wwPDB EM Validation Summary Report

Oct 5, 2024 – 11:26 AM EDT

PDB ID	:	5KPV
EMDB ID	:	EMD-8280
Title	:	Structure of RelA bound to ribosome in presence of A/R tRNA (Structure II)
Authors	:	Loveland, A.B.; Bah, E.; Madireddy, R.; Zhang, Y.; Brilot, A.F.; Grigorieff, N.; Korostelev, A.A.
Deposited on	:	2016-07-05
Resolution	:	4.10 Å(reported)

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

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

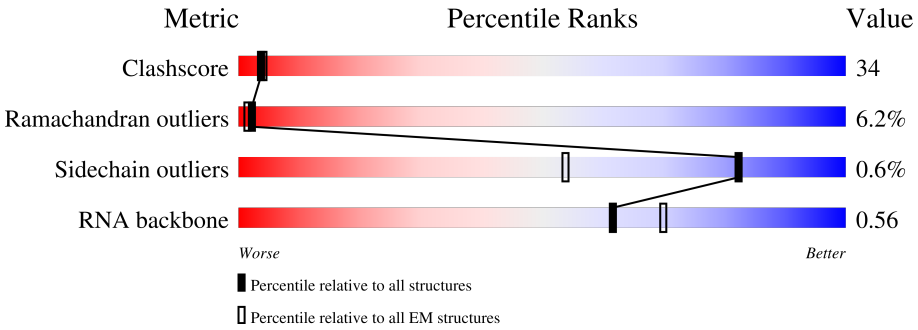
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.10 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	273	43% 53%
2	B	209	45% 53%
3	C	201	39% 55% 6%
4	D	179	34% 62%
5	E	177	46% 52%
6	F	149	42% 37% 54% 9%
7	G	165	25% 21% 52% 6% 21%

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Mol	Chain	Length	Quality of chain
8	H	142	14% 27% 67% 5%
9	I	142	44% 54%
10	J	123	37% 61%
11	K	144	43% 53%
12	L	136	49% 47%
13	M	127	43% 47% 5% 6%
14	N	117	35% 63%
15	O	115	42% 56%
16	P	118	41% 56%
17	Q	103	30% 62% 8%
18	R	110	46% 50%
19	S	100	39% 51% 7%
20	T	104	25% 68% 5%
21	U	94	36% 61%
22	V	85	52% 35% 12%
23	W	78	44% 55%
24	X	63	29% 63% 8%
25	Y	59	44% 54%
26	Z	70	37% 49% 9% 6%
27	1	57	32% 58% 9%
28	2	55	47% 44% 9%
29	3	46	46% 52%
30	4	65	46% 51%
31	5	38	34% 55% 11%
32	6	241	17% 37% 49% 10%

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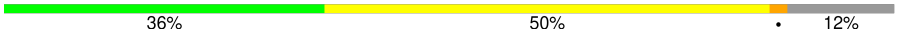
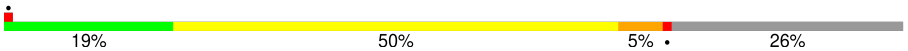
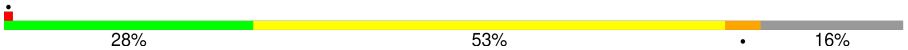
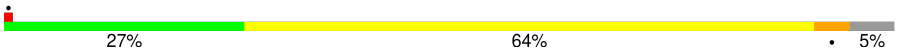
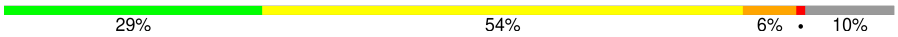
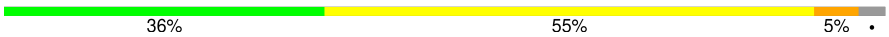
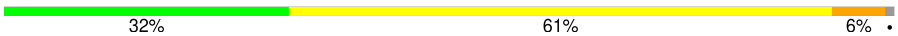
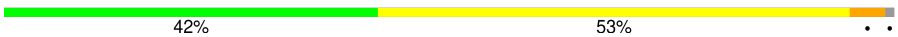
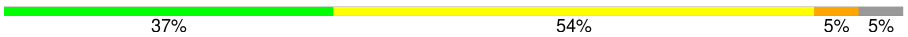
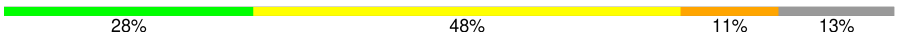
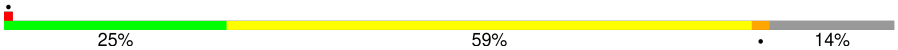
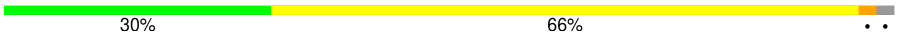
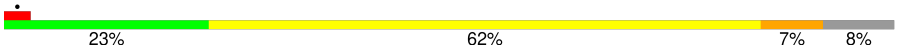
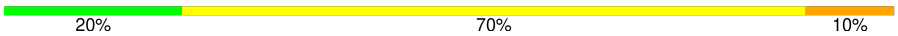
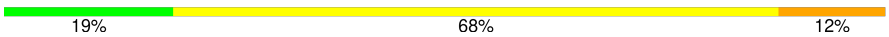
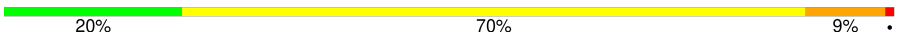
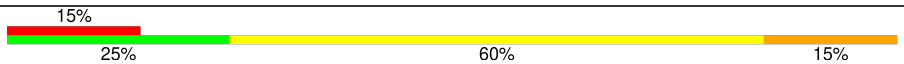
Mol	Chain	Length	Quality of chain
33	7	233	
34	8	206	
35	9	167	
36	10	135	
37	11	179	
38	12	130	
39	13	130	
40	14	103	
41	15	129	
42	16	124	
43	17	118	
44	18	101	
45	19	89	
46	20	82	
47	21	84	
48	22	75	
49	23	92	
50	24	87	
51	25	71	
52	26	1539	
53	27	2903	
54	28	120	
55	29	20	
56	30	76	
57	31	77	

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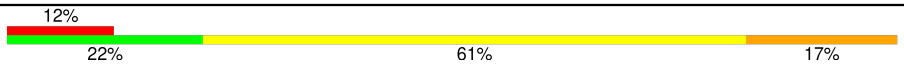
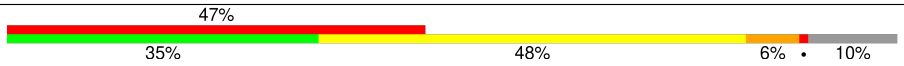
Mol	Chain	Length	Quality of chain
58	32	77	
59	33	750	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 154603 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 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	10	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	11	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	12	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	13	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	14	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	15	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	16	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	17	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	18	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	19	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	20	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	21	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	22	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	23	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	24	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	25	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	26	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	27	2903	Total	C	N	O	P	0	0
			62322	27801	11468	20150	2903		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
27	747	C	U	conflict	GB 802133627
27	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	28	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
28	120	A	-	conflict	GB 1028475309

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	29	20	Total	C	N	O	P	0	0
			432	195	86	132	19		

- Molecule 56 is a RNA chain called A-site tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	30	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 57 is a RNA chain called P-site tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	31	77	Total	C	N	O	P	0	0
			1644	732	297	538	77		

- Molecule 58 is a RNA chain called E-site tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	32	77	Total	C	N	O	P	0	0
			1643	732	297	537	77		

- Molecule 59 is a protein called GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	33	675	Total	C	N	O	S	0	0
			4911	3070	904	915	22		

There are 7 discrepancies between the modelled and reference sequences:

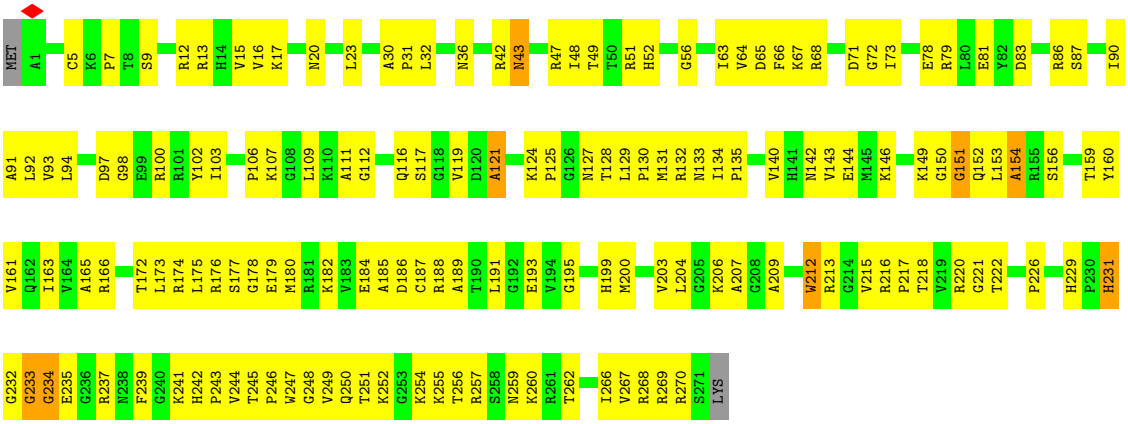
Chain	Residue	Modelled	Actual	Comment	Reference
33	-5	MET	-	expression tag	UNP P0AG20
33	-4	HIS	-	expression tag	UNP P0AG20
33	-3	HIS	-	expression tag	UNP P0AG20
33	-2	HIS	-	expression tag	UNP P0AG20
33	-1	HIS	-	expression tag	UNP P0AG20
33	0	HIS	-	expression tag	UNP P0AG20
33	1	HIS	-	expression tag	UNP P0AG20

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.

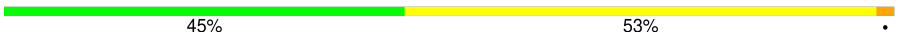
• Molecule 1: 50S ribosomal protein L2

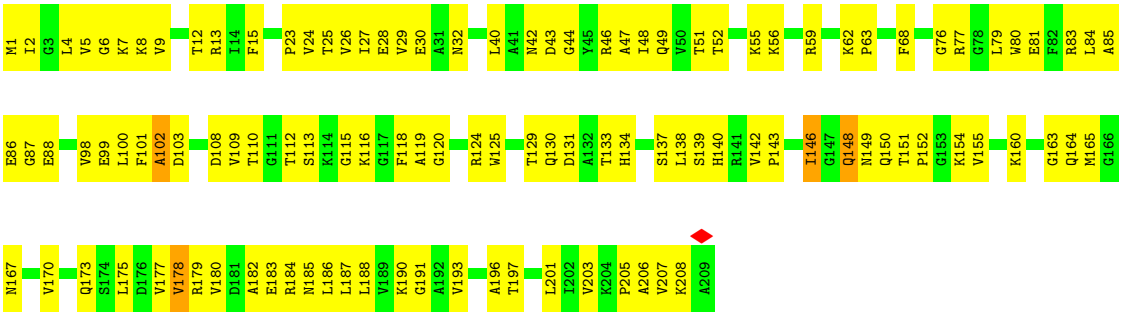
Chain A:



• Molecule 2: 50S ribosomal protein L3

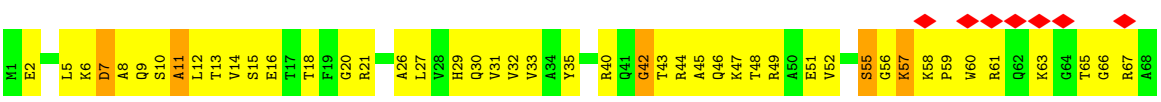
Chain B:

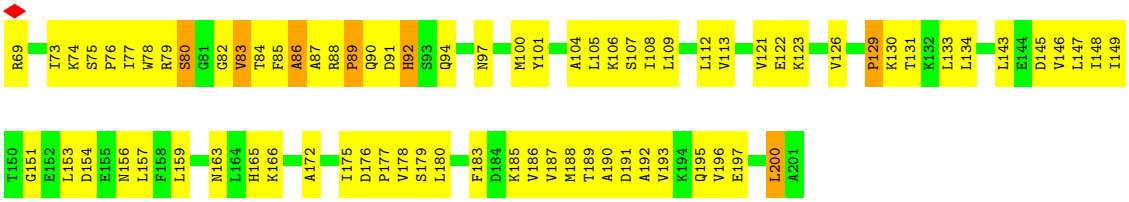




• Molecule 3: 50S ribosomal protein L4

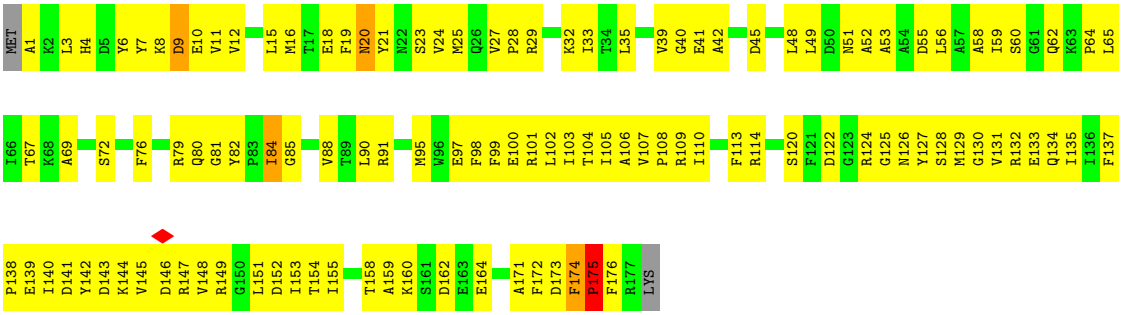
Chain C:





• Molecule 4: 50S ribosomal protein L5

Chain D:

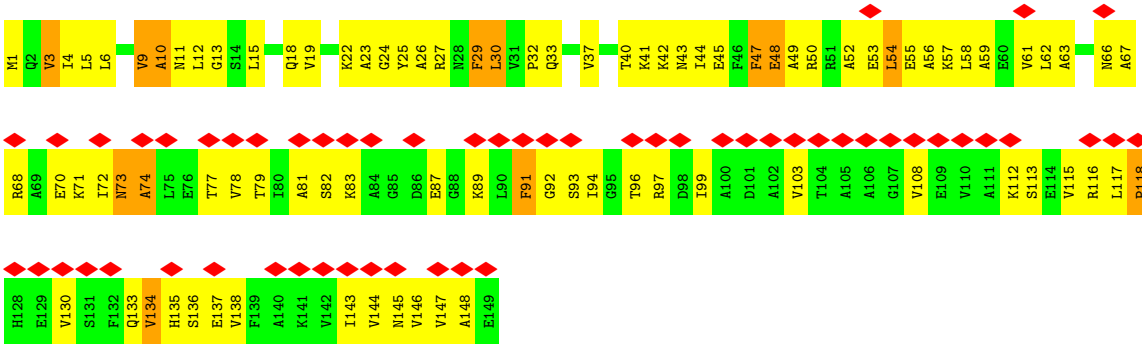


• Molecule 5: 50S ribosomal protein L6

Chain E:

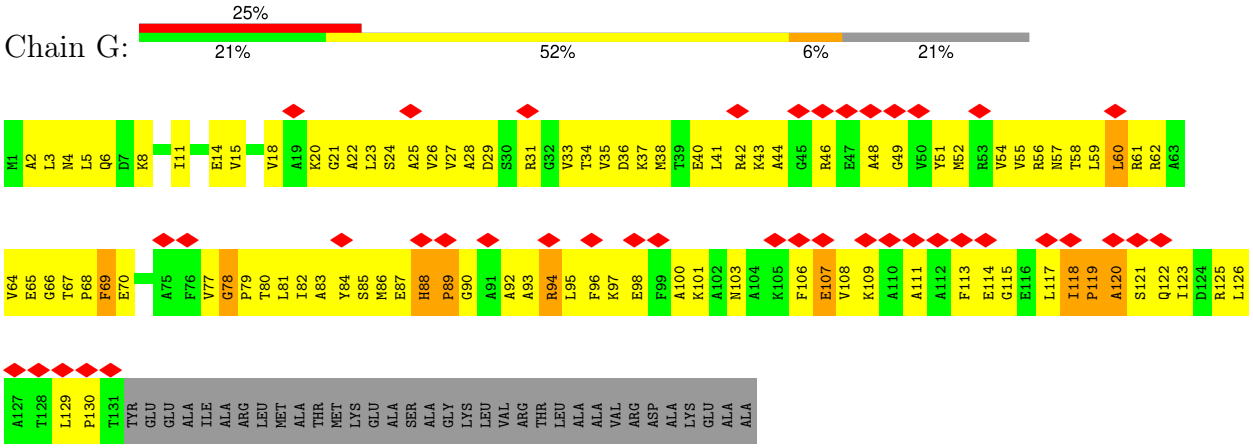
• Molecule 6: 50S ribosomal protein L9

Chain F:



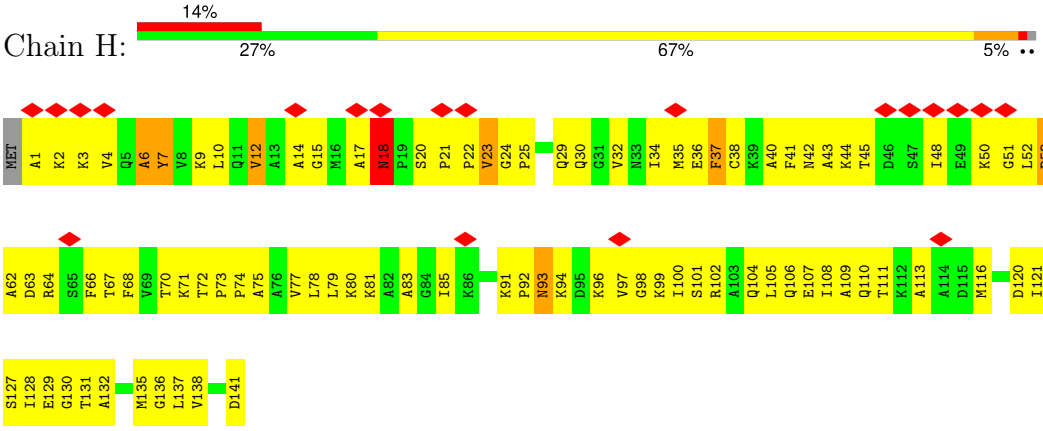
• Molecule 7: 50S ribosomal protein L10

Chain G:



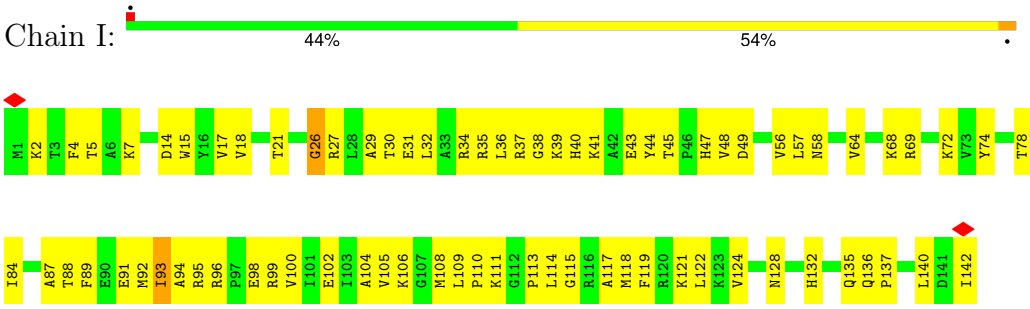
• Molecule 8: 50S ribosomal protein L11

Chain H:



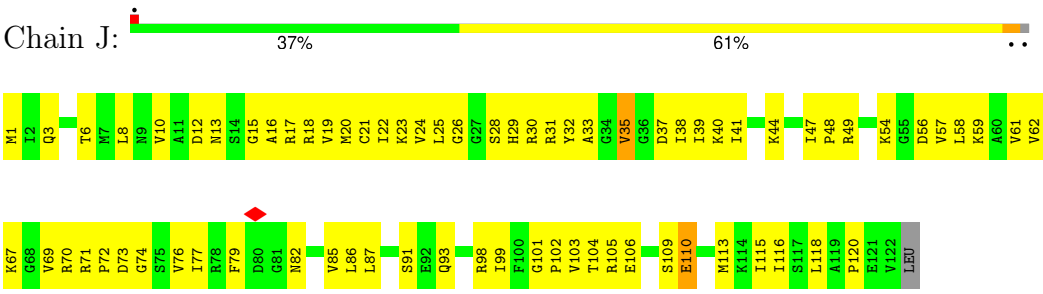
• Molecule 9: 50S ribosomal protein L13

Chain I:



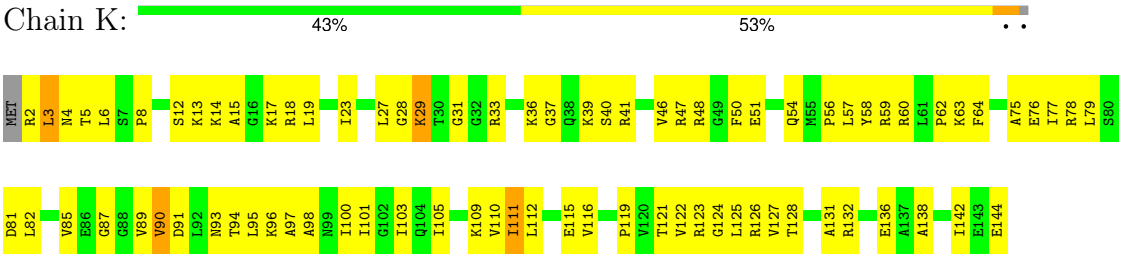
• Molecule 10: 50S ribosomal protein L14

Chain J:



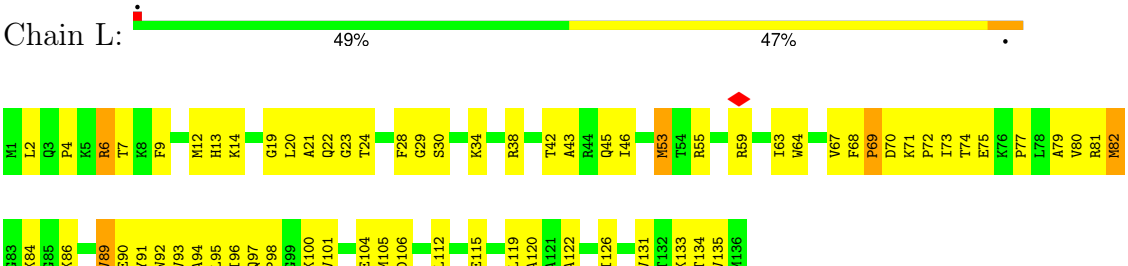
• Molecule 11: 50S ribosomal protein L15

Chain K:



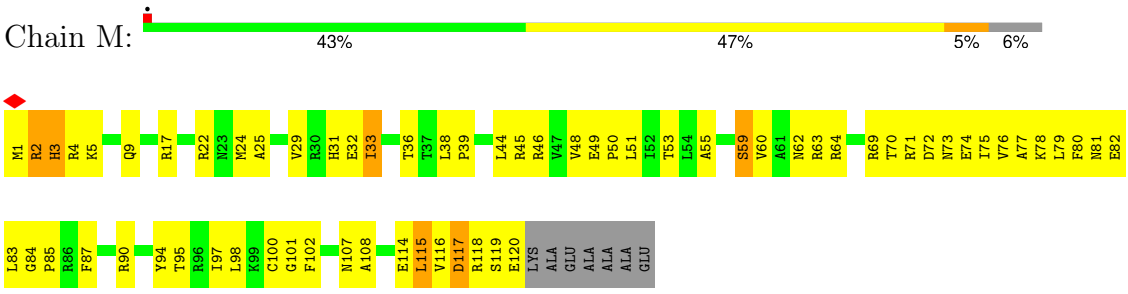
• Molecule 12: 50S ribosomal protein L16

Chain L:



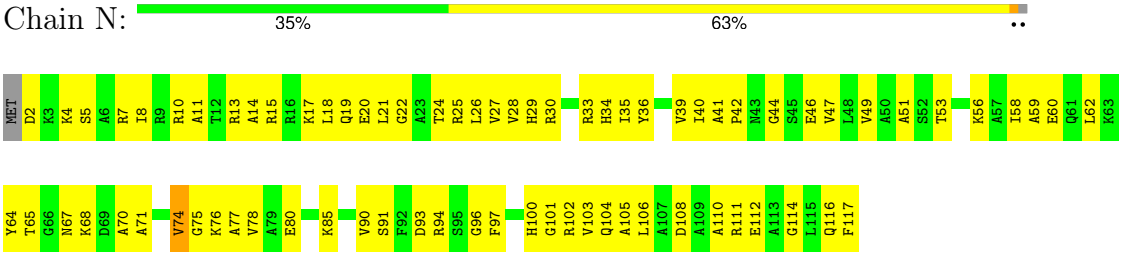
• Molecule 13: 50S ribosomal protein L17

Chain M:



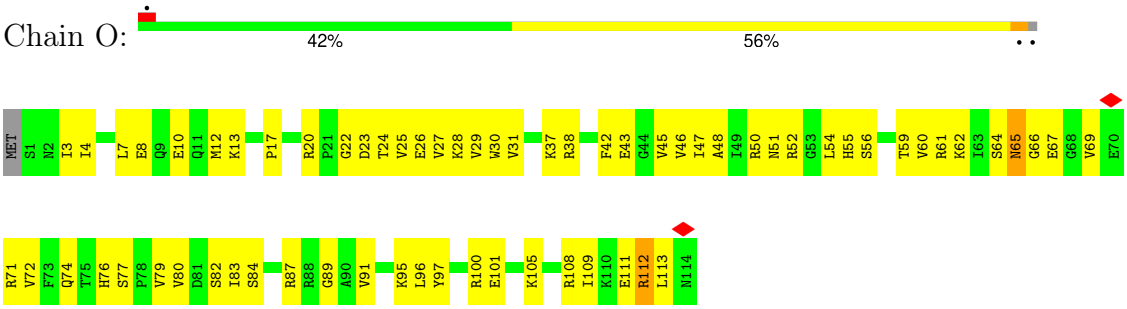
• Molecule 14: 50S ribosomal protein L18

Chain N:



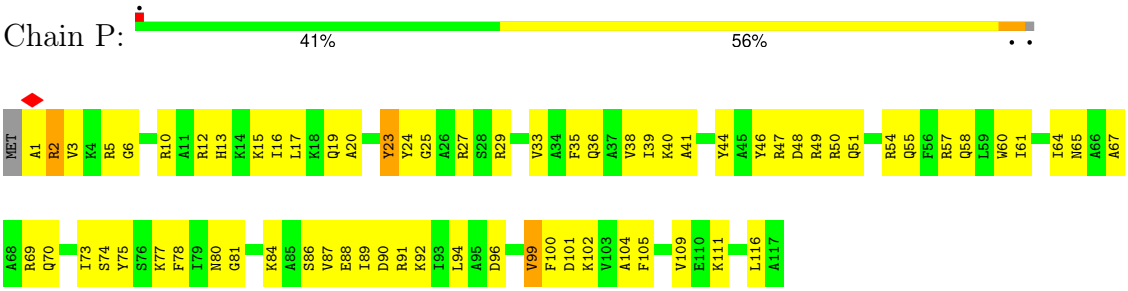
• Molecule 15: 50S ribosomal protein L19

Chain O:



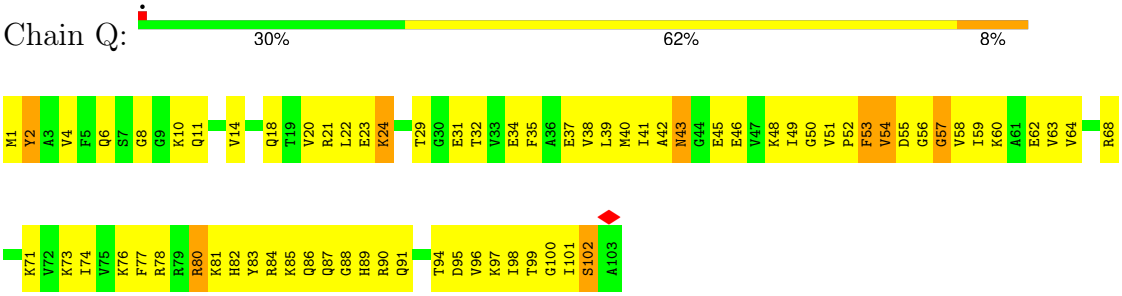
• Molecule 16: 50S ribosomal protein L20

Chain P:



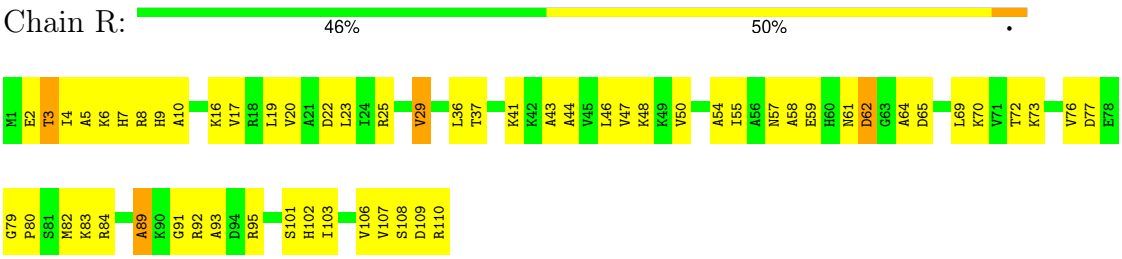
• Molecule 17: 50S ribosomal protein L21

Chain Q:



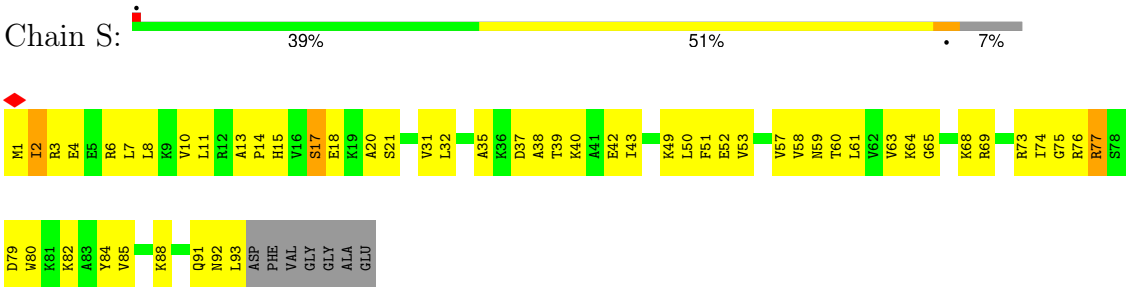
• Molecule 18: 50S ribosomal protein L22

Chain R:



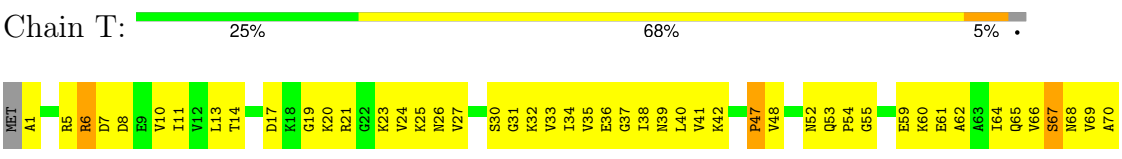
• Molecule 19: 50S ribosomal protein L23

Chain S:



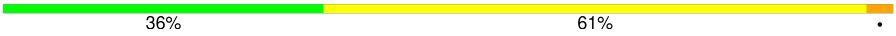
• Molecule 20: 50S ribosomal protein L24

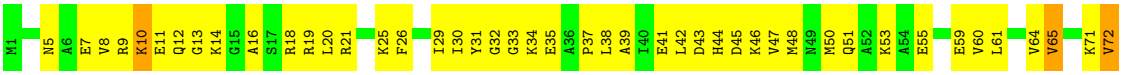
Chain T:

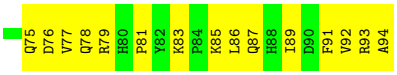


• Molecule 21: 50S ribosomal protein L25

Chain U:

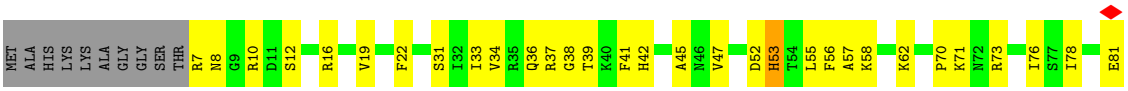






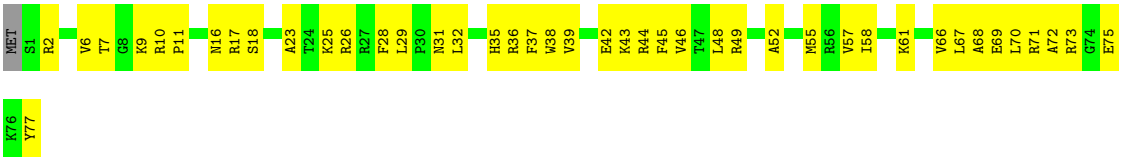
• Molecule 22: 50S ribosomal protein L27

Chain V:



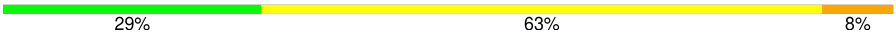
• Molecule 23: 50S ribosomal protein L28

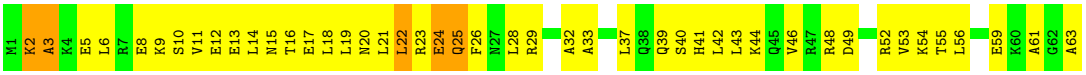
Chain W:



• Molecule 24: 50S ribosomal protein L29

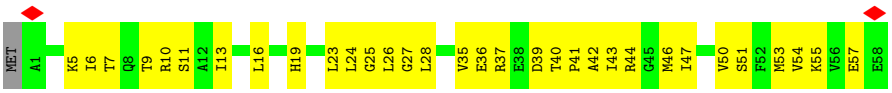
Chain X:





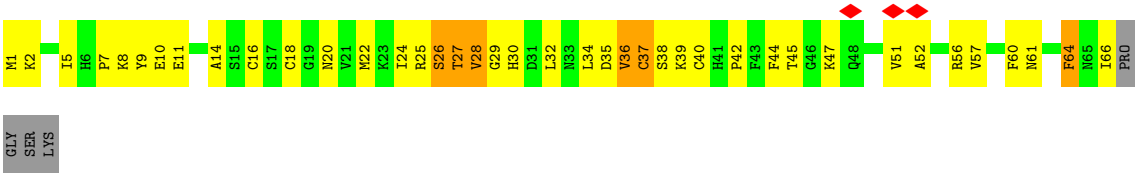
• Molecule 25: 50S ribosomal protein L30

