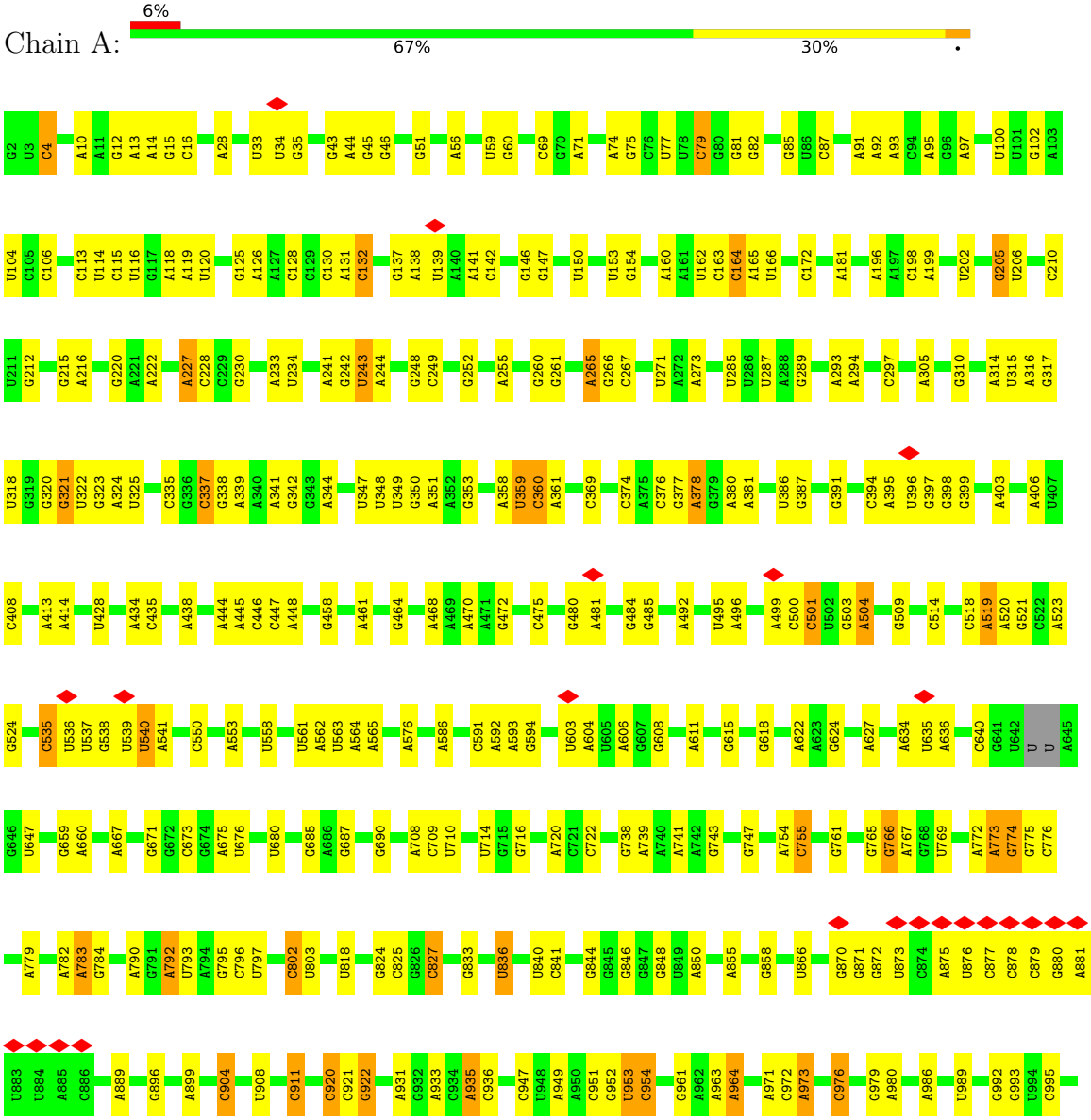
• Molecule 21: 30S ribosomal protein S21

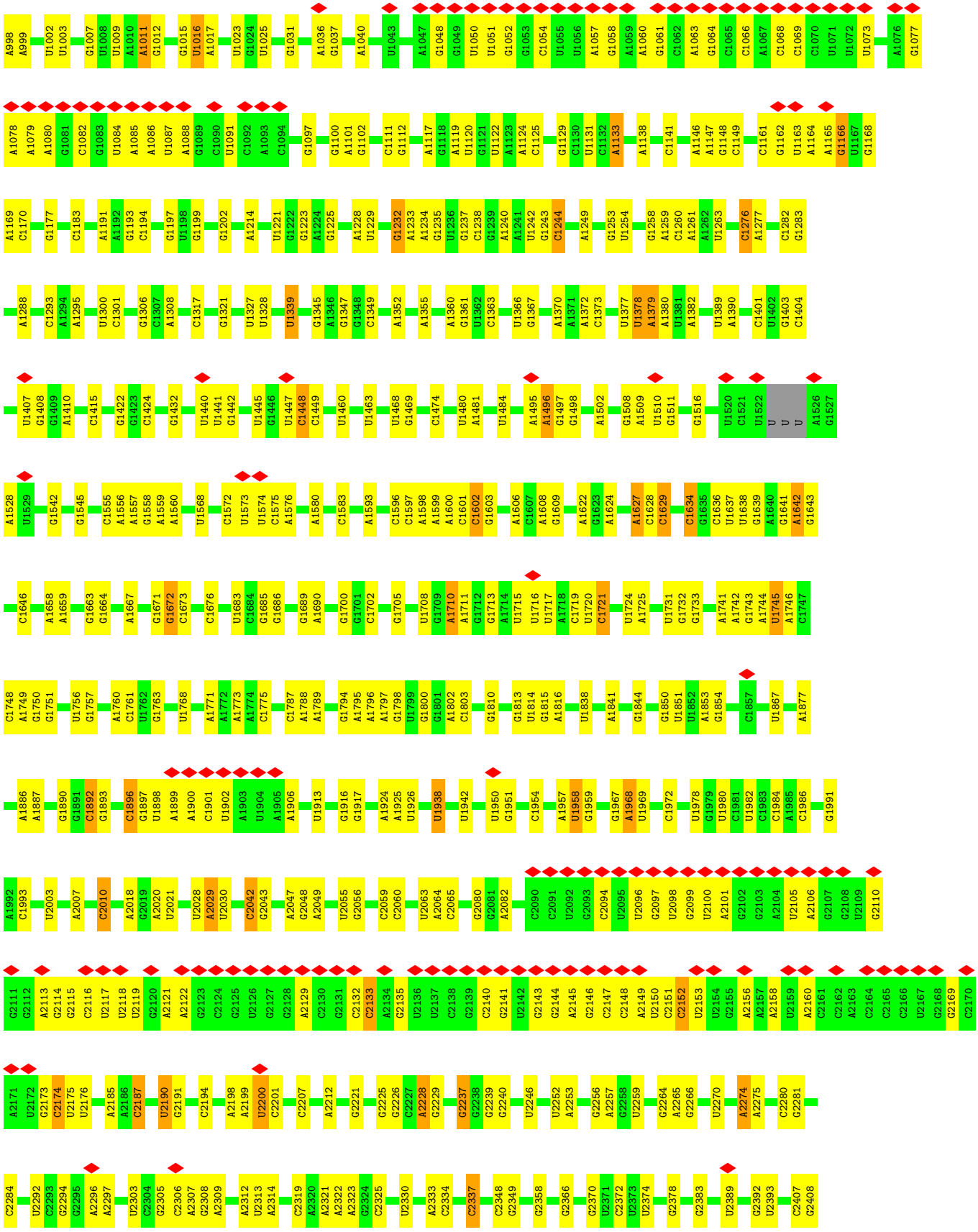
Chain u:



• Molecule 22: 23S ribosomal RNA

Chain A:




A998 A999 U1002 U1003 G1007 U1008 U1009 A1010 A1011 G1012 G1015 U1016 A1017 U1023 G1024 U1025 G1031 A1036 G1037 A1040 U1043 A1047 G1048 G1049 U1050 U1051 G1052 G1053 C1054 U1055 U1056 A1057 G1058 A1059 A1060 G1061 C1062 A1063 G1064 C1065 C1066 A1067 C1068 C1069 C1070 U1071 U1072 U1073 A1076 G1077
A1078 A1079 A1080 G1081 C1082 G1083 U1084 A1085 A1086 U1087 A1088 G1089 C1090 U1091 C1092 A1093 C1094 G1097 G1100 A1101 G1102 C1111 G1112 A1117 G1118 A1119 U1120 G1121 U1122 A1123 A1124 C1125 G1129 C1130 U1131 C1132 A1133 A1138 C1141 A1146 A1147 G1148 C1149 C1161 G1162 U1163 A1164 A1165 G1166 U1167 G1168
A1169 C1170 G1177 C1183 A1191 A1192 G1193 C1194 G1197 U1198 G1199 G1202 A1214 U1221 G1222 G1223 A1224 G1225 A1228 U1229 G1232 A1233 A1234 G1235 U1236 G1237 C1238 G1239 A1240 A1241 U1242 G1243 C1244 A1249 G1253 U1254 G1258 A1259 C1260 A1261 A1262 U1263 C1276 A1277 C1282 G1283
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U1407 G1408 G1409 A1410 C1415 G1422 G1423 C1424 G1432 U1440 U1441 G1442 U1445 G1446 U1447 C1448 C1449 U1460 U1463 U1468 G1469 C1474 U1480 A1481 U1484 A1495 A1496 G1497 G1498 A1502 G1508 A1509 U1510 G1511 G1516 U1520 C1521 U1522 U U U A1526 G1527
A1528 U1529 G1542 G1545 C1555 A1556 A1557 G1558 A1559 A1560 U1568 C1572 U1573 U1574 C1575 A1576 A1580 C1583 A1593 C1596 C1597 A1598 A1599 A1600 C1601 C1602 G1603 A1606 C1607 A1608 G1609 A1622 G1623 A1624 A1627 C1628 C1629 C1634 G1635 C1636 U1637 U1638 G1639 A1640 G1641 A1642 G1643
C1646 A1658 A1659 G1663 G1664 A1667 G1671 G1672 C1673 C1676 U1683 C1684 G1685 G1686 G1689 A1690 G1700 G1701 C1702 G1705 U1708 G1709 A1710 A1711 G1712 G1713 A1714 U1715 U1716 U1717 A1718 C1719 U1720 C1721 U1724 A1725 U1731 G1732 G1733 A1741 A1742 G1743 A1744 U1745 A1746 C1747
C1748 A1749 G1750 G1751 U1756 G1757 A1760 C1761 U1762 G1763 U1768 A1771 A1772 A1773 A1774 C1775 C1787 A1788 A1789 G1794 A1795 A1796 A1797 G1798 U1799 G1800 G1801 A1802 C1803 G1810 G1813 U1814 G1815 A1816 U1838 A1841 G1844 G1850 U1851 U1852 A1853 G1854 C1857 U1867 A1877
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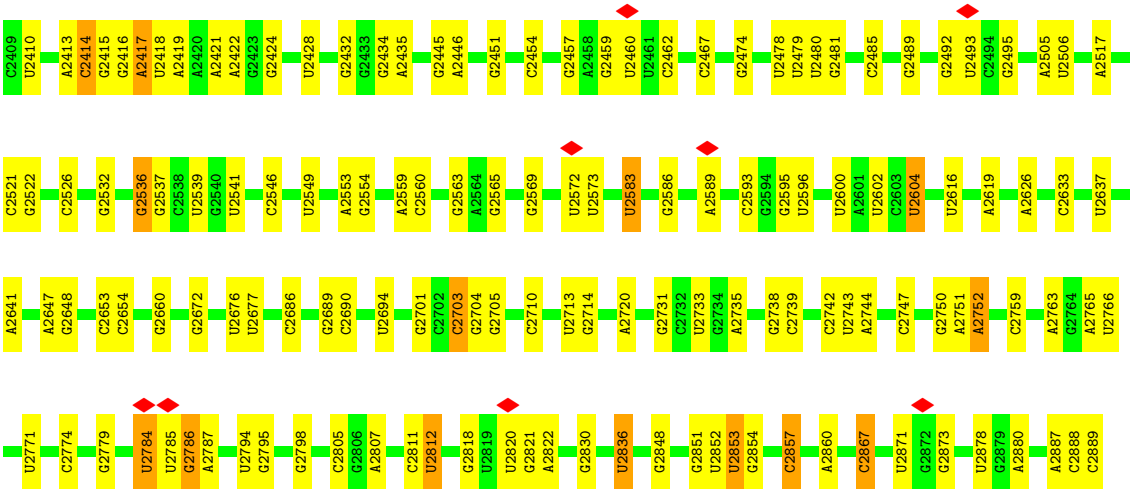
A1992 C1993 U2003 A2007 C2010 A2018 G2019 A2020 U2021 U2028 A2029 U2030 C2042 G2043 A2047 G2048 A2049 U2055 G2056 C2059 C2060 U2063 A2064 C2065 G2080 G2081 A2082 C2090 C2091 U2092 G2093 C2094 U2095 U2096 G2097 U2098 G2099 U2100 A2101 G2102 G2103 A2104 U2105 A2106 G2107 G2108 U2109 G2110
G2111 C2112 A2113 G2114 G2115 C2116 U2117 U2118 U2119 G2120 A2121 A2122 G2123 C2124 G2125 U2126 G2127 G2128 A2129 C2130 G2131 C2132 C2133 A2134 G2135 U2136 U2137 C2138 G2139 C2140 G2141 U2142 G2143 G2144 A2145 G2146 C2147 C2148 A2149 U2150 C2151 C2152 U2153 U2154 C2155 A2156 A2157 A2158 U2159 A2160 C2161 C2162 A2163 C2164 C2165 C2166 U2167 G2168 C2169 C2170
A2171 U2172 G2173 C2174 U2175 U2176 A2185 A2186 C2187 U2190 G2191 C2194 A2198 A2199 U2200 C2201 C2207 A2212 G2221 G2225 G2226 C2227 A2228 G2229 G2237 G2238 G2239 G2240 U2246 U2252 A2253 G2256 A2257 G2258 U2259 G2264 A2265 G2266 U2270 A2274 A2275 C2280 G2281
C2284 U2292 C2293 G2294 G2295 A2296 A2297 U2303 C2304 G2305 C2306 A2307 G2308 A2309 A2312 U2313 A2314 C2319 A2320 A2321 A2322 A2323 G2324 C2325 U2330 A2333 C2334 C2337 C2348 G2349 G2358 G2366 G2370 U2371 C2372 U2373 U2374 G2378 G2383 U2389 G2392 U2393 C2407 G2408

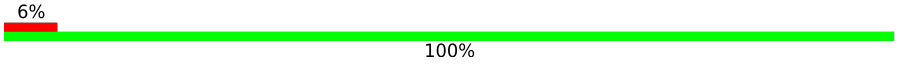


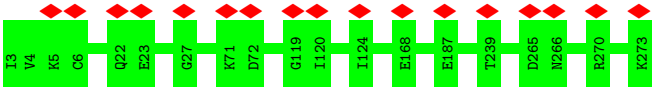
• Molecule 23: 5S ribosomal RNA

Chain B:

• Molecule 24: 50S ribosomal protein L2

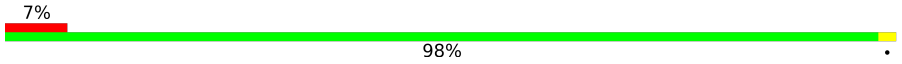
Chain C:

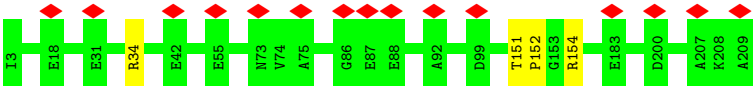




• Molecule 25: 50S ribosomal protein L3

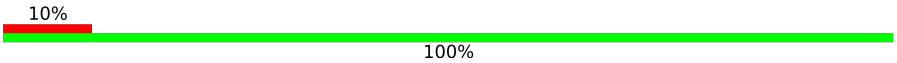
Chain D:

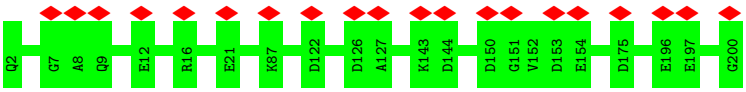




• Molecule 26: 50S ribosomal protein L4

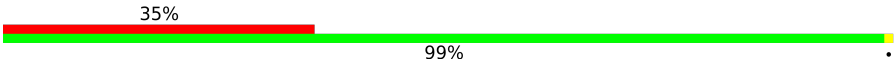
Chain E:

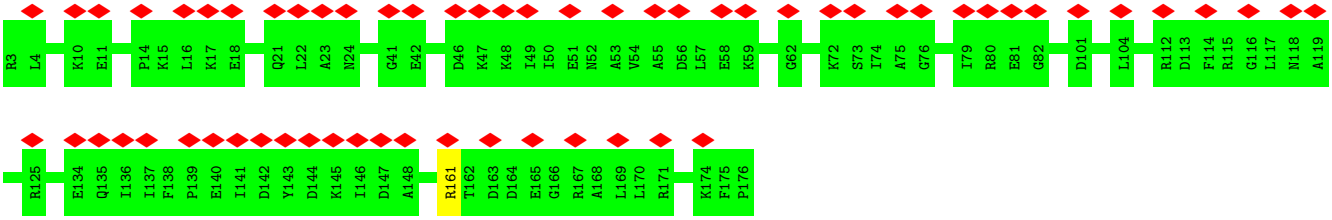




• Molecule 27: 50S ribosomal protein L5

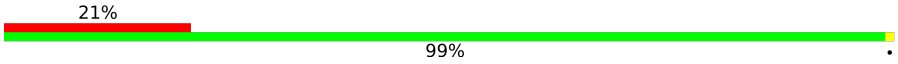
Chain F:

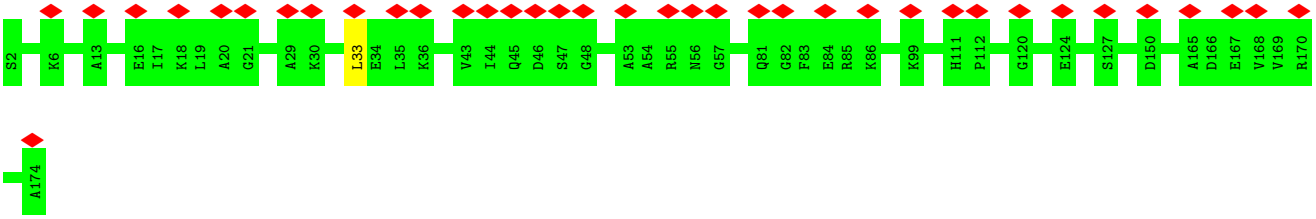




• Molecule 28: 50S ribosomal protein L6

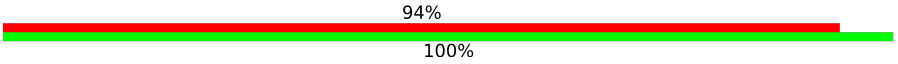
Chain G:

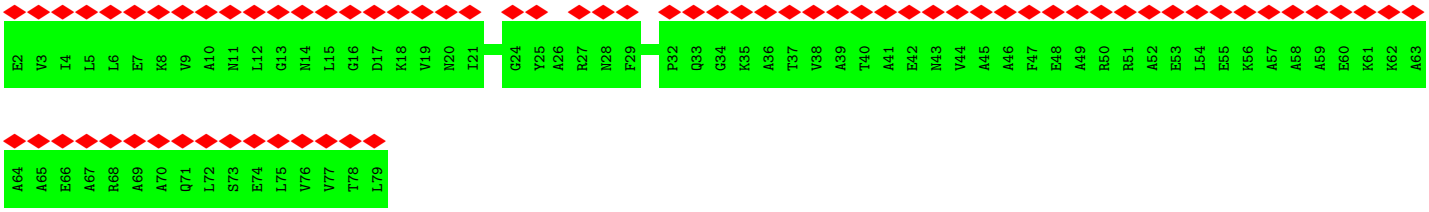




• Molecule 29: 50S ribosomal protein L9

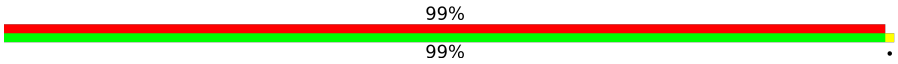
Chain H:

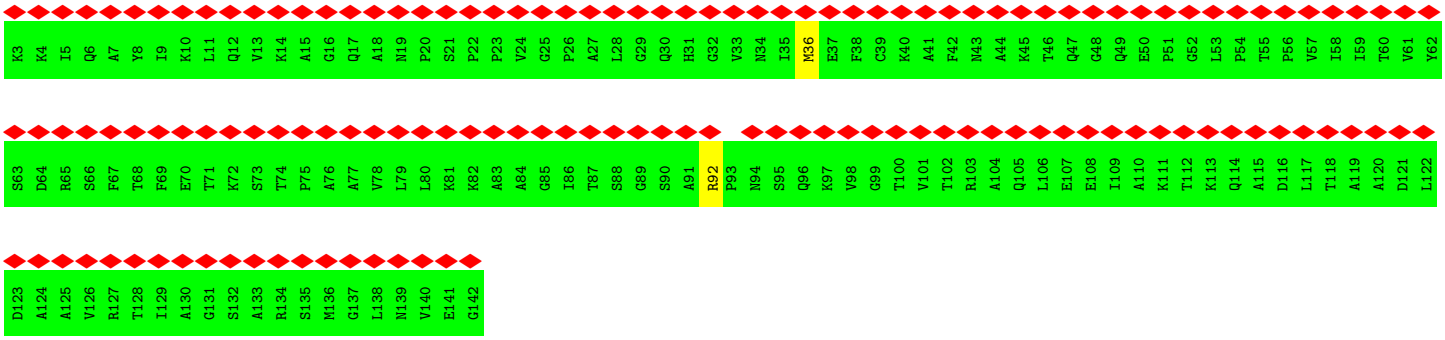




• Molecule 30: 50S ribosomal protein L11

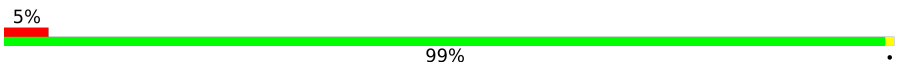
Chain I:

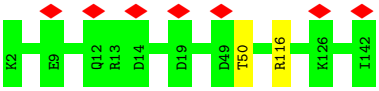




• Molecule 31: 50S ribosomal protein L13

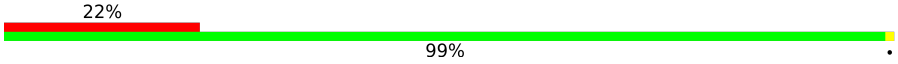
Chain J:

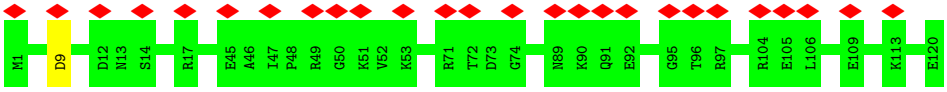




• Molecule 32: 50S ribosomal protein L14

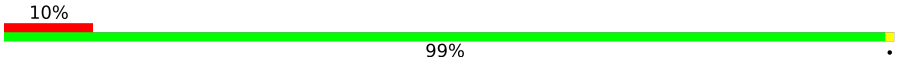
Chain K:

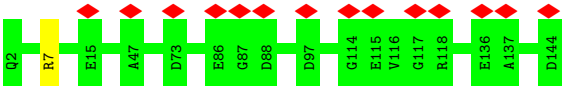




• Molecule 33: 50S ribosomal protein L15

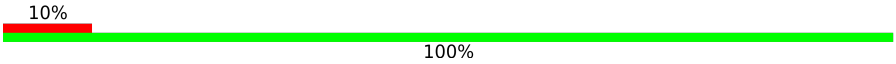
Chain L:

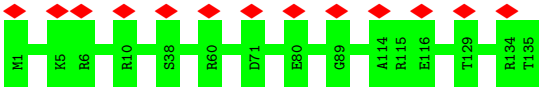




• Molecule 34: 50S ribosomal protein L16

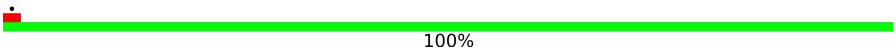
Chain M:

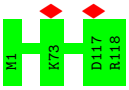




• Molecule 35: 50S ribosomal protein L17

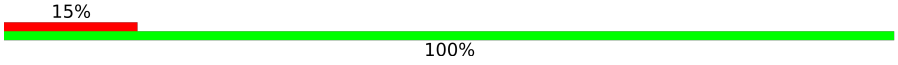
Chain N:

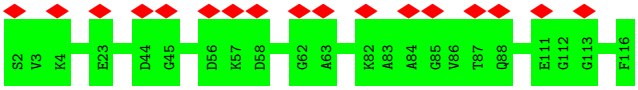




• Molecule 36: 50S ribosomal protein L18

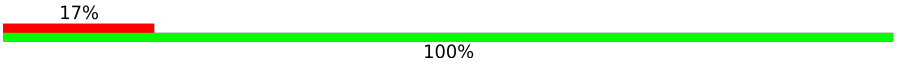
Chain O:

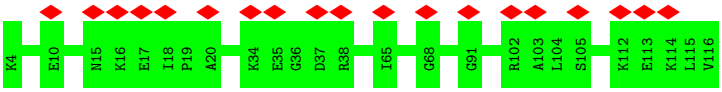




• Molecule 37: 50S ribosomal protein L19

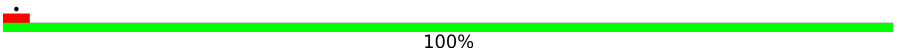
Chain P:

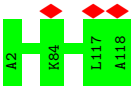




• Molecule 38: 50S ribosomal protein L20

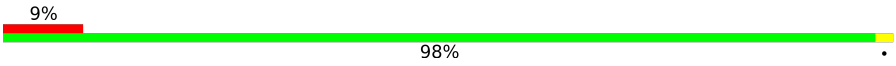
Chain Q:

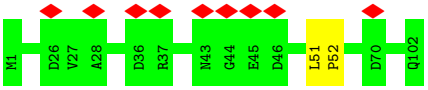




• Molecule 39: 50S ribosomal protein L21

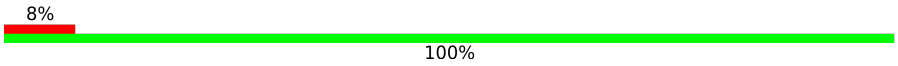
Chain R:

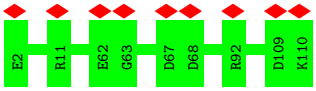




• Molecule 40: 50S ribosomal protein L22

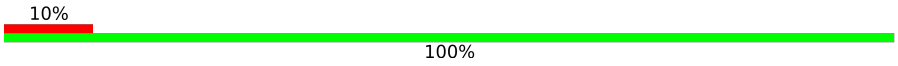
Chain S:

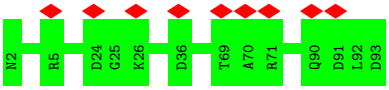




• Molecule 41: 50S ribosomal protein L23

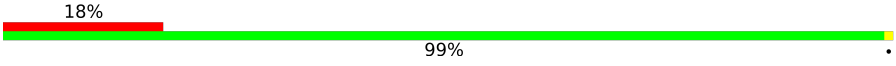
Chain T:

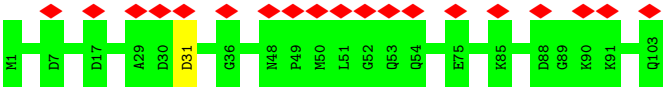




• Molecule 42: 50S ribosomal protein L24

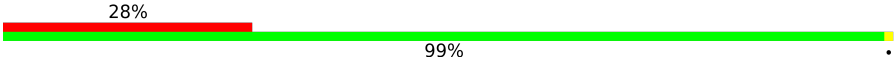
Chain U:

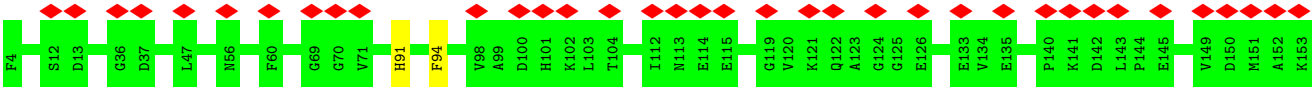


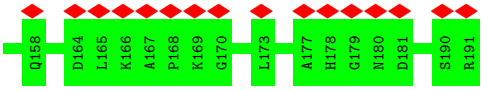


• Molecule 43: 50S ribosomal protein L25

Chain V:

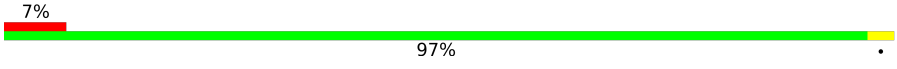


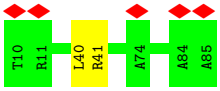




• Molecule 44: 50S ribosomal protein L27

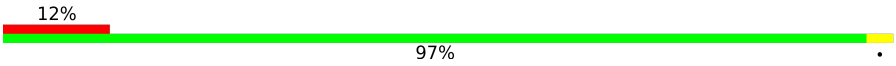
Chain W:

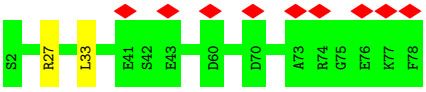




• Molecule 45: 50S ribosomal protein L28

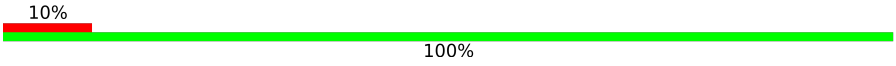
Chain X:

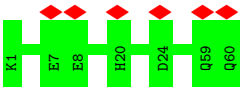




• Molecule 46: Ribosomal protein uL29

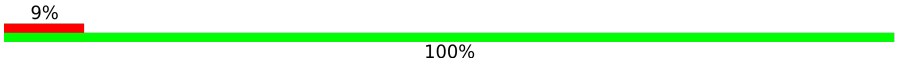
Chain Y:

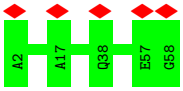




• Molecule 47: 50S ribosomal protein L30

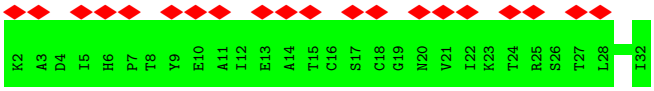
Chain Z:





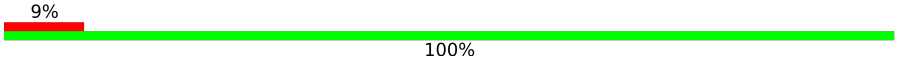
• Molecule 48: 50S ribosomal protein L31

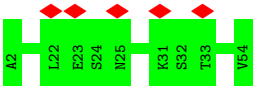
Chain 1:



• Molecule 49: 50S ribosomal protein L32

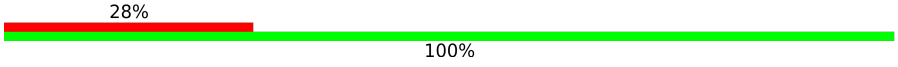
Chain 2:

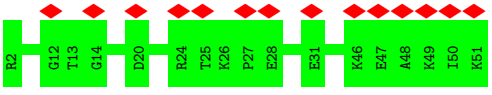




• Molecule 50: 50S ribosomal protein L33

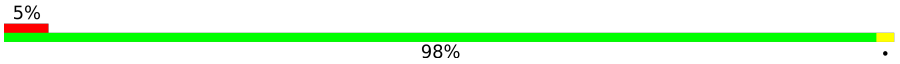
Chain 3:

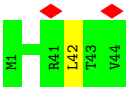




• Molecule 51: 50S ribosomal protein L34

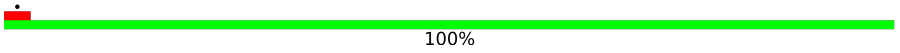
Chain 4:

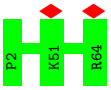




• Molecule 52: 50S ribosomal protein L35

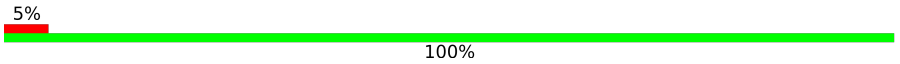
Chain 5:

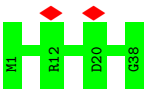




• Molecule 53: 50S ribosomal protein L36

Chain 6:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.474	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0731	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.86	0/36667	1.01	109/57202 (0.2%)
2	b	0.30	0/1850	0.53	0/2486
3	c	0.36	0/1656	0.58	0/2232
4	d	0.40	0/1622	0.55	0/2171
5	e	0.44	0/1159	0.63	0/1559
6	f	0.38	0/867	0.53	0/1167
7	g	0.29	0/1207	0.52	0/1616
8	h	0.42	0/993	0.54	0/1332
9	i	0.37	0/1006	0.57	0/1347
10	j	0.35	0/775	0.58	1/1046 (0.1%)
11	k	0.36	0/854	0.51	0/1159
12	l	0.43	0/963	0.60	0/1292
13	m	0.29	0/867	0.54	0/1165
14	n	0.35	0/788	0.53	0/1048
15	o	0.37	0/693	0.50	0/926
16	p	0.47	0/621	0.57	0/837
17	q	0.44	0/627	0.59	0/844
18	r	0.40	0/566	0.55	0/763
19	s	0.30	0/649	0.54	0/874
20	t	0.35	0/662	0.50	0/881
21	u	0.35	0/524	0.48	0/689
22	A	0.94	3/69275 (0.0%)	1.12	357/108063 (0.3%)
23	B	0.69	0/2789	1.02	7/4345 (0.2%)
24	C	0.39	0/2084	0.58	0/2800
25	D	0.44	0/1572	0.61	0/2118
26	E	0.37	0/1529	0.59	0/2060
27	F	0.30	0/1304	0.58	0/1766
28	G	0.33	0/1311	0.56	0/1767
29	H	0.27	0/580	0.45	0/781
30	I	0.29	0/1041	0.57	0/1408
31	J	0.42	0/1148	0.54	0/1549
32	K	0.38	0/931	0.64	1/1247 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	L	0.36	0/1067	0.62	0/1422
34	M	0.41	0/1089	0.55	0/1456
35	N	0.38	0/960	0.60	0/1282
36	O	0.33	0/888	0.55	0/1183
37	P	0.40	0/900	0.56	0/1203
38	Q	0.45	0/946	0.57	0/1257
39	R	0.36	0/814	0.60	0/1091
40	S	0.35	0/829	0.54	0/1104
41	T	0.39	0/710	0.60	0/953
42	U	0.35	0/809	0.65	1/1079 (0.1%)
43	V	0.35	0/1420	0.61	0/1927
44	W	0.40	0/582	0.68	0/773
45	X	0.36	0/637	0.60	1/849 (0.1%)
46	Y	0.32	0/471	0.55	0/630
47	Z	0.36	0/449	0.60	0/602
48	1	0.28	0/235	0.54	0/318
49	2	0.38	0/429	0.59	0/572
50	3	0.35	0/425	0.62	0/566
51	4	0.41	0/379	0.61	0/496
52	5	0.36	0/511	0.65	0/668
53	6	0.38	0/304	0.55	0/399
All	All	0.79	3/154034 (0.0%)	0.97	477/230370 (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
10	j	0	1
25	D	0	1
39	R	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1011	A	N9-C4	-6.33	1.34	1.37
22	A	1133	A	N9-C4	-5.72	1.34	1.37
22	A	519	A	N9-C4	-5.59	1.34	1.37

