Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 04:12 PM EST

PDB ID	:	3J9Y
EMDB ID	:	EMD-6311
Title	:	Cryo-EM structure of tetracycline resistance protein TetM bound to a translating E.coli ribosome
Authors	:	Arenz, S.; Nguyen, F.; Beckmann, R.; Wilson, D.N.
Deposited on	:	2015-03-23
Resolution	:	3.90 Å(reported)
Based on initial model	:	5AFI

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

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

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

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

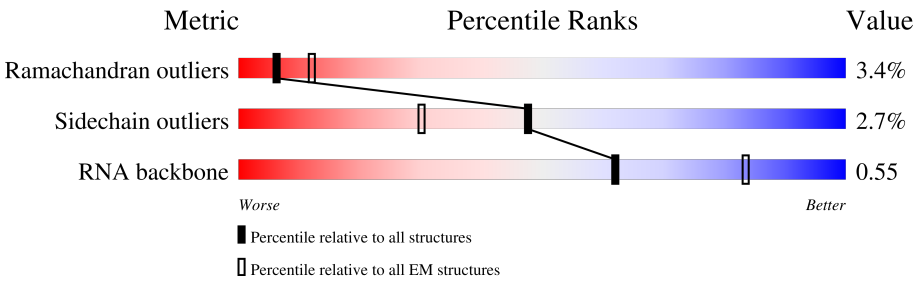
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	1539	8% 83% 17% •
2	b	240	74% 85% 6% 9%
3	d	206	71% 92% 8%
4	e	167	43% 84% 10% • 6%
5	f	135	38% 68% • • 26%
6	h	130	35% 96% • •
7	k	129	56% 84% 6% 10%
8	l	124	69% 93% 6% •

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Mol	Chain	Length	Quality of chain
9	o	89	36% 91% 8%
10	p	82	52% 93% 7%
11	q	84	52% 86% 10% 5%
12	r	75	28% 79% 8% 13%
13	t	87	43% 93% 5%
14	u	71	86% 82% 10% 8%
15	v	78	21% 73% 23%
16	x	11	27% 73% 9% 18%
17	w	639	28% 96%
18	c	233	45% 85% 12%
19	g	179	56% 78% 7% 16%
20	i	130	49% 88% 10%
21	j	103	65% 87% 8% 5%
22	m	118	43% 91% 6%
23	n	102	37% 90% 9%
24	s	92	36% 85% 14%
25	A	2903	7% 79% 20%
26	B	120	7% 84% 16%
27	C	273	19% 95% 5%
28	D	209	32% 98%
29	E	201	38% 94% 6%
30	F	179	59% 92% 7%
31	G	177	57% 97%
32	H	149	90% 97%
33	I	142	96% 91% 8%

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Mol	Chain	Length	Quality of chain
34	J	142	26% 97%
35	K	123	37% 93% 7%
36	L	144	40% 90% 9%
37	M	136	29% 97%
38	N	127	29% 91% 6%
39	O	117	44% 97%
40	P	115	40% 96%
41	Q	118	18% 97%
42	R	103	41% 97%
43	S	110	29% 93% 6%
44	T	100	41% 88% 7%
45	U	104	56% 94%
46	V	94	44% 97%
47	W	85	20% 86% 12%
48	X	78	32% 97%
49	Y	63	56% 97%
50	Z	59	24% 98%
51	0	57	30% 93% 5%
52	1	55	91% 89% 9%
53	2	46	15% 100%
54	3	65	23% 95%
55	4	38	18% 100%
56	5	165	73% 73% 6% 21%
57	6	70	77% 91% 6%
58	7	69	96% 99%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 148915 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	1539	33029	14738	6052	10700	1539	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	218	1704	1081	305	311	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	205	1643	1026	315	298	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	157	1141	709	218	208	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	100	817	515	148	148	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	h	129	979	616	173	184	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	k	116	869	535	173	158	3	0	0

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	l	123	955	590	196	165	4	0	0

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	o	88	714	439	144	130	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	p	82	649	406	128	114	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	q	80	648	411	121	113	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	r	65	504	317	96	91	0	0

- Molecule 13 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	t	85	665	411	137	114	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	u	65	495	307	100	87	1	0	0

- Molecule 15 is a RNA chain called P-site fMet-tRNAfMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
15	v	77	1644	733	297	536	77	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	77	FME	-	modified residue	GB 147949

- Molecule 16 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	x	9	189	85	31	64	9	0	0

- Molecule 17 is a protein called Tetracycline resistance protein TetM.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	w	639	2590	1308	640	642	0	0

- Molecule 18 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	c	206	1624	1028	305	288	3	0	0

- Molecule 19 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	g	151	1181	735	227	215	4	0	0

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	i	127	1022	634	206	179	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	j	98	786	493	150	142	1	0	0

- Molecule 22 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	m	114	883	546	178	156	3	0	0

- Molecule 23 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	s	79	637	408	120	107	2	0	0

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	A	2900	62276	27788	11460	20128	2900	0	0

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	B	120	2572	1145	471	836	120	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	C	271	2082	1288	423	364	7	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	D	209	1565	979	288	294	4	0	0

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	E	201	1552	974	283	290	5	0	0

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	G	176	1323	832	243	246	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	H	149	1111	699	197	214	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	I	141	1032	651	179	196	6	0	0

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	J	142	1129	714	212	199	4	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	K	122	938	587	180	165	6	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	L	143	1045	649	206	189	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	M	136	1074	686	205	177	6	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	N	120	960	593	196	166	5	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	R	103	816	516	153	145	2	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	S	110	857	532	166	156	3	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	T	93	738	466	139	131	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	V	94	753	479	137	134	3	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	W	75	575	356	116	102	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Y	63	509	313	99	95	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Z	58	449	281	87	79	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	0	56	444	269	94	80	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	1	50	409	263	75	71	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	2	46	377	228	90	57	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	3	64	504	323	105	74	2	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	4	38	302	185	65	48	4	0	0

- Molecule 56 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	5	131	988	625	175	183	5	0	0

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	6	66	522	323	99	94	6	0	0

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

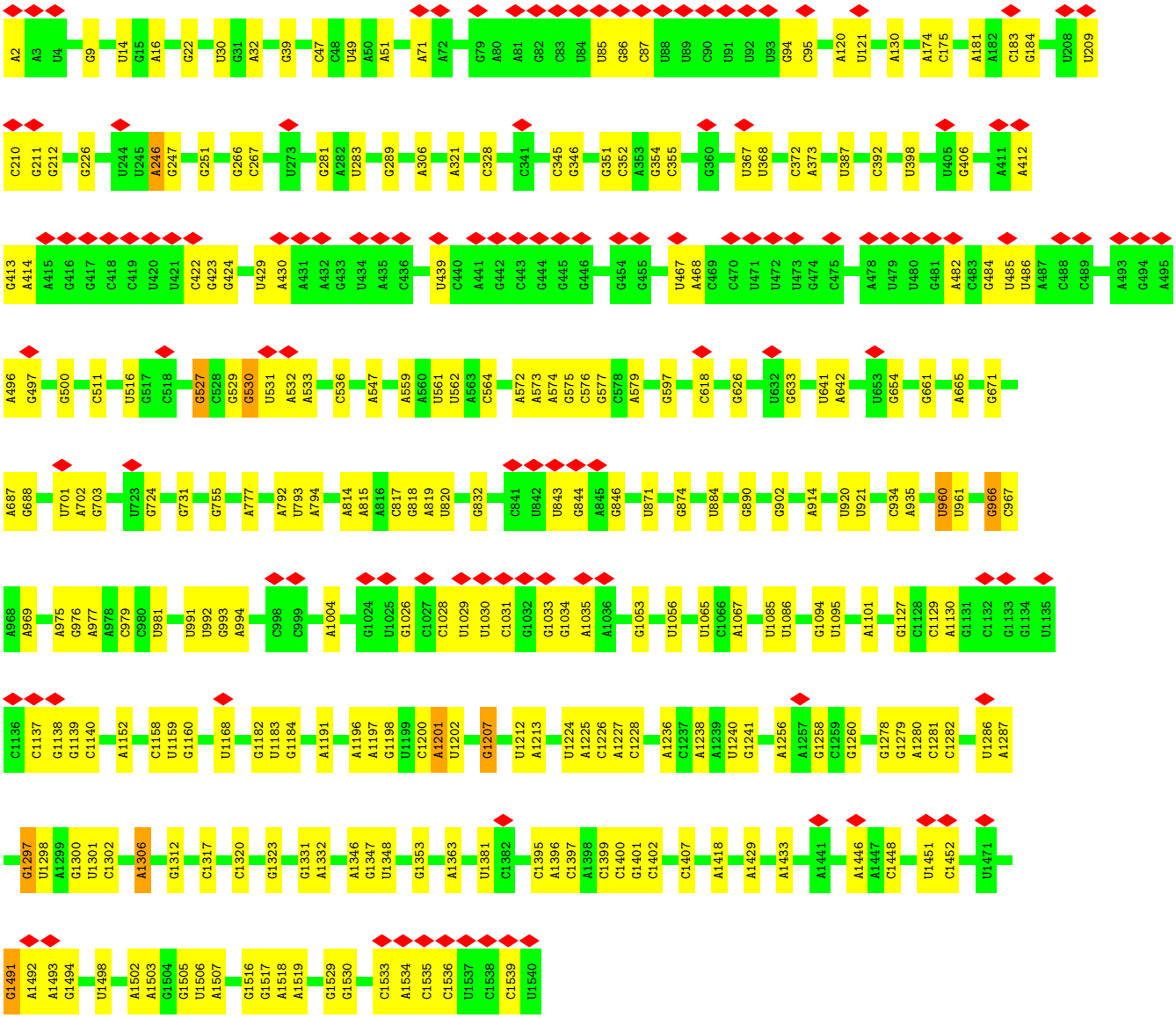
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	7	69	276	138	69	69	0	0

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.

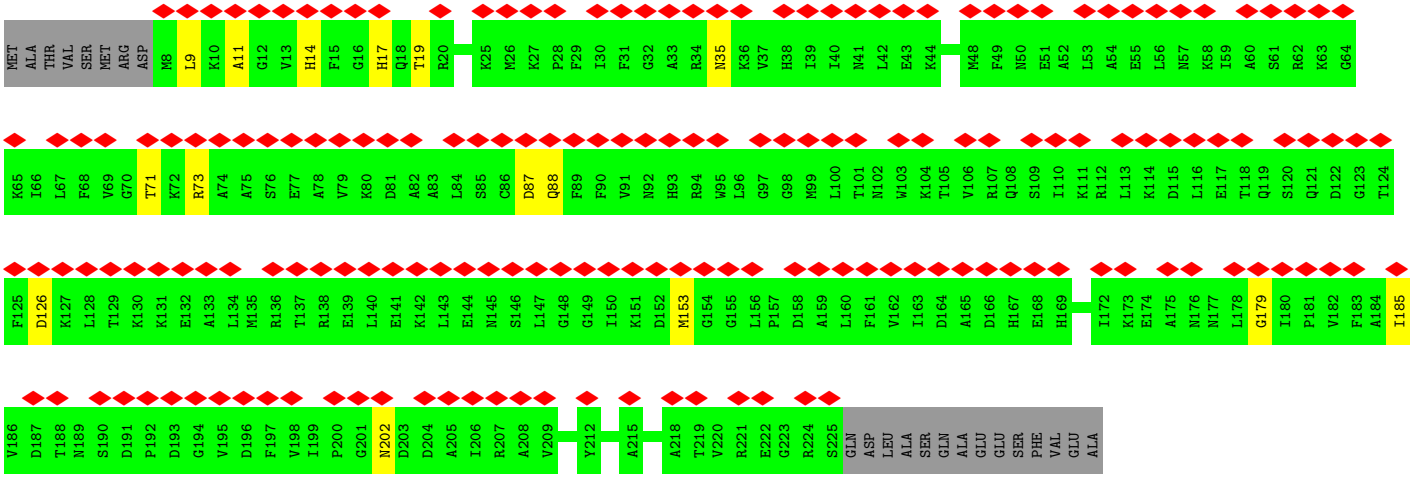
- Molecule 1: 16S ribosomal RNA

Chain a:



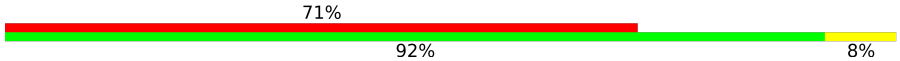
- Molecule 2: 30S ribosomal protein S2

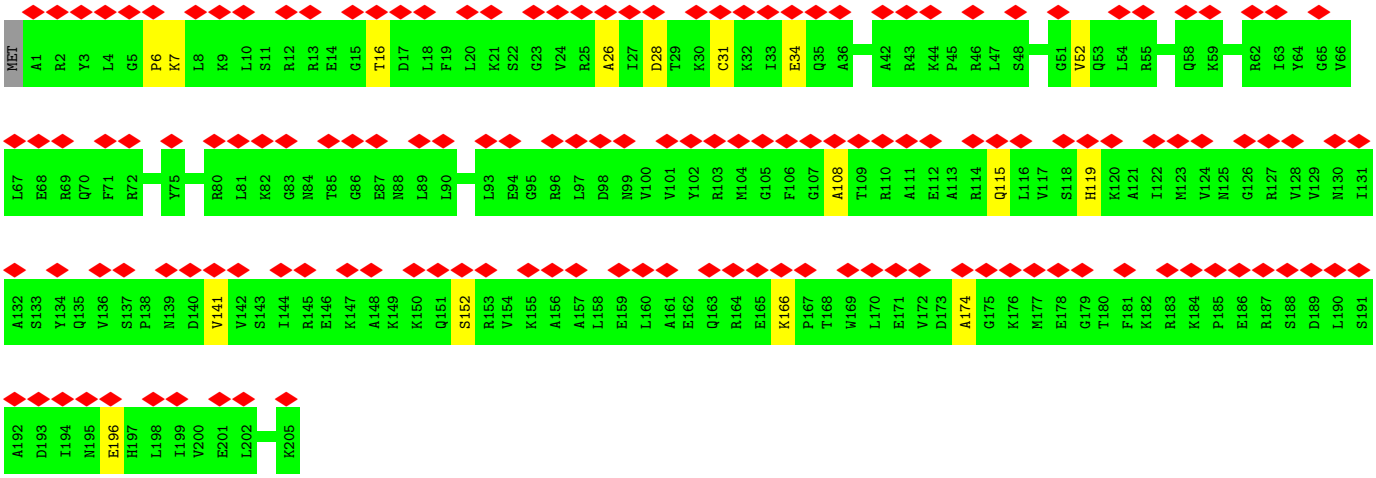
Chain b:



- Molecule 3: 30S ribosomal protein S4

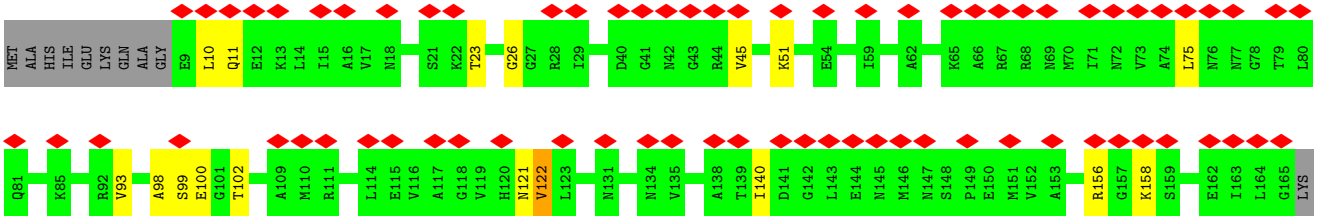
Chain d:





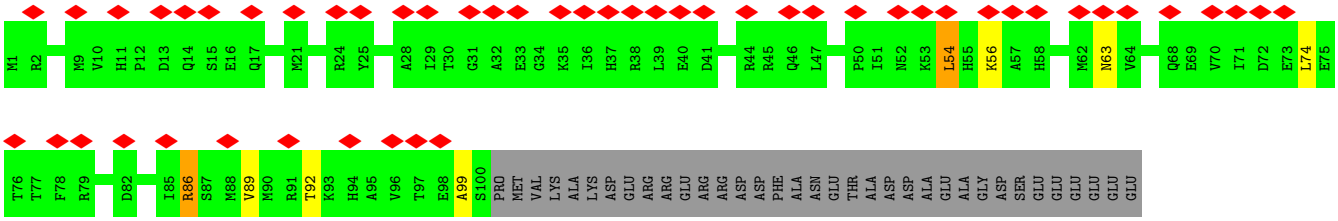
- Molecule 4: 30S ribosomal protein S5

Chain e:



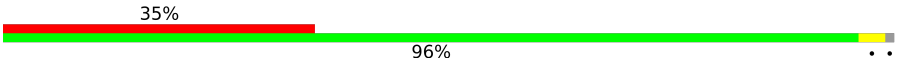
- Molecule 5: 30S ribosomal protein S6

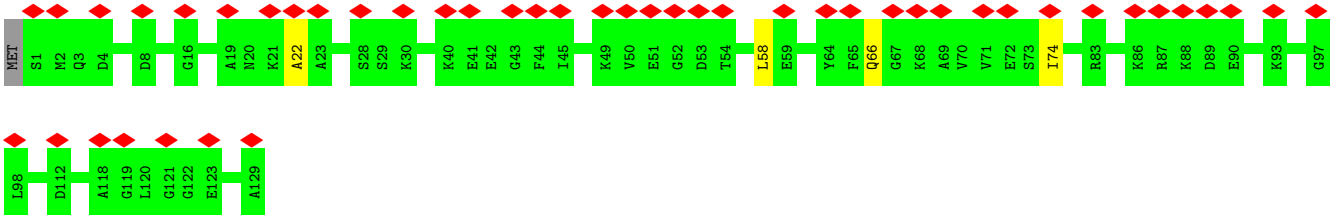
Chain f:



- Molecule 6: 30S ribosomal protein S8

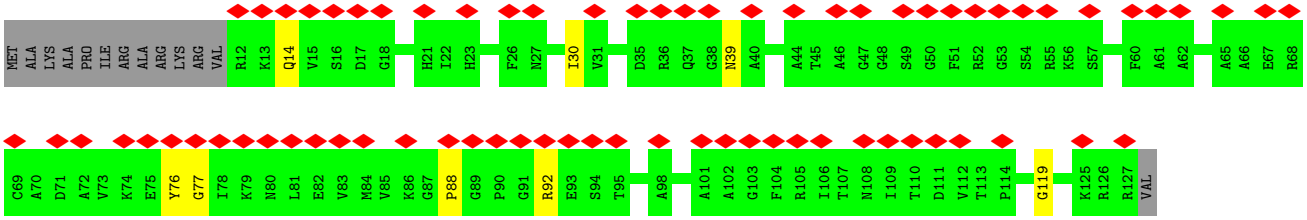
Chain h:





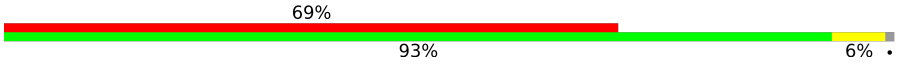
- Molecule 7: 30S ribosomal protein S11

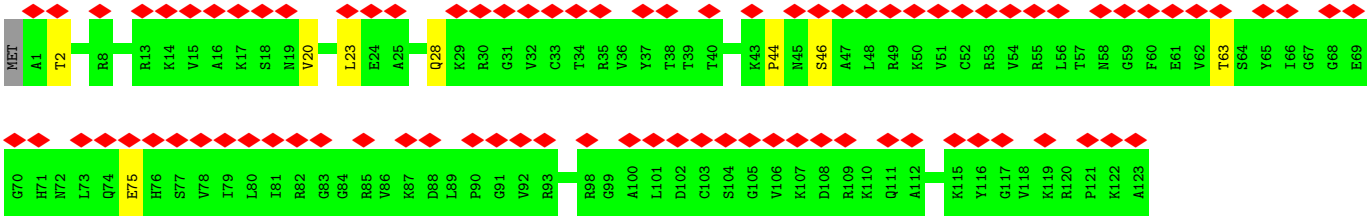
Chain k:



- Molecule 8: 30S ribosomal protein S12

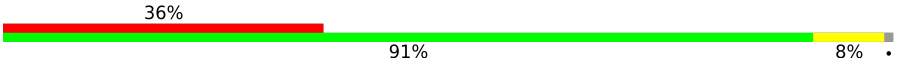
Chain l:

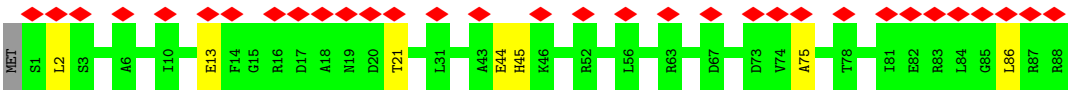




- Molecule 9: 30S ribosomal protein S15

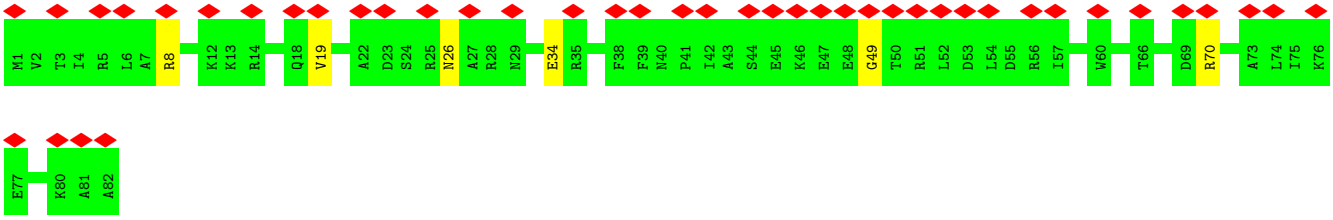
Chain o:





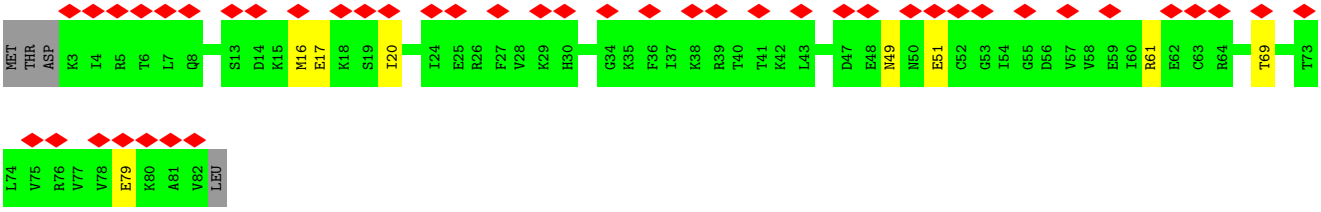
- Molecule 10: 30S ribosomal protein S16

Chain p: 52% 93% 7%



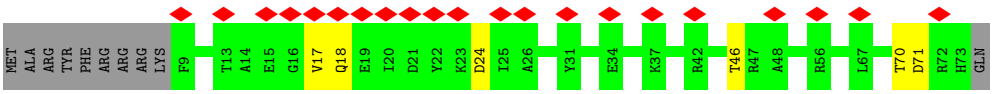
- Molecule 11: 30S ribosomal protein S17

Chain q: 52% 86% 10% 5%



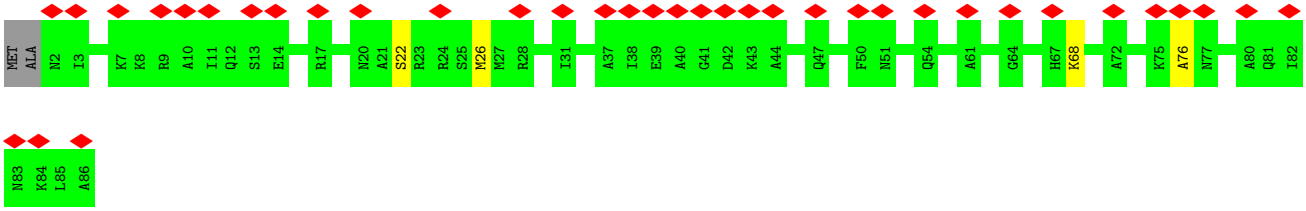
- Molecule 12: 30S ribosomal protein S18

Chain r: 28% 79% 8% 13%



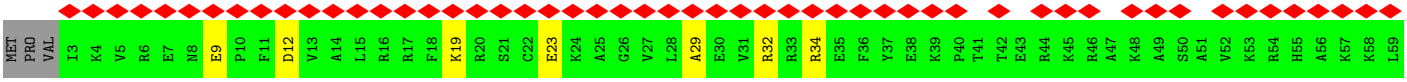
- Molecule 13: 30S ribosomal protein S20

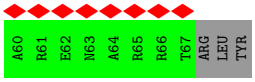
Chain t: 43% 93% 5%



- Molecule 14: 30S ribosomal protein S21

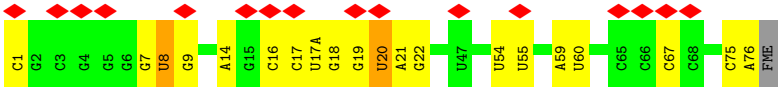
Chain u: 86% 82% 10% 8%





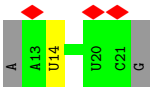
- Molecule 15: P-site fMet-tRNAfMet

Chain v:



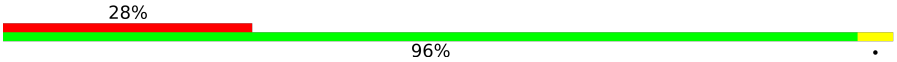
- Molecule 16: mRNA

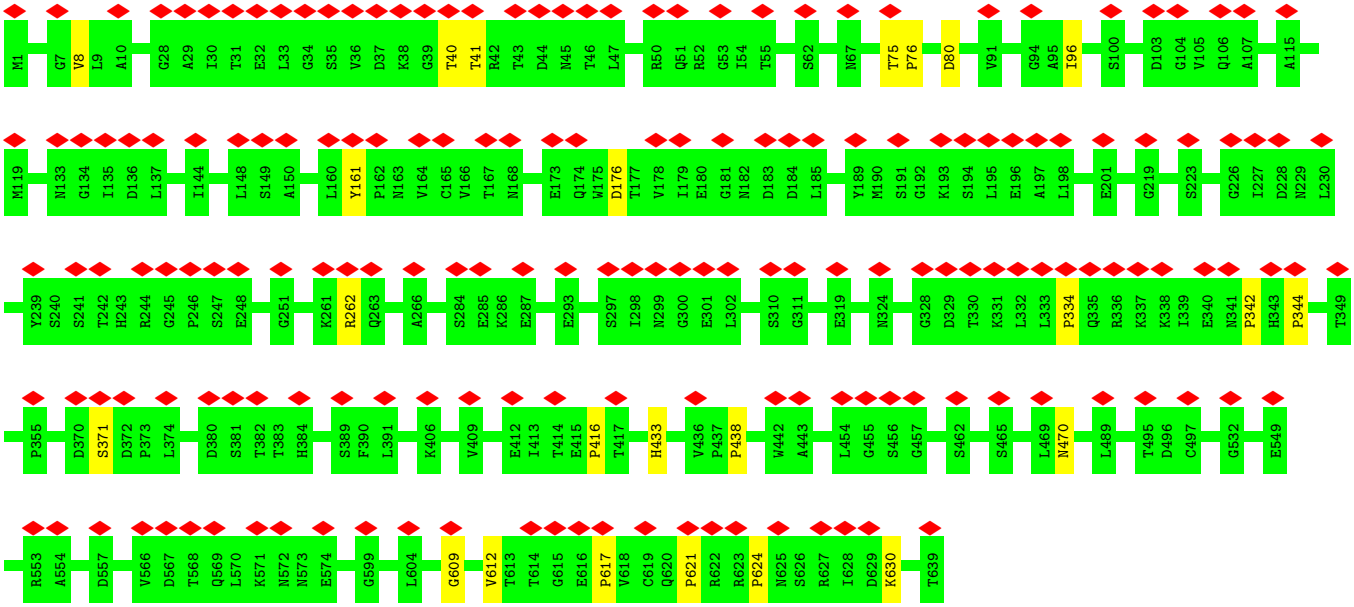
Chain x:



- Molecule 17: Tetracycline resistance protein TetM

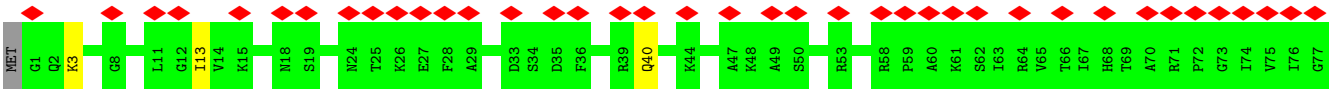
Chain w:

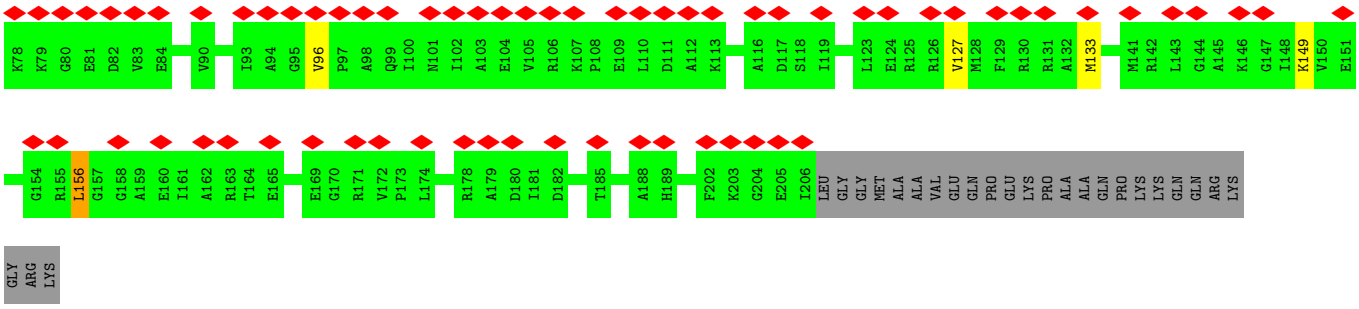




- Molecule 18: 30S ribosomal protein S3

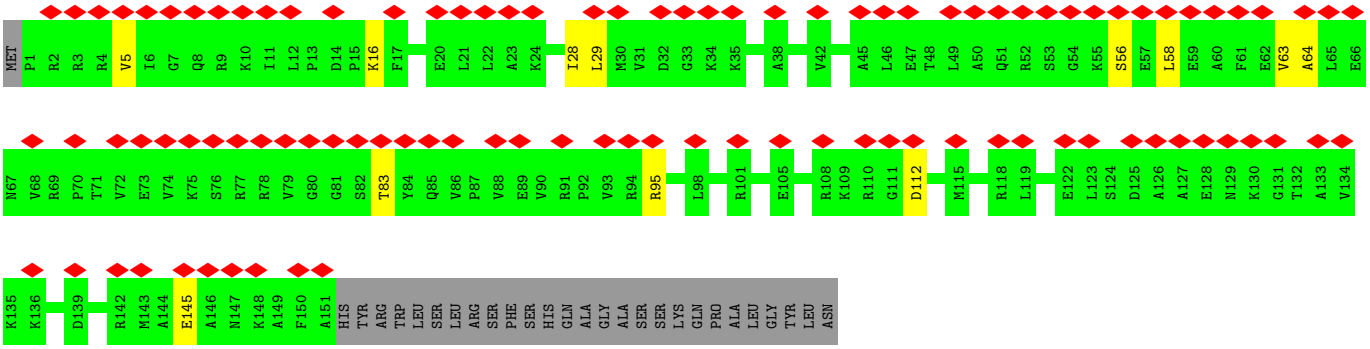
Chain c:





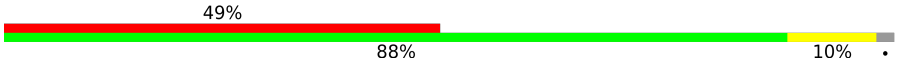
- Molecule 19: 30S ribosomal protein S7

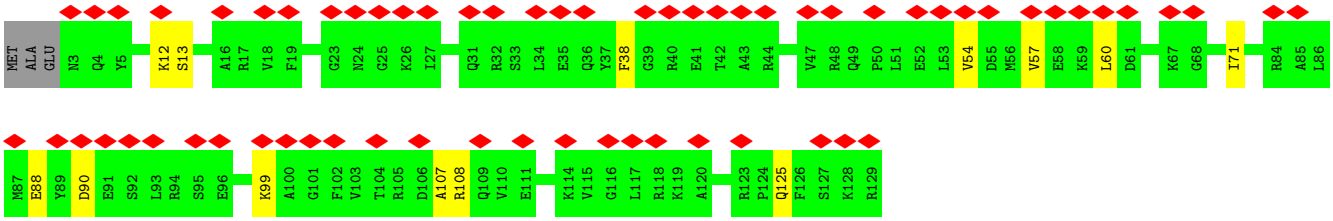
Chain g:



- Molecule 20: 30S ribosomal protein S9

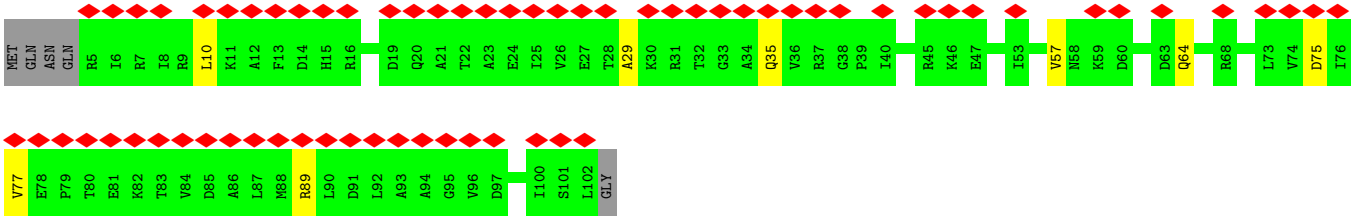
Chain i:





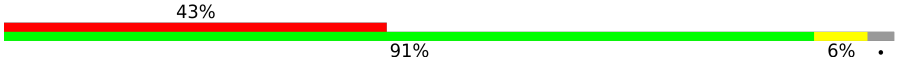
- Molecule 21: 30S ribosomal protein S10

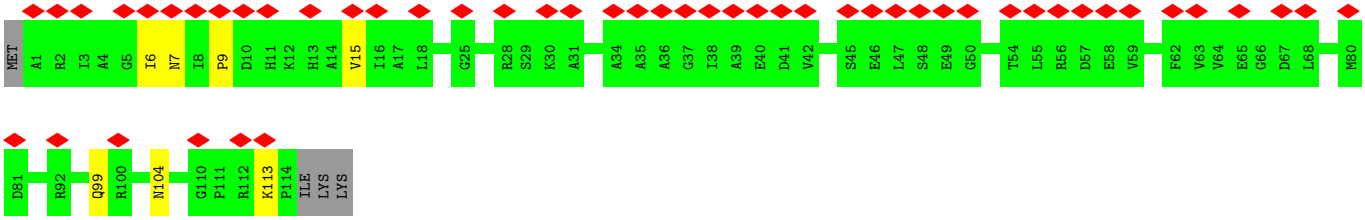
Chain j:



- Molecule 22: 30S ribosomal protein S13

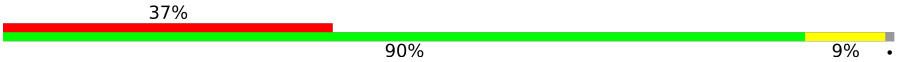
Chain m:

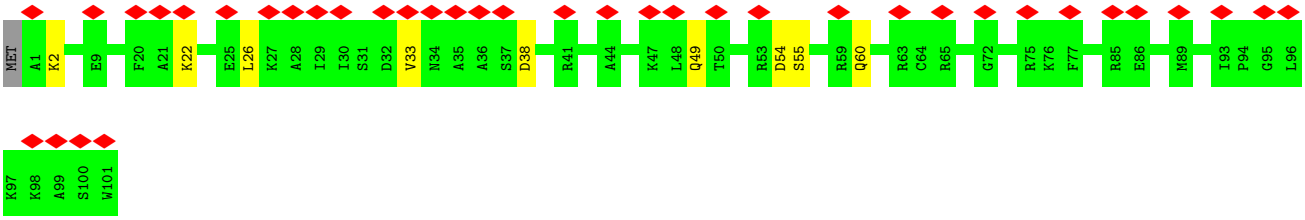




• Molecule 23: 30S ribosomal protein S14

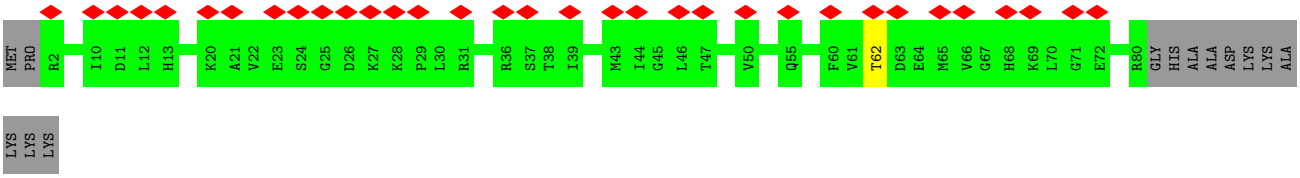
Chain n:





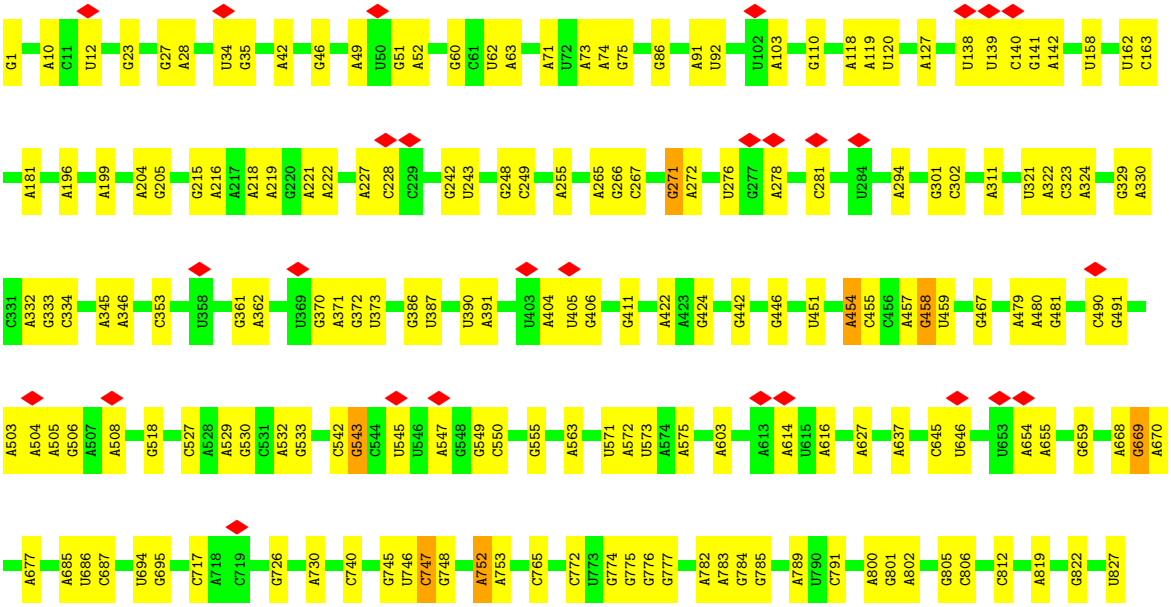
• Molecule 24: 30S ribosomal protein S19

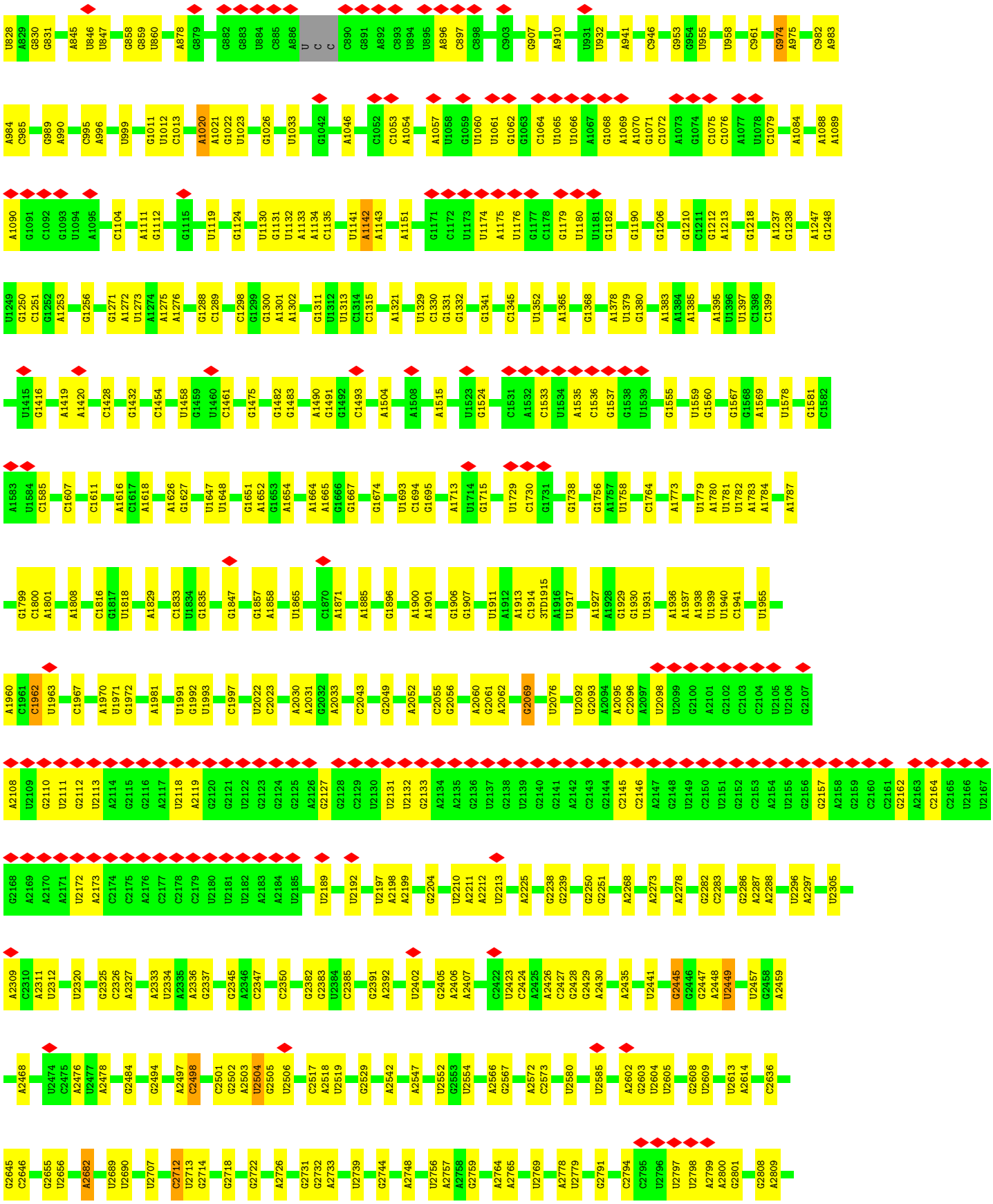
Chain s:



• Molecule 25: 23S ribosomal RNA

Chain A:

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A984 C985 G989 A990 C995 A996 U999 G1011 U1012 C1013 A1020 A1021 G1022 U1023 G1026 U1033 G1042 A1046 C1052 C1053 A1054 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1084 A1088 A1089
A1090 G1091 C1092 G1093 U1094 A1095 C1104 A1111 G1112 G1115 U1119 G1124 U1130 G1131 U1132 A1133 A1134 C1135 U1141 A1142 A1143 A1151 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 G1190 G1206 G1210 C1211 G1212 A1213 G1218 A1237 G1238 A1247 G1248
U1249 G1250 C1251 G1252 A1253 G1256 G1271 A1272 U1273 A1274 A1275 A1276 G1288 C1289 C1298 G1299 G1300 A1301 A1302 G1311 U1312 U1313 C1314 C1315 A1321 U1329 C1330 G1331 G1332 G1341 C1345 U1352 A1365 G1368 A1378 U1379 G1380 A1383 A1384 A1385 A1395 U1396 U1397 C1398 C1399
U1415 G1416 A1419 A1420 C1428 G1432 C1454 U1458 G1459 U1460 C1461 G1475 G1482 G1483 A1490 G1491 G1492 C1493 A1504 A1508 A1515 U1523 G1524 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1555 U1559 G1560 G1567 G1568 A1569 U1578 G1581 C1582
A1583 U1584 C1585 C1607 C1611 A1616 C1617 A1618 A1626 G1627 U1647 U1648 G1651 A1652 G1653 A1654 A1664 A1665 G1666 G1667 G1674 U1693 C1694 G1695 A1713 U1714 G1715 U1729 C1730 G1731 G1738 G1756 A1757 U1758 C1764 A1773 U1779 A1780 U1781 U1782 A1783 A1784 A1787
G1799 C1800 A1801 A1808 C1816 G1817 U1818 A1829 C1833 U1834 G1835 G1847 G1857 A1858 U1865 C1870 A1871 A1885 G1896 A1900 A1901 G1906 G1907 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1927 A1928 G1929 G1930 U1931 A1936 A1937 A1938 U1939 U1940 C1941 U1955
A1960 C1961 C1962 U1963 C1967 A1970 U1971 G1972 A1981 U1991 G1992 U1993 C1997 U2022 C2023 A2030 A2031 G2032 A2033 C2043 G2049 A2052 C2055 G2056 A2060 G2061 A2062 G2069 U2076 U2092 G2093 A2094 A2095 C2096 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107
A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 C2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167
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A2309 C2310 A2311 U2312 U2320 G2325 C2326 A2327 A2333 U2334 A2335 A2336 G2337 G2345 A2346 C2347 C2350 G2382 G2383 U2384 C2385 G2391 A2392 U2402 G2405 A2406 A2407 C2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 A2435 U2441 G2445 G2446 G2447 A2448 U2449 U2457 G2458 A2459
A2468 U2474 C2475 A2476 U2477 A2478 G2484 G2494 A2497 C2498 C2501 G2502 A2503 U2504 G2505 U2506 C2517 A2518 U2519 G2529 A2542 A2547 U2552 G2553 U2554 A2566 G2567 A2572 C2573 U2580 U2585 A2602 G2603 U2604 U2605 G2608 U2609 U2613 A2614 C2636
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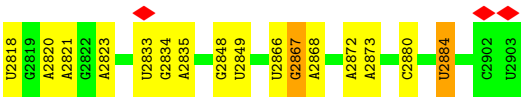
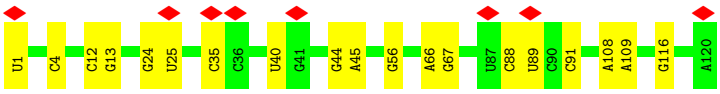


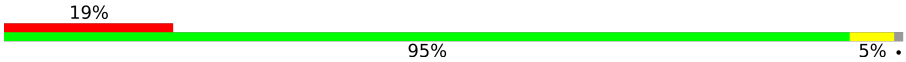
• Molecule 26: 5S ribosomal RNA

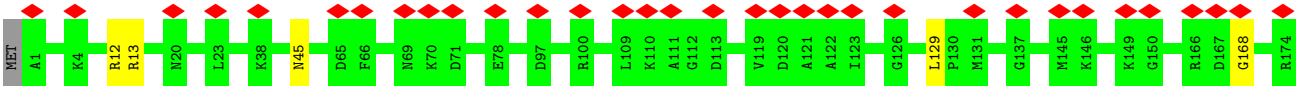
Chain B:



• Molecule 27: 50S ribosomal protein L2

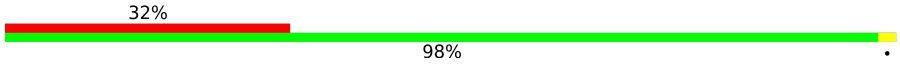
Chain C:

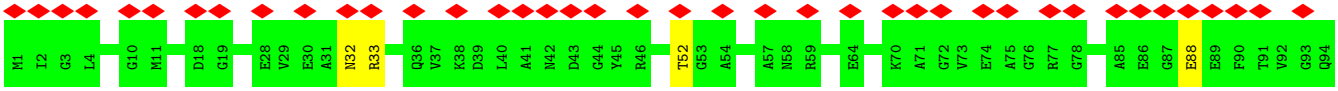


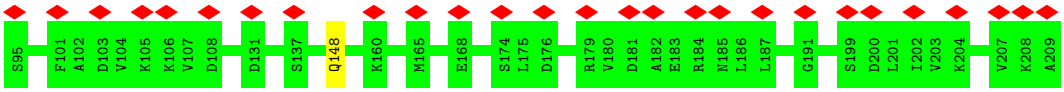


• Molecule 28: 50S ribosomal protein L3

Chain D:

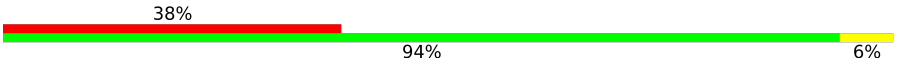


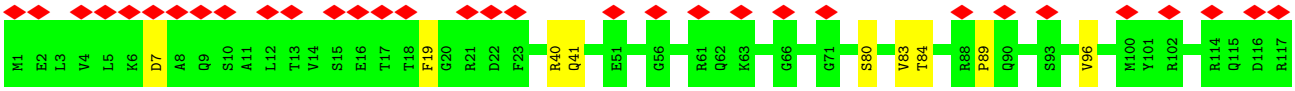


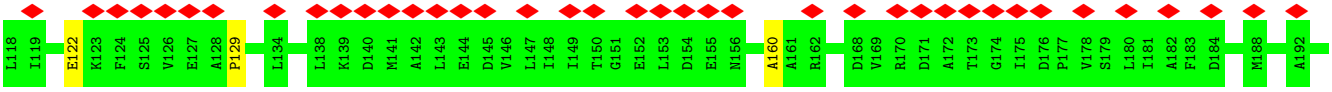


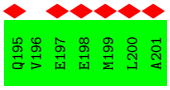
• Molecule 29: 50S ribosomal protein L4

Chain E:



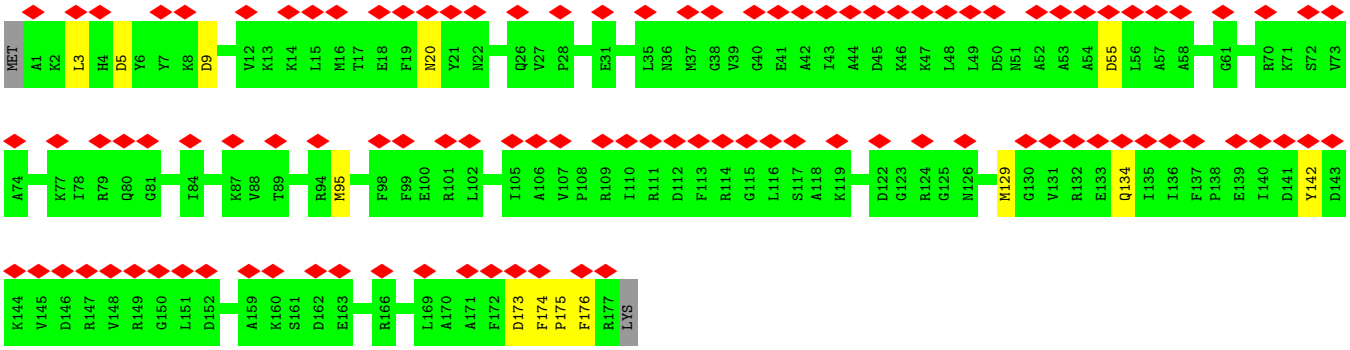






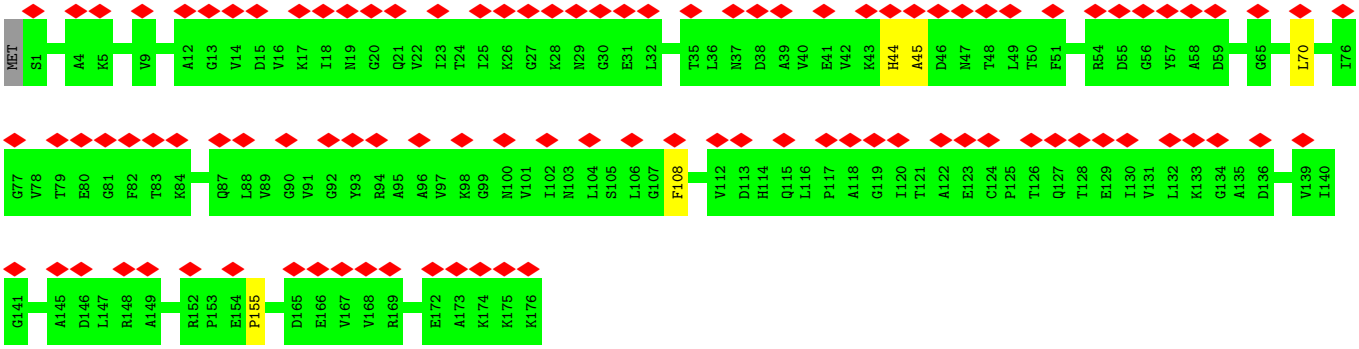
• Molecule 30: 50S ribosomal protein L5

Chain F: 59% 92% 7%



- Molecule 31: 50S ribosomal protein L6

Chain G: 57% 97%

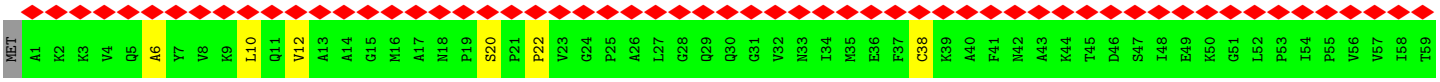


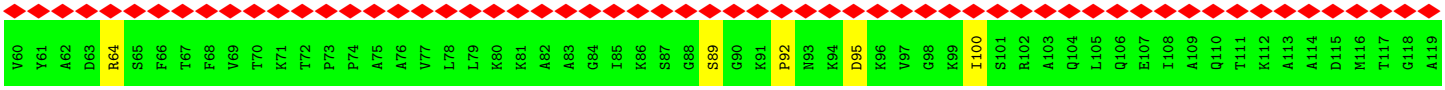
- Molecule 32: 50S ribosomal protein L9

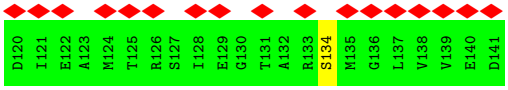
Chain H: 90% 97%

- Molecule 33: 50S ribosomal protein L11

Chain I: 96% 91% 8%

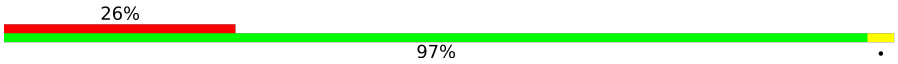


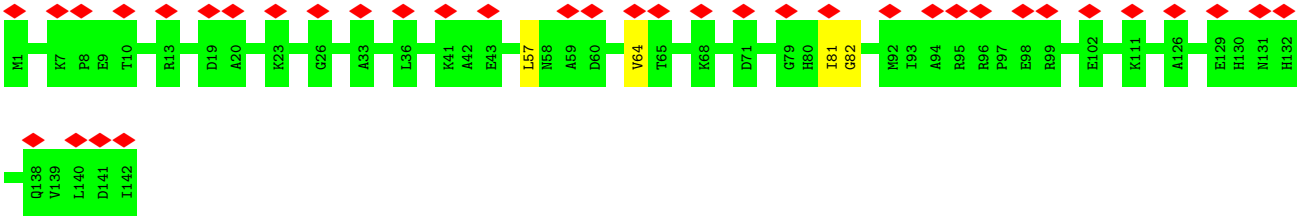




- Molecule 34: 50S ribosomal protein L13

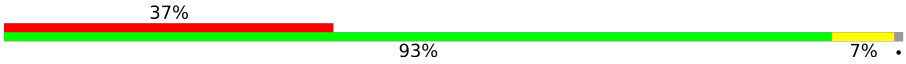
Chain J:

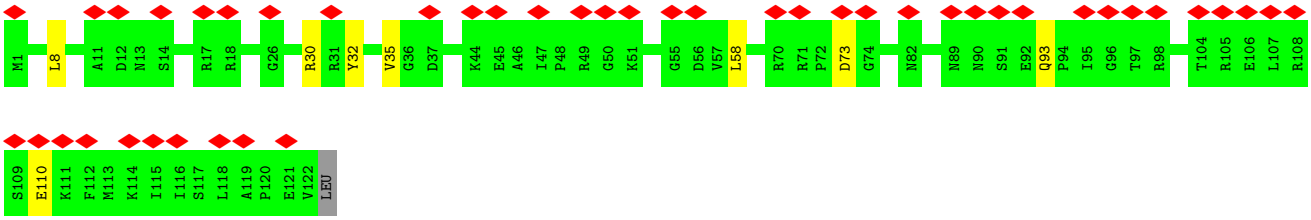




- Molecule 35: 50S ribosomal protein L14

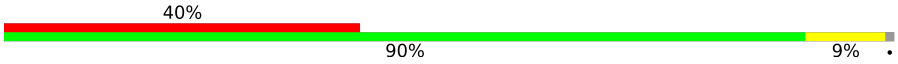
Chain K:

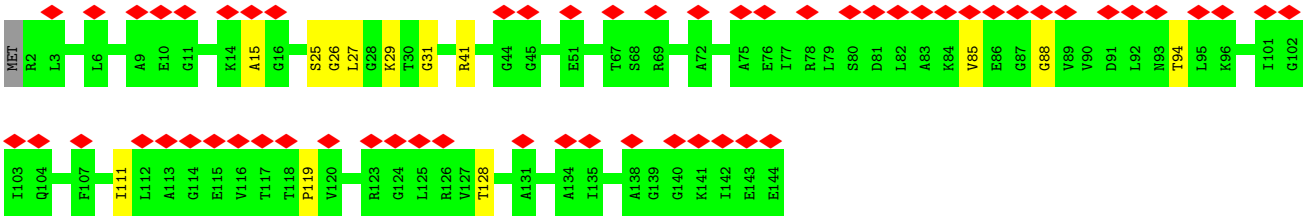




- Molecule 36: 50S ribosomal protein L15

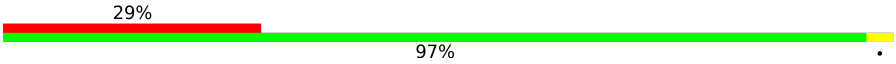
Chain L:

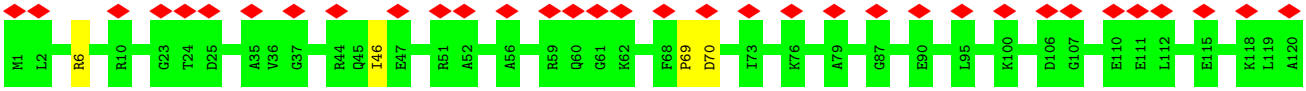


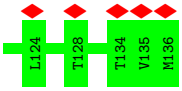


- Molecule 37: 50S ribosomal protein L16

Chain M:

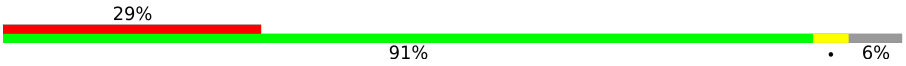


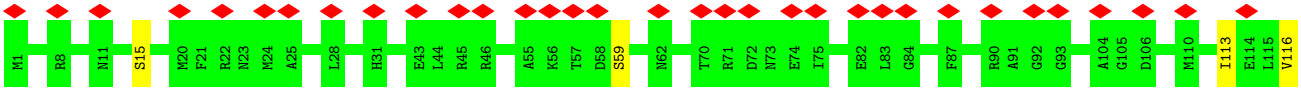


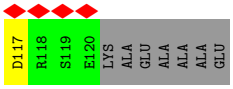


• Molecule 38: 50S ribosomal protein L17

Chain N:

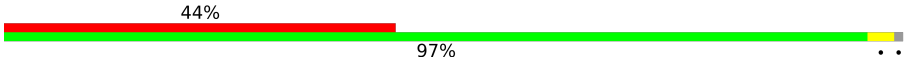


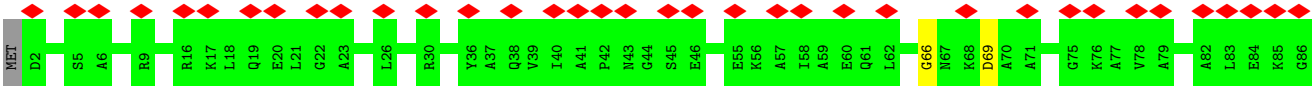


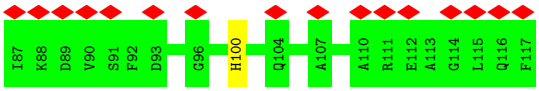


• Molecule 39: 50S ribosomal protein L18

Chain O:

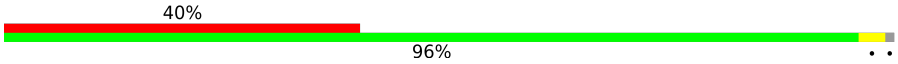


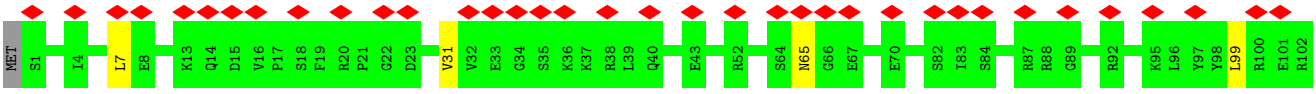


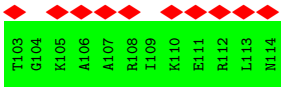


• Molecule 40: 50S ribosomal protein L19

Chain P:

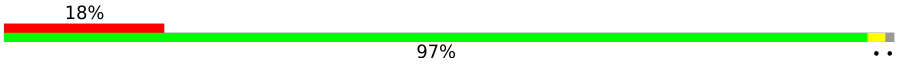


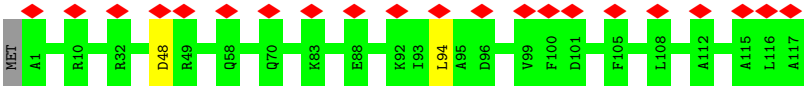




• Molecule 41: 50S ribosomal protein L20

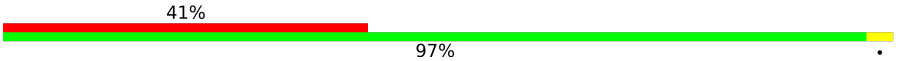
Chain Q:

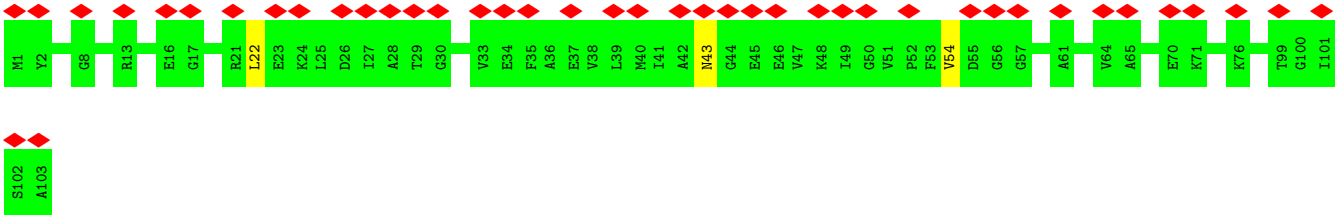




• Molecule 42: 50S ribosomal protein L21

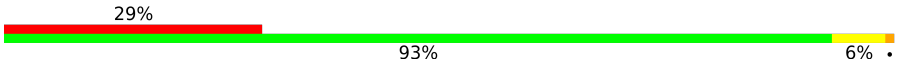
Chain R:

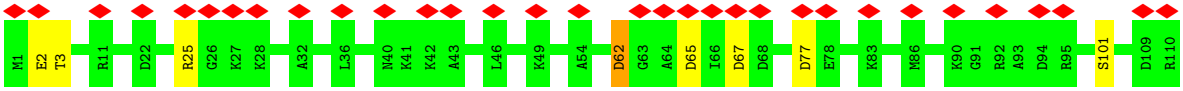




- Molecule 43: 50S ribosomal protein L22

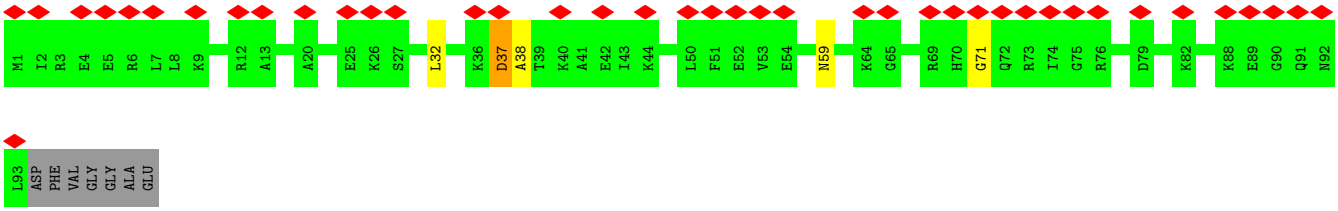
Chain S:





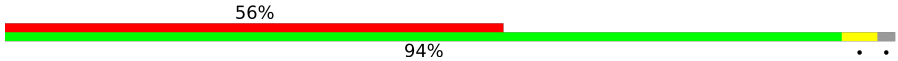
- Molecule 44: 50S ribosomal protein L23

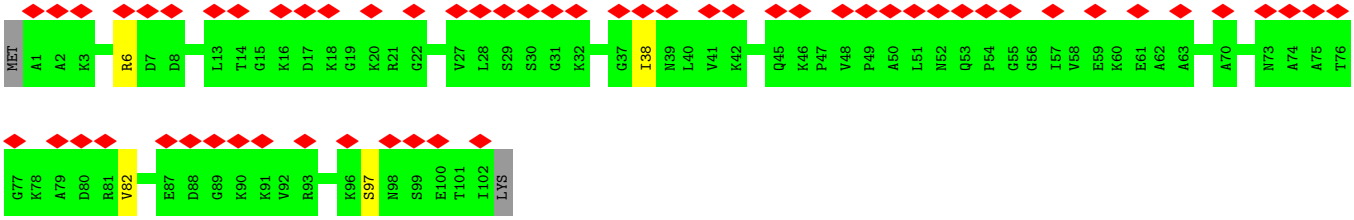
Chain T:



- Molecule 45: 50S ribosomal protein L24

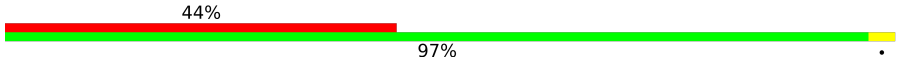
Chain U:

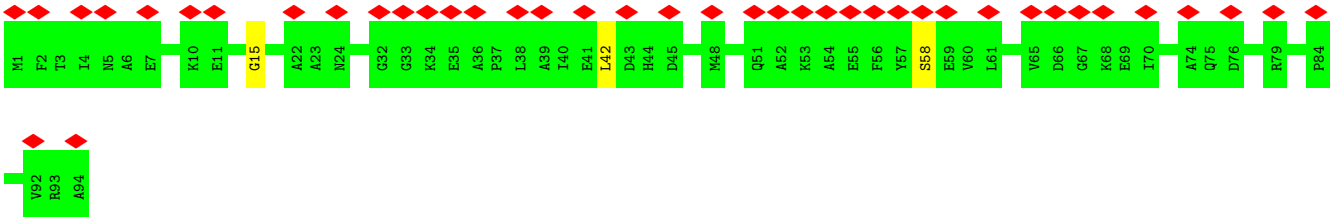




- Molecule 46: 50S ribosomal protein L25

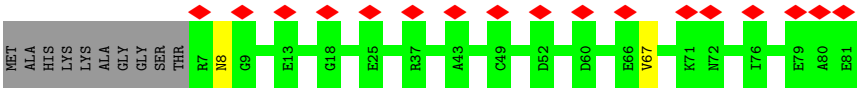
Chain V:





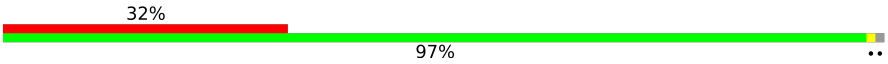
- Molecule 47: 50S ribosomal protein L27

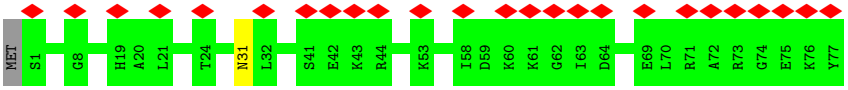
Chain W:



- Molecule 48: 50S ribosomal protein L28

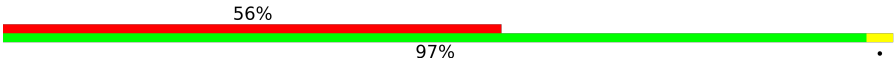
Chain X:

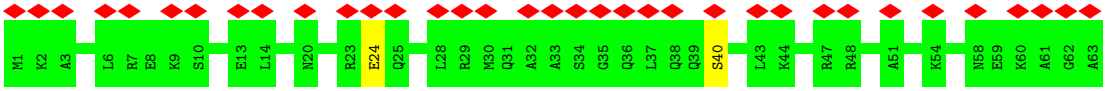




- Molecule 49: 50S ribosomal protein L29

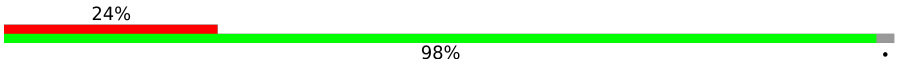
Chain Y:

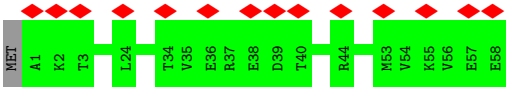




- Molecule 50: 50S ribosomal protein L30

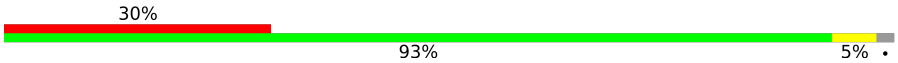
Chain Z:

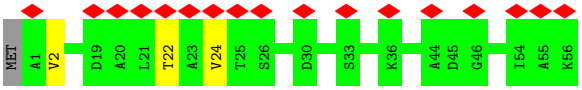




- Molecule 51: 50S ribosomal protein L32

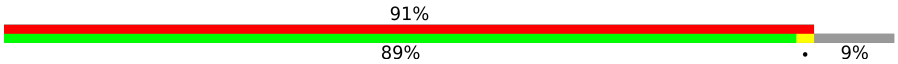
Chain 0:





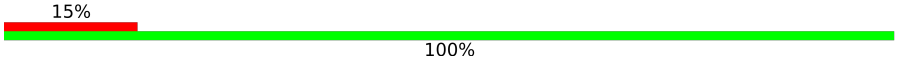
- Molecule 52: 50S ribosomal protein L33

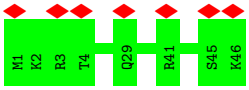
Chain 1:



- Molecule 53: 50S ribosomal protein L34

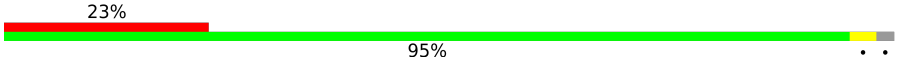
Chain 2:

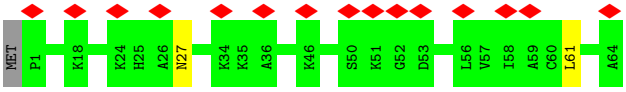




- Molecule 54: 50S ribosomal protein L35

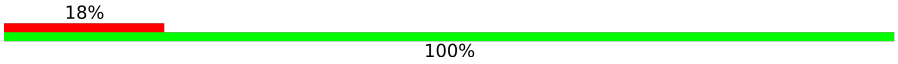
Chain 3:

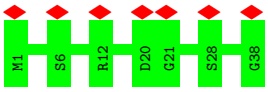




- Molecule 55: 50S ribosomal protein L36

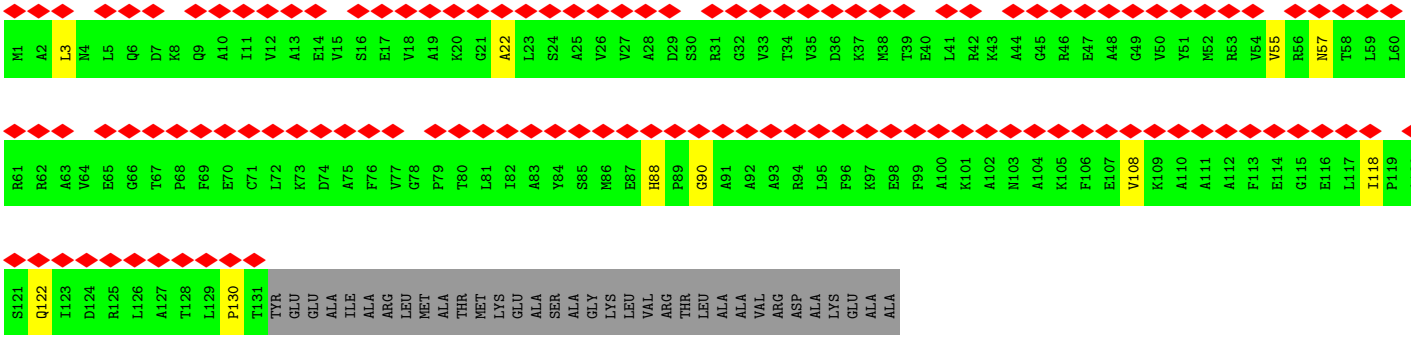
Chain 4:





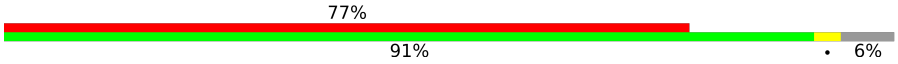
- Molecule 56: 50S ribosomal protein L10

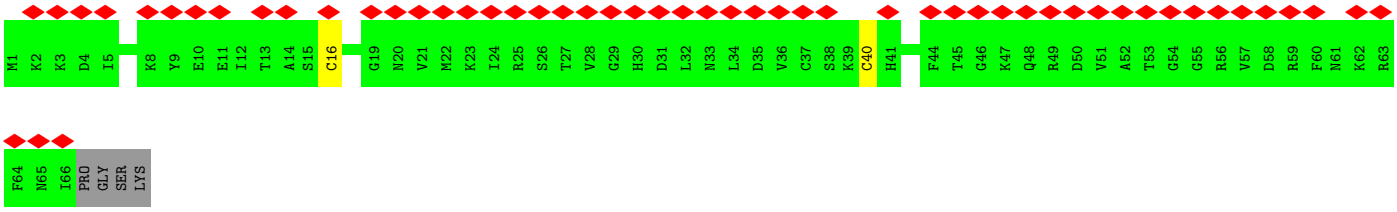
Chain 5:



- Molecule 57: 50S ribosomal protein L31

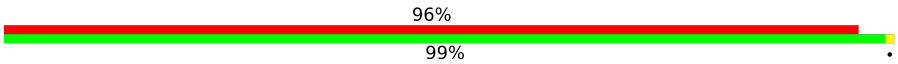
Chain 6:

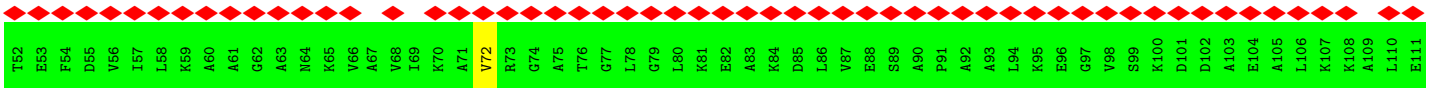


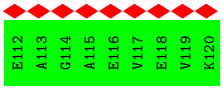


- Molecule 58: 50S ribosomal protein L7/L12

Chain 7:






E112
A113
G114
A115
E116
V117
E118
V119
K120

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	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: OMG, UR3, 5MC, 6MZ, 5MU, 4SU, MA6, 7MG, OMU, 2MG, H2U, 1MG, PSU, 4OC, 2MA, 3TD, OMC

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	0.39	1/36701 (0.0%)	0.85	12/57246 (0.0%)
2	b	0.30	0/1735	0.44	0/2338
3	d	0.28	0/1665	0.44	0/2227
4	e	0.32	0/1154	0.46	0/1554
5	f	0.35	0/835	0.48	0/1128
6	h	0.27	0/989	0.45	0/1326
7	k	0.28	0/885	0.48	0/1195
8	l	0.29	0/969	0.47	0/1300
9	o	0.32	0/722	0.44	0/964
10	p	0.33	0/659	0.46	0/884
11	q	0.28	0/657	0.46	0/881
12	r	0.28	0/511	0.43	0/689
13	t	0.38	0/671	0.48	0/888
14	u	0.29	0/500	0.42	0/668
15	v	0.42	1/1747 (0.1%)	0.82	0/2721
16	x	0.58	1/210 (0.5%)	0.78	0/324
17	w	0.17	0/2594	0.35	0/3251
18	c	0.32	0/1651	0.46	0/2225
19	g	0.36	0/1195	0.50	0/1602
20	i	0.27	0/1034	0.45	0/1375
21	j	0.36	0/796	0.54	0/1077
22	m	0.36	0/892	0.50	0/1193
23	n	0.27	0/811	0.40	0/1081
24	s	0.28	0/652	0.44	0/877
25	A	0.47	1/69174 (0.0%)	0.90	51/107910 (0.0%)
26	B	0.38	1/2876 (0.0%)	0.86	0/4483
27	C	0.31	0/2121	0.47	0/2852
28	D	0.34	0/1586	0.48	0/2134
29	E	0.26	0/1571	0.41	0/2113
30	F	0.31	0/1434	0.47	0/1926
31	G	0.35	0/1343	0.47	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	H	0.23	0/1122	0.40	0/1515
33	I	0.23	0/1046	0.44	0/1410
34	J	0.29	0/1152	0.43	0/1551
35	K	0.28	0/947	0.41	0/1268
36	L	0.26	0/1054	0.45	0/1403
37	M	0.32	0/1093	0.46	0/1460
38	N	0.28	0/973	0.44	0/1301
39	O	0.33	0/902	0.44	0/1209
40	P	0.28	0/929	0.43	0/1242
41	Q	0.34	0/960	0.43	0/1278
42	R	0.34	0/829	0.52	0/1107
43	S	0.28	0/864	0.47	0/1156
44	T	0.29	0/744	0.45	0/994
45	U	0.35	0/787	0.44	0/1051
46	V	0.31	0/766	0.45	0/1025
47	W	0.33	0/582	0.47	0/769
48	X	0.28	0/635	0.40	0/848
49	Y	0.33	0/510	0.46	0/677
50	Z	0.25	0/453	0.41	0/605
51	0	0.26	0/450	0.41	0/599
52	1	0.26	0/416	0.41	0/554
53	2	0.29	0/380	0.44	0/498
54	3	0.27	0/513	0.43	0/676
55	4	0.28	0/303	0.41	0/397
56	5	0.25	0/1001	0.45	0/1350
57	6	0.33	0/531	0.54	0/709
58	7	0.33	0/275	0.73	0/342
All	All	0.40	5/160557 (0.0%)	0.79	63/239242 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	1	U	OP3-P	-10.61	1.48	1.61
15	v	1	C	OP3-P	-10.59	1.48	1.61
25	A	1	G	OP3-P	-10.57	1.48	1.61
1	a	2	A	OP3-P	-10.49	1.48	1.61
16	x	14	U	C1'-N1	5.54	1.57	1.48

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	974	G	N1-C6-O6	9.38	125.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1936	A	N1-C6-N6	9.08	124.05	118.60
25	A	1936	A	C2-N3-C4	-7.41	106.90	110.60
25	A	783	A	N7-C8-N9	7.26	117.43	113.80
1	a	1297	G	P-O3'-C3'	7.22	128.36	119.70
25	A	783	A	C5-N7-C8	-7.16	100.32	103.90
25	A	62	U	C2-N1-C1'	6.97	126.06	117.70
1	a	530	G	P-O5'-C5'	-6.91	109.85	120.90
25	A	974	G	C6-C5-N7	-6.75	126.35	130.40
1	a	1491	G	C4'-C3'-O3'	6.63	126.26	113.00
25	A	62	U	N1-C2-O2	6.49	127.34	122.80
25	A	984	A	C2-N3-C4	-6.48	107.36	110.60
25	A	1779	U	C5-C6-N1	-6.48	119.46	122.70
25	A	783	A	N1-C6-N6	6.47	122.48	118.60
25	A	2884	U	C2-N1-C1'	6.39	125.37	117.70
25	A	2884	U	N1-C2-O2	6.24	127.17	122.80
25	A	2076	U	C2-N1-C1'	6.08	125.00	117.70
25	A	1313	U	C2-N1-C1'	5.96	124.85	117.70
25	A	62	U	N3-C2-O2	-5.94	118.04	122.20
25	A	2682	A	C8-N9-C4	5.77	108.11	105.80
25	A	974	G	N7-C8-N9	5.71	115.96	113.10
1	a	529	G	O3'-P-O5'	-5.70	93.17	104.00
1	a	1158	C	C2-N1-C1'	5.66	125.02	118.80
25	A	2501	C	C2-N1-C1'	-5.64	112.59	118.80
25	A	2884	U	N3-C2-O2	-5.62	118.27	122.20
1	a	246	A	P-O3'-C3'	5.60	126.42	119.70
25	A	458	G	C4-N9-C1'	-5.60	119.22	126.50
25	A	2542	A	C8-N9-C4	5.60	108.04	105.80
25	A	2867	G	C6-C5-N7	5.51	133.71	130.40
25	A	2867	G	C4-N9-C1'	-5.50	119.35	126.50
25	A	2867	G	N3-C4-N9	-5.49	122.70	126.00
25	A	669	G	C8-N9-C1'	-5.49	119.86	127.00
25	A	974	G	C4-C5-N7	5.44	112.98	110.80
25	A	783	A	C8-N9-C4	-5.41	103.64	105.80
25	A	783	A	C5-C6-N1	-5.40	115.00	117.70
25	A	1142	A	OP1-P-O3'	5.38	117.05	105.20
25	A	1936	A	C4-C5-N7	5.34	113.37	110.70
25	A	752	A	P-O3'-C3'	5.33	126.09	119.70
25	A	1936	A	C5-N7-C8	-5.29	101.25	103.90
25	A	2501	C	C5-C6-N1	-5.29	118.36	121.00
25	A	669	G	C4-N9-C1'	5.26	133.34	126.50
25	A	1020	A	P-O3'-C3'	5.21	125.95	119.70
1	a	1201	A	P-O3'-C3'	5.17	125.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2712	C	P-O3'-C3'	5.15	125.88	119.70
25	A	271	G	OP1-P-O3'	5.15	116.53	105.20
1	a	1158	C	N1-C2-O2	5.15	121.99	118.90
25	A	783	A	C2-N3-C4	-5.15	108.03	110.60
25	A	974	G	C5-C6-O6	-5.15	125.51	128.60
25	A	2759	G	N1-C2-N3	5.12	126.97	123.90
1	a	1306	A	N7-C8-N9	5.11	116.35	113.80
25	A	1475	G	OP2-P-O3'	5.10	116.41	105.20
25	A	974	G	C5-C6-N1	-5.09	108.96	111.50
25	A	451	U	C5-C6-N1	-5.08	120.16	122.70
25	A	1652	A	C8-N9-C4	5.08	107.83	105.80
1	a	246	A	OP1-P-O3'	5.08	116.37	105.20
1	a	16	A	C8-N9-C4	5.07	107.83	105.80
25	A	458	G	O4'-C1'-N9	5.04	112.23	108.20
25	A	543	G	C5-C6-O6	-5.04	125.58	128.60
25	A	1313	U	N1-C2-O2	5.03	126.32	122.80
25	A	1936	A	C6-C5-N7	-5.02	128.79	132.30
25	A	454	A	OP2-P-O3'	5.02	116.23	105.20
25	A	2076	U	N1-C2-O2	5.01	126.31	122.80
1	a	960	U	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

There are no planarity outliers.

