wwPDB EM Validation Summary Report

Nov 11, 2026 – 10:39 AM JST

PDB ID	:	24NM / pdb_000024nm
EMDB ID	:	EMD-69697
Title	:	P/E-tRNA bound M. smegmatis 70S ribosome in complex with RRF (RRI I)
Authors	:	Sengupta, J.; Dhur, A.; Baid, P.; Srinivasan, K.
Deposited on	:	2026-03-12
Resolution	:	4.50 Å(reported)
Based on initial model	:	5O61

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

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

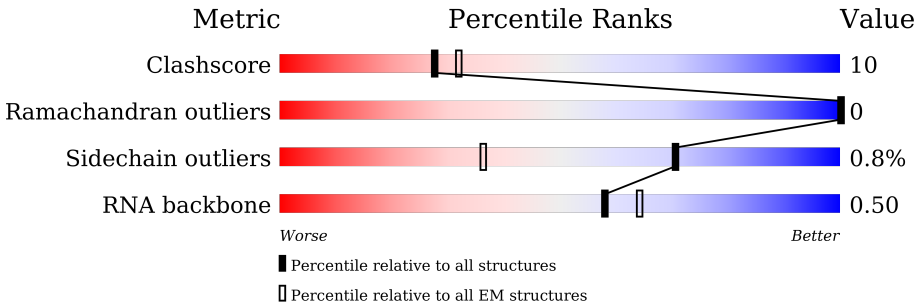
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

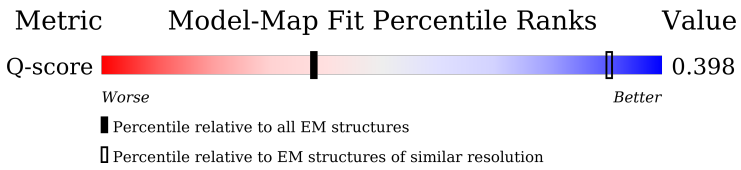
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	2	77	6% 44% 44% 12%
2	3	24	8% 71% 25% .
3	4	4	25% 25% 75%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	5	185	39% 72% 28%
5	6	235	87% 89% 11%
6	A	1528	44% 46% 9%
7	B	118	54% 38% 8%
8	C	275	7% 48% 27% 24%
9	D	201	6% 54% 45%
10	E	214	5% 57% 25% 16%
11	F	96	63% 38%
12	G	156	17% 62% 37%
13	H	132	64% 35%
14	I	150	6% 40% 44% 16%
15	J	101	19% 55% 43%
16	K	138	62% 21% 17%
17	L	124	63% 35%
18	M	124	9% 48% 45% 6%
19	N	61	56% 43%
20	O	89	53% 46%
21	P	156	44% 29% 28%
22	Q	98	64% 32%
23	R	84	56% 21% 23%
24	S	93	12% 57% 31% 12%
25	T	86	62% 37%
26	U	100	78% 19%
27	V	277	81% 54% 28% 18%
28	W	215	74% 15% 11%

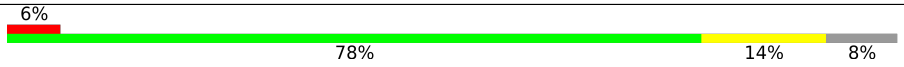
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	X	88	68% 20% 10%
30	Y	64	83% 16%
31	Z	77	71% 12% 17%
32	a	61	79% 18%
33	b	57	72% 21% 5%
34	c	55	67% 22% 11%
35	d	47	91% 6%
36	e	64	80% 19%
37	f	37	84% 16%
38	g	75	47% 17% 36%
39	i	278	82% 17%
40	j	217	83% 15%
41	k	215	83% 13%
42	l	187	6% 61% 36%
43	m	179	7% 80% 18%
44	n	151	36% 81% 19%
45	o	142	73% 61% 30% 6%
46	p	175	65% 54% 18% 28%
47	q	147	88% 11%
48	r	122	85% 15%
49	s	147	83% 16%
50	t	138	82% 17%
51	u	199	47% 13% 41%
52	v	127	73% 24%
53	w	113	85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	x	129	
55	y	103	
56	z	153	
57	1	105	
58	h	3120	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 152926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	77	1644	732	297	538	77	0	0

- Molecule 2 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	3	23	189	111	50	28	0	0

- Molecule 3 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	4	84	38	14	28	4	0	0

- Molecule 4 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	185	1459	894	265	295	5	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	235	1759	1098	317	340	4	0	0

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	1511	32439	14448	5930	10550	1511	0	0

- Molecule 7 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	180	Total	C	N	O	S	0	0
			1296	812	245	235	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	155	Total	C	N	O	S	0	0
			1232	768	241	221	2		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	I	126	Total 994	C 630	N 194	O 170	0	0

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	99	Total 788	C 495	N 146	O 144	S 3	0	0

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	115	Total 855	C 528	N 170	O 156	S 1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total 958	C 594	N 197	O 165	S 2	0	0

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	116	Total 935	C 572	N 191	O 169	S 3	0	0

- Molecule 19 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	60	Total 477	C 302	N 97	O 73	S 5	0	0

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	O	88	Total 720	C 449	N 147	O 124	0	0

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	P	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 23 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 27 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 28 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	192	Total 1428	C 881	N 255	O 292	0	0

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	X	79	Total 586	C 361	N 123	O 102	0	0

- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	63	Total 470	C 283	N 103	O 80	S 4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	64	Total 531	C 324	N 103	O 103	S 1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	a	59	Total 474	C 292	N 95	O 87	0	0

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	54	Total 423	C 260	N 93	O 69	S 1	0	0

- Molecule 34 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	49	Total 405	C 248	N 82	O 71	S 4	0	0

- Molecule 35 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 36 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	e	63	Total	C	N	O	0	0
			502	302	115	85		

- Molecule 37 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 38 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 39 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 40 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 41 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 42 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 43 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 44 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 45 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 46 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 47 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 48 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 49 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	145	Total 1078	C 676	N 205	O 194	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	136	Total 1092	C 690	N 213	O 187	S 2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	118	Total 928	C 583	N 180	O 163	S 2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	v	126	Total 956	C 586	N 199	O 171	0	0

- Molecule 53 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	113	Total 907	C 570	N 171	O 165	S 1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	x	124	Total 988	C 613	N 203	O 172	0	0

- Molecule 55 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	y	100	Total 754	C 478	N 137	O 139	0	0

- Molecule 56 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	z	114	Total 873	C 543	N 171	O 159	0	0

- Molecule 57 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	1	97	Total 732	C 456	N 137	O 137	S 2	0	0

- Molecule 58 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	h	3084	Total 66232	C 29522	N 12183	O 21443	P 3084	0	0

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
59	F	1	Total 1	Mg 1	0
59	R	1	Total 1	Mg 1	0
59	i	2	Total 2	Mg 2	0
59	j	1	Total 1	Mg 1	0
59	l	1	Total 1	Mg 1	0
59	t	1	Total 1	Mg 1	0
59	z	1	Total 1	Mg 1	0
59	h	4	Total 4	Mg 4	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
60	N	1	Total 1	Zn 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
60	R	1	Total Zn 1 1	0
60	Y	1	Total Zn 1 1	0
60	c	1	Total Zn 1 1	0
60	f	1	Total Zn 1 1	0
60	g	1	Total Zn 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: P/E-tRNA

Chain 2:

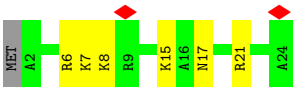




• Molecule 2: 50S ribosomal protein bL37

Chain 3:





• Molecule 3: mRNA fragment

Chain 4:

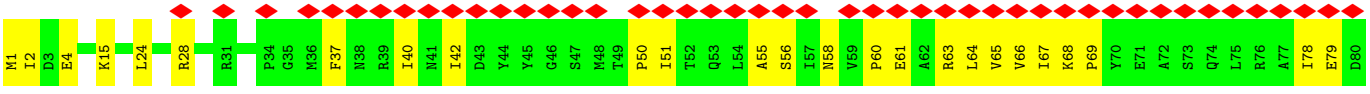


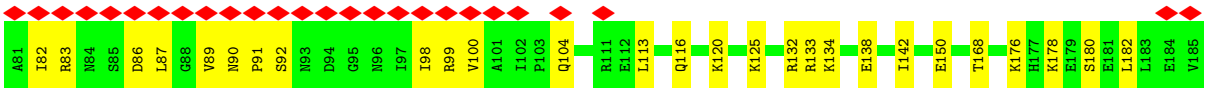


• Molecule 4: Ribosome-recycling factor

Chain 5:



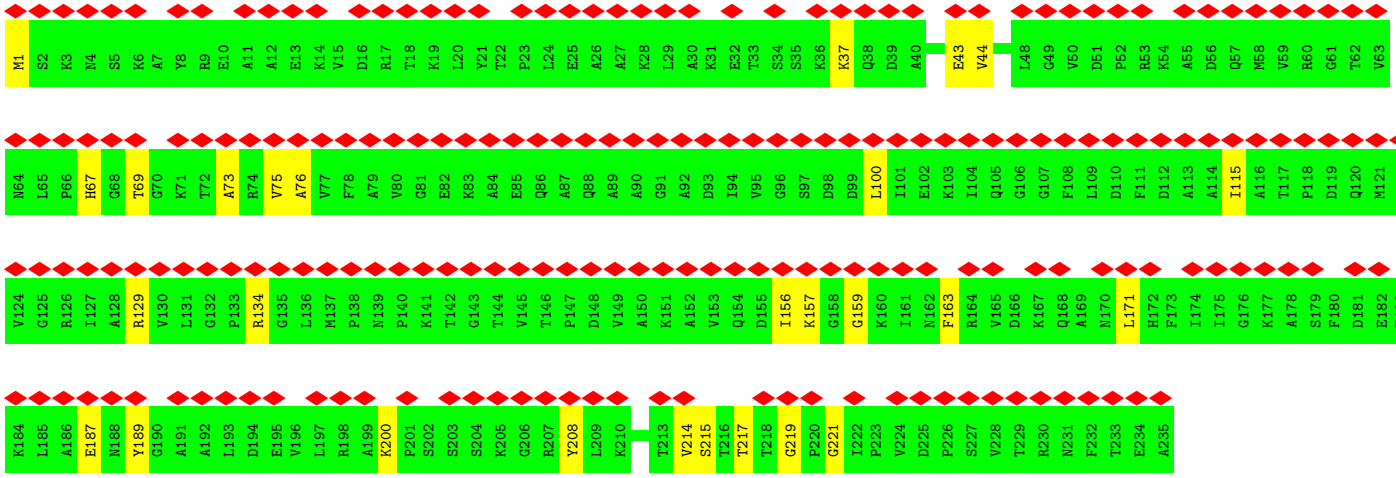




• Molecule 5: Large ribosomal subunit protein uL1

Chain 6:

