Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 08:43 PM EST

PDB ID	:	3JCD
EMDB ID	:	EMD-6549
Title	:	Structure of Escherichia coli EF4 in posttranslocational ribosomes (Post EF4)
Authors	:	Zhang, D.; Yan, K.; Liu, G.; Song, G.; Luo, J.; Shi, Y.; Cheng, E.; Wu, S.; Jiang, T.; Low, J.; Gao, N.; Qin, Y.
Deposited on	:	2015-12-01
Resolution	:	3.70 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 ⓘ symbol.

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

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

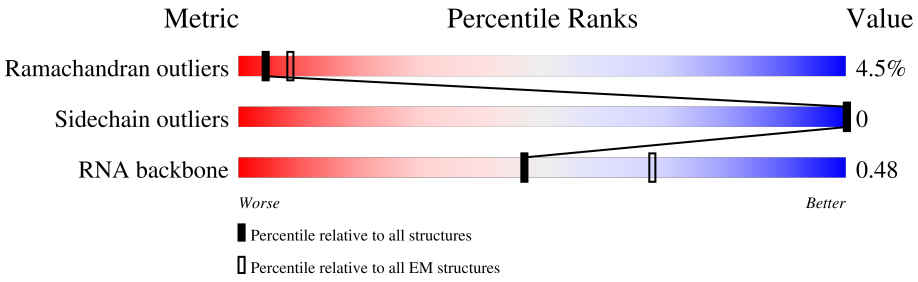
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	b	241	45% 85% 5% 10%
2	c	233	42% 85% • 12%
3	d	206	46% 95% •
4	e	167	50% 87% • 10%
5	f	135	23% 70% 6% 24%
6	g	179	40% 81% • 16%
7	h	130	39% 98% ••
8	i	130	34% 95% • •

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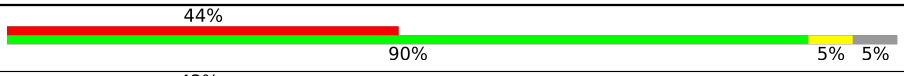
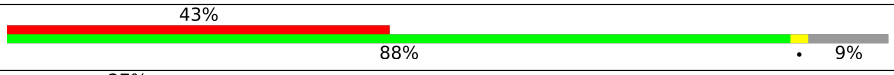
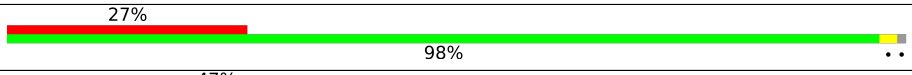
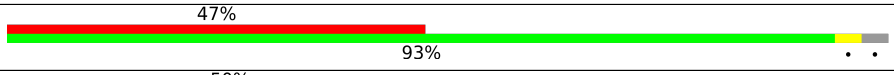
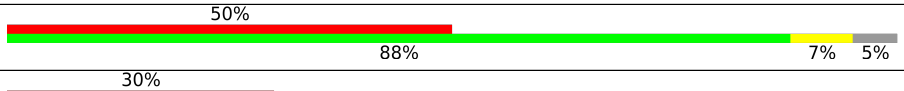
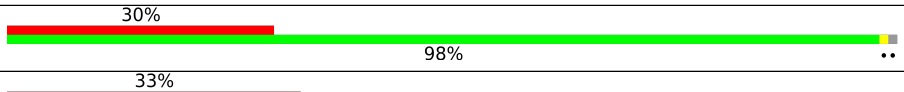
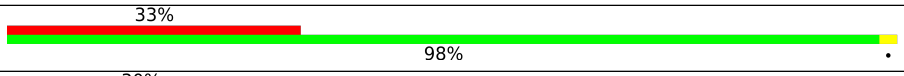
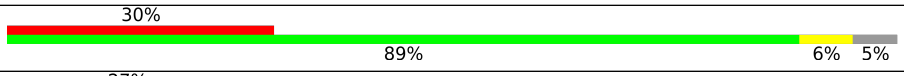
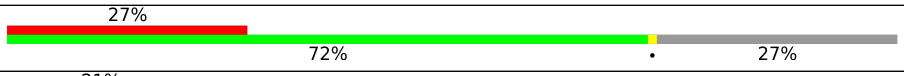
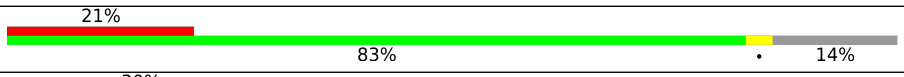
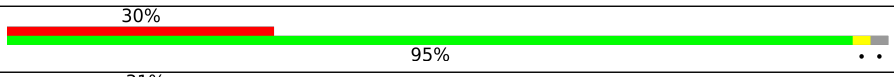
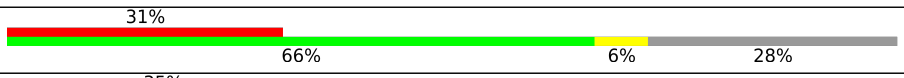
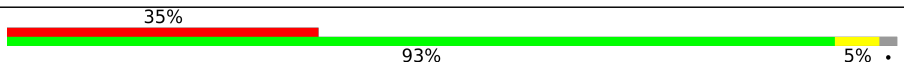
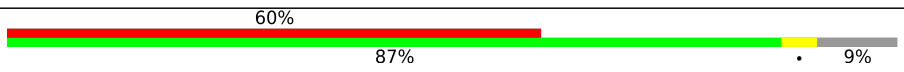
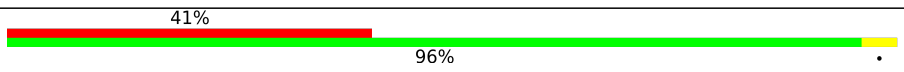
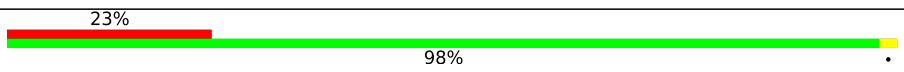
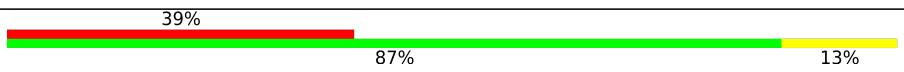
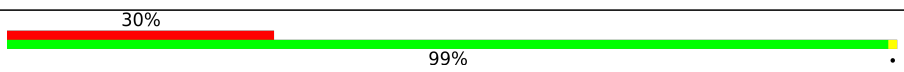
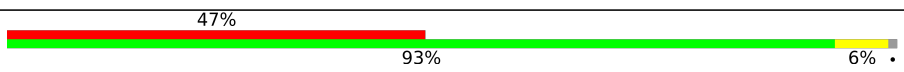
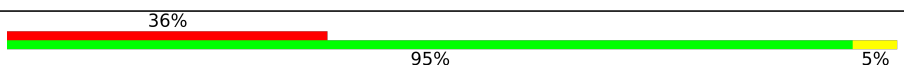
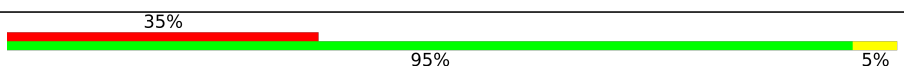
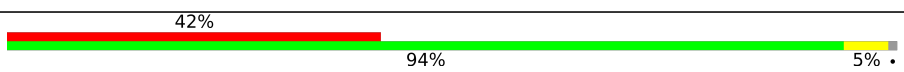
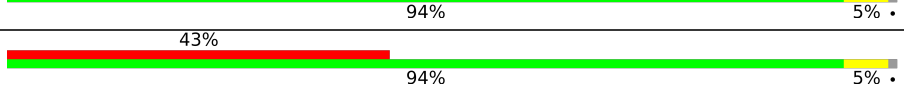
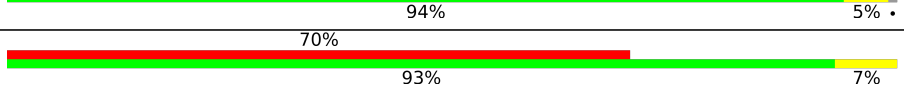
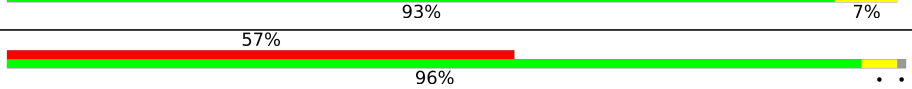
Mol	Chain	Length	Quality of chain
9	j	103	
10	k	129	
11	l	124	
12	m	118	
13	n	101	
14	o	89	
15	p	82	
16	q	84	
17	r	75	
18	s	92	
19	t	87	
20	u	71	
21	0	57	
22	1	55	
23	2	46	
24	3	64	
25	4	38	
26	5	234	
27	C	273	
28	D	209	
29	E	201	
30	F	179	
31	G	177	
32	H	149	
33	I	142	

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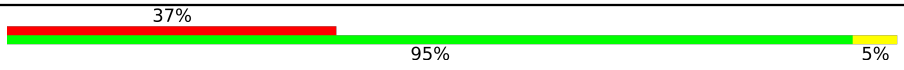
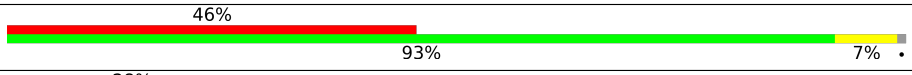
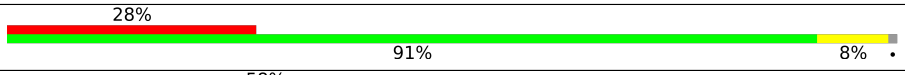
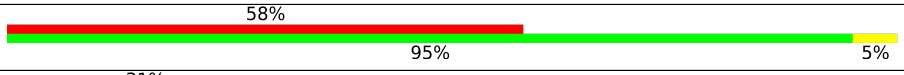
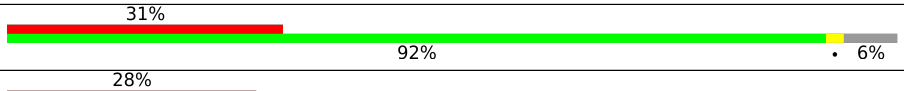
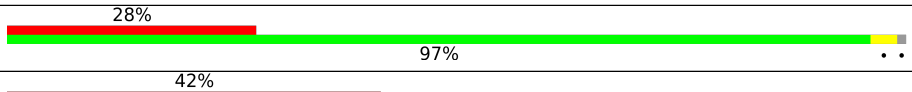
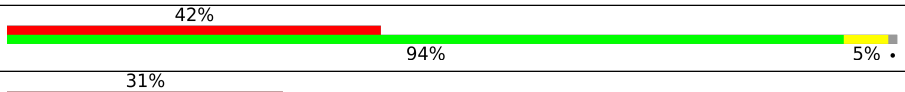
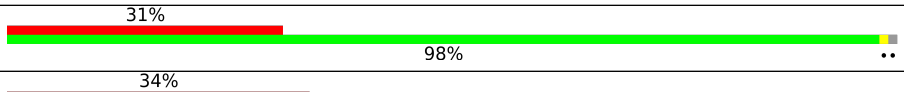
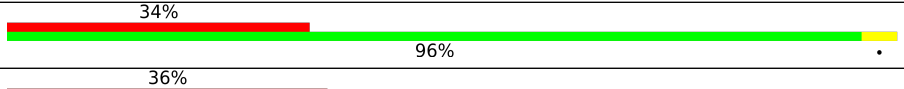
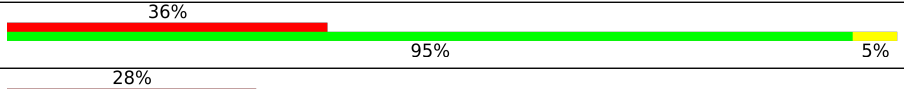
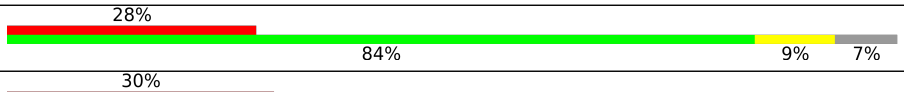
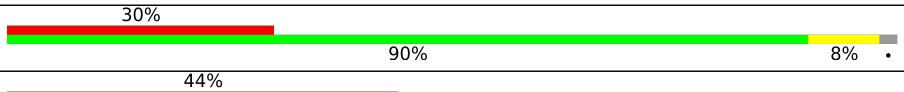
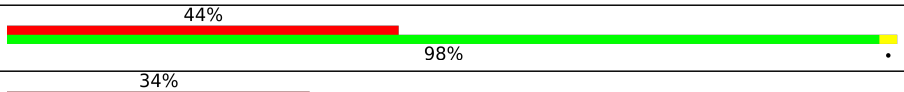
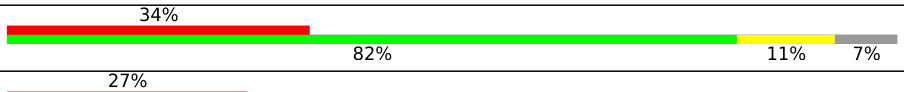
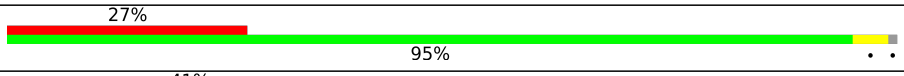
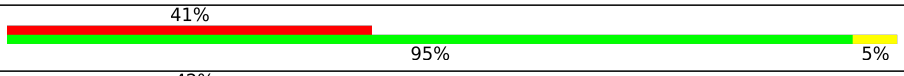
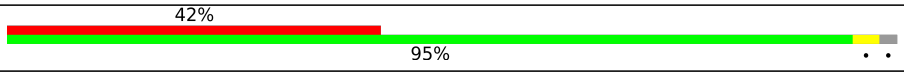
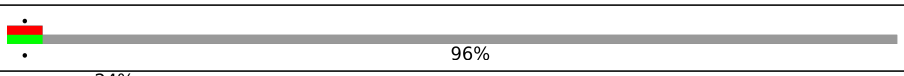
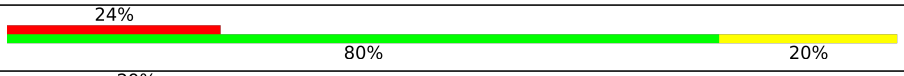
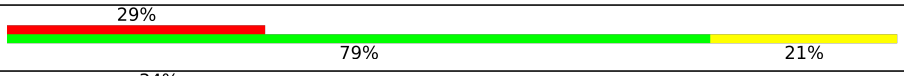
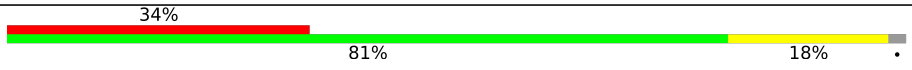
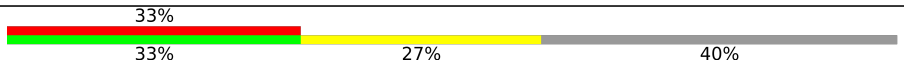
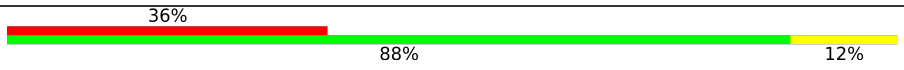
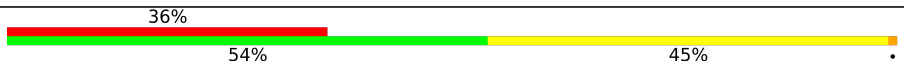
Mol	Chain	Length	Quality of chain
34	J	142	
35	K	123	
36	L	144	
37	M	136	
38	N	127	
39	O	117	
40	P	115	
41	Q	118	
42	R	103	
43	S	110	
44	T	100	
45	U	104	
46	V	94	
47	W	85	
48	X	78	
49	Y	63	
50	Z	59	
51	x	599	
52	a	1533	
53	A	2904	
54	B	120	
55	7	15	
56	8	76	
56	9	76	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 147815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

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

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	150	1105	687	211	201	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	102	832	525	150	150	7	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	r	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 22 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 24 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 25 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

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

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

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

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

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

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

- Molecule 51 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	26	Total	C	N	O	S	0	0
			214	134	43	35	2		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	2903	Total	C	N	O	P	0	0
			62320	27801	11467	20149	2903		

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	9	Total	C	N	O	P	0	0
			191	86	34	62	9		

- Molecule 56 is a RNA chain called tRNA.

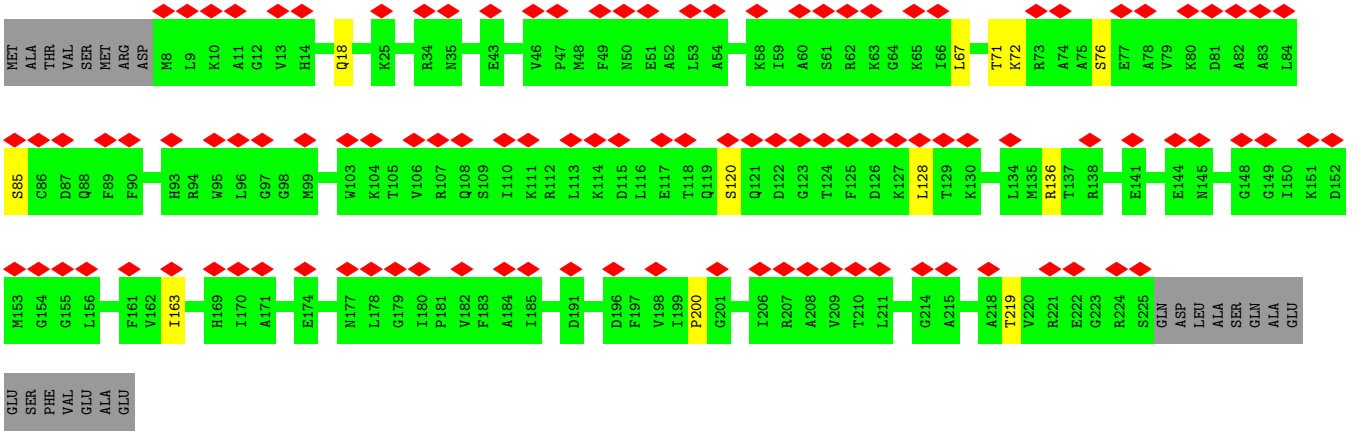
Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		
56	9	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

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.