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	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	2 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	2	24
4	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	1	21
5	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1	20
6	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	6	37
7	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2	22
8	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3	27
9	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	1	21
10	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	5	36
11	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1	19
12	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	15
13	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	6	37
14	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	15
17	w	637/639 (100%)	562 (88%)	51 (8%)	24 (4%)	3	28
18	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	15	52
19	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	18
20	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	1	19
21	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	1	19
22	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	2	25
23	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2	23
24	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
27	C	269/273 (98%)	242 (90%)	22 (8%)	5 (2%)	8	41
28	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	15	52
29	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	3	30
30	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	3	31
31	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	4	33
32	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	5	35
33	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	19
34	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11	46
35	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	5	36
36	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	15
37	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	5	36
39	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	17	54
40	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	17	54
41	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
42	R	101/103 (98%)	81 (80%)	18 (18%)	2 (2%)	7	40
43	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	21
44	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	4	31
45	U	100/104 (96%)	81 (81%)	16 (16%)	3 (3%)	4	33
46	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	6	38
47	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	11	46
48	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	12	48
49	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	44
50	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
51	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	8	41
52	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
53	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	9	44
55	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
56	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2	22
57	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	9	44
58	7	67/69 (97%)	58 (87%)	8 (12%)	1 (2%)	10	45
All	All	6551/6928 (95%)	5610 (86%)	716 (11%)	225 (3%)	6	31

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	e	122	VAL
5	f	63	ASN
10	p	8	ARG
11	q	79	GLU
12	r	17	VAL
17	w	76	PRO
17	w	80	ASP
17	w	176	ASP
17	w	334	PRO

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Mol	Chain	Res	Type
17	w	342	PRO
17	w	344	PRO
17	w	416	PRO
17	w	433	HIS
17	w	438	PRO
17	w	612	VAL
17	w	617	PRO
17	w	624	PRO
18	c	156	LEU
20	i	12	LYS
20	i	71	ILE
21	j	57	VAL
21	j	75	ASP
21	j	89	ARG
27	C	204	LEU
30	F	175	PRO
31	G	108	PHE
34	J	81	ILE
35	K	93	GLN
36	L	15	ALA
36	L	85	VAL
36	L	128	THR
43	S	67	ASP
45	U	6	ARG
45	U	97	SER
48	X	31	ASN
54	3	27	ASN
2	b	17	HIS
2	b	19	THR
2	b	179	GLY
3	d	26	ALA
3	d	108	ALA
4	e	23	THR
4	e	93	VAL
6	h	66	GLN
7	k	76	TYR
7	k	77	GLY
7	k	88	PRO
8	l	75	GLU
9	o	21	THR
9	o	45	HIS
11	q	17	GLU

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Mol	Chain	Res	Type
11	q	49	ASN
12	r	46	THR
13	t	68	LYS
14	u	12	ASP
17	w	41	THR
17	w	96	ILE
18	c	13	ILE
19	g	16	LYS
19	g	56	SER
19	g	63	VAL
19	g	112	ASP
19	g	145	GLU
20	i	57	VAL
21	j	29	ALA
21	j	77	VAL
22	m	104	ASN
23	n	54	ASP
27	C	195	GLY
27	C	231	HIS
32	H	9	VAL
33	I	89	SER
33	I	92	PRO
35	K	35	VAL
35	K	110	GLU
36	L	29	LYS
36	L	31	GLY
36	L	111	ILE
37	M	70	ASP
39	O	66	GLY
40	P	65	ASN
42	R	43	ASN
42	R	54	VAL
43	S	2	GLU
43	S	3	THR
44	T	37	ASP
44	T	38	ALA
44	T	71	GLY
49	Y	24	GLU
56	5	55	VAL
2	b	73	ARG
2	b	87	ASP
2	b	153	MET

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Mol	Chain	Res	Type
3	d	7	LYS
3	d	31	CYS
3	d	152	SER
3	d	166	LYS
3	d	174	ALA
4	e	98	ALA
4	e	99	SER
4	e	121	ASN
5	f	54	LEU
5	f	92	THR
6	h	74	ILE
7	k	14	GLN
8	l	2	THR
8	l	46	SER
9	o	2	LEU
9	o	13	GLU
10	p	49	GLY
11	q	16	MET
13	t	76	ALA
14	u	29	ALA
14	u	32	ARG
14	u	34	ARG
17	w	8	VAL
17	w	371	SER
19	g	64	ALA
19	g	95	ARG
20	i	90	ASP
20	i	107	ALA
20	i	125	GLN
21	j	35	GLN
22	m	6	ILE
22	m	7	ASN
22	m	113	LYS
23	n	22	LYS
23	n	38	ASP
23	n	55	SER
27	C	239	PHE
29	E	89	PRO
29	E	122	GLU
31	G	44	HIS
31	G	45	ALA
32	H	15	LEU

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Mol	Chain	Res	Type
33	I	12	VAL
33	I	64	ARG
36	L	88	GLY
37	M	6	ARG
38	N	59	SER
43	S	62	ASP
56	5	88	HIS
56	5	118	ILE
57	6	40	CYS
2	b	11	ALA
2	b	88	GLN
2	b	126	ASP
4	e	100	GLU
4	e	102	THR
5	f	56	LYS
5	f	86	ARG
5	f	99	ALA
6	h	22	ALA
7	k	92	ARG
8	l	23	LEU
9	o	75	ALA
12	r	18	GLN
12	r	71	ASP
17	w	40	THR
17	w	262	ARG
17	w	470	ASN
19	g	29	LEU
20	i	99	LYS
28	D	32	ASN
29	E	80	SER
29	E	160	ALA
30	F	20	ASN
30	F	142	TYR
30	F	173	ASP
30	F	176	PHE
32	H	2	GLN
33	I	6	ALA
33	I	20	SER
36	L	25	SER
38	N	117	ASP
43	S	65	ASP
46	V	58	SER

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Mol	Chain	Res	Type
47	W	8	ASN
51	0	2	VAL
56	5	22	ALA
56	5	90	GLY
56	5	130	PRO
58	7	72	VAL
2	b	14	HIS
3	d	34	GLU
12	r	70	THR
17	w	161	TYR
17	w	609	GLY
17	w	630	LYS
23	n	2	LYS
29	E	84	THR
30	F	174	PHE
31	G	70	LEU
32	H	3	VAL
33	I	22	PRO
33	I	100	ILE
34	J	82	GLY
36	L	94	THR
3	d	6	PRO
3	d	28	ASP
20	i	13	SER
28	D	148	GLN
29	E	83	VAL
33	I	38	CYS
36	L	119	PRO
43	S	101	SER
7	k	119	GLY
8	l	44	PRO
17	w	75	THR
27	C	168	GLY
36	L	26	GLY
37	M	69	PRO
38	N	116	VAL
11	q	20	ILE
14	u	9	GLU
45	U	38	ILE
19	g	5	VAL
29	E	129	PRO
46	V	15	GLY

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Mol	Chain	Res	Type
56	5	108	VAL
17	w	621	PRO
19	g	28	ILE
4	e	26	GLY
22	m	9	PRO
31	G	155	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	180/198 (91%)	175 (97%)	5 (3%)	43	66
3	d	172/173 (99%)	166 (96%)	6 (4%)	36	62
4	e	114/126 (90%)	105 (92%)	9 (8%)	12	41
5	f	87/116 (75%)	83 (95%)	4 (5%)	27	55
6	h	104/105 (99%)	103 (99%)	1 (1%)	76	86
7	k	89/99 (90%)	87 (98%)	2 (2%)	52	71
8	l	103/104 (99%)	100 (97%)	3 (3%)	42	65
9	o	76/77 (99%)	74 (97%)	2 (3%)	46	68
10	p	65/65 (100%)	61 (94%)	4 (6%)	18	48
11	q	74/78 (95%)	71 (96%)	3 (4%)	30	58
12	r	48/65 (74%)	47 (98%)	1 (2%)	53	73
13	t	65/66 (98%)	63 (97%)	2 (3%)	40	64
14	u	44/61 (72%)	42 (96%)	2 (4%)	27	56
17	w	6/576 (1%)	6 (100%)	0	100	100
18	c	170/190 (90%)	163 (96%)	7 (4%)	30	58
19	g	124/147 (84%)	122 (98%)	2 (2%)	62	79
20	i	105/107 (98%)	100 (95%)	5 (5%)	25	54
21	j	86/90 (96%)	84 (98%)	2 (2%)	50	71
22	m	92/96 (96%)	90 (98%)	2 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	n	79/84 (94%)	75 (95%)	4 (5%)	24	53
24	s	70/79 (89%)	69 (99%)	1 (1%)	67	81
27	C	216/218 (99%)	208 (96%)	8 (4%)	34	60
28	D	164/164 (100%)	161 (98%)	3 (2%)	59	77
29	E	165/165 (100%)	160 (97%)	5 (3%)	41	64
30	F	148/150 (99%)	141 (95%)	7 (5%)	26	55
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	I	109/110 (99%)	106 (97%)	3 (3%)	43	66
34	J	116/116 (100%)	114 (98%)	2 (2%)	60	78
35	K	103/104 (99%)	98 (95%)	5 (5%)	25	54
36	L	102/103 (99%)	100 (98%)	2 (2%)	55	74
37	M	109/109 (100%)	108 (99%)	1 (1%)	78	87
38	N	100/103 (97%)	98 (98%)	2 (2%)	55	74
39	O	86/87 (99%)	84 (98%)	2 (2%)	50	71
40	P	99/100 (99%)	96 (97%)	3 (3%)	41	64
41	Q	89/90 (99%)	87 (98%)	2 (2%)	52	71
42	R	84/84 (100%)	83 (99%)	1 (1%)	71	83
43	S	93/93 (100%)	90 (97%)	3 (3%)	39	63
44	T	80/84 (95%)	77 (96%)	3 (4%)	33	59
45	U	83/85 (98%)	82 (99%)	1 (1%)	71	83
46	V	78/78 (100%)	77 (99%)	1 (1%)	69	82
47	W	57/63 (90%)	56 (98%)	1 (2%)	59	77
48	X	67/68 (98%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	54 (98%)	1 (2%)	59	77
50	Z	48/49 (98%)	48 (100%)	0	100	100
51	0	47/48 (98%)	45 (96%)	2 (4%)	29	57
52	1	45/49 (92%)	44 (98%)	1 (2%)	52	71
53	2	38/38 (100%)	38 (100%)	0	100	100
54	3	51/52 (98%)	50 (98%)	1 (2%)	55	74
55	4	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	5	100/123 (81%)	97 (97%)	3 (3%)	41	64
57	6	59/62 (95%)	58 (98%)	1 (2%)	60	78
All	All	4829/5638 (86%)	4698 (97%)	131 (3%)	48	67

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	9	LEU
2	b	35	ASN
2	b	71	THR
2	b	185	ILE
2	b	202	ASN
3	d	16	THR
3	d	52	VAL
3	d	115	GLN
3	d	119	HIS
3	d	141	VAL
3	d	196	GLU
4	e	10	LEU
4	e	11	GLN
4	e	45	VAL
4	e	51	LYS
4	e	75	LEU
4	e	122	VAL
4	e	140	ILE
4	e	156	ARG
4	e	158	LYS
5	f	54	LEU
5	f	74	LEU
5	f	86	ARG
5	f	89	VAL
6	h	58	LEU
7	k	30	ILE
7	k	39	ASN
8	l	20	VAL
8	l	28	GLN
8	l	63	THR
9	o	44	GLU
9	o	86	LEU
10	p	19	VAL
10	p	26	ASN

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Mol	Chain	Res	Type
10	p	34	GLU
10	p	70	ARG
11	q	51	GLU
11	q	61	ARG
11	q	69	THR
12	r	24	ASP
13	t	22	SER
13	t	26	MET
14	u	19	LYS
14	u	23	GLU
18	c	3	LYS
18	c	40	GLN
18	c	96	VAL
18	c	127	VAL
18	c	133	MET
18	c	149	LYS
18	c	156	LEU
19	g	58	LEU
19	g	83	THR
20	i	38	PHE
20	i	54	VAL
20	i	60	LEU
20	i	88	GLU
20	i	108	ARG
21	j	10	LEU
21	j	64	GLN
22	m	15	VAL
22	m	99	GLN
23	n	26	LEU
23	n	33	VAL
23	n	49	GLN
23	n	60	GLN
24	s	62	THR
27	C	12	ARG
27	C	13	ARG
27	C	45	ASN
27	C	129	LEU
27	C	181	ARG
27	C	206	LYS
27	C	212	TRP
27	C	257	ARG
28	D	33	ARG

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Mol	Chain	Res	Type
28	D	52	THR
28	D	88	GLU
29	E	7	ASP
29	E	19	PHE
29	E	40	ARG
29	E	41	GLN
29	E	96	VAL
30	F	3	LEU
30	F	5	ASP
30	F	9	ASP
30	F	55	ASP
30	F	95	MET
30	F	129	MET
30	F	134	GLN
33	I	10	LEU
33	I	95	ASP
33	I	134	SER
34	J	57	LEU
34	J	64	VAL
35	K	8	LEU
35	K	30	ARG
35	K	32	TYR
35	K	58	LEU
35	K	73	ASP
36	L	27	LEU
36	L	41	ARG
37	M	46	ILE
38	N	15	SER
38	N	113	ILE
39	O	69	ASP
39	O	100	HIS
40	P	7	LEU
40	P	31	VAL
40	P	99	LEU
41	Q	48	ASP
41	Q	94	LEU
42	R	22	LEU
43	S	25	ARG
43	S	62	ASP
43	S	77	ASP
44	T	32	LEU
44	T	37	ASP

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Mol	Chain	Res	Type
44	T	59	ASN
45	U	82	VAL
46	V	42	LEU
47	W	67	VAL
49	Y	40	SER
51	0	22	THR
51	0	24	VAL
52	1	46	VAL
54	3	61	LEU
56	5	3	LEU
56	5	57	ASN
56	5	122	GLN
57	6	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	202	ASN
3	d	70	GLN
3	d	119	HIS
3	d	135	GLN
5	f	11	HIS
7	k	39	ASN
8	l	76	HIS
9	o	45	HIS
10	p	26	ASN
11	q	30	HIS
12	r	51	GLN
18	c	40	GLN
19	g	141	HIS
21	j	64	GLN
21	j	70	HIS
22	m	90	HIS
23	n	49	GLN
24	s	51	HIS
24	s	56	HIS
27	C	196	ASN
28	D	49	GLN
28	D	149	ASN
30	F	134	GLN
31	G	103	ASN
31	G	138	GLN

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Mol	Chain	Res	Type
34	J	40	HIS
41	Q	71	ASN
43	S	61	ASN
45	U	65	GLN
51	0	5	ASN
57	6	65	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	254 (16%)	0
15	v	76/78 (97%)	17 (22%)	0
16	x	8/11 (72%)	0	0
25	A	2894/2903 (99%)	542 (18%)	91 (3%)
26	B	119/120 (99%)	17 (14%)	4 (3%)
All	All	4632/4651 (99%)	830 (17%)	95 (2%)

All (830) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A
1	a	39	G
1	a	47	C
1	a	49	U
1	a	51	A
1	a	71	A
1	a	85	U
1	a	86	G
1	a	87	C
1	a	94	G
1	a	95	C
1	a	120	A
1	a	121	U
1	a	130	A
1	a	174	A
1	a	175	C
1	a	181	A

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Mol	Chain	Res	Type
1	a	183	C
1	a	184	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	246	A
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	306	A
1	a	321	A
1	a	328	C
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	355	C
1	a	367	U
1	a	368	U
1	a	372	C
1	a	373	A
1	a	387	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	439	U
1	a	467	U

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Mol	Chain	Res	Type
1	a	468	A
1	a	482	A
1	a	484	G
1	a	485	U
1	a	486	U
1	a	496	A
1	a	497	G
1	a	500	G
1	a	511	C
1	a	527	7MG
1	a	530	G
1	a	531	U
1	a	532	A
1	a	533	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	597	G
1	a	618	C
1	a	626	G
1	a	633	G
1	a	641	U
1	a	642	A
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	688	G
1	a	701	U
1	a	702	A
1	a	703	G

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Mol	Chain	Res	Type
1	a	724	G
1	a	731	G
1	a	755	G
1	a	777	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	871	U
1	a	874	G
1	a	884	U
1	a	890	G
1	a	902	G
1	a	914	A
1	a	920	U
1	a	921	U
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	979	C
1	a	981	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1004	A
1	a	1026	G

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Mol	Chain	Res	Type
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1056	U
1	a	1065	U
1	a	1067	A
1	a	1085	U
1	a	1086	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1127	G
1	a	1129	C
1	a	1130	A
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1152	A
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1198	G
1	a	1200	C
1	a	1201	A
1	a	1202	U
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1224	U
1	a	1225	A

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Mol	Chain	Res	Type
1	a	1226	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1331	G
1	a	1332	A
1	a	1346	A
1	a	1347	G
1	a	1348	U
1	a	1353	G
1	a	1363	A
1	a	1381	U
1	a	1395	C
1	a	1396	A
1	a	1397	C
1	a	1399	C
1	a	1400	C
1	a	1401	G
1	a	1418	A

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Mol	Chain	Res	Type
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1448	C
1	a	1451	U
1	a	1452	C
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1502	A
1	a	1503	A
1	a	1505	G
1	a	1506	U
1	a	1507	A
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
15	v	7	G
15	v	8	4SU
15	v	9	G
15	v	14	A
15	v	16	C
15	v	17	C
15	v	17(A)	U
15	v	18	G
15	v	19	G
15	v	20	H2U
15	v	21	A
15	v	22	G
15	v	59	A
15	v	60	U
15	v	67	C
15	v	75	C
15	v	76	A
25	A	10	A
25	A	12	U

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Mol	Chain	Res	Type
25	A	23	G
25	A	27	G
25	A	28	A
25	A	34	U
25	A	35	G
25	A	42	A
25	A	46	G
25	A	49	A
25	A	51	G
25	A	52	A
25	A	60	G
25	A	63	A
25	A	71	A
25	A	73	A
25	A	74	A
25	A	75	G
25	A	91	A
25	A	92	U
25	A	103	A
25	A	110	G
25	A	118	A
25	A	119	A
25	A	120	U
25	A	127	A
25	A	138	U
25	A	139	U
25	A	140	C
25	A	141	G
25	A	142	A
25	A	158	U
25	A	162	U
25	A	163	C
25	A	181	A
25	A	196	A
25	A	199	A
25	A	204	A
25	A	205	G
25	A	215	G
25	A	216	A
25	A	218	A
25	A	219	A
25	A	221	A

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Mol	Chain	Res	Type
25	A	222	A
25	A	227	A
25	A	228	C
25	A	242	G
25	A	243	U
25	A	248	G
25	A	249	C
25	A	255	A
25	A	265	A
25	A	266	G
25	A	267	C
25	A	272	A
25	A	276	U
25	A	278	A
25	A	281	C
25	A	294	A
25	A	301	G
25	A	302	C
25	A	311	A
25	A	321	U
25	A	322	A
25	A	323	C
25	A	324	A
25	A	329	G
25	A	330	A
25	A	333	G
25	A	334	C
25	A	346	A
25	A	353	C
25	A	361	G
25	A	362	A
25	A	370	G
25	A	371	A
25	A	372	G
25	A	373	U
25	A	386	G
25	A	387	U
25	A	390	U
25	A	391	A
25	A	404	A
25	A	405	U
25	A	406	G

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Mol	Chain	Res	Type
25	A	411	G
25	A	422	A
25	A	424	G
25	A	442	G
25	A	446	G
25	A	454	A
25	A	455	C
25	A	457	A
25	A	458	G
25	A	459	U
25	A	467	G
25	A	480	A
25	A	481	G
25	A	490	C
25	A	491	G
25	A	504	A
25	A	505	A
25	A	506	G
25	A	508	A
25	A	518	G
25	A	527	C
25	A	529	A
25	A	530	G
25	A	532	A
25	A	533	G
25	A	542	C
25	A	543	G
25	A	545	U
25	A	547	A
25	A	550	C
25	A	555	G
25	A	563	A
25	A	572	A
25	A	573	U
25	A	575	A
25	A	603	A
25	A	614	A
25	A	616	A
25	A	627	A
25	A	637	A
25	A	645	C
25	A	646	U