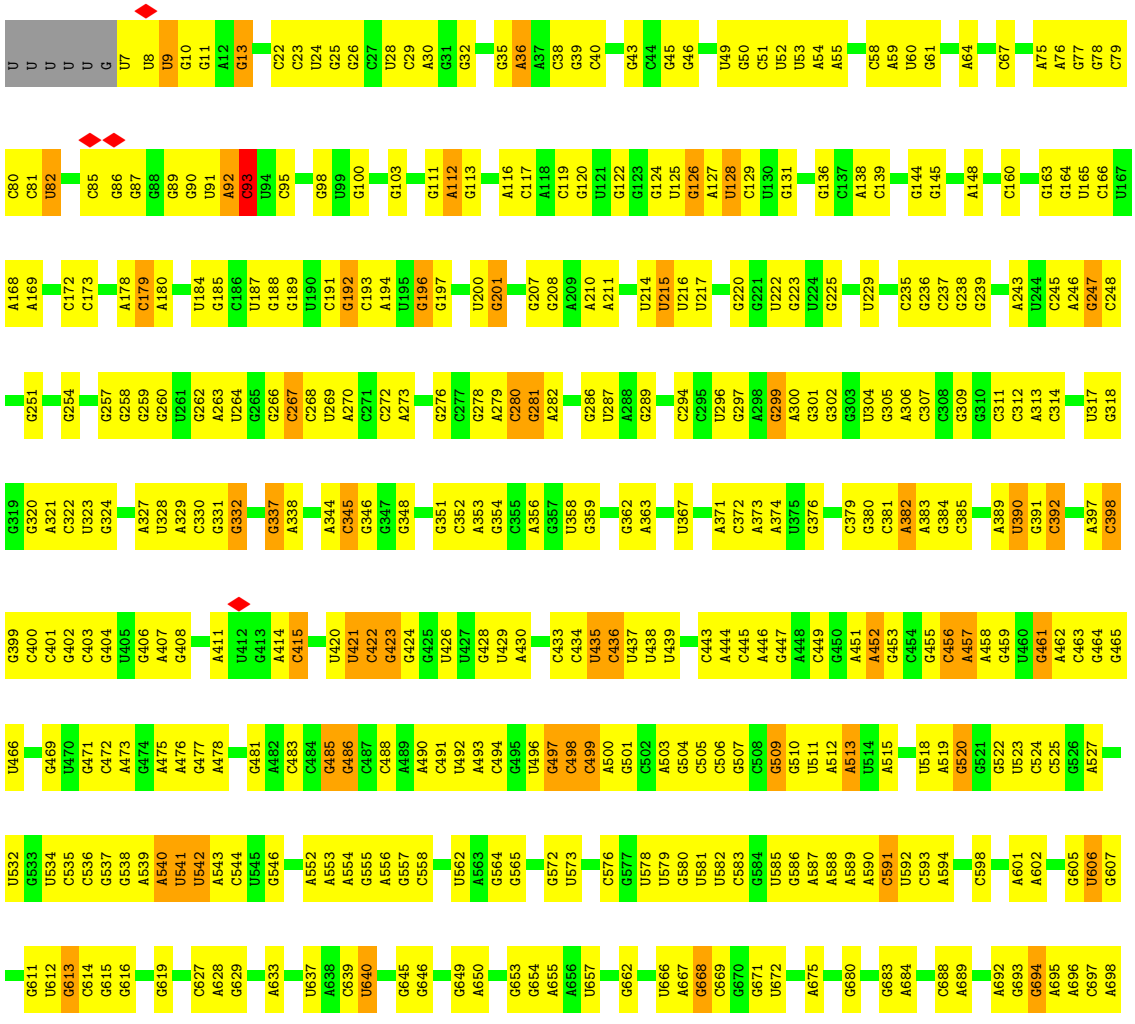


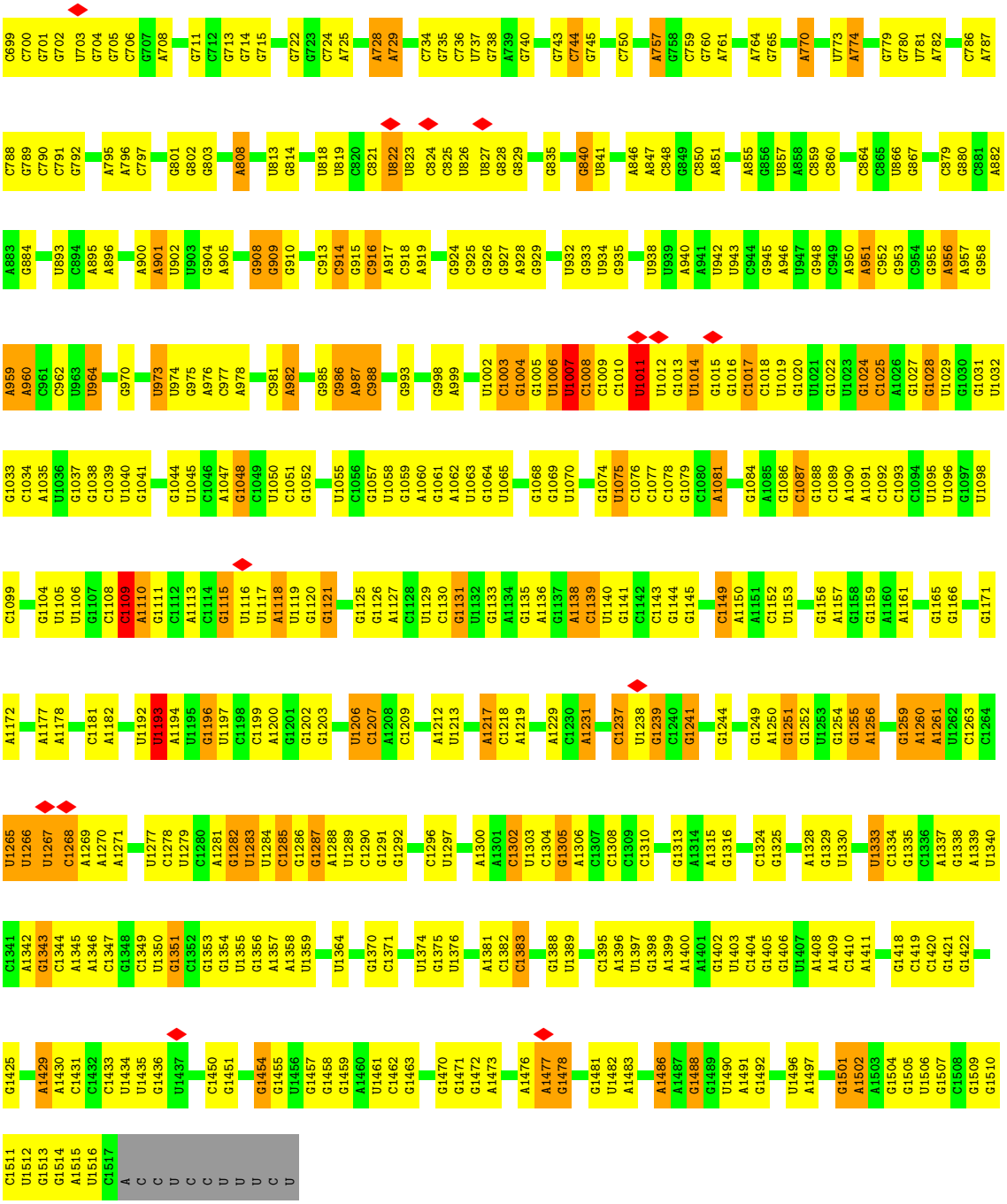


• Molecule 6: 16S ribosomal RNA

Chain A:

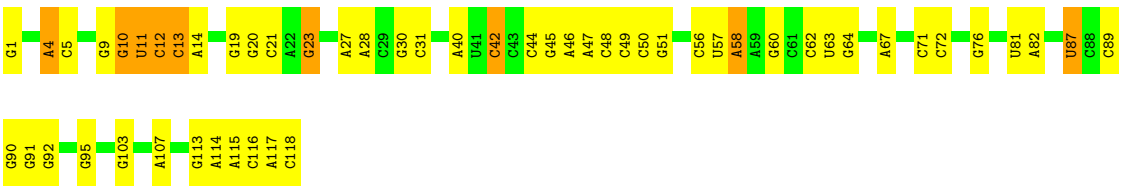




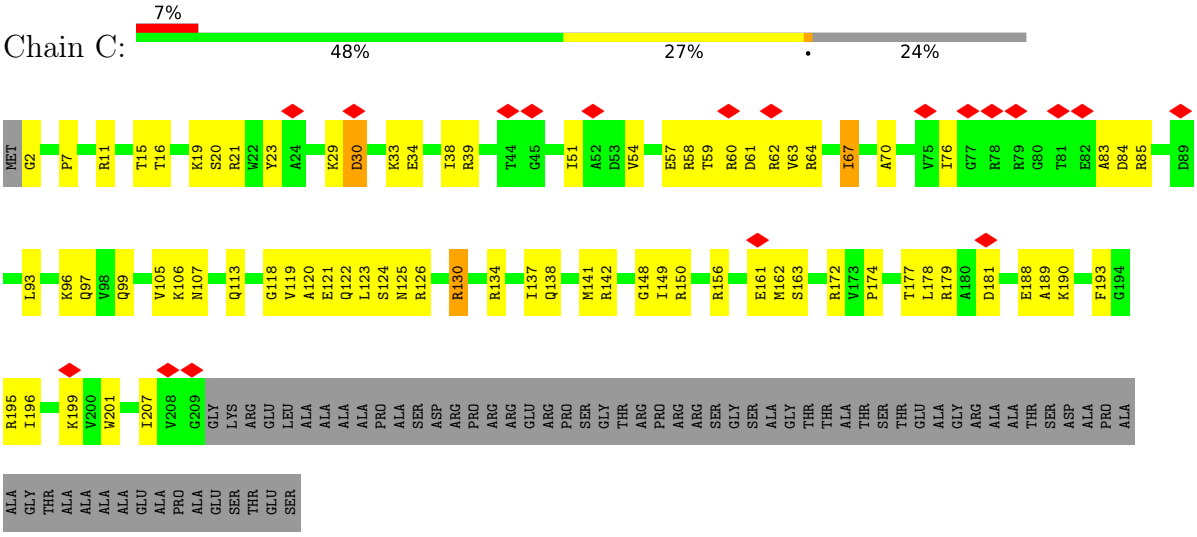


• Molecule 7: 5S ribosomal RNA

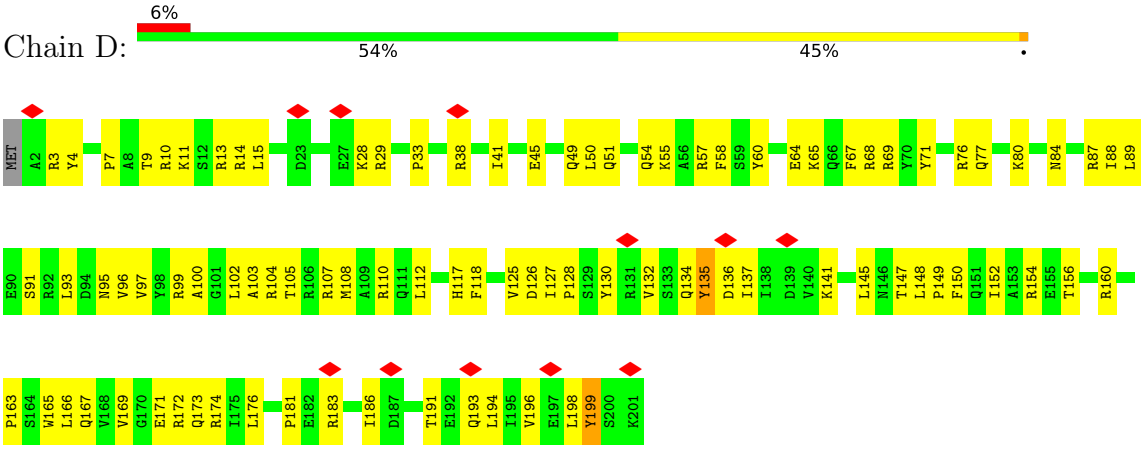
Chain B:



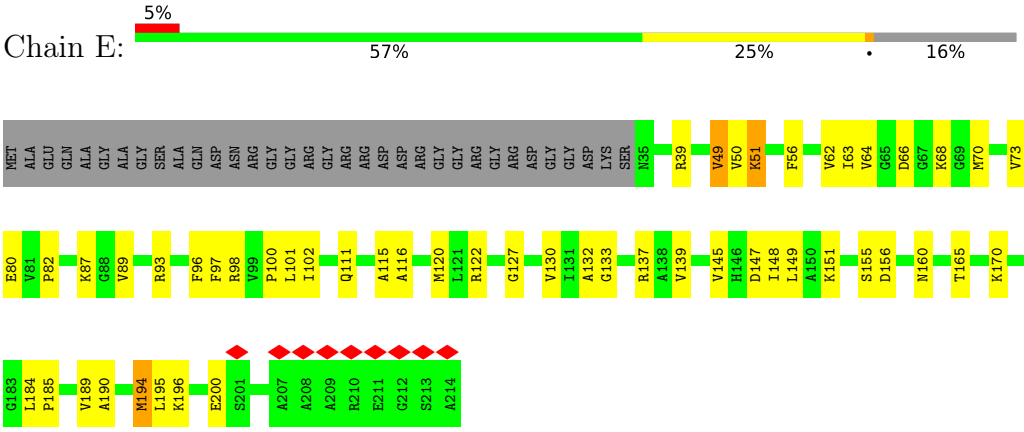
• Molecule 8: 30S ribosomal protein S3



• Molecule 9: 30S ribosomal protein S4

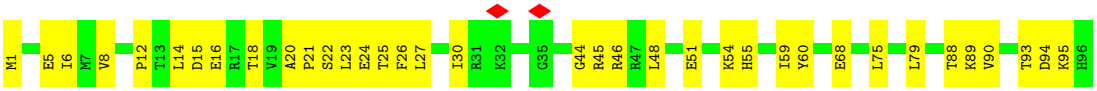


• Molecule 10: 30S ribosomal protein S5



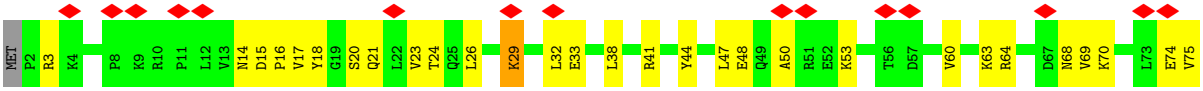
• Molecule 11: Small ribosomal subunit protein bS6

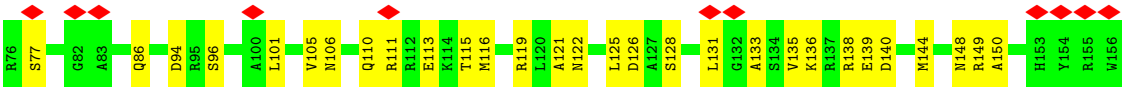




• Molecule 12: 30S ribosomal protein S7

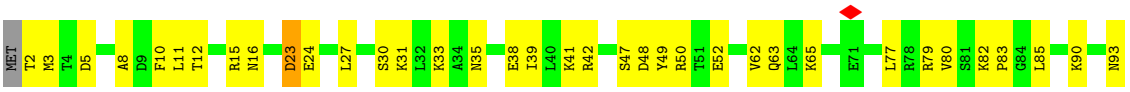


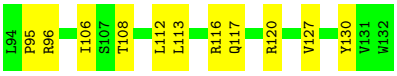




• Molecule 13: 30S ribosomal protein S8

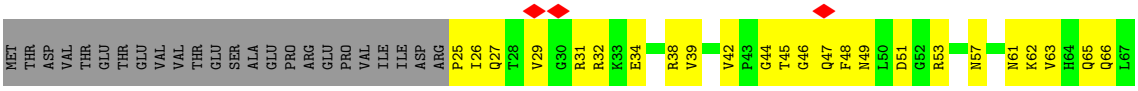






• Molecule 14: 30S ribosomal protein S9

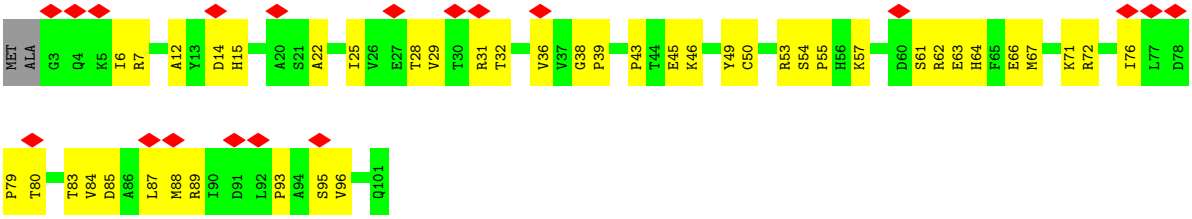






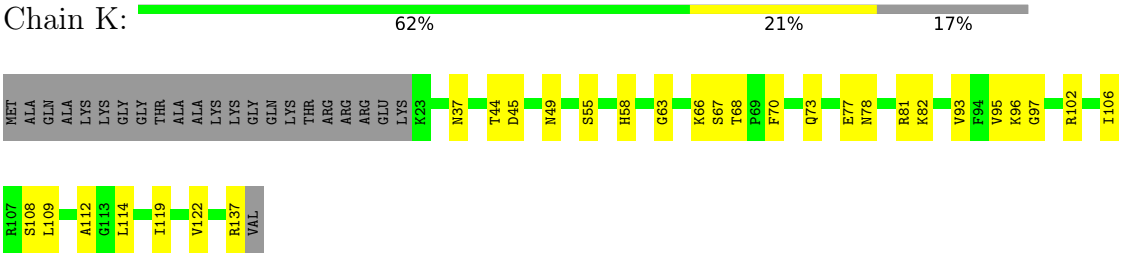
• Molecule 15: 30S ribosomal protein S10





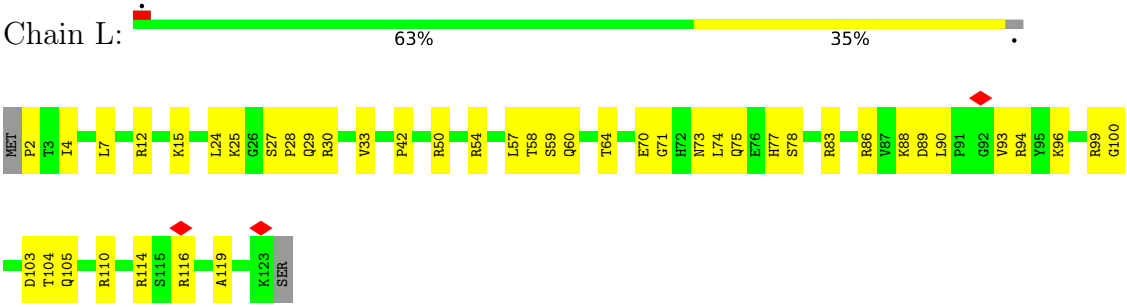
• Molecule 16: 30S ribosomal protein S11

Chain K:



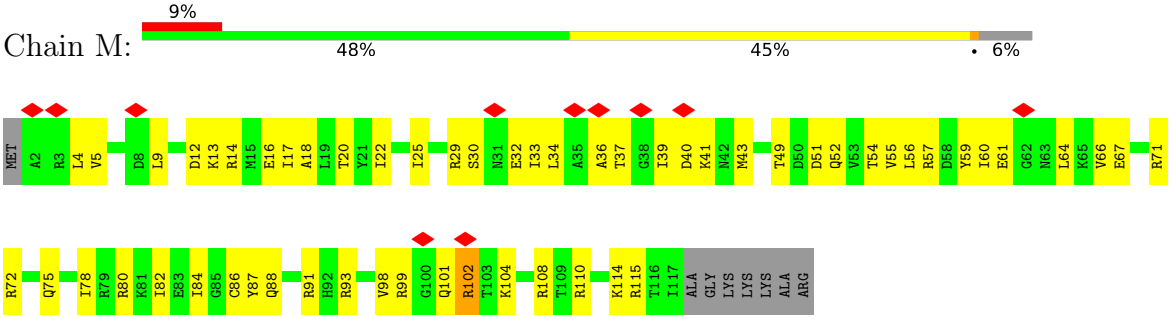
• Molecule 17: 30S ribosomal protein S12