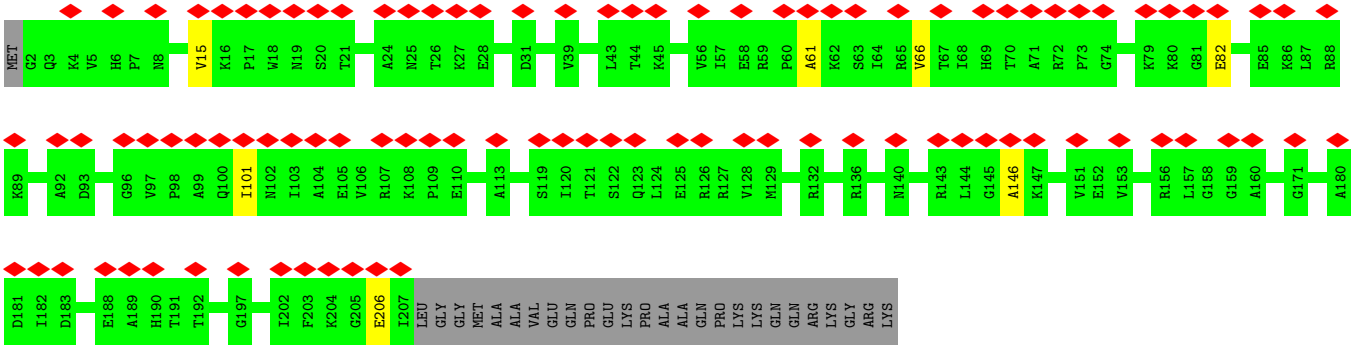
• Molecule 1: 30S ribosomal protein S2

Chain b:



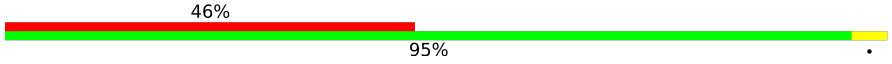
• Molecule 2: 30S ribosomal protein S3

Chain c:

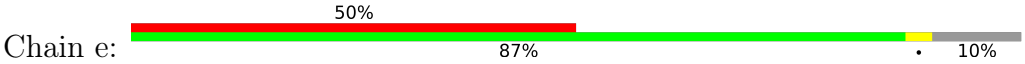


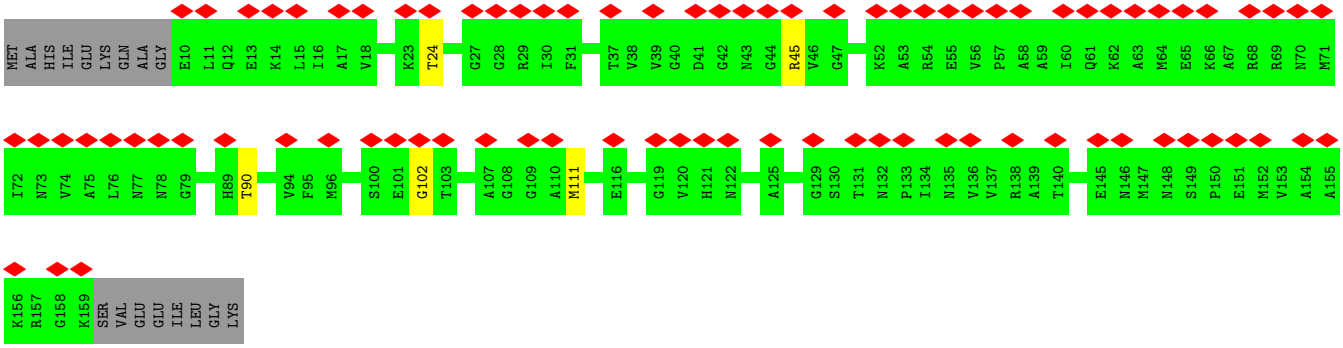
• Molecule 3: 30S ribosomal protein S4

Chain d:

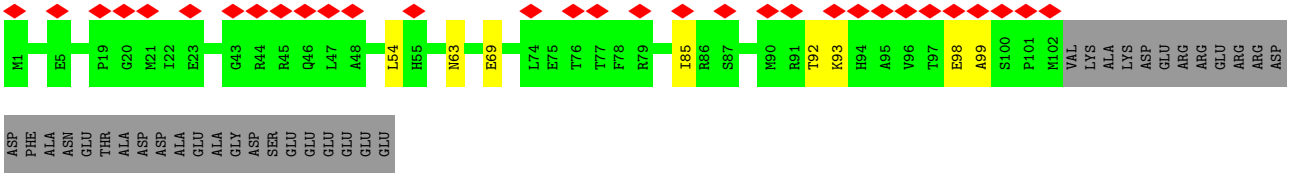


• Molecule 4: 30S ribosomal protein S5

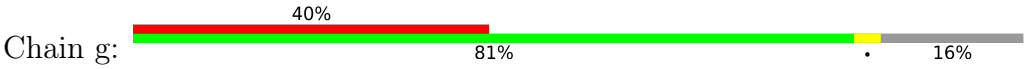


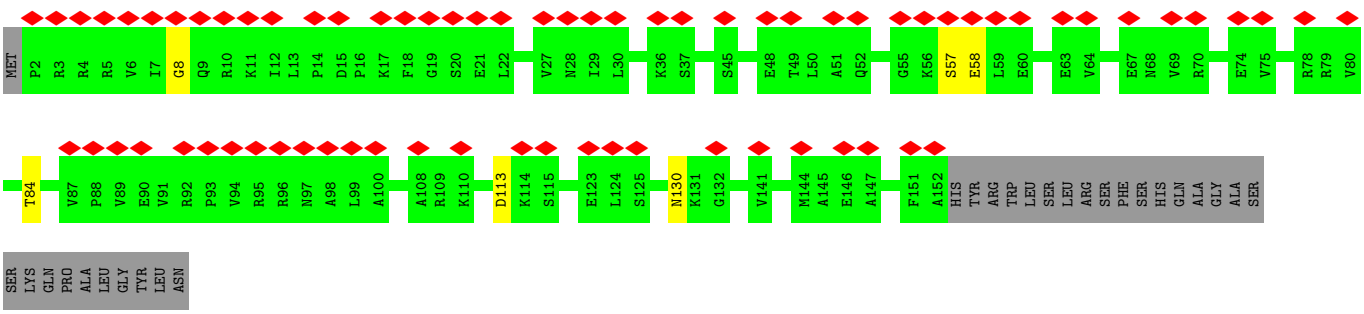


• Molecule 5: 30S ribosomal protein S6



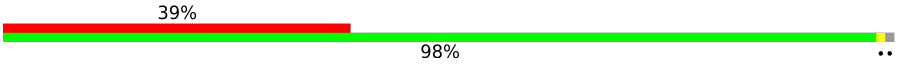
• Molecule 6: 30S ribosomal protein S7

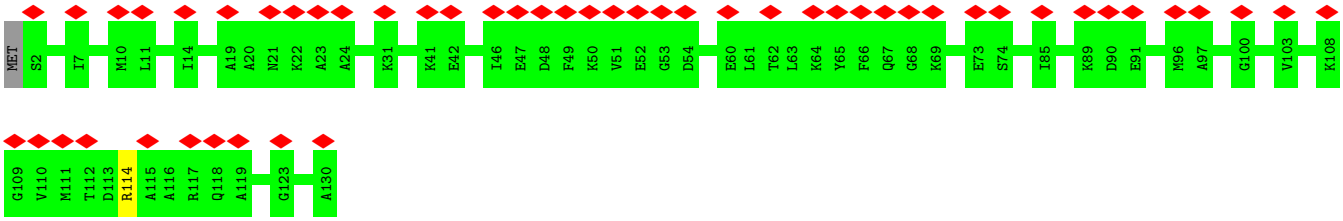




• Molecule 7: 30S ribosomal protein S8

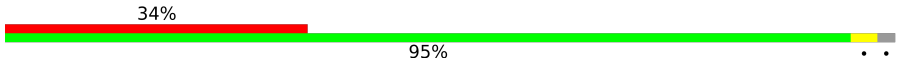
Chain h:

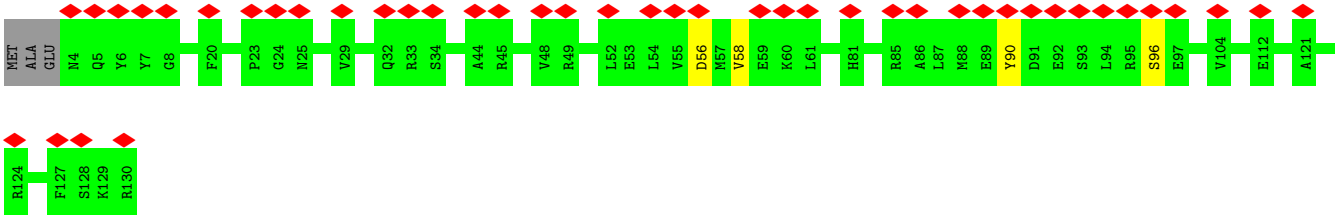




• Molecule 8: 30S ribosomal protein S9

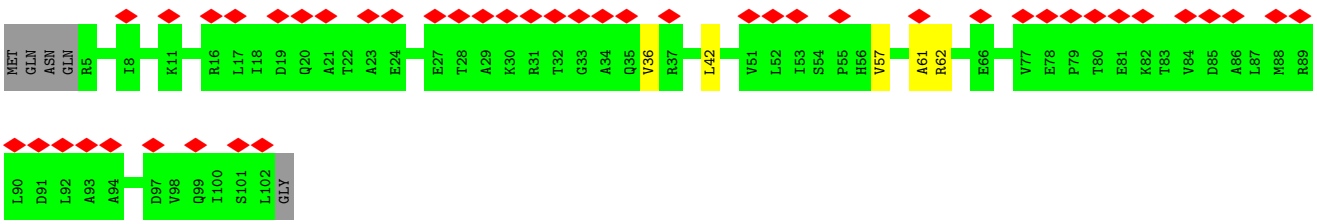
Chain i:





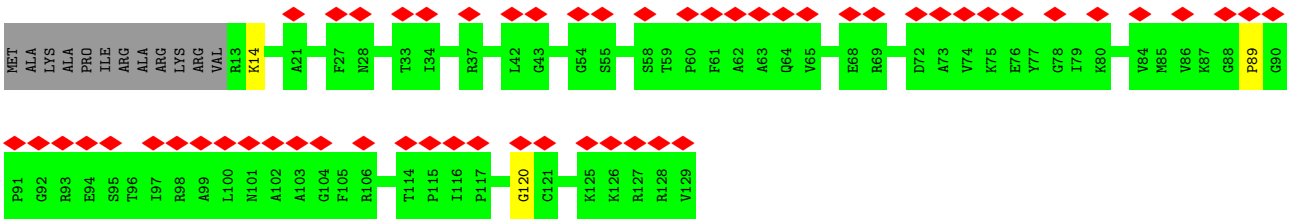
• Molecule 9: 30S ribosomal protein S10

Chain j:



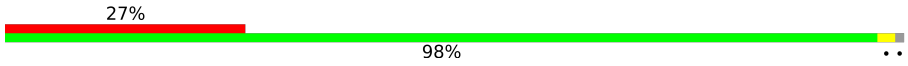
• Molecule 10: 30S ribosomal protein S11

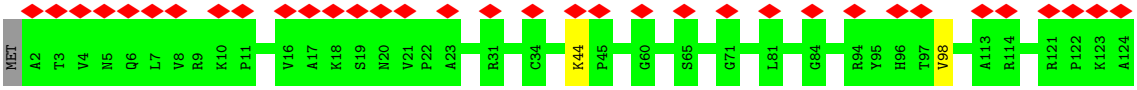
Chain k:



• Molecule 11: 30S ribosomal protein S12

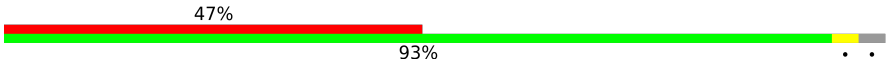
Chain l:

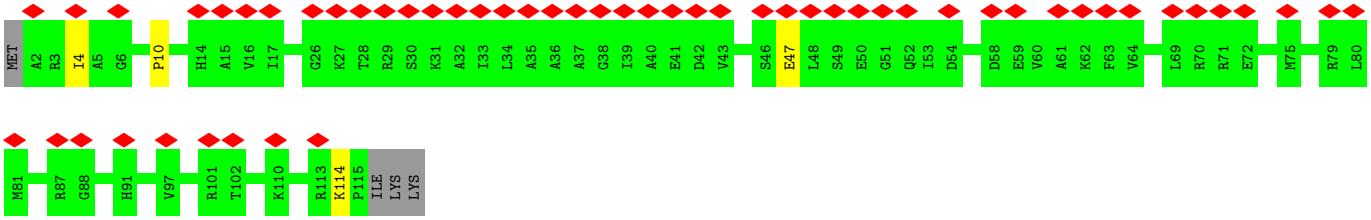




• Molecule 12: 30S ribosomal protein S13

Chain m:



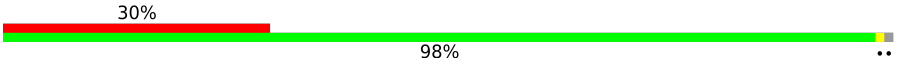


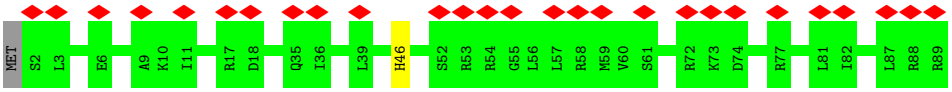
• Molecule 13: 30S ribosomal protein S14

Chain n:

• Molecule 14: 30S ribosomal protein S15

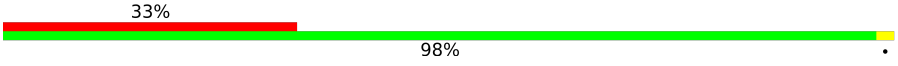
Chain o:

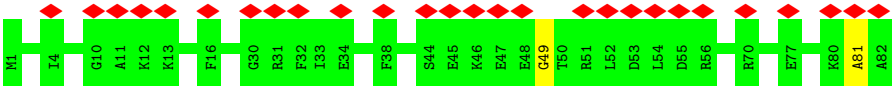




• Molecule 15: 30S ribosomal protein S16

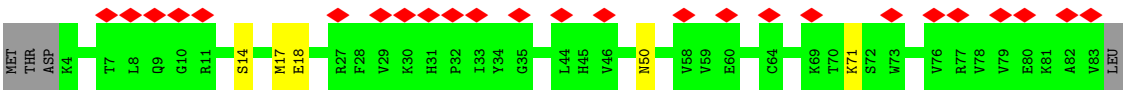
Chain p:





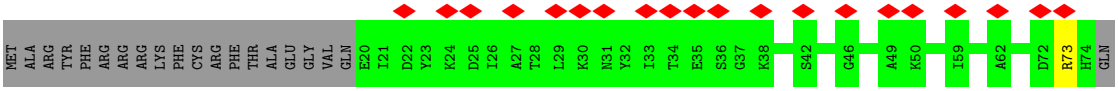
• Molecule 16: 30S ribosomal protein S17

Chain q:

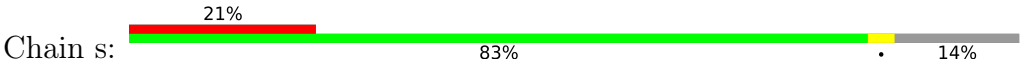


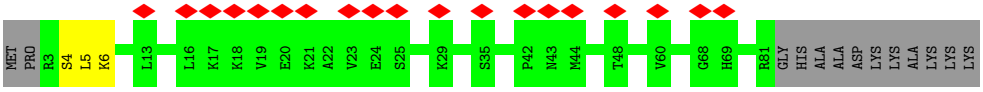
• Molecule 17: 30S ribosomal protein S18

Chain r:

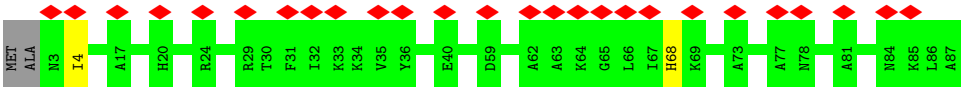


• Molecule 18: 30S ribosomal protein S19

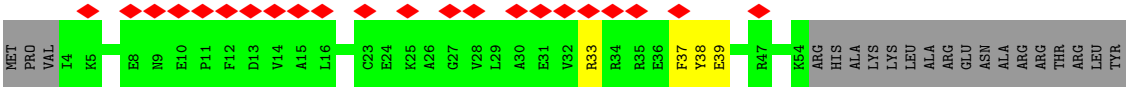




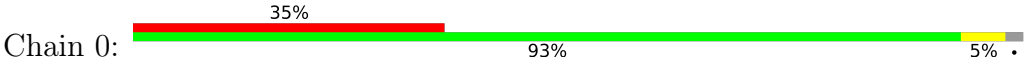
• Molecule 19: 30S ribosomal protein S20

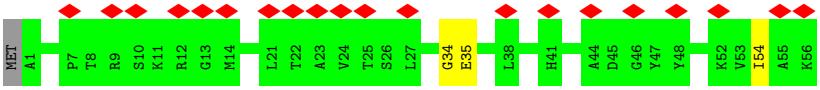


• Molecule 20: 30S ribosomal protein S21

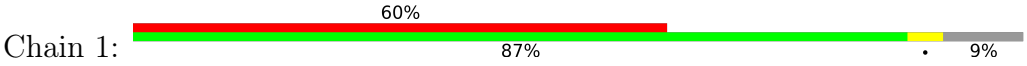


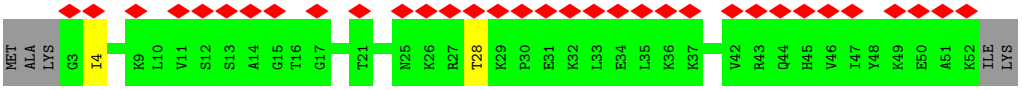
• Molecule 21: 50S ribosomal protein L32



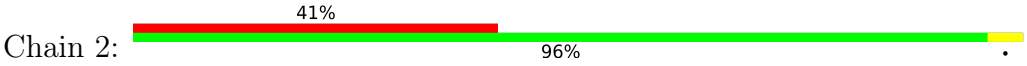


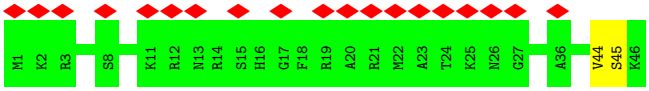
• Molecule 22: 50S ribosomal protein L33





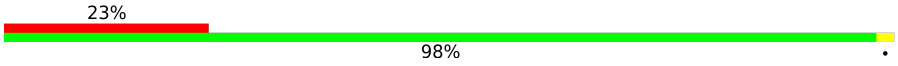
• Molecule 23: 50S ribosomal protein L34

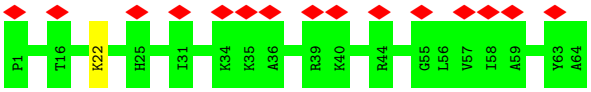




• Molecule 24: 50S ribosomal protein L35

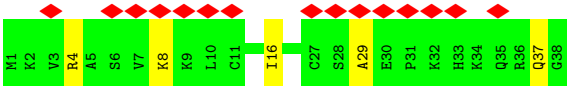
Chain 3:





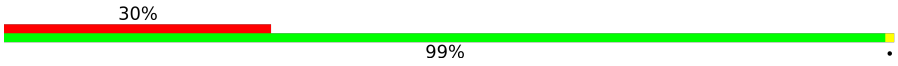
• Molecule 25: 50S ribosomal protein L36

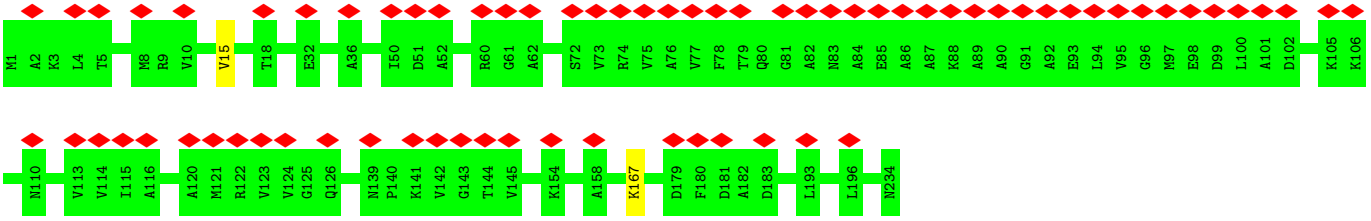
Chain 4:



• Molecule 26: 50S ribosomal protein L1

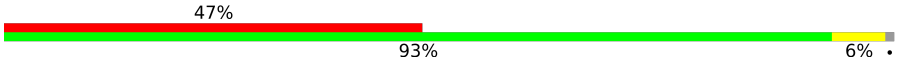
Chain 5:

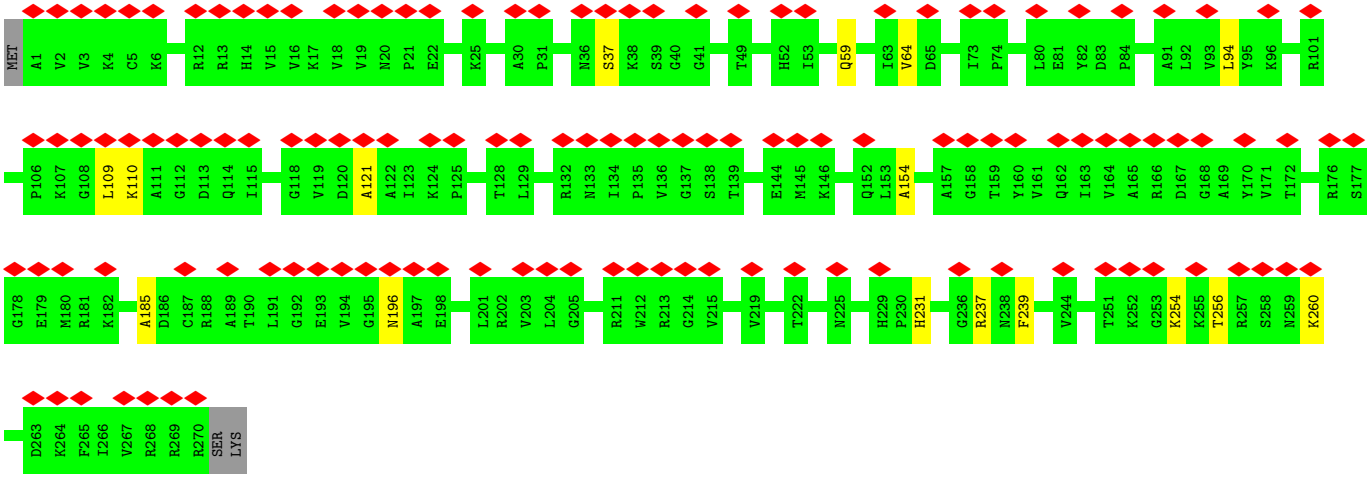




• Molecule 27: 50S ribosomal protein L2

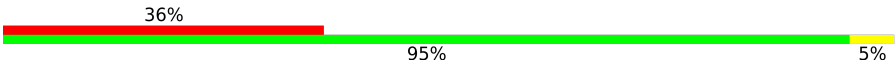
Chain C:

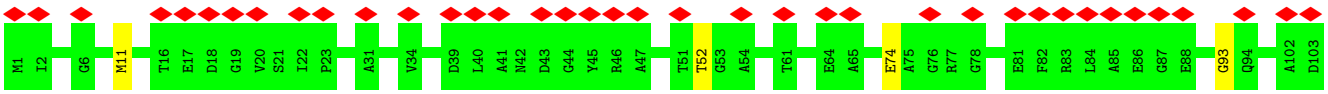


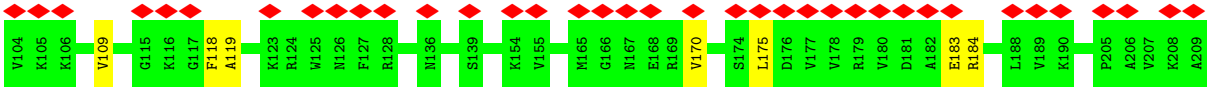


• Molecule 28: 50S ribosomal protein L3

Chain D:

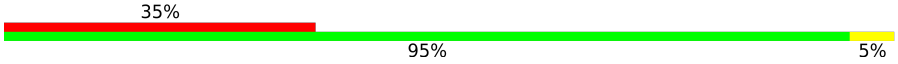


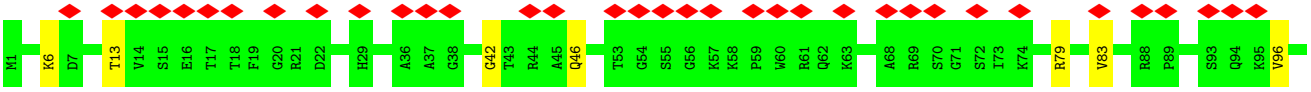


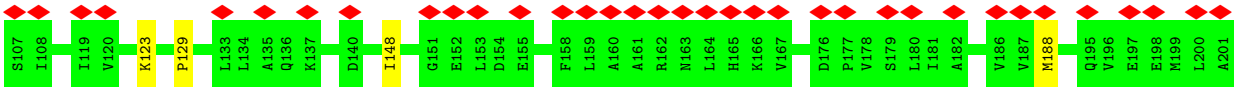


• Molecule 29: 50S ribosomal protein L4

Chain E:

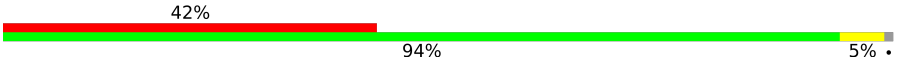


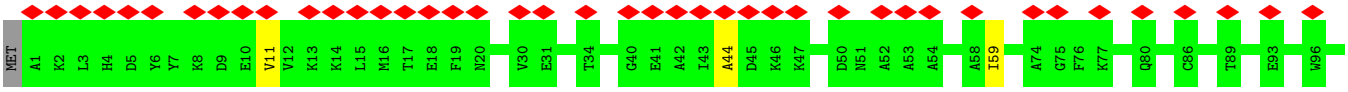


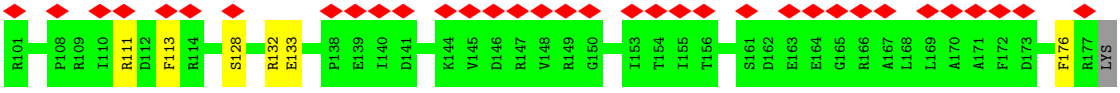


• Molecule 30: 50S ribosomal protein L5

Chain F:

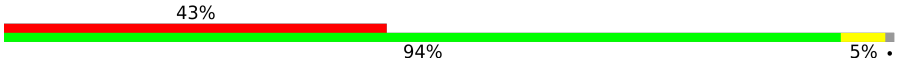


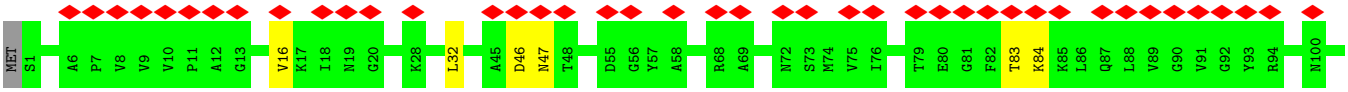


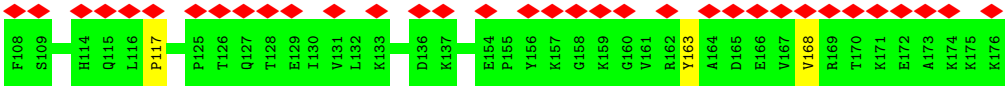


• Molecule 31: 50S ribosomal protein L6

Chain G:

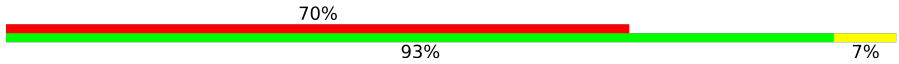


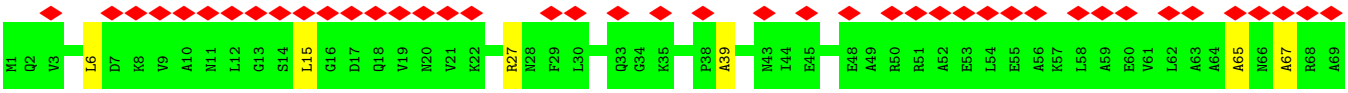


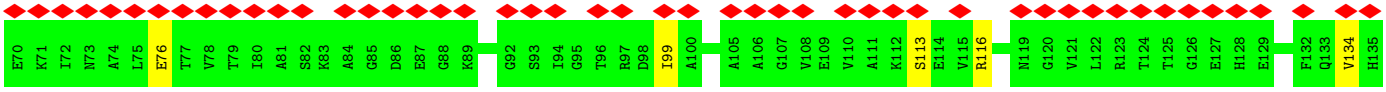


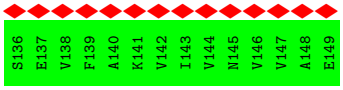
• Molecule 32: 50S ribosomal protein L9

Chain H:



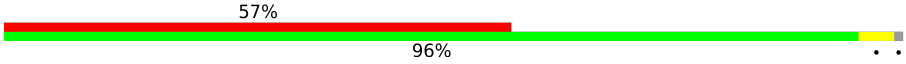


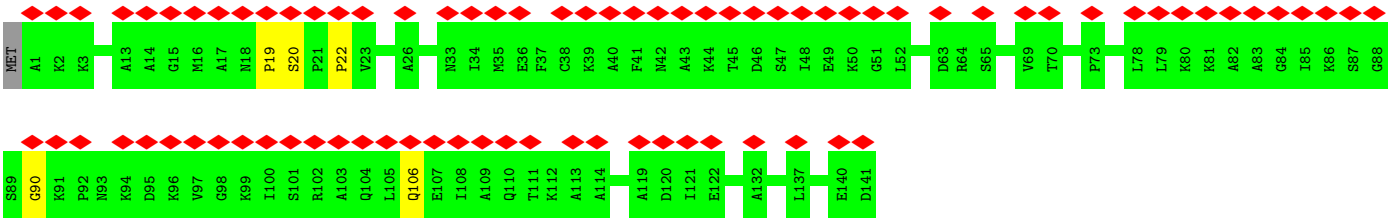




• Molecule 33: 50S ribosomal protein L11

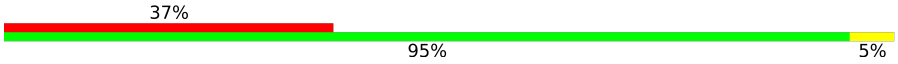
Chain I:

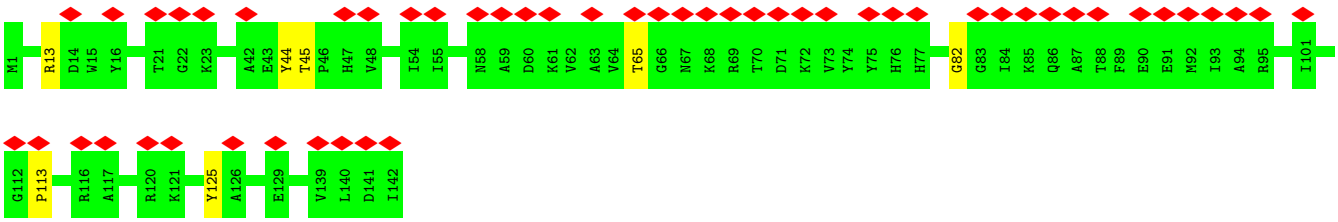




• Molecule 34: 50S ribosomal protein L13

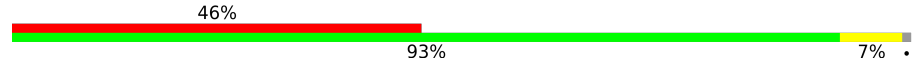
Chain J:

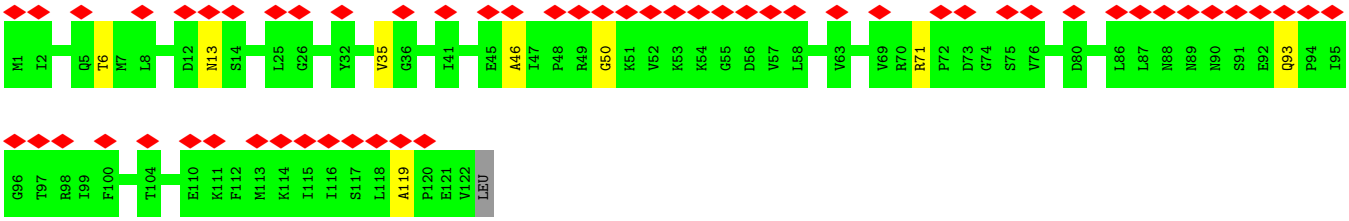




• Molecule 35: 50S ribosomal protein L14

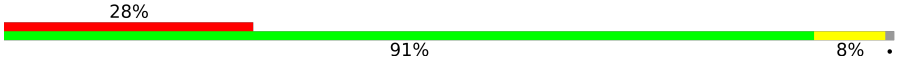
Chain K:

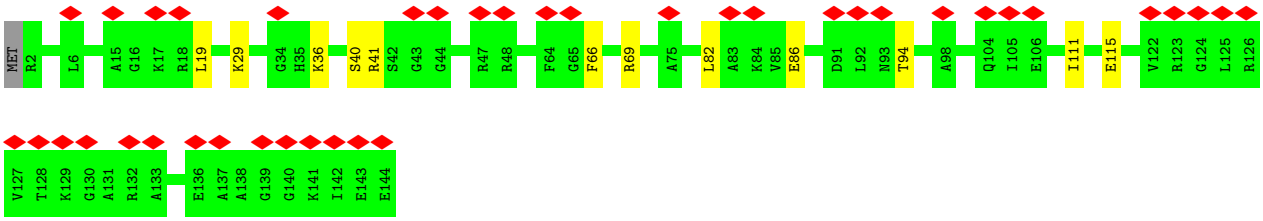




• Molecule 36: 50S ribosomal protein L15

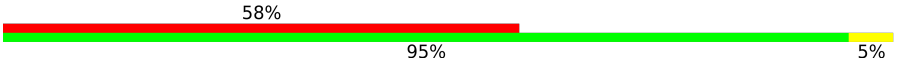
Chain L:

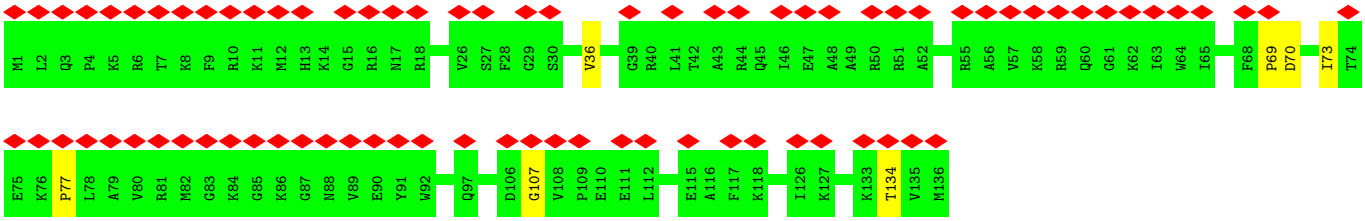




• Molecule 37: 50S ribosomal protein L16

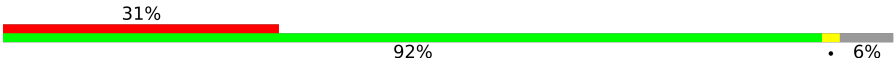
Chain M:

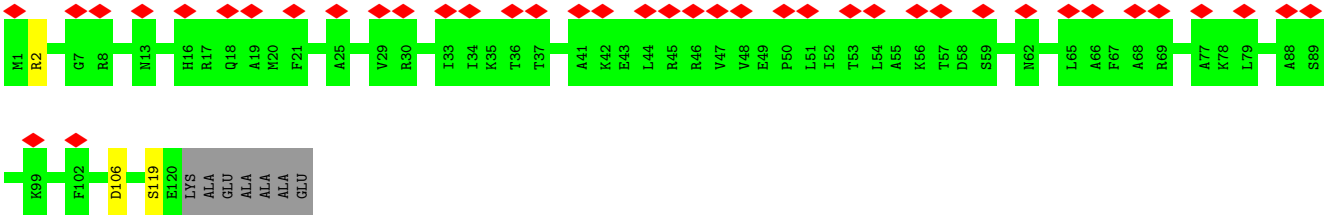




• Molecule 38: 50S ribosomal protein L17

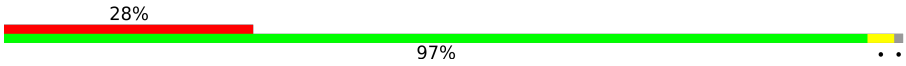
Chain N:

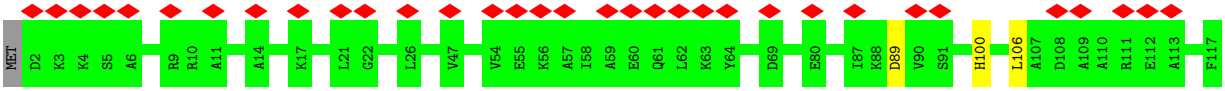




• Molecule 39: 50S ribosomal protein L18

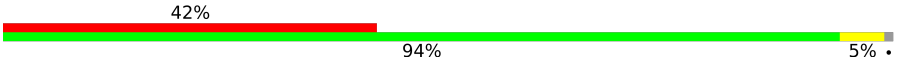
Chain O:

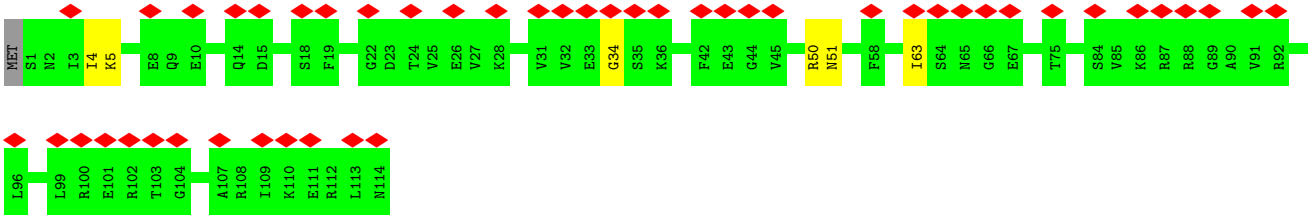




• Molecule 40: 50S ribosomal protein L19

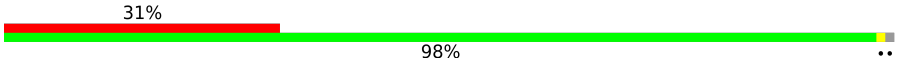
Chain P:

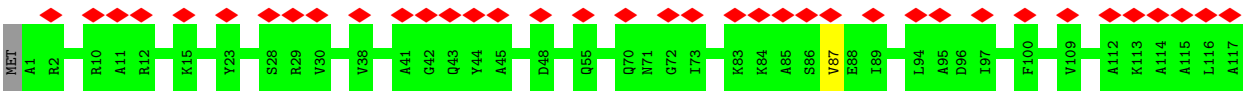




• Molecule 41: 50S ribosomal protein L20

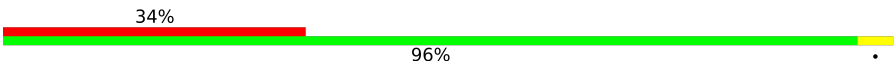
Chain Q:

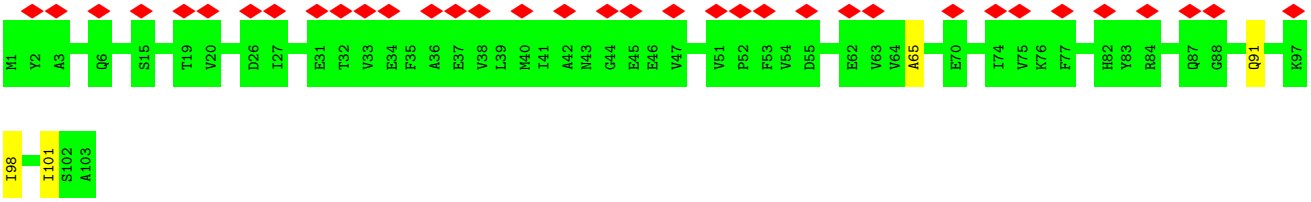




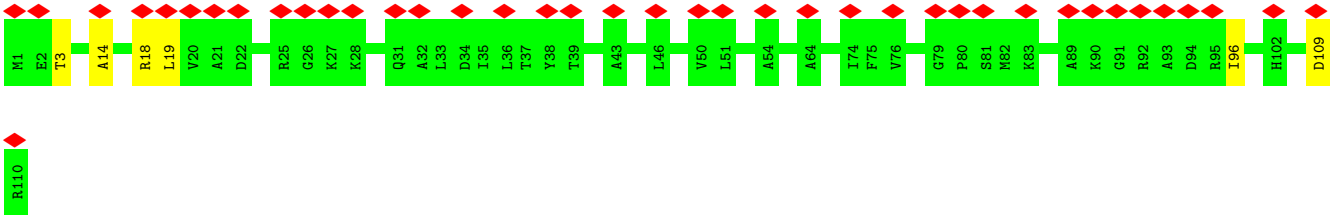
• Molecule 42: 50S ribosomal protein L21

Chain R:

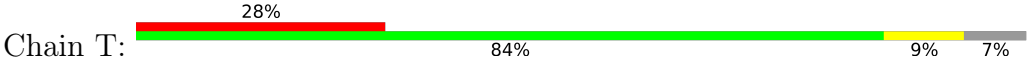


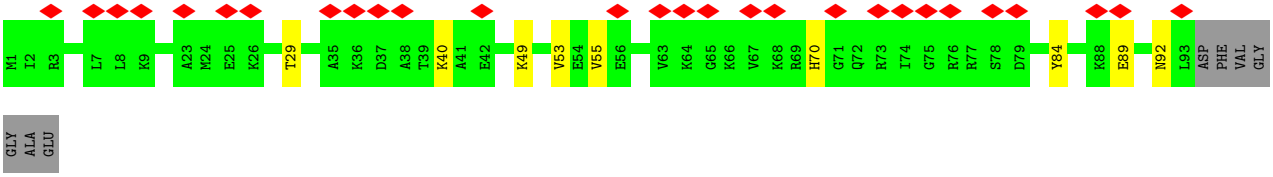


• Molecule 43: 50S ribosomal protein L22

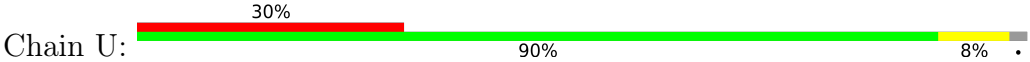


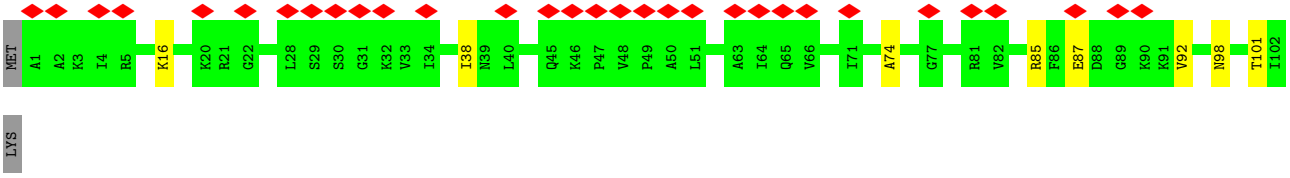
• Molecule 44: 50S ribosomal protein L23