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Mol	Chain	Res	Type
25	A	654	A
25	A	655	A
25	A	659	G
25	A	668	A
25	A	669	G
25	A	670	A
25	A	677	A
25	A	685	A
25	A	686	U
25	A	687	C
25	A	694	U
25	A	695	G
25	A	717	C
25	A	726	G
25	A	730	A
25	A	740	C
25	A	747	5MC
25	A	748	G
25	A	752	A
25	A	753	A
25	A	765	C
25	A	772	C
25	A	775	G
25	A	776	G
25	A	777	G
25	A	782	A
25	A	784	G
25	A	785	G
25	A	789	A
25	A	791	C
25	A	801	G
25	A	802	A
25	A	805	G
25	A	806	C
25	A	812	C
25	A	819	A
25	A	822	G
25	A	827	U
25	A	828	U
25	A	830	G
25	A	831	G
25	A	845	A

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Mol	Chain	Res	Type
25	A	846	U
25	A	847	U
25	A	858	G
25	A	859	G
25	A	860	U
25	A	878	A
25	A	896	A
25	A	897	C
25	A	907	G
25	A	910	A
25	A	932	U
25	A	941	A
25	A	946	C
25	A	953	G
25	A	958	U
25	A	961	C
25	A	974	G
25	A	975	A
25	A	982	C
25	A	983	A
25	A	985	C
25	A	989	G
25	A	990	A
25	A	995	C
25	A	996	A
25	A	999	U
25	A	1011	G
25	A	1012	U
25	A	1013	C
25	A	1021	A
25	A	1022	G
25	A	1023	U
25	A	1026	G
25	A	1033	U
25	A	1046	A
25	A	1053	C
25	A	1054	A
25	A	1057	A
25	A	1060	U
25	A	1061	U
25	A	1062	G
25	A	1064	C

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Mol	Chain	Res	Type
25	A	1065	U
25	A	1066	U
25	A	1068	G
25	A	1069	A
25	A	1070	A
25	A	1071	G
25	A	1072	C
25	A	1075	C
25	A	1076	C
25	A	1079	C
25	A	1084	A
25	A	1088	A
25	A	1089	A
25	A	1090	A
25	A	1104	C
25	A	1111	A
25	A	1112	G
25	A	1119	U
25	A	1130	U
25	A	1131	G
25	A	1132	U
25	A	1134	A
25	A	1135	C
25	A	1142	A
25	A	1143	A
25	A	1151	A
25	A	1174	U
25	A	1175	A
25	A	1176	U
25	A	1179	G
25	A	1180	U
25	A	1206	G
25	A	1212	G
25	A	1213	A
25	A	1218	G
25	A	1237	A
25	A	1238	G
25	A	1247	A
25	A	1248	G
25	A	1250	G
25	A	1251	C
25	A	1253	A

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Mol	Chain	Res	Type
25	A	1256	G
25	A	1271	G
25	A	1272	A
25	A	1273	U
25	A	1276	A
25	A	1289	C
25	A	1298	C
25	A	1300	G
25	A	1301	A
25	A	1302	A
25	A	1311	G
25	A	1315	C
25	A	1321	A
25	A	1329	U
25	A	1330	C
25	A	1332	G
25	A	1341	G
25	A	1345	C
25	A	1352	U
25	A	1365	A
25	A	1368	G
25	A	1378	A
25	A	1379	U
25	A	1380	G
25	A	1383	A
25	A	1385	A
25	A	1395	A
25	A	1397	U
25	A	1416	G
25	A	1419	A
25	A	1420	A
25	A	1428	C
25	A	1454	C
25	A	1458	U
25	A	1461	C
25	A	1482	G
25	A	1483	G
25	A	1490	A
25	A	1491	G
25	A	1493	C
25	A	1504	A
25	A	1515	A

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Mol	Chain	Res	Type
25	A	1524	G
25	A	1533	C
25	A	1535	A
25	A	1536	C
25	A	1537	G
25	A	1555	G
25	A	1559	U
25	A	1560	G
25	A	1567	G
25	A	1569	A
25	A	1578	U
25	A	1581	G
25	A	1585	C
25	A	1607	C
25	A	1611	C
25	A	1616	A
25	A	1627	G
25	A	1647	U
25	A	1648	U
25	A	1651	G
25	A	1654	A
25	A	1664	A
25	A	1665	A
25	A	1667	G
25	A	1674	G
25	A	1694	C
25	A	1695	G
25	A	1715	G
25	A	1729	U
25	A	1730	C
25	A	1738	G
25	A	1756	G
25	A	1758	U
25	A	1764	C
25	A	1773	A
25	A	1780	A
25	A	1781	U
25	A	1782	U
25	A	1784	A
25	A	1787	A
25	A	1800	C
25	A	1801	A

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Mol	Chain	Res	Type
25	A	1808	A
25	A	1816	C
25	A	1818	U
25	A	1829	A
25	A	1833	C
25	A	1847	G
25	A	1858	A
25	A	1865	U
25	A	1871	A
25	A	1885	A
25	A	1896	G
25	A	1900	A
25	A	1901	A
25	A	1906	G
25	A	1907	G
25	A	1913	A
25	A	1914	C
25	A	1927	A
25	A	1929	G
25	A	1930	G
25	A	1931	U
25	A	1937	A
25	A	1938	A
25	A	1940	U
25	A	1941	C
25	A	1955	U
25	A	1960	A
25	A	1962	5MC
25	A	1963	U
25	A	1967	C
25	A	1970	A
25	A	1971	U
25	A	1972	G
25	A	1981	A
25	A	1991	U
25	A	1992	G
25	A	1993	U
25	A	1997	C
25	A	2022	U
25	A	2023	C
25	A	2031	A
25	A	2033	A

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Mol	Chain	Res	Type
25	A	2043	C
25	A	2049	G
25	A	2052	A
25	A	2055	C
25	A	2056	G
25	A	2060	A
25	A	2061	G
25	A	2062	A
25	A	2069	7MG
25	A	2093	G
25	A	2095	A
25	A	2096	C
25	A	2098	U
25	A	2108	A
25	A	2110	G
25	A	2111	U
25	A	2112	G
25	A	2113	U
25	A	2118	U
25	A	2119	A
25	A	2127	G
25	A	2131	U
25	A	2132	U
25	A	2133	G
25	A	2145	C
25	A	2146	C
25	A	2157	G
25	A	2162	G
25	A	2164	C
25	A	2172	U
25	A	2173	A
25	A	2189	U
25	A	2192	U
25	A	2198	A
25	A	2199	A
25	A	2204	G
25	A	2211	A
25	A	2212	A
25	A	2213	U
25	A	2225	A
25	A	2238	G
25	A	2239	G

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Mol	Chain	Res	Type
25	A	2250	G
25	A	2268	A
25	A	2273	A
25	A	2278	A
25	A	2283	C
25	A	2287	A
25	A	2288	A
25	A	2297	A
25	A	2305	U
25	A	2309	A
25	A	2311	A
25	A	2312	U
25	A	2320	U
25	A	2325	G
25	A	2327	A
25	A	2334	U
25	A	2336	A
25	A	2337	G
25	A	2345	G
25	A	2347	C
25	A	2350	C
25	A	2382	G
25	A	2383	G
25	A	2385	C
25	A	2391	G
25	A	2392	A
25	A	2402	U
25	A	2406	A
25	A	2407	A
25	A	2423	U
25	A	2424	C
25	A	2426	A
25	A	2427	C
25	A	2428	G
25	A	2429	G
25	A	2430	A
25	A	2435	A
25	A	2441	U
25	A	2445	2MG
25	A	2447	G
25	A	2448	A
25	A	2449	H2U

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Mol	Chain	Res	Type
25	A	2459	A
25	A	2468	A
25	A	2476	A
25	A	2478	A
25	A	2484	G
25	A	2494	G
25	A	2497	A
25	A	2498	OMC
25	A	2502	G
25	A	2504	PSU
25	A	2505	G
25	A	2506	U
25	A	2517	C
25	A	2518	A
25	A	2519	U
25	A	2529	G
25	A	2547	A
25	A	2554	U
25	A	2567	G
25	A	2572	A
25	A	2573	C
25	A	2585	U
25	A	2602	A
25	A	2603	G
25	A	2608	G
25	A	2609	U
25	A	2613	U
25	A	2614	A
25	A	2636	C
25	A	2645	G
25	A	2646	C
25	A	2655	G
25	A	2656	U
25	A	2682	A
25	A	2689	U
25	A	2690	U
25	A	2707	U
25	A	2712	C
25	A	2713	U
25	A	2714	G
25	A	2718	G
25	A	2722	G

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Mol	Chain	Res	Type
25	A	2726	A
25	A	2731	G
25	A	2732	G
25	A	2733	A
25	A	2739	U
25	A	2744	G
25	A	2748	A
25	A	2757	A
25	A	2764	A
25	A	2765	A
25	A	2769	U
25	A	2778	A
25	A	2779	U
25	A	2791	G
25	A	2794	C
25	A	2797	U
25	A	2799	A
25	A	2800	A
25	A	2801	G
25	A	2808	G
25	A	2809	A
25	A	2818	U
25	A	2820	A
25	A	2821	A
25	A	2823	A
25	A	2833	U
25	A	2834	G
25	A	2835	A
25	A	2848	G
25	A	2849	U
25	A	2867	G
25	A	2868	A
25	A	2872	A
25	A	2873	A
25	A	2880	C
25	A	2884	U
26	B	4	C
26	B	12	C
26	B	13	G
26	B	24	G
26	B	25	U
26	B	35	C

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Mol	Chain	Res	Type
26	B	40	U
26	B	44	G
26	B	45	A
26	B	56	G
26	B	67	G
26	B	88	C
26	B	89	U
26	B	91	C
26	B	108	A
26	B	109	A
26	B	116	G

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	51	G
25	A	86	G
25	A	204	A
25	A	227	A
25	A	242	G
25	A	265	A
25	A	271	G
25	A	301	G
25	A	311	A
25	A	321	U
25	A	332	A
25	A	345	A
25	A	372	G
25	A	386	G
25	A	390	U
25	A	446	G
25	A	454	A
25	A	458	G
25	A	479	A
25	A	480	A
25	A	490	C
25	A	503	A
25	A	530	G
25	A	549	G
25	A	571	U
25	A	637	A
25	A	685	A

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Mol	Chain	Res	Type
25	A	686	U
25	A	747	5MC
25	A	752	A
25	A	774	G
25	A	776	G
25	A	800	A
25	A	830	G
25	A	858	G
25	A	859	G
25	A	974	G
25	A	1012	U
25	A	1020	A
25	A	1022	G
25	A	1070	A
25	A	1089	A
25	A	1111	A
25	A	1124	G
25	A	1130	U
25	A	1133	A
25	A	1134	A
25	A	1141	U
25	A	1142	A
25	A	1182	G
25	A	1190	G
25	A	1210	G
25	A	1212	G
25	A	1275	A
25	A	1288	G
25	A	1300	G
25	A	1331	G
25	A	1378	A
25	A	1399	C
25	A	1432	G
25	A	1626	A
25	A	1693	U
25	A	1713	A
25	A	1783	A
25	A	1799	G
25	A	1857	G
25	A	1930	G
25	A	1940	U
25	A	2060	A

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Mol	Chain	Res	Type
25	A	2092	U
25	A	2197	U
25	A	2210	U
25	A	2282	G
25	A	2286	G
25	A	2296	U
25	A	2326	C
25	A	2333	A
25	A	2391	G
25	A	2405	G
25	A	2406	A
25	A	2517	C
25	A	2518	A
25	A	2566	A
25	A	2614	A
25	A	2655	G
25	A	2712	C
25	A	2756	U
25	A	2798	U
25	A	2808	G
25	A	2820	A
25	A	2866	U
26	B	24	G
26	B	56	G
26	B	66	A
26	B	88	C

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

39 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	$\#\|Z\| > 2$
15	4SU	v	8	15	18,21,22	1.69	4 (22%)	26,30,33	2.29	5 (19%)
15	H2U	v	20	15	18,21,22	0.91	2 (11%)	21,30,33	1.60	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	2MG	A	1835	25	18,26,27	1.01	1 (5%)	16,38,41	1.26	3 (18%)
25	PSU	A	2504	25	18,21,22	1.34	2 (11%)	22,30,33	1.81	3 (13%)
25	PSU	A	2580	25	18,21,22	1.42	2 (11%)	22,30,33	2.02	4 (18%)
15	PSU	v	55	15	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
25	2MG	A	2445	25	18,26,27	1.00	1 (5%)	16,38,41	1.14	2 (12%)
25	PSU	A	1911	25	18,21,22	1.32	2 (11%)	22,30,33	1.96	4 (18%)
25	PSU	A	1917	25	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
25	OMU	A	2552	25	19,22,23	1.21	3 (15%)	26,31,34	2.17	7 (26%)
1	MA6	a	1519	1	19,26,27	0.96	1 (5%)	18,38,41	1.94	6 (33%)
25	2MA	A	2503	25	17,25,26	1.01	1 (5%)	17,37,40	0.98	2 (11%)
1	7MG	a	527	1	22,26,27	1.36	4 (18%)	29,39,42	2.45	7 (24%)
25	6MZ	A	2030	25	18,25,26	0.92	1 (5%)	16,36,39	2.49	4 (25%)
25	H2U	A	2449	25	18,21,22	0.91	2 (11%)	21,30,33	1.67	3 (14%)
25	OMC	A	2498	25	19,22,23	0.83	1 (5%)	26,31,34	0.87	0
25	7MG	A	2069	25	22,26,27	1.41	4 (18%)	29,39,42	2.51	7 (24%)
1	UR3	a	1498	1	19,22,23	0.93	0	26,32,35	1.58	3 (11%)
1	2MG	a	966	1	18,26,27	0.87	1 (5%)	16,38,41	1.17	2 (12%)
25	5MU	A	1939	25	19,22,23	1.36	4 (21%)	28,32,35	2.26	6 (21%)
1	4OC	a	1402	1	20,23,24	1.67	4 (20%)	26,32,35	2.37	10 (38%)
25	3TD	A	1915	25	18,22,23	1.22	2 (11%)	22,32,35	1.93	3 (13%)
1	5MC	a	967	1	18,22,23	0.98	1 (5%)	26,32,35	1.07	2 (7%)
25	5MC	A	747	25	18,22,23	0.97	2 (11%)	26,32,35	1.38	3 (11%)
25	PSU	A	955	25	18,21,22	1.42	4 (22%)	22,30,33	2.00	4 (18%)
25	PSU	A	2604	25	18,21,22	1.37	3 (16%)	22,30,33	1.91	4 (18%)
15	5MU	v	54	15	19,22,23	1.39	5 (26%)	28,32,35	2.22	5 (17%)
25	5MC	A	1962	25	18,22,23	0.97	2 (11%)	26,32,35	1.10	2 (7%)
25	PSU	A	2605	25	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
1	5MC	a	1407	1	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
1	2MG	a	1516	1	18,26,27	0.88	1 (5%)	16,38,41	1.12	2 (12%)
25	PSU	A	2457	25	18,21,22	1.34	3 (16%)	22,30,33	2.05	4 (18%)
1	MA6	a	1518	1	19,26,27	1.12	2 (10%)	18,38,41	1.95	4 (22%)
25	6MZ	A	1618	25	18,25,26	0.98	1 (5%)	16,36,39	2.26	4 (25%)
1	2MG	a	1207	1	18,26,27	0.95	1 (5%)	16,38,41	1.15	2 (12%)
1	PSU	a	516	1	18,21,22	1.45	4 (22%)	22,30,33	2.12	5 (22%)
25	PSU	A	746	25	18,21,22	1.32	2 (11%)	22,30,33	1.83	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	1MG	A	745	25	18,26,27	0.80	0	19,39,42	1.07	1 (5%)
25	OMG	A	2251	15,25	18,26,27	1.03	1 (5%)	19,38,41	1.01	1 (5%)

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
15	4SU	v	8	15	-	0/7/25/26	0/2/2/2
15	H2U	v	20	15	-	1/7/38/39	0/2/2/2
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	A	2504	25	-	2/7/25/26	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
15	PSU	v	55	15	-	2/7/25/26	0/2/2/2
25	2MG	A	2445	25	-	2/5/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	2/9/27/28	0/2/2/2
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
25	2MA	A	2503	25	-	1/3/25/26	0/3/3/3
1	7MG	a	527	1	-	3/7/37/38	0/3/3/3
25	6MZ	A	2030	25	-	2/5/27/28	0/3/3/3
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	OMC	A	2498	25	-	1/9/27/28	0/2/2/2
25	7MG	A	2069	25	-	1/7/37/38	0/3/3/3
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/5/27/28	0/3/3/3
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	3/9/29/30	0/2/2/2
25	3TD	A	1915	25	-	3/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
25	5MC	A	747	25	-	0/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
15	5MU	v	54	15	-	0/7/25/26	0/2/2/2
25	5MC	A	1962	25	-	1/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	4/7/29/30	0/3/3/3
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
1	2MG	a	1207	1	-	2/5/27/28	0/3/3/3
1	PSU	a	516	1	-	2/7/25/26	0/2/2/2
25	PSU	A	746	25	-	1/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
25	OMG	A	2251	15,25	-	0/5/27/28	0/3/3/3

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	v	8	4SU	C4-S4	-4.44	1.60	1.68
1	a	1402	4OC	O3'-C3'	4.33	1.53	1.43
1	a	1402	4OC	C6-C5	3.84	1.44	1.35
25	A	2069	7MG	C4-N9	-3.84	1.33	1.37
1	a	527	7MG	C4-N9	-3.64	1.33	1.37
25	A	1915	3TD	C10-N3	3.35	1.53	1.47
25	A	1835	2MG	C6-N1	-3.26	1.33	1.37
25	A	2251	OMG	C6-N1	-3.18	1.33	1.37
25	A	1911	PSU	C6-C5	3.18	1.39	1.35
25	A	1618	6MZ	C5-C4	3.17	1.49	1.40
15	v	55	PSU	C6-C5	3.17	1.39	1.35
1	a	516	PSU	C4-N3	-3.13	1.33	1.38
25	A	955	PSU	C4-N3	-3.11	1.33	1.38
15	v	8	4SU	C4-N3	-3.08	1.34	1.37
25	A	2580	PSU	C4-N3	-3.07	1.33	1.38
25	A	1917	PSU	C6-C5	3.03	1.38	1.35
25	A	2605	PSU	C6-C5	3.00	1.38	1.35
1	a	967	5MC	C6-C5	2.99	1.39	1.34
25	A	2605	PSU	C4-N3	-2.96	1.33	1.38
25	A	2604	PSU	C4-N3	-2.92	1.33	1.38
25	A	1939	5MU	C4-N3	-2.92	1.33	1.38
25	A	2069	7MG	C5-N7	-2.90	1.32	1.35
25	A	2030	6MZ	C5-C4	2.89	1.48	1.40
25	A	1939	5MU	C6-N1	-2.88	1.33	1.38
25	A	746	PSU	C4-N3	-2.81	1.33	1.38
25	A	2504	PSU	C4-N3	-2.75	1.33	1.38
15	v	54	5MU	C6-C5	2.75	1.39	1.34
25	A	2457	PSU	C4-N3	-2.74	1.33	1.38
1	a	1518	MA6	C5-C4	2.74	1.48	1.40
25	A	1962	5MC	C6-N1	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	527	7MG	C5-C4	2.73	1.47	1.38
15	v	55	PSU	C4-N3	-2.72	1.33	1.38
25	A	746	PSU	C6-C5	2.72	1.38	1.35
25	A	2445	2MG	C6-N1	-2.69	1.33	1.37
25	A	2504	PSU	C6-C5	2.67	1.38	1.35
1	a	1407	5MC	C6-N1	-2.63	1.33	1.38
1	a	1402	4OC	C1'-N1	2.62	1.55	1.47
25	A	1917	PSU	C4-N3	-2.59	1.34	1.38
15	v	54	5MU	C4-N3	-2.59	1.34	1.38
25	A	747	5MC	C6-C5	2.56	1.38	1.34
25	A	2605	PSU	C2-N3	-2.56	1.33	1.37
1	a	516	PSU	C6-C5	2.56	1.38	1.35
25	A	2604	PSU	C6-C5	2.54	1.38	1.35
25	A	2604	PSU	C2-N3	-2.53	1.33	1.37
25	A	2552	OMU	C4-N3	-2.51	1.34	1.38
25	A	747	5MC	C6-N1	-2.50	1.33	1.38
25	A	2069	7MG	C5-C4	2.50	1.46	1.38
15	v	20	H2U	C2-N3	-2.47	1.33	1.38
25	A	2457	PSU	C6-C5	2.46	1.38	1.35
25	A	1939	5MU	C6-C5	2.46	1.38	1.34
1	a	966	2MG	C6-N1	-2.45	1.34	1.37
25	A	1939	5MU	C2-N3	-2.44	1.33	1.38
25	A	1915	3TD	C4-N3	-2.43	1.35	1.40
25	A	2449	H2U	C2-N3	-2.42	1.33	1.38
25	A	2580	PSU	C6-C5	2.42	1.38	1.35
15	v	54	5MU	C2-N1	2.42	1.42	1.38
25	A	1911	PSU	C4-N3	-2.39	1.34	1.38
1	a	1207	2MG	C6-N1	-2.39	1.34	1.37
1	a	527	7MG	C6-N1	-2.38	1.34	1.38
1	a	1407	5MC	C6-C5	2.36	1.38	1.34
15	v	8	4SU	C2-N1	2.32	1.42	1.38
1	a	516	PSU	C2-N3	-2.32	1.33	1.37
25	A	955	PSU	C2-N3	-2.30	1.33	1.37
15	v	8	4SU	C5-C4	-2.29	1.39	1.42
15	v	54	5MU	C6-N1	-2.28	1.34	1.38
25	A	1962	5MC	C6-C5	2.28	1.38	1.34
25	A	2449	H2U	C4-N3	-2.27	1.33	1.37
1	a	1518	MA6	C6-N1	2.27	1.36	1.33
25	A	2503	2MA	C2-N3	2.26	1.36	1.31
25	A	2069	7MG	C6-N1	-2.26	1.34	1.38
25	A	955	PSU	C2-N1	-2.24	1.33	1.36
1	a	527	7MG	C5-N7	-2.24	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	v	20	H2U	C4-N3	-2.23	1.33	1.37
1	a	1519	MA6	C5-C4	2.20	1.46	1.40
1	a	516	PSU	O4'-C1'	-2.20	1.40	1.43
1	a	1402	4OC	C2'-C1'	2.13	1.58	1.53
25	A	2552	OMU	C2-N1	2.10	1.41	1.38
25	A	2552	OMU	C2-N3	-2.09	1.34	1.38
25	A	955	PSU	C6-C5	2.08	1.37	1.35
1	a	1516	2MG	C6-N1	-2.08	1.34	1.37
25	A	2498	OMC	C6-N1	-2.07	1.33	1.38
15	v	54	5MU	C2-N3	-2.05	1.34	1.38
25	A	2457	PSU	C2-N1	-2.00	1.34	1.36

