Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 06:23 am GMT

PDB ID	:	6H4N
EMDB ID	:	EMD-0137
Title	:	Structure of a hibernating 100S ribosome reveals an inactive conformation of the ribosomal protein S1 - 70S Hibernating E. coli Ribosome
Authors	:	Beckert, B.; Turk, M.; Czech, A.; Berninghausen, O.; Beckmann, R.; Ignatova, Z.; Plitzko, J.; Wilson, N.D.
Deposited on	:	2018-07-22
Resolution	:	3.00 Å(reported)

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

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

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

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

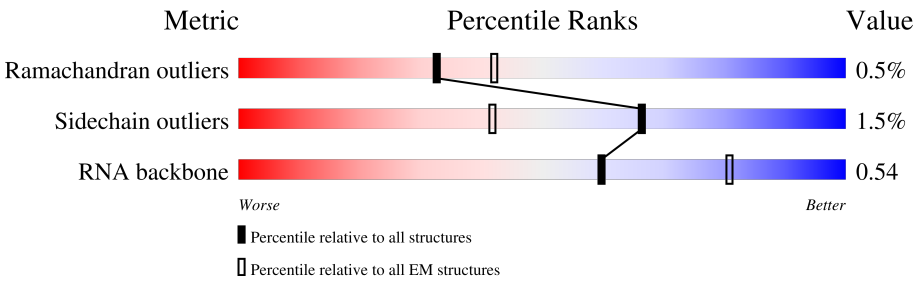
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.00 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	1534	7% 81% 18% •
2	b	218	62% 98% •
3	c	206	33% 99% •
4	d	205	34% 97% •
5	e	157	17% 97% •
6	f	100	35% 100%
7	g	161	41% 94% 6% •
8	h	129	20% 98% •

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Mol	Chain	Length	Quality of chain
9	i	127	31% 96%
10	j	98	48% 99%
11	k	116	26% 97%
12	l	123	26% 98%
13	m	114	39% 98%
14	n	101	30% 98%
15	o	88	23% 98%
16	p	82	23% 98%
17	q	80	40% 99%
18	r	65	20% 100%
19	s	79	32% 100%
20	t	85	22% 98%
21	u	65	74% 91% 9%
22	A	2903	11% 77% 22%
23	B	120	7% 80% 18%
24	C	271	11% 99%
25	D	209	16% 98%
26	E	201	38% 99%
27	F	177	44% 99%
28	G	176	47% 98%
29	H	149	89% 98%
30	J	142	19% 99%
31	K	122	22% 99%
32	L	143	19% 99%
33	M	136	14% 96%

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Mol	Chain	Length	Quality of chain
34	N	120	8% 98%
35	O	116	23% 99%
36	P	114	24% 99%
37	Q	117	9% 100%
38	R	103	23% 98%
39	S	110	20% 98%
40	T	93	34% 99%
41	U	102	43% 100%
42	V	94	28% 100%
43	W	75	9% 96%
44	X	77	22% 97%
45	Y	63	48% 97%
46	Z	58	14% 97%
47	0	56	29% 100%
48	1	50	30% 100%
49	2	46	9% 100%
50	3	64	6% 94% 6%
51	4	38	18% 100%
52	6	66	73% 100%
53	w	77	86% 48% 40% 12%
54	v	55	65% 91% 9%
55	y	557	63% 57% 5% 37%
56	x	95	29% 94% 6%
57	I	5	100% 40% 40% 20%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 147282 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	1534	32916	14680	6039	10663	1534	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 S3.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	161	1266	791	243	228	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	154	ALA	ARG	conflict	UNP P02359
g	161	ALA	PHE	conflict	UNP P02359

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	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 15 is a protein called 30S ribosomal protein S15.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	A	2900	62261	27774	11460	20127	2900	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 1036415628
A	1847	G	A	conflict	GB 1036415628
A	2069	A	G	conflict	GB 1036415628

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	-	expression tag	GB 1393501787

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	0	56	444	269	94	80	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	1	50	409	263	75	71	0	0

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	2	46	377	228	90	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	3	64	504	323	105	74	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	4	38	302	185	65	48	4	0	0

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	6	66	522	323	99	94	6	0	0

- Molecule 53 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	w	77	1642	732	296	537	77	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	29	U	G	conflict	GB 1063812051
w	41	A	C	conflict	GB 1063812051

- Molecule 54 is a protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	v	55	453	275	96	77	5	0	0

- Molecule 55 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	y	351	2180	1339	397	441	3	0	0

- Molecule 56 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	95	754	474	133	145	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	57	ASP	ASN	conflict	UNP P0AFX0
x	61	LEU	ILE	conflict	UNP P0AFX0

- Molecule 57 is a RNA chain called RNA (5'-R(P*CP*UP*CP*CP*U)-3').

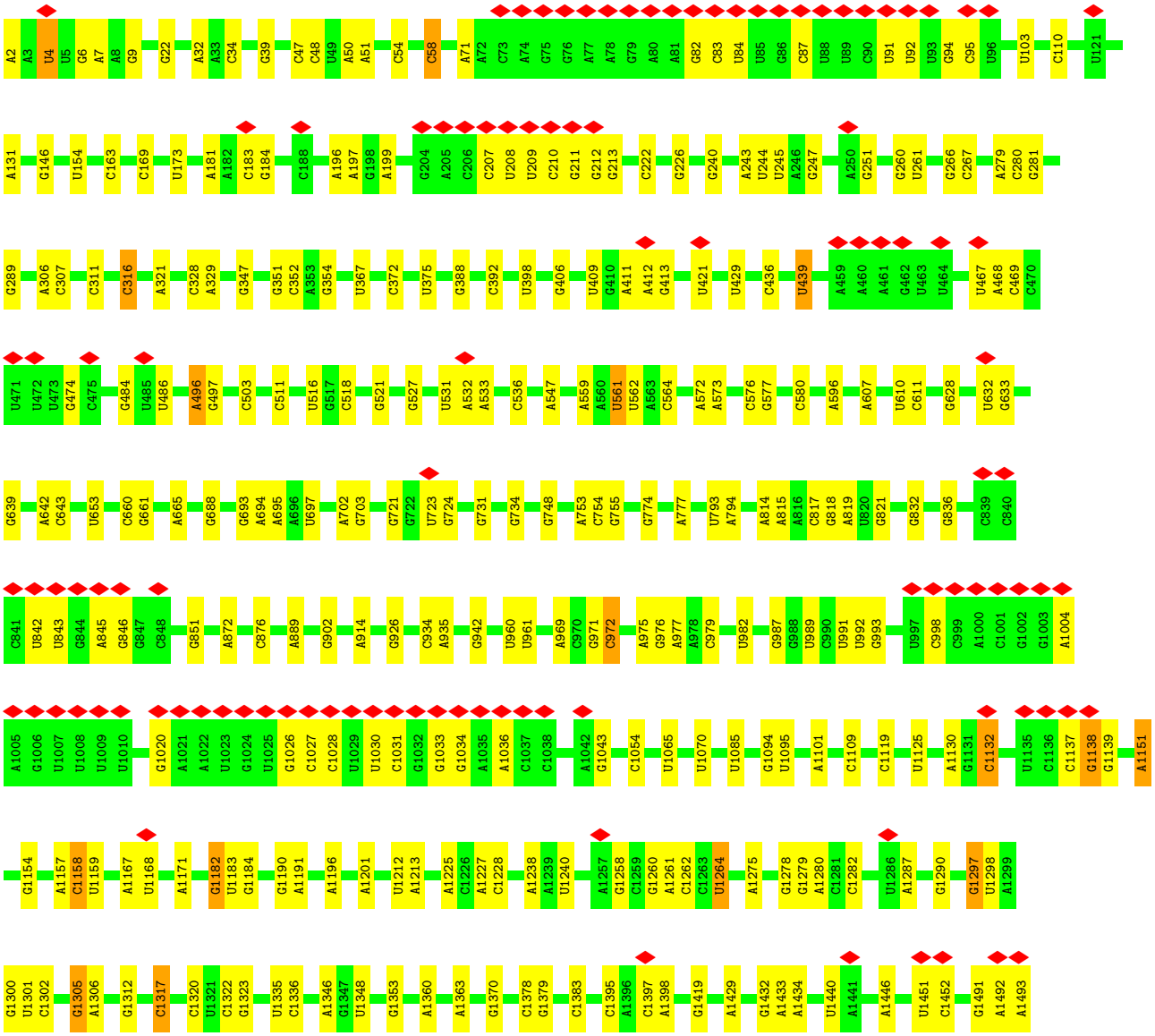
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	I	5	100	45	13	37	5	0	0

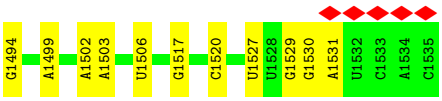
3 Residue-property plots (i)

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

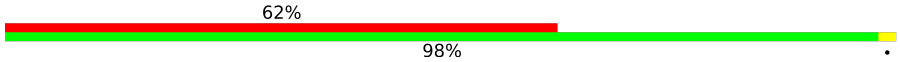
Chain a: 7% 81% 18%

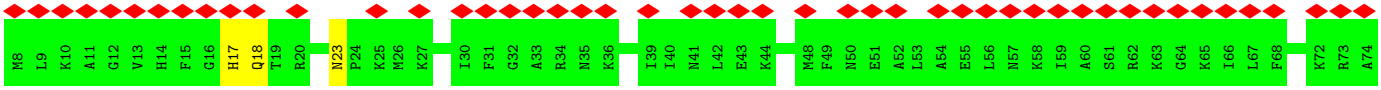


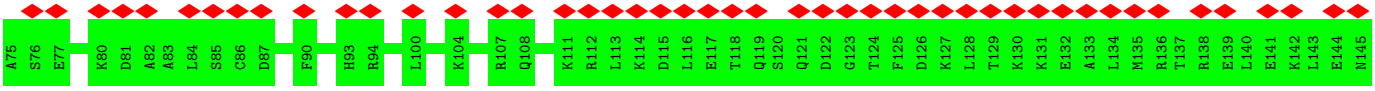


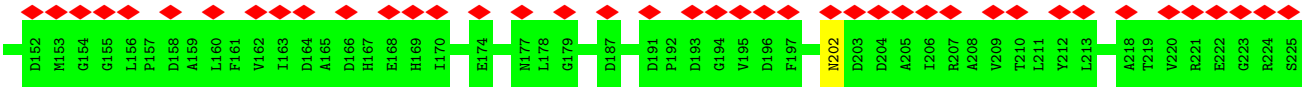
• Molecule 2: 30S ribosomal protein S2

Chain b:



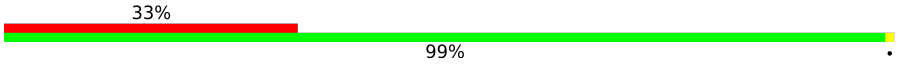


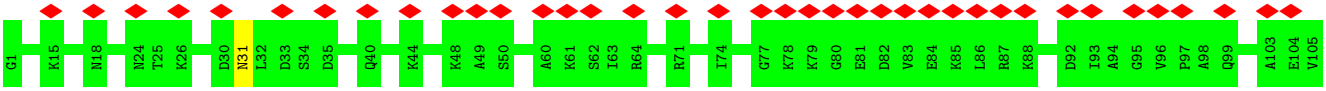


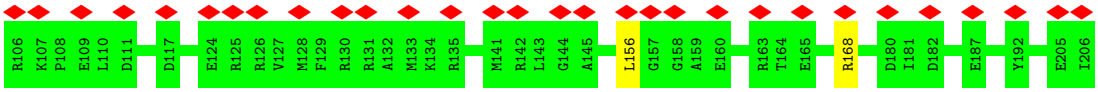


• Molecule 3: 30S ribosomal protein S3

Chain c:

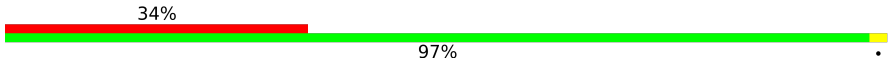


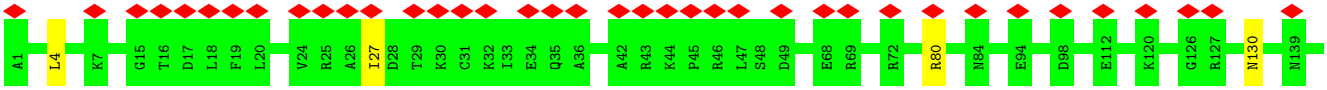


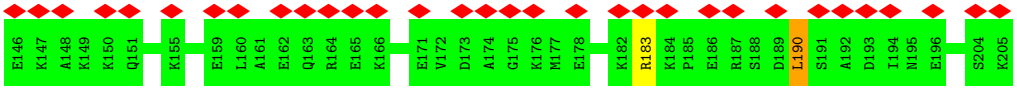


• Molecule 4: 30S ribosomal protein S4

Chain d:

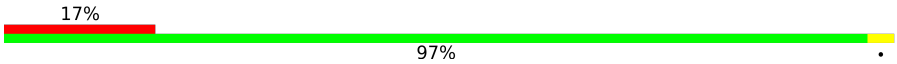






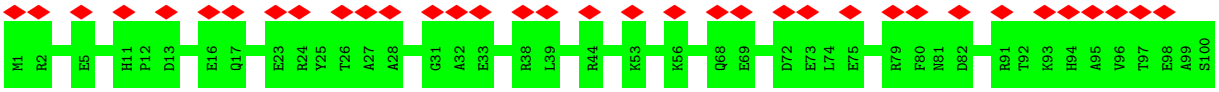
• Molecule 5: 30S ribosomal protein S5

Chain e:



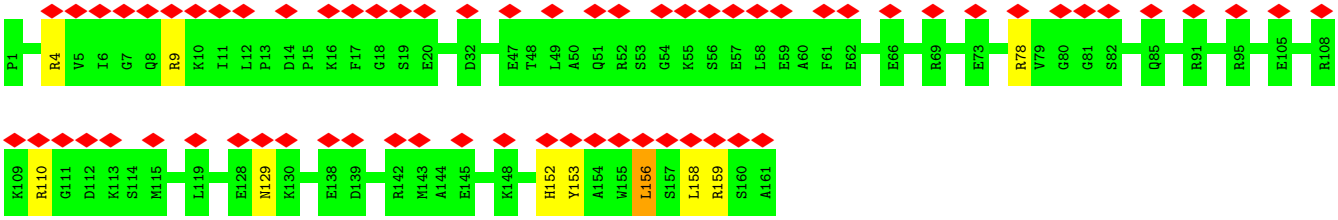
• Molecule 6: 30S ribosomal protein S6

Chain f: 35% 100%



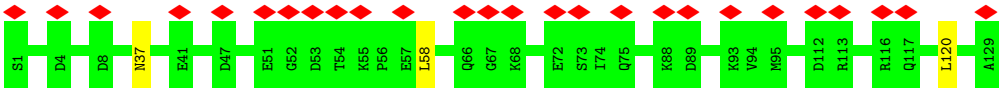
• Molecule 7: 30S ribosomal protein S7

Chain g: 41% 94% 6%



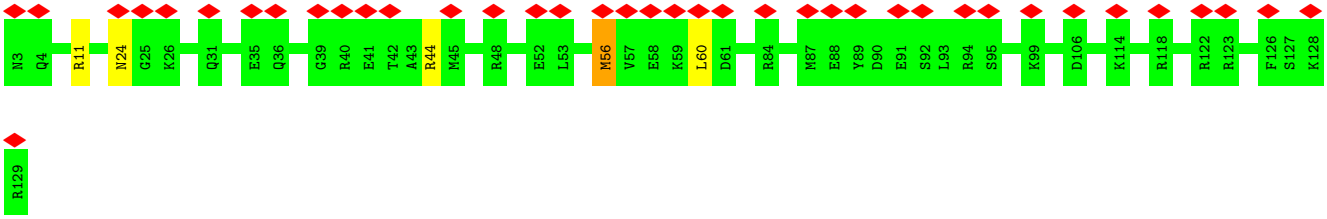
• Molecule 8: 30S ribosomal protein S8

Chain h: 20% 98%



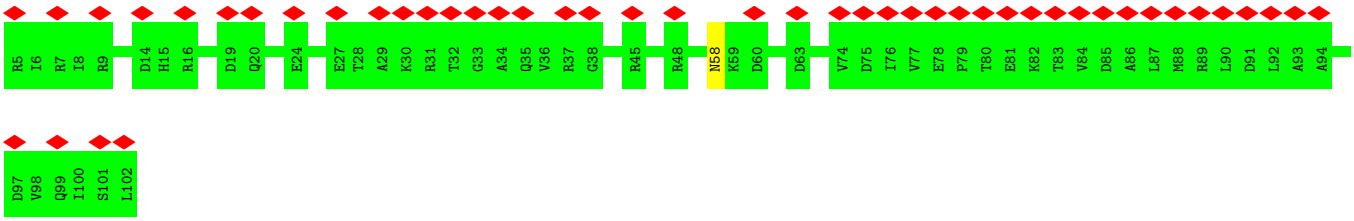
• Molecule 9: 30S ribosomal protein S9

Chain i: 31% 96%



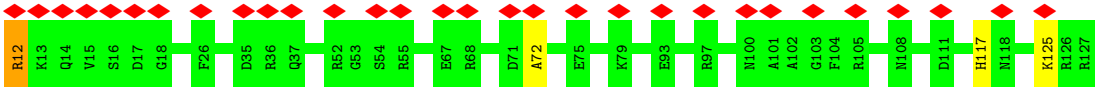
• Molecule 10: 30S ribosomal protein S10

Chain j: 48% 99%



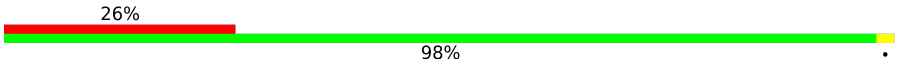
• Molecule 11: 30S ribosomal protein S11

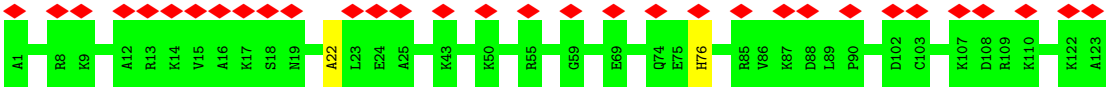
Chain k: 26% 97%



• Molecule 12: 30S ribosomal protein S12

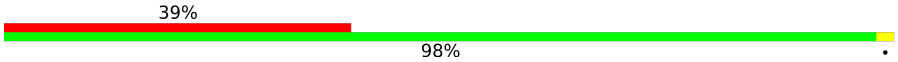
Chain l:

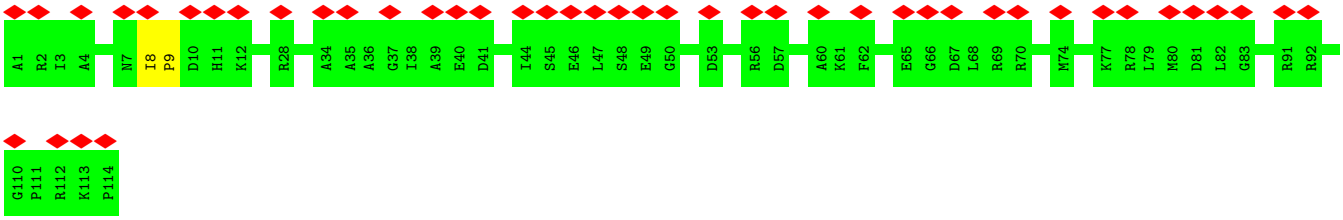




• Molecule 13: 30S ribosomal protein S13

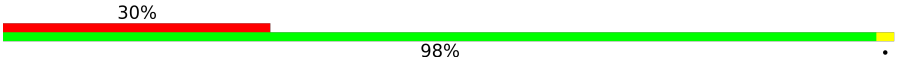
Chain m:

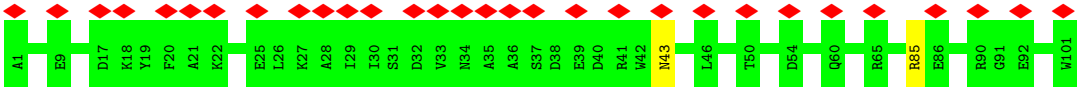




• Molecule 14: 30S ribosomal protein S14

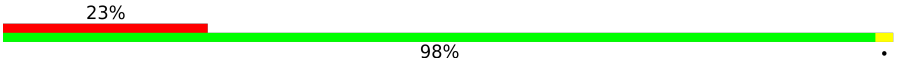
Chain n:

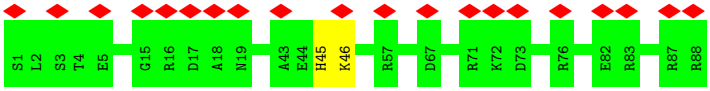




• Molecule 15: 30S ribosomal protein S15

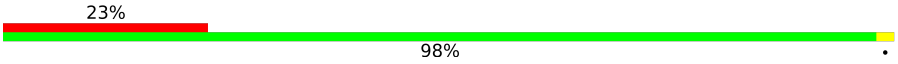
Chain o:

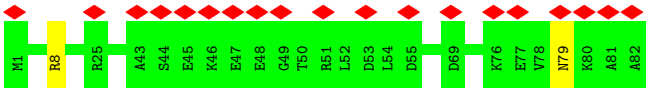




• Molecule 16: 30S ribosomal protein S16

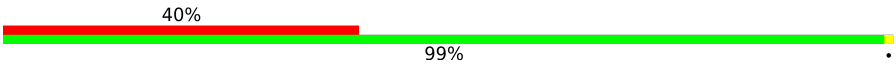
Chain p:

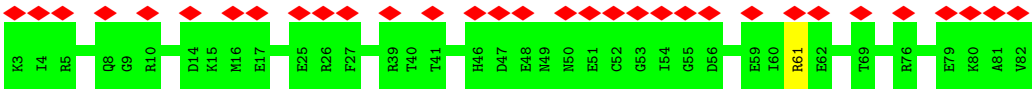




• Molecule 17: 30S ribosomal protein S17

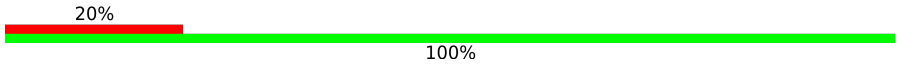
Chain q:

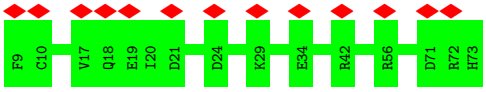




- Molecule 18: 30S ribosomal protein S18

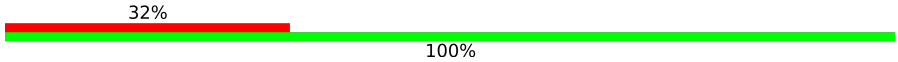
Chain r:

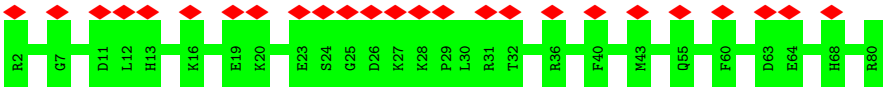




- Molecule 19: 30S ribosomal protein S19

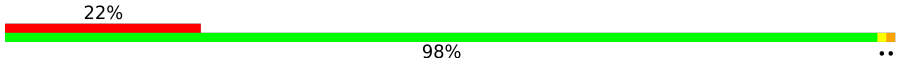
Chain s:

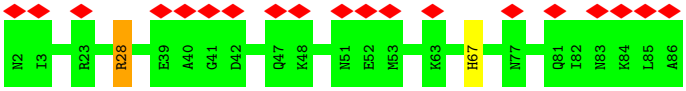




- Molecule 20: 30S ribosomal protein S20

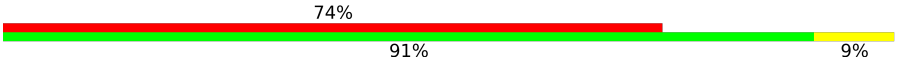
Chain t:

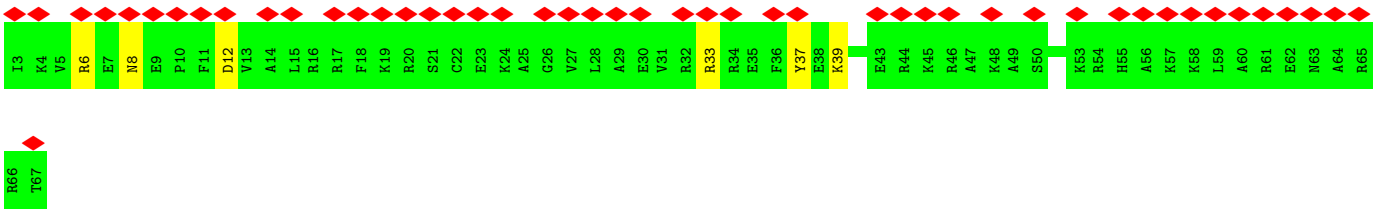




- Molecule 21: 30S ribosomal protein S21

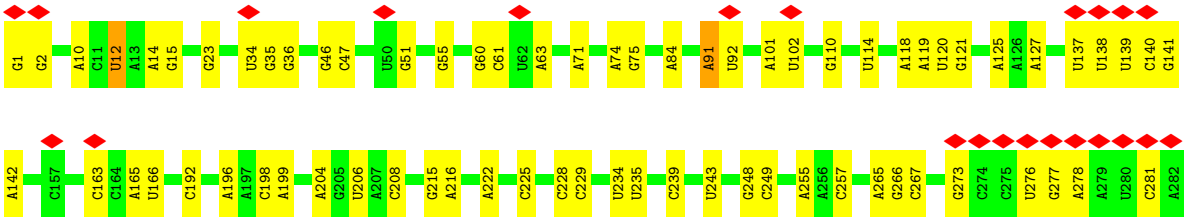
Chain u:

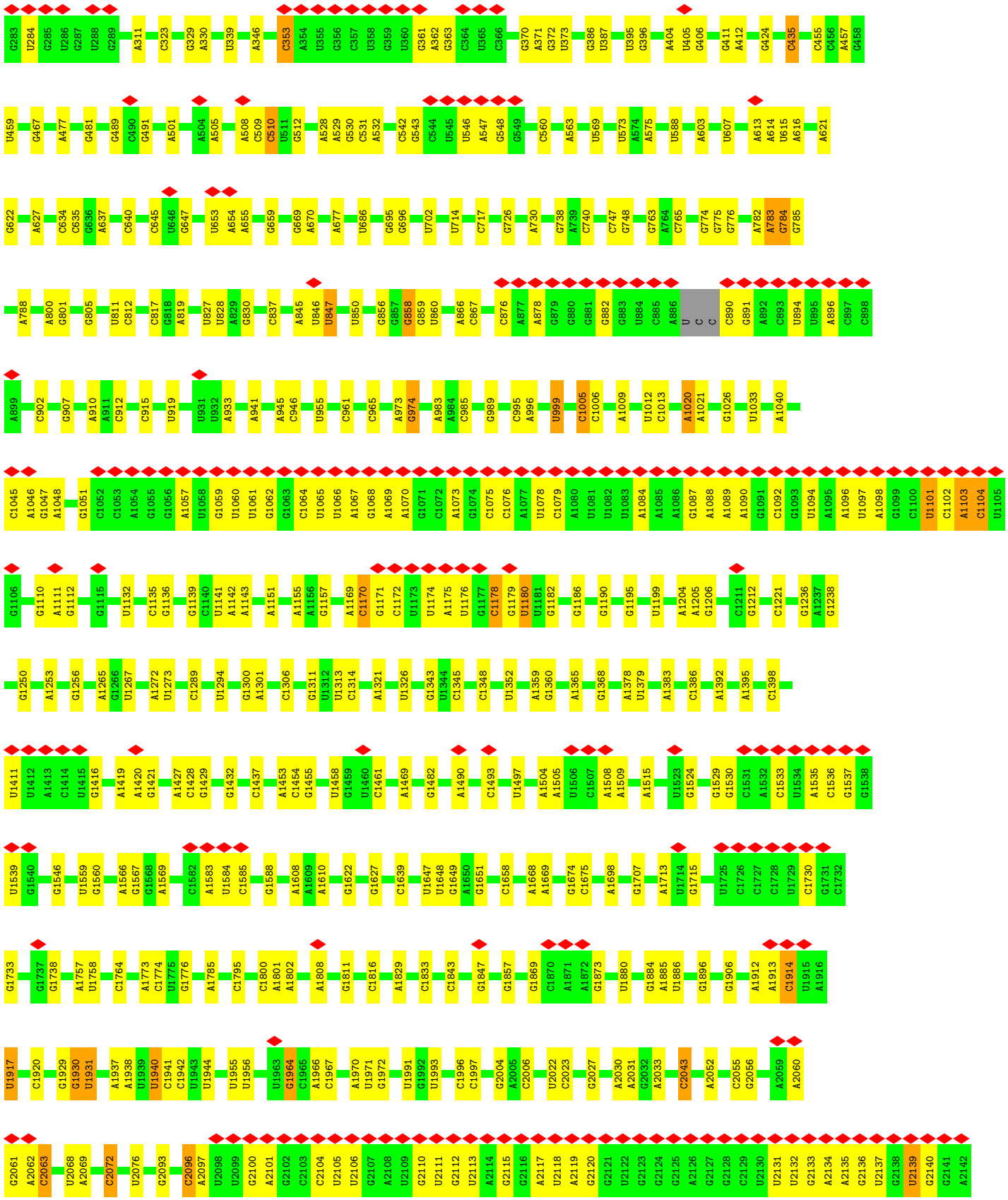


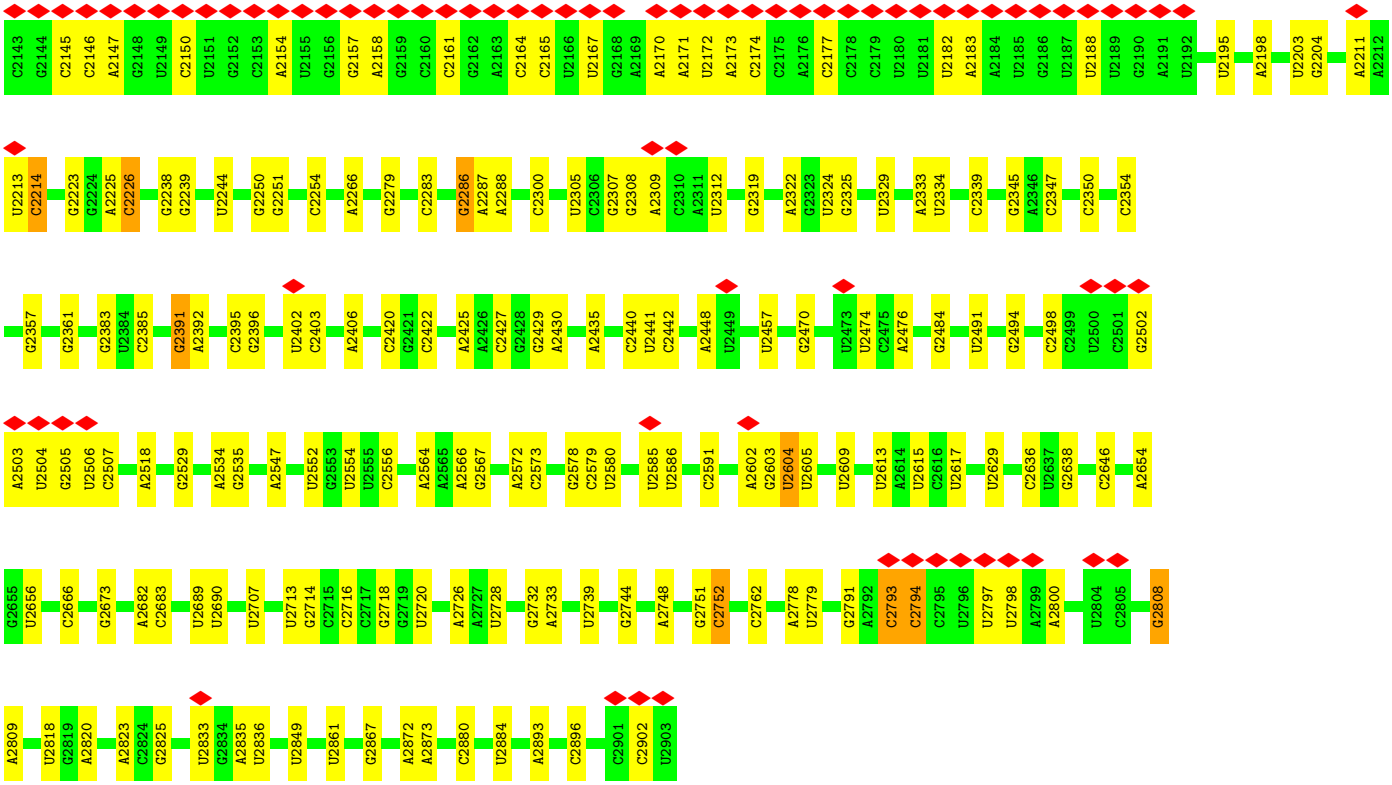


- Molecule 22: 23S ribosomal RNA

Chain A:

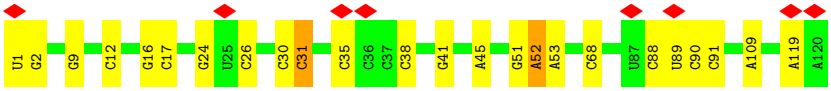



G283 U284 G285 U286 G287 U288 G289 A311 C323 G329 A330 U339 A346 C353 A354 U355 G356 C357 U358 G359 U360 G361 A362 G363 C364 U365 C366 G370 A371 G372 U373 G386 U387 U395 G396 A404 U405 G406 G411 A412 G424 C435 C455 C456 A457 G458
U459 G467 A477 G481 G489 C490 G491 A501 A504 A505 A508 C509 C510 U511 G512 A528 A529 G530 C531 A532 C542 G543 C544 U545 U546 A547 G548 G549 C560 A563 U569 U573 A574 A575 U588 A603 U607 A613 A614 U615 A616 A621
G622 A627 C634 C635 G636 A637 C640 G645 U646 G647 U653 A654 A655 G659 G669 A670 A677 U686 G695 G696 U702 U714 C717 G726 A730 G738 A739 C740 C747 G748 G763 A764 C765 G774 G775 G776 A782 A783 G784 G785
A788 A800 G801 G805 U811 C812 C817 G818 A819 U827 U828 A829 G830 C837 A845 U846 U847 U850 G856 G857 G858 G859 U860 A866 C867 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A886 U C C C890 G891 A892 C893 U894 U895 A896 C897 C898
A899 C902 G907 A910 A911 C912 C915 U919 U931 U932 A933 A941 A945 C946 U955 C961 C965 A973 G974 A983 A984 C985 G989 C995 A996 U999 C1005 C1006 A1009 U1012 C1013 A1020 A1021 G1026 U1033 A1040
C1045 A1046 G1047 A1048 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105
G1106 G1110 A1111 G1112 G1115 U1132 C1135 G1136 G1139 C1140 U1141 A1142 A1143 A1151 A1155 A1156 G1157 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 G1186 G1190 G1195 U1199 A1204 A1205 G1206 C1211 G1212 C1221 G1236 A1237 G1238
G1250 A1253 G1256 A1265 G1266 U1267 A1272 U1273 C1289 U1294 G1300 A1301 C1306 G1311 U1312 U1313 C1314 A1321 U1326 G1343 U1344 C1345 C1348 U1352 A1359 G1360 A1365 G1368 A1378 U1379 A1383 C1386 A1392 A1395 C1398
U1411 U1412 A1413 C1414 U1415 G1416 A1419 A1420 G1421 A1427 C1428 G1429 G1432 C1437 A1453 C1454 G1455 U1458 G1459 U1460 C1461 A1469 G1482 A1490 C1493 U1497 A1504 A1505 U1506 C1507 A1508 A1509 A1515 U1523 G1524 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538
U1539 G1540 G1546 U1559 G1560 A1566 G1567 G1568 A1569 C1582 A1583 U1584 C1585 G1588 A1608 A1609 A1610 G1622 G1627 C1639 U1647 U1648 G1649 A1650 G1651 C1658 A1668 A1669 G1674 C1675 A1698 G1707 A1713 U1714 G1715 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732
G1733 G1737 G1738 A1757 U1758 C1764 A1773 C1774 U1775 G1776 A1785 C1795 C1800 A1801 A1802 A1808 G1811 C1816 A1829 C1833 C1843 G1847 G1857 G1869 C1870 A1871 A1872 G1873 U1880 G1884 A1885 U1886 G1896 G1906 A1912 A1913 C1914 U1915 A1916
U1917 C1920 G1929 G1930 U1931 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 U1955 U1956 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 U1991 G1992 U1993 C1996 C1997 G2004 A2005 C2006 U2022 C2023 G2027 A2030 A2031 G2032 A2033 C2043 A2052 C2055 G2056 A2059 A2060
G2061 A2062 C2063 U2068 A2069 C2072 U2076 G2093 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



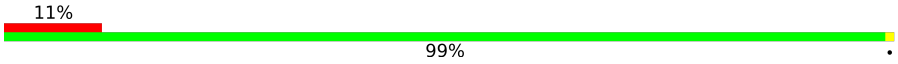
- Molecule 23: 5S ribosomal RNA

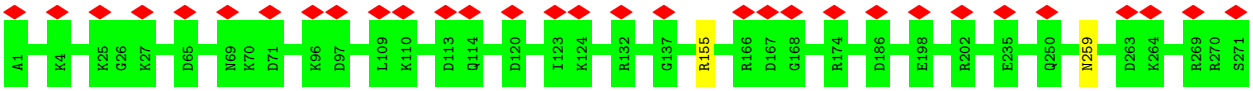
Chain B:



- Molecule 24: 50S ribosomal protein L2

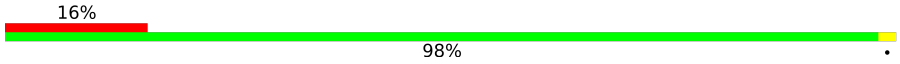
Chain C:

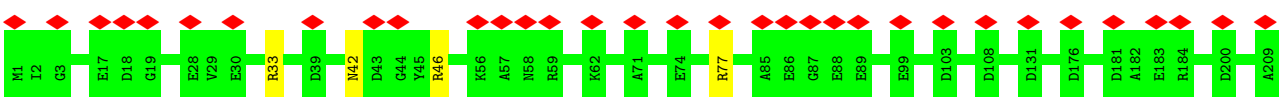




- Molecule 25: 50S ribosomal protein L3

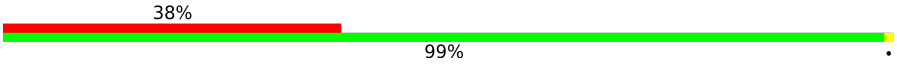
Chain D:

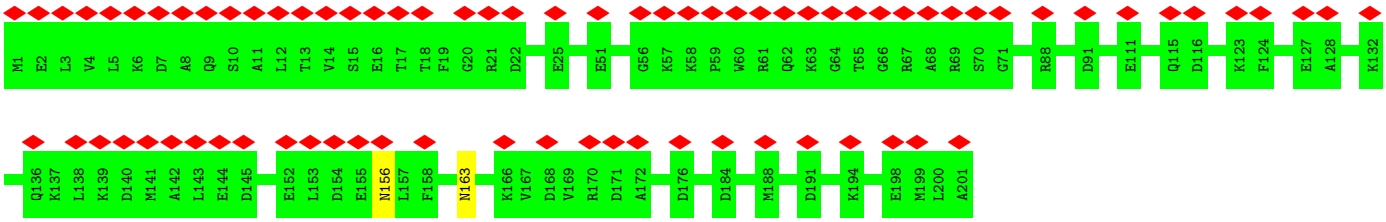




- Molecule 26: 50S ribosomal protein L4

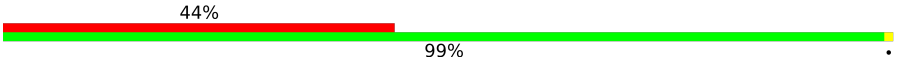
Chain E:

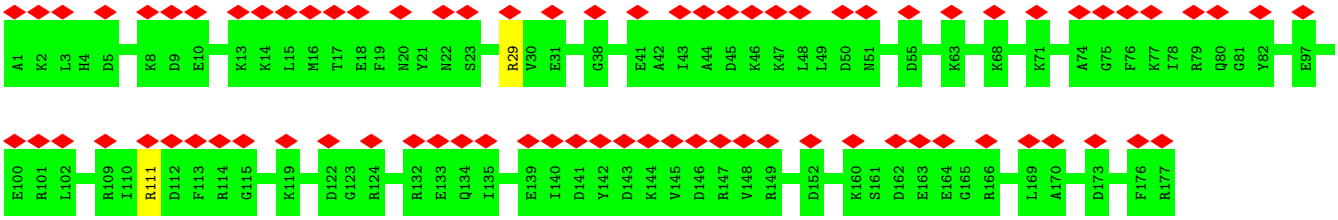




- Molecule 27: 50S ribosomal protein L5

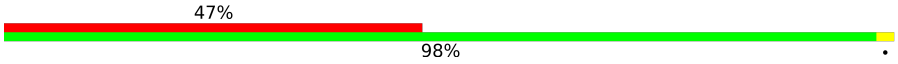
Chain F:

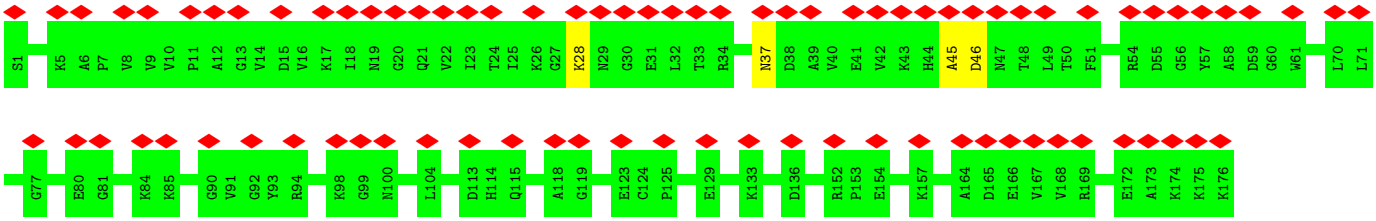




- Molecule 28: 50S ribosomal protein L6

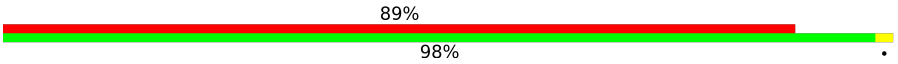
Chain G:

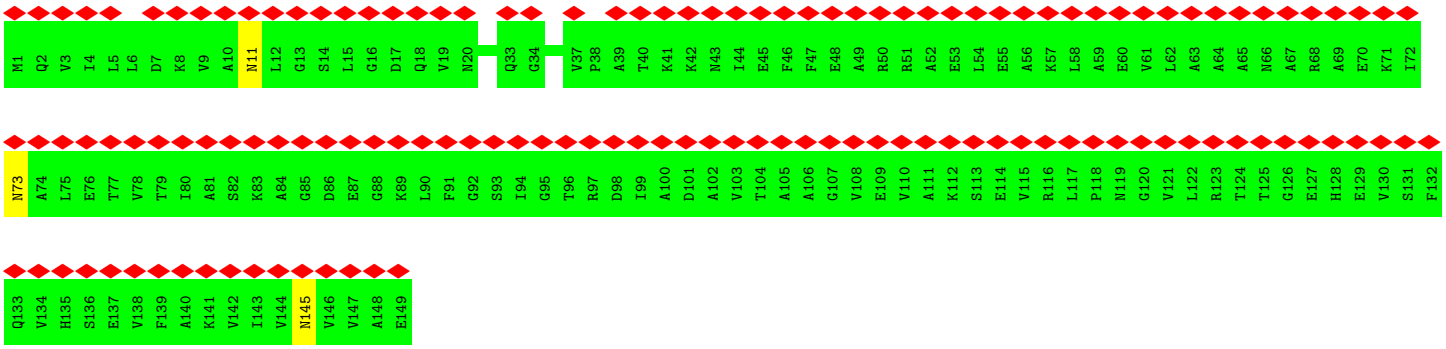




- Molecule 29: 50S ribosomal protein L9

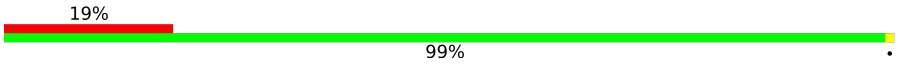
Chain H:

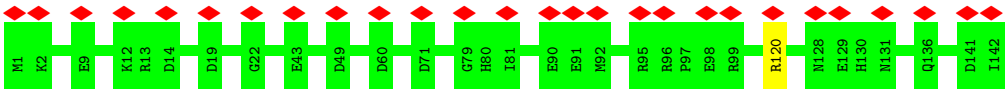




- Molecule 30: 50S ribosomal protein L13

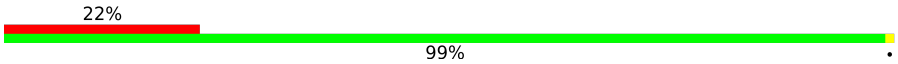
Chain J:

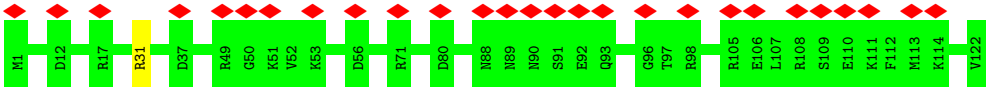




• Molecule 31: 50S ribosomal protein L14

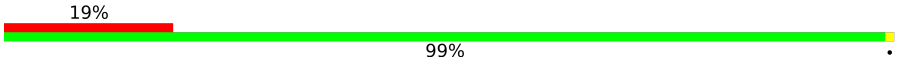
Chain K:

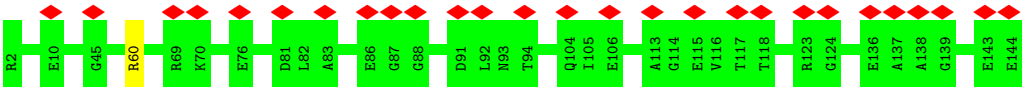




• Molecule 32: 50S ribosomal protein L15

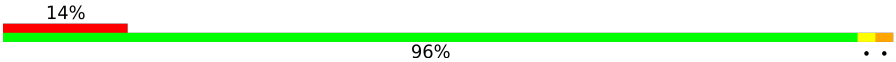
Chain L:

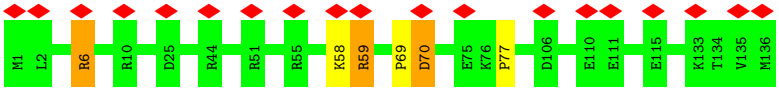




• Molecule 33: 50S ribosomal protein L16

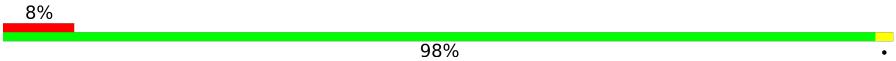
Chain M:

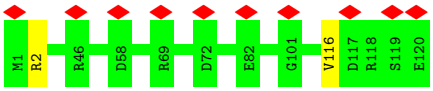




• Molecule 34: 50S ribosomal protein L17

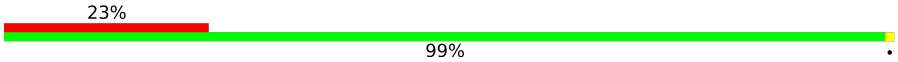
Chain N:

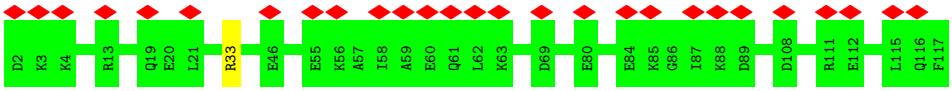




• Molecule 35: 50S ribosomal protein L18

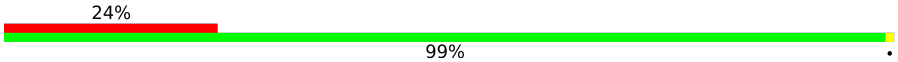
Chain O:

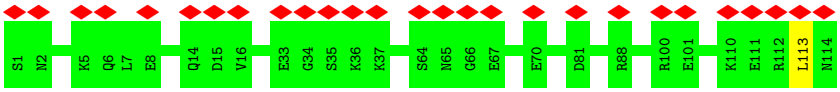




• Molecule 36: 50S ribosomal protein L19

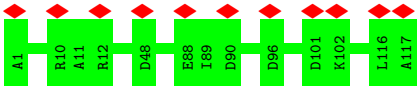
Chain P:





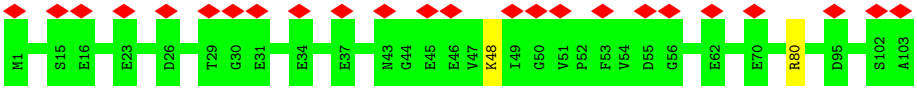
• Molecule 37: 50S ribosomal protein L20

Chain Q: 9% 100%



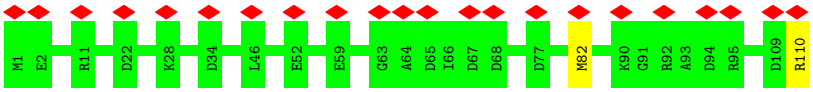
• Molecule 38: 50S ribosomal protein L21

Chain R: 23% 98%



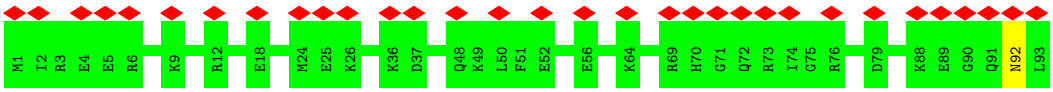
• Molecule 39: 50S ribosomal protein L22

Chain S: 20% 98%



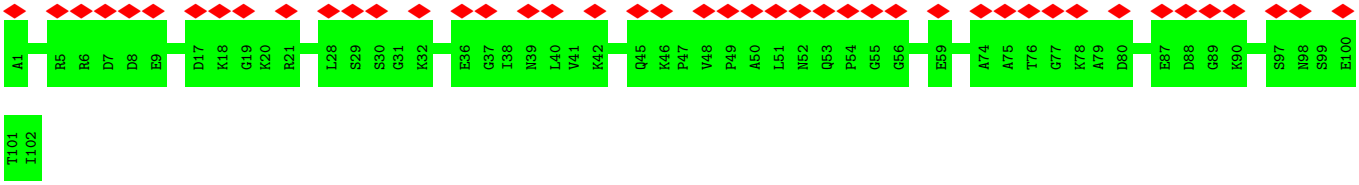
• Molecule 40: 50S ribosomal protein L23

Chain T: 34% 99%



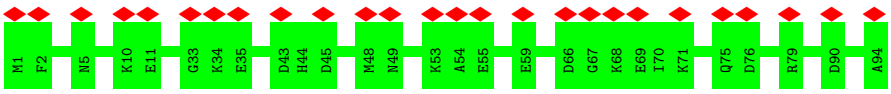
• Molecule 41: 50S ribosomal protein L24

Chain U: 43% 100%



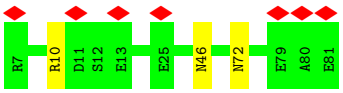
• Molecule 42: 50S ribosomal protein L25

Chain V: 28% 100%



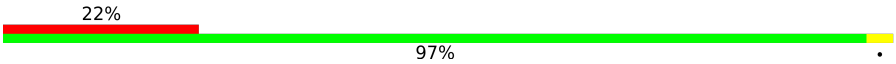
• Molecule 43: 50S ribosomal protein L27

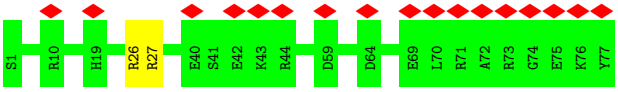
Chain W: 9% 96%



• Molecule 44: 50S ribosomal protein L28

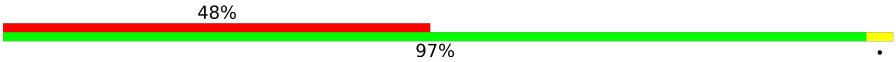
Chain X:

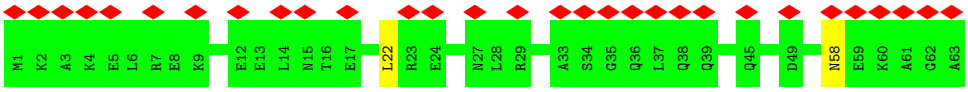




• Molecule 45: 50S ribosomal protein L29

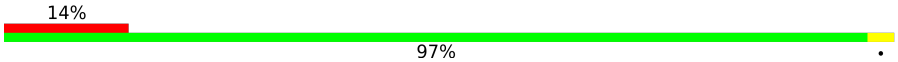
Chain Y:

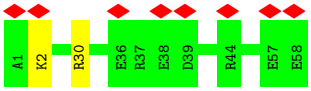




• Molecule 46: 50S ribosomal protein L30

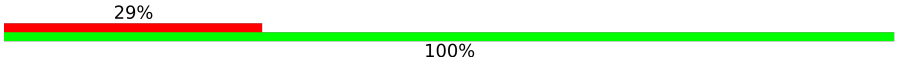
Chain Z:

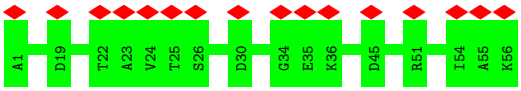




• Molecule 47: 50S ribosomal protein L32

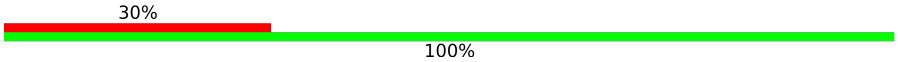
Chain 0:

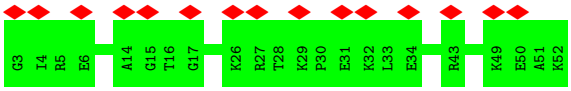




• Molecule 48: 50S ribosomal protein L33

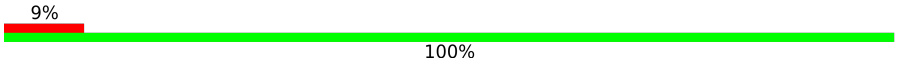
Chain 1:

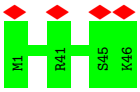




• Molecule 49: 50S ribosomal protein L34

Chain 2:





• Molecule 50: 50S ribosomal protein L35

Chain 3: 6% 94% 6%

P1 K15 H30 I31 K51 G52 D53 L56 L61 A64

- Molecule 51: 50S ribosomal protein L36

Chain 4: 18% 100%

M1 R12 M13 D20 G21 S28 A29 E30 G38

- Molecule 52: 50S ribosomal protein L31

Chain 6: 73% 100%

M1 K2 K3 D4 I5 K8 Y9 E10 E11 A14 S17 C18 G19 N20 V21 M22 K23 I24 R25 G29 H30 D31 L32 N33 L34 D35 K39 C40 H41 P42 F43 F44 T45 G46 K47 Q48 R49 D50 V51 A52 T53 G54 G55 R56 V57 D58 R59 F60 N61 K62 R63 F64 N65 I66

- Molecule 53: tRNA

Chain w: 86% 48% 40% 12%

C1 G2 C3 G4 G5 G6 G7 U8 G9 G10 A11 G12 C13 A14 G15 C16 C17 U117 G18 G19 U20 A21 G22 C23 U24 C25 G26 U27 C28 U29 G30 G31 C32 U33 C34 A35 U36 A37 A38 C39 C40 A44 G45 A46 U47 C48 G49 U50 C51 G52 G53 U54 U55 C56 A57 A58 A59 U60 C61

C62 G63 G64 C65 C66 C67 C68 C69 G70 C71 A72 A73 C74 C75 A76

- Molecule 54: Ribosome modulation factor

Chain v: 65% 91% 9%

M1 K2 R3 R6 D7 R8 L9 E10 R15 A22 G23 R24 S25 K26 E27 M28 C29 P30 Y31 Q32 T33 L34 N35 Q36 R37 S38 L41 G42 R45 M48 A49 D50 R51 V52 V53 M54 A55

- Molecule 55: 30S ribosomal protein S1

Chain y: 63% 57% 5% • 37%

MET THR E3 S4 F5 A6 Q7 L8 F9 E10 E11 S12 L13 K14 E15 I16 E17 T18 R19 P20 G21 S22 I23 V24 R25 G26 V27 V28 V29 A30 I31 D32 K33 D34 V35 V36 L37 V38 D39 A40 G41 L42 K43 S44 E45 S46 A47 I48 P49 A50 E51 Q52 F53 K54 N55 A56 Q57 G58 E59 L60

E61 I62 Q63 V64 G65 D66 E67 V68 D69 V70 A71 L72 D73 A74 V75 E76 D77 G78 F79 G80 E81 T82 L83 L84 S85 R86 E87 K88 A89 K90 R91 H92 E93 A94 W95 I96 T97 L98 E99 K100 A101 Y102 E103 D104 A105 E106 T107 V108 T109 G110 V111 I112 N113 G114 K115 V116 K117 G118 G119 F120

T121 V122 E123 L124 N125 G126 I127 R128 A129 F130 L131 P132 G133 S134 L135 V136 D137 V138 R139 P140 V141 R142 D143 T144 L145 H146 L147 E148 G149 K150 E151 L152 E153 F154 K155 V156 I157 K158 L159 D160 Q161 K162 R163 N164 N165 V166 V167 V168 S169 R170 R171 A172 V173 I174 E175 S176 GLU ASN SER ALA

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

ILE THR VAL LYS VAL LEU LYS PHE ASP ARG GLU ARG THR ARG VAL SER LEU GLY LEU LYS GLN LEU GLY E264 D265 P266 W267 V268 A269 I270 A271 K272 R273 Y274 P275 E276 G277 T278 K279 L280 T281 G282 R283 V284 T285 N286 L287 T288 D289 Y290 G291 C292 F293 V294 E295 I296 E297 E298 G299 V300