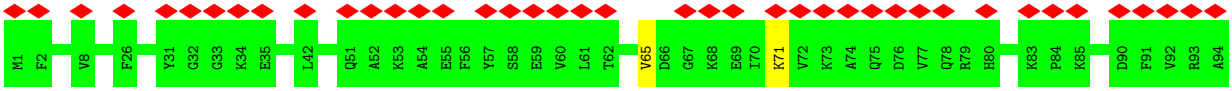


• Molecule 45: 50S ribosomal protein L24

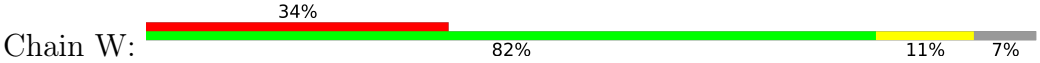


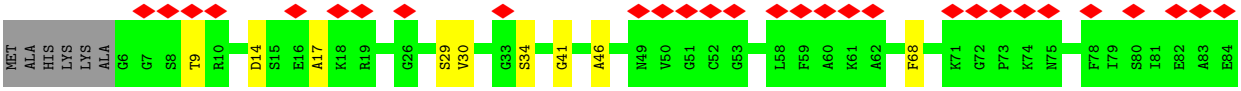


• Molecule 46: 50S ribosomal protein L25



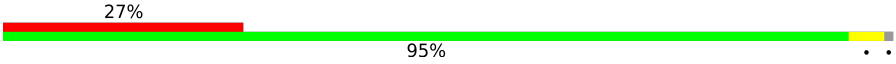
• Molecule 47: 50S ribosomal protein L27

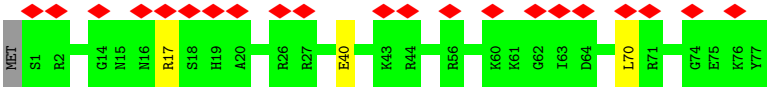




• Molecule 48: 50S ribosomal protein L28

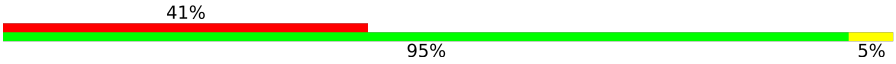
Chain X:

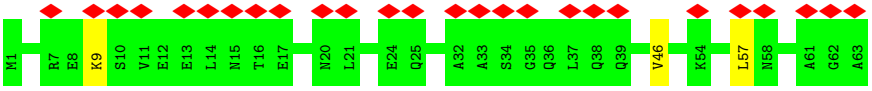




• Molecule 49: 50S ribosomal protein L29

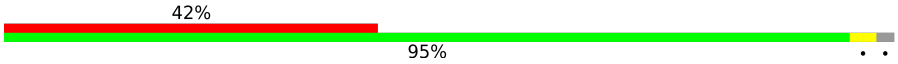
Chain Y:

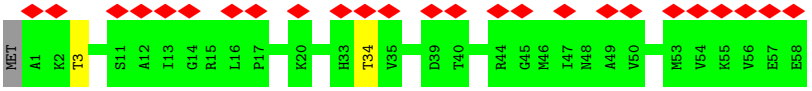




• Molecule 50: 50S ribosomal protein L30

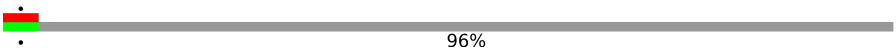
Chain Z:

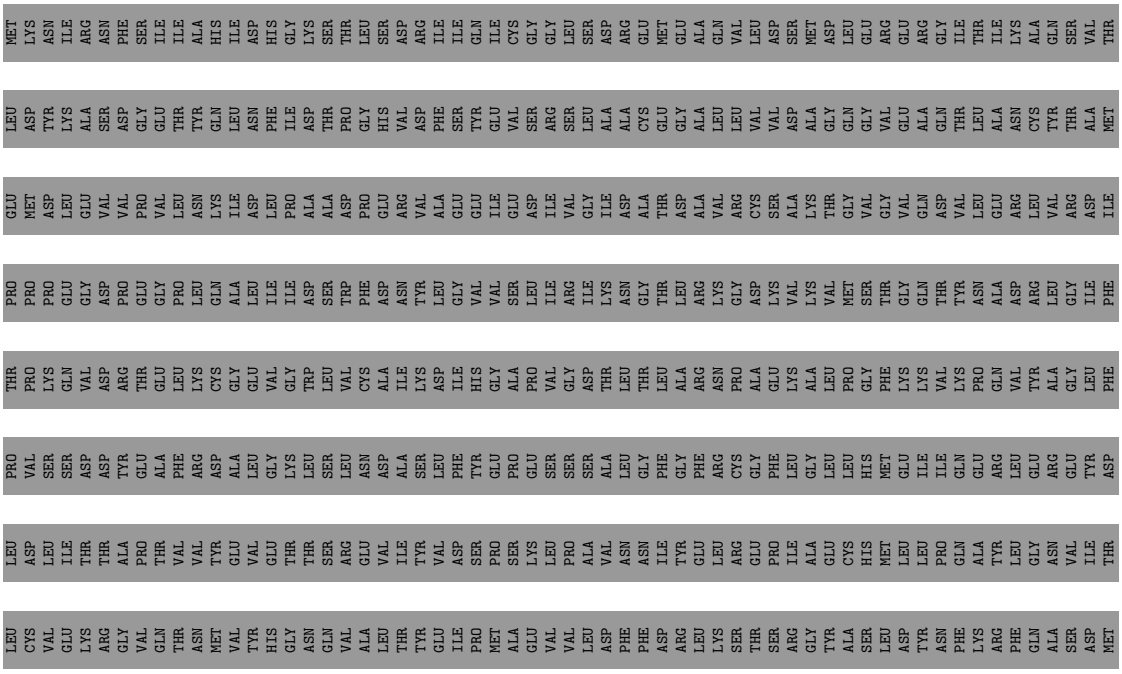


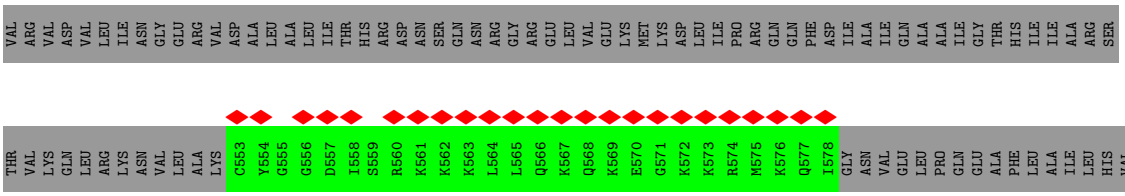


• Molecule 51: Elongation factor 4

Chain x:

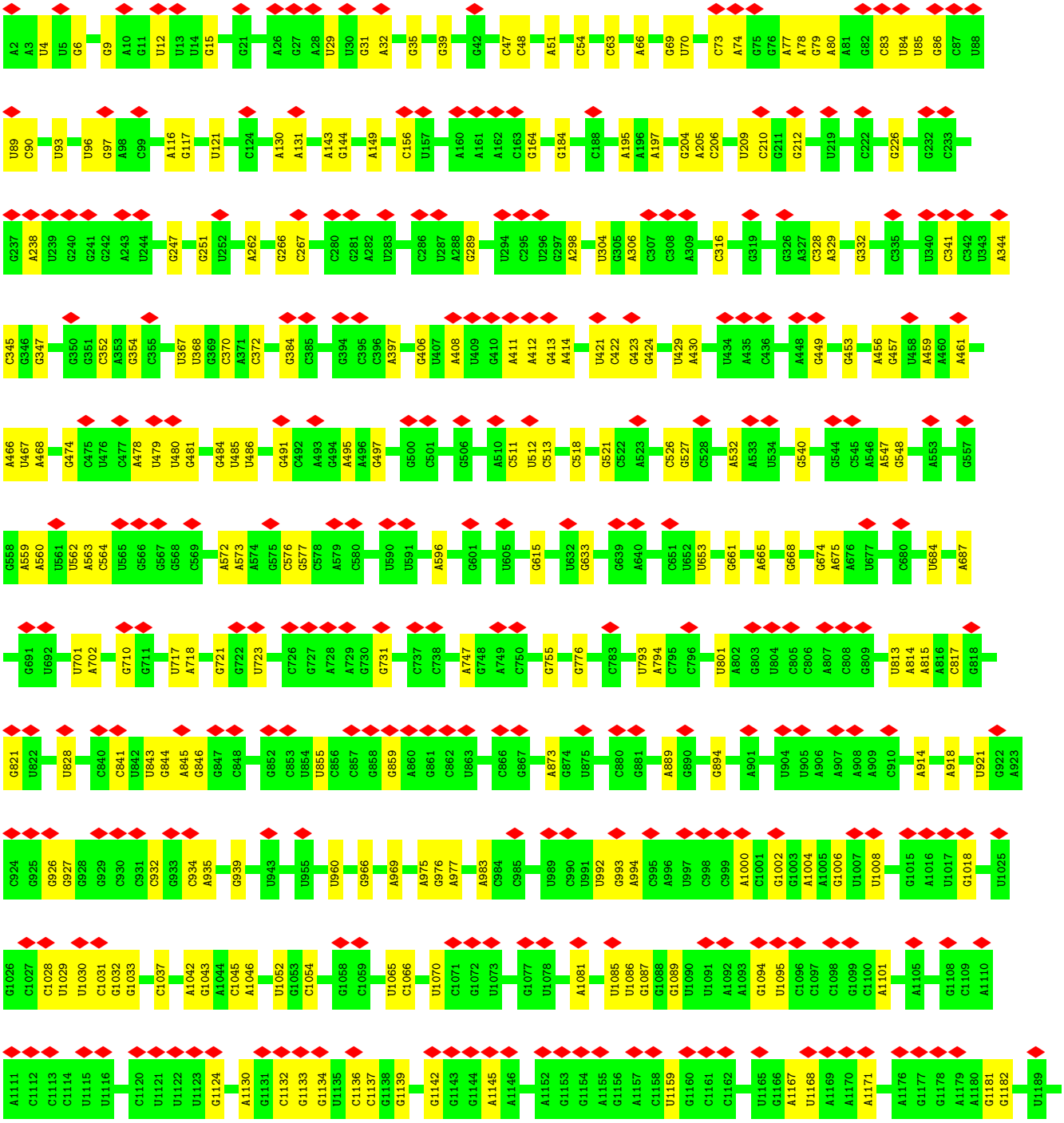


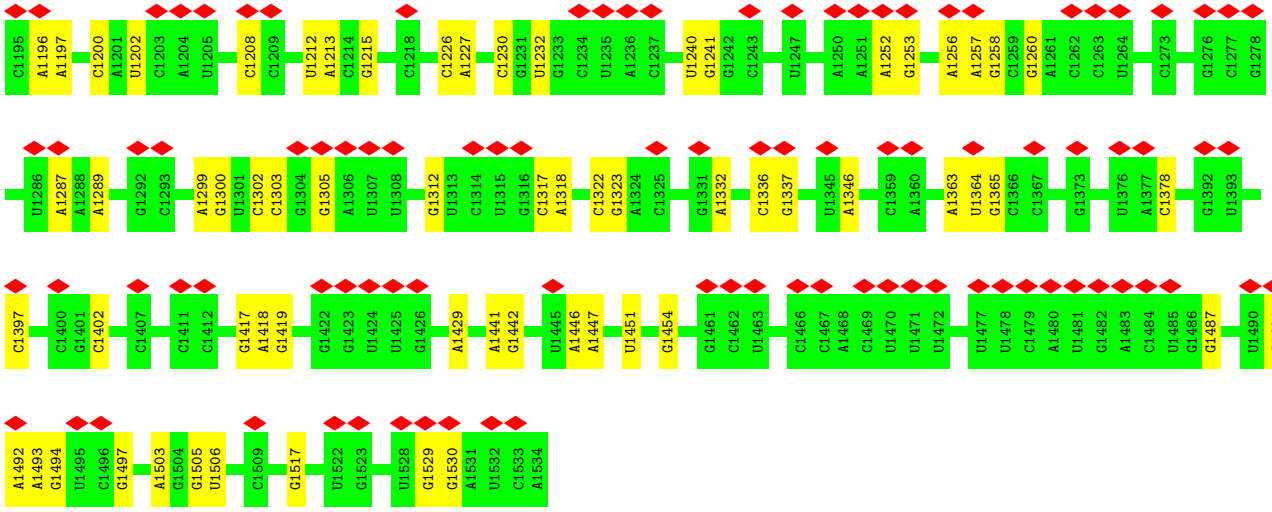




• Molecule 52: 16S ribosomal RNA

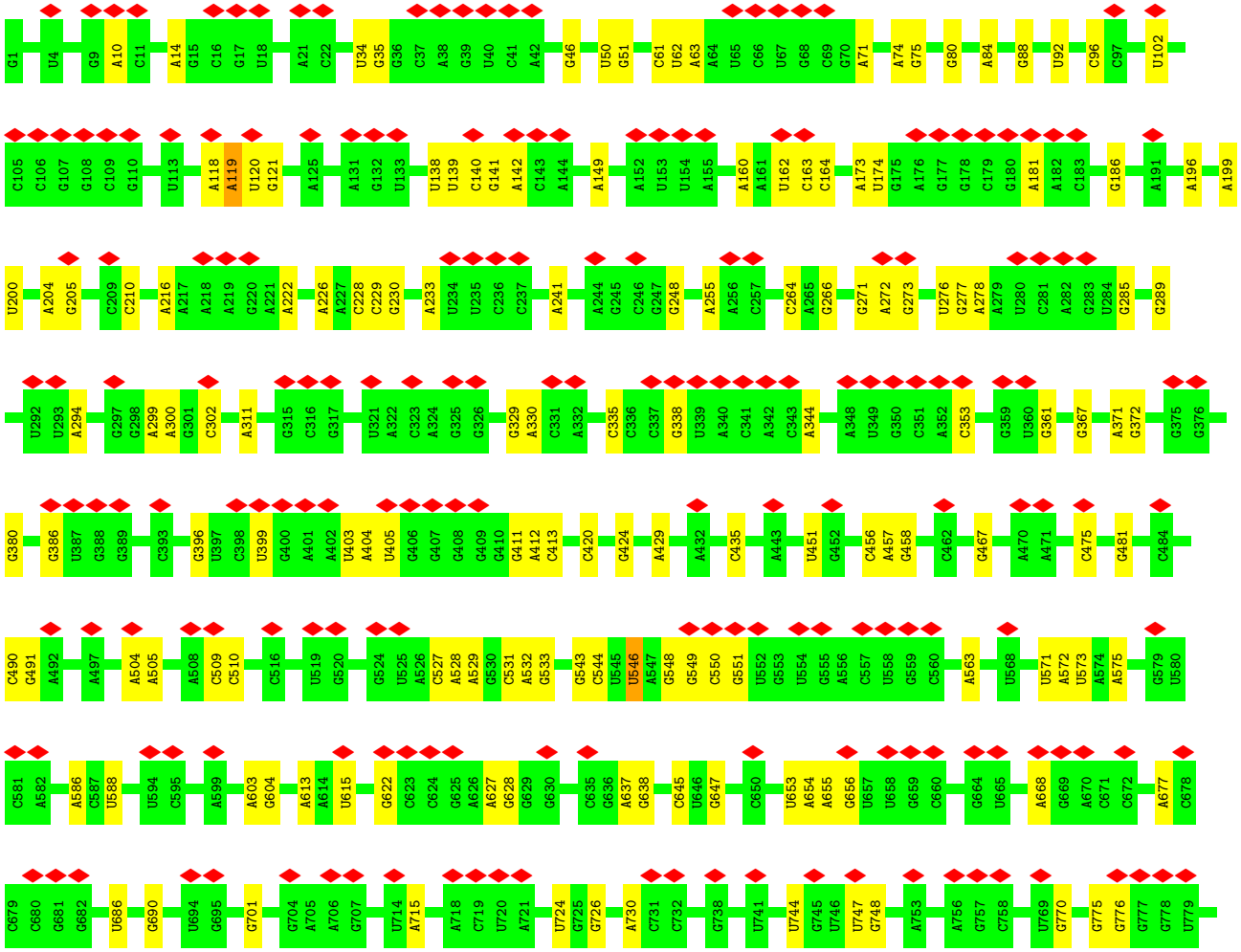
Chain a:

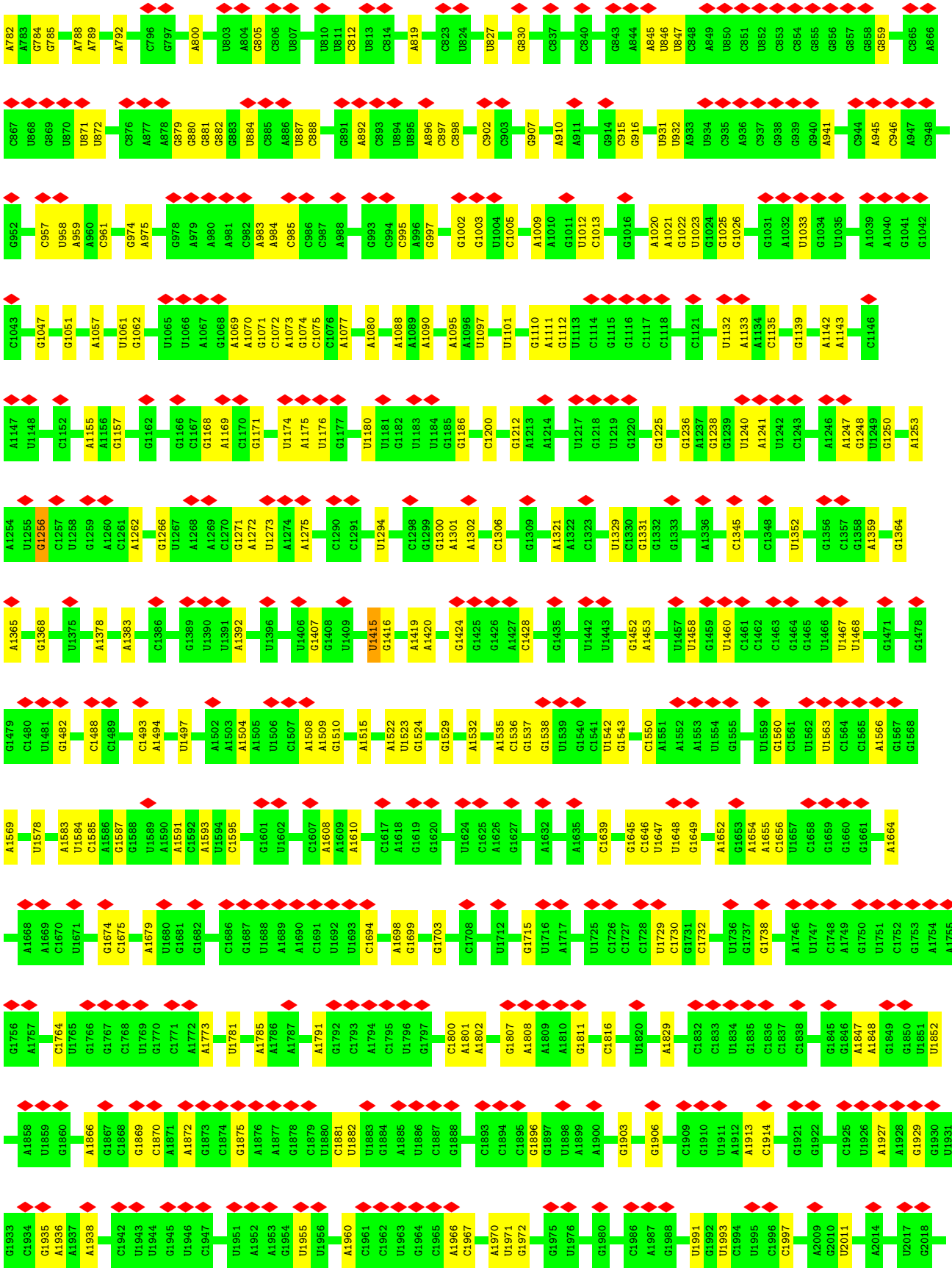


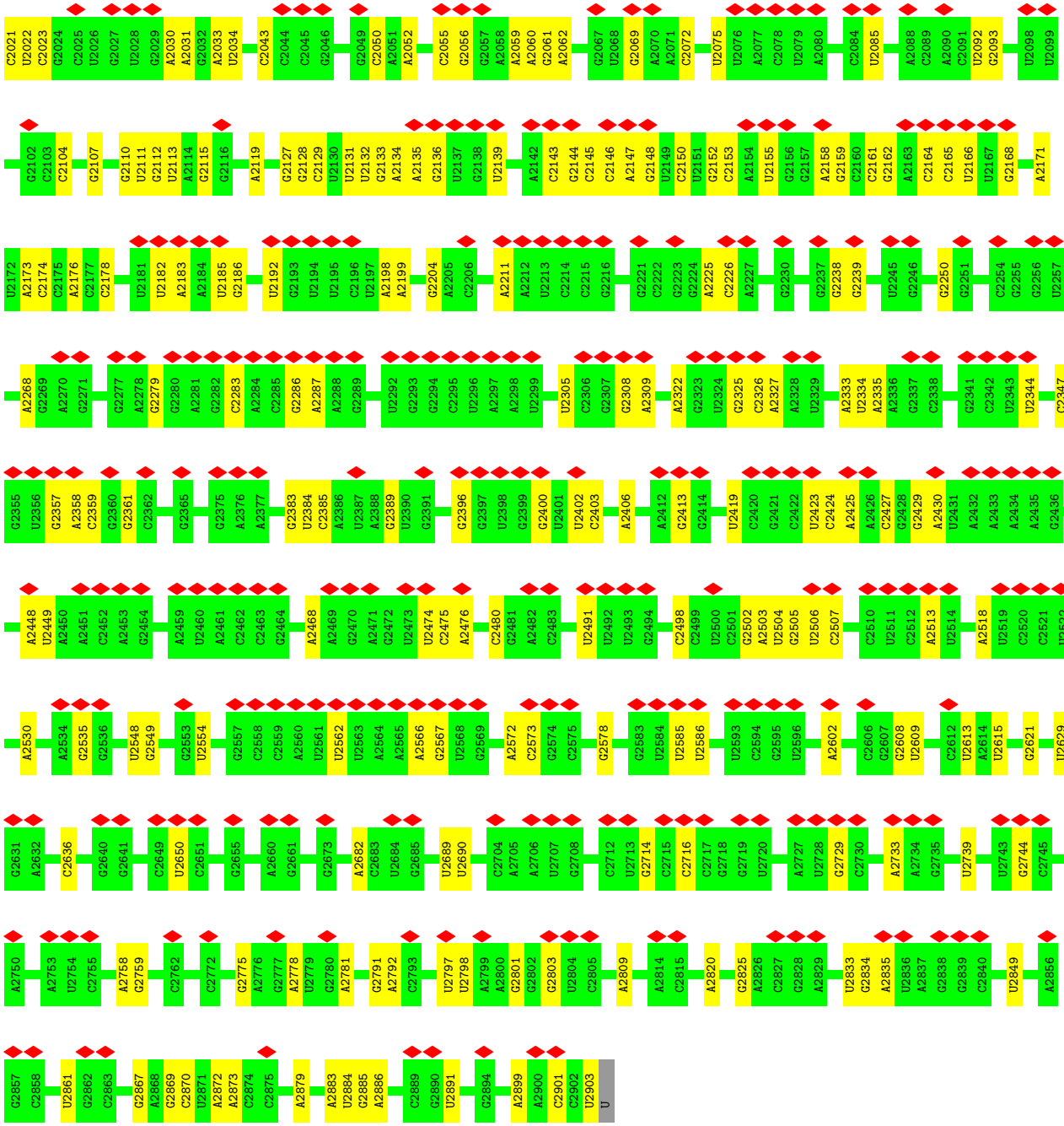


• Molecule 53: 23S ribosomal RNA

Chain A:

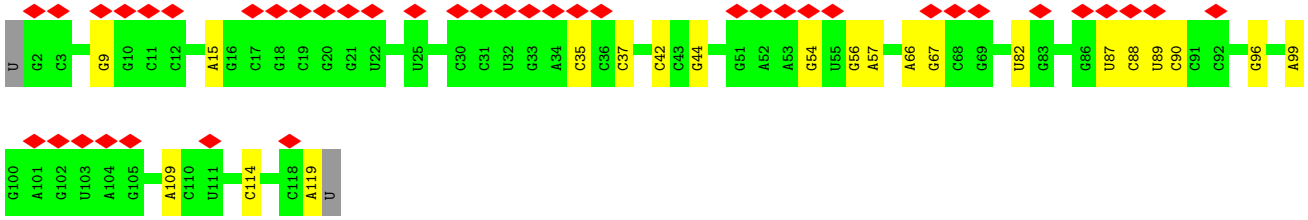



A782 A783 G784 G785 A788 A789 A792 C796 G797 A800 U803 A804 G805 C806 U807 U810 U811 C812 U813 C814 A819 C823 U824 U827 G830 C837 C840 G843 A844 A845 U846 U847 C848 A849 U850 C851 U852 C853 C854 G855 G856 G857 G858 G859 C865 A866
C867 U868 G869 U870 U871 U872 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A886 U887 C888 C891 A892 C893 U894 U895 A896 C897 C898 C902 C903 G907 A910 A911 G914 C915 G916 U931 U932 A933 U934 C935 A936 C937 G938 G939 G940 A941 C944 A945 C946 A947 C948
G952 C957 U958 A959 A960 C961 G974 A975 G978 A979 A980 A981 C982 A983 A984 C985 C986 C987 A988 G993 C994 C995 A996 G997 G1002 G1003 U1004 C1005 A1009 A1010 G1011 U1012 C1013 G1016 A1020 A1021 G1022 U1023 G1024 G1025 G1026 G1031 A1032 U1033 G1034 U1035 A1039 A1040 G1041 G1042
C1043 G1047 G1051 A1057 U1061 G1062 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 A1080 A1088 A1089 A1090 A1095 A1096 U1097 U1101 G1110 A1111 G1112 U1113 C1114 G1115 G1116 C1117 C1118 C1121 U1132 A1133 A1134 C1135 G1139 A1142 A1143 C1146
A1147 U1148 C1152 A1155 A1156 G1157 G1162 G1166 C1167 G1168 A1169 C1170 G1171 U1174 A1175 U1176 G1177 U1180 U1181 G1182 U1183 U1184 G1185 G1186 C1200 G1212 A1213 A1214 U1217 G1218 U1219 G1220 G1225 G1236 A1237 G1238 G1239 U1240 A1241 U1242 C1243 A1246 A1247 G1248 U1249 G1250 A1253
A1254 U1255 G1256 C1257 U1258 G1259 A1260 C1261 A1262 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 C1290 C1291 U1294 C1298 G1299 G1300 A1301 A1302 C1306 G1309 A1321 A1322 C1323 U1329 C1330 G1331 G1332 G1333 A1336 C1345 C1348 U1352 G1356 C1357 G1358 A1359 G1364
A1365 G1368 U1375 A1378 A1383 C1386 G1389 U1390 U1391 A1392 U1396 G1406 G1407 G1408 U1409 U1415 G1416 A1419 A1420 G1424 G1425 G1426 A1427 C1428 G1435 U1442 U1443 G1452 A1453 U1457 U1458 G1459 U1460 C1461 C1462 C1463 G1464 G1465 U1466 U1467 U1468 G1471 G1478
G1479 C1480 U1481 G1482 C1488 C1489 C1493 A1494 U1497 A1502 A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 A1515 A1522 U1523 G1524 G1529 A1532 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 C1550 A1551 A1552 A1553 U1554 G1555 U1559 G1560 C1561 U1562 U1563 C1564 C1565 A1566 G1567 G1568
A1569 U1578 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 G1601 U1602 C1607 A1608 A1609 A1610 C1617 A1618 G1619 G1620 U1624 C1625 A1626 G1627 A1632 A1635 C1639 G1645 C1646 U1647 U1648 G1649 A1652 G1653 A1654 A1655 C1656 U1657 C1658 G1659 G1660 G1661 A1664
A1668 A1669 C1670 U1671 G1674 C1675 A1679 U1680 G1681 G1682 C1686 G1687 U1688 A1689 A1690 C1691 U1692 U1693 C1694 A1698 G1699 G1703 C1708 U1712 G1715 U1716 A1717 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 U1736 G1737 G1738 A1746 U1747 C1748 A1749 G1750 U1751 C1752 G1753 A1754 A1755
G1756 A1757 C1764 U1765 G1766 G1767 C1768 U1769 G1770 C1771 A1772 A1773 U1781 A1785 A1786 A1787 A1791 G1792 C1793 A1794 C1795 U1796 G1797 C1800 A1801 A1802 G1807 A1808 A1809 A1810 G1811 C1816 U1820 A1829 C1832 C1833 U1834 G1835 C1836 C1837 C1838 G1845 G1846 A1847 A1848 G1849 G1850 U1851 U1852
A1858 U1859 G1860 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 A1877 G1878 C1879 U1880 C1881 U1882 U1883 G1884 A1885 U1886 C1887 G1888 C1893 C1894 C1895 G1896 G1897 U1898 A1899 A1900 G1903 G1906 C1909 G1910 U1911 A1912 A1913 C1914 G1921 G1922 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932
G1933 C1934 G1935 A1936 A1937 A1938 C1942 U1943 U1944 G1945 U1946 C1947 U1951 A1952 A1953 G1954 U1955 U1956 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1975 U1976 G1980 C1986 A1987 G1988 U1991 G1992 U1993 C1994 U1995 C1996 C1997 A2009 G2010 U2011 A2014 U2017 G2018



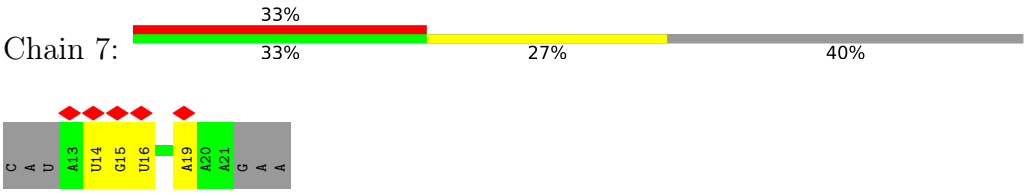
• Molecule 54: 5S ribosomal RNA

Chain B:



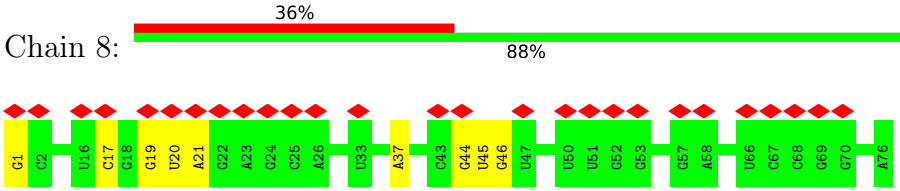
• Molecule 55: mRNA

Chain 7:



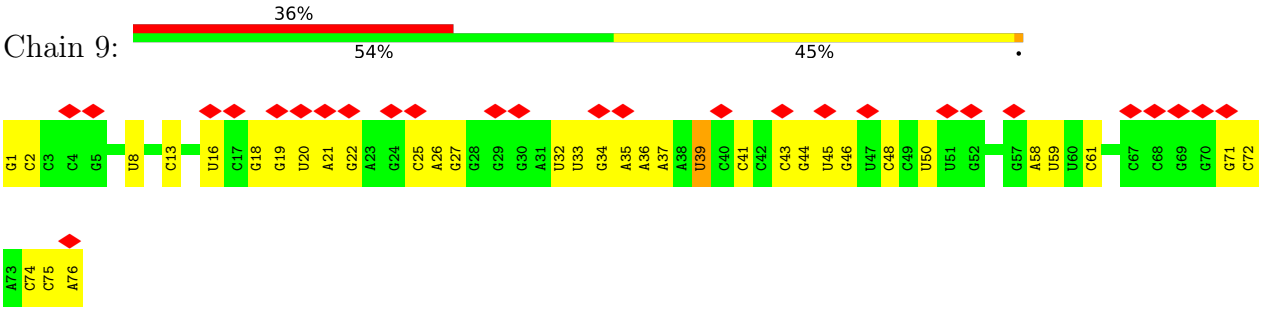
• Molecule 56: tRNA

Chain 8:



• Molecule 56: tRNA

Chain 9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18772	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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	b	0.30	0/1735	0.55	0/2338
2	c	0.34	0/1651	0.50	0/2225
3	d	0.32	0/1665	0.52	0/2227
4	e	0.35	0/1118	0.54	0/1504
5	f	0.33	0/851	0.56	0/1150
6	g	0.32	0/1195	0.50	0/1602
7	h	0.36	0/989	0.53	0/1326
8	i	0.32	0/1034	0.52	0/1375
9	j	0.31	0/796	0.57	0/1077
10	k	0.35	0/893	0.52	0/1205
11	l	0.35	0/969	0.54	0/1300
12	m	0.32	0/892	0.56	0/1193
13	n	0.33	0/785	0.52	0/1043
14	o	0.35	0/722	0.51	0/964
15	p	0.34	0/659	0.48	0/884
16	q	0.33	0/657	0.55	0/881
17	r	0.36	0/462	0.48	0/621
18	s	0.30	0/652	0.50	0/877
19	t	0.36	0/671	0.51	0/888
20	u	0.34	0/430	0.56	0/570
21	0	0.36	0/450	0.52	0/599
22	1	0.36	0/416	0.58	0/554
23	2	0.36	0/380	0.52	0/498
24	3	0.38	0/513	0.56	0/676
25	4	0.32	0/303	0.54	0/397
26	5	0.27	0/1748	0.60	0/2355
27	C	0.39	0/2115	0.58	1/2844 (0.0%)
28	D	0.37	0/1586	0.57	0/2134
29	E	0.34	0/1571	0.54	0/2113
30	F	0.32	0/1434	0.53	0/1926
31	G	0.31	0/1343	0.53	0/1816
32	H	0.30	0/1122	0.59	0/1515
33	I	0.26	0/1046	0.54	0/1410
34	J	0.39	0/1152	0.56	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	K	0.40	0/947	0.57	0/1268
36	L	0.33	0/1054	0.56	0/1403
37	M	0.36	0/1093	0.57	0/1460
38	N	0.38	0/973	0.55	0/1301
39	O	0.31	0/902	0.51	1/1209 (0.1%)
40	P	0.37	0/929	0.56	0/1242
41	Q	0.43	0/960	0.51	0/1278
42	R	0.35	0/829	0.53	0/1107
43	S	0.37	0/864	0.55	0/1156
44	T	0.36	0/744	0.61	0/994
45	U	0.33	0/787	0.57	0/1051
46	V	0.33	0/766	0.50	0/1025
47	W	0.35	0/603	0.64	0/797
48	X	0.37	0/635	0.56	0/848
49	Y	0.32	0/510	0.51	0/677
50	Z	0.32	0/453	0.57	0/605
51	x	0.31	0/214	0.54	0/275
52	a	0.52	0/36834	0.77	0/57462
53	A	0.58	0/69799	0.81	6/108892 (0.0%)
54	B	0.46	0/2828	0.77	0/4410
55	7	0.48	0/213	0.91	0/329
56	8	0.51	1/1813 (0.1%)	0.79	0/2823
56	9	0.39	1/1813 (0.1%)	0.83	3/2823 (0.1%)
All	All	0.50	2/160568 (0.0%)	0.74	11/240073 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
20	u	0	1
31	G	0	1
35	K	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	9	1	G	OP3-P	-10.74	1.48	1.61
56	8	1	G	OP3-P	-10.71	1.48	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	9	39	U	C2-N1-C1'	7.25	126.40	117.70
56	9	39	U	N1-C2-O2	7.22	127.85	122.80
56	9	39	U	N3-C2-O2	-6.07	117.95	122.20
53	A	1415	U	C2-N1-C1'	6.02	124.92	117.70
39	O	106	LEU	CA-CB-CG	5.67	128.34	115.30
27	C	109	LEU	CA-CB-CG	5.49	127.93	115.30
53	A	1415	U	N1-C2-O2	5.38	126.56	122.80
53	A	546	U	C2-N1-C1'	5.37	124.15	117.70
53	A	1256	G	C4-N9-C1'	5.31	133.40	126.50
53	A	119	A	P-O3'-C3'	5.25	126.00	119.70
53	A	1256	G	C8-N9-C1'	-5.13	120.33	127.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	G	83	THR	Peptide
35	K	71	ARG	Peptide
20	u	39	GLU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	b	216/241 (90%)	181 (84%)	23 (11%)	12 (6%)	2 19
2	c	204/233 (88%)	190 (93%)	7 (3%)	7 (3%)	3 30
3	d	203/206 (98%)	179 (88%)	15 (7%)	9 (4%)	2 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	e	148/167 (89%)	128 (86%)	15 (10%)	5 (3%)	3	30
5	f	100/135 (74%)	79 (79%)	13 (13%)	8 (8%)	1	12
6	g	149/179 (83%)	125 (84%)	18 (12%)	6 (4%)	3	26
7	h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	19	56
8	i	125/130 (96%)	109 (87%)	12 (10%)	4 (3%)	4	31
9	j	96/103 (93%)	78 (81%)	13 (14%)	5 (5%)	2	21
10	k	115/129 (89%)	104 (90%)	8 (7%)	3 (3%)	5	34
11	l	121/124 (98%)	105 (87%)	14 (12%)	2 (2%)	9	42
12	m	112/118 (95%)	103 (92%)	5 (4%)	4 (4%)	3	29
13	n	92/101 (91%)	77 (84%)	8 (9%)	7 (8%)	1	13
14	o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13	48
15	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5	35
16	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1	17
17	r	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	8	40
18	s	77/92 (84%)	68 (88%)	6 (8%)	3 (4%)	3	27
19	t	83/87 (95%)	80 (96%)	1 (1%)	2 (2%)	6	35
20	u	49/71 (69%)	36 (74%)	10 (20%)	3 (6%)	1	18
21	0	54/57 (95%)	49 (91%)	2 (4%)	3 (6%)	2	19
22	1	48/55 (87%)	43 (90%)	3 (6%)	2 (4%)	3	25
23	2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	23
24	3	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	43
25	4	36/38 (95%)	29 (81%)	2 (6%)	5 (14%)	0	3
26	5	232/234 (99%)	198 (85%)	32 (14%)	2 (1%)	17	54
27	C	268/273 (98%)	233 (87%)	20 (8%)	15 (6%)	2	19
28	D	207/209 (99%)	168 (81%)	28 (14%)	11 (5%)	2	21
29	E	199/201 (99%)	170 (85%)	18 (9%)	11 (6%)	2	20
30	F	175/179 (98%)	153 (87%)	13 (7%)	9 (5%)	2	21
31	G	174/177 (98%)	142 (82%)	24 (14%)	8 (5%)	2	23
32	H	147/149 (99%)	114 (78%)	22 (15%)	11 (8%)	1	13
33	I	139/142 (98%)	121 (87%)	13 (9%)	5 (4%)	3	29
34	J	140/142 (99%)	120 (86%)	13 (9%)	7 (5%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	K	120/123 (98%)	96 (80%)	17 (14%)	7 (6%)	1 19
36	L	141/144 (98%)	115 (82%)	14 (10%)	12 (8%)	1 10
37	M	134/136 (98%)	114 (85%)	13 (10%)	7 (5%)	2 21
38	N	118/127 (93%)	105 (89%)	10 (8%)	3 (2%)	5 35
39	O	114/117 (97%)	105 (92%)	7 (6%)	2 (2%)	8 41
40	P	112/115 (97%)	98 (88%)	8 (7%)	6 (5%)	2 20
41	Q	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17 54
42	R	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	3 26
43	S	108/110 (98%)	93 (86%)	9 (8%)	6 (6%)	2 19
44	T	91/100 (91%)	65 (71%)	17 (19%)	9 (10%)	0 8
45	U	100/104 (96%)	79 (79%)	13 (13%)	8 (8%)	1 12
46	V	92/94 (98%)	84 (91%)	6 (6%)	2 (2%)	6 37
47	W	77/85 (91%)	55 (71%)	13 (17%)	9 (12%)	0 5
48	X	75/78 (96%)	65 (87%)	7 (9%)	3 (4%)	3 26
49	Y	61/63 (97%)	51 (84%)	7 (12%)	3 (5%)	2 22
50	Z	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	3 29
51	x	24/599 (4%)	23 (96%)	1 (4%)	0	100 100
All	All	5878/6817 (86%)	5045 (86%)	567 (10%)	266 (4%)	4 23

All (266) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	72	LYS
1	b	163	ILE
3	d	151	LYS
5	f	63	ASN
5	f	93	LYS
5	f	98	GLU
8	i	58	VAL
12	m	4	ILE
13	n	29	ALA
13	n	52	PRO
16	q	50	ASN
22	1	4	ILE
24	3	22	LYS
25	4	8	LYS