The worst 5 of 477 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	359	U	N3-C2-O2	-10.61	114.77	122.20
22	A	359	U	N1-C2-O2	10.16	129.91	122.80
22	A	359	U	C2-N1-C1'	10.01	129.72	117.70
22	A	1448	C	C6-N1-C2	-9.89	116.34	120.30
1	a	104	C	C2-N1-C1'	9.72	129.49	118.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	D	151	THR	Peptide
39	R	51	LEU	Peptide
10	j	56	HIS	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	
2	b	230/239 (96%)	211 (92%)	19 (8%)	0	100	100
3	c	203/205 (99%)	180 (89%)	23 (11%)	0	100	100
4	d	203/205 (99%)	185 (91%)	18 (9%)	0	100	100
5	e	154/156 (99%)	133 (86%)	21 (14%)	0	100	100
6	f	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
7	g	152/154 (99%)	141 (93%)	11 (7%)	0	100	100
8	h	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
9	i	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
10	j	94/96 (98%)	85 (90%)	9 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	k	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
12	l	119/121 (98%)	100 (84%)	19 (16%)	0	100	100
13	m	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
14	n	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
15	o	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
16	p	76/78 (97%)	70 (92%)	6 (8%)	0	100	100
17	q	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
18	r	69/71 (97%)	65 (94%)	4 (6%)	0	100	100
19	s	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
20	t	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
21	u	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
24	C	269/271 (99%)	241 (90%)	28 (10%)	0	100	100
25	D	205/207 (99%)	179 (87%)	25 (12%)	1 (0%)	29	63
26	E	197/199 (99%)	188 (95%)	9 (5%)	0	100	100
27	F	172/174 (99%)	154 (90%)	18 (10%)	0	100	100
28	G	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
29	H	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
30	I	138/140 (99%)	118 (86%)	20 (14%)	0	100	100
31	J	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
32	K	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
33	L	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
34	M	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
35	N	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
36	O	113/115 (98%)	104 (92%)	9 (8%)	0	100	100
37	P	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
38	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
39	R	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	15	49
40	S	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
41	T	90/92 (98%)	80 (89%)	10 (11%)	0	100	100
42	U	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
43	V	186/188 (99%)	169 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	W	74/76 (97%)	55 (74%)	19 (26%)	0	100	100
45	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
46	Y	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
47	Z	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
48	1	29/31 (94%)	24 (83%)	5 (17%)	0	100	100
49	2	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
50	3	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
51	4	43/44 (98%)	38 (88%)	5 (12%)	0	100	100
52	5	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
53	6	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
All	All	5676/5785 (98%)	5184 (91%)	490 (9%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	R	52	PRO
25	D	152	PRO

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	
2	b	191/197 (97%)	190 (100%)	1 (0%)	88	93
3	c	165/171 (96%)	165 (100%)	0	100	100
4	d	166/173 (96%)	164 (99%)	2 (1%)	71	84
5	e	114/115 (99%)	111 (97%)	3 (3%)	46	73
6	f	88/90 (98%)	87 (99%)	1 (1%)	73	86
7	g	116/120 (97%)	114 (98%)	2 (2%)	60	80
8	h	108/108 (100%)	108 (100%)	0	100	100
9	i	102/102 (100%)	99 (97%)	3 (3%)	42	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	j	85/85 (100%)	83 (98%)	2 (2%)	49 75
11	k	84/87 (97%)	84 (100%)	0	100 100
12	l	105/105 (100%)	102 (97%)	3 (3%)	42 71
13	m	92/92 (100%)	88 (96%)	4 (4%)	29 62
14	n	78/80 (98%)	78 (100%)	0	100 100
15	o	73/73 (100%)	73 (100%)	0	100 100
16	p	61/63 (97%)	61 (100%)	0	100 100
17	q	70/70 (100%)	67 (96%)	3 (4%)	29 62
18	r	54/61 (88%)	52 (96%)	2 (4%)	34 64
19	s	69/71 (97%)	68 (99%)	1 (1%)	67 83
20	t	67/68 (98%)	66 (98%)	1 (2%)	65 82
21	u	51/52 (98%)	50 (98%)	1 (2%)	55 78
24	C	206/212 (97%)	206 (100%)	0	100 100
25	D	157/159 (99%)	155 (99%)	2 (1%)	69 83
26	E	155/157 (99%)	155 (100%)	0	100 100
27	F	124/149 (83%)	123 (99%)	1 (1%)	81 90
28	G	133/137 (97%)	132 (99%)	1 (1%)	81 90
29	H	55/55 (100%)	55 (100%)	0	100 100
30	I	108/108 (100%)	106 (98%)	2 (2%)	57 79
31	J	118/118 (100%)	116 (98%)	2 (2%)	60 80
32	K	100/100 (100%)	100 (100%)	0	100 100
33	L	104/105 (99%)	103 (99%)	1 (1%)	76 87
34	M	108/108 (100%)	108 (100%)	0	100 100
35	N	97/97 (100%)	97 (100%)	0	100 100
36	O	86/86 (100%)	86 (100%)	0	100 100
37	P	94/95 (99%)	94 (100%)	0	100 100
38	Q	87/87 (100%)	87 (100%)	0	100 100
39	R	82/86 (95%)	82 (100%)	0	100 100
40	S	86/86 (100%)	86 (100%)	0	100 100
41	T	73/77 (95%)	73 (100%)	0	100 100
42	U	88/88 (100%)	88 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	V	144/153 (94%)	142 (99%)	2 (1%)	67 83
44	W	56/56 (100%)	54 (96%)	2 (4%)	35 65
45	X	65/66 (98%)	64 (98%)	1 (2%)	65 82
46	Y	51/53 (96%)	51 (100%)	0	100 100
47	Z	48/48 (100%)	48 (100%)	0	100 100
48	1	27/27 (100%)	27 (100%)	0	100 100
49	2	46/46 (100%)	46 (100%)	0	100 100
50	3	46/46 (100%)	46 (100%)	0	100 100
51	4	38/37 (103%)	37 (97%)	1 (3%)	46 73
52	5	54/54 (100%)	54 (100%)	0	100 100
53	6	33/34 (97%)	33 (100%)	0	100 100
All	All	4608/4713 (98%)	4564 (99%)	44 (1%)	77 87

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	u	45	ARG
31	J	50	THR
25	D	34	ARG
28	G	33	LEU
33	L	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
26	E	91	HIS
32	K	91	GLN
27	F	52	ASN
30	I	17	GLN
37	P	7	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1525/1526 (99%)	365 (23%)	0
22	A	2880/2888 (99%)	824 (28%)	46 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	B	116/117 (99%)	25 (21%)	4 (3%)
All	All	4521/4531 (99%)	1214 (26%)	50 (1%)

5 of 1214 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	3	A
1	a	6	G
1	a	7	A
1	a	9	G
1	a	16	A

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	1642	A
22	A	2029	A
23	B	66	A
22	A	1672	G
22	A	1741	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 172 ligands modelled in this entry, 172 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)

There are no chain breaks in this entry.

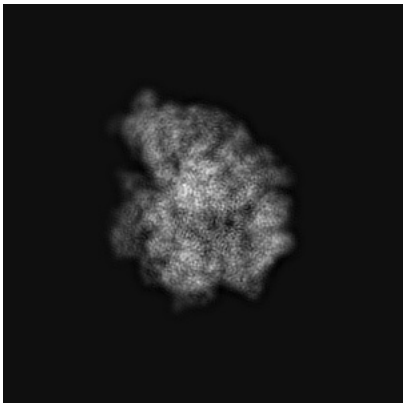
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10285. These allow visual inspection of the internal detail of the map and identification of artifacts.