E301 G302 L303 V304 H305 V306 S307 E308 M309 D310 W311 T312 N313 K314 N315 I316 H317 P318 S319 K320 V321 V322 N323 V324 G325 D326 V327 V328 E329 V330 M331 V332 L333 D334 I335 D336 E337 E338 R339 R340 R341 I342 S343 L344 G345 L346 K347 Q348 C349 K350 A351 N352 P353 W354 Q355 Q356 F357 A358 E359 T360

H361 N362 K363 G364 D365 R366 V367 E368 G369 K370 I371 K372 S373 I374 T375 D376 F377 G378 I379 F380 I381 G382 L383 D384 G385 G386 I387 D388 G389 L390 V391 H392 L393 S394 D395 I396 S397 W398 N399 V400 A401 G402 E403 E404 A405 V406 R407 E408 Y409 K410 K411 G412 D413 E414 I415 A416 A417 V418 V419 L420

Q421 V422 D423 A424 E425 R426 E427 R428 I429 S430 L431 G432 V433 K434 Q435 L436 A437 E438 D439 P440 PHE ASN ASN TRP VAL ALA LEU ASN LYS LYS GLY ALA ILE VAL THR GLY LYS VAL THR ALA VAL ASP ALA LYS GLY ALA THR VAL GLU LEU ALA ASP GLY VAL GLU GLY TYR LEU ARG ALA

SER GLU ALA SER ARG ASP ARG VAL GLU ASP ALA THR LEU VAL LEU SER VAL GLY ASP GLU VAL GLU ALA LYS PHE THR GLY VAL ASP ARG LYS ASN ARG ALA ILE SER LEU SER VAL ARG ALA LYS ASP GLU ALA ASP GLU LYS ASP ALA ILE ALA THR VAL ASN LYS GLN GLU ASP ALA

ASN PHE SER ASN ASN ALA MET ALA GLU ALA PHE LYS ALA ALA ALA LYS GLY GLU

- Molecule 56: Ribosome hibernation promoting factor

Chain x: 29% 94% 6%

M1 Q2 L3 N8 N9 V10 E11 E14 A15 L16 R17 E18 A25 K26 L27 E28 Q29 Y30 K42 V43 E44 K45 V46 D51 E60 E66 G67 Q68 D69 D79 R83 D90 K91 Q94 H95

- Molecule 57: RNA (5'-R(P*CP*UP*CP*CP*U)-3')

Chain I: 100% 40% 40% 20%

C1536 U1537 C1538 C1539 U1540

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	188304	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.439	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.912, 398.912, 398.912	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.76	1/36857 (0.0%)	1.04	93/57496 (0.2%)
2	b	0.36	0/1735	0.62	0/2338
3	c	0.40	0/1651	0.59	1/2225 (0.0%)
4	d	0.38	0/1665	0.64	2/2227 (0.1%)
5	e	0.41	0/1154	0.66	0/1554
6	f	0.39	0/835	0.64	0/1128
7	g	0.36	0/1284	0.66	1/1724 (0.1%)
8	h	0.38	0/989	0.60	1/1326 (0.1%)
9	i	0.40	0/1034	0.65	0/1375
10	j	0.38	0/796	0.63	0/1077
11	k	0.39	0/885	0.67	0/1195
12	l	0.41	0/969	0.63	0/1300
13	m	0.34	0/892	0.63	0/1193
14	n	0.37	0/811	0.55	0/1081
15	o	0.35	0/722	0.61	0/964
16	p	0.42	0/659	0.60	0/884
17	q	0.37	0/657	0.63	0/881
18	r	0.40	0/511	0.55	0/689
19	s	0.40	0/652	0.63	0/877
20	t	0.33	0/671	0.58	1/888 (0.1%)
21	u	0.45	0/500	0.85	1/668 (0.1%)
22	A	0.81	2/69733 (0.0%)	1.07	266/108786 (0.2%)
23	B	0.72	1/2876 (0.0%)	1.09	10/4483 (0.2%)
24	C	0.46	0/2121	0.61	0/2852
25	D	0.42	0/1586	0.58	0/2134
26	E	0.38	0/1571	0.53	0/2113
27	F	0.37	0/1434	0.60	0/1926
28	G	0.35	0/1343	0.56	0/1816
29	H	0.32	0/1122	0.58	0/1515
30	J	0.42	0/1152	0.57	0/1551
31	K	0.41	0/947	0.62	0/1268
32	L	0.42	0/1054	0.65	0/1403
33	M	0.41	0/1093	0.62	2/1460 (0.1%)
34	N	0.39	0/973	0.63	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	O	0.37	0/902	0.54	0/1209
36	P	0.42	0/929	0.62	1/1242 (0.1%)
37	Q	0.46	0/960	0.53	0/1278
38	R	0.43	0/829	0.62	0/1107
39	S	0.42	0/864	0.59	0/1156
40	T	0.37	0/744	0.60	0/994
41	U	0.37	0/787	0.61	0/1051
42	V	0.40	0/766	0.59	0/1025
43	W	0.42	0/582	0.52	0/769
44	X	0.42	0/635	0.56	0/848
45	Y	0.34	0/510	0.63	1/677 (0.1%)
46	Z	0.36	0/453	0.58	0/605
47	0	0.38	0/450	0.59	0/599
48	1	0.38	0/416	0.58	0/554
49	2	0.40	0/380	0.57	0/498
50	3	0.41	0/513	0.68	2/676 (0.3%)
51	4	0.44	0/303	0.59	0/397
52	6	0.33	0/531	0.58	0/709
53	w	0.54	1/1833 (0.1%)	1.28	26/2851 (0.9%)
54	v	0.36	0/460	0.65	0/611
55	y	0.50	1/2196 (0.0%)	0.98	13/3006 (0.4%)
56	x	1.05	1/764 (0.1%)	1.20	6/1028 (0.6%)
57	I	0.77	0/109	1.49	1/166 (0.6%)
All	All	0.70	7/159850 (0.0%)	0.97	428/238754 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
4	d	0	2
7	g	0	4
9	i	0	1
11	k	0	4
12	l	0	2
13	m	0	1
15	o	0	1
20	t	0	1
21	u	0	3
28	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	M	0	1
34	N	0	1
35	O	0	1
50	3	0	1
54	v	0	2
55	y	0	6
All	All	0	33

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	x	2	GLN	C-N	-27.49	0.70	1.34
23	B	1	U	OP3-P	-10.69	1.48	1.61
22	A	1	G	OP3-P	-10.66	1.48	1.61
53	w	1	C	OP3-P	-10.51	1.48	1.61
1	a	2	A	OP3-P	-10.49	1.48	1.61
55	y	169	SER	N-CA	7.46	1.61	1.46
22	A	528	A	N9-C4	-5.80	1.34	1.37