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Mol	Chain	Res	Type
28	D	170	VAL
29	E	79	ARG
31	G	16	VAL
31	G	47	ASN
31	G	84	LYS
31	G	168	VAL
32	H	65	ALA
32	H	67	ALA
32	H	99	ILE
33	I	22	PRO
34	J	44	TYR
40	P	50	ARG
43	S	96	ILE
43	S	109	ASP
44	T	29	THR
44	T	40	LYS
45	U	92	VAL
1	b	18	GLN
1	b	76	SER
1	b	85	SER
1	b	120	SER
1	b	136	ARG
2	c	206	GLU
3	d	24	GLY
3	d	32	CYS
3	d	125	VAL
4	e	90	THR
5	f	69	GLU
5	f	92	THR
6	g	113	ASP
6	g	130	ASN
8	i	90	TYR
8	i	96	SER
9	j	61	ALA
12	m	10	PRO
12	m	47	GLU
13	n	23	LYS
13	n	53	ARG
16	q	14	SER
16	q	71	LYS
19	t	4	ILE
19	t	68	HIS

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Mol	Chain	Res	Type
21	0	34	GLY
21	0	35	GLU
25	4	4	ARG
25	4	29	ALA
26	5	167	LYS
27	C	231	HIS
27	C	239	PHE
28	D	11	MET
28	D	74	GLU
28	D	93	GLY
28	D	175	LEU
28	D	184	ARG
29	E	148	ILE
30	F	11	VAL
30	F	44	ALA
30	F	59	ILE
30	F	111	ARG
30	F	176	PHE
31	G	117	PRO
31	G	163	TYR
32	H	27	ARG
32	H	76	GLU
32	H	134	VAL
33	I	90	GLY
34	J	45	THR
34	J	65	THR
35	K	13	ASN
36	L	29	LYS
36	L	111	ILE
37	M	69	PRO
40	P	4	ILE
40	P	5	LYS
43	S	14	ALA
43	S	18	ARG
44	T	55	VAL
44	T	89	GLU
45	U	87	GLU
45	U	98	ASN
47	W	9	THR
47	W	17	ALA
48	X	17	ARG
50	Z	34	THR

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Mol	Chain	Res	Type
1	b	67	LEU
1	b	200	PRO
2	c	61	ALA
2	c	82	GLU
2	c	146	ALA
3	d	5	LEU
3	d	27	ALA
4	e	24	THR
4	e	45	ARG
5	f	54	LEU
6	g	58	GLU
9	j	57	VAL
10	k	120	GLY
12	m	114	LYS
15	p	81	ALA
18	s	4	SER
18	s	5	LEU
18	s	6	LYS
23	2	45	SER
27	C	37	SER
27	C	94	LEU
27	C	110	LYS
27	C	121	ALA
27	C	185	ALA
27	C	237	ARG
27	C	256	THR
27	C	260	LYS
29	E	6	LYS
29	E	13	THR
30	F	133	GLU
31	G	32	LEU
32	H	116	ARG
33	I	19	PRO
34	J	82	GLY
34	J	125	TYR
35	K	6	THR
35	K	46	ALA
36	L	69	ARG
36	L	82	LEU
36	L	86	GLU
37	M	70	ASP
37	M	107	GLY

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Mol	Chain	Res	Type
37	M	134	THR
40	P	51	ASN
41	Q	87	VAL
42	R	65	ALA
42	R	91	GLN
43	S	3	THR
43	S	19	LEU
44	T	49	LYS
45	U	16	LYS
45	U	74	ALA
45	U	101	THR
46	V	65	VAL
46	V	71	LYS
47	W	29	SER
47	W	41	GLY
47	W	68	PHE
49	Y	57	LEU
5	f	99	ALA
6	g	84	THR
7	h	114	ARG
9	j	36	VAL
9	j	62	ARG
13	n	3	LYS
14	o	46	HIS
15	p	49	GLY
16	q	17	MET
17	r	73	ARG
20	u	33	ARG
20	u	37	PHE
27	C	64	VAL
27	C	154	ALA
27	C	196	ASN
27	C	254	LYS
28	D	52	THR
29	E	42	GLY
29	E	46	GLN
29	E	96	VAL
29	E	123	LYS
29	E	188	MET
30	F	128	SER
30	F	132	ARG
31	G	46	ASP

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Mol	Chain	Res	Type
32	H	6	LEU
32	H	15	LEU
32	H	113	SER
35	K	93	GLN
35	K	119	ALA
36	L	36	LYS
36	L	40	SER
36	L	41	ARG
36	L	115	GLU
37	M	73	ILE
38	N	106	ASP
39	O	89	ASP
39	O	100	HIS
40	P	63	ILE
44	T	70	HIS
45	U	38	ILE
47	W	34	SER
48	X	40	GLU
48	X	70	LEU
49	Y	9	LYS
50	Z	3	THR
1	b	219	THR
2	c	66	VAL
2	c	101	ILE
3	d	33	LYS
6	g	57	SER
8	i	56	ASP
10	k	89	PRO
11	l	98	VAL
13	n	70	PRO
13	n	92	GLU
16	q	18	GLU
21	0	54	ILE
22	1	28	THR
23	2	44	VAL
25	4	16	ILE
25	4	37	GLN
27	C	59	GLN
28	D	109	VAL
28	D	118	PHE
28	D	119	ALA
29	E	83	VAL

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Mol	Chain	Res	Type
32	H	39	ALA
33	I	20	SER
33	I	106	GLN
34	J	13	ARG
34	J	113	PRO
35	K	50	GLY
36	L	19	LEU
36	L	94	THR
37	M	77	PRO
38	N	2	ARG
38	N	119	SER
42	R	98	ILE
44	T	84	TYR
44	T	92	ASN
45	U	85	ARG
47	W	14	ASP
1	b	71	THR
1	b	128	LEU
3	d	36	GLN
4	e	111	MET
5	f	85	ILE
10	k	14	LYS
20	u	38	TYR
28	D	183	GLU
30	F	113	PHE
36	L	66	PHE
42	R	101	ILE
47	W	46	ALA
3	d	167	LYS
6	g	8	GLY
35	K	35	VAL
44	T	53	VAL
9	j	42	LEU
11	l	44	LYS
26	5	15	VAL
40	P	34	GLY
47	W	30	VAL
2	c	15	VAL
4	e	102	GLY
49	Y	46	VAL
29	E	129	PRO
37	M	36	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	180/199 (90%)	180 (100%)	0	100	100
2	c	170/190 (90%)	170 (100%)	0	100	100
3	d	172/173 (99%)	172 (100%)	0	100	100
4	e	113/126 (90%)	113 (100%)	0	100	100
5	f	89/116 (77%)	89 (100%)	0	100	100
6	g	124/147 (84%)	124 (100%)	0	100	100
7	h	104/105 (99%)	104 (100%)	0	100	100
8	i	105/107 (98%)	105 (100%)	0	100	100
9	j	86/90 (96%)	86 (100%)	0	100	100
10	k	90/99 (91%)	90 (100%)	0	100	100
11	l	103/104 (99%)	103 (100%)	0	100	100
12	m	92/96 (96%)	92 (100%)	0	100	100
13	n	79/84 (94%)	79 (100%)	0	100	100
14	o	76/77 (99%)	76 (100%)	0	100	100
15	p	65/65 (100%)	65 (100%)	0	100	100
16	q	74/78 (95%)	74 (100%)	0	100	100
17	r	48/65 (74%)	48 (100%)	0	100	100
18	s	70/79 (89%)	70 (100%)	0	100	100
19	t	65/66 (98%)	65 (100%)	0	100	100
20	u	44/61 (72%)	44 (100%)	0	100	100
21	0	47/48 (98%)	47 (100%)	0	100	100
22	1	45/49 (92%)	45 (100%)	0	100	100
23	2	38/38 (100%)	38 (100%)	0	100	100
24	3	51/51 (100%)	51 (100%)	0	100	100
25	4	34/34 (100%)	34 (100%)	0	100	100
26	5	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	C	215/218 (99%)	215 (100%)	0	100	100
28	D	164/164 (100%)	164 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/150 (99%)	148 (100%)	0	100	100
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	I	109/110 (99%)	109 (100%)	0	100	100
34	J	116/116 (100%)	116 (100%)	0	100	100
35	K	103/104 (99%)	103 (100%)	0	100	100
36	L	102/103 (99%)	102 (100%)	0	100	100
37	M	109/109 (100%)	109 (100%)	0	100	100
38	N	100/103 (97%)	100 (100%)	0	100	100
39	O	86/87 (99%)	86 (100%)	0	100	100
40	P	99/100 (99%)	99 (100%)	0	100	100
41	Q	89/90 (99%)	89 (100%)	0	100	100
42	R	84/84 (100%)	84 (100%)	0	100	100
43	S	93/93 (100%)	93 (100%)	0	100	100
44	T	80/84 (95%)	80 (100%)	0	100	100
45	U	83/85 (98%)	83 (100%)	0	100	100
46	V	78/78 (100%)	78 (100%)	0	100	100
47	W	59/63 (94%)	59 (100%)	0	100	100
48	X	67/68 (98%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	55 (100%)	0	100	100
50	Z	48/49 (98%)	48 (100%)	0	100	100
51	x	23/511 (4%)	23 (100%)	0	100	100
All	All	4871/5569 (88%)	4871 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	c	69	HIS

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Mol	Chain	Res	Type
2	c	139	GLN
3	d	120	HIS
3	d	152	GLN
4	e	121	HIS
5	f	3	HIS
5	f	55	HIS
5	f	63	ASN
6	g	86	GLN
6	g	148	ASN
7	h	76	GLN
8	i	32	GLN
9	j	56	HIS
10	k	22	HIS
12	m	14	HIS
16	q	45	HIS
16	q	51	ASN
18	s	57	HIS
21	0	5	ASN
23	2	6	GLN
24	3	23	HIS
25	4	37	GLN
26	5	83	ASN
26	5	155	ASN
26	5	234	ASN
27	C	52	HIS
27	C	57	HIS
27	C	199	HIS
27	C	259	ASN
28	D	32	ASN
28	D	49	GLN
28	D	130	GLN
28	D	164	GLN
29	E	41	GLN
29	E	165	HIS
30	F	51	ASN
31	G	21	GLN
31	G	87	GLN
31	G	110	HIS
31	G	138	GLN
32	H	2	GLN
32	H	18	GLN
32	H	135	HIS

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Mol	Chain	Res	Type
34	J	40	HIS
34	J	135	GLN
39	O	34	HIS
40	P	40	GLN
41	Q	36	GLN
41	Q	43	GLN
42	R	66	HIS
44	T	70	HIS
44	T	91	GLN
45	U	65	GLN
49	Y	27	ASN
49	Y	41	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	a	1532/1533 (99%)	301 (19%)	0
53	A	2902/2904 (99%)	597 (20%)	16 (0%)
54	B	117/120 (97%)	21 (17%)	0
55	7	8/15 (53%)	4 (50%)	0
56	8	75/76 (98%)	8 (10%)	2 (2%)
56	9	75/76 (98%)	33 (44%)	1 (1%)
All	All	4709/4724 (99%)	964 (20%)	19 (0%)

All (964) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	a	4	U
52	a	6	G
52	a	9	G
52	a	12	U
52	a	15	G
52	a	29	U
52	a	31	G
52	a	32	A
52	a	35	G
52	a	39	G
52	a	47	C
52	a	48	C
52	a	51	A
52	a	54	C

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Mol	Chain	Res	Type
52	a	63	C
52	a	66	A
52	a	69	G
52	a	70	U
52	a	73	C
52	a	74	A
52	a	77	A
52	a	78	A
52	a	79	G
52	a	80	A
52	a	83	C
52	a	84	U
52	a	85	U
52	a	86	G
52	a	89	U
52	a	90	C
52	a	93	U
52	a	96	U
52	a	97	G
52	a	116	A
52	a	117	G
52	a	121	U
52	a	130	A
52	a	131	A
52	a	143	A
52	a	144	G
52	a	149	A
52	a	156	C
52	a	164	G
52	a	184	G
52	a	195	A
52	a	197	A
52	a	204	G
52	a	205	A
52	a	206	C
52	a	209	U
52	a	210	C
52	a	212	G
52	a	226	G
52	a	238	A
52	a	247	G
52	a	251	G

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Mol	Chain	Res	Type
52	a	262	A
52	a	266	G
52	a	267	C
52	a	289	G
52	a	298	A
52	a	304	U
52	a	306	A
52	a	316	C
52	a	328	C
52	a	329	A
52	a	332	G
52	a	341	C
52	a	344	A
52	a	345	C
52	a	347	G
52	a	352	C
52	a	354	G
52	a	367	U
52	a	368	U
52	a	370	C
52	a	372	C
52	a	384	G
52	a	397	A
52	a	406	G
52	a	408	A
52	a	411	A
52	a	412	A
52	a	413	G
52	a	414	A
52	a	421	U
52	a	422	C
52	a	423	G
52	a	424	G
52	a	429	U
52	a	430	A
52	a	449	G
52	a	453	G
52	a	456	A
52	a	457	G
52	a	459	A
52	a	461	A
52	a	466	A

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Mol	Chain	Res	Type
52	a	467	U
52	a	468	A
52	a	474	G
52	a	478	A
52	a	479	U
52	a	480	U
52	a	481	G
52	a	484	G
52	a	485	U
52	a	486	U
52	a	491	G
52	a	495	A
52	a	497	G
52	a	511	C
52	a	512	U
52	a	513	C
52	a	518	C
52	a	521	G
52	a	526	C
52	a	527	G
52	a	532	A
52	a	540	G
52	a	547	A
52	a	548	G
52	a	559	A
52	a	560	A
52	a	562	U
52	a	563	A
52	a	564	C
52	a	572	A
52	a	573	A
52	a	576	C
52	a	577	G
52	a	596	A
52	a	615	G
52	a	633	G
52	a	653	U
52	a	661	G
52	a	665	A
52	a	668	G
52	a	674	G
52	a	675	A

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Mol	Chain	Res	Type
52	a	684	U
52	a	687	A
52	a	701	U
52	a	702	A
52	a	710	G
52	a	717	U
52	a	718	A
52	a	721	G
52	a	723	U
52	a	731	G
52	a	747	A
52	a	755	G
52	a	776	G
52	a	793	U
52	a	794	A
52	a	801	U
52	a	813	U
52	a	814	A
52	a	815	A
52	a	817	C
52	a	821	G
52	a	828	U
52	a	841	C
52	a	843	U
52	a	844	G
52	a	845	A
52	a	846	G
52	a	855	U
52	a	859	G
52	a	873	A
52	a	889	A
52	a	894	G
52	a	914	A
52	a	918	A
52	a	921	U
52	a	926	G
52	a	927	G
52	a	932	C
52	a	934	C
52	a	935	A
52	a	939	G
52	a	960	U

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Mol	Chain	Res	Type
52	a	966	G
52	a	969	A
52	a	975	A
52	a	976	G
52	a	977	A
52	a	983	A
52	a	992	U
52	a	993	G
52	a	994	A
52	a	1000	A
52	a	1002	G
52	a	1004	A
52	a	1006	G
52	a	1008	U
52	a	1018	G
52	a	1028	C
52	a	1029	U
52	a	1030	U
52	a	1031	C
52	a	1032	G
52	a	1033	G
52	a	1037	C
52	a	1042	A
52	a	1043	G
52	a	1045	C
52	a	1046	A
52	a	1052	U
52	a	1054	C
52	a	1065	U
52	a	1066	C
52	a	1070	U
52	a	1081	A
52	a	1085	U
52	a	1086	U
52	a	1087	G
52	a	1089	G
52	a	1094	G
52	a	1095	U
52	a	1101	A
52	a	1124	G
52	a	1130	A
52	a	1132	C

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Mol	Chain	Res	Type
52	a	1133	G
52	a	1134	G
52	a	1136	C
52	a	1137	C
52	a	1139	G
52	a	1142	G
52	a	1145	A
52	a	1159	U
52	a	1167	A
52	a	1168	U
52	a	1171	A
52	a	1181	G
52	a	1182	G
52	a	1196	A
52	a	1197	A
52	a	1200	C
52	a	1202	U
52	a	1208	C
52	a	1212	U
52	a	1213	A
52	a	1215	G
52	a	1226	C
52	a	1227	A
52	a	1230	C
52	a	1232	U
52	a	1240	U
52	a	1241	G
52	a	1252	A
52	a	1253	G
52	a	1256	A
52	a	1257	A
52	a	1258	G
52	a	1260	G
52	a	1287	A
52	a	1289	A
52	a	1299	A
52	a	1300	G
52	a	1302	C
52	a	1303	C
52	a	1305	G
52	a	1312	G
52	a	1317	C

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Mol	Chain	Res	Type
52	a	1318	A
52	a	1322	C
52	a	1323	G
52	a	1332	A
52	a	1336	C
52	a	1337	G
52	a	1346	A
52	a	1363	A
52	a	1364	U
52	a	1365	G
52	a	1378	C
52	a	1397	C
52	a	1402	C
52	a	1417	G
52	a	1418	A
52	a	1419	G
52	a	1429	A
52	a	1441	A
52	a	1442	G
52	a	1446	A
52	a	1447	A
52	a	1451	U
52	a	1454	G
52	a	1487	G
52	a	1491	G
52	a	1492	A
52	a	1493	A
52	a	1494	G
52	a	1497	G
52	a	1503	A
52	a	1505	G
52	a	1506	U
52	a	1517	G
52	a	1529	G
52	a	1530	G
53	A	10	A
53	A	14	A
53	A	34	U
53	A	35	G
53	A	46	G
53	A	50	U
53	A	51	G

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Mol	Chain	Res	Type
53	A	61	C
53	A	62	U
53	A	63	A
53	A	71	A
53	A	74	A
53	A	75	G
53	A	80	G
53	A	84	A
53	A	88	G
53	A	92	U
53	A	96	C
53	A	102	U
53	A	118	A
53	A	120	U
53	A	121	G
53	A	138	U
53	A	139	U
53	A	140	C
53	A	141	G
53	A	142	A
53	A	149	A
53	A	160	A
53	A	162	U
53	A	163	C
53	A	164	C
53	A	173	A
53	A	174	U
53	A	181	A
53	A	186	G
53	A	196	A
53	A	199	A
53	A	200	U
53	A	204	A
53	A	205	G
53	A	210	C
53	A	216	A
53	A	222	A
53	A	226	A
53	A	228	C
53	A	229	C
53	A	230	G
53	A	233	A

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Mol	Chain	Res	Type
53	A	241	A
53	A	248	G
53	A	255	A
53	A	264	C
53	A	266	G
53	A	271	G
53	A	272	A
53	A	273	G
53	A	276	U
53	A	277	G
53	A	278	A
53	A	285	G
53	A	289	G
53	A	294	A
53	A	299	A
53	A	300	A
53	A	302	C
53	A	311	A
53	A	329	G
53	A	330	A
53	A	335	C
53	A	338	G
53	A	353	C
53	A	361	G
53	A	367	G
53	A	371	A
53	A	372	G
53	A	380	G
53	A	386	G
53	A	396	G
53	A	399	U
53	A	404	A
53	A	405	U
53	A	411	G
53	A	412	A
53	A	413	C
53	A	420	C
53	A	424	G
53	A	429	A
53	A	435	C
53	A	451	U
53	A	456	C

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Mol	Chain	Res	Type
53	A	457	A
53	A	458	G
53	A	467	G
53	A	475	C
53	A	481	G
53	A	490	C
53	A	491	G
53	A	504	A
53	A	505	A
53	A	509	C
53	A	510	C
53	A	528	A
53	A	529	A
53	A	531	C
53	A	532	A
53	A	533	G
53	A	543	G
53	A	544	C
53	A	546	U
53	A	548	G
53	A	549	G
53	A	550	C
53	A	551	G
53	A	563	A
53	A	571	U
53	A	572	A
53	A	573	U
53	A	575	A
53	A	586	A
53	A	588	U
53	A	603	A
53	A	604	G
53	A	613	A
53	A	615	U
53	A	622	G
53	A	627	A
53	A	628	G
53	A	637	A
53	A	638	G
53	A	645	C
53	A	647	G
53	A	653	U

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Mol	Chain	Res	Type
53	A	654	A
53	A	655	A
53	A	656	G
53	A	668	A
53	A	677	A
53	A	686	U
53	A	690	G
53	A	701	G
53	A	715	A
53	A	724	U
53	A	726	G
53	A	730	A
53	A	744	U
53	A	747	U
53	A	748	G
53	A	770	G
53	A	775	G
53	A	776	G
53	A	782	A
53	A	784	G
53	A	785	G
53	A	788	A
53	A	789	A
53	A	792	A
53	A	800	A
53	A	805	G
53	A	812	C
53	A	819	A
53	A	827	U
53	A	830	G
53	A	845	A
53	A	846	U
53	A	847	U
53	A	859	G
53	A	871	U
53	A	872	U
53	A	879	G
53	A	880	G
53	A	881	G
53	A	882	G
53	A	884	U
53	A	887	U