Chain L:



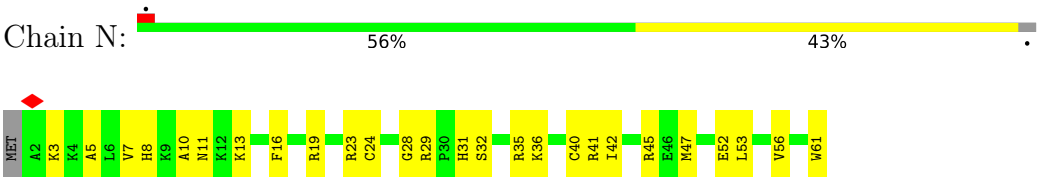
• Molecule 18: 30S ribosomal protein S13

Chain M:



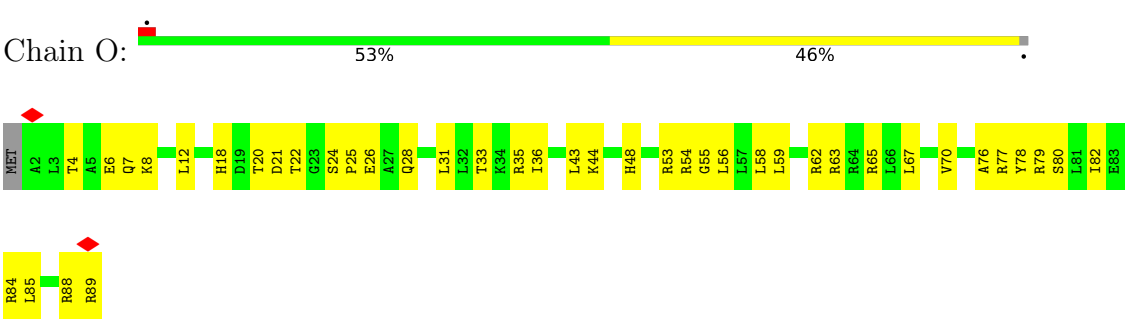
• Molecule 19: 30S ribosomal protein S14 type Z

Chain N:



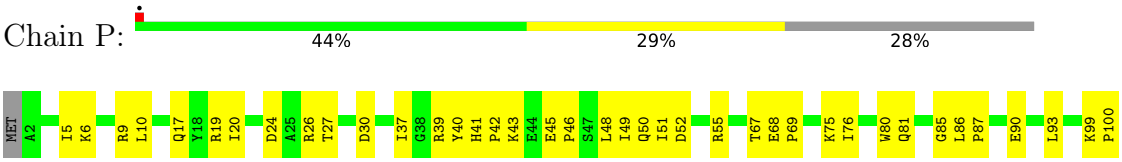
• Molecule 20: 30S ribosomal protein S15

Chain O:



• Molecule 21: 30S ribosomal protein S16

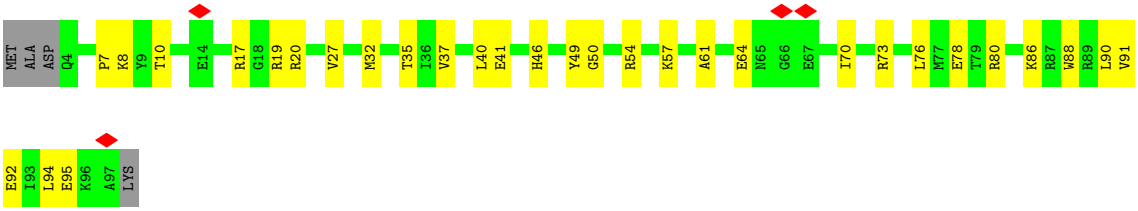
Chain P:



• Molecule 22: 30S ribosomal protein S17

Chain Q:

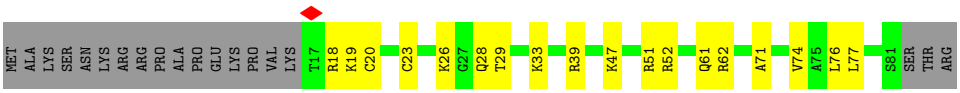




• Molecule 23: 30S ribosomal protein S18 2

Chain R:

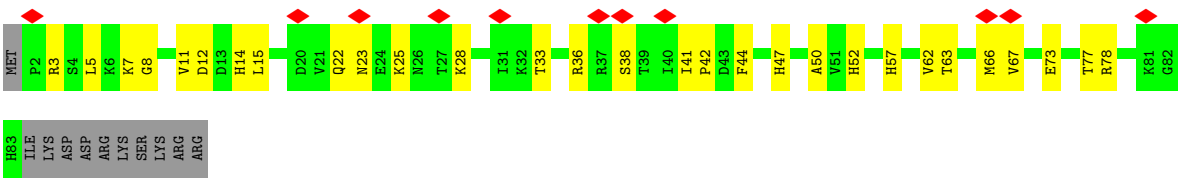




• Molecule 24: 30S ribosomal protein S19

Chain S:

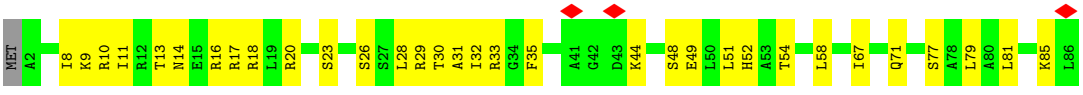




• Molecule 25: 30S ribosomal protein S20

Chain T:

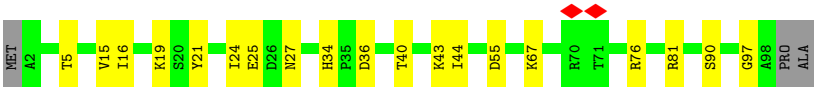




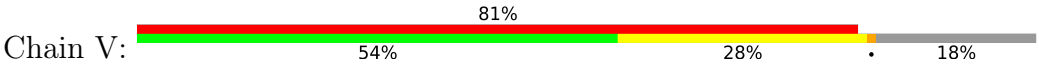
• Molecule 26: 50S ribosomal protein L23

Chain U:





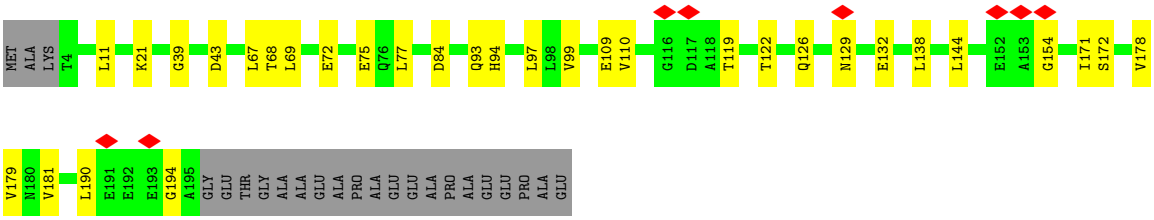
• Molecule 27: 30S ribosomal protein S2





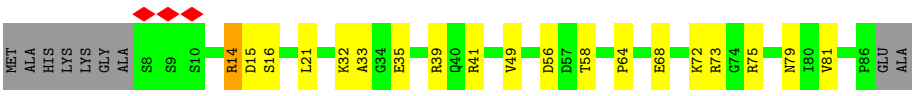
• Molecule 28: 50S ribosomal protein L25



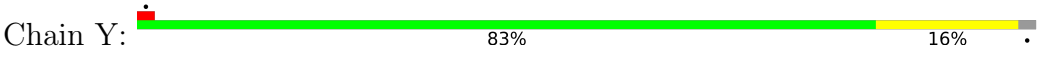


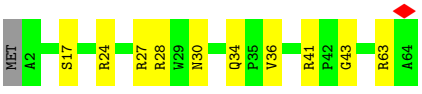
• Molecule 29: 50S ribosomal protein L27





• Molecule 30: 50S ribosomal protein L28

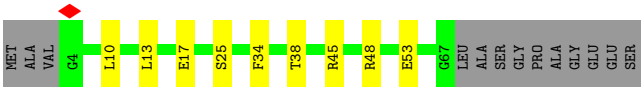




• Molecule 31: 50S ribosomal protein L29

Chain Z:

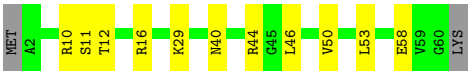




• Molecule 32: 50S ribosomal protein L30

Chain a:

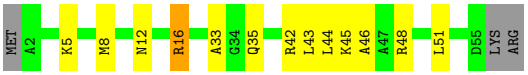




• Molecule 33: 50S ribosomal protein L32

Chain b:

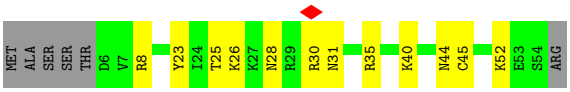




• Molecule 34: 50S ribosomal protein L33 1

Chain c:

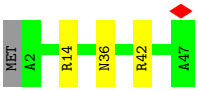




• Molecule 35: 50S ribosomal protein L34

Chain d:

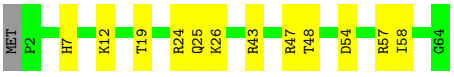




• Molecule 36: 50S ribosomal protein L35

Chain e:

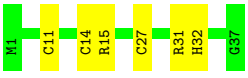




• Molecule 37: 50S ribosomal protein L36

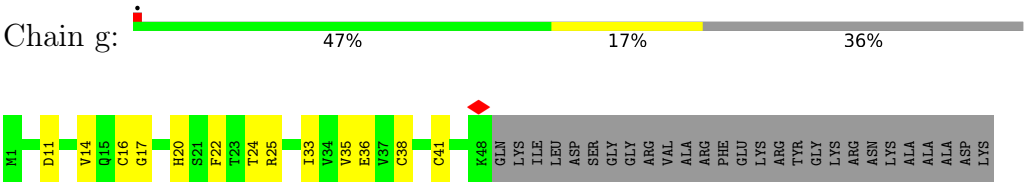
Chain f:





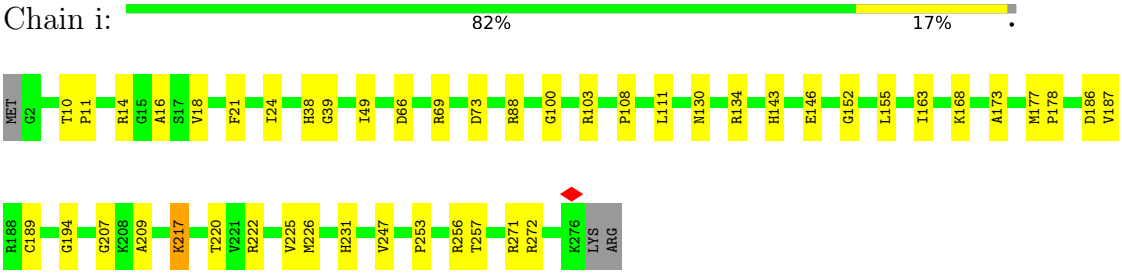
• Molecule 38: 50S ribosomal protein L31

Chain g:



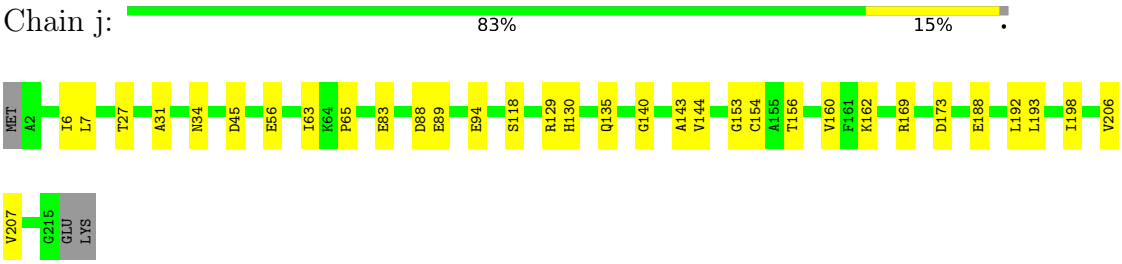
• Molecule 39: 50S ribosomal protein L2

Chain i:



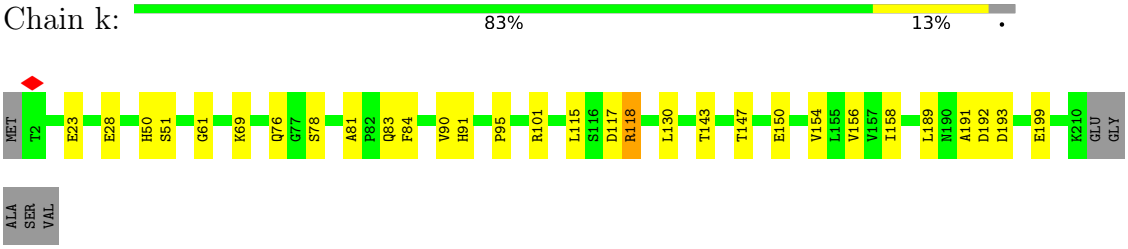
• Molecule 40: 50S ribosomal protein L3

Chain j:



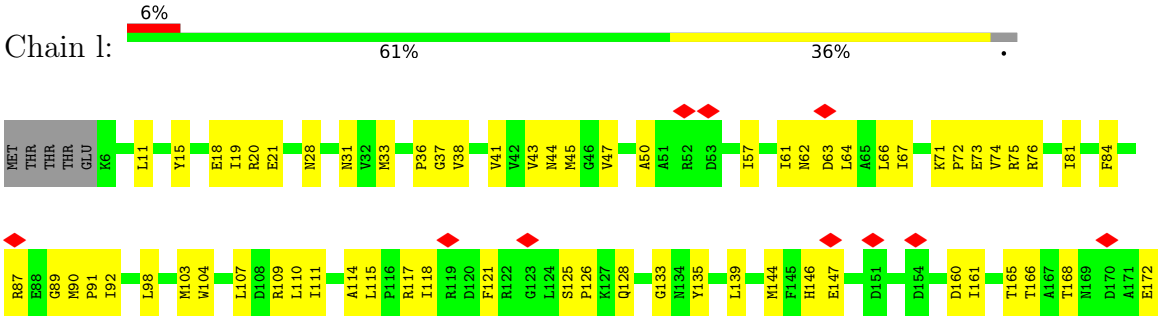
• Molecule 41: 50S ribosomal protein L4

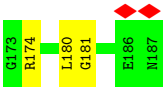
Chain k:



• Molecule 42: 50S ribosomal protein L5

Chain l:

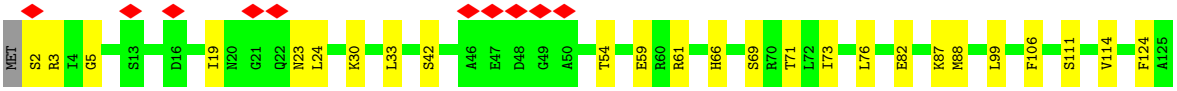


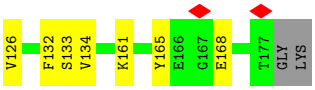


• Molecule 43: 50S ribosomal protein L6

Chain m:



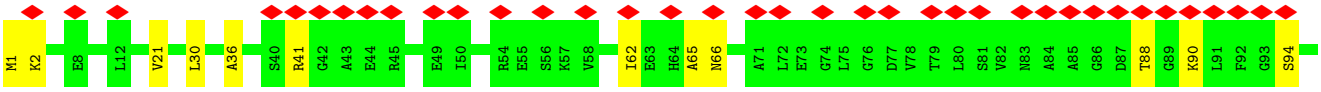


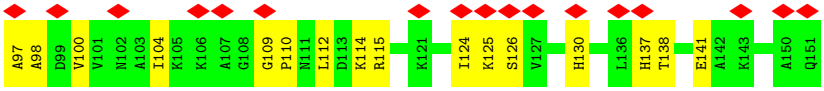


• Molecule 44: 50S ribosomal protein L9

Chain n:



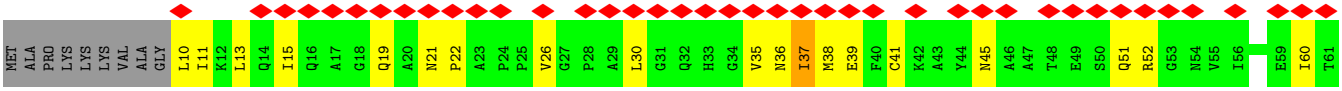


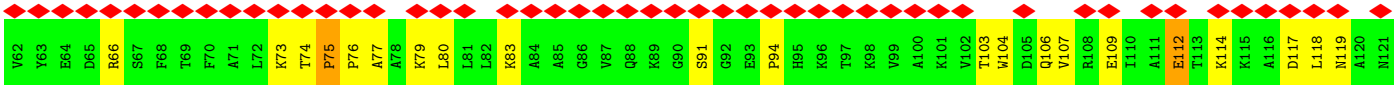


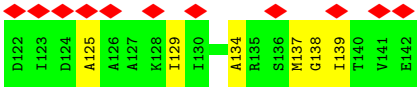
• Molecule 45: 50S ribosomal protein L11

Chain o:







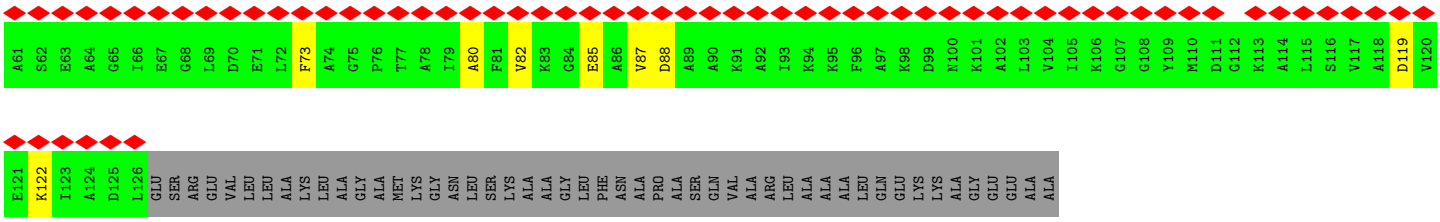


• Molecule 46: 50S ribosomal protein L10

Chain p:







• Molecule 47: 50S ribosomal protein L13

Chain q:





• Molecule 48: 50S ribosomal protein L14

Chain r:





• Molecule 49: 50S ribosomal protein L15

Chain s:

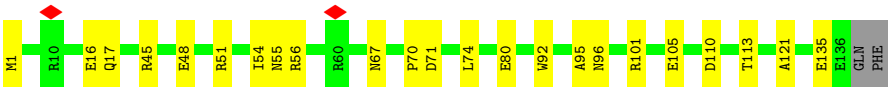




• Molecule 50: 50S ribosomal protein L16

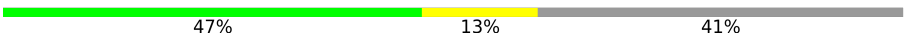
Chain t:

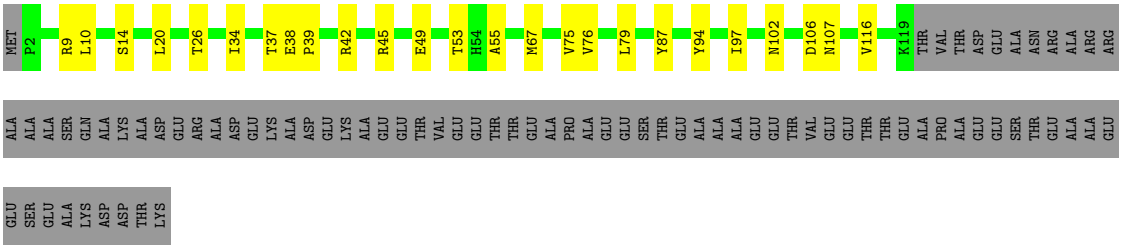




• Molecule 51: 50S ribosomal protein L17

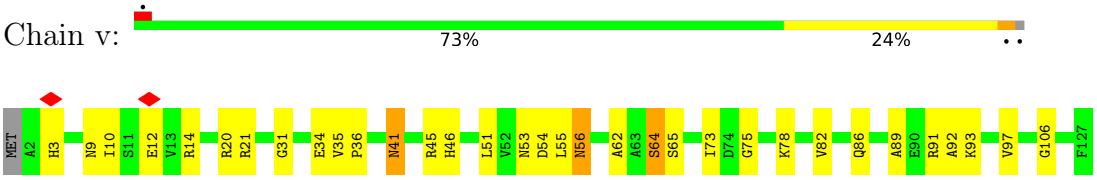
Chain u:





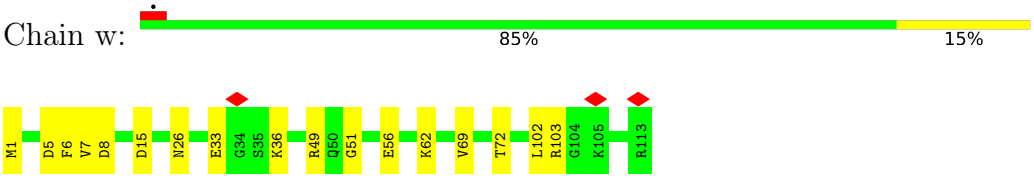
• Molecule 52: 50S ribosomal protein L18

Chain v:



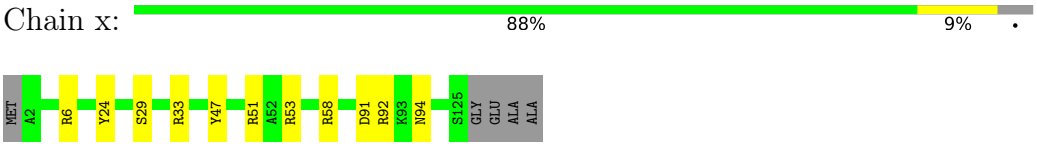
• Molecule 53: 50S ribosomal protein L19

Chain w:



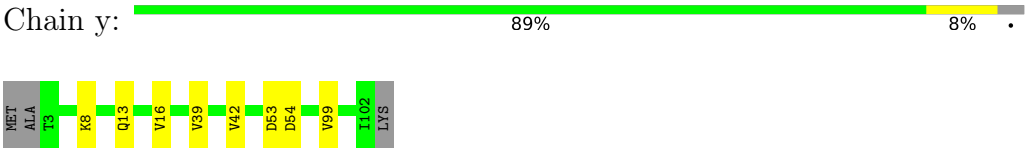
• Molecule 54: 50S ribosomal protein L20

Chain x:



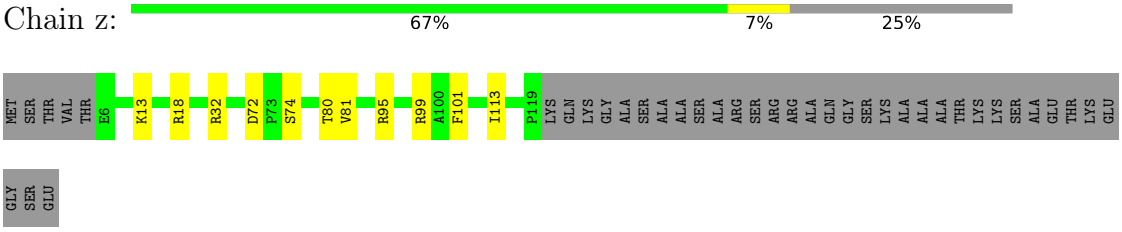
• Molecule 55: 50S ribosomal protein L21

Chain y:



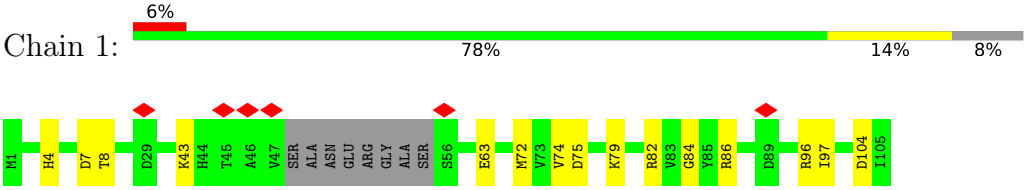
• Molecule 56: 50S ribosomal protein L22

Chain z:



• Molecule 57: Large ribosomal subunit protein uL24

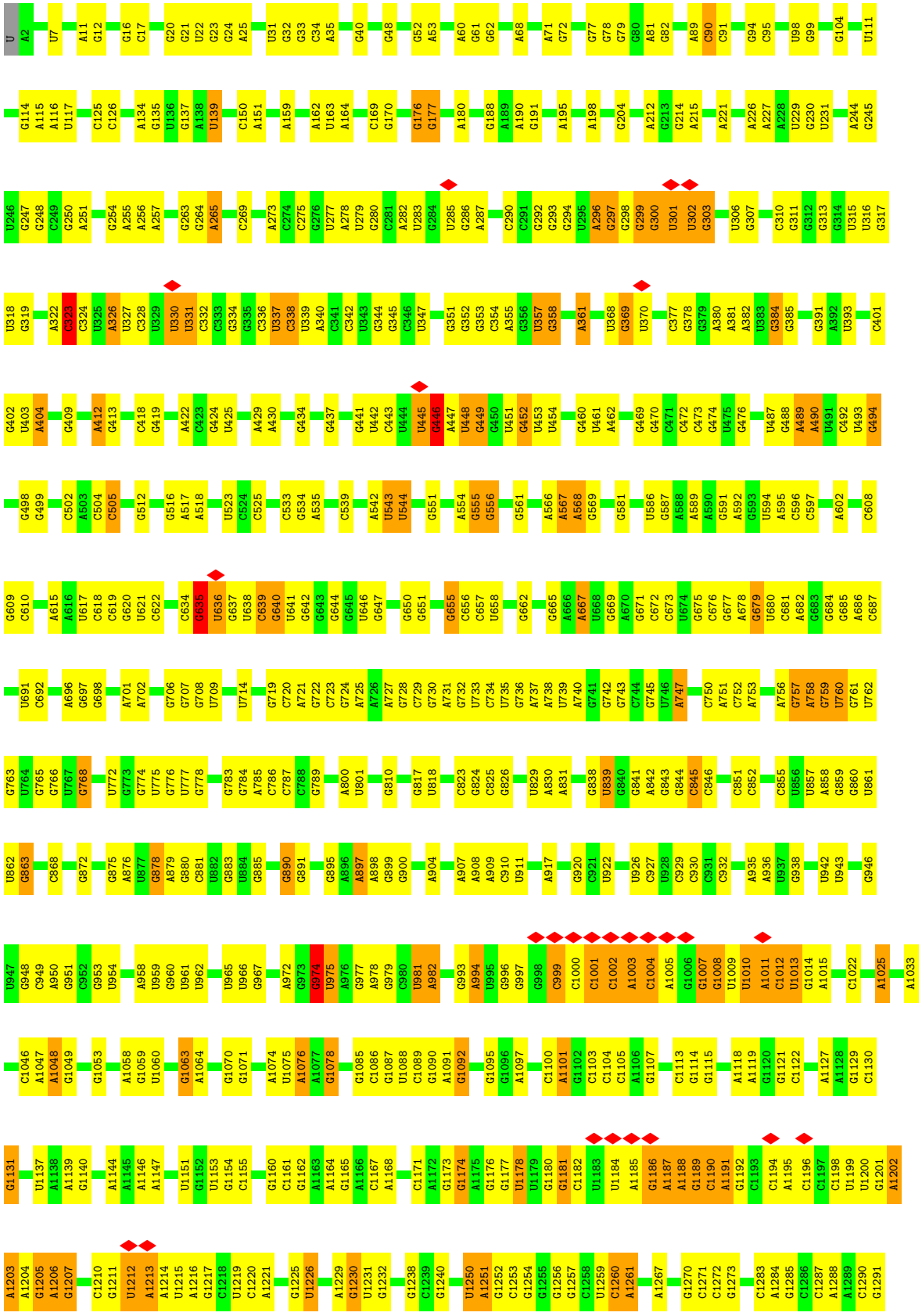
Chain 1:

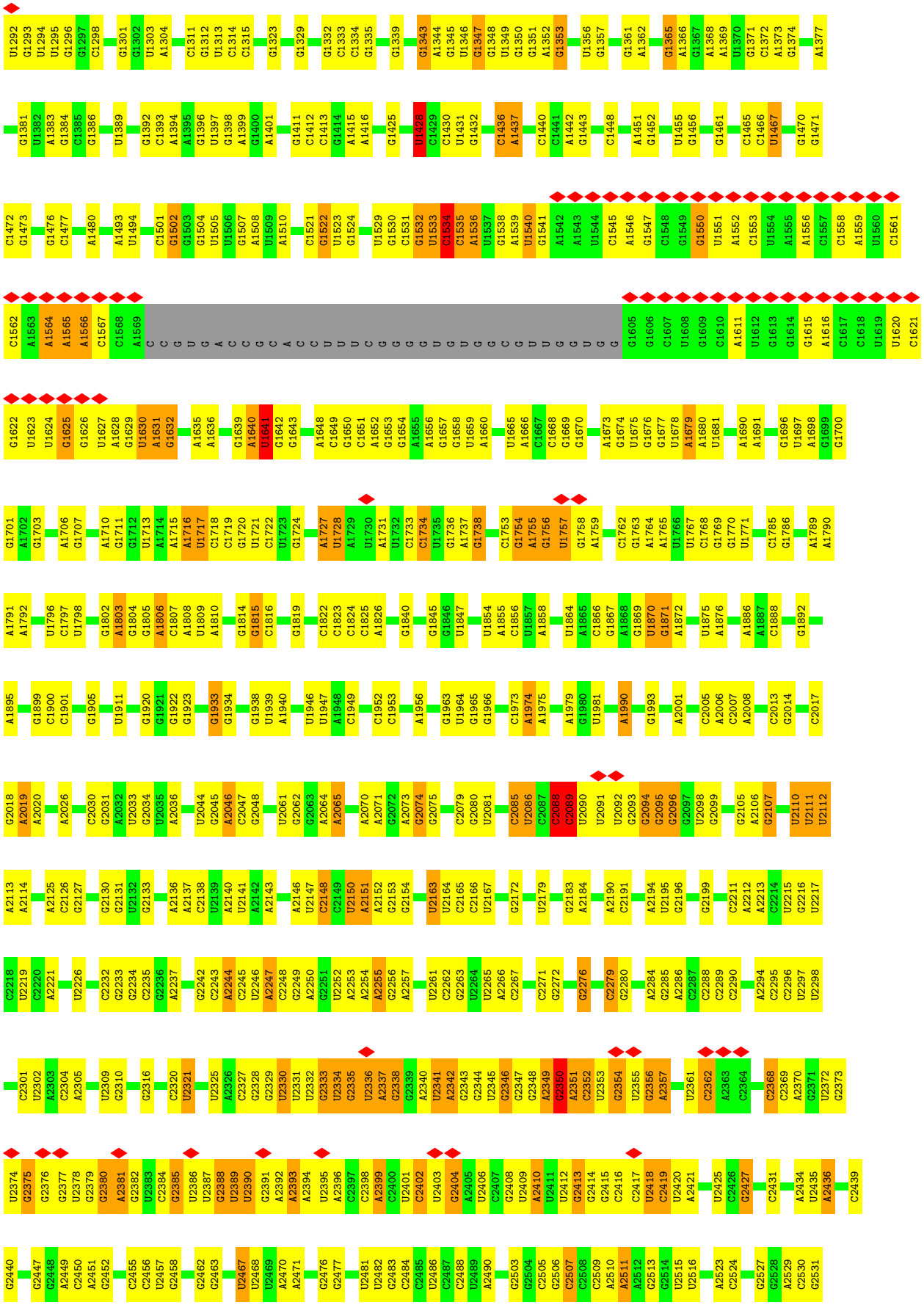


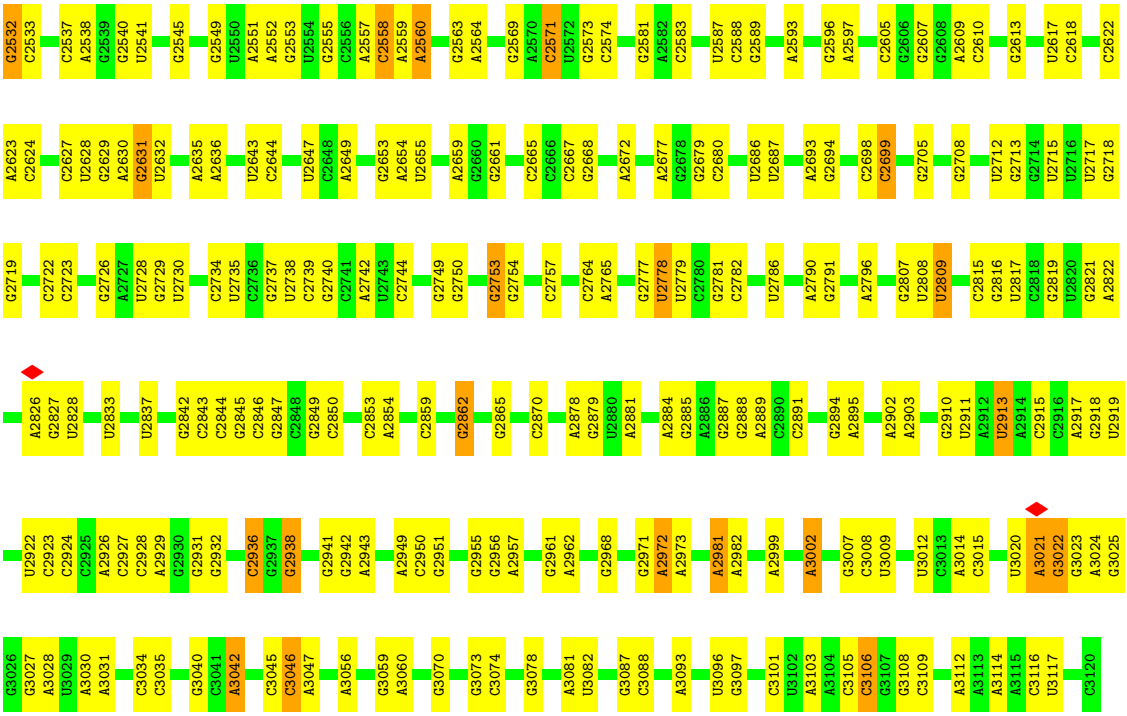
• Molecule 58: 23S ribosomal RNA

Chain h:








G2532 C2533
C2537 A2538 G2539 G2540 U2541
G2545
G2549 U2550 A2551 A2552 G2553 U2554 G2555 C2556 A2557 C2558 A2559 A2560
G2563 A2564
G2569 A2570 C2571 U2572 G2573 C2574
G2581 A2582 C2583
U2587 C2588 G2589
A2593
G2596 A2597
C2605 G2606 G2607 G2608 A2609 C2610
G2613
U2617 C2618
C2622
A2623 C2624
C2627 U2628 G2629 A2630 G2631 U2632
A2635 A2636
U2643 C2644
U2647 C2648 A2649
G2653 A2654 U2655
A2659 G2660 G2661
C2665 C2666 C2667 G2668
A2672
A2677 G2678 G2679 C2680
U2686 U2687
A2693 G2694
C2698 C2699
G2705
G2708
U2712 G2713 G2714 U2715 U2716 U2717 G2718
G2719
C2722 C2723
G2726 A2727 U2728 G2729 U2730
C2734 U2735 C2736 G2737 U2738 C2739 G2740 C2741 A2742 U2743 C2744
G2749 G2750
G2753 G2754
C2757
C2764 A2765
G2777 U2778 U2779 C2780 G2781 C2782
U2786
A2790 G2791
A2796
G2807 U2808 U2809
C2815 G2816 U2817 C2818 G2819 U2820 G2821 A2822
A2826 G2827 U2828
U2833
U2837
G2842 C2843 C2844 G2845 C2846 G2847 C2848 G2849 C2850
C2853 A2854
C2859
G2862
G2865
C2870
A2878 G2879 U2880 A2881
A2884 G2885 A2886 G2887 G2888 A2889 C2890 C2891
G2894 A2895
A2902 A2903
G2910 U2911 A2912 U2913 A2914 C2915 C2916 A2917 G2918 U2919
U2922 C2923 C2924 C2925 A2926 C2927 C2928 A2929 G2930 G2931 G2932
C2936 G2937 G2938
G2941 G2942 A2943
A2949 C2950 G2951
G2955 G2956 A2957
G2961 A2962
G2968
G2971 A2972 A2973
A2981 A2982
A2999
A3002
G3007 C3008 U3009
U3012 C3013 A3014 C3015
U3020 A3021 G3022 G3023 A3024 G3025
G3026 G3027 A3028 U3029 A3030 A3031
C3034 C3035
G3040 C3041 A3042
C3045 C3046 A3047
A3056
G3059 A3060
G3070
G3073 C3074
G3078
A3081 U3082
G3087 C3088
A3093
U3096 G3097
C3101 U3102 A3103 A3104 C3105 C3106 G3107 G3108 C3109
A3112 A3113 A3114 A3115 C3116 U3117
C3120

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20.82	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0243	Depositor
Map size (Å)	449.40002, 449.40002, 449.40002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.46	0/1836	0.81	2/2859 (0.1%)
2	3	0.18	0/191	0.34	0/247
3	4	0.73	0/93	0.98	0/142
4	5	0.18	0/1472	0.41	2/1976 (0.1%)
5	6	0.15	0/1783	0.31	0/2404
6	A	0.51	0/36309	0.82	21/56657 (0.0%)
7	B	0.40	0/2821	0.74	0/4396
8	C	0.18	0/1684	0.38	0/2261
9	D	0.19	0/1672	0.41	0/2251
10	E	0.21	0/1312	0.42	0/1772
11	F	0.32	1/782 (0.1%)	0.46	0/1059
12	G	0.18	0/1252	0.39	0/1690
13	H	0.21	0/1025	0.41	0/1385
14	I	0.18	0/1012	0.39	0/1362
15	J	0.25	0/802	0.47	0/1086
16	K	0.21	0/873	0.40	0/1180
17	L	0.23	0/969	0.42	0/1294
18	M	0.17	0/942	0.44	0/1260
19	N	0.21	0/488	0.42	0/650
20	O	0.17	0/729	0.36	0/977
21	P	0.20	0/908	0.45	0/1226
22	Q	0.17	0/759	0.38	0/1016
23	R	0.23	0/518	0.39	0/693
24	S	0.23	0/680	0.41	0/915
25	T	0.21	0/663	0.37	0/882
26	U	0.19	0/766	0.31	0/1030
27	V	0.20	0/1822	0.35	0/2457
28	W	0.20	0/1443	0.32	0/1970
29	X	0.24	0/595	0.40	0/798
30	Y	0.19	0/478	0.28	0/641
31	Z	0.16	0/534	0.26	0/713
32	a	0.21	0/477	0.36	0/640

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.24	0/427	0.35	0/572
34	c	0.16	0/413	0.26	0/553
35	d	0.19	0/380	0.30	0/500
36	e	0.19	0/507	0.33	0/672
37	f	0.17	0/303	0.27	0/401
38	g	0.14	0/372	0.36	0/503
39	i	0.25	0/2153	0.36	0/2895
40	j	0.20	0/1609	0.32	0/2165
41	k	0.20	0/1592	0.32	0/2153
42	l	0.16	0/1467	0.38	0/1973
43	m	0.15	0/1369	0.32	0/1848
44	n	0.13	0/1027	0.38	0/1398
45	o	0.25	0/1006	0.60	3/1364 (0.2%)
46	p	0.10	0/925	0.29	0/1246
47	q	0.19	0/1157	0.28	0/1567
48	r	0.20	0/946	0.32	0/1268
49	s	0.21	0/1091	0.40	0/1457
50	t	0.19	0/1118	0.34	0/1506
51	u	0.20	0/945	0.36	0/1267
52	v	0.16	0/966	0.29	0/1298
53	w	0.20	0/921	0.34	0/1236
54	x	0.20	0/1000	0.29	0/1341
55	y	0.18	0/764	0.32	0/1030
56	z	0.19	0/887	0.33	0/1204
57	1	0.20	0/738	0.28	0/987
58	h	0.49	0/74164	0.80	42/115718 (0.0%)
All	All	0.43	1/165937 (0.0%)	0.71	70/248011 (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
9	D	0	1
13	H	0	1
17	L	0	1
18	M	0	1
19	N	0	1
29	X	0	1
33	b	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	93	THR	C-N	-6.31	1.24	1.33

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	o	75	PRO	CA-N-CD	-9.98	98.03	112.00
45	o	75	PRO	N-CD-CG	-8.93	89.81	103.20
58	h	338	C	N3-C2-O2	-8.80	115.74	121.90
58	h	2245	C	C2-N1-C1'	8.48	128.13	118.80
4	5	50	PRO	CA-N-CD	-8.35	100.31	112.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	D	69	ARG	Sidechain
13	H	96	ARG	Sidechain
17	L	86	ARG	Sidechain
18	M	102	ARG	Sidechain
19	N	29	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1644	0	836	25	0
2	3	189	0	205	6	0
3	4	84	0	43	5	0
4	5	1459	0	1478	39	0
5	6	1759	0	1818	23	0
6	A	32439	0	16321	530	0
7	B	2522	0	1285	36	0
8	C	1660	0	1707	64	0
9	D	1641	0	1668	78	0
10	E	1296	0	1360	48	0
11	F	771	0	797	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	1232	0	1282	42	0
13	H	1010	0	1046	36	0
14	I	994	0	1050	53	0
15	J	788	0	819	34	0
16	K	855	0	863	24	0
17	L	958	0	1045	44	0
18	M	935	0	986	49	0
19	N	477	0	499	25	0
20	O	720	0	760	37	0
21	P	891	0	935	50	0
22	Q	748	0	795	29	0
23	R	513	0	537	15	0
24	S	662	0	677	24	0
25	T	660	0	712	25	0
26	U	756	0	802	13	0
27	V	1793	0	1839	57	0
28	W	1428	0	1443	20	0
29	X	586	0	601	14	0
30	Y	470	0	480	7	0
31	Z	531	0	541	6	0
32	a	474	0	500	9	0
33	b	423	0	463	8	0
34	c	405	0	407	8	0
35	d	377	0	411	3	0
36	e	502	0	541	10	0
37	f	299	0	321	5	0
38	g	364	0	348	13	0
39	i	2110	0	2165	34	0
40	j	1587	0	1630	24	0
41	k	1569	0	1607	21	0
42	l	1445	0	1475	56	0
43	m	1348	0	1399	21	0
44	n	1018	0	988	21	0
45	o	990	0	1021	37	0
46	p	918	0	959	23	0
47	q	1130	0	1167	13	0
48	r	938	0	1000	14	0
49	s	1078	0	1151	22	0
50	t	1092	0	1128	17	0
51	u	928	0	972	14	0
52	v	956	0	991	20	0
53	w	907	0	938	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	x	988	0	1038	10	0
55	y	754	0	802	5	0
56	z	873	0	909	7	0
57	1	732	0	782	11	0
58	h	66232	0	33325	816	0
59	F	1	0	0	0	0
59	R	1	0	0	0	0
59	h	4	0	0	0	0
59	i	2	0	0	0	0
59	j	1	0	0	0	0
59	l	1	0	0	0	0
59	t	1	0	0	0	0
59	z	1	0	0	0	0
60	N	1	0	0	0	0
60	R	1	0	0	0	0
60	Y	1	0	0	0	0
60	c	1	0	0	0	0
60	f	1	0	0	0	0
60	g	1	0	0	0	0
All	All	152926	0	103668	2435	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 2435 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:V:155:GLN:NE2	27:V:157:VAL:O	1.69	1.24
27:V:155:GLN:HE22	27:V:157:VAL:C	1.68	0.99
27:V:66:THR:OG1	27:V:155:GLN:CG	2.20	0.90
58:h:1755:A:H2'	58:h:1758:G:H1	1.37	0.88
58:h:2356:G:H2'	58:h:2380:G:H1	1.38	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3	21/24 (88%)	21 (100%)	0	0	100	100
4	5	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
5	6	233/235 (99%)	230 (99%)	3 (1%)	0	100	100
8	C	206/275 (75%)	195 (95%)	11 (5%)	0	100	100
9	D	198/201 (98%)	187 (94%)	11 (6%)	0	100	100
10	E	178/214 (83%)	166 (93%)	12 (7%)	0	100	100
11	F	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
12	G	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
13	H	129/132 (98%)	123 (95%)	6 (5%)	0	100	100
14	I	124/150 (83%)	112 (90%)	12 (10%)	0	100	100
15	J	97/101 (96%)	89 (92%)	8 (8%)	0	100	100
16	K	113/138 (82%)	105 (93%)	8 (7%)	0	100	100
17	L	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
18	M	114/124 (92%)	105 (92%)	9 (8%)	0	100	100
19	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
20	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	P	111/156 (71%)	103 (93%)	8 (7%)	0	100	100
22	Q	92/98 (94%)	89 (97%)	3 (3%)	0	100	100
23	R	63/84 (75%)	60 (95%)	3 (5%)	0	100	100
24	S	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
25	T	83/86 (96%)	83 (100%)	0	0	100	100
26	U	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
27	V	226/277 (82%)	214 (95%)	12 (5%)	0	100	100
28	W	190/215 (88%)	183 (96%)	7 (4%)	0	100	100
29	X	77/88 (88%)	71 (92%)	6 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Y	61/64 (95%)	54 (88%)	7 (12%)	0	100	100
31	Z	62/77 (80%)	61 (98%)	1 (2%)	0	100	100
32	a	57/61 (93%)	54 (95%)	3 (5%)	0	100	100
33	b	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
34	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
35	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
36	e	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
37	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
38	g	46/75 (61%)	42 (91%)	4 (9%)	0	100	100
39	i	273/278 (98%)	257 (94%)	16 (6%)	0	100	100
40	j	212/217 (98%)	200 (94%)	12 (6%)	0	100	100
41	k	207/215 (96%)	202 (98%)	5 (2%)	0	100	100
42	l	180/187 (96%)	169 (94%)	11 (6%)	0	100	100
43	m	174/179 (97%)	171 (98%)	3 (2%)	0	100	100
44	n	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
45	o	131/142 (92%)	123 (94%)	8 (6%)	0	100	100
46	p	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
47	q	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
48	r	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
49	s	143/147 (97%)	132 (92%)	11 (8%)	0	100	100
50	t	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
51	u	116/199 (58%)	112 (97%)	4 (3%)	0	100	100
52	v	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
53	w	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
54	x	122/129 (95%)	121 (99%)	1 (1%)	0	100	100
55	y	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
56	z	112/153 (73%)	110 (98%)	2 (2%)	0	100	100
57	1	93/105 (89%)	90 (97%)	3 (3%)	0	100	100
All	All	6356/7066 (90%)	6060 (95%)	296 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	18/19 (95%)	18 (100%)	0	100	100
4	5	160/160 (100%)	160 (100%)	0	100	100
5	6	184/184 (100%)	184 (100%)	0	100	100
8	C	170/212 (80%)	167 (98%)	3 (2%)	51	67
9	D	175/176 (99%)	172 (98%)	3 (2%)	53	67
10	E	127/147 (86%)	124 (98%)	3 (2%)	43	63
11	F	85/85 (100%)	84 (99%)	1 (1%)	63	73
12	G	131/132 (99%)	130 (99%)	1 (1%)	73	77
13	H	107/108 (99%)	106 (99%)	1 (1%)	70	76
14	I	102/125 (82%)	101 (99%)	1 (1%)	68	76
15	J	89/90 (99%)	87 (98%)	2 (2%)	45	64
16	K	89/105 (85%)	89 (100%)	0	100	100
17	L	103/105 (98%)	103 (100%)	0	100	100
18	M	99/104 (95%)	98 (99%)	1 (1%)	68	76
19	N	49/50 (98%)	49 (100%)	0	100	100
20	O	76/77 (99%)	76 (100%)	0	100	100
21	P	92/118 (78%)	92 (100%)	0	100	100
22	Q	80/83 (96%)	79 (99%)	1 (1%)	61	72
23	R	55/72 (76%)	55 (100%)	0	100	100
24	S	73/84 (87%)	72 (99%)	1 (1%)	59	71
25	T	69/70 (99%)	69 (100%)	0	100	100
26	U	83/85 (98%)	82 (99%)	1 (1%)	63	73
27	V	191/218 (88%)	185 (97%)	6 (3%)	35	56
28	W	155/168 (92%)	155 (100%)	0	100	100
29	X	58/63 (92%)	57 (98%)	1 (2%)	53	67
30	Y	50/51 (98%)	50 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Z	58/66 (88%)	58 (100%)	0	100	100
32	a	52/54 (96%)	52 (100%)	0	100	100
33	b	43/46 (94%)	42 (98%)	1 (2%)	44	63
34	c	47/52 (90%)	47 (100%)	0	100	100
35	d	35/36 (97%)	35 (100%)	0	100	100
36	e	53/54 (98%)	53 (100%)	0	100	100
37	f	35/35 (100%)	35 (100%)	0	100	100
38	g	43/63 (68%)	43 (100%)	0	100	100
39	i	215/218 (99%)	213 (99%)	2 (1%)	70	76
40	j	160/163 (98%)	160 (100%)	0	100	100
41	k	169/173 (98%)	167 (99%)	2 (1%)	63	73
42	l	151/156 (97%)	151 (100%)	0	100	100
43	m	148/150 (99%)	148 (100%)	0	100	100
44	n	90/116 (78%)	89 (99%)	1 (1%)	65	74
45	o	102/108 (94%)	100 (98%)	2 (2%)	48	65
46	p	89/120 (74%)	89 (100%)	0	100	100
47	q	119/120 (99%)	119 (100%)	0	100	100
48	r	100/100 (100%)	100 (100%)	0	100	100
49	s	112/114 (98%)	112 (100%)	0	100	100
50	t	114/116 (98%)	114 (100%)	0	100	100
51	u	97/158 (61%)	94 (97%)	3 (3%)	35	56
52	v	93/94 (99%)	90 (97%)	3 (3%)	34	55
53	w	100/100 (100%)	98 (98%)	2 (2%)	48	65
54	x	97/99 (98%)	97 (100%)	0	100	100
55	y	81/83 (98%)	81 (100%)	0	100	100
56	z	90/117 (77%)	90 (100%)	0	100	100
57	1	81/86 (94%)	81 (100%)	0	100	100
All	All	5244/5688 (92%)	5202 (99%)	42 (1%)	70	77