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2069	7MG	N9-C4-N3	8.58	138.30	125.47
1	a	527	7MG	N9-C4-N3	8.55	138.26	125.47
25	A	2030	6MZ	C2-N1-C6	7.19	122.75	116.59
15	v	8	4SU	C4-N3-C2	-6.87	120.67	127.34
1	a	516	PSU	N1-C2-N3	6.73	122.76	115.13
25	A	1915	3TD	N1-C2-N3	6.50	121.27	116.14
25	A	2580	PSU	N1-C2-N3	6.50	122.49	115.13
25	A	2457	PSU	N1-C2-N3	6.33	122.31	115.13
25	A	955	PSU	N1-C2-N3	6.22	122.18	115.13
25	A	1911	PSU	N1-C2-N3	6.08	122.02	115.13
25	A	2449	H2U	C4-N3-C2	-6.04	120.78	125.79
25	A	1618	6MZ	C2-N1-C6	6.03	121.76	116.59
25	A	1917	PSU	N1-C2-N3	5.98	121.91	115.13
1	a	1498	UR3	C4-N3-C2	-5.97	118.94	124.56
25	A	2604	PSU	N1-C2-N3	5.85	121.75	115.13
25	A	2069	7MG	N9-C8-N7	-5.84	95.03	103.38
15	v	20	H2U	C4-N3-C2	-5.81	120.97	125.79
25	A	2605	PSU	N1-C2-N3	5.80	121.70	115.13
25	A	2504	PSU	N1-C2-N3	5.79	121.69	115.13
15	v	8	4SU	C5-C4-N3	5.75	120.03	114.69
25	A	1939	5MU	C4-N3-C2	-5.71	119.96	127.35
15	v	55	PSU	N1-C2-N3	5.71	121.60	115.13
25	A	746	PSU	N1-C2-N3	5.65	121.53	115.13
15	v	54	5MU	O4-C4-C5	-5.41	118.63	124.90
15	v	54	5MU	C4-N3-C2	-5.39	120.38	127.35
1	a	527	7MG	N9-C8-N7	-5.36	95.72	103.38
1	a	1402	4OC	O3'-C3'-C2'	5.31	126.26	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2552	OMU	C4-N3-C2	-5.13	119.81	126.58
15	v	54	5MU	C5-C4-N3	5.06	119.63	115.31
25	A	1618	6MZ	C9-N6-C6	-5.04	118.53	122.87
25	A	1939	5MU	N3-C2-N1	4.97	121.48	114.89
25	A	1939	5MU	C5-C4-N3	4.95	119.54	115.31
1	a	527	7MG	C5-C4-N3	-4.94	118.72	128.13
25	A	2030	6MZ	C9-N6-C6	-4.90	118.65	122.87
25	A	2069	7MG	C5-C4-N3	-4.86	118.86	128.13
15	v	54	5MU	N3-C2-N1	4.80	121.26	114.89
25	A	2552	OMU	N3-C2-N1	4.75	121.19	114.89
25	A	1939	5MU	C5-C6-N1	-4.65	118.55	123.34
25	A	2552	OMU	C1'-N1-C2	4.62	125.93	117.57
1	a	516	PSU	C4-N3-C2	-4.46	119.92	126.34
25	A	1939	5MU	O4-C4-C5	-4.45	119.75	124.90
1	a	1518	MA6	C10-N6-C6	-4.45	106.05	119.51
1	a	1402	4OC	C6-N1-C2	-4.44	112.80	120.49
25	A	955	PSU	C4-N3-C2	-4.39	120.02	126.34
25	A	2604	PSU	C4-N3-C2	-4.36	120.06	126.34
15	v	8	4SU	N3-C2-N1	4.33	120.64	114.89
15	v	8	4SU	C5-C4-S4	-4.28	118.95	124.47
25	A	2457	PSU	C4-N3-C2	-4.23	120.24	126.34
25	A	1911	PSU	C4-N3-C2	-4.23	120.25	126.34
25	A	2457	PSU	O2-C2-N1	-4.15	118.22	122.79
25	A	1915	3TD	C4-N3-C2	-4.15	120.10	124.61
25	A	746	PSU	C4-N3-C2	-4.08	120.46	126.34
1	a	1519	MA6	N3-C2-N1	-4.00	122.42	128.68
25	A	2069	7MG	C2-N3-C4	4.00	119.42	112.30
25	A	2552	OMU	C5-C4-N3	3.98	120.79	114.84
1	a	527	7MG	C2-N3-C4	3.88	119.20	112.30
25	A	955	PSU	O2-C2-N1	-3.84	118.56	122.79
25	A	2580	PSU	C4-N3-C2	-3.82	120.83	126.34
15	v	54	5MU	C5-C6-N1	-3.79	119.44	123.34
15	v	55	PSU	C4-N3-C2	-3.78	120.89	126.34
1	a	1402	4OC	C3'-C2'-C1'	3.72	109.88	102.89
1	a	516	PSU	O2-C2-N1	-3.71	118.70	122.79
25	A	1917	PSU	C4-N3-C2	-3.69	121.03	126.34
25	A	2605	PSU	C4-N3-C2	-3.66	121.07	126.34
25	A	1939	5MU	O2-C2-N1	-3.63	117.97	122.79
1	a	1518	MA6	N1-C6-N6	3.60	120.85	117.06
25	A	2504	PSU	O2-C2-N1	-3.60	118.83	122.79
25	A	2504	PSU	C4-N3-C2	-3.59	121.17	126.34
1	a	1518	MA6	N3-C2-N1	-3.58	123.09	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1407	5MC	C5-C6-N1	-3.55	119.68	123.34
25	A	2580	PSU	O2-C2-N1	-3.52	118.92	122.79
25	A	747	5MC	C5-C6-N1	-3.45	119.79	123.34
25	A	1911	PSU	O2-C2-N1	-3.44	119.00	122.79
1	a	1519	MA6	C10-N6-C6	-3.44	109.11	119.51
1	a	1519	MA6	C9-N6-C6	-3.37	109.30	119.51
1	a	1402	4OC	O2-C2-N3	-3.36	116.86	122.33
25	A	1917	PSU	O2-C2-N1	-3.30	119.15	122.79
25	A	2552	OMU	O4-C4-C5	-3.29	119.38	125.16
1	a	1402	4OC	O3'-C3'-C4'	3.21	120.33	111.05
25	A	746	PSU	O2-C2-N1	-3.21	119.26	122.79
1	a	1402	4OC	O4'-C1'-C2'	-3.21	100.94	106.57
1	a	1402	4OC	C2'-C1'-N1	3.19	120.43	114.22
1	a	1402	4OC	O4'-C1'-N1	3.15	115.56	108.36
1	a	1518	MA6	C9-N6-C6	-3.09	110.16	119.51
1	a	1498	UR3	C1'-N1-C2	3.07	122.18	116.99
25	A	1618	6MZ	N3-C2-N1	-3.04	123.92	128.68
1	a	1519	MA6	N1-C6-N6	3.04	120.25	117.06
25	A	1962	5MC	C5-C4-N3	-2.95	118.49	121.67
25	A	2030	6MZ	C4-C5-N7	-2.94	106.33	109.40
15	v	55	PSU	O2-C2-N1	-2.94	119.55	122.79
25	A	2030	6MZ	N3-C2-N1	-2.88	124.17	128.68
1	a	1519	MA6	C10-N6-C9	-2.87	106.86	116.12
25	A	1915	3TD	C10-N3-C4	2.85	122.05	117.69
1	a	967	5MC	C5-C6-N1	-2.81	120.45	123.34
1	a	1402	4OC	N1-C2-N3	2.80	123.91	118.81
25	A	1835	2MG	C5-C6-N1	2.77	118.84	113.95
25	A	1962	5MC	C5-C6-N1	-2.75	120.51	123.34
25	A	2069	7MG	C5-C4-N9	-2.72	102.82	106.35
25	A	2552	OMU	C1'-N1-C6	-2.66	115.03	120.84
25	A	745	1MG	C8-N7-C5	2.63	108.01	102.99
25	A	2604	PSU	C5-C6-N1	-2.57	118.25	122.11
1	a	527	7MG	C5-C4-N9	-2.57	103.01	106.35
1	a	1407	5MC	C5-C4-N3	-2.56	118.91	121.67
25	A	747	5MC	C5-C4-N3	-2.54	118.94	121.67
1	a	966	2MG	C5-C6-N1	2.53	118.42	113.95
1	a	527	7MG	C5-C6-N1	2.52	115.44	110.99
1	a	1519	MA6	C4-C5-N7	-2.52	106.78	109.40
25	A	1618	6MZ	C4-C5-N7	-2.50	106.80	109.40
25	A	2580	PSU	C5-C6-N1	-2.50	118.36	122.11
25	A	2503	2MA	C8-N7-C5	2.48	107.72	102.99
25	A	2604	PSU	O2-C2-N1	-2.40	120.15	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1207	2MG	C5-C6-N1	2.37	118.14	113.95
25	A	2069	7MG	O6-C6-C5	-2.37	121.73	127.54
25	A	2457	PSU	C5-C6-N1	-2.37	118.56	122.11
1	a	967	5MC	C5-C4-N3	-2.36	119.13	121.67
1	a	966	2MG	C8-N7-C5	2.33	107.43	102.99
1	a	516	PSU	O4'-C1'-C2'	2.31	108.41	105.14
25	A	2445	2MG	O6-C6-C5	-2.31	119.86	124.37
25	A	2605	PSU	O2-C2-N1	-2.31	120.25	122.79
15	v	8	4SU	C1'-N1-C2	2.31	121.75	117.57
25	A	2449	H2U	O4-C4-N3	2.30	123.93	120.28
25	A	2069	7MG	C5-C6-N1	2.27	115.00	110.99
1	a	527	7MG	O6-C6-C5	-2.27	121.97	127.54
25	A	2503	2MA	C5-C6-N1	2.27	117.93	114.02
25	A	2605	PSU	C6-C5-C4	-2.27	116.61	118.20
25	A	1835	2MG	O6-C6-C5	-2.26	119.96	124.37
25	A	1835	2MG	C8-N7-C5	2.24	107.25	102.99
25	A	2449	H2U	C5-C6-N1	-2.24	104.25	111.61
1	a	516	PSU	C5-C6-N1	-2.20	118.80	122.11
25	A	2251	OMG	C8-N7-C5	2.18	107.15	102.99
1	a	1516	2MG	C5-C6-N1	2.18	117.81	113.95
25	A	746	PSU	C5-C6-N1	-2.16	118.86	122.11
1	a	1516	2MG	O6-C6-C5	-2.15	120.18	124.37
15	v	20	H2U	N3-C2-N1	2.12	118.90	116.65
1	a	1402	4OC	C1'-N1-C6	2.11	125.45	120.84
25	A	2445	2MG	C5-C6-N1	2.11	117.68	113.95
25	A	955	PSU	C5-C6-N1	-2.11	118.95	122.11
1	a	1207	2MG	C8-N7-C5	2.10	106.98	102.99
25	A	1911	PSU	C5-C6-N1	-2.09	118.97	122.11
25	A	747	5MC	C3'-C2'-C1'	2.04	105.30	101.43
25	A	2552	OMU	O2-C2-N3	-2.01	117.75	121.50
1	a	1407	5MC	O2-C2-N3	-2.01	119.06	122.33
1	a	1498	UR3	C3U-N3-C2	2.01	120.83	117.31

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	7MG	C3'-C4'-C5'-O5'
1	a	1207	2MG	O4'-C4'-C5'-O5'
1	a	1207	2MG	C3'-C4'-C5'-O5'
1	a	1402	4OC	C1'-C2'-O2'-CM2
1	a	1518	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	a	1518	MA6	C5-C6-N6-C10
1	a	1518	MA6	N1-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C9
15	v	55	PSU	O4'-C1'-C5-C4
15	v	55	PSU	O4'-C1'-C5-C6
25	A	1915	3TD	C2'-C1'-C5-C4
25	A	1915	3TD	O4'-C1'-C5-C4
25	A	1915	3TD	O4'-C1'-C5-C6
25	A	2030	6MZ	O4'-C4'-C5'-O5'
25	A	2445	2MG	O4'-C4'-C5'-O5'
25	A	2445	2MG	C3'-C4'-C5'-O5'
25	A	2552	OMU	O4'-C1'-N1-C2
25	A	2552	OMU	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1402	4OC	O4'-C4'-C5'-O5'
25	A	2504	PSU	O4'-C4'-C5'-O5'
1	a	966	2MG	O4'-C4'-C5'-O5'
1	a	1402	4OC	C3'-C4'-C5'-O5'
25	A	2030	6MZ	C3'-C4'-C5'-O5'
25	A	2504	PSU	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	966	2MG	C3'-C4'-C5'-O5'
1	a	527	7MG	O4'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C9
25	A	2503	2MA	O4'-C4'-C5'-O5'
25	A	1962	5MC	C4'-C5'-O5'-P
15	v	20	H2U	C4'-C5'-O5'-P
1	a	527	7MG	C4'-C5'-O5'-P
1	a	516	PSU	O4'-C1'-C5-C4
1	a	516	PSU	O4'-C1'-C5-C6
25	A	746	PSU	O4'-C1'-C5-C6
25	A	2069	7MG	O4'-C4'-C5'-O5'
25	A	2498	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

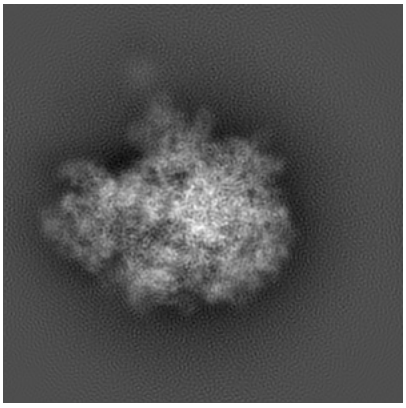
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6311. These allow visual inspection of the internal detail of the map and identification of artifacts.

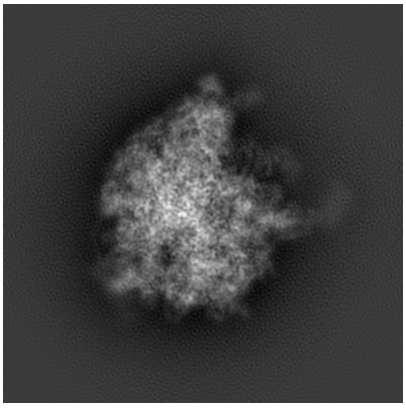
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

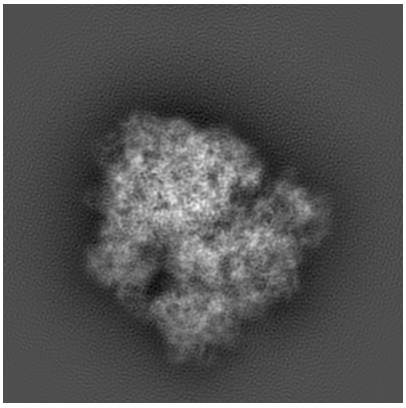
6.1.1 Primary map



X



Y

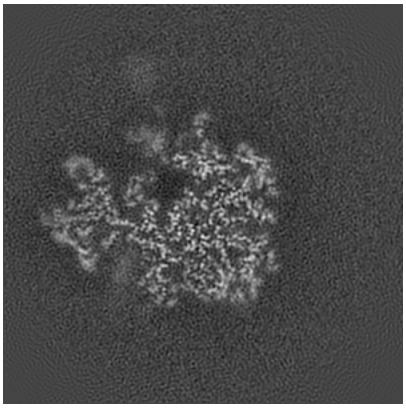


Z

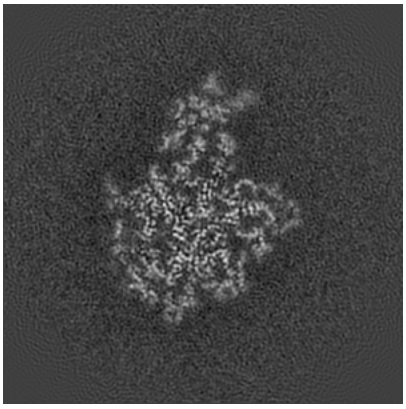
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

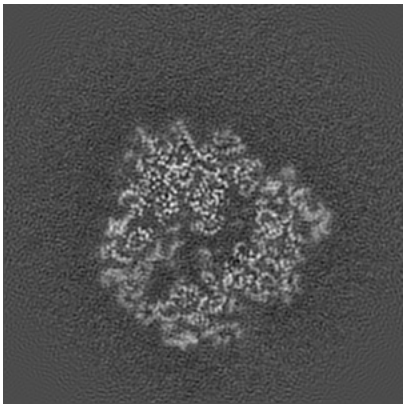
6.2.1 Primary map



X Index: 184



Y Index: 184

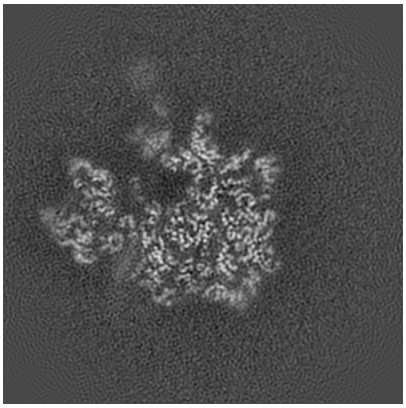


Z Index: 184

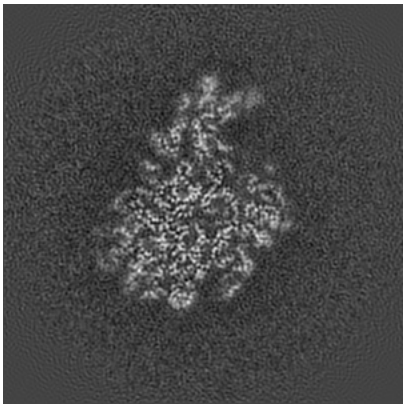
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

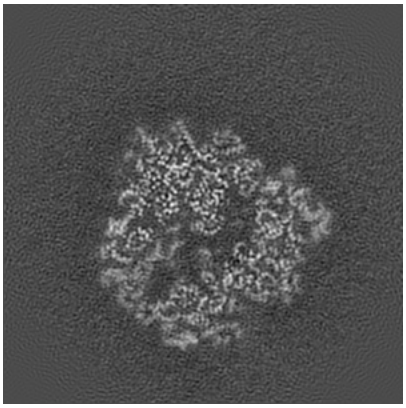
6.3.1 Primary map



X Index: 180



Y Index: 176

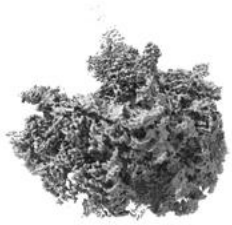


Z Index: 184

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 0.0025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