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Mol	Chain	Res	Type
53	A	888	C
53	A	892	A
53	A	896	A
53	A	897	C
53	A	898	C
53	A	902	C
53	A	907	G
53	A	910	A
53	A	915	C
53	A	916	G
53	A	931	U
53	A	932	U
53	A	941	A
53	A	945	A
53	A	946	C
53	A	957	C
53	A	958	U
53	A	959	A
53	A	961	C
53	A	974	G
53	A	975	A
53	A	983	A
53	A	984	A
53	A	985	C
53	A	995	C
53	A	997	G
53	A	1002	G
53	A	1003	G
53	A	1005	C
53	A	1009	A
53	A	1012	U
53	A	1013	C
53	A	1021	A
53	A	1022	G
53	A	1023	U
53	A	1026	G
53	A	1033	U
53	A	1047	G
53	A	1051	G
53	A	1057	A
53	A	1061	U
53	A	1062	G

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Mol	Chain	Res	Type
53	A	1069	A
53	A	1070	A
53	A	1071	G
53	A	1072	C
53	A	1073	A
53	A	1074	G
53	A	1075	C
53	A	1077	A
53	A	1080	A
53	A	1088	A
53	A	1090	A
53	A	1095	A
53	A	1097	U
53	A	1101	U
53	A	1110	G
53	A	1111	A
53	A	1112	G
53	A	1132	U
53	A	1133	A
53	A	1135	C
53	A	1139	G
53	A	1142	A
53	A	1143	A
53	A	1155	A
53	A	1157	G
53	A	1168	G
53	A	1169	A
53	A	1171	G
53	A	1174	U
53	A	1175	A
53	A	1176	U
53	A	1180	U
53	A	1186	G
53	A	1200	C
53	A	1212	G
53	A	1225	G
53	A	1236	G
53	A	1238	G
53	A	1240	U
53	A	1241	A
53	A	1247	A
53	A	1248	G

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Mol	Chain	Res	Type
53	A	1250	G
53	A	1253	A
53	A	1256	G
53	A	1262	A
53	A	1266	G
53	A	1271	G
53	A	1272	A
53	A	1273	U
53	A	1275	A
53	A	1294	U
53	A	1300	G
53	A	1301	A
53	A	1302	A
53	A	1306	C
53	A	1321	A
53	A	1329	U
53	A	1345	C
53	A	1352	U
53	A	1359	A
53	A	1364	G
53	A	1365	A
53	A	1368	G
53	A	1378	A
53	A	1383	A
53	A	1392	A
53	A	1407	G
53	A	1415	U
53	A	1416	G
53	A	1419	A
53	A	1420	A
53	A	1424	G
53	A	1428	C
53	A	1452	G
53	A	1453	A
53	A	1458	U
53	A	1460	U
53	A	1467	U
53	A	1468	U
53	A	1482	G
53	A	1488	C
53	A	1493	C
53	A	1494	A

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Mol	Chain	Res	Type
53	A	1497	U
53	A	1504	A
53	A	1508	A
53	A	1509	A
53	A	1510	G
53	A	1515	A
53	A	1522	A
53	A	1523	U
53	A	1524	G
53	A	1529	G
53	A	1532	A
53	A	1535	A
53	A	1536	C
53	A	1537	G
53	A	1538	G
53	A	1542	U
53	A	1543	G
53	A	1550	C
53	A	1560	G
53	A	1563	U
53	A	1566	A
53	A	1569	A
53	A	1578	U
53	A	1583	A
53	A	1584	U
53	A	1585	C
53	A	1587	G
53	A	1591	A
53	A	1593	A
53	A	1595	C
53	A	1608	A
53	A	1610	A
53	A	1639	C
53	A	1645	G
53	A	1646	C
53	A	1647	U
53	A	1648	U
53	A	1649	G
53	A	1652	A
53	A	1654	A
53	A	1655	A
53	A	1656	C

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Mol	Chain	Res	Type
53	A	1664	A
53	A	1674	G
53	A	1675	C
53	A	1679	A
53	A	1694	C
53	A	1698	A
53	A	1699	G
53	A	1703	G
53	A	1715	G
53	A	1729	U
53	A	1730	C
53	A	1732	C
53	A	1738	G
53	A	1764	C
53	A	1773	A
53	A	1781	U
53	A	1785	A
53	A	1791	A
53	A	1800	C
53	A	1801	A
53	A	1802	A
53	A	1807	G
53	A	1808	A
53	A	1811	G
53	A	1816	C
53	A	1829	A
53	A	1848	A
53	A	1852	U
53	A	1866	A
53	A	1869	G
53	A	1870	C
53	A	1872	A
53	A	1875	G
53	A	1881	C
53	A	1882	U
53	A	1896	G
53	A	1903	G
53	A	1906	G
53	A	1913	A
53	A	1914	C
53	A	1927	A
53	A	1929	G

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Mol	Chain	Res	Type
53	A	1936	A
53	A	1938	A
53	A	1955	U
53	A	1960	A
53	A	1966	A
53	A	1967	C
53	A	1970	A
53	A	1971	U
53	A	1972	G
53	A	1991	U
53	A	1993	U
53	A	1997	C
53	A	2011	U
53	A	2021	C
53	A	2022	U
53	A	2023	C
53	A	2030	A
53	A	2031	A
53	A	2033	A
53	A	2034	U
53	A	2043	C
53	A	2050	C
53	A	2052	A
53	A	2055	C
53	A	2056	G
53	A	2059	A
53	A	2060	A
53	A	2061	G
53	A	2062	A
53	A	2069	G
53	A	2072	C
53	A	2075	U
53	A	2085	U
53	A	2092	U
53	A	2093	G
53	A	2104	C
53	A	2107	G
53	A	2110	G
53	A	2111	U
53	A	2112	G
53	A	2113	U
53	A	2115	G

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Mol	Chain	Res	Type
53	A	2119	A
53	A	2127	G
53	A	2128	G
53	A	2129	C
53	A	2131	U
53	A	2132	U
53	A	2133	G
53	A	2134	A
53	A	2135	A
53	A	2136	G
53	A	2139	U
53	A	2143	C
53	A	2144	G
53	A	2145	C
53	A	2146	C
53	A	2147	A
53	A	2148	G
53	A	2150	C
53	A	2152	G
53	A	2153	C
53	A	2155	U
53	A	2158	A
53	A	2159	G
53	A	2161	C
53	A	2162	G
53	A	2164	C
53	A	2165	C
53	A	2166	U
53	A	2168	G
53	A	2171	A
53	A	2173	A
53	A	2174	C
53	A	2176	A
53	A	2178	C
53	A	2182	U
53	A	2183	A
53	A	2185	U
53	A	2186	G
53	A	2192	U
53	A	2198	A
53	A	2199	A
53	A	2204	G

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Mol	Chain	Res	Type
53	A	2211	A
53	A	2225	A
53	A	2226	C
53	A	2238	G
53	A	2239	G
53	A	2250	G
53	A	2268	A
53	A	2279	G
53	A	2283	C
53	A	2286	G
53	A	2287	A
53	A	2305	U
53	A	2308	G
53	A	2309	A
53	A	2322	A
53	A	2325	G
53	A	2327	A
53	A	2333	A
53	A	2334	U
53	A	2335	A
53	A	2344	U
53	A	2347	C
53	A	2353	G
53	A	2354	C
53	A	2357	G
53	A	2358	A
53	A	2359	C
53	A	2361	G
53	A	2383	G
53	A	2384	U
53	A	2385	C
53	A	2389	G
53	A	2396	G
53	A	2400	G
53	A	2402	U
53	A	2403	C
53	A	2406	A
53	A	2413	G
53	A	2419	U
53	A	2423	U
53	A	2424	C
53	A	2425	A

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Mol	Chain	Res	Type
53	A	2427	C
53	A	2429	G
53	A	2430	A
53	A	2441	U
53	A	2448	A
53	A	2449	U
53	A	2468	A
53	A	2475	C
53	A	2476	A
53	A	2480	C
53	A	2491	U
53	A	2498	C
53	A	2502	G
53	A	2503	A
53	A	2504	U
53	A	2505	G
53	A	2506	U
53	A	2507	C
53	A	2513	A
53	A	2518	A
53	A	2530	A
53	A	2535	G
53	A	2548	U
53	A	2549	G
53	A	2554	U
53	A	2562	U
53	A	2566	A
53	A	2567	G
53	A	2572	A
53	A	2573	C
53	A	2578	G
53	A	2585	U
53	A	2586	U
53	A	2602	A
53	A	2608	G
53	A	2609	U
53	A	2613	U
53	A	2615	U
53	A	2621	G
53	A	2629	U
53	A	2630	G
53	A	2636	C

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Mol	Chain	Res	Type
53	A	2650	U
53	A	2682	A
53	A	2689	U
53	A	2690	U
53	A	2714	G
53	A	2716	C
53	A	2729	G
53	A	2733	A
53	A	2739	U
53	A	2744	G
53	A	2748	A
53	A	2758	A
53	A	2759	G
53	A	2775	G
53	A	2778	A
53	A	2781	A
53	A	2791	G
53	A	2792	A
53	A	2797	U
53	A	2798	U
53	A	2801	G
53	A	2803	G
53	A	2809	A
53	A	2820	A
53	A	2825	G
53	A	2833	U
53	A	2834	G
53	A	2835	A
53	A	2849	U
53	A	2861	U
53	A	2867	G
53	A	2869	G
53	A	2870	C
53	A	2872	A
53	A	2873	A
53	A	2879	A
53	A	2883	A
53	A	2884	U
53	A	2885	G
53	A	2886	A
53	A	2891	U
53	A	2899	A

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Mol	Chain	Res	Type
53	A	2901	C
53	A	2903	U
54	B	9	G
54	B	15	A
54	B	35	C
54	B	37	C
54	B	42	C
54	B	44	G
54	B	54	G
54	B	56	G
54	B	57	A
54	B	66	A
54	B	67	G
54	B	82	U
54	B	87	U
54	B	88	C
54	B	89	U
54	B	90	C
54	B	96	G
54	B	99	A
54	B	109	A
54	B	114	C
54	B	119	A
55	7	14	U
55	7	15	G
55	7	16	U
55	7	19	A
56	8	17	C
56	8	19	G
56	8	20	U
56	8	21	A
56	8	37	A
56	8	44	G
56	8	45	U
56	8	46	G
56	9	2	C
56	9	8	U
56	9	13	C
56	9	16	U
56	9	18	G
56	9	19	G
56	9	20	U

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Mol	Chain	Res	Type
56	9	21	A
56	9	22	G
56	9	25	C
56	9	26	A
56	9	27	G
56	9	32	U
56	9	33	U
56	9	34	G
56	9	35	A
56	9	36	A
56	9	37	A
56	9	39	U
56	9	41	C
56	9	43	C
56	9	44	G
56	9	45	U
56	9	46	G
56	9	48	C
56	9	50	U
56	9	58	A
56	9	59	U
56	9	61	C
56	9	72	C
56	9	74	C
56	9	75	C
56	9	76	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A	119	A
53	A	271	G
53	A	344	A
53	A	403	U
53	A	404	A
53	A	527	C
53	A	784	G
53	A	880	G
53	A	1020	A
53	A	1025	G
53	A	1331	G
53	A	1847	A

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Mol	Chain	Res	Type
53	A	1935	G
53	A	2326	C
53	A	2423	U
53	A	2474	U
56	8	20	U
56	8	45	U
56	9	71	G

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)

There are no chain breaks in this entry.

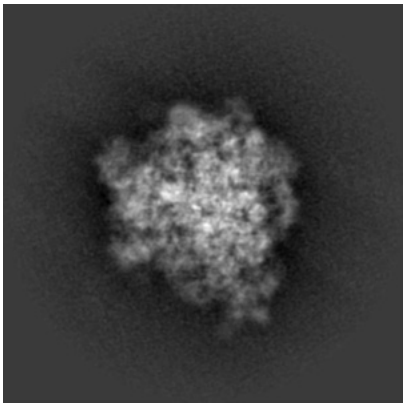
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6549. These allow visual inspection of the internal detail of the map and identification of artifacts.

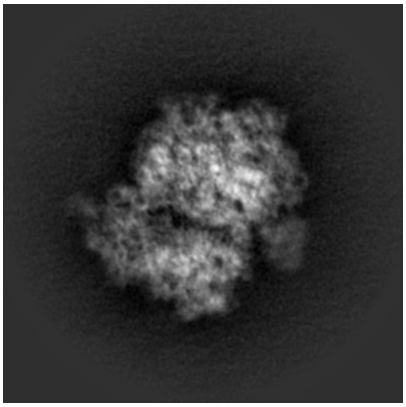
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

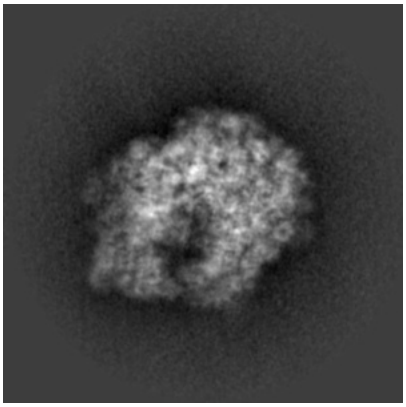
6.1.1 Primary map



X



Y

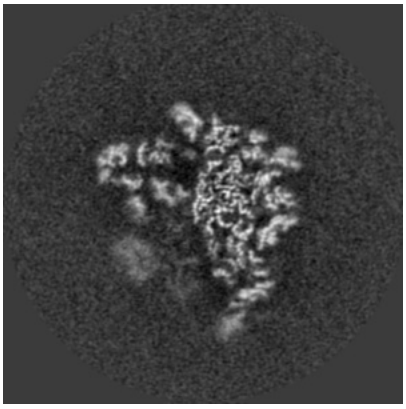


Z

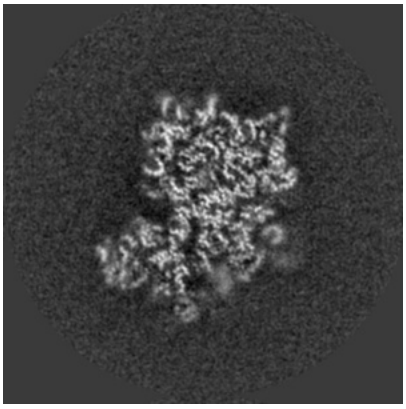
The images above show the map projected in three orthogonal directions.

6.2 Central slices

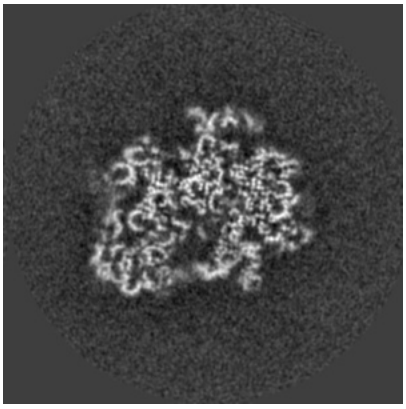
6.2.1 Primary map



X Index: 160



Y Index: 160

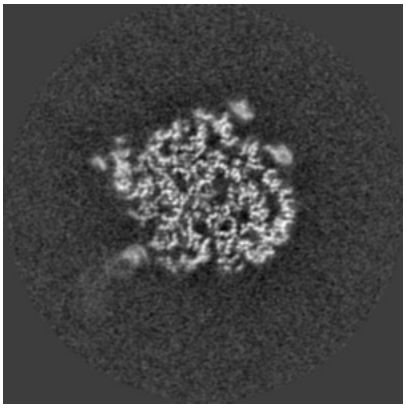


Z Index: 160

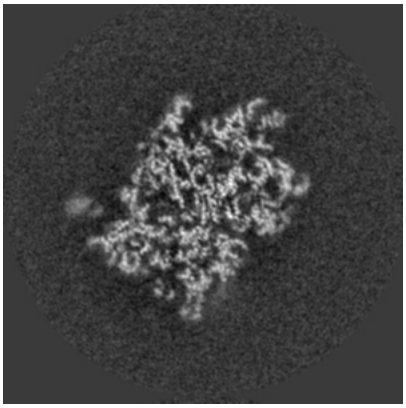
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

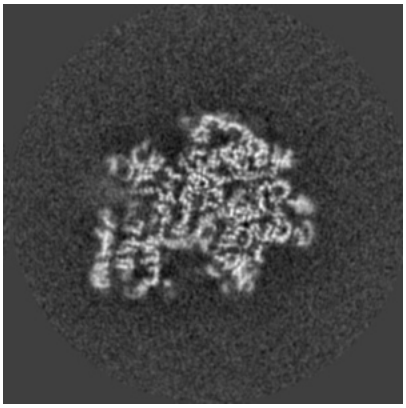
6.3.1 Primary map



X Index: 185



Y Index: 178



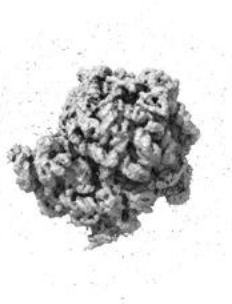
Z Index: 167

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 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

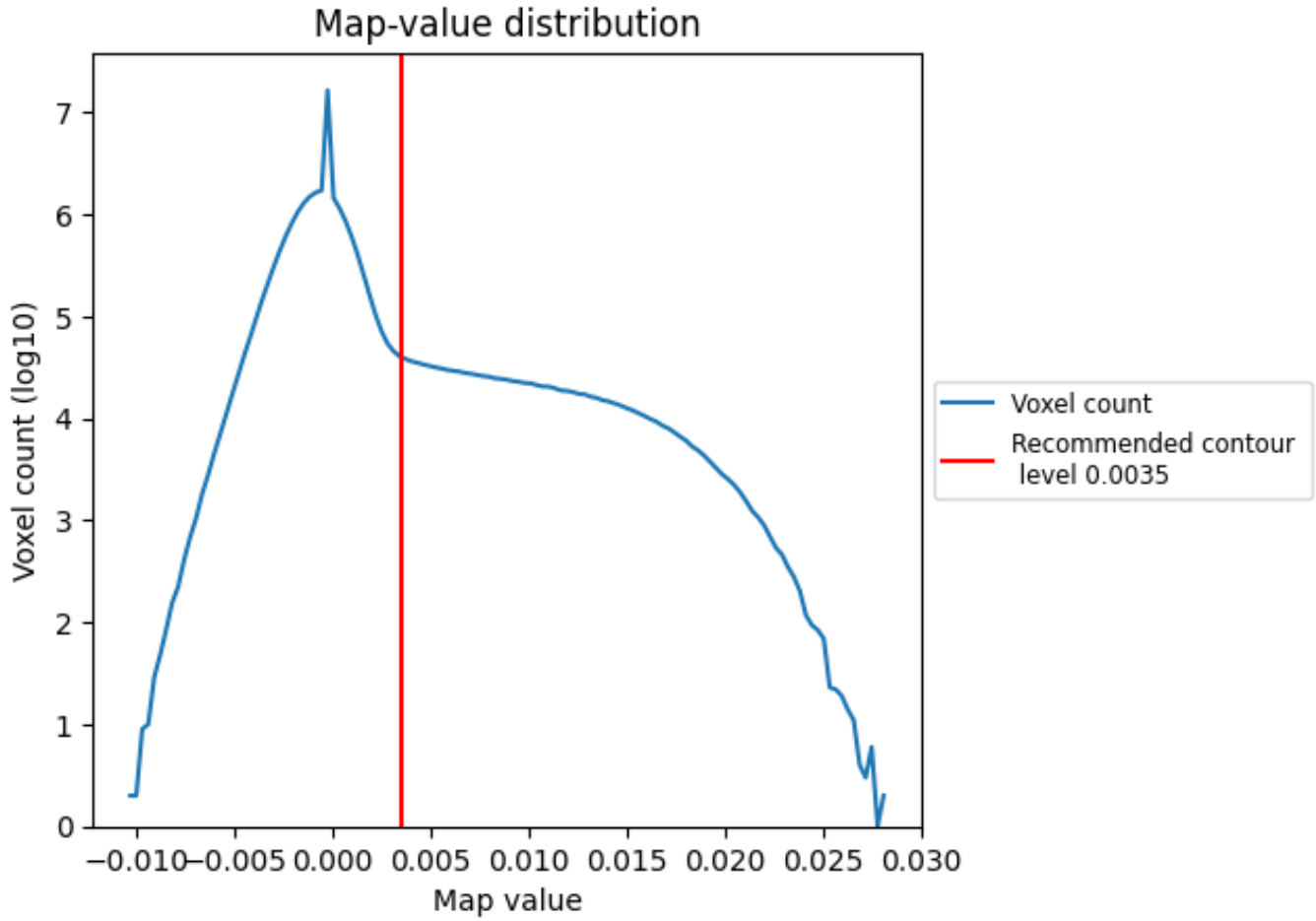
6.5 Mask visualisation (i)