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	x	3	LEU	O-C-N	-23.60	84.94	122.70
56	x	3	LEU	CA-C-N	16.62	153.77	117.20
1	a	516	U	N3-C2-O2	-10.93	114.55	122.20
1	a	961	U	N3-C2-O2	-10.54	114.82	122.20
22	A	2580	U	N3-C2-O2	-10.52	114.84	122.20
55	y	169	SER	N-CA-C	9.97	137.92	111.00
22	A	1917	U	N3-C2-O2	-9.77	115.36	122.20
22	A	1092	C	N1-C2-O2	9.60	124.66	118.90
22	A	955	U	N3-C2-O2	-9.47	115.57	122.20
22	A	2604	U	N3-C2-O2	-9.30	115.69	122.20
22	A	1914	C	C2-N1-C1'	9.25	128.98	118.80
22	A	1914	C	N1-C2-O2	9.14	124.38	118.90
56	x	3	LEU	C-N-CA	9.07	144.38	121.70
22	A	1005	C	C2-N1-C1'	8.98	128.68	118.80
22	A	890	C	N1-C2-O2	8.90	124.24	118.90
22	A	2580	U	N1-C2-O2	8.87	129.01	122.80
22	A	1313	U	C2-N1-C1'	8.82	128.29	117.70
1	a	58	C	C6-N1-C2	-8.80	116.78	120.30
21	u	12	ASP	CB-CG-OD1	8.78	126.21	118.30
55	y	88	LYS	C-N-CA	8.76	143.60	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	2457	U	N3-C2-O2	-8.74	116.08	122.20
22	A	890	C	C2-N1-C1'	8.70	128.37	118.80
53	w	68	C	C2-N1-C1'	8.66	128.33	118.80
22	A	1313	U	N1-C2-O2	8.55	128.78	122.80
22	A	1092	C	N3-C2-O2	-8.51	115.94	121.90
53	w	25	C	N1-C2-O2	8.42	123.95	118.90
22	A	2063	C	C6-N1-C2	-8.38	116.95	120.30
1	a	516	U	N1-C2-O2	8.36	128.65	122.80
22	A	1774	C	N3-C2-O2	-8.13	116.21	121.90
22	A	1917	U	N1-C2-O2	8.11	128.48	122.80
22	A	2457	U	C2-N1-C1'	8.10	127.42	117.70
22	A	1917	U	C2-N1-C1'	8.06	127.38	117.70
22	A	510	C	N1-C2-O2	8.06	123.73	118.90
22	A	1313	U	N3-C2-O2	-8.05	116.56	122.20
22	A	2604	U	N1-C2-O2	8.01	128.41	122.80
22	A	12	U	C2-N1-C1'	8.00	127.30	117.70
22	A	1956	U	N3-C2-O2	-7.92	116.66	122.20
53	w	56	C	C2-N1-C1'	7.91	127.50	118.80
1	a	169	C	N1-C2-O2	7.88	123.63	118.90
22	A	890	C	C6-N1-C2	-7.83	117.17	120.30
22	A	837	C	N1-C2-O2	7.77	123.56	118.90
22	A	234	U	N3-C2-O2	-7.68	116.83	122.20
22	A	955	U	N1-C2-O2	7.61	128.13	122.80
22	A	2457	U	N1-C2-O2	7.58	128.11	122.80
22	A	955	U	C2-N1-C1'	7.58	126.79	117.70
53	w	56	C	C5-C6-N1	7.57	124.79	121.00
22	A	1348	C	N1-C2-O2	7.55	123.43	118.90
22	A	2605	U	C2-N1-C1'	7.55	126.76	117.70
4	d	4	LEU	CA-CB-CG	7.51	132.58	115.30
55	y	305	HIS	N-CA-C	7.46	131.16	111.00
1	a	516	U	C2-N1-C1'	7.45	126.64	117.70
22	A	2096	C	C2-N1-C1'	7.44	126.98	118.80
22	A	2605	U	N3-C2-O2	-7.44	116.99	122.20
22	A	890	C	C5-C6-N1	7.43	124.72	121.00
23	B	31	C	C2-N1-C1'	7.41	126.95	118.80
1	a	307	C	N1-C2-O2	7.41	123.35	118.90
22	A	2617	U	N3-C2-O2	-7.40	117.02	122.20
22	A	512	G	O4'-C1'-N9	7.40	114.12	108.20
22	A	2604	U	C2-N1-C1'	7.38	126.56	117.70
22	A	2139	U	N3-C2-O2	-7.37	117.04	122.20
22	A	2226	C	N1-C2-O2	7.32	123.29	118.90
53	w	25	C	N3-C2-O2	-7.30	116.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1956	U	N1-C2-O2	7.29	127.90	122.80
53	w	56	C	C6-N1-C2	-7.23	117.41	120.30
22	A	542	C	C2-N1-C1'	7.22	126.74	118.80
22	A	2580	U	C2-N1-C1'	7.18	126.32	117.70
22	A	1914	C	N3-C2-O2	-7.18	116.87	121.90
1	a	58	C	C5-C6-N1	7.18	124.59	121.00
1	a	1158	C	C2-N1-C1'	7.17	126.69	118.80
1	a	979	C	N1-C2-O2	7.12	123.17	118.90
22	A	1005	C	C6-N1-C2	-7.11	117.46	120.30
53	w	56	C	N1-C2-O2	7.09	123.15	118.90
22	A	2072	C	C2-N1-C1'	7.06	126.57	118.80
1	a	611	C	N1-C2-O2	7.06	123.14	118.90
1	a	1125	U	N1-C2-O2	7.06	127.74	122.80
22	A	510	C	C2-N1-C1'	7.04	126.55	118.80
22	A	837	C	N3-C2-O2	-7.04	116.97	121.90
55	y	440	PRO	N-CA-CB	7.01	111.71	103.30
22	A	137	U	N3-C2-O2	-7.00	117.30	122.20
22	A	1170	C	N1-C2-O2	6.99	123.09	118.90
22	A	2072	C	C5-C6-N1	6.98	124.49	121.00
1	a	1125	U	N3-C2-O2	-6.97	117.32	122.20
22	A	1178	C	N1-C2-O2	6.96	123.08	118.90
1	a	979	C	N3-C2-O2	-6.96	117.03	121.90
36	P	113	LEU	CA-CB-CG	6.95	131.28	115.30
22	A	1170	C	C2-N1-C1'	6.94	126.44	118.80
1	a	961	U	N1-C2-N3	6.91	119.04	114.90
22	A	1314	C	C2-N1-C1'	6.88	126.37	118.80
55	y	104	ASP	N-CA-C	-6.88	92.43	111.00
22	A	2104	C	N1-C2-O2	6.87	123.02	118.90
22	A	1005	C	C5-C6-N1	6.86	124.43	121.00
1	a	1301	U	C2-N1-C1'	6.85	125.92	117.70
1	a	307	C	N3-C2-O2	-6.83	117.12	121.90
22	A	2312	U	C5-C6-N1	6.82	126.11	122.70
22	A	2063	C	C2-N1-C1'	6.81	126.29	118.80
22	A	1092	C	C2-N1-C1'	6.80	126.28	118.80
22	A	974	G	C4-N9-C1'	6.74	135.27	126.50
1	a	169	C	N3-C2-O2	-6.71	117.20	121.90
1	a	1297	G	P-O3'-C3'	6.71	127.75	119.70
7	g	156	LEU	CA-CB-CG	6.70	130.71	115.30
23	B	31	C	C6-N1-C2	-6.70	117.62	120.30
1	a	1305	G	P-O3'-C3'	6.68	127.72	119.70
22	A	837	C	C6-N1-C2	-6.67	117.63	120.30
22	A	2043	C	C2-N1-C1'	6.67	126.14	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1294	U	N3-C2-O2	-6.66	117.54	122.20
22	A	1020	A	P-O3'-C3'	6.65	127.68	119.70
22	A	1880	U	N3-C2-O2	-6.63	117.56	122.20
22	A	1940	U	P-O3'-C3'	6.62	127.64	119.70
22	A	2096	C	C6-N1-C2	-6.62	117.65	120.30
22	A	137	U	N1-C2-O2	6.61	127.43	122.80
1	a	1432	G	P-O3'-C3'	6.60	127.62	119.70
53	w	20	U	P-O3'-C3'	6.59	127.61	119.70
22	A	912	C	C2-N1-C1'	6.58	126.04	118.80
22	A	1930	G	P-O3'-C3'	6.58	127.60	119.70
1	a	92	U	C2-N1-C1'	6.56	125.57	117.70
22	A	867	C	N1-C2-O2	6.54	122.82	118.90
22	A	2063	C	N1-C2-O2	6.47	122.78	118.90
22	A	1178	C	N3-C2-O2	-6.47	117.37	121.90
22	A	1005	C	N1-C2-O2	6.45	122.77	118.90
1	a	961	U	C2-N3-C4	-6.43	123.14	127.00
53	w	51	C	C2-N1-C1'	6.42	125.87	118.80
1	a	1262	C	N1-C2-O2	6.42	122.75	118.90
22	A	1774	C	N1-C2-O2	6.42	122.75	118.90
22	A	2063	C	N3-C2-O2	-6.40	117.42	121.90
1	a	92	U	N1-C2-O2	6.40	127.28	122.80
22	A	1914	C	C6-N1-C1'	-6.40	113.12	120.80
3	c	156	LEU	CA-CB-CG	6.40	130.01	115.30
23	B	30	C	C6-N1-C2	-6.40	117.74	120.30
22	A	114	U	C2-N1-C1'	6.39	125.37	117.70
22	A	257	C	N1-C2-O2	6.39	122.73	118.90
1	a	1348	U	N1-C2-O2	6.37	127.26	122.80
22	A	1931	U	N1-C2-O2	6.37	127.26	122.80
22	A	91	A	P-O3'-C3'	6.36	127.33	119.70
22	A	635	C	C6-N1-C2	-6.35	117.76	120.30
22	A	12	U	N3-C2-O2	-6.34	117.76	122.20
22	A	2300	C	C2-N1-C1'	6.33	125.77	118.80
22	A	890	C	N3-C2-O2	-6.33	117.47	121.90
22	A	2442	C	N1-C2-O2	6.32	122.69	118.90
22	A	1508	A	O4'-C1'-N9	6.32	113.26	108.20
50	3	61	LEU	CA-CB-CG	6.32	129.83	115.30
22	A	1313	U	C6-N1-C1'	-6.32	112.35	121.20
22	A	2139	U	N1-C2-O2	6.30	127.21	122.80
53	w	73	A	O5'-P-OP1	6.29	118.25	110.70
22	A	1092	C	C6-N1-C2	-6.29	117.78	120.30
22	A	2808	G	P-O3'-C3'	6.28	127.24	119.70
22	A	435	C	N1-C2-O2	6.28	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	169	C	C6-N1-C2	-6.26	117.80	120.30
22	A	2793	C	C2-N1-C1'	6.25	125.67	118.80
22	A	2354	C	C6-N1-C2	-6.24	117.80	120.30
22	A	1920	C	C6-N1-C2	-6.24	117.80	120.30
22	A	1267	U	N1-C2-O2	6.24	127.16	122.80
22	A	2617	U	N1-C2-O2	6.24	127.17	122.80
22	A	2072	C	C6-N1-C2	-6.22	117.81	120.30
22	A	1314	C	C6-N1-C2	-6.22	117.81	120.30
1	a	1317	C	N1-C2-O2	6.21	122.62	118.90
53	w	68	C	C6-N1-C2	-6.20	117.82	120.30
22	A	783	A	C5-N7-C8	-6.19	100.80	103.90
22	A	234	U	N1-C2-O2	6.18	127.12	122.80
22	A	2226	C	N3-C2-O2	-6.18	117.58	121.90
22	A	847	U	N3-C2-O2	-6.17	117.88	122.20
56	x	2	GLN	O-C-N	6.14	132.52	122.70
22	A	965	C	C6-N1-C2	-6.13	117.85	120.30
22	A	1102	C	N3-C2-O2	-6.13	117.61	121.90
22	A	2214	C	N1-C2-O2	6.11	122.57	118.90
1	a	610	U	N1-C2-O2	6.11	127.08	122.80
1	a	58	C	C2-N1-C1'	6.10	125.51	118.80
22	A	1267	U	N3-C2-O2	-6.10	117.93	122.20
53	w	25	C	C6-N1-C2	-6.10	117.86	120.30
22	A	1180	U	C2-N1-C1'	6.10	125.02	117.70
56	x	2	GLN	C-N-CA	-6.09	106.48	121.70
1	a	998	C	N3-C2-O2	-6.07	117.65	121.90
22	A	2072	C	N1-C2-O2	6.07	122.54	118.90
22	A	1993	U	N1-C2-O2	6.05	127.04	122.80
1	a	316	C	C2-N1-C1'	6.05	125.46	118.80
22	A	858	G	P-O3'-C3'	6.05	126.96	119.70
22	A	902	C	C2-N1-C1'	6.04	125.45	118.80
22	A	1993	U	N3-C2-O2	-6.04	117.97	122.20
1	a	754	C	C2-N1-C1'	6.03	125.44	118.80
1	a	610	U	N3-C2-O2	-6.03	117.98	122.20
1	a	1138	G	C4-N9-C1'	6.02	134.33	126.50
22	A	2104	C	N3-C2-O2	-6.02	117.68	121.90
53	w	53	G	P-O3'-C3'	6.02	126.93	119.70
22	A	1914	C	C6-N1-C2	-6.01	117.89	120.30
22	A	2605	U	N1-C2-O2	5.99	126.99	122.80
53	w	3	C	C2-N1-C1'	5.99	125.39	118.80
22	A	1348	C	N3-C2-O2	-5.98	117.71	121.90
55	y	353	PRO	N-CA-CB	5.98	110.47	103.30
22	A	1880	U	N1-C2-O2	5.97	126.98	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	17	C	C2-N1-C1'	5.96	125.36	118.80
55	y	140	PRO	N-CA-CB	5.96	110.45	103.30
22	A	2214	C	N3-C2-O2	-5.95	117.73	121.90
1	a	536	C	C2-N1-C1'	5.95	125.34	118.80
22	A	1079	C	N1-C2-O2	5.94	122.47	118.90
22	A	208	C	C6-N1-C2	-5.94	117.92	120.30
22	A	1221	C	C2-N1-C1'	5.93	125.33	118.80
22	A	783	A	N7-C8-N9	5.92	116.76	113.80
22	A	1005	C	C6-N1-C1'	-5.92	113.70	120.80
22	A	2636	C	C2-N1-C1'	5.92	125.31	118.80
23	B	52	A	P-O3'-C3'	5.91	126.80	119.70
55	y	330	VAL	N-CA-C	5.90	126.92	111.00
1	a	1138	G	N3-C4-C5	-5.89	125.65	128.60
22	A	339	U	N3-C2-O2	-5.88	118.08	122.20
22	A	1102	C	N1-C2-O2	5.88	122.43	118.90
53	w	68	C	C6-N1-C1'	-5.88	113.75	120.80
1	a	611	C	N3-C2-O2	-5.86	117.80	121.90
22	A	2683	C	C6-N1-C2	-5.85	117.96	120.30
55	y	132	PRO	N-CA-CB	5.85	110.32	103.30
22	A	2139	U	C2-N1-C1'	5.85	124.72	117.70
22	A	607	U	N3-C2-O2	-5.84	118.11	122.20
45	Y	22	LEU	CA-CB-CG	5.84	128.73	115.30
22	A	1348	C	C2-N1-C1'	5.83	125.22	118.80
22	A	206	U	N1-C2-O2	5.83	126.88	122.80
22	A	2195	U	N3-C2-O2	-5.83	118.12	122.20
55	y	168	VAL	C-N-CA	5.83	136.26	121.70
1	a	1158	C	N1-C2-O2	5.82	122.39	118.90
22	A	2656	U	N1-C2-O2	5.82	126.87	122.80
1	a	1190	G	P-O3'-C3'	5.82	126.68	119.70
22	A	1314	C	C5-C6-N1	5.82	123.91	121.00
22	A	2739	U	N3-C2-O2	-5.82	118.13	122.20
22	A	640	C	C5-C6-N1	5.81	123.91	121.00
53	w	37	A	O5'-P-OP1	5.81	117.67	110.70
1	a	311	C	C6-N1-C2	-5.80	117.98	120.30
1	a	561	U	P-O3'-C3'	5.80	126.66	119.70
22	A	1993	U	C2-N1-C1'	5.79	124.65	117.70
22	A	2244	U	N3-C4-O4	5.78	123.45	119.40
1	a	103	U	N3-C2-O2	-5.78	118.16	122.20
22	A	1103	A	OP1-P-O3'	5.78	117.91	105.20
1	a	1182	G	P-O3'-C3'	5.77	126.63	119.70
22	A	2457	U	C6-N1-C1'	-5.77	113.12	121.20
22	A	459	U	N3-C2-O2	-5.77	118.16	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1343	G	C4-N9-C1'	5.76	133.99	126.50
22	A	1920	C	C5-C6-N1	5.75	123.88	121.00
1	a	1109	C	N3-C2-O2	-5.74	117.88	121.90
1	a	169	C	C2-N1-C1'	5.73	125.10	118.80
22	A	2063	C	C5-C6-N1	5.72	123.86	121.00
22	A	12	U	N1-C2-O2	5.71	126.80	122.80
22	A	974	G	N7-C8-N9	5.71	115.96	113.10
1	a	503	C	C6-N1-C2	-5.71	118.02	120.30
1	a	1348	U	N3-C2-O2	-5.71	118.21	122.20
22	A	2329	U	C5-C6-N1	5.70	125.55	122.70
55	y	344	LEU	CA-CB-CG	5.70	128.42	115.30
22	A	2474	U	C2-N1-C1'	5.68	124.51	117.70
22	A	1157	G	C6-C5-N7	-5.67	127.00	130.40
22	A	2552	U	N3-C2-O2	-5.67	118.23	122.20
22	A	634	C	C6-N1-C2	-5.67	118.03	120.30
22	A	2104	C	C6-N1-C2	-5.66	118.04	120.30
23	B	17	C	C6-N1-C2	-5.66	118.04	120.30
1	a	660	C	C2-N1-C1'	5.65	125.01	118.80
22	A	542	C	C6-N1-C2	-5.64	118.04	120.30
22	A	459	U	N1-C2-O2	5.63	126.74	122.80
1	a	697	U	N3-C2-O2	-5.62	118.27	122.20
1	a	1301	U	N1-C2-O2	5.62	126.73	122.80
22	A	2339	C	C2-N1-C1'	5.61	124.97	118.80
53	w	68	C	N1-C2-O2	5.61	122.27	118.90
22	A	999	U	N3-C2-O2	-5.61	118.28	122.20
22	A	847	U	N1-C2-O2	5.60	126.72	122.80
22	A	2683	C	N1-C2-O2	5.60	122.26	118.90
1	a	998	C	N1-C2-O2	5.60	122.26	118.90
22	A	860	U	N1-C2-O2	5.60	126.72	122.80
22	A	1289	C	C2-N1-C1'	5.60	124.96	118.80
33	M	70	ASP	CB-CG-OD1	5.60	123.34	118.30
22	A	1306	C	C2-N1-C1'	5.59	124.95	118.80
22	A	1931	U	C2-N1-C1'	5.58	124.40	117.70
1	a	1109	C	N1-C2-O2	5.58	122.25	118.90
22	A	192	C	C6-N1-C2	-5.58	118.07	120.30
22	A	1101	U	N3-C2-O2	-5.58	118.30	122.20
22	A	2794	C	C2-N1-C1'	5.58	124.93	118.80
22	A	965	C	C2-N1-C1'	5.57	124.93	118.80
22	A	1914	C	C5-C6-N1	5.57	123.79	121.00
22	A	860	U	N3-C2-O2	-5.57	118.30	122.20
22	A	257	C	N3-C2-O2	-5.57	118.00	121.90
22	A	2474	U	N1-C2-O2	5.57	126.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	974	G	C4-C5-N7	5.56	113.02	110.80
1	a	436	C	C2-N1-C1'	5.56	124.91	118.80
22	A	1931	U	N3-C2-O2	-5.56	118.31	122.20
22	A	2244	U	C5-C4-O4	-5.55	122.57	125.90
1	a	1262	C	N3-C2-O2	-5.54	118.02	121.90
56	x	2	GLN	CA-C-N	-5.54	105.00	117.20
1	a	643	C	C6-N1-C2	-5.54	118.08	120.30
22	A	1101	U	N1-C2-O2	5.53	126.67	122.80
1	a	439	U	N3-C2-O2	-5.53	118.33	122.20
22	A	198	C	C5-C6-N1	5.53	123.76	121.00
22	A	915	C	C2-N1-C1'	5.52	124.88	118.80
22	A	2161	C	N3-C2-O2	-5.52	118.03	121.90
22	A	1795	C	C6-N1-C2	-5.52	118.09	120.30
22	A	850	U	N3-C2-O2	-5.50	118.35	122.20
53	w	3	C	N1-C2-O2	5.50	122.20	118.90
22	A	510	C	C5-C6-N1	5.50	123.75	121.00
22	A	1294	U	N1-C2-O2	5.50	126.65	122.80
53	w	13	C	C2-N1-C1'	5.50	124.85	118.80
1	a	611	C	C6-N1-C2	-5.50	118.10	120.30
1	a	1317	C	N3-C2-O2	-5.49	118.06	121.90
4	d	190	LEU	CA-CB-CG	5.49	127.93	115.30
22	A	1843	C	C5-C6-N1	5.48	123.74	121.00
22	A	1940	U	OP2-P-O3'	5.48	117.25	105.20
1	a	1383	C	N1-C2-O2	5.47	122.19	118.90
23	B	31	C	C5-C6-N1	5.47	123.74	121.00
20	t	67	HIS	C-N-CA	5.46	135.36	121.70
22	A	2720	U	N3-C2-O2	-5.46	118.38	122.20
22	A	2656	U	N3-C2-O2	-5.45	118.39	122.20
53	w	32	C	N1-C2-O2	5.45	122.17	118.90
22	A	783	A	C8-N9-C4	-5.45	103.62	105.80
22	A	2666	C	N1-C2-O2	5.44	122.16	118.90
1	a	979	C	C6-N1-C2	-5.44	118.12	120.30
1	a	972	C	C6-N1-C2	-5.42	118.13	120.30
22	A	890	C	C2-N3-C4	5.42	122.61	119.90
22	A	1931	U	C5-C6-N1	5.41	125.41	122.70
22	A	784	G	P-O3'-C3'	5.41	126.19	119.70
22	A	2391	G	P-O3'-C3'	5.40	126.18	119.70
22	A	560	C	C6-N1-C2	-5.40	118.14	120.30
22	A	1104	C	C6-N1-C2	-5.40	118.14	120.30
22	A	974	G	C8-N9-C1'	-5.39	119.99	127.00
22	A	1170	C	N3-C2-O2	-5.39	118.13	121.90
22	A	2474	U	N3-C2-O2	-5.39	118.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	2552	U	C2-N1-C1'	5.39	124.17	117.70
1	a	516	U	C6-N1-C2	-5.38	117.77	121.00
23	B	30	C	C5-C6-N1	5.38	123.69	121.00
22	A	2076	U	C2-N1-C1'	5.38	124.16	117.70
1	a	611	C	C2-N1-C1'	5.38	124.72	118.80
1	a	110	C	N1-C2-O2	5.37	122.12	118.90
22	A	2043	C	C5-C6-N1	5.37	123.69	121.00
23	B	26	C	N1-C2-O2	5.37	122.12	118.90
1	a	1151	A	O4'-C1'-N9	5.37	112.49	108.20
22	A	2579	C	C6-N1-C2	-5.37	118.15	120.30
22	A	890	C	C6-N1-C1'	-5.36	114.37	120.80
1	a	4	U	C2-N1-C1'	5.36	124.13	117.70
1	a	92	U	N3-C2-O2	-5.34	118.47	122.20
22	A	12	U	C5-C6-N1	5.33	125.37	122.70
22	A	1221	C	N1-C2-O2	5.33	122.09	118.90
22	A	882	G	N3-C4-N9	5.32	129.19	126.00
22	A	1157	G	C4-N9-C1'	5.31	133.40	126.50
22	A	1348	C	C6-N1-C2	-5.31	118.18	120.30
22	A	47	C	C6-N1-C2	-5.30	118.18	120.30
22	A	1795	C	C5-C6-N1	5.30	123.65	121.00
22	A	206	U	N3-C2-O2	-5.29	118.49	122.20
22	A	1585	C	N1-C2-O2	5.29	122.07	118.90
1	a	1264	U	N3-C2-O2	-5.29	118.50	122.20
1	a	1190	G	OP2-P-O3'	5.29	116.83	105.20
22	A	702	U	C2-N1-C1'	5.28	124.04	117.70
22	A	1343	G	C8-N9-C1'	-5.28	120.13	127.00
22	A	1658	C	C6-N1-C2	-5.28	118.19	120.30
1	a	697	U	N1-C2-O2	5.28	126.50	122.80
22	A	2096	C	C5-C6-N1	5.28	123.64	121.00
1	a	469	C	N1-C2-O2	5.28	122.07	118.90
1	a	516	U	C5-C4-O4	5.27	129.06	125.90
22	A	208	C	C5-C6-N1	5.27	123.63	121.00
22	A	2226	C	C2-N1-C1'	5.26	124.59	118.80
1	a	1301	U	N3-C2-O2	-5.26	118.52	122.20
1	a	409	U	N3-C2-O2	-5.26	118.52	122.20
22	A	2106	U	C2-N1-C1'	5.25	124.00	117.70
23	B	12	C	C2-N1-C1'	5.25	124.57	118.80
22	A	12	U	C6-N1-C2	-5.23	117.86	121.00
22	A	2286	G	P-O3'-C3'	5.23	125.98	119.70
22	A	2591	C	C6-N1-C2	-5.23	118.21	120.30
1	a	4	U	N1-C2-O2	5.22	126.45	122.80
1	a	34	C	C5-C6-N1	5.22	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1178	C	C6-N1-C2	-5.22	118.21	120.30
8	h	58	LEU	CA-CB-CG	5.21	127.30	115.30
1	a	1109	C	C6-N1-C2	-5.20	118.22	120.30
22	A	353	C	C2-N1-C1'	5.20	124.52	118.80
22	A	1886	U	N1-C2-O2	5.20	126.44	122.80
22	A	2556	C	N1-C2-O2	5.20	122.02	118.90
22	A	353	C	C6-N1-C2	-5.20	118.22	120.30
1	a	1264	U	N1-C2-O2	5.20	126.44	122.80
22	A	817	C	C6-N1-C2	-5.20	118.22	120.30
22	A	435	C	N3-C2-O2	-5.19	118.27	121.90
22	A	640	C	C6-N1-C2	-5.19	118.22	120.30
57	I	1537	U	P-O3'-C3'	5.18	125.92	119.70
22	A	1157	G	C4-C5-N7	5.18	112.87	110.80
22	A	2752	C	N1-C2-O2	5.18	122.00	118.90
1	a	54	C	N1-C2-O2	5.17	122.00	118.90
22	A	965	C	C5-C6-N1	5.17	123.59	121.00
22	A	1076	C	C6-N1-C2	-5.17	118.23	120.30
53	w	68	C	C5-C6-N1	5.16	123.58	121.00
22	A	974	G	C6-C5-N7	-5.16	127.31	130.40
22	A	1326	U	N1-C2-O2	5.16	126.41	122.80
1	a	1138	G	N3-C4-N9	5.15	129.09	126.00
1	a	1158	C	C6-N1-C1'	-5.15	114.62	120.80
55	y	169	SER	N-CA-CB	-5.15	102.78	110.50
53	w	34	C	C5-C6-N1	5.14	123.57	121.00
1	a	1132	C	N1-C2-O2	5.14	121.99	118.90
22	A	370	G	O4'-C1'-N9	-5.14	104.09	108.20
22	A	1398	C	C2-N1-C1'	5.14	124.46	118.80
22	A	1157	G	C8-N9-C1'	-5.14	120.32	127.00
22	A	2896	C	C5-C6-N1	5.14	123.57	121.00
33	M	6	ARG	CA-CB-CG	5.13	124.69	113.40
22	A	1348	C	C5-C6-N1	5.13	123.57	121.00
22	A	2656	U	C5-C6-N1	5.13	125.27	122.70
22	A	192	C	C5-C6-N1	5.13	123.56	121.00
1	a	516	U	O4'-C1'-N1	5.12	112.30	108.20
22	A	1157	G	N3-C4-N9	5.12	129.07	126.00
22	A	243	U	N1-C2-O2	5.12	126.38	122.80
22	A	510	C	N3-C2-O2	-5.11	118.32	121.90
22	A	2442	C	N3-C2-O2	-5.10	118.33	121.90
50	3	56	LEU	CA-CB-CG	5.10	127.03	115.30
53	w	29	U	C2-N1-C1'	5.09	123.81	117.70
22	A	2825	G	C4-N9-C1'	5.09	133.12	126.50
22	A	955	U	O4'-C1'-N1	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	542	C	C5-C6-N1	5.08	123.54	121.00
22	A	1669	A	C4-N9-C1'	5.08	135.45	126.30
53	w	51	C	N1-C2-O2	5.08	121.95	118.90
1	a	580	C	C5-C6-N1	5.08	123.54	121.00
53	w	29	U	N1-C2-O2	5.08	126.36	122.80
22	A	2113	U	N1-C2-O2	5.08	126.35	122.80
22	A	1843	C	C6-N1-C2	-5.07	118.27	120.30
53	w	24	U	C2-N1-C1'	5.07	123.78	117.70
22	A	1964	G	O4'-C1'-N9	-5.07	104.15	108.20
22	A	2339	C	C6-N1-C2	-5.07	118.27	120.30
22	A	2395	C	C6-N1-C2	-5.07	118.27	120.30
1	a	979	C	C2-N1-C1'	5.05	124.35	118.80
55	y	332	VAL	N-CA-C	5.05	124.63	111.00
1	a	1119	C	C5-C6-N1	5.04	123.52	121.00
1	a	496	A	O4'-C1'-N9	5.04	112.23	108.20
22	A	955	U	C6-N1-C1'	-5.03	114.15	121.20
1	a	1125	U	C2-N1-C1'	5.03	123.74	117.70
22	A	1199	U	C5-C6-N1	5.03	125.22	122.70
22	A	2006	C	C5-C6-N1	5.03	123.52	121.00
1	a	1317	C	C2-N1-C1'	5.03	124.33	118.80
22	A	235	U	N3-C2-O2	-5.02	118.69	122.20
22	A	1774	C	C6-N1-C2	-5.02	118.29	120.30
22	A	867	C	N3-C2-O2	-5.02	118.39	121.90
22	A	2254	C	N1-C2-O2	5.02	121.91	118.90
22	A	1170	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1440	U	C2-N1-C1'	5.01	123.71	117.70
22	A	243	U	N3-C2-O2	-5.01	118.69	122.20
1	a	1520	C	C2-N1-C1'	5.01	124.31	118.80
1	a	439	U	N1-C2-O2	5.00	126.30	122.80
22	A	2312	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	3	30	HIS	Peptide
28	G	45	ALA	Peptide
33	M	58	LYS	Peptide
34	N	116	VAL	Peptide
35	O	33	ARG	Peptide
2	b	17	HIS	Peptide
4	d	190	LEU	Peptide