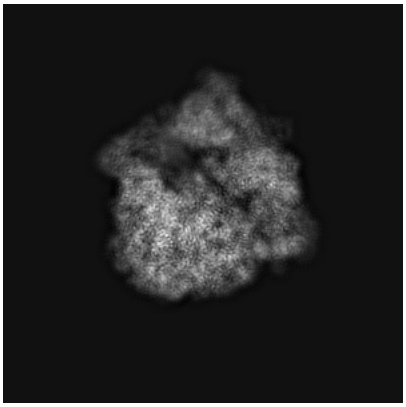
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

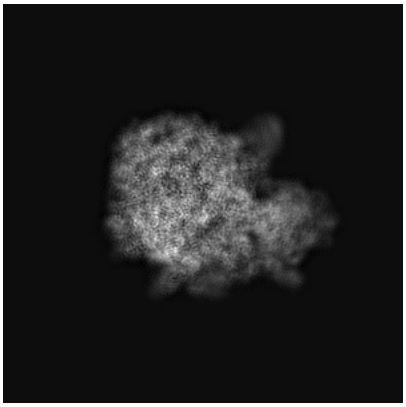
6.1.1 Primary map



X



Y

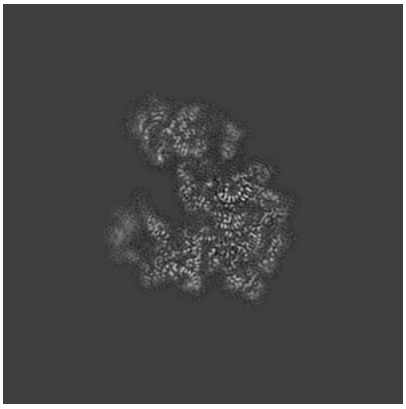


Z

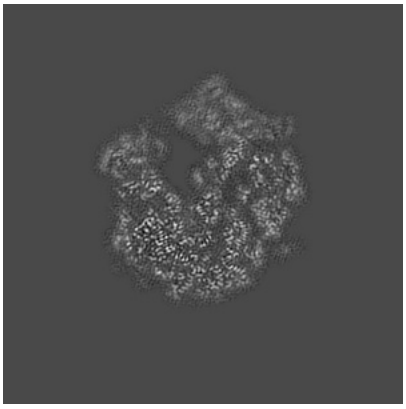
The images above show the map projected in three orthogonal directions.

6.2 Central slices

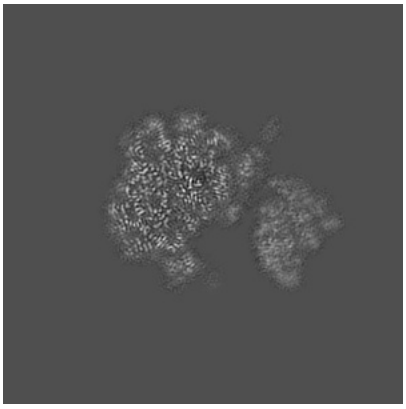
6.2.1 Primary map



X Index: 200



Y Index: 200

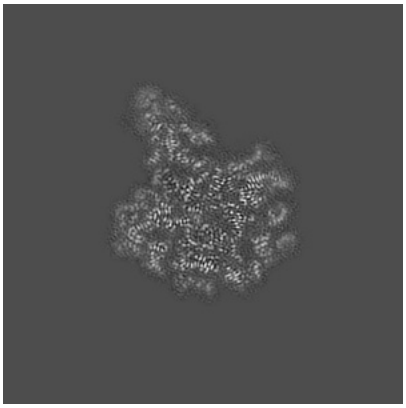


Z Index: 200

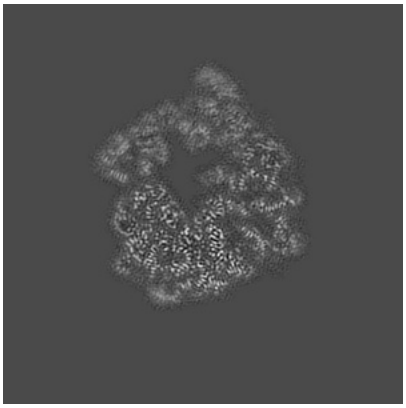
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

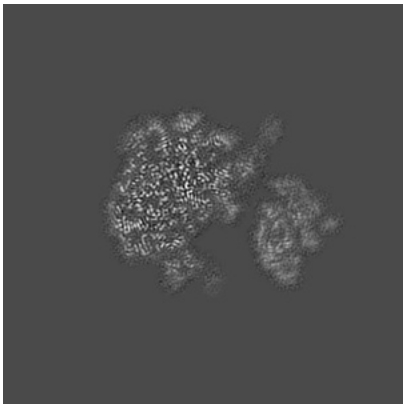
6.3.1 Primary map



X Index: 172



Y Index: 181

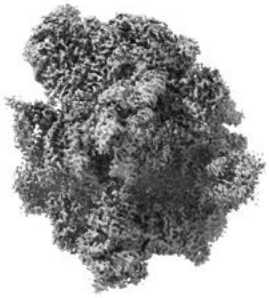


Z Index: 198

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

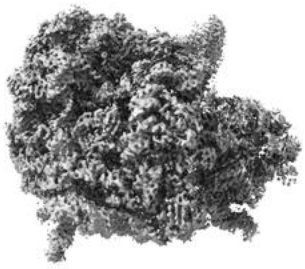
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0731. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

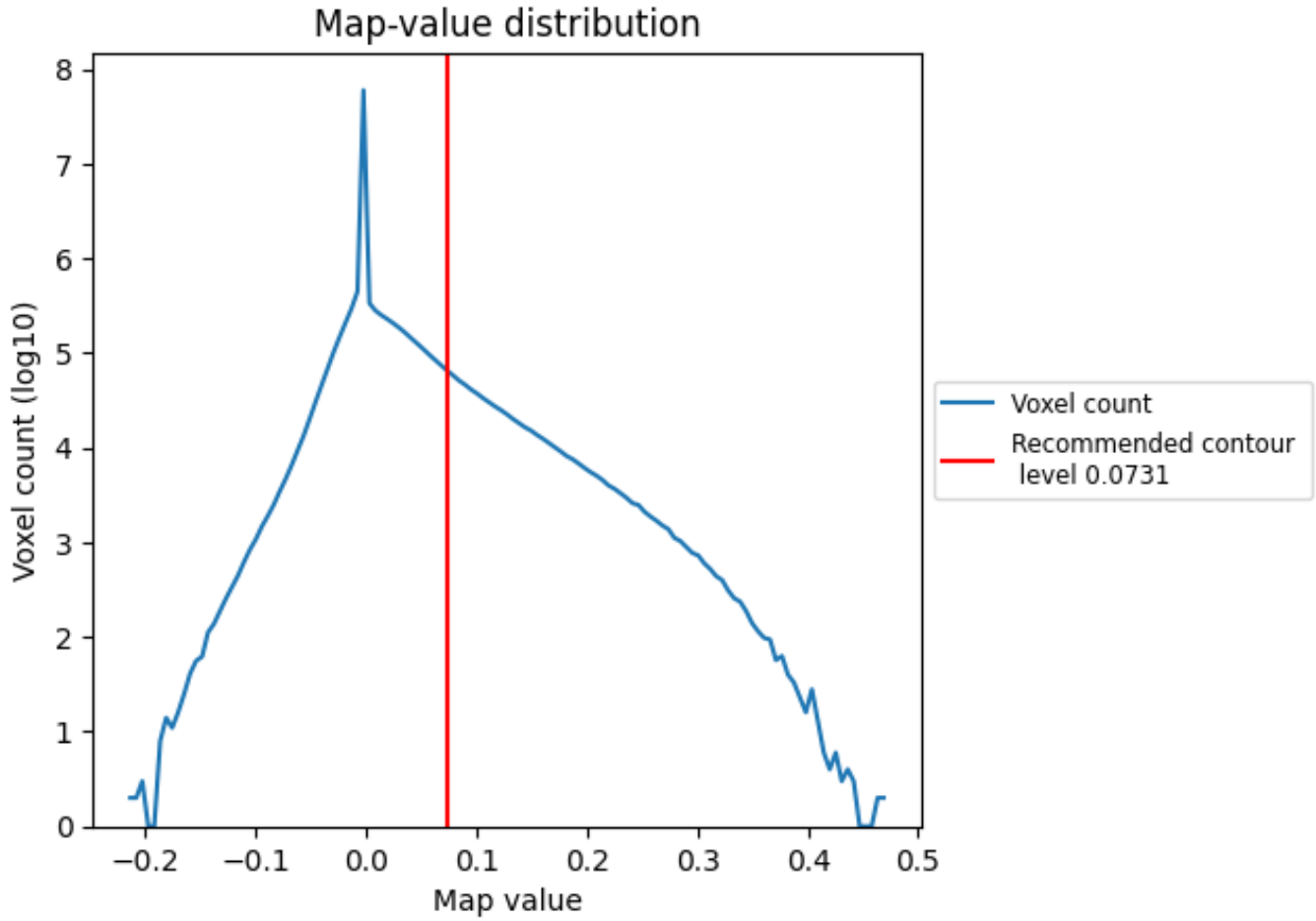
6.5 Mask visualisation (i)