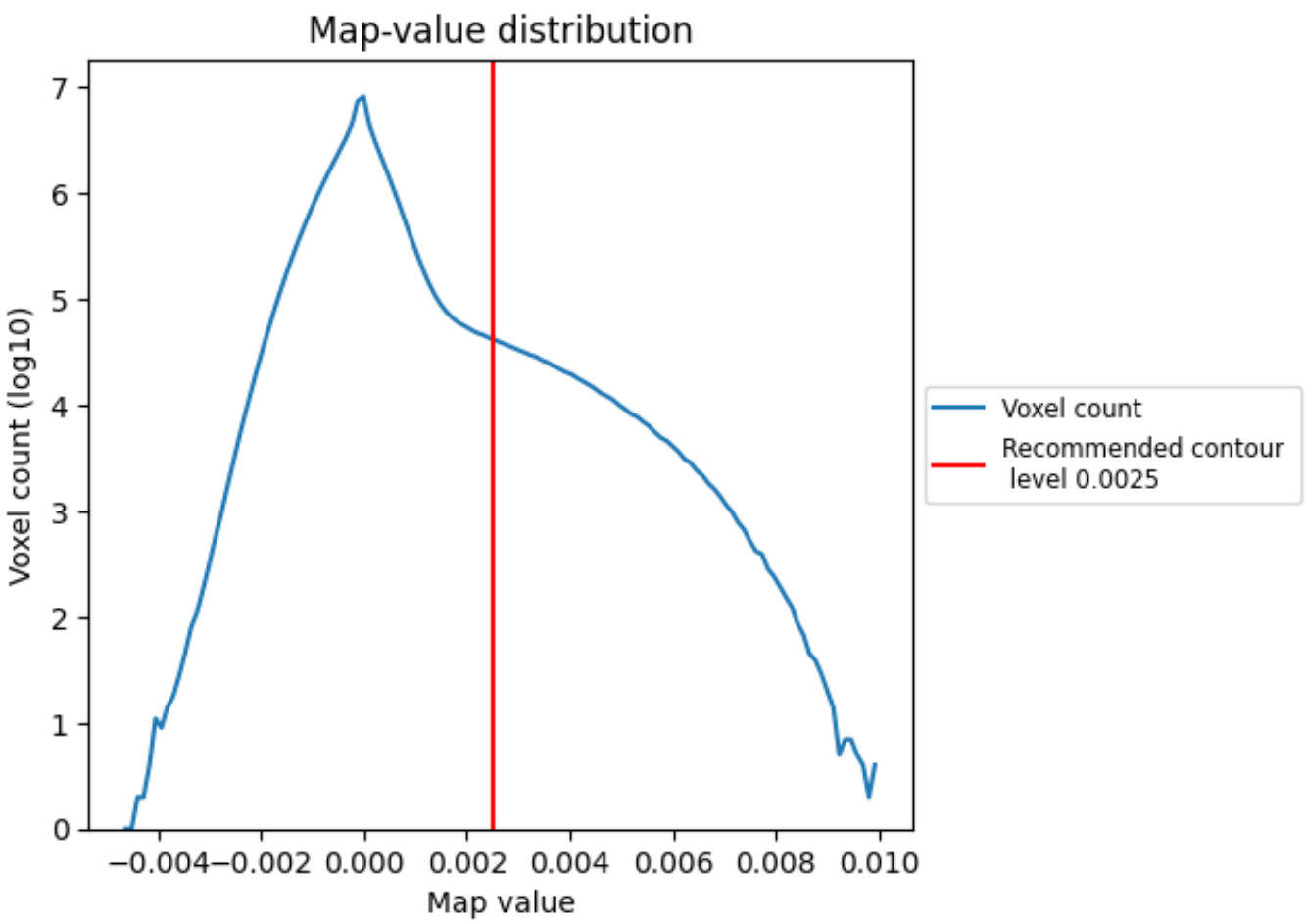
6.5 Mask visualisation (i)

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

7 Map analysis (i)

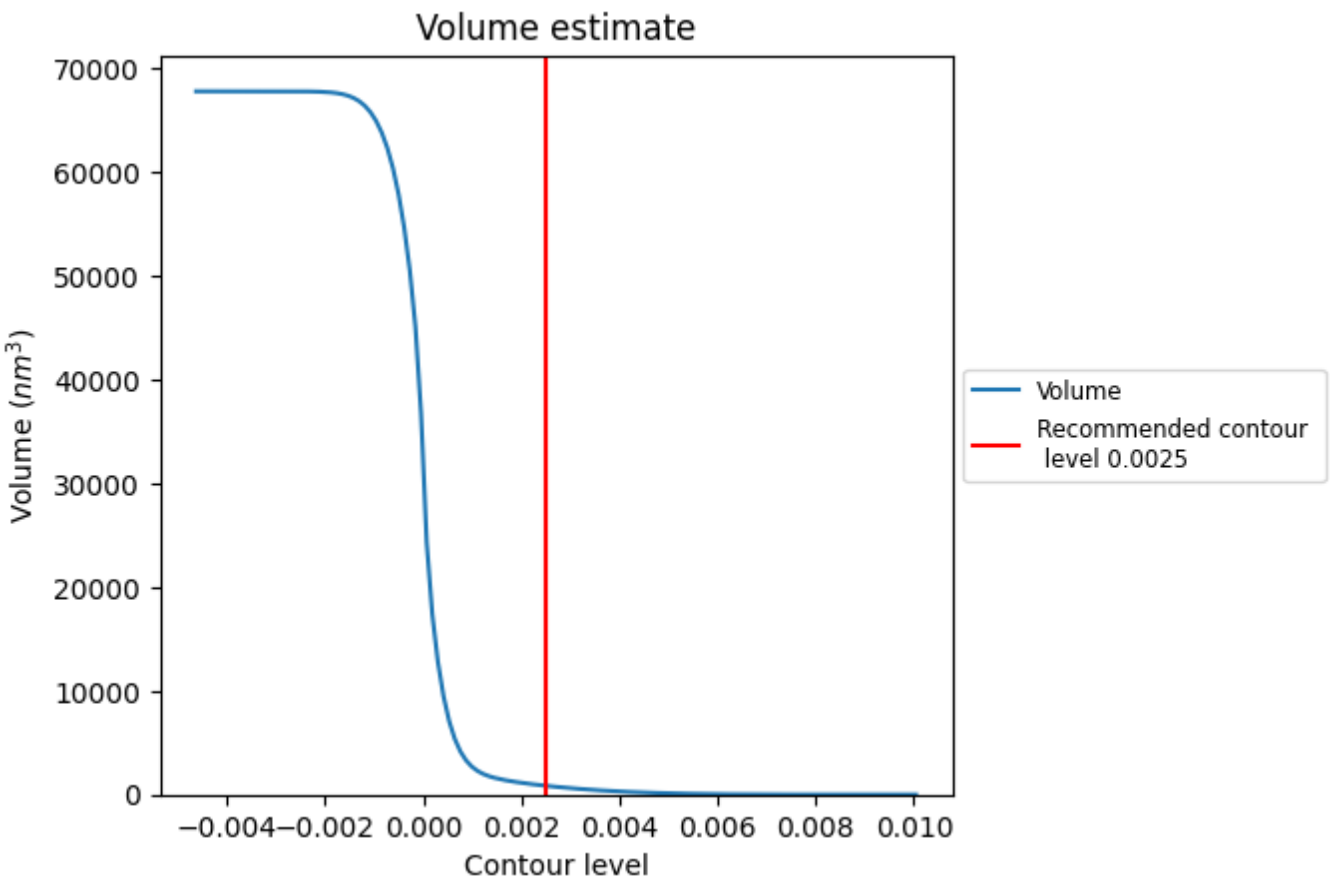
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

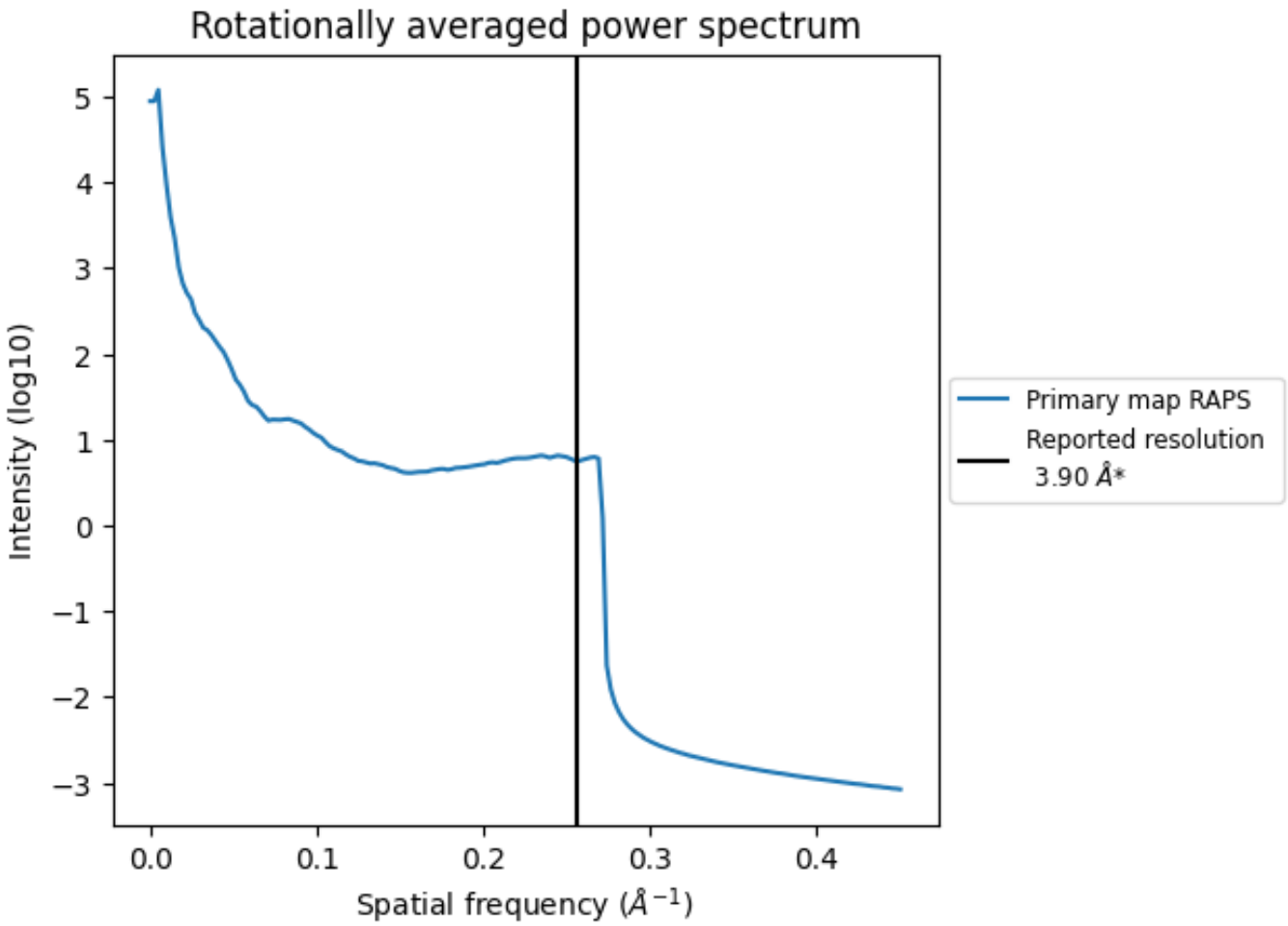
7.2 Volume estimate (i)



The volume at the recommended contour level is 847 nm^3; this corresponds to an approximate mass of 765 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 0.256 Å^{-1}

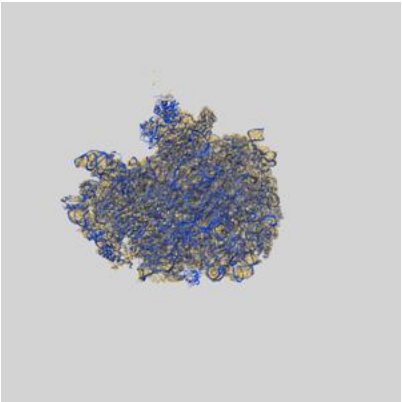
8 Fourier-Shell correlation (i)

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

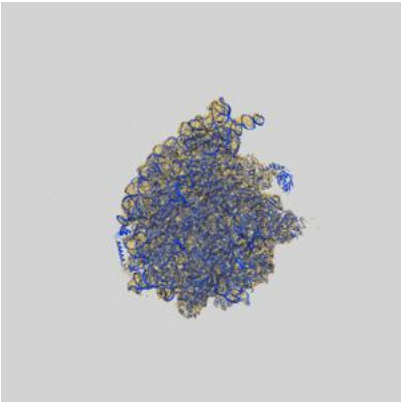
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6311 and PDB model 3J9Y. Per-residue inclusion information can be found in section 3 on page 14.

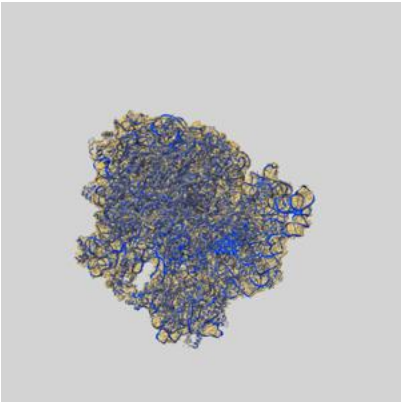
9.1 Map-model overlay (i)



X



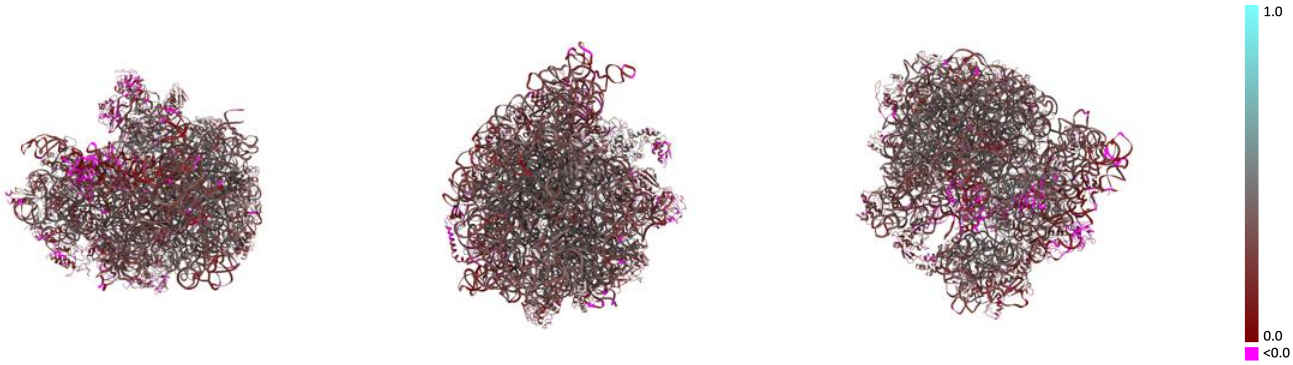
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0025 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.

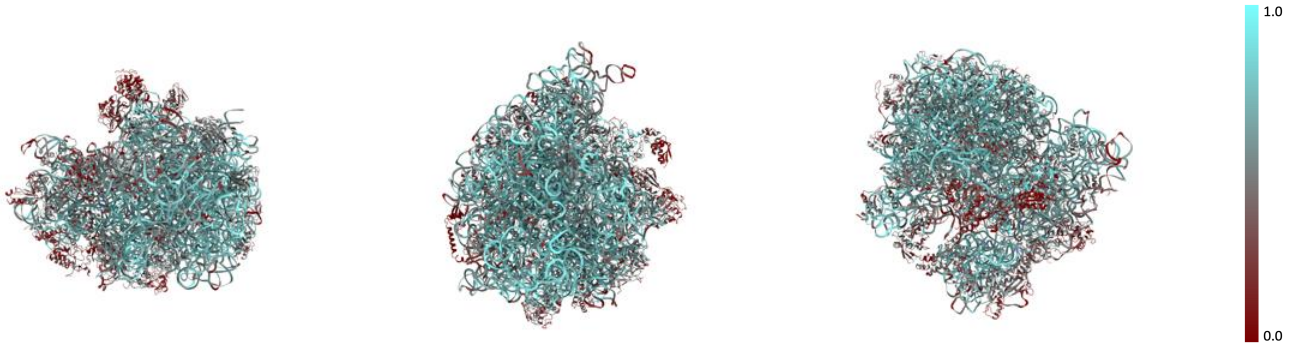
9.2 Q-score mapped to coordinate model (i)



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.

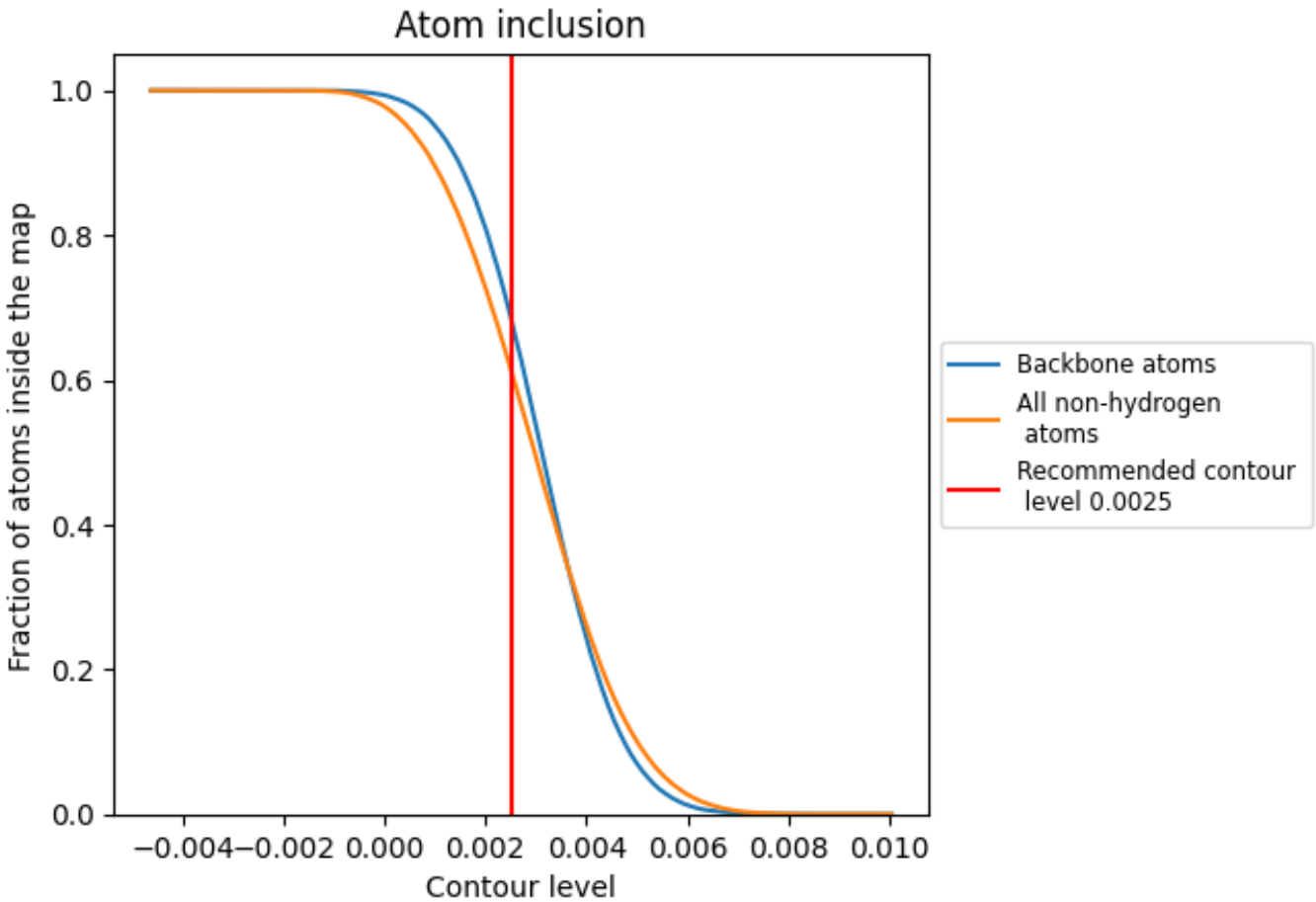
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0025).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.3090
0	0.5280	0.3330
1	0.0200	0.2110
2	0.5775	0.3730
3	0.5458	0.3920
4	0.5719	0.3390
5	0.0878	0.0610
6	0.2270	0.1460
7	0.0471	0.0810
A	0.7371	0.3470
B	0.7084	0.3020
C	0.5580	0.3710
D	0.4876	0.3260
E	0.4474	0.2970
F	0.3664	0.2340
G	0.3462	0.2370
H	0.0885	0.1440
I	0.0685	0.0950
J	0.5091	0.3230
K	0.4644	0.3460
L	0.4596	0.3160
M	0.4875	0.3640
N	0.5347	0.3520
O	0.4438	0.2670
P	0.4527	0.3140
Q	0.5683	0.3550
R	0.4454	0.3010
S	0.4928	0.3260
T	0.4266	0.3070
U	0.3651	0.2580
V	0.4336	0.2890
W	0.5206	0.3530
X	0.4925	0.3440
Y	0.3964	0.2170
Z	0.4828	0.3330

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Chain	Atom inclusion	Q-score
a	0.6890	0.3000
b	0.2412	0.1730
c	0.4094	0.2980
d	0.2635	0.0730
e	0.4227	0.2640
f	0.4083	0.2110
g	0.3330	0.2490
h	0.4583	0.2970
i	0.3892	0.2650
j	0.3022	0.2490
k	0.3503	0.1950
l	0.2942	0.1340
m	0.4230	0.2770
n	0.4531	0.3180
o	0.4841	0.2870
p	0.3955	0.1970
q	0.3829	0.2310
r	0.4763	0.3050
s	0.4332	0.2790
t	0.4431	0.2370
u	0.1387	0.1780
v	0.5560	0.2840
w	0.5713	0.3570
x	0.5185	0.2760