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Mol	Chain	Res	Type	Group
4	d	27	ILE	Peptide
7	g	110	ARG	Peptide
7	g	152	HIS	Peptide
7	g	158	LEU	Peptide
7	g	4	ARG	Peptide
9	i	56	MET	Peptide
11	k	117	HIS	Peptide
11	k	12	ARG	Peptide
11	k	125	LYS	Peptide
11	k	72	ALA	Peptide
12	l	22	ALA	Peptide
12	l	76	HIS	Peptide
13	m	8	ILE	Peptide
15	o	45	HIS	Peptide
20	t	28	ARG	Peptide
21	u	39	LYS	Peptide
21	u	6	ARG	Peptide
21	u	8	ASN	Peptide
54	v	26	LYS	Peptide
54	v	6	ARG	Peptide
55	y	274	TYR	Peptide
55	y	391	VAL	Peptide
55	y	417	ALA	Peptide
55	y	419	VAL	Peptide
55	y	81	GLU	Peptide
55	y	82	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	216/218 (99%)	182 (84%)	33 (15%)	1 (0%)	29	68
3	c	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
4	d	203/205 (99%)	181 (89%)	22 (11%)	0	100	100
5	e	155/157 (99%)	142 (92%)	13 (8%)	0	100	100
6	f	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
7	g	159/161 (99%)	137 (86%)	21 (13%)	1 (1%)	25	64
8	h	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	i	125/127 (98%)	102 (82%)	23 (18%)	0	100	100
10	j	96/98 (98%)	82 (85%)	13 (14%)	1 (1%)	15	53
11	k	114/116 (98%)	97 (85%)	17 (15%)	0	100	100
12	l	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
13	m	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	17	55
14	n	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
15	o	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	48
16	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	q	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
18	r	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
19	s	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
20	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
21	u	63/65 (97%)	46 (73%)	16 (25%)	1 (2%)	9	40
24	C	269/271 (99%)	244 (91%)	25 (9%)	0	100	100
25	D	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
26	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
27	F	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
28	G	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	25	64
29	H	147/149 (99%)	127 (86%)	20 (14%)	0	100	100
30	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
31	K	120/122 (98%)	103 (86%)	17 (14%)	0	100	100
32	L	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
33	M	134/136 (98%)	126 (94%)	4 (3%)	4 (3%)	4	24
34	N	118/120 (98%)	108 (92%)	10 (8%)	0	100	100
35	O	114/116 (98%)	103 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	P	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
37	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
38	R	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
39	S	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
40	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
41	U	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
42	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	W	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
44	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
45	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
46	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
47	0	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
48	1	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
49	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
50	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	40
51	4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	6	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
54	v	53/55 (96%)	43 (81%)	9 (17%)	1 (2%)	8	36
55	y	347/557 (62%)	253 (73%)	75 (22%)	19 (6%)	2	10
56	x	93/95 (98%)	85 (91%)	7 (8%)	1 (1%)	14	50
All	All	6082/6394 (95%)	5435 (89%)	614 (10%)	33 (0%)	32	68

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
21	u	37	TYR
55	y	139	ARG
55	y	153	GLU
55	y	169	SER
55	y	306	VAL
55	y	379	ILE
55	y	387	ILE
15	o	46	LYS
55	y	104	ASP

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Mol	Chain	Res	Type
55	y	108	VAL
55	y	309	MET
55	y	333	LEU
55	y	360	THR
55	y	397	SER
7	g	153	TYR
54	v	7	ASP
55	y	76	GLU
55	y	142	ARG
55	y	349	CYS
28	G	46	ASP
33	M	70	ASP
50	3	31	ILE
55	y	82	THR
33	M	59	ARG
33	M	77	PRO
55	y	70	VAL
55	y	439	ASP
10	j	58	ASN
33	M	69	PRO
55	y	391	VAL
13	m	9	PRO
56	x	46	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/180 (100%)	178 (99%)	2 (1%)	73	90
3	c	170/170 (100%)	168 (99%)	2 (1%)	71	90
4	d	172/172 (100%)	169 (98%)	3 (2%)	60	85
5	e	114/119 (96%)	110 (96%)	4 (4%)	36	71
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	132/132 (100%)	127 (96%)	5 (4%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	104/104 (100%)	102 (98%)	2 (2%)	57	84
9	i	105/105 (100%)	100 (95%)	5 (5%)	25	62
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	88 (99%)	1 (1%)	73	90
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	77 (98%)	2 (2%)	47	79
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	63 (97%)	2 (3%)	40	75
17	q	74/74 (100%)	73 (99%)	1 (1%)	67	88
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	64 (98%)	1 (2%)	65	87
21	u	44/55 (80%)	43 (98%)	1 (2%)	50	80
24	C	216/216 (100%)	214 (99%)	2 (1%)	78	92
25	D	164/164 (100%)	160 (98%)	4 (2%)	49	79
26	E	165/165 (100%)	163 (99%)	2 (1%)	71	90
27	F	148/148 (100%)	146 (99%)	2 (1%)	67	88
28	G	137/137 (100%)	135 (98%)	2 (2%)	65	87
29	H	114/114 (100%)	111 (97%)	3 (3%)	46	78
30	J	116/116 (100%)	115 (99%)	1 (1%)	78	92
31	K	103/103 (100%)	102 (99%)	1 (1%)	76	91
32	L	102/102 (100%)	101 (99%)	1 (1%)	76	91
33	M	109/109 (100%)	107 (98%)	2 (2%)	59	85
34	N	100/100 (100%)	99 (99%)	1 (1%)	76	91
35	O	86/86 (100%)	86 (100%)	0	100	100
36	P	99/99 (100%)	99 (100%)	0	100	100
37	Q	89/89 (100%)	89 (100%)	0	100	100
38	R	84/84 (100%)	82 (98%)	2 (2%)	49	79
39	S	93/93 (100%)	91 (98%)	2 (2%)	52	81
40	T	80/80 (100%)	79 (99%)	1 (1%)	69	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	U	83/83 (100%)	83 (100%)	0	100	100
42	V	78/78 (100%)	78 (100%)	0	100	100
43	W	57/57 (100%)	54 (95%)	3 (5%)	22	58
44	X	67/67 (100%)	65 (97%)	2 (3%)	41	75
45	Y	55/55 (100%)	54 (98%)	1 (2%)	59	85
46	Z	48/48 (100%)	46 (96%)	2 (4%)	30	66
47	0	47/47 (100%)	47 (100%)	0	100	100
48	1	45/45 (100%)	45 (100%)	0	100	100
49	2	38/38 (100%)	38 (100%)	0	100	100
50	3	51/51 (100%)	51 (100%)	0	100	100
51	4	34/34 (100%)	34 (100%)	0	100	100
52	6	59/59 (100%)	59 (100%)	0	100	100
54	v	44/44 (100%)	42 (96%)	2 (4%)	27	64
55	y	137/461 (30%)	134 (98%)	3 (2%)	52	81
56	x	80/81 (99%)	77 (96%)	3 (4%)	33	69
All	All	4883/5236 (93%)	4810 (98%)	73 (2%)	66	87

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	23	ASN
2	b	202	ASN
3	c	31	ASN
3	c	168	ARG
4	d	80	ARG
4	d	130	ASN
4	d	183	ARG
5	e	45	VAL
5	e	69	ASN
5	e	92	ARG
5	e	151	MET
7	g	9	ARG
7	g	78	ARG
7	g	129	ASN
7	g	156	LEU
7	g	159	ARG
8	h	37	ASN

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Mol	Chain	Res	Type
8	h	120	LEU
9	i	11	ARG
9	i	24	ASN
9	i	44	ARG
9	i	56	MET
9	i	60	LEU
11	k	12	ARG
14	n	43	ASN
14	n	85	ARG
16	p	8	ARG
16	p	79	ASN
17	q	61	ARG
20	t	28	ARG
21	u	33	ARG
24	C	155	ARG
24	C	259	ASN
25	D	33	ARG
25	D	42	ASN
25	D	46	ARG
25	D	77	ARG
26	E	156	ASN
26	E	163	ASN
27	F	29	ARG
27	F	111	ARG
28	G	28	LYS
28	G	37	ASN
29	H	11	ASN
29	H	73	ASN
29	H	145	ASN
30	J	120	ARG
31	K	31	ARG
32	L	60	ARG
33	M	6	ARG
33	M	59	ARG
34	N	2	ARG
38	R	48	LYS
38	R	80	ARG
39	S	82	MET
39	S	110	ARG
40	T	92	ASN
43	W	10	ARG
43	W	46	ASN

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Mol	Chain	Res	Type
43	W	72	ASN
44	X	26	ARG
44	X	27	ARG
45	Y	58	ASN
46	Z	2	LYS
46	Z	30	ARG
54	v	3	ARG
54	v	8	ARG
55	y	54	LYS
55	y	273	ARG
55	y	305	HIS
56	x	27	LEU
56	x	28	GLU
56	x	29	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	18	GLN
2	b	23	ASN
2	b	202	ASN
3	c	31	ASN
3	c	139	ASN
3	c	189	HIS
4	d	99	ASN
4	d	115	GLN
5	e	69	ASN
6	f	3	HIS
6	f	55	HIS
7	g	51	GLN
7	g	129	ASN
8	h	37	ASN
9	i	4	GLN
9	i	24	ASN
9	i	31	GLN
9	i	36	GLN
9	i	125	GLN
12	l	28	GLN
14	n	43	ASN
15	o	45	HIS
16	p	18	GLN
16	p	63	GLN

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Mol	Chain	Res	Type
16	p	79	ASN
17	q	8	GLN
17	q	30	HIS
19	s	68	HIS
20	t	20	ASN
20	t	47	GLN
20	t	51	ASN
24	C	85	ASN
24	C	238	ASN
24	C	259	ASN
25	D	42	ASN
25	D	150	GLN
25	D	164	GLN
26	E	156	ASN
26	E	163	ASN
28	G	110	HIS
29	H	11	ASN
29	H	73	ASN
29	H	135	HIS
29	H	145	ASN
30	J	40	HIS
30	J	58	ASN
31	K	29	HIS
35	O	38	GLN
36	P	11	GLN
36	P	40	GLN
37	Q	36	GLN
37	Q	43	GLN
38	R	18	GLN
38	R	89	HIS
38	R	91	GLN
39	S	61	ASN
40	T	92	ASN
41	U	68	ASN
42	V	49	ASN
43	W	8	ASN
43	W	46	ASN
43	W	72	ASN
47	0	5	ASN
47	0	41	HIS
49	2	26	ASN
50	3	42	HIS

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Mol	Chain	Res	Type
51	4	35	GLN
54	v	18	GLN
56	x	2	GLN
56	x	36	GLN
56	x	55	HIS
56	x	88	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1533/1534 (99%)	260 (16%)	0
22	A	2898/2903 (99%)	569 (19%)	13 (0%)
23	B	119/120 (99%)	18 (15%)	1 (0%)
53	w	75/77 (97%)	34 (45%)	0
57	I	4/5 (80%)	2 (50%)	2 (50%)
All	All	4629/4639 (99%)	883 (19%)	16 (0%)

All (883) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	6	G
1	a	7	A
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	58	C
1	a	71	A
1	a	82	G
1	a	83	C
1	a	84	U
1	a	87	C
1	a	91	U
1	a	94	G
1	a	95	C
1	a	131	A

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Mol	Chain	Res	Type
1	a	146	G
1	a	154	U
1	a	163	C
1	a	173	U
1	a	181	A
1	a	183	C
1	a	184	G
1	a	196	A
1	a	197	A
1	a	199	A
1	a	207	C
1	a	208	U
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	213	G
1	a	222	C
1	a	226	G
1	a	240	G
1	a	243	A
1	a	244	U
1	a	245	U
1	a	247	G
1	a	251	G
1	a	260	G
1	a	261	U
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	281	G
1	a	289	G
1	a	306	A
1	a	316	C
1	a	321	A
1	a	328	C
1	a	329	A
1	a	347	G
1	a	351	G
1	a	352	C
1	a	354	G

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Mol	Chain	Res	Type
1	a	367	U
1	a	372	C
1	a	375	U
1	a	388	G
1	a	392	C
1	a	398	U
1	a	406	G
1	a	411	A
1	a	412	A
1	a	413	G
1	a	421	U
1	a	429	U
1	a	439	U
1	a	467	U
1	a	468	A
1	a	474	G
1	a	484	G
1	a	486	U
1	a	496	A
1	a	497	G
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G
1	a	531	U
1	a	532	A
1	a	533	A
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	576	C
1	a	577	G
1	a	596	A
1	a	607	A
1	a	628	G
1	a	632	U
1	a	633	G
1	a	639	G

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Mol	Chain	Res	Type
1	a	642	A
1	a	653	U
1	a	661	G
1	a	665	A
1	a	688	G
1	a	693	G
1	a	694	A
1	a	695	A
1	a	702	A
1	a	703	G
1	a	721	G
1	a	723	U
1	a	724	G
1	a	731	G
1	a	734	G
1	a	748	G
1	a	753	A
1	a	755	G
1	a	774	G
1	a	777	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	821	G
1	a	832	G
1	a	836	G
1	a	842	U
1	a	843	U
1	a	845	A
1	a	846	G
1	a	851	G
1	a	872	A
1	a	876	C
1	a	889	A
1	a	902	G
1	a	914	A
1	a	926	G
1	a	934	C

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Mol	Chain	Res	Type
1	a	935	A
1	a	942	G
1	a	960	U
1	a	969	A
1	a	971	G
1	a	972	C
1	a	975	A
1	a	976	G
1	a	977	A
1	a	982	U
1	a	987	G
1	a	989	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	1004	A
1	a	1020	G
1	a	1026	G
1	a	1027	C
1	a	1028	C
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1036	A
1	a	1043	G
1	a	1054	C
1	a	1065	U
1	a	1070	U
1	a	1085	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1130	A
1	a	1132	C
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1151	A
1	a	1154	G
1	a	1157	A
1	a	1158	C

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Mol	Chain	Res	Type
1	a	1159	U
1	a	1167	A
1	a	1168	U
1	a	1171	A
1	a	1182	G
1	a	1183	U
1	a	1184	G
1	a	1191	A
1	a	1196	A
1	a	1201	A
1	a	1212	U
1	a	1213	A
1	a	1225	A
1	a	1227	A
1	a	1228	C
1	a	1238	A
1	a	1240	U
1	a	1258	G
1	a	1260	G
1	a	1261	A
1	a	1264	U
1	a	1275	A
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1282	C
1	a	1287	A
1	a	1290	G
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1302	C
1	a	1305	G
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1322	C
1	a	1323	G
1	a	1335	U
1	a	1336	C
1	a	1346	A

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Mol	Chain	Res	Type
1	a	1353	G
1	a	1360	A
1	a	1363	A
1	a	1370	G
1	a	1378	C
1	a	1379	G
1	a	1395	C
1	a	1397	C
1	a	1398	A
1	a	1419	G
1	a	1429	A
1	a	1433	A
1	a	1434	A
1	a	1446	A
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	1499	A
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1527	U
1	a	1529	G
1	a	1530	G
1	a	1531	A
22	A	2	G
22	A	10	A
22	A	12	U
22	A	14	A
22	A	15	G
22	A	23	G
22	A	34	U
22	A	35	G
22	A	36	G
22	A	46	G
22	A	51	G
22	A	55	G
22	A	60	G

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Mol	Chain	Res	Type
22	A	61	C
22	A	63	A
22	A	71	A
22	A	74	A
22	A	75	G
22	A	84	A
22	A	91	A
22	A	92	U
22	A	101	A
22	A	102	U
22	A	110	G
22	A	118	A
22	A	119	A
22	A	120	U
22	A	121	G
22	A	125	A
22	A	127	A
22	A	138	U
22	A	139	U
22	A	140	C
22	A	141	G
22	A	142	A
22	A	163	C
22	A	165	A
22	A	166	U
22	A	196	A
22	A	199	A
22	A	204	A
22	A	215	G
22	A	216	A
22	A	222	A
22	A	225	C
22	A	228	C
22	A	229	C
22	A	239	C
22	A	248	G
22	A	249	C
22	A	255	A
22	A	265	A
22	A	266	G
22	A	267	C
22	A	273	G

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Mol	Chain	Res	Type
22	A	276	U
22	A	277	G
22	A	278	A
22	A	281	C
22	A	284	U
22	A	311	A
22	A	323	C
22	A	329	G
22	A	330	A
22	A	346	A
22	A	353	C
22	A	361	G
22	A	362	A
22	A	363	G
22	A	371	A
22	A	372	G
22	A	373	U
22	A	386	G
22	A	387	U
22	A	395	U
22	A	396	G
22	A	404	A
22	A	405	U
22	A	406	G
22	A	411	G
22	A	412	A
22	A	424	G
22	A	435	C
22	A	455	C
22	A	457	A
22	A	467	G
22	A	477	A
22	A	481	G
22	A	489	G
22	A	491	G
22	A	501	A
22	A	505	A
22	A	508	A
22	A	509	C
22	A	510	C
22	A	529	A
22	A	530	G

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Mol	Chain	Res	Type
22	A	531	C
22	A	532	A
22	A	543	G
22	A	546	U
22	A	547	A
22	A	548	G
22	A	563	A
22	A	569	U
22	A	573	U
22	A	575	A
22	A	588	U
22	A	603	A
22	A	613	A
22	A	614	A
22	A	615	U
22	A	616	A
22	A	621	A
22	A	622	G
22	A	627	A
22	A	637	A
22	A	645	C
22	A	647	G
22	A	653	U
22	A	654	A
22	A	655	A
22	A	659	G
22	A	669	G
22	A	670	A
22	A	677	A
22	A	686	U
22	A	695	G
22	A	696	G
22	A	714	U
22	A	717	C
22	A	726	G
22	A	730	A
22	A	738	G
22	A	740	C
22	A	747	C
22	A	748	G
22	A	763	G
22	A	765	C

Continued on next page...