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

7 Map analysis

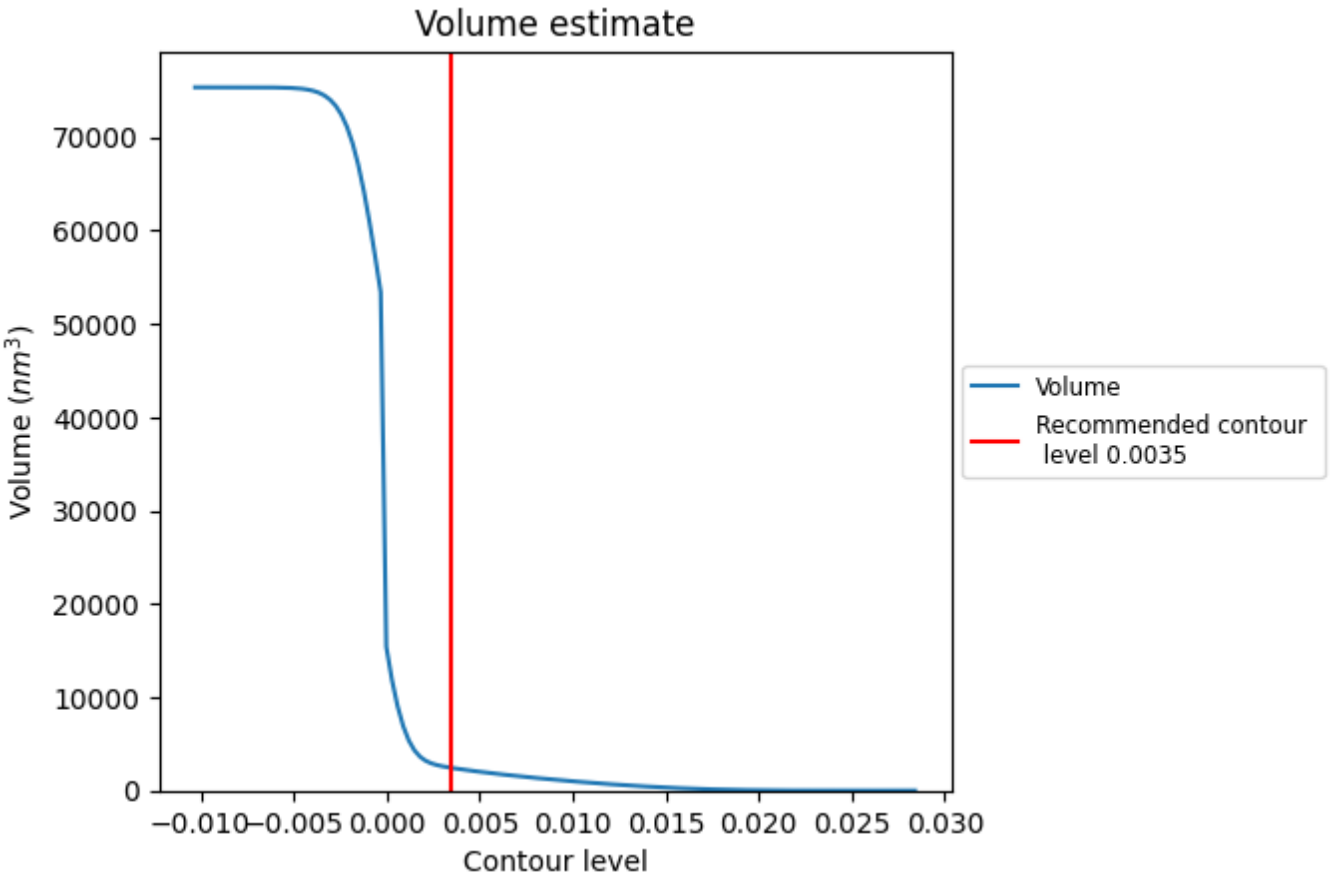
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

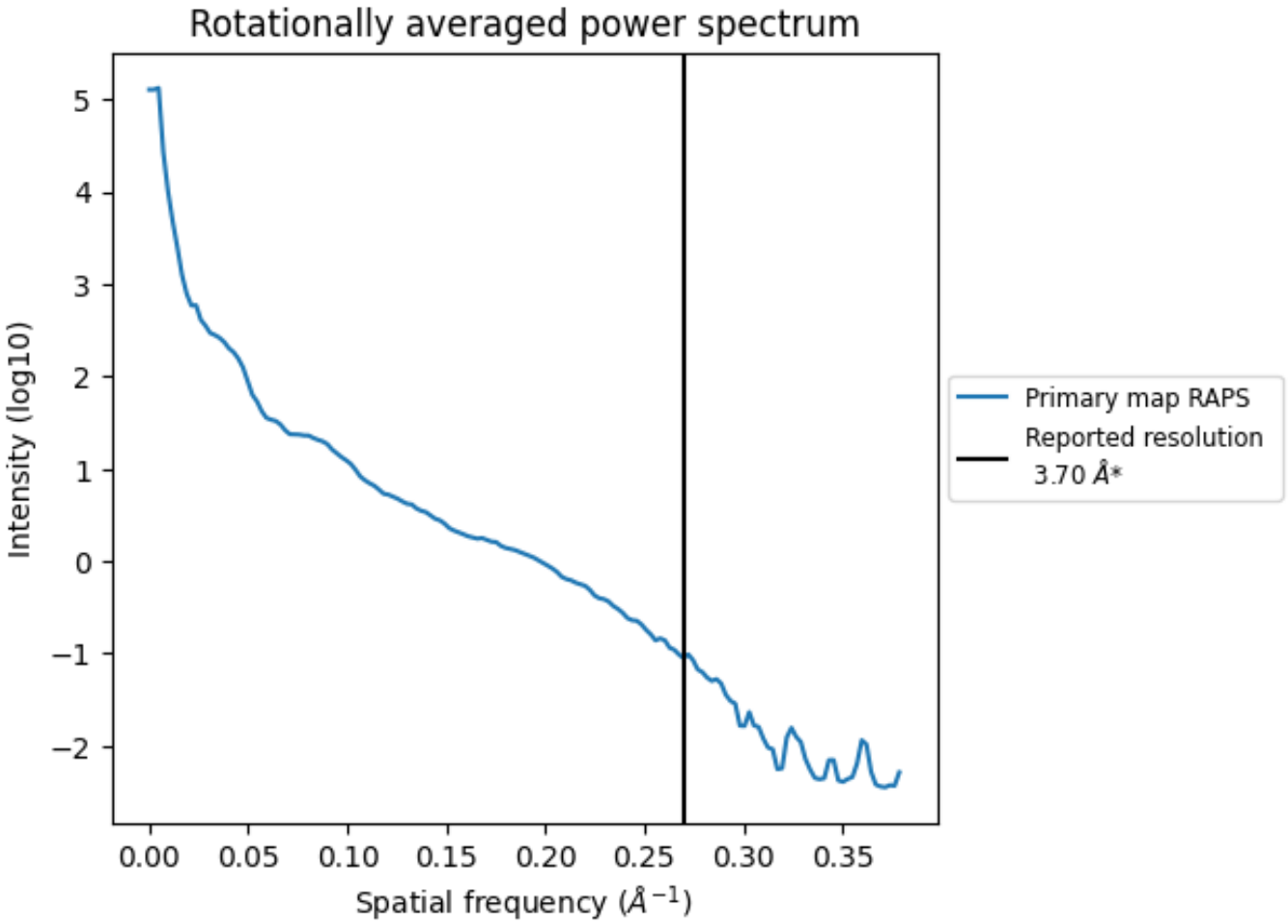
7.2 Volume estimate



The volume at the recommended contour level is 2427 nm^3; this corresponds to an approximate mass of 2193 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)

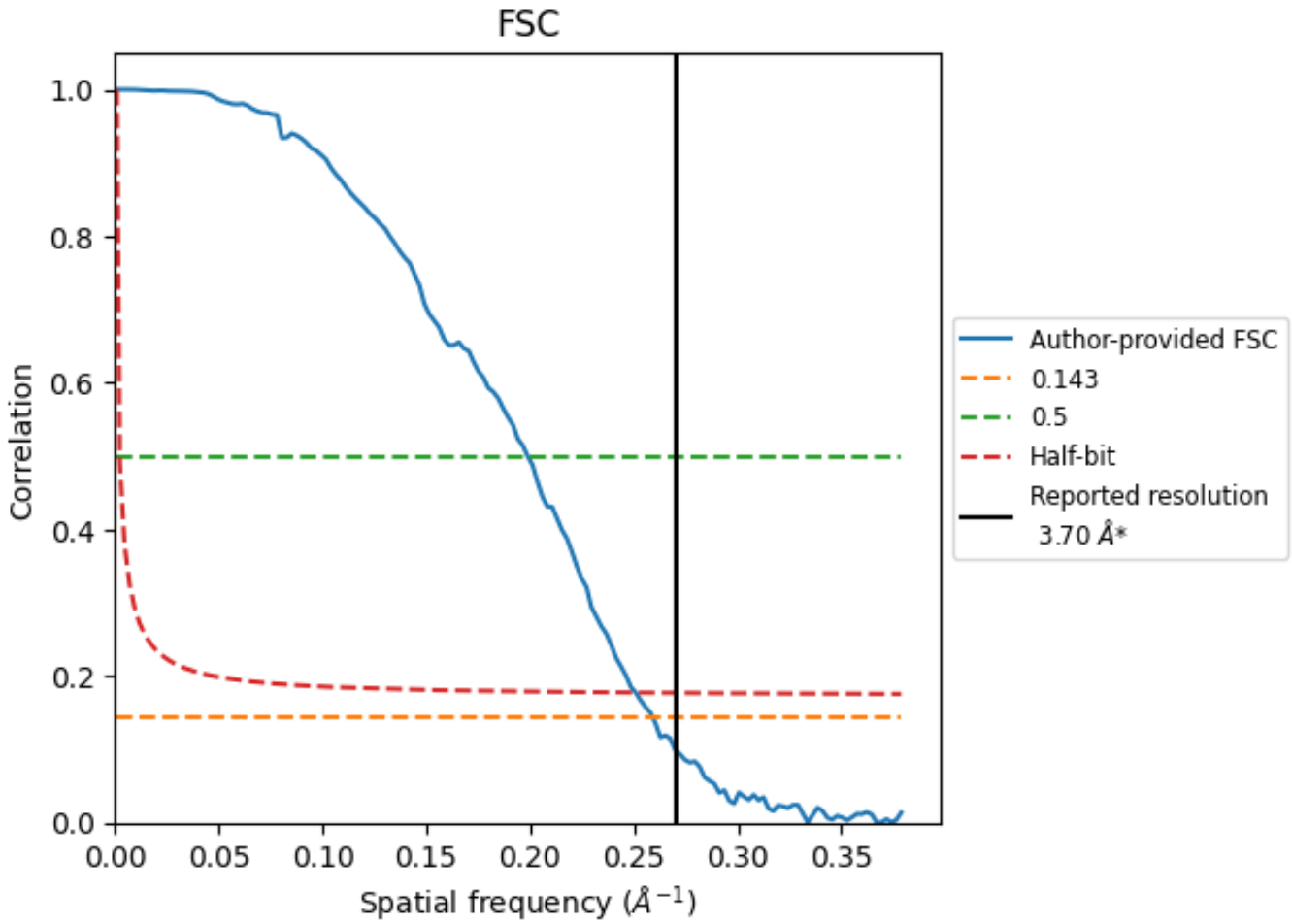


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

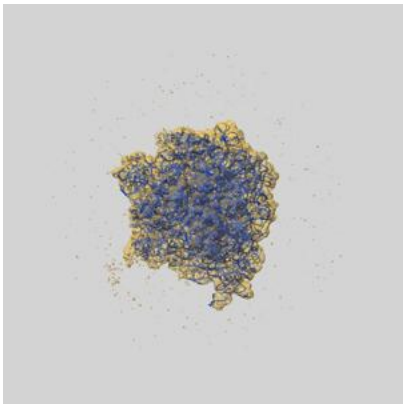
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.86	5.03	3.98
Unmasked-calculated*	-	-	-

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

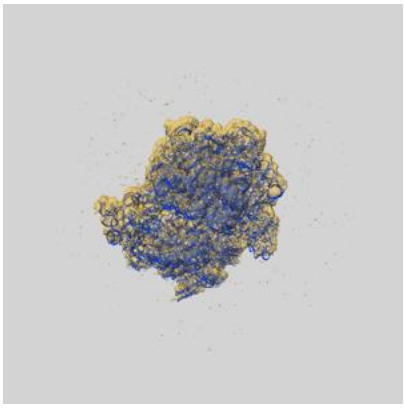
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6549 and PDB model 3JCD. Per-residue inclusion information can be found in section 3 on page 14.

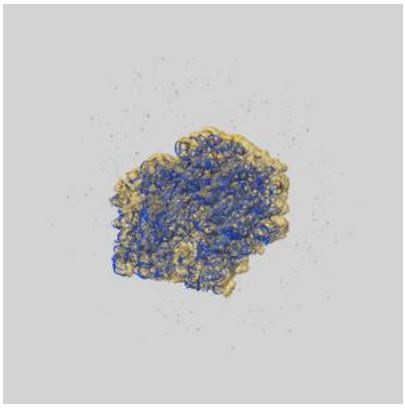
9.1 Map-model overlay



X



Y



Z

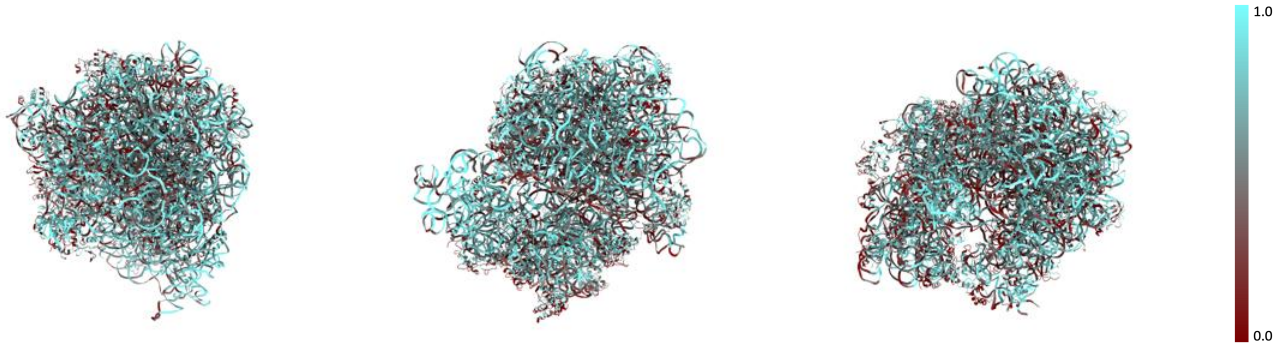
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

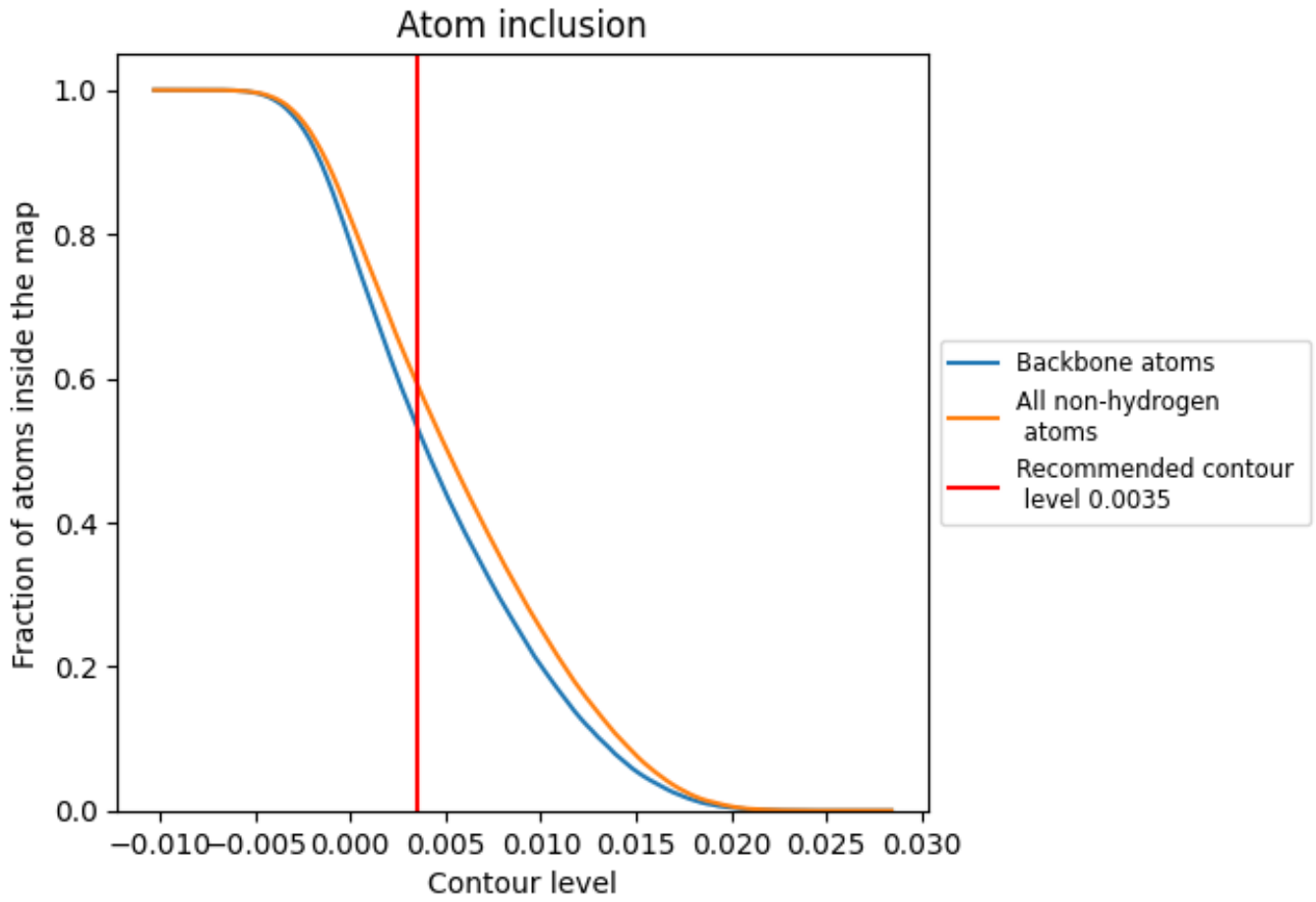
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0035).

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5922	-0.0090
0	0.5491	-0.0360
1	0.3142	-0.0230
2	0.5099	-0.0410
3	0.6660	-0.0270
4	0.4795	-0.0150
5	0.6300	0.0140
7	0.4136	-0.0520
8	0.5514	-0.0050
9	0.5779	0.0000
A	0.6102	-0.0110
B	0.5994	-0.0120
C	0.4642	0.0000
D	0.5442	-0.0090
E	0.5632	0.0040
F	0.5040	-0.0110
G	0.5143	-0.0030
H	0.2993	0.0010
I	0.3982	0.0020
J	0.5482	-0.0380
K	0.4381	0.0030
L	0.6289	0.0130
M	0.3791	-0.0370
N	0.6085	-0.0160
O	0.6732	0.0110
P	0.4955	-0.0160
Q	0.6068	-0.0210
R	0.5910	-0.0250
S	0.5837	-0.0010
T	0.5720	-0.0090
U	0.6310	0.0030
V	0.4946	0.0040
W	0.6017	-0.0170
X	0.6040	-0.0110
Y	0.5493	-0.0290

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Chain	Atom inclusion	Q-score
Z	0.4943	-0.0240
a	0.6578	-0.0050
b	0.4555	-0.0090
c	0.4417	-0.0260
d	0.4667	-0.0240
e	0.4183	-0.0140
f	0.6017	0.0060
g	0.4869	-0.0360
h	0.5177	0.0140
i	0.5536	-0.0090
j	0.4796	0.0130
k	0.4818	-0.0170
l	0.6493	-0.0000
m	0.4536	-0.0300
n	0.4266	-0.0300
o	0.6377	-0.0380
p	0.6252	0.0420
q	0.5807	-0.0220
r	0.5482	-0.0020
s	0.6876	-0.0120
t	0.6262	-0.0280
u	0.4803	0.0160
x	0.0909	-0.0350