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

7 Map analysis

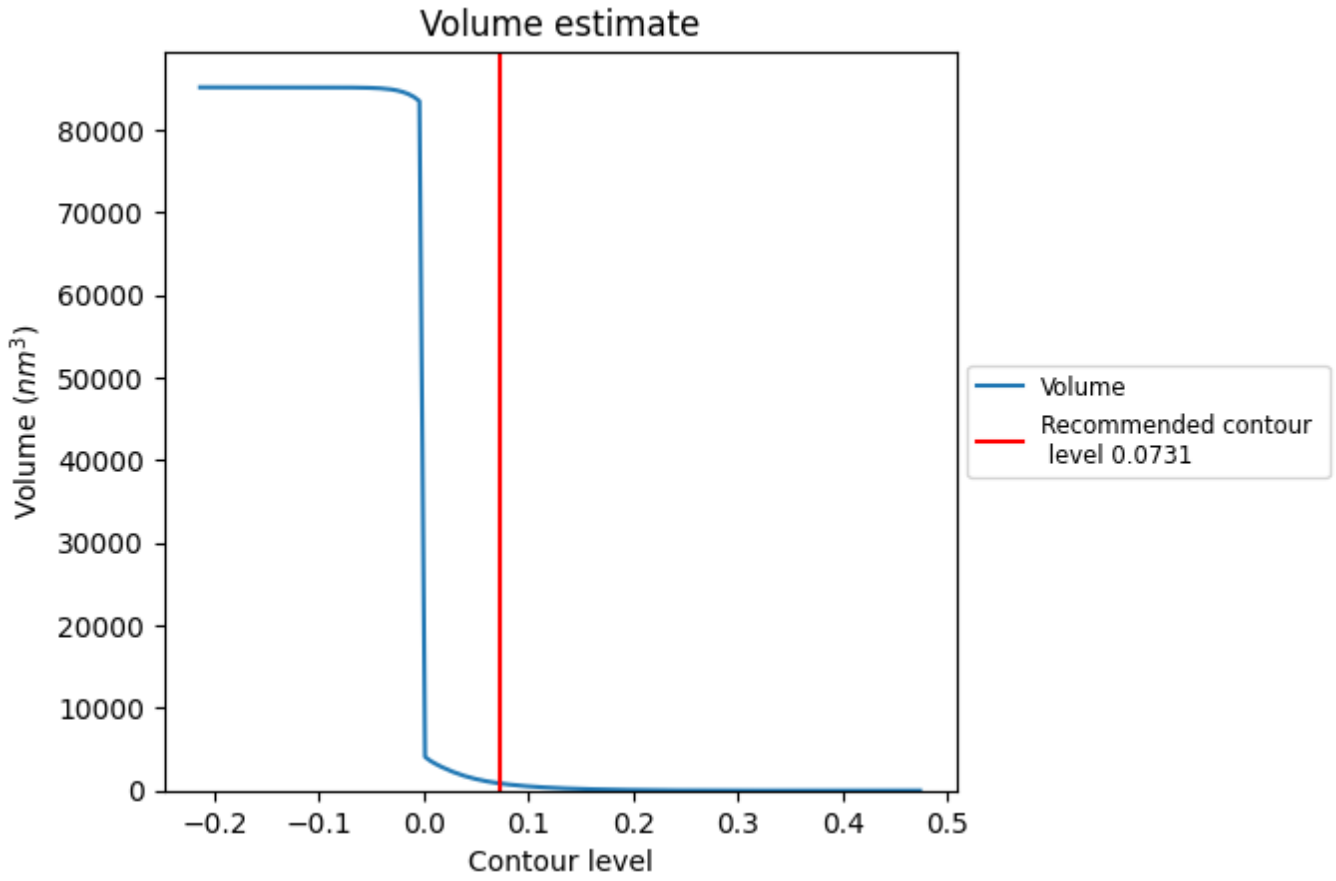
This section contains the results of statistical analysis of the map.

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.

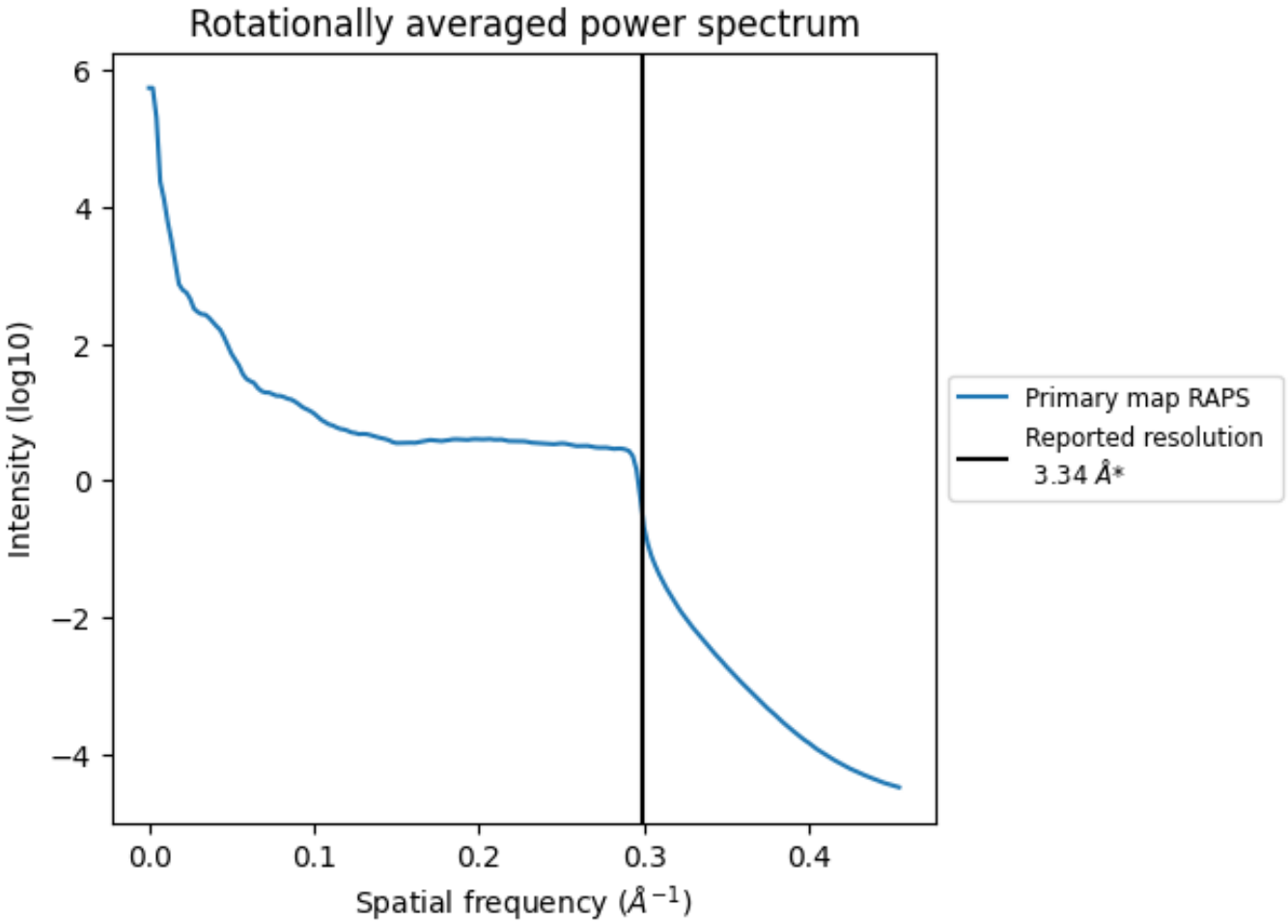
7.2 Volume estimate (i)



The volume at the recommended contour level is 860 nm^3; this corresponds to an approximate mass of 777 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 0.299 Å^{-1}

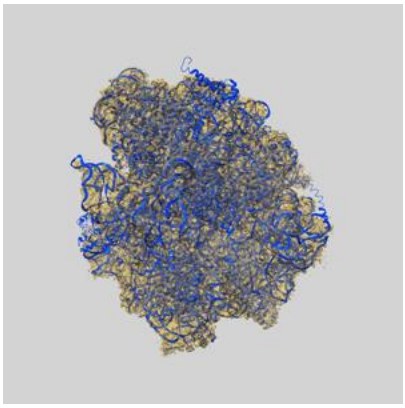
8 Fourier-Shell correlation (i)

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

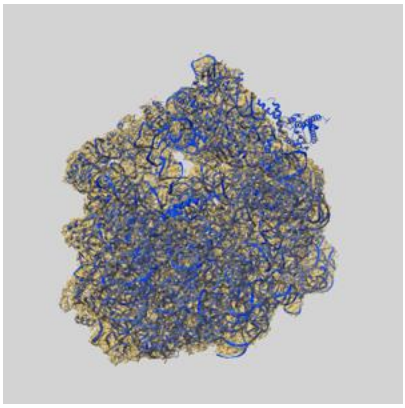
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10285 and PDB model 6SPG. Per-residue inclusion information can be found in section 3 on page 14.