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Mol	Chain	Res	Type
22	A	774	G
22	A	775	G
22	A	776	G
22	A	782	A
22	A	783	A
22	A	784	G
22	A	785	G
22	A	788	A
22	A	800	A
22	A	801	G
22	A	805	G
22	A	811	U
22	A	812	C
22	A	819	A
22	A	827	U
22	A	828	U
22	A	830	G
22	A	845	A
22	A	846	U
22	A	847	U
22	A	856	G
22	A	858	G
22	A	859	G
22	A	866	A
22	A	876	C
22	A	878	A
22	A	891	G
22	A	894	U
22	A	896	A
22	A	907	G
22	A	910	A
22	A	919	U
22	A	933	A
22	A	941	A
22	A	945	A
22	A	946	C
22	A	961	C
22	A	973	A
22	A	974	G
22	A	983	A
22	A	985	C
22	A	989	G

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Mol	Chain	Res	Type
22	A	995	C
22	A	996	A
22	A	999	U
22	A	1005	C
22	A	1006	C
22	A	1009	A
22	A	1012	U
22	A	1013	C
22	A	1021	A
22	A	1026	G
22	A	1033	U
22	A	1040	A
22	A	1045	C
22	A	1046	A
22	A	1047	G
22	A	1048	A
22	A	1051	G
22	A	1057	A
22	A	1059	G
22	A	1060	U
22	A	1061	U
22	A	1062	G
22	A	1064	C
22	A	1065	U
22	A	1066	U
22	A	1067	A
22	A	1068	G
22	A	1069	A
22	A	1070	A
22	A	1073	A
22	A	1075	C
22	A	1078	U
22	A	1084	A
22	A	1087	G
22	A	1088	A
22	A	1089	A
22	A	1090	A
22	A	1094	U
22	A	1096	A
22	A	1097	U
22	A	1098	A
22	A	1101	U

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Mol	Chain	Res	Type
22	A	1103	A
22	A	1104	C
22	A	1110	G
22	A	1111	A
22	A	1112	G
22	A	1132	U
22	A	1135	C
22	A	1136	G
22	A	1139	G
22	A	1141	U
22	A	1142	A
22	A	1143	A
22	A	1151	A
22	A	1155	A
22	A	1169	A
22	A	1170	C
22	A	1171	G
22	A	1172	C
22	A	1174	U
22	A	1175	A
22	A	1176	U
22	A	1178	C
22	A	1179	G
22	A	1180	U
22	A	1186	G
22	A	1195	G
22	A	1204	A
22	A	1205	A
22	A	1206	G
22	A	1212	G
22	A	1236	G
22	A	1238	G
22	A	1250	G
22	A	1253	A
22	A	1256	G
22	A	1265	A
22	A	1272	A
22	A	1273	U
22	A	1300	G
22	A	1301	A
22	A	1311	G
22	A	1321	A

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Mol	Chain	Res	Type
22	A	1345	C
22	A	1352	U
22	A	1359	A
22	A	1360	G
22	A	1365	A
22	A	1368	G
22	A	1378	A
22	A	1379	U
22	A	1383	A
22	A	1386	C
22	A	1392	A
22	A	1395	A
22	A	1411	U
22	A	1416	G
22	A	1419	A
22	A	1420	A
22	A	1421	G
22	A	1427	A
22	A	1428	C
22	A	1429	G
22	A	1437	C
22	A	1453	A
22	A	1454	C
22	A	1455	G
22	A	1458	U
22	A	1461	C
22	A	1469	A
22	A	1482	G
22	A	1490	A
22	A	1493	C
22	A	1497	U
22	A	1504	A
22	A	1505	A
22	A	1509	A
22	A	1515	A
22	A	1524	G
22	A	1529	G
22	A	1530	G
22	A	1533	C
22	A	1535	A
22	A	1536	C
22	A	1537	G

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Mol	Chain	Res	Type
22	A	1539	U
22	A	1546	G
22	A	1559	U
22	A	1560	G
22	A	1566	A
22	A	1567	G
22	A	1569	A
22	A	1583	A
22	A	1584	U
22	A	1588	G
22	A	1608	A
22	A	1610	A
22	A	1622	G
22	A	1627	G
22	A	1639	C
22	A	1647	U
22	A	1648	U
22	A	1649	G
22	A	1651	G
22	A	1668	A
22	A	1674	G
22	A	1675	C
22	A	1698	A
22	A	1707	G
22	A	1713	A
22	A	1715	G
22	A	1730	C
22	A	1733	G
22	A	1738	G
22	A	1757	A
22	A	1758	U
22	A	1764	C
22	A	1773	A
22	A	1776	G
22	A	1785	A
22	A	1800	C
22	A	1801	A
22	A	1802	A
22	A	1808	A
22	A	1811	G
22	A	1816	C
22	A	1829	A

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Mol	Chain	Res	Type
22	A	1833	C
22	A	1847	G
22	A	1857	G
22	A	1869	G
22	A	1873	G
22	A	1884	G
22	A	1885	A
22	A	1896	G
22	A	1906	G
22	A	1912	A
22	A	1913	A
22	A	1914	C
22	A	1917	U
22	A	1929	G
22	A	1930	G
22	A	1931	U
22	A	1937	A
22	A	1938	A
22	A	1940	U
22	A	1941	C
22	A	1942	C
22	A	1944	U
22	A	1955	U
22	A	1964	G
22	A	1966	A
22	A	1967	C
22	A	1970	A
22	A	1971	U
22	A	1972	G
22	A	1991	U
22	A	1996	C
22	A	1997	C
22	A	2004	G
22	A	2022	U
22	A	2023	C
22	A	2027	G
22	A	2030	A
22	A	2031	A
22	A	2033	A
22	A	2043	C
22	A	2052	A
22	A	2055	C

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Mol	Chain	Res	Type
22	A	2056	G
22	A	2060	A
22	A	2061	G
22	A	2062	A
22	A	2063	C
22	A	2068	U
22	A	2069	A
22	A	2072	C
22	A	2093	G
22	A	2096	C
22	A	2097	A
22	A	2100	G
22	A	2101	A
22	A	2105	U
22	A	2110	G
22	A	2111	U
22	A	2112	G
22	A	2115	G
22	A	2117	A
22	A	2118	U
22	A	2119	A
22	A	2120	G
22	A	2131	U
22	A	2132	U
22	A	2133	G
22	A	2134	A
22	A	2135	A
22	A	2136	G
22	A	2137	U
22	A	2139	U
22	A	2140	G
22	A	2145	C
22	A	2146	C
22	A	2147	A
22	A	2150	C
22	A	2154	A
22	A	2157	G
22	A	2158	A
22	A	2164	C
22	A	2165	C
22	A	2167	U
22	A	2170	A

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Mol	Chain	Res	Type
22	A	2171	A
22	A	2172	U
22	A	2173	A
22	A	2174	C
22	A	2177	C
22	A	2182	U
22	A	2183	A
22	A	2188	U
22	A	2198	A
22	A	2203	U
22	A	2204	G
22	A	2211	A
22	A	2213	U
22	A	2214	C
22	A	2223	G
22	A	2225	A
22	A	2226	C
22	A	2238	G
22	A	2239	G
22	A	2250	G
22	A	2251	G
22	A	2266	A
22	A	2279	G
22	A	2283	C
22	A	2287	A
22	A	2288	A
22	A	2305	U
22	A	2307	G
22	A	2308	G
22	A	2309	A
22	A	2319	G
22	A	2322	A
22	A	2325	G
22	A	2333	A
22	A	2334	U
22	A	2345	G
22	A	2347	C
22	A	2350	C
22	A	2357	G
22	A	2361	G
22	A	2383	G
22	A	2385	C

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Mol	Chain	Res	Type
22	A	2392	A
22	A	2396	G
22	A	2402	U
22	A	2403	C
22	A	2406	A
22	A	2420	C
22	A	2422	C
22	A	2425	A
22	A	2427	C
22	A	2429	G
22	A	2430	A
22	A	2435	A
22	A	2440	C
22	A	2441	U
22	A	2448	A
22	A	2470	G
22	A	2476	A
22	A	2484	G
22	A	2491	U
22	A	2494	G
22	A	2498	C
22	A	2502	G
22	A	2503	A
22	A	2504	U
22	A	2505	G
22	A	2506	U
22	A	2507	C
22	A	2518	A
22	A	2529	G
22	A	2534	A
22	A	2535	G
22	A	2547	A
22	A	2554	U
22	A	2564	A
22	A	2566	A
22	A	2567	G
22	A	2572	A
22	A	2573	C
22	A	2578	G
22	A	2585	U
22	A	2586	U
22	A	2602	A

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Mol	Chain	Res	Type
22	A	2603	G
22	A	2604	U
22	A	2609	U
22	A	2613	U
22	A	2615	U
22	A	2629	U
22	A	2638	G
22	A	2646	C
22	A	2654	A
22	A	2673	G
22	A	2682	A
22	A	2689	U
22	A	2690	U
22	A	2707	U
22	A	2713	U
22	A	2714	G
22	A	2716	C
22	A	2718	G
22	A	2726	A
22	A	2728	U
22	A	2732	G
22	A	2733	A
22	A	2744	G
22	A	2748	A
22	A	2751	G
22	A	2752	C
22	A	2762	C
22	A	2778	A
22	A	2779	U
22	A	2791	G
22	A	2793	C
22	A	2794	C
22	A	2797	U
22	A	2798	U
22	A	2800	A
22	A	2808	G
22	A	2809	A
22	A	2818	U
22	A	2820	A
22	A	2823	A
22	A	2833	U
22	A	2835	A

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Mol	Chain	Res	Type
22	A	2836	U
22	A	2849	U
22	A	2861	U
22	A	2867	G
22	A	2872	A
22	A	2873	A
22	A	2880	C
22	A	2884	U
22	A	2893	A
22	A	2902	C
23	B	2	G
23	B	9	G
23	B	16	G
23	B	24	G
23	B	31	C
23	B	35	C
23	B	38	C
23	B	41	G
23	B	45	A
23	B	51	G
23	B	53	A
23	B	68	C
23	B	88	C
23	B	89	U
23	B	90	C
23	B	91	C
23	B	109	A
23	B	119	A
53	w	4	G
53	w	7	G
53	w	8	U
53	w	9	G
53	w	13	C
53	w	16	C
53	w	17	C
53	w	18	G
53	w	19	G
53	w	20	U
53	w	21	A
53	w	22	G
53	w	24	U
53	w	25	C

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Mol	Chain	Res	Type
53	w	26	G
53	w	27	U
53	w	28	C
53	w	30	G
53	w	37	A
53	w	38	A
53	w	46	A
53	w	47	U
53	w	48	C
53	w	49	G
53	w	52	G
53	w	53	G
53	w	54	U
53	w	56	C
53	w	68	C
53	w	69	C
53	w	73	A
53	w	74	C
53	w	75	C
53	w	76	A
57	I	1538	C
57	I	1539	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	91	A
22	A	784	G
22	A	858	G
22	A	1020	A
22	A	1182	G
22	A	1190	G
22	A	1432	G
22	A	1930	G
22	A	1940	U
22	A	2286	G
22	A	2324	U
22	A	2391	G
22	A	2808	G
23	B	52	A
57	I	1537	U
57	I	1538	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	w	1
56	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	17:C	O3'	117:U	P	3.73
1	x	2:GLN	C	3:LEU	N	0.70

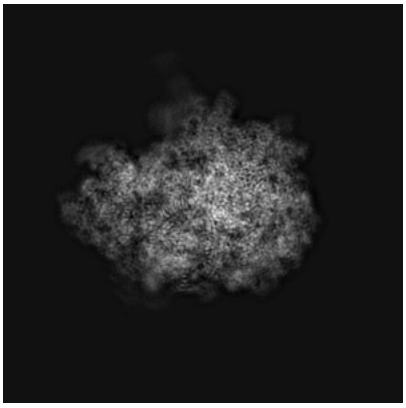
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0137. These allow visual inspection of the internal detail of the map and identification of artifacts.

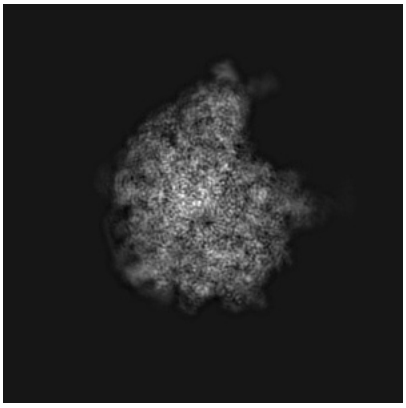
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

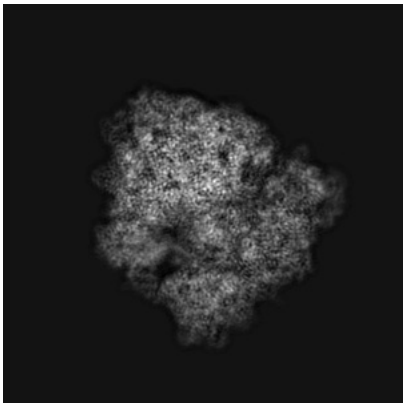
6.1.1 Primary map



X



Y

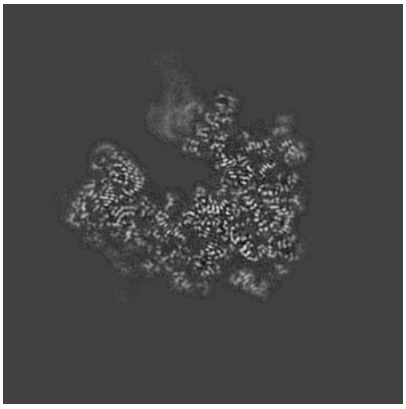


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 184

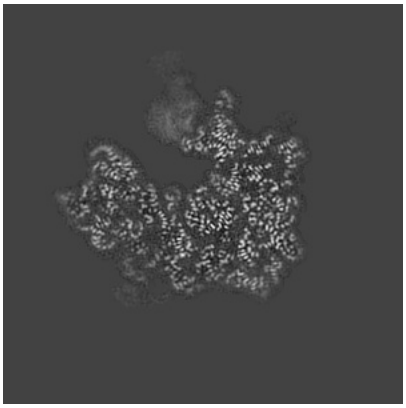
Y Index: 184

Z Index: 184

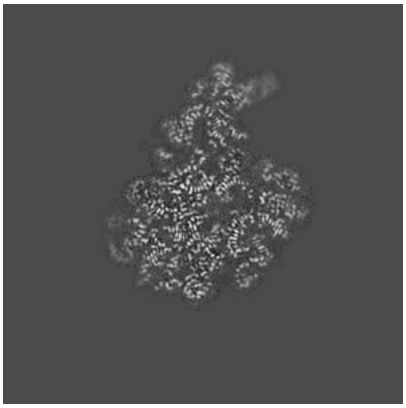
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

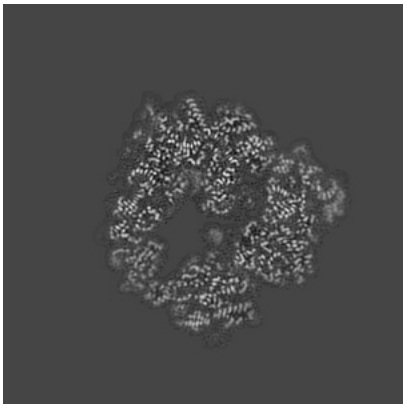
6.3.1 Primary map



X Index: 189



Y Index: 194



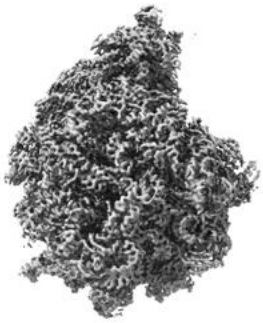
Z Index: 198

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

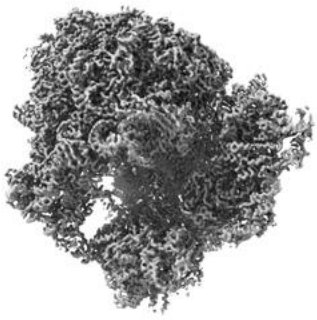
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

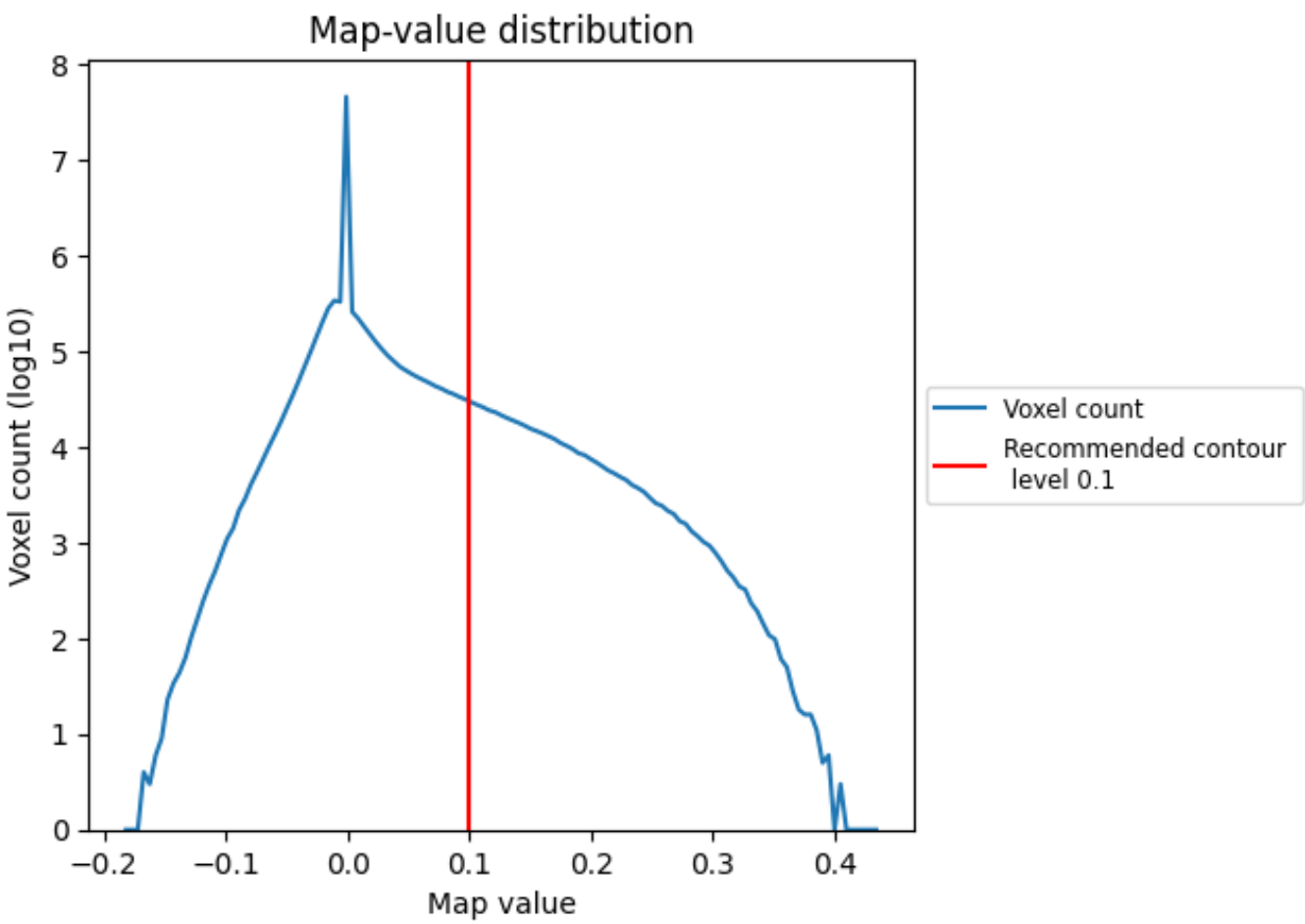
6.5 Mask visualisation (i)

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

7 Map analysis (i)

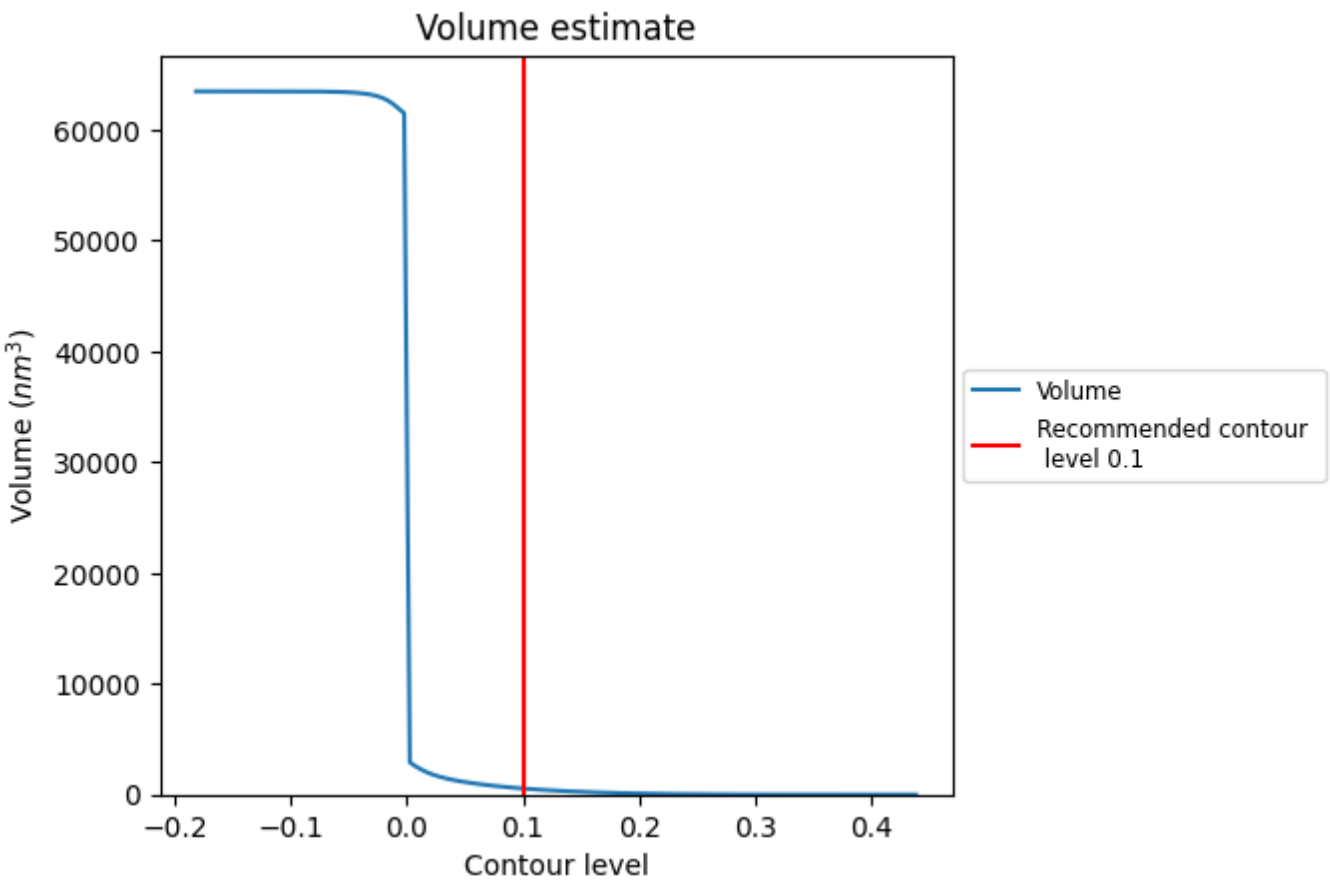
This section contains the results of statistical analysis of the map.