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	i	217	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	u	34	ILE
41	k	28	GLU
45	o	37	ILE
52	v	41	ASN

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

Mol	Chain	Res	Type
39	i	87	ASN
45	o	14	GLN
39	i	164	GLN
43	m	86	GLN
45	o	45	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	76/77 (98%)	20 (26%)	0
3	4	3/4 (75%)	2 (66%)	0
58	h	3082/3120 (98%)	584 (18%)	0
6	A	1510/1528 (98%)	328 (21%)	19 (1%)
7	B	117/118 (99%)	18 (15%)	1 (0%)
All	All	4788/4847 (98%)	952 (19%)	20 (0%)

5 of 952 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	G
1	2	9	G
1	2	17	C
1	2	18	U
1	2	19	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1259	G
6	A	1477	A
7	B	10	G
6	A	1482	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	895	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

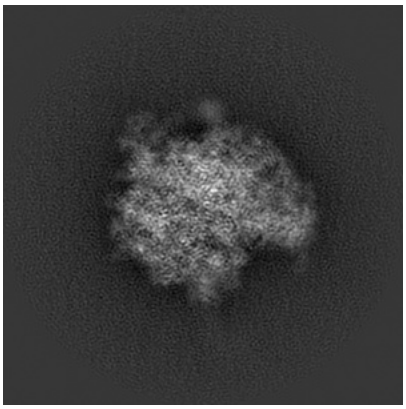
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69697. These allow visual inspection of the internal detail of the map and identification of artifacts.

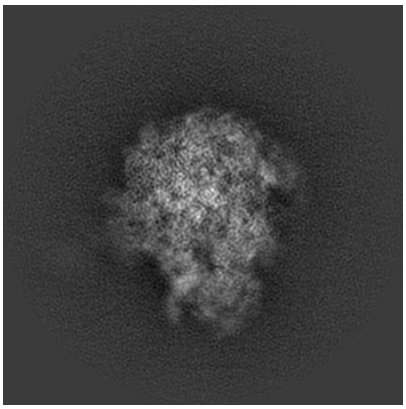
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

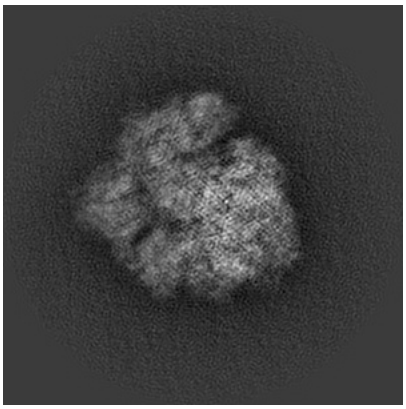
6.1.1 Primary map



X

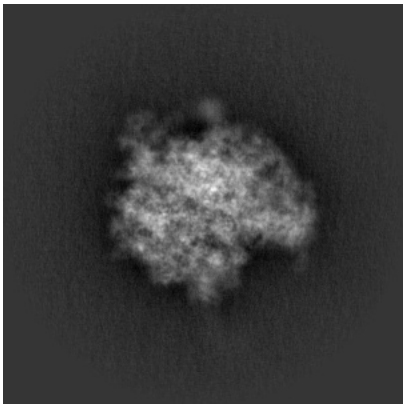


Y

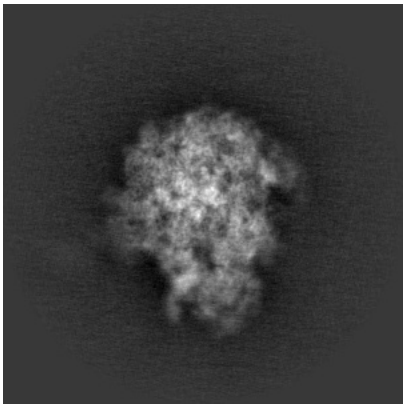


Z

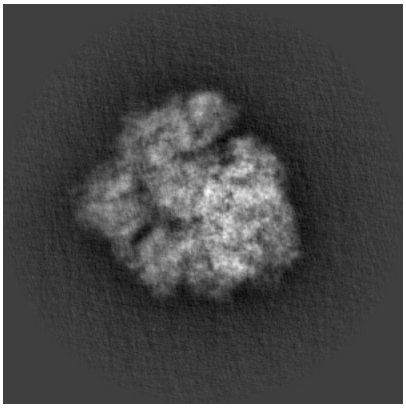
6.1.2 Raw map



X



Y

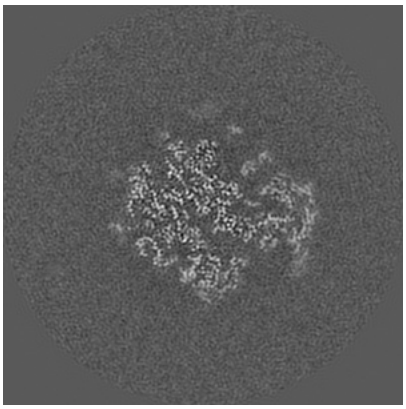


Z

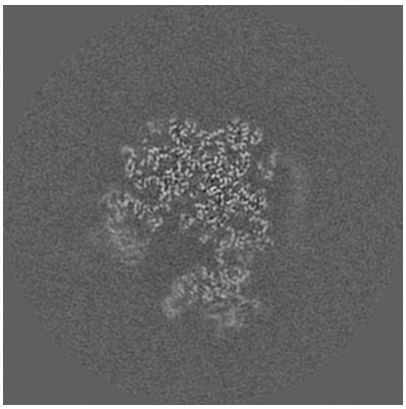
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

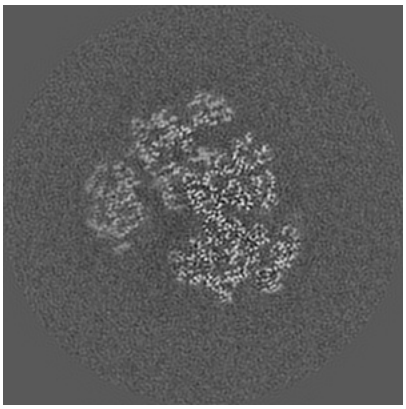
6.2.1 Primary map



X Index: 210

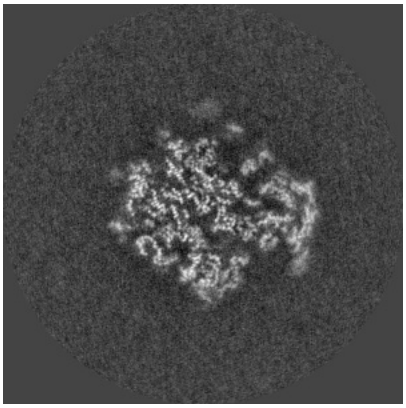


Y Index: 210

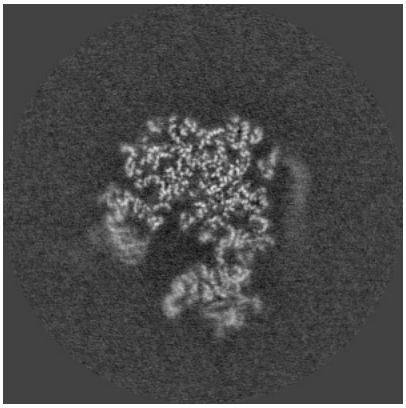


Z Index: 210

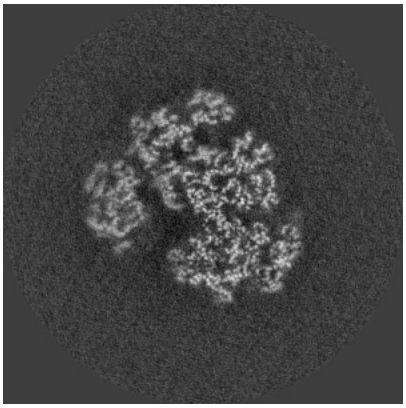
6.2.2 Raw map



X Index: 210



Y Index: 210

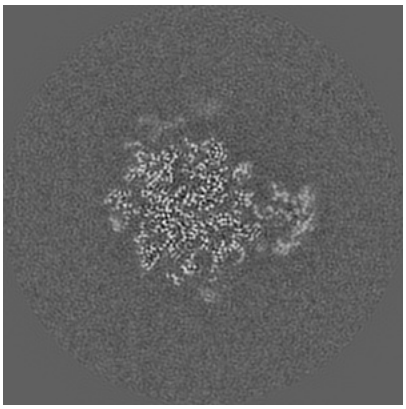


Z Index: 210

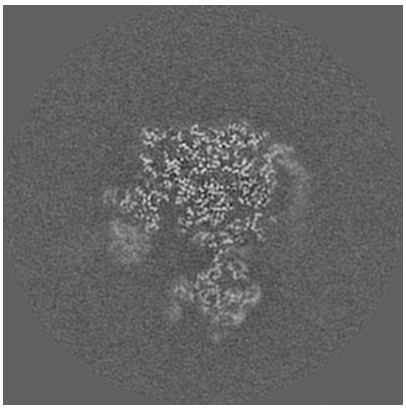
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

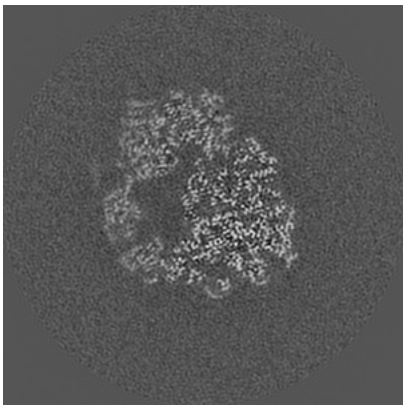
6.3.1 Primary map



X Index: 225

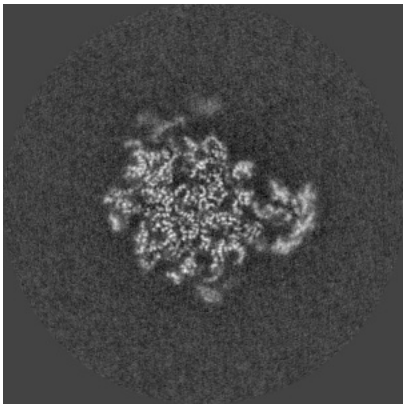


Y Index: 219

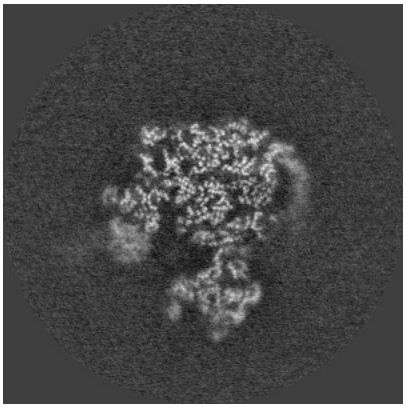


Z Index: 197

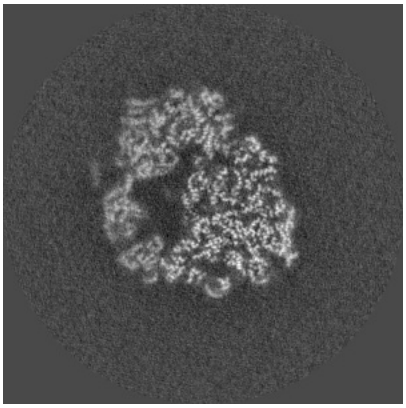
6.3.2 Raw map



X Index: 224



Y Index: 219

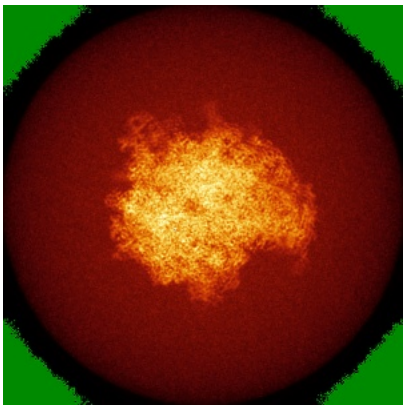


Z Index: 197

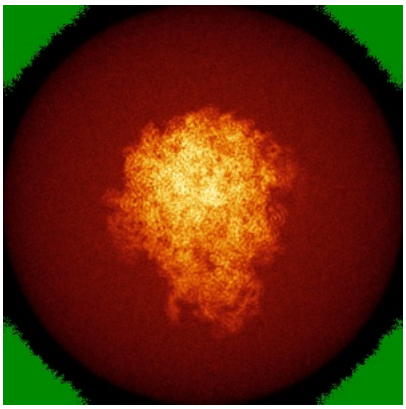
The images above show the largest variance slices of the map in three orthogonal directions.