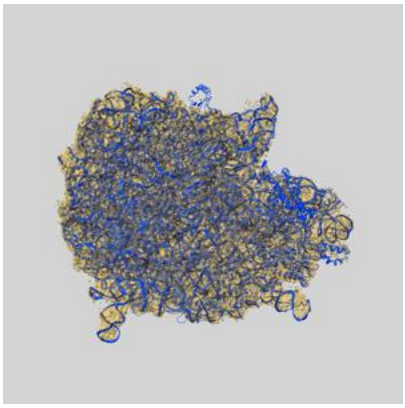
9.1 Map-model overlay



X



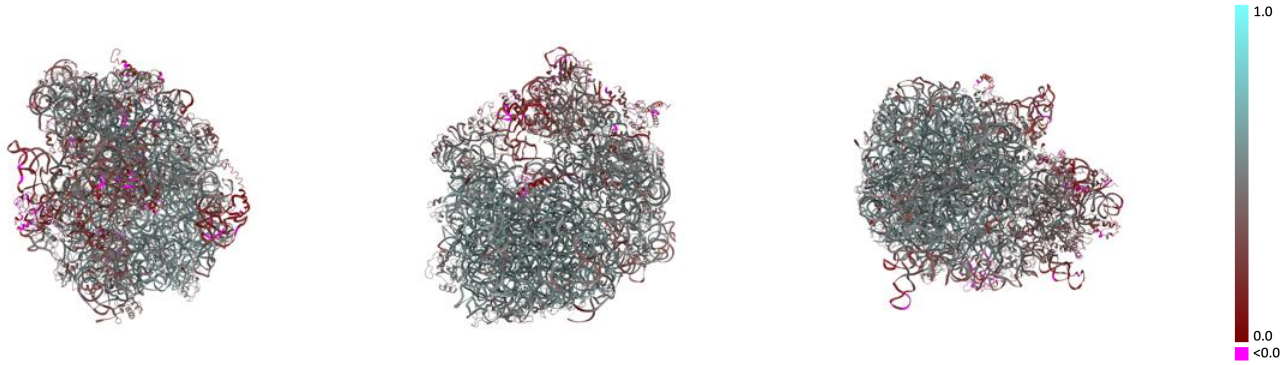
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0731 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.

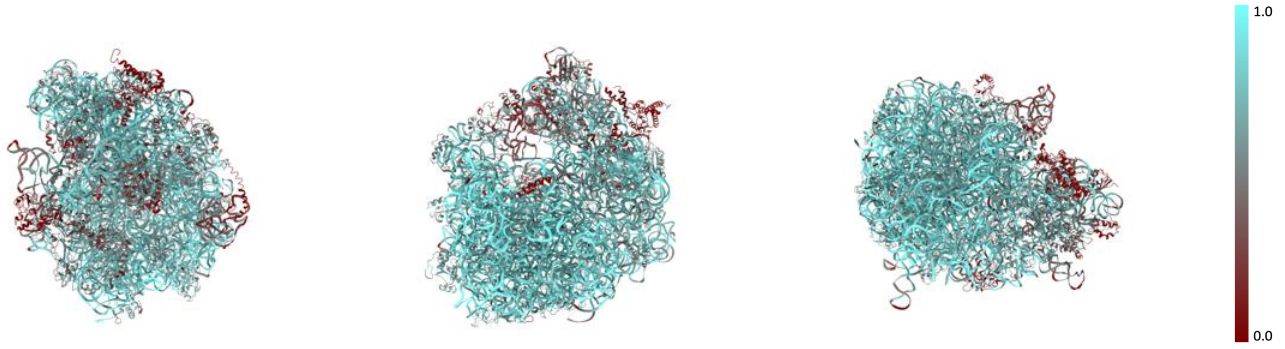
9.2 Q-score mapped to coordinate model



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.

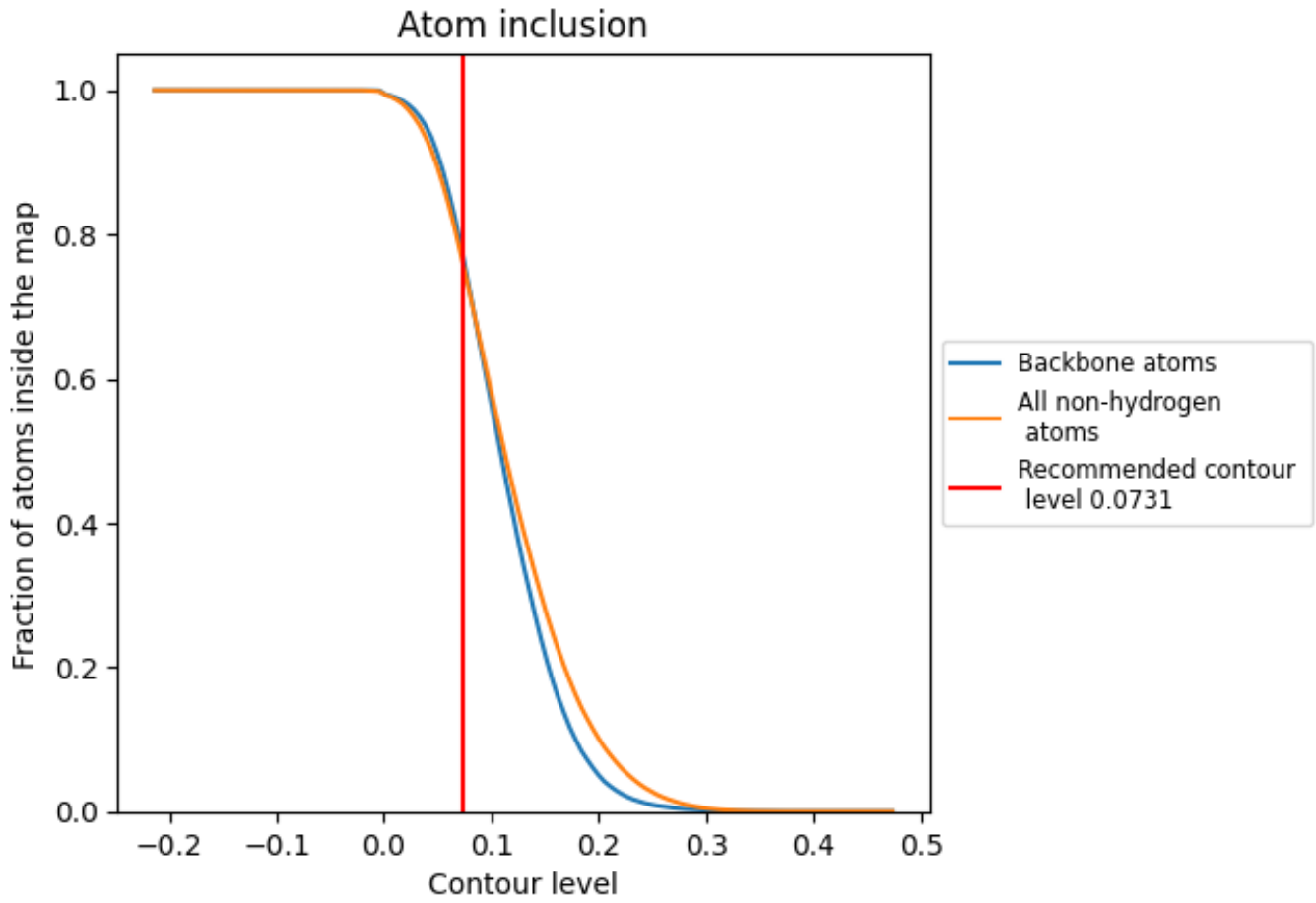
9.3 Atom inclusion mapped to coordinate model



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 (0.0731).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.0731) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7638	0.4680
1	0.3100	0.2040
2	0.7255	0.4890
3	0.5848	0.4370
4	0.7813	0.5540
5	0.7286	0.5340
6	0.7405	0.5280
A	0.8694	0.5150
B	0.8658	0.4590
C	0.7328	0.5270
D	0.7646	0.5160
E	0.7128	0.5070
F	0.5048	0.3360
G	0.5812	0.4190
H	0.0634	0.1670
I	0.0217	0.0610
J	0.7500	0.5160
K	0.6343	0.4910
L	0.7167	0.4960
M	0.6838	0.5070
N	0.7791	0.5280
O	0.6420	0.4240
P	0.6632	0.4910
Q	0.7998	0.5380
R	0.7267	0.5050
S	0.6890	0.5120
T	0.6681	0.4960
U	0.6315	0.4290
V	0.5493	0.4370
W	0.7750	0.5120
X	0.7105	0.5070
Y	0.7162	0.4810
Z	0.7021	0.5120
a	0.8209	0.4470
b	0.0858	0.2710

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Chain	Atom inclusion	Q-score
c	0.4537	0.3630
d	0.5748	0.4100
e	0.5996	0.4350
f	0.5187	0.3580
g	0.2528	0.2470
h	0.6397	0.4680
i	0.3491	0.2610
j	0.3110	0.2880
k	0.5814	0.4300
l	0.5958	0.4610
m	0.3176	0.2210
n	0.4592	0.3570
o	0.6447	0.4480
p	0.7223	0.4740
q	0.6187	0.4380
r	0.5456	0.4150
s	0.2882	0.2430
t	0.6928	0.4610
u	0.3279	0.3450