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.

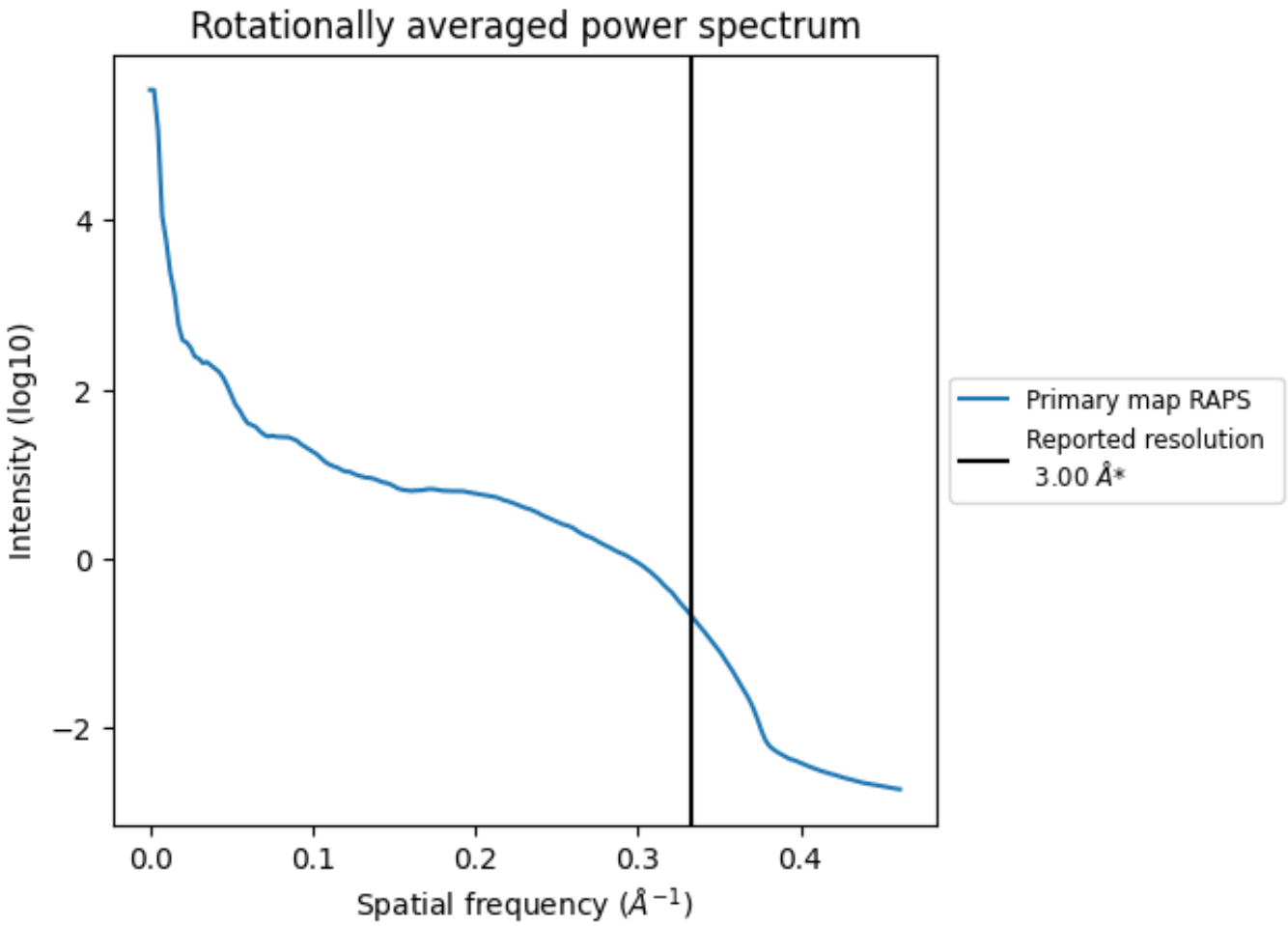
7.2 Volume estimate (i)



The volume at the recommended contour level is 547 nm^3; this corresponds to an approximate mass of 494 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)

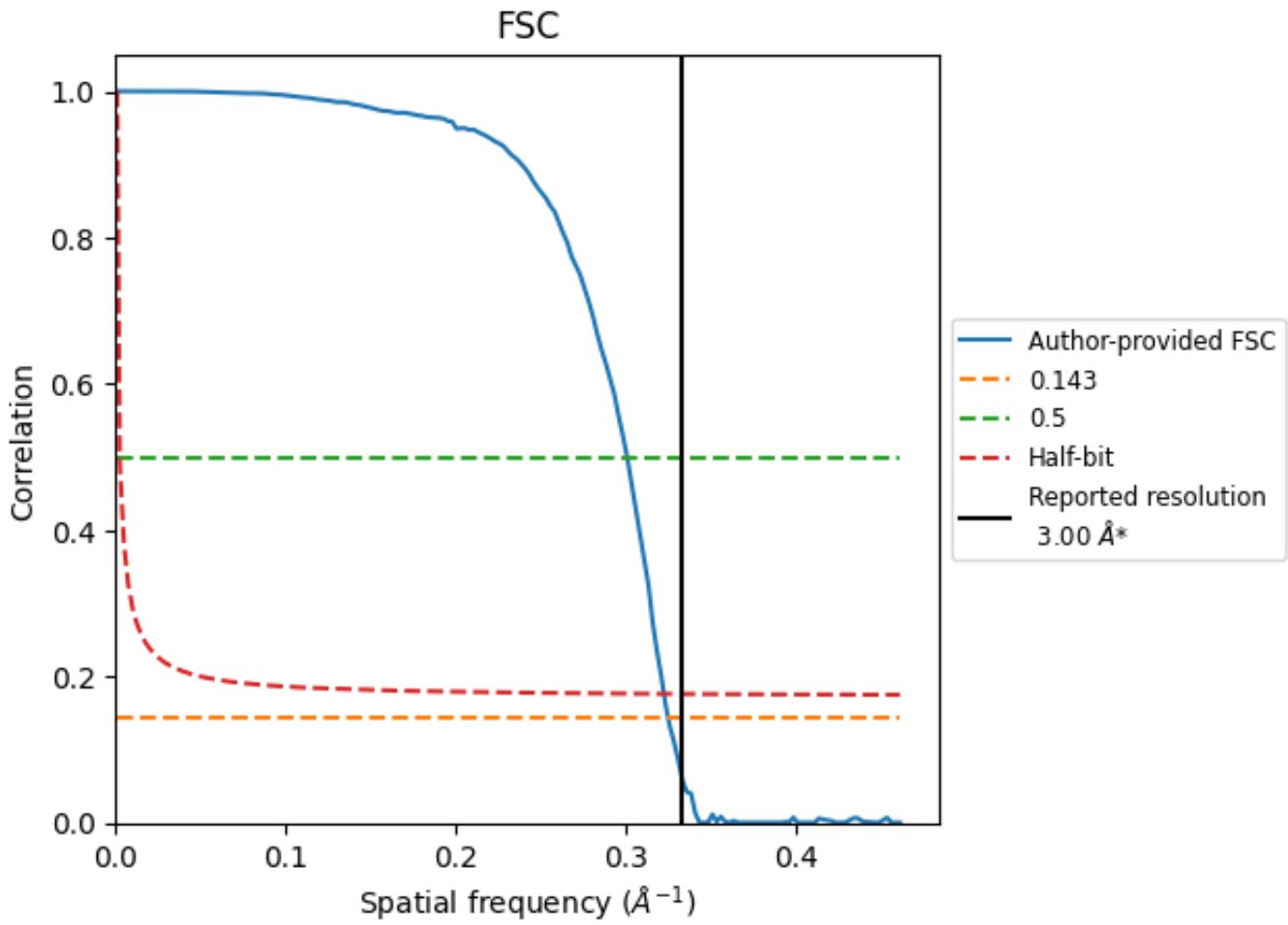


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

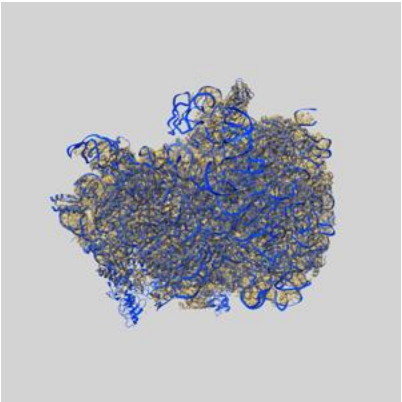
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.08	3.32	3.10
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

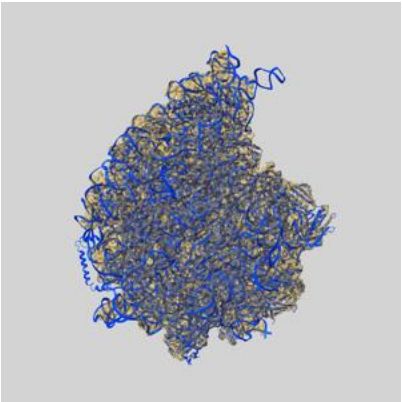
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0137 and PDB model 6H4N. Per-residue inclusion information can be found in section 3 on page 15.

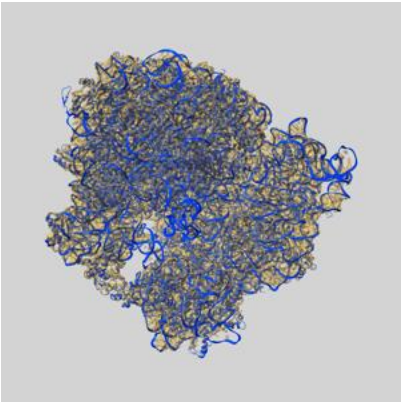
9.1 Map-model overlay (i)



X



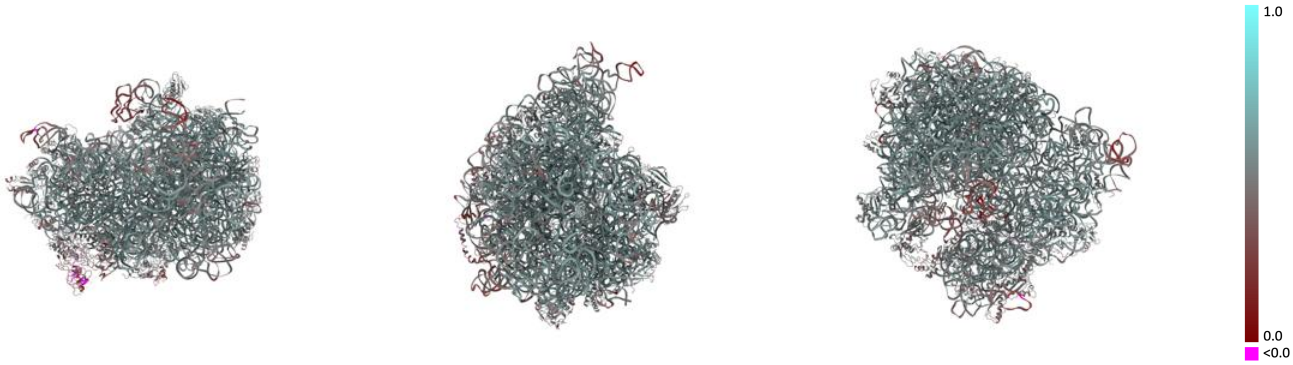
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

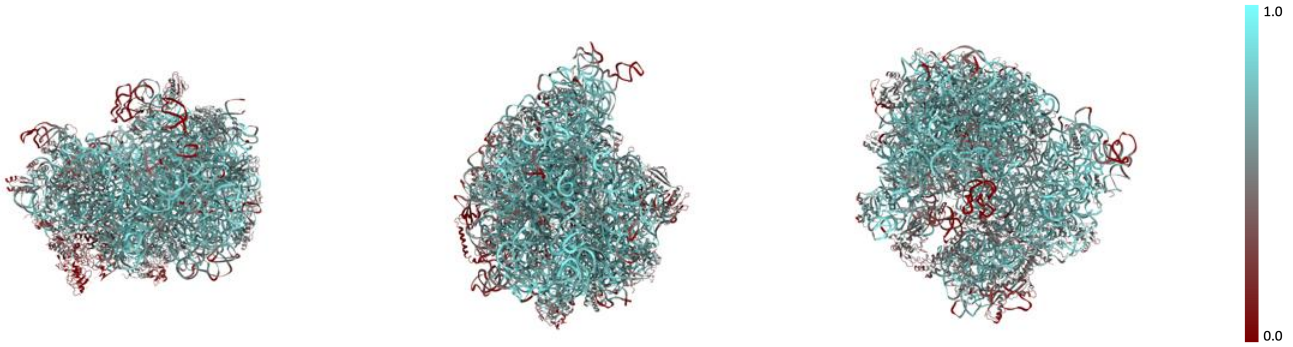
9.2 Q-score mapped to coordinate model (i)



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.

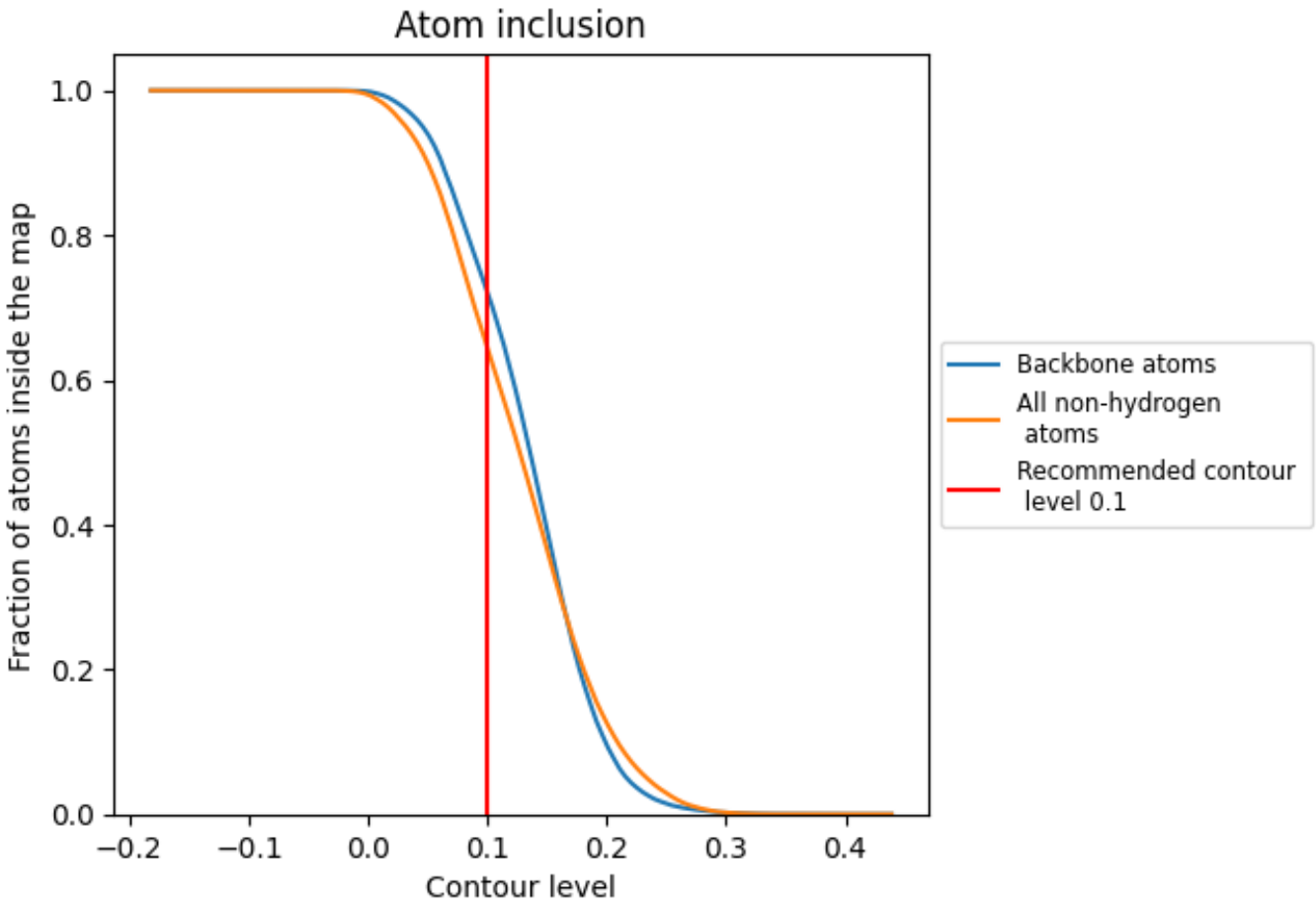
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 65% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6451	0.5230
0	0.5748	0.5230
1	0.5411	0.5190
2	0.6648	0.5640
3	0.6558	0.5590
4	0.5411	0.5290
6	0.2838	0.4060
A	0.7288	0.5420
B	0.7208	0.5370
C	0.6181	0.5530
D	0.5813	0.5460
E	0.4414	0.4960
F	0.4202	0.4670
G	0.3878	0.4800
H	0.0885	0.3740
I	0.0900	0.4400
J	0.5800	0.5360
K	0.5312	0.5270
L	0.5620	0.5140
M	0.5720	0.5380
N	0.6171	0.5400
O	0.5481	0.5020
P	0.5462	0.5290
Q	0.6487	0.5450
R	0.5408	0.5150
S	0.5347	0.5190
T	0.4834	0.5070
U	0.4211	0.4860
V	0.5257	0.5110
W	0.6279	0.5570
X	0.5624	0.5380
Y	0.4185	0.4440
Z	0.5675	0.5360
a	0.7437	0.5430
b	0.3469	0.4460

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Chain	Atom inclusion	Q-score
c	0.5044	0.4930
d	0.4792	0.4900
e	0.5559	0.5140
f	0.4812	0.4620
g	0.4302	0.4610
h	0.5406	0.5210
i	0.5005	0.4820
j	0.4179	0.4640
k	0.5101	0.5010
l	0.5396	0.5230
m	0.4430	0.4640
n	0.5247	0.4920
o	0.5377	0.4940
p	0.5486	0.5030
q	0.4446	0.4920
r	0.5794	0.5260
s	0.4831	0.4860
t	0.4954	0.4880
u	0.2710	0.3150
v	0.3318	0.4630
w	0.2503	0.4010
x	0.4886	0.4810
y	0.0065	0.2690