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

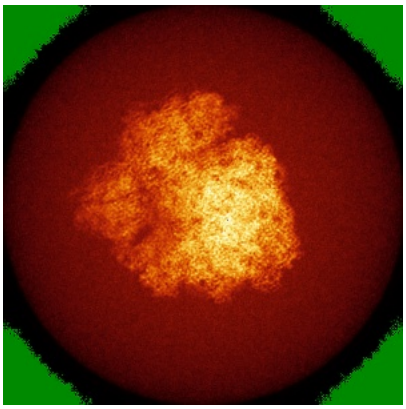
6.4.1 Primary map



X

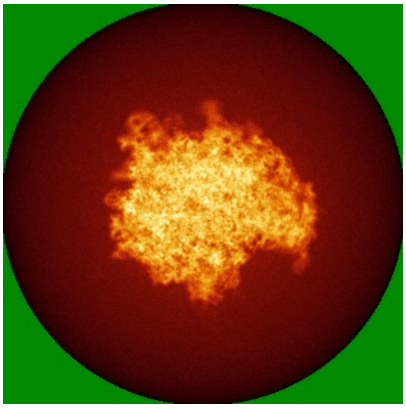


Y

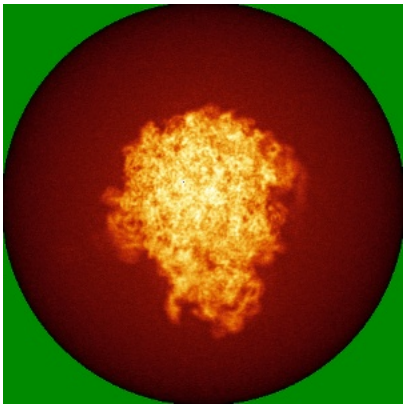


Z

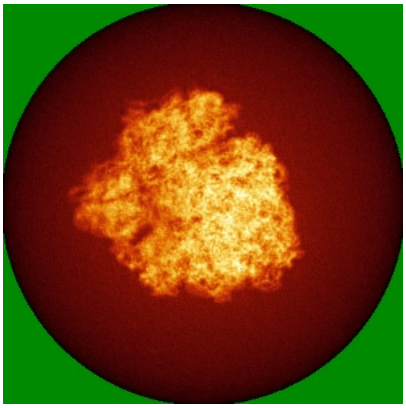
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

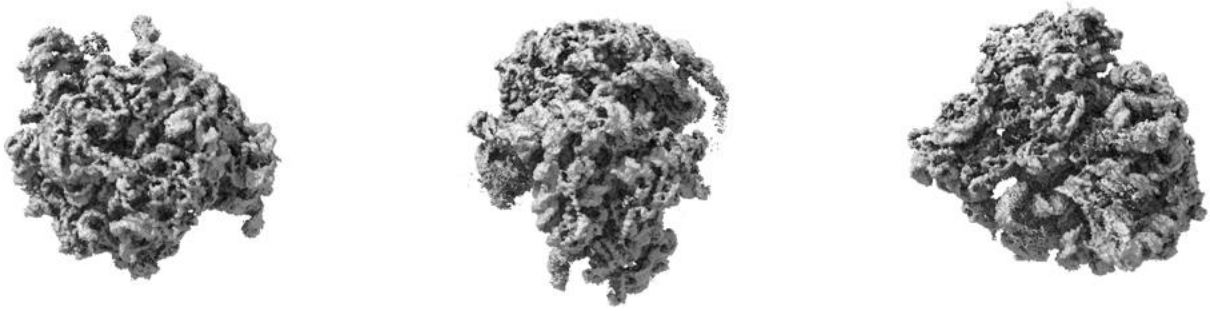
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

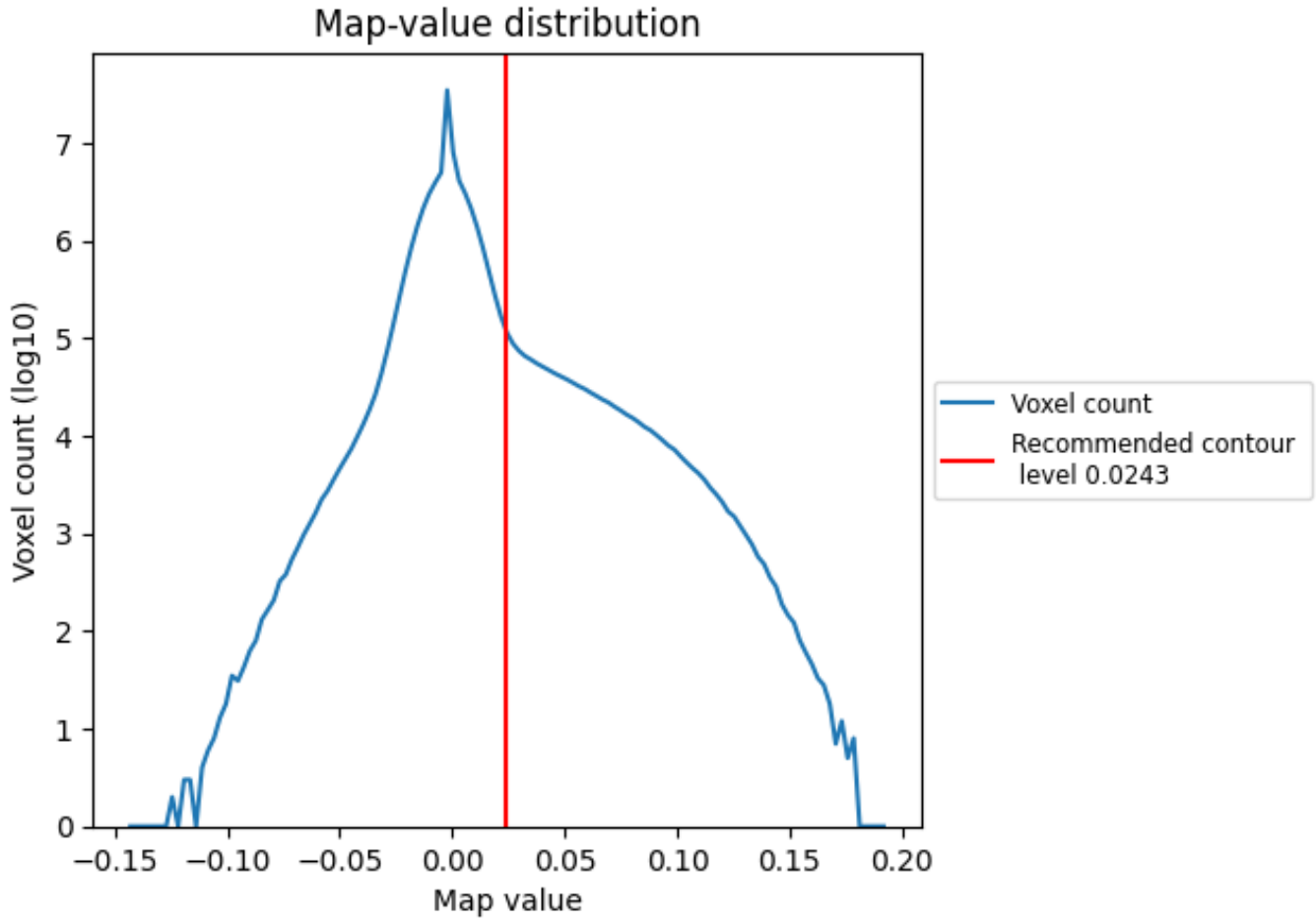
6.6 Mask visualisation (i)

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

7 Map analysis

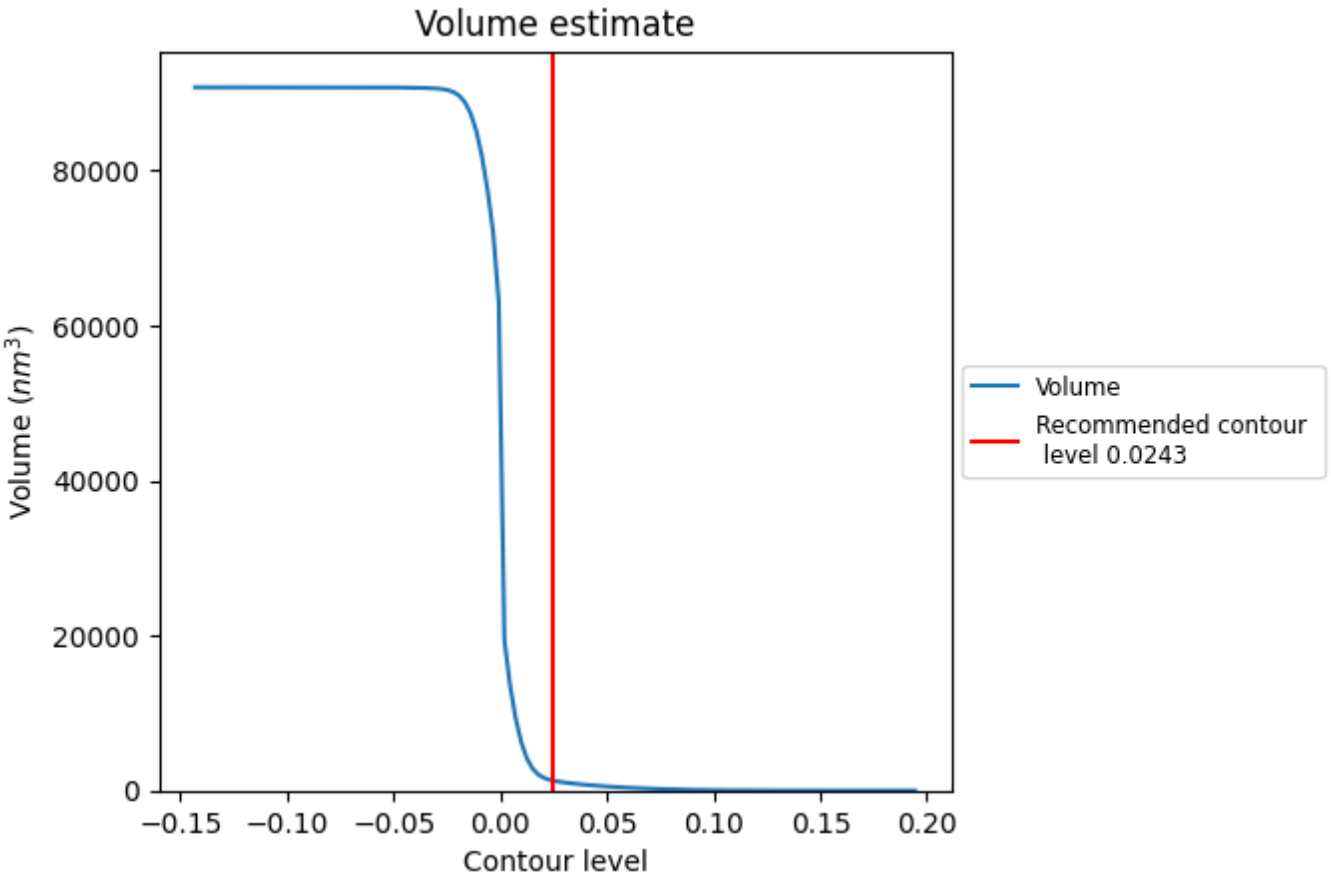
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

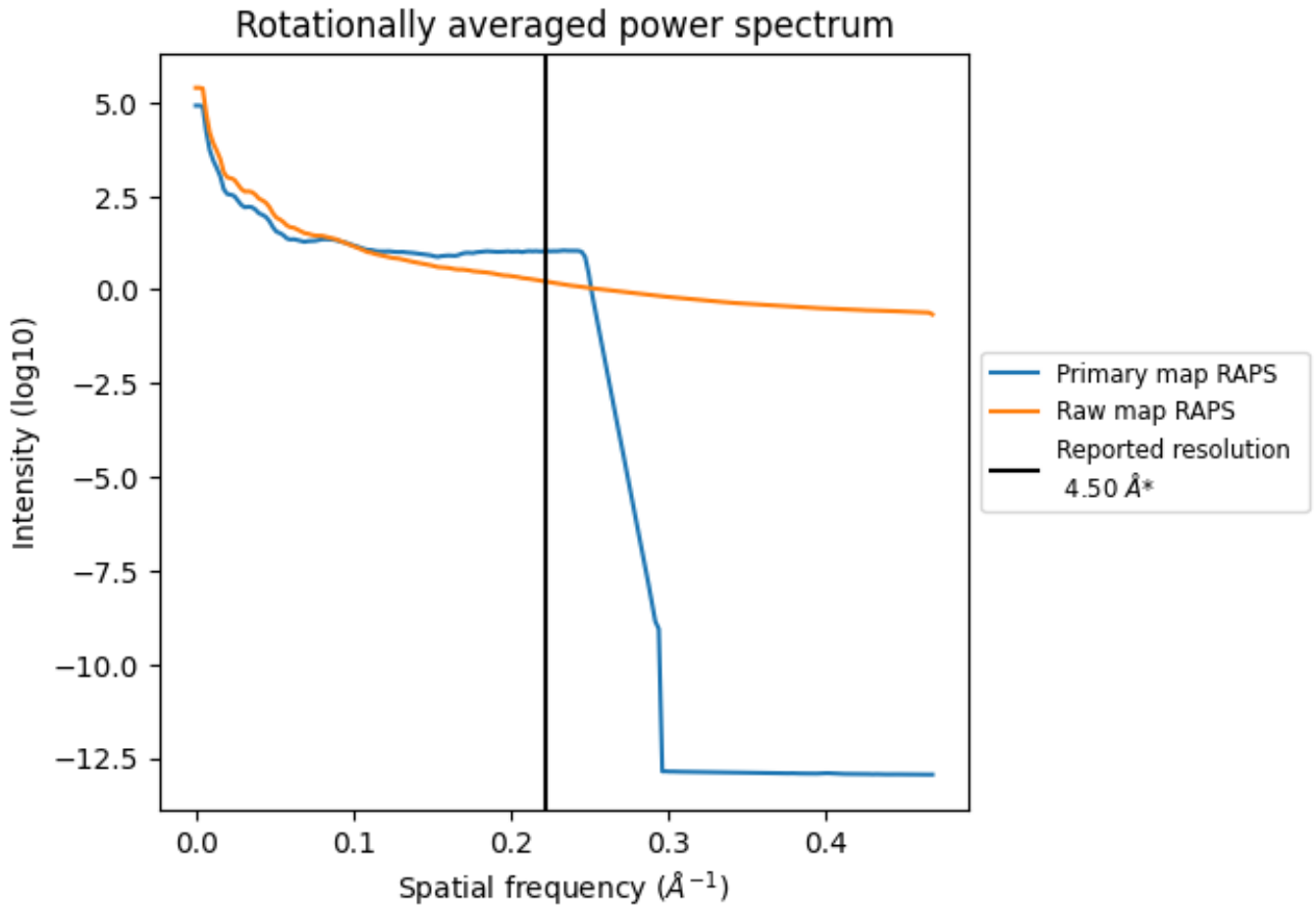
7.2 Volume estimate (i)



The volume at the recommended contour level is 1311 nm^3; this corresponds to an approximate mass of 1184 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)

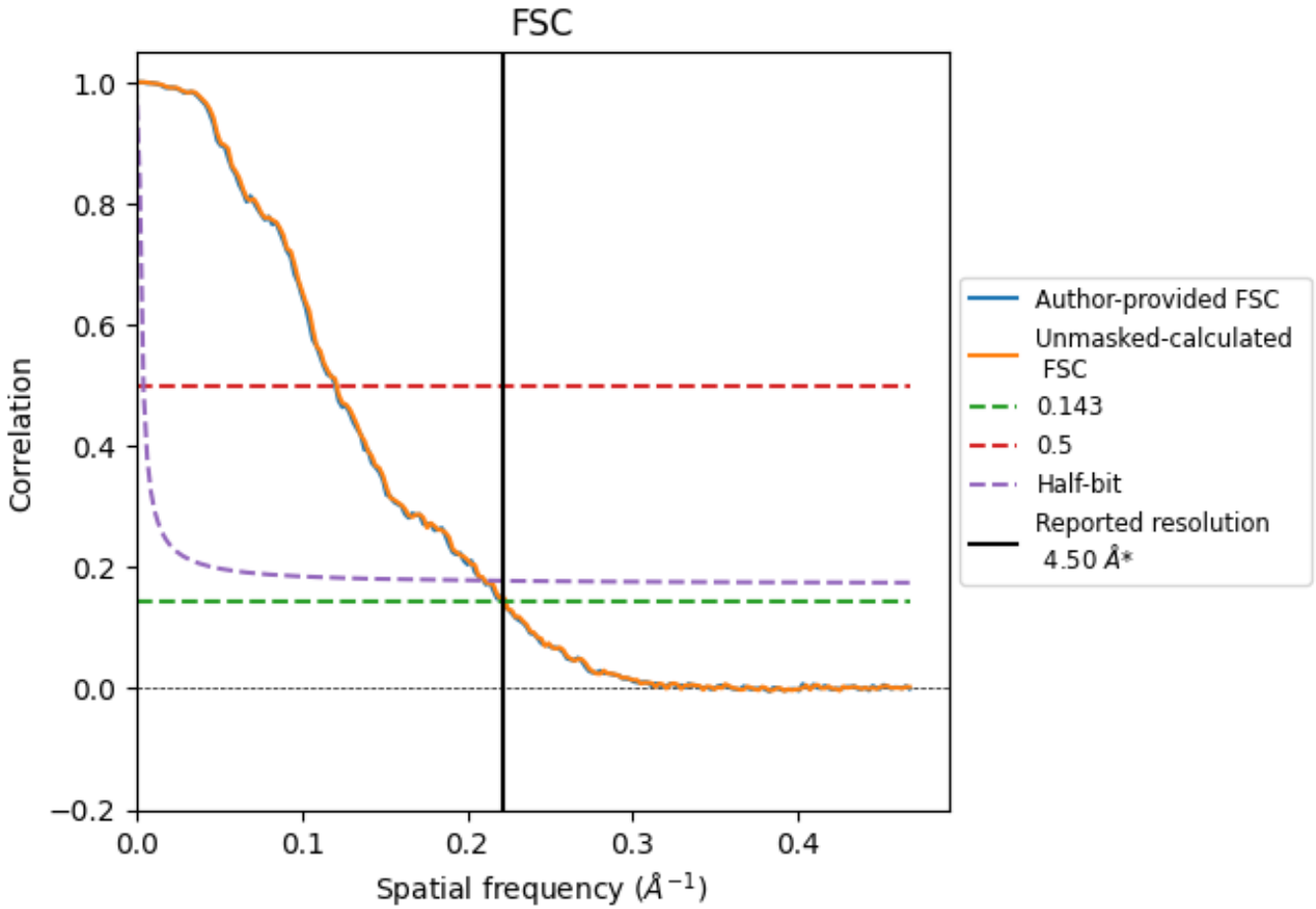


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

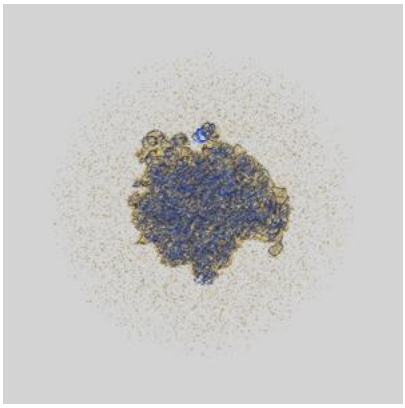
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.51	8.31	4.76
Unmasked-calculated*	4.48	8.26	4.75

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

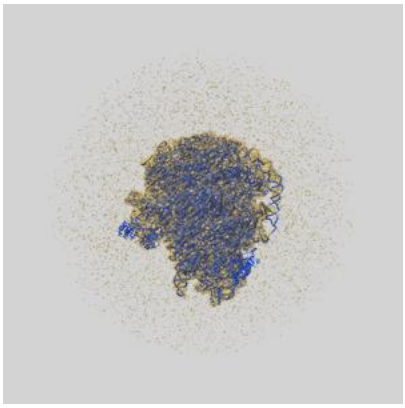
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-69697 and PDB model 24NM. Per-residue inclusion information can be found in section 3 on page 16.

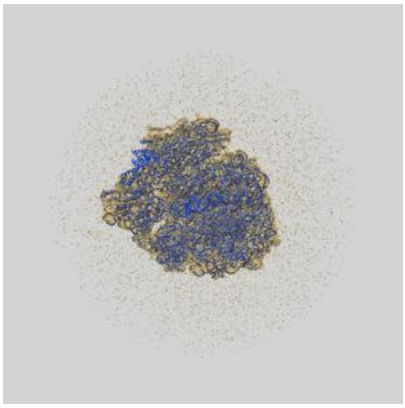
9.1 Map-model overlay



X



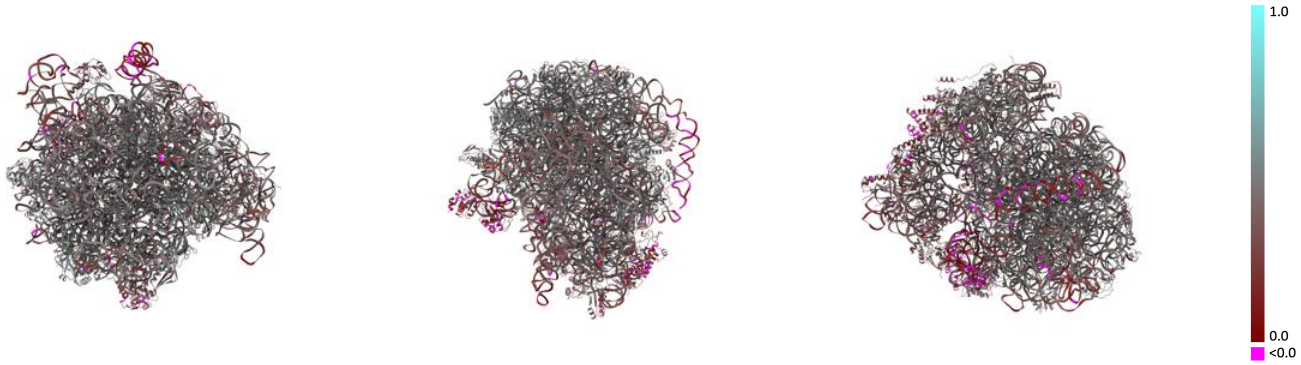
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

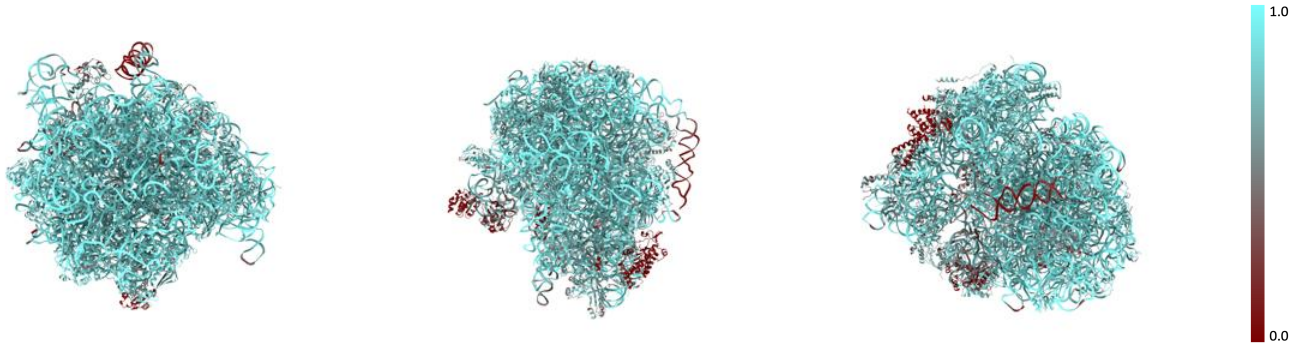
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

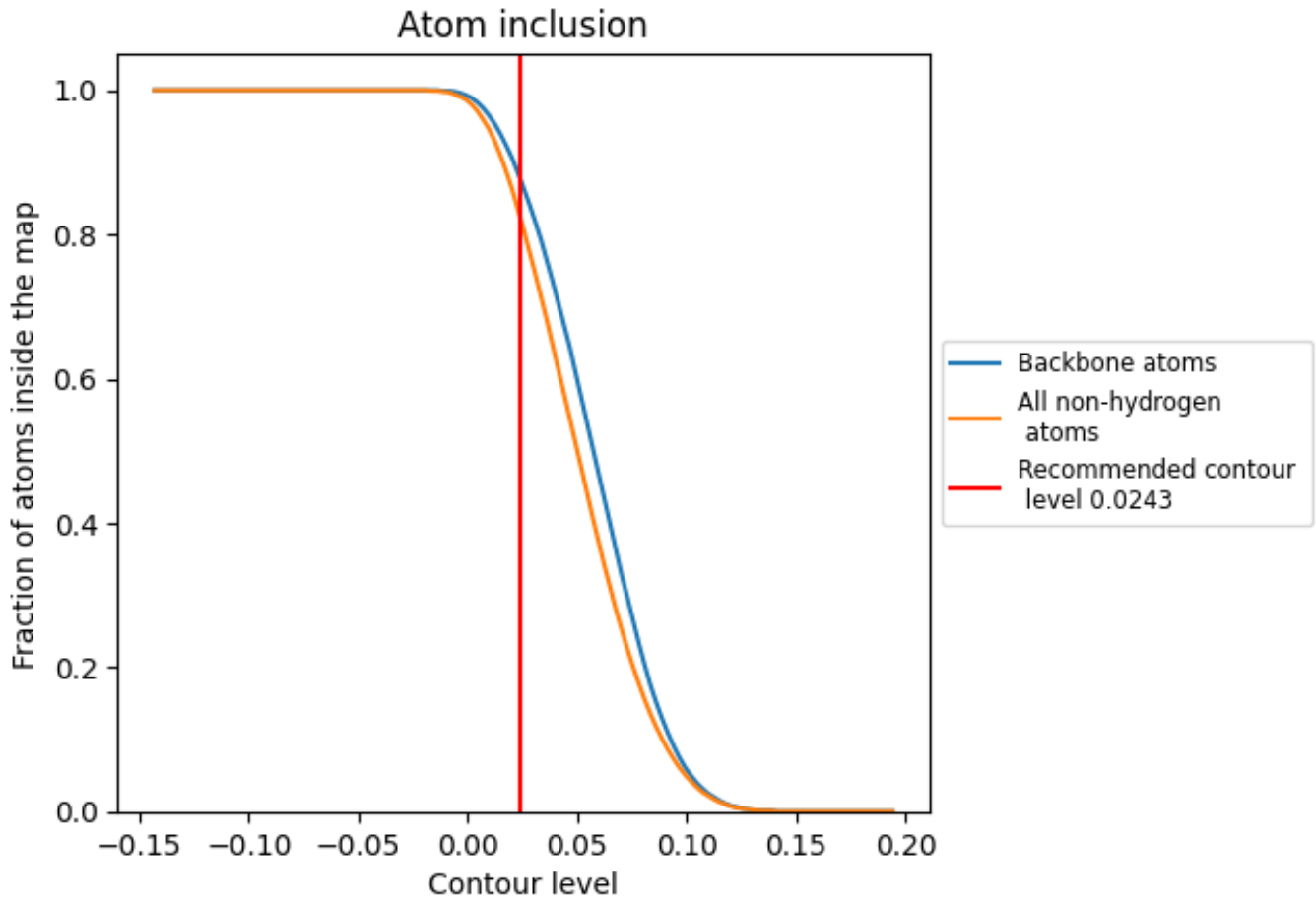
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0243).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.0243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.3980
1	0.7600	0.4310
2	0.7650	0.3330
3	0.7210	0.4680
4	0.6430	0.2210
5	0.4590	0.3060
6	0.1830	0.0940
A	0.8910	0.3890
B	0.9240	0.4070
C	0.6890	0.3980
D	0.7040	0.3790
E	0.7600	0.4330
F	0.7560	0.4320
G	0.6400	0.3480
H	0.8360	0.4620
I	0.7090	0.3820
J	0.6390	0.3440
K	0.8090	0.4680
L	0.7830	0.4730
M	0.6990	0.3890
N	0.7990	0.4350
O	0.8140	0.4400
P	0.7930	0.4210
Q	0.7700	0.4240
R	0.8490	0.4590
S	0.6790	0.3480
T	0.7840	0.3990
U	0.8040	0.4530
V	0.0440	0.2200
W	0.7480	0.4250
X	0.8150	0.4720
Y	0.8300	0.4860
Z	0.8180	0.4260
a	0.8260	0.4700
b	0.8330	0.4640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.8200	0.4700
d	0.8420	0.4830
e	0.8310	0.4960
f	0.8260	0.4710
g	0.7400	0.3390
h	0.8790	0.4040
i	0.8250	0.4780
j	0.8500	0.4830
k	0.8430	0.4630
l	0.7160	0.3560
m	0.7750	0.3940
n	0.5330	0.3370
o	0.2350	0.1330
p	0.1110	0.1390
q	0.8540	0.4810
r	0.7850	0.4700
s	0.8400	0.4650
t	0.8040	0.4690
u	0.8310	0.4680
v	0.8210	0.4290
w	0.7790	0.4510
x	0.8470	0.4610
y	0.8690	0.4950
z	0.8360	0.4800