Chain Y:



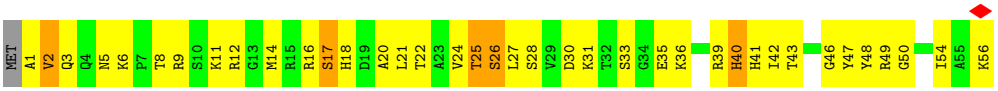
• Molecule 26: 50S ribosomal protein L31

Chain Z:



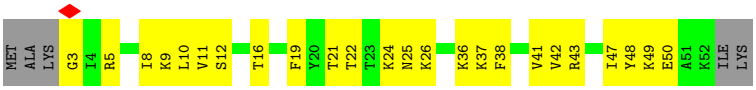
• Molecule 27: 50S ribosomal protein L32

Chain 1:



• Molecule 28: 50S ribosomal protein L33

Chain 2:

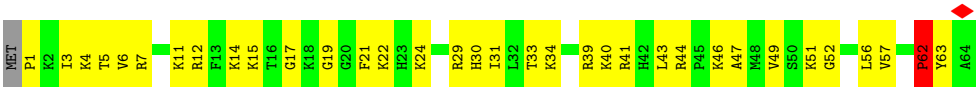


• Molecule 29: 50S ribosomal protein L34

Chain 3:

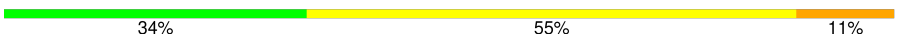
• Molecule 30: 50S ribosomal protein L35

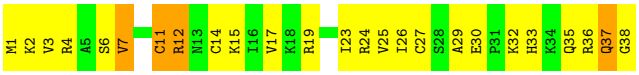
Chain 4:



• Molecule 31: 50S ribosomal protein L36

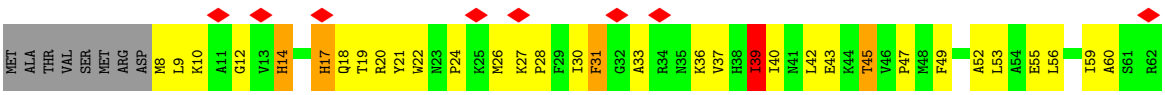
Chain 5:

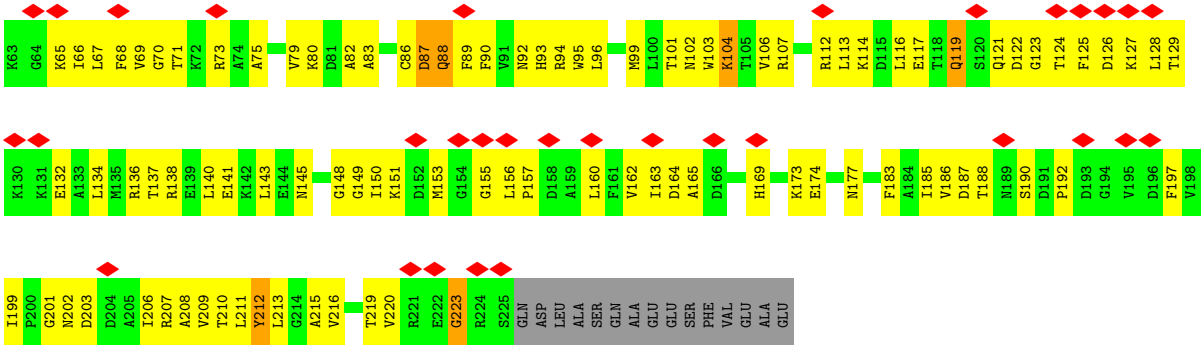




• Molecule 32: 30S ribosomal protein S2

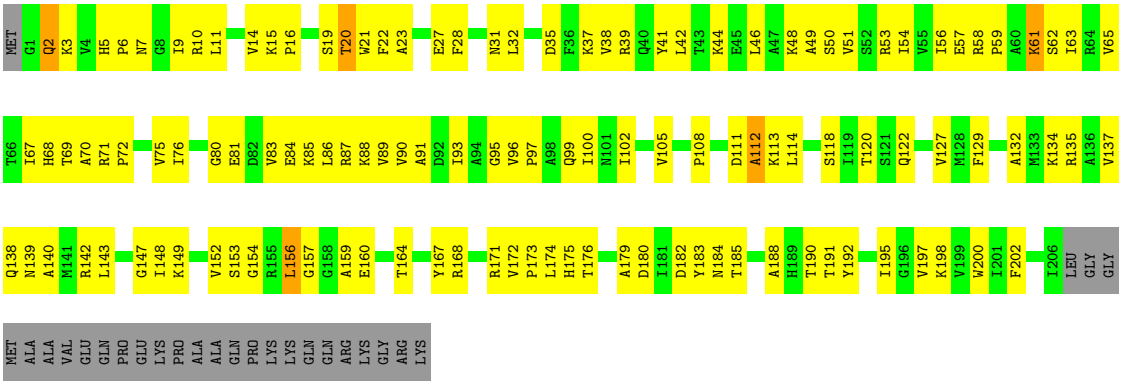
Chain 6:





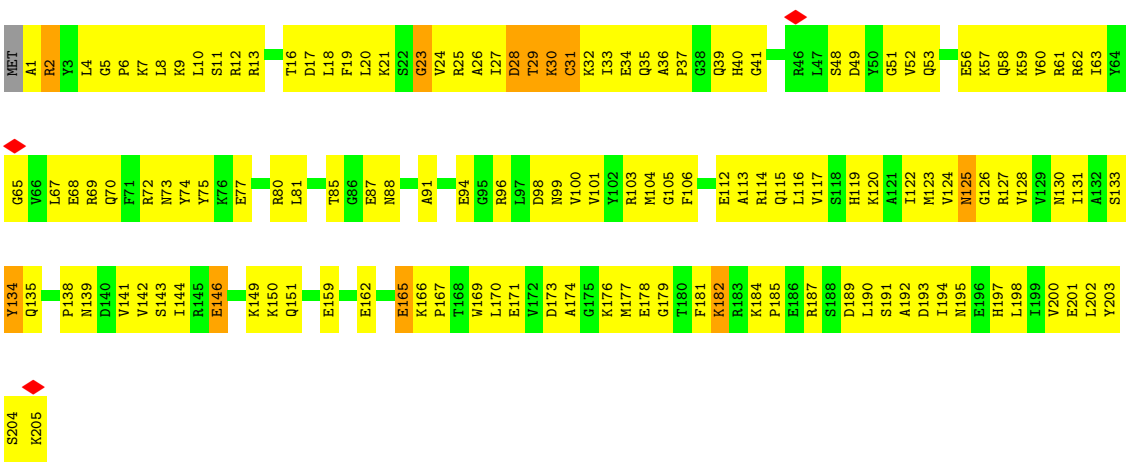
• Molecule 33: 30S ribosomal protein S3

Chain 7:



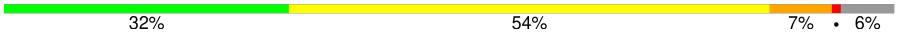
• Molecule 34: 30S ribosomal protein S4

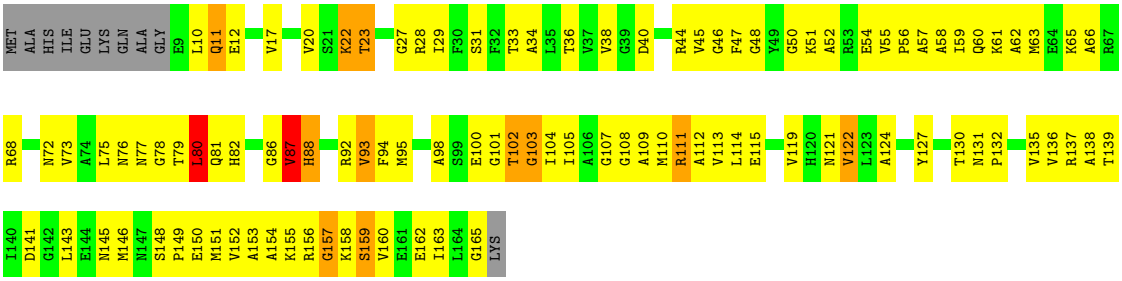
Chain 8:



• Molecule 35: 30S ribosomal protein S5

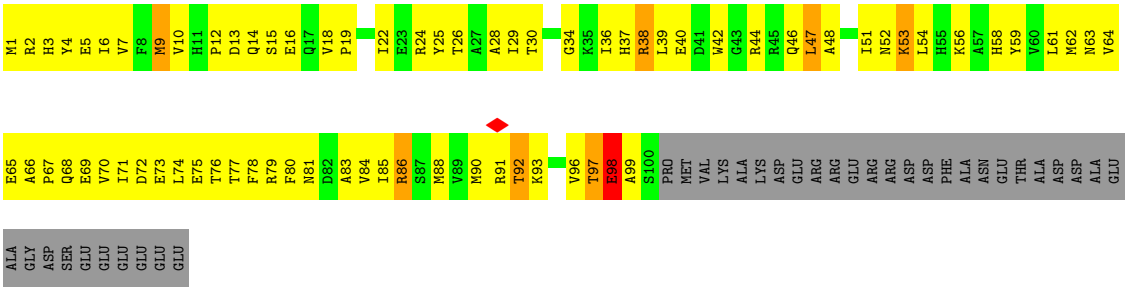
Chain 9:





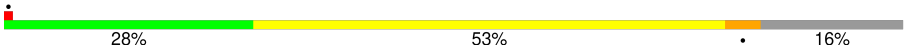
• Molecule 36: 30S ribosomal protein S6

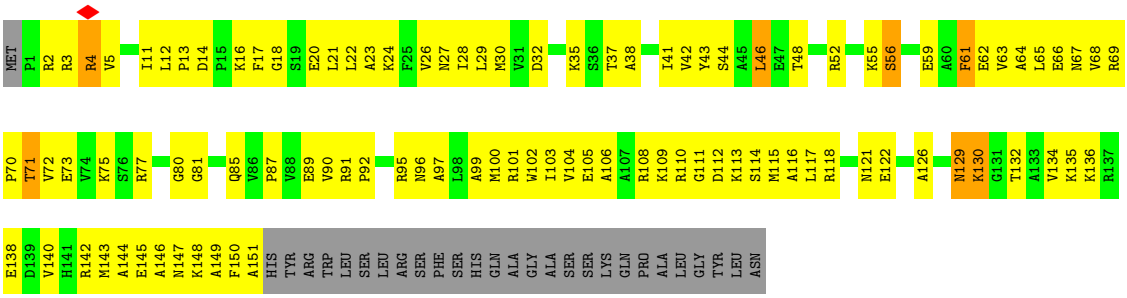
Chain 10:



• Molecule 37: 30S ribosomal protein S7

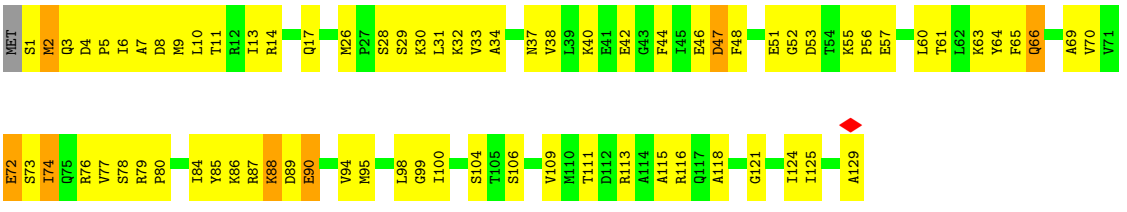
Chain 11:





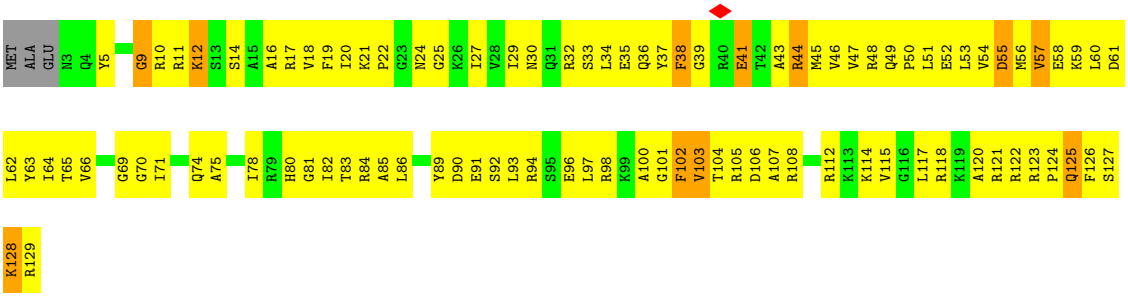
• Molecule 38: 30S ribosomal protein S8

Chain 12:



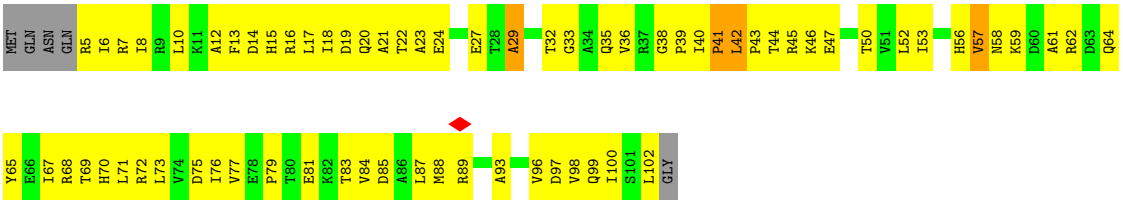
• Molecule 39: 30S ribosomal protein S9

Chain 13:



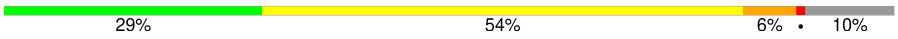
• Molecule 40: 30S ribosomal protein S10

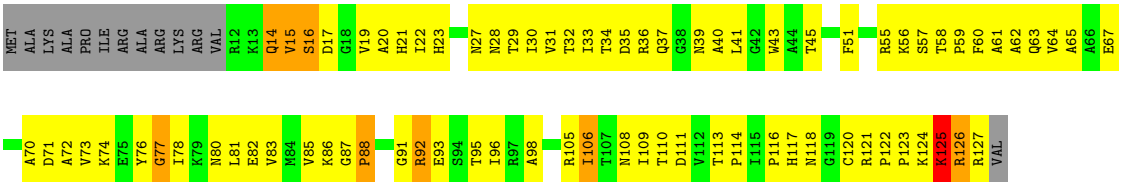
Chain 14:



• Molecule 41: 30S ribosomal protein S11

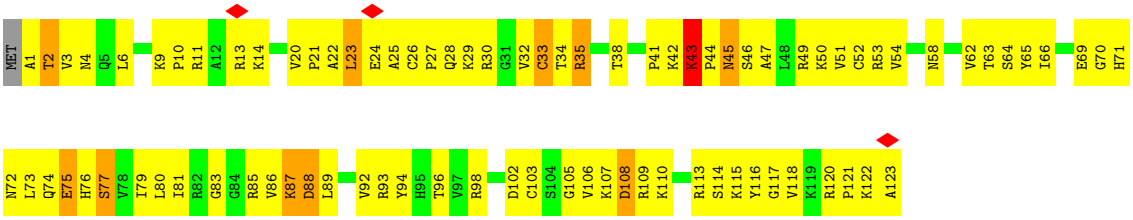
Chain 15:





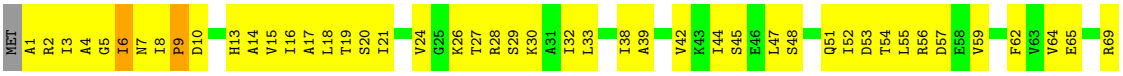
• Molecule 42: 30S ribosomal protein S12

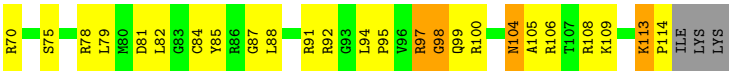
Chain 16:



• Molecule 43: 30S ribosomal protein S13

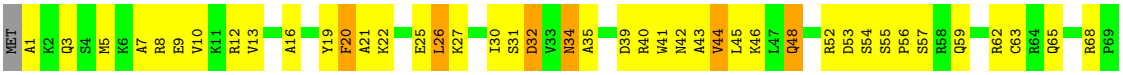
Chain 17:

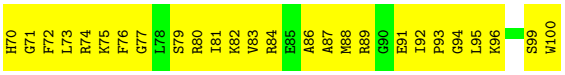




• Molecule 44: 30S ribosomal protein S14

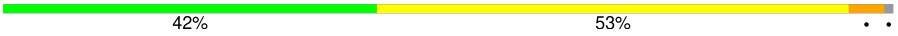
Chain 18:

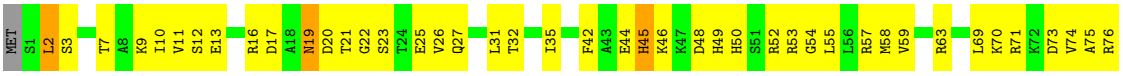


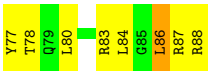


• Molecule 45: 30S ribosomal protein S15

Chain 19:





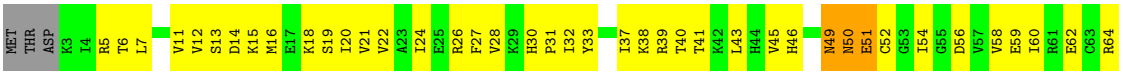


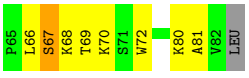
• Molecule 46: 30S ribosomal protein S16

Chain 20:

• Molecule 47: 30S ribosomal protein S17

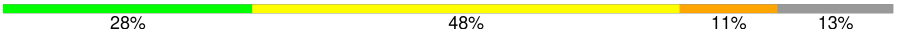
Chain 21:





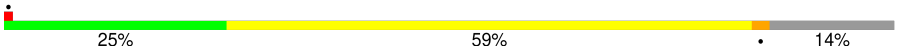
• Molecule 48: 30S ribosomal protein S18

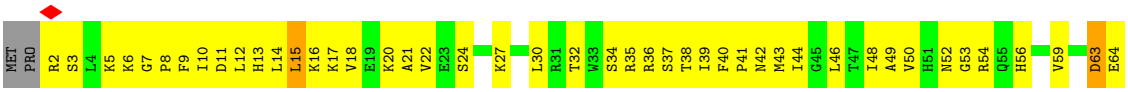
Chain 22:

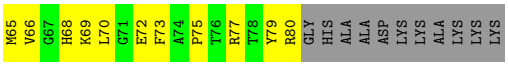


• Molecule 49: 30S ribosomal protein S19

Chain 23:





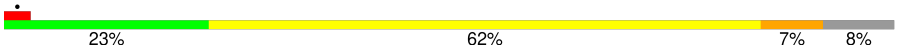


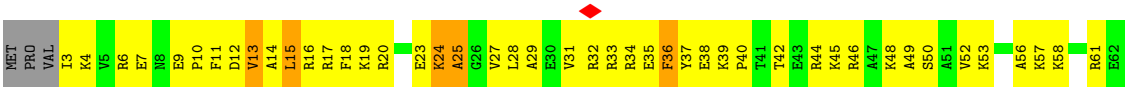
• Molecule 50: 30S ribosomal protein S20

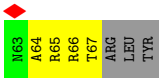
Chain 24:

• Molecule 51: 30S ribosomal protein S21

Chain 25:

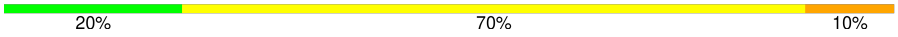


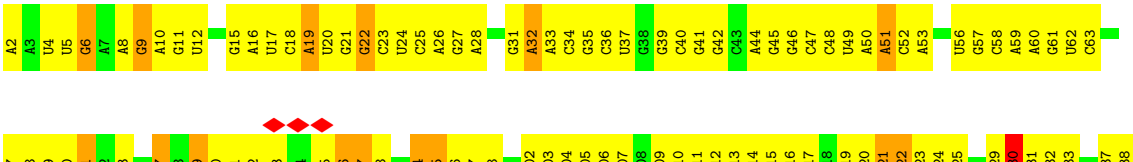


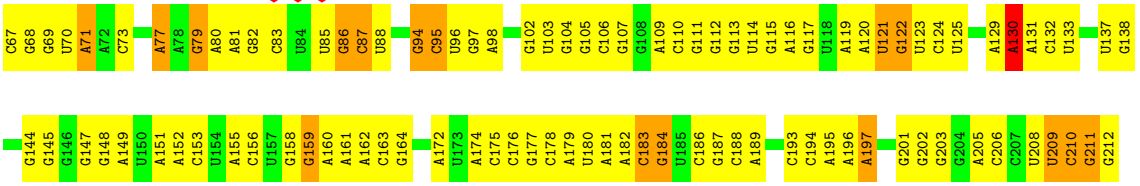


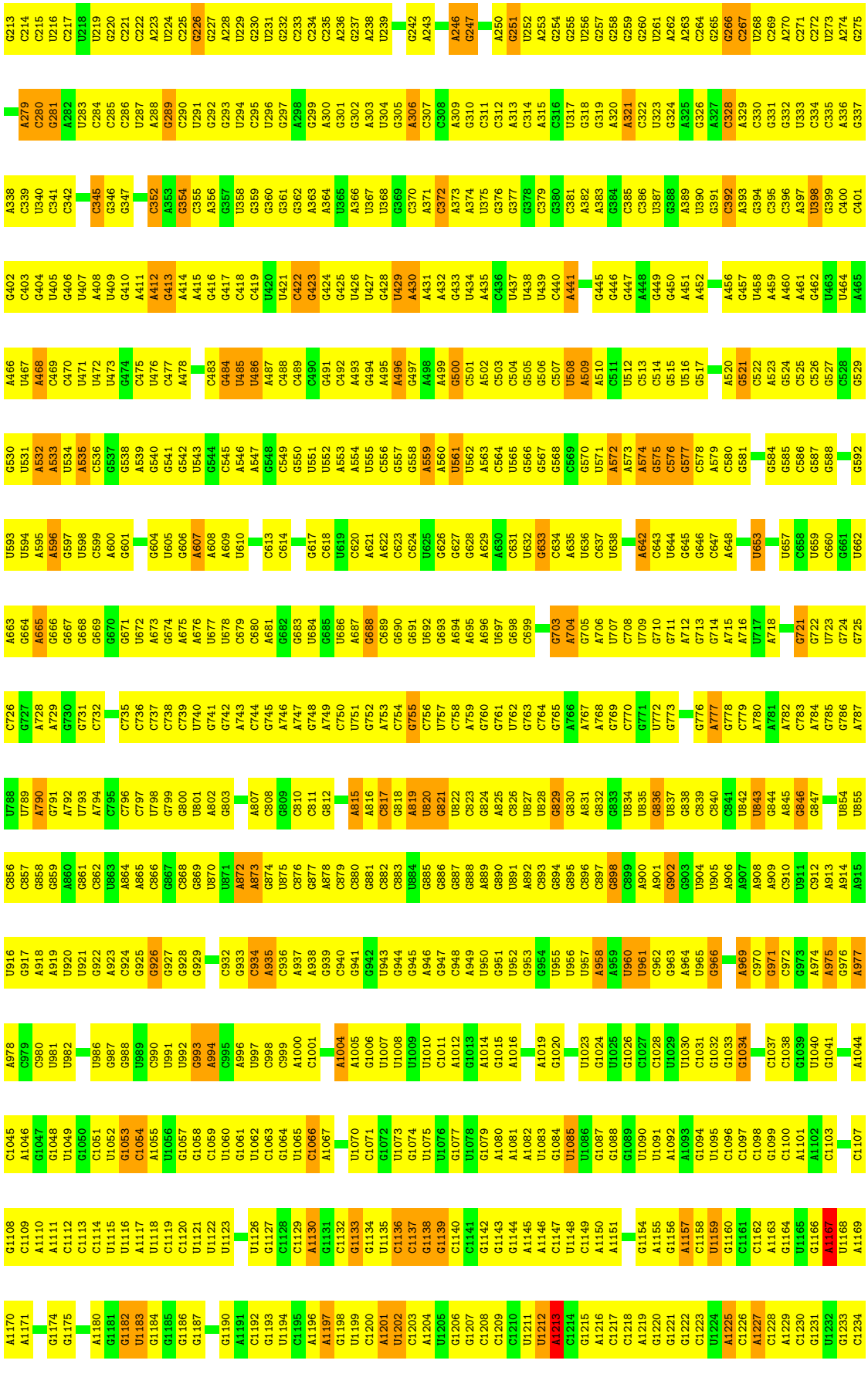
• Molecule 52: 16S ribosomal RNA

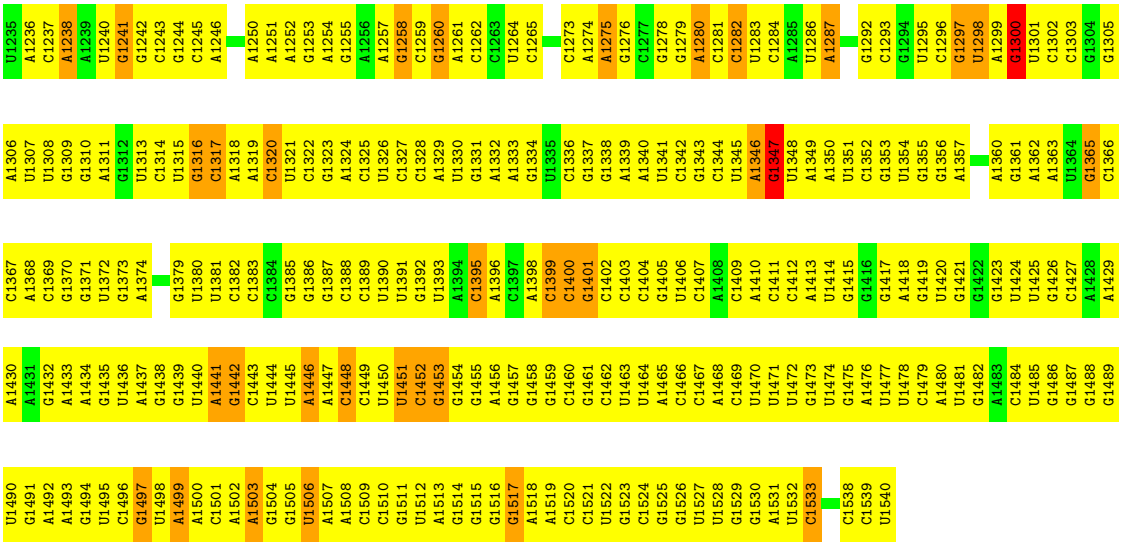
Chain 26:





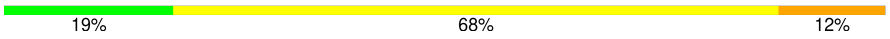


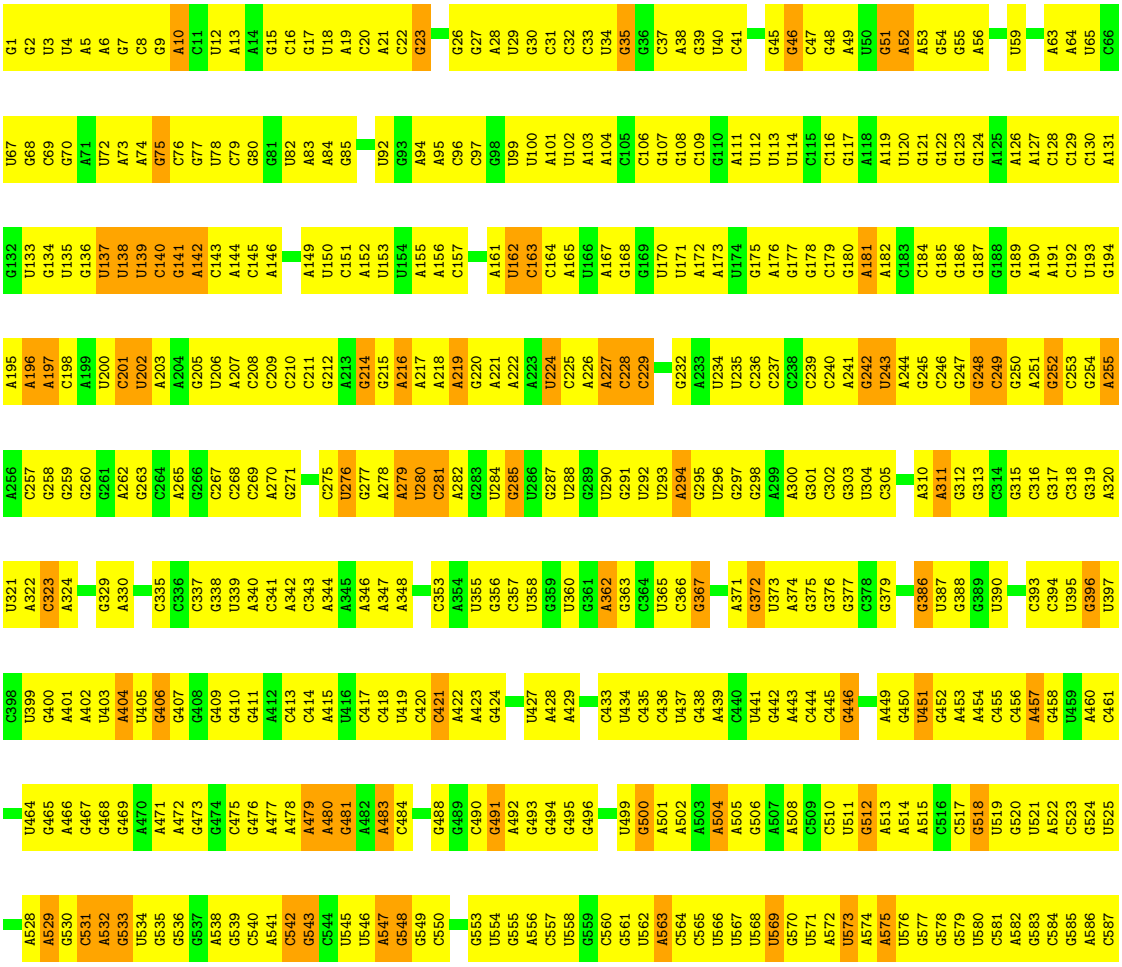


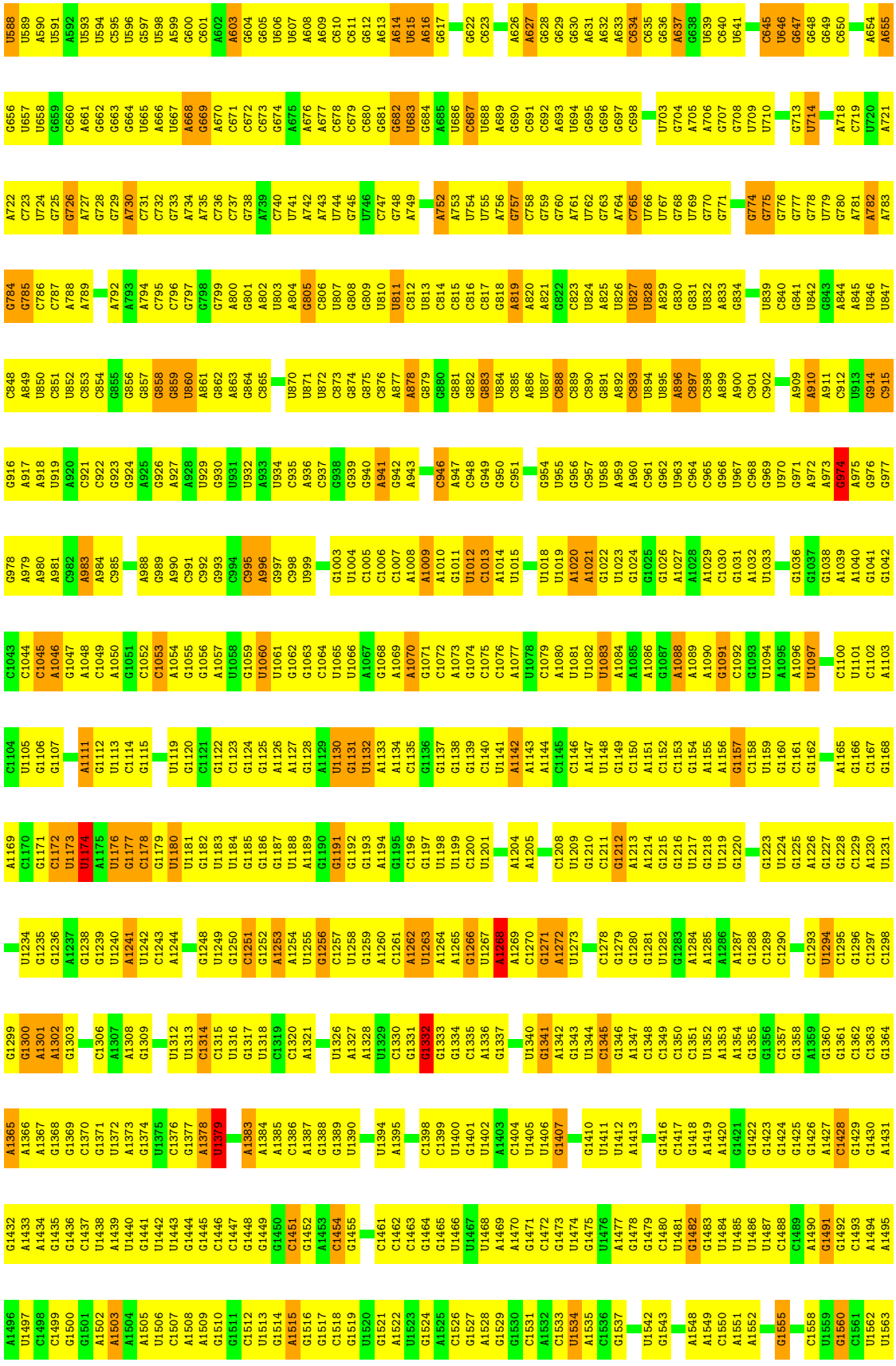


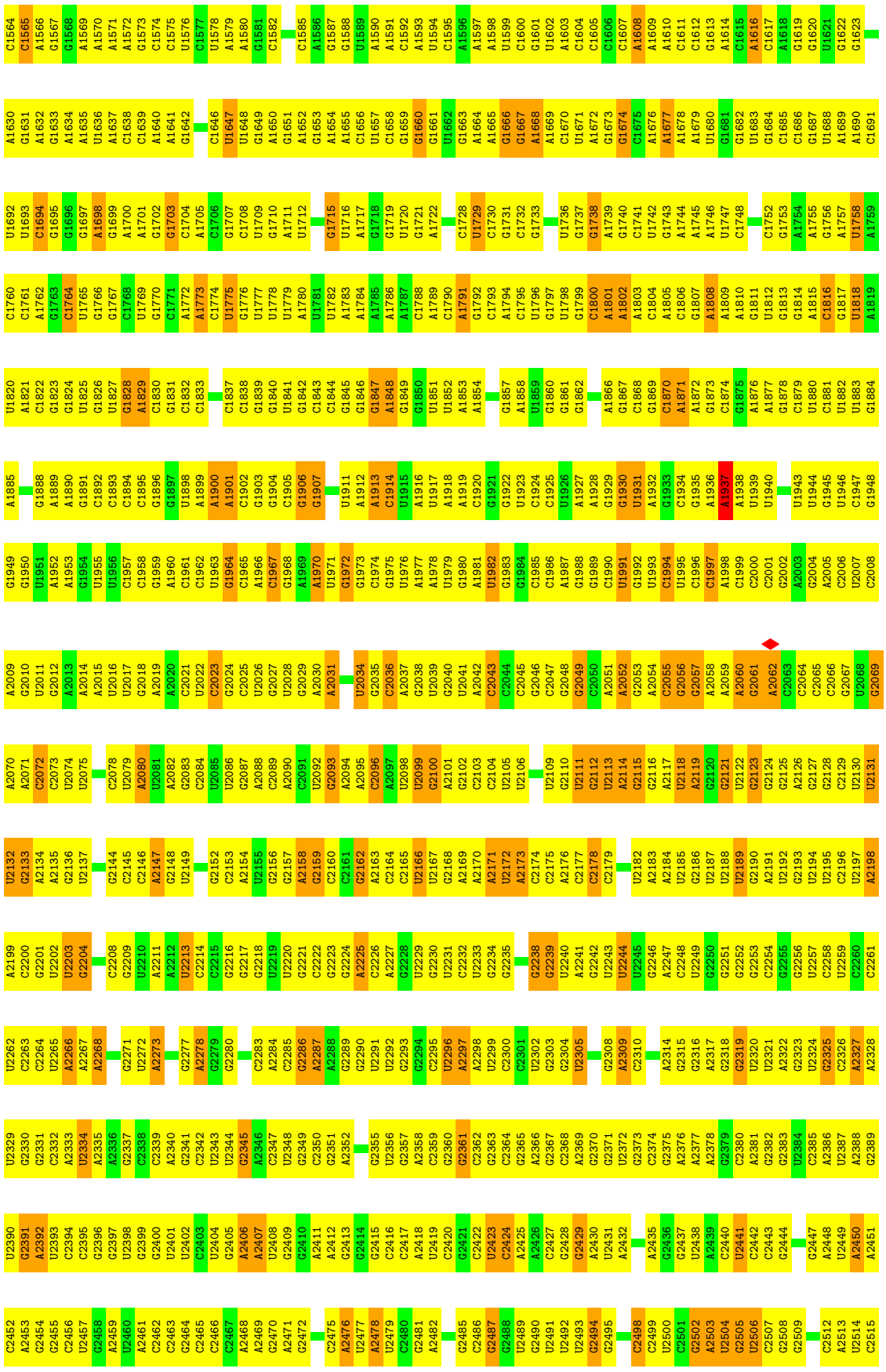
• Molecule 53: 23S ribosomal RNA

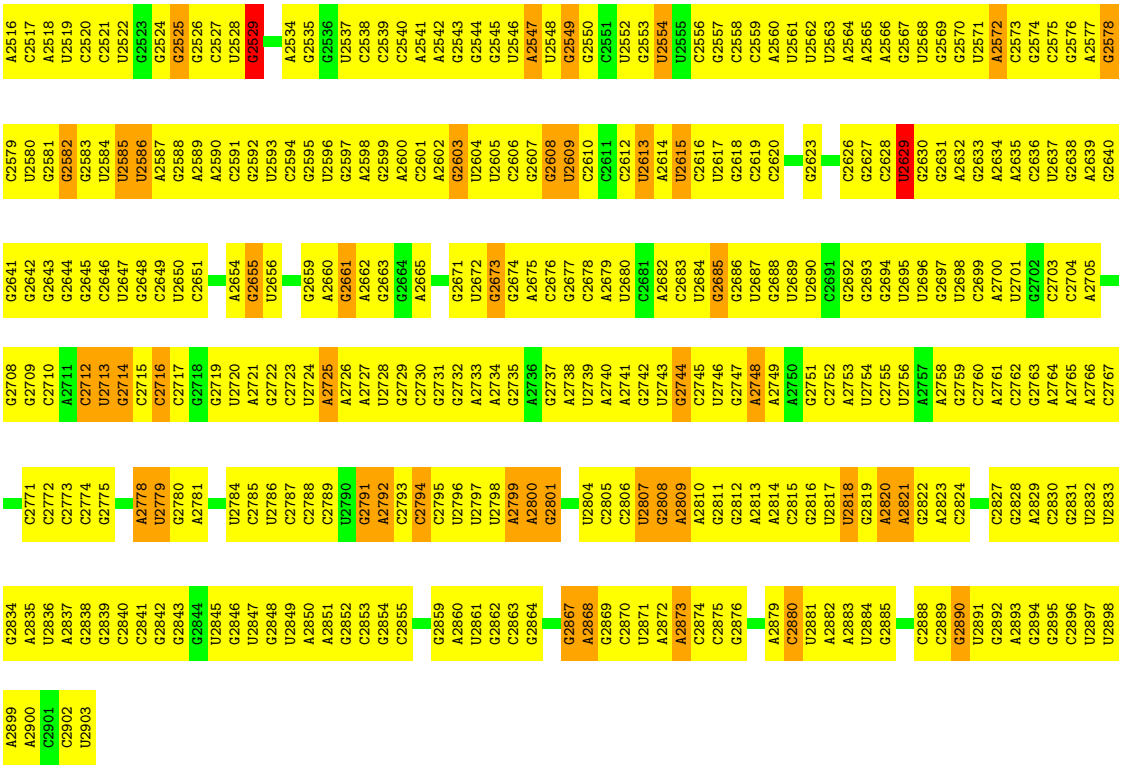
Chain 27:





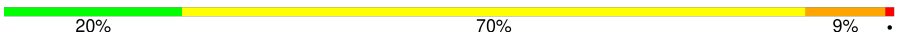


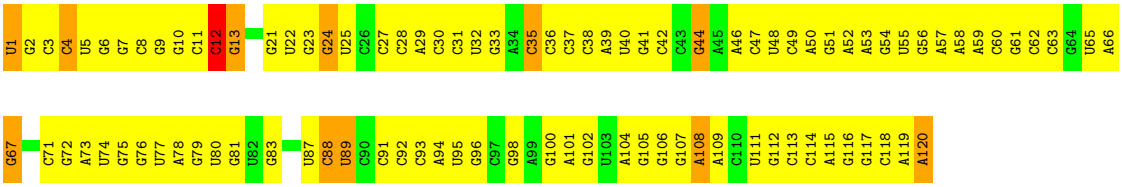




- Molecule 54: 5S ribosomal RNA

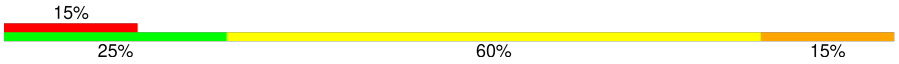
Chain 28:

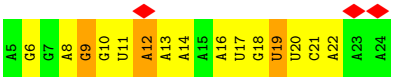




- Molecule 55: mRNA

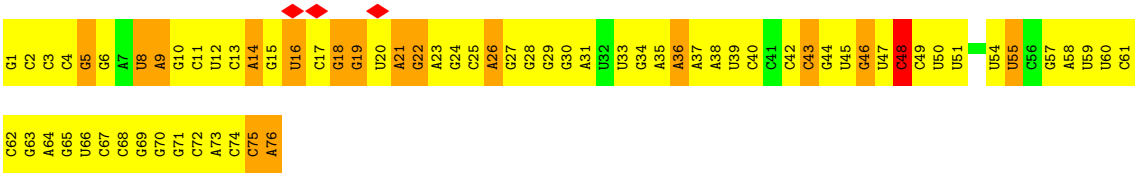
Chain 29:





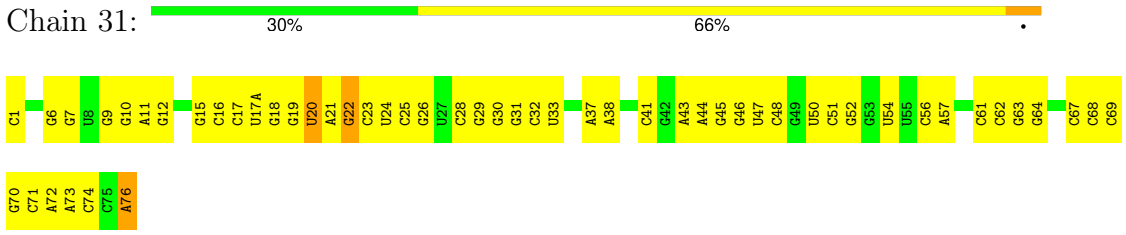
- Molecule 56: A-site tRNAPhe

Chain 30:



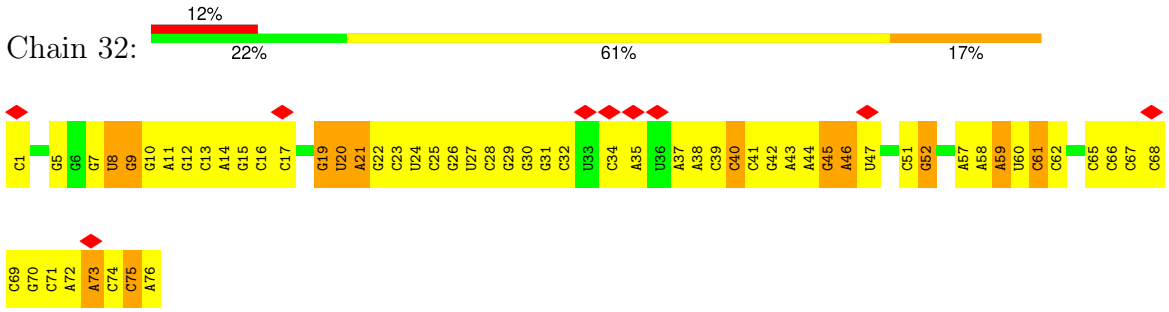
• Molecule 57: P-site tRNAfMet

Chain 31:



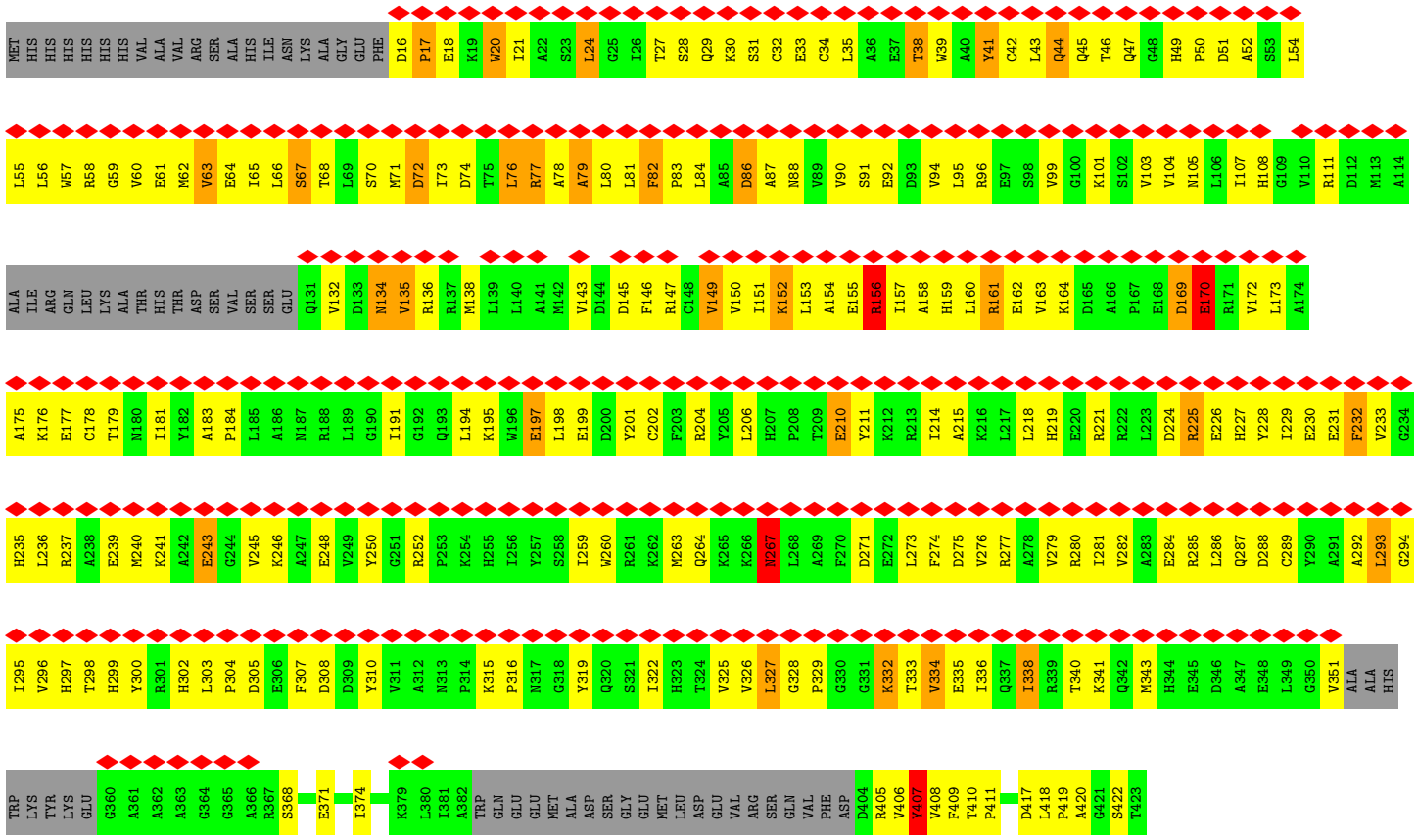
• Molecule 58: E-site tRNAfMet

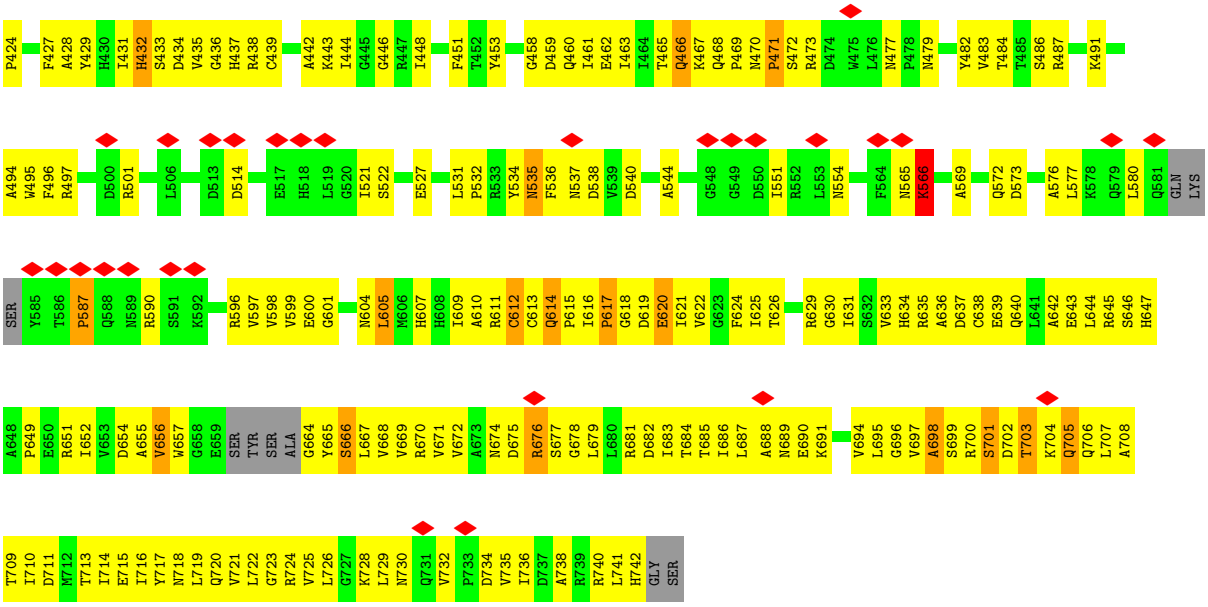
Chain 32:



• Molecule 59: GTP pyrophosphokinase

Chain 33:




P424 F427 A428 Y429 H430 I431 H432 S433 D434 V435 G436 H437 R438 C439 A442 K443 I444 G445 G446 R447 I448 F451 T452 Y453 G458 D459 Q460 I461 E462 I463 I464 T465 Q466 K467 Q468 P469 N470 P471 S472 R473 D474 W475 L476 M477 P478 N479 Y482 V483 T484 T485 S486 R487 K491
A494 W495 F496 R497 D500 R501 L506 D513 D514 E517 H518 L519 G520 I521 S522 E527 L531 P532 R533 Y534 N535 F536 N537 D538 V539 D540 A544 G548 G549 D550 I551 R552 L553 N554 F564 N565 K566 A569 Q572 D573 A576 L577 K578 Q579 L580 Q581 GLN LYS
SER Y585 T586 P587 Q588 N589 R590 S591 K592 R596 V597 V598 V599 E600 G601 N604 L605 M606 H607 H608 I609 A610 R611 C612 C613 Q614 P615 I616 P617 G618 D619 E620 I621 V622 G623 F624 I625 T626 R629 G630 I631 S632 V633 H634 R635 A636 D637 C638 E639 Q640 L641 A642 E643 L644 R645 S646 H647
A648 P649 E650 R651 I652 V653 D654 A655 V656 W657 G658 E659 SER TYR SER ALA G664 Y665 S666 L667 V668 V669 R670 V671 V672 A673 N674 D675 R676 S677 G678 L679 L680 R681 D682 I683 T684 T685 I686 L687 A688 N689 E690 K691 V694 L695 G696 V697 A698 S699 R700 S701 D702 T703 K704 Q705 Q706 L707 A708
T709 I710 D711 M712 T713 I714 E715 I716 Y717 N718 L719 Q720 V721 L722 G723 R724 V725 L726 G727 K728 L729 N730 Q731 V732 P733 D734 V735 I736 D737 A738 R739 R740 L741 H742 GLY SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46935	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	30488	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.155	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/2121	0.71	0/2852
2	B	0.37	0/1586	0.70	0/2134
3	C	0.39	0/1571	0.70	0/2113
4	D	0.35	0/1434	0.62	0/1926
5	E	0.32	0/1343	0.65	0/1816
6	F	0.40	0/1122	0.66	0/1515
7	G	0.45	0/1001	0.79	3/1350 (0.2%)
8	H	0.42	0/1046	0.79	1/1410 (0.1%)
9	I	0.33	0/1152	0.64	0/1551
10	J	0.32	0/947	0.68	0/1268
11	K	0.34	0/1054	0.71	1/1403 (0.1%)
12	L	0.36	0/1093	0.64	0/1460
13	M	0.35	0/973	0.65	1/1301 (0.1%)
14	N	0.33	0/902	0.63	0/1209
15	O	0.35	0/929	0.67	0/1242
16	P	0.38	0/960	0.60	0/1278
17	Q	0.36	0/829	0.79	1/1107 (0.1%)
18	R	0.32	0/864	0.67	0/1156
19	S	0.34	0/744	0.76	0/994
20	T	0.35	0/787	0.68	0/1051
21	U	0.35	0/766	0.66	1/1025 (0.1%)
22	V	0.39	0/582	0.68	0/769
23	W	0.34	0/635	0.65	0/848
24	X	0.32	0/510	0.62	0/677
25	Y	0.33	0/453	0.68	0/605
26	Z	0.40	0/531	0.76	0/709
27	1	0.31	0/450	0.71	0/599
28	2	0.38	0/416	0.68	0/554
29	3	0.39	0/380	0.67	0/498
30	4	0.35	0/513	0.62	0/676
31	5	0.33	0/303	0.74	0/397
32	6	0.40	0/1735	0.67	1/2338 (0.0%)
33	7	0.35	0/1651	0.64	0/2225
34	8	0.33	0/1665	0.68	2/2227 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	9	0.33	0/1169	0.67	0/1573
36	10	0.35	0/835	0.75	1/1128 (0.1%)
37	11	0.32	0/1195	0.62	0/1602
38	12	0.35	0/989	0.70	0/1326
39	13	0.35	0/1034	0.71	0/1375
40	14	0.35	0/796	0.71	1/1077 (0.1%)
41	15	0.36	0/885	0.73	1/1195 (0.1%)
42	16	0.36	0/969	0.76	1/1300 (0.1%)
43	17	0.31	0/892	0.70	0/1193
44	18	0.46	0/817	0.61	0/1088
45	19	0.32	0/722	0.58	0/964
46	20	0.37	0/659	0.71	0/884
47	21	0.35	0/657	0.72	0/881
48	22	0.38	0/544	0.62	0/731
49	23	0.36	0/652	0.72	0/877
50	24	0.33	0/671	0.55	0/888
51	25	0.41	0/550	0.73	1/728 (0.1%)
52	26	0.51	1/36967 (0.0%)	0.72	4/57666 (0.0%)
53	27	0.54	3/69801 (0.0%)	0.72	7/108894 (0.0%)
54	28	0.41	1/2876 (0.0%)	0.71	1/4483 (0.0%)
55	29	0.97	0/486	0.74	0/757
56	30	0.65	1/1813 (0.1%)	0.77	0/2823
57	31	0.44	1/1836 (0.1%)	0.70	0/2859
58	32	0.89	2/1835 (0.1%)	0.77	1/2857 (0.0%)
59	33	0.65	6/4985 (0.1%)	1.09	37/6770 (0.5%)
All	All	0.50	15/167683 (0.0%)	0.72	66/250202 (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
52	26	0	13
53	27	0	34
56	30	0	1
59	33	0	3
All	All	0	51

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	33	156	ARG	CZ-NH2	-10.66	1.19	1.33
59	33	152	LYS	CD-CE	-7.76	1.31	1.51
53	27	1379	U	O3'-P	-7.76	1.51	1.61
59	33	17	PRO	CA-CB	-7.25	1.39	1.53
52	26	2	A	OP3-P	-7.00	1.52	1.61

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	33	156	ARG	NE-CZ-NH1	19.76	130.18	120.30
59	33	156	ARG	NH1-CZ-NH2	-13.83	104.19	119.40
59	33	17	PRO	N-CA-CB	-11.16	89.90	103.30
59	33	17	PRO	CA-CB-CG	10.28	124.33	104.80
59	33	63	VAL	CG1-CB-CG2	-9.25	96.11	110.90

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	26	130	A	Sidechain
52	26	159	G	Sidechain
52	26	266	G	Sidechain
52	26	820	U	Sidechain
52	26	88	U	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	A	2082	0	2157	183	0
2	B	1565	0	1616	121	0
3	C	1552	0	1619	137	0
4	D	1410	0	1447	150	0
5	E	1323	0	1374	88	0
6	F	1111	0	1148	83	0
7	G	988	0	1025	124	0
8	H	1032	0	1088	136	0
9	I	1129	0	1162	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	938	0	1012	90	0
11	K	1045	0	1117	89	0
12	L	1074	0	1157	70	0
13	M	960	0	1000	75	0
14	N	892	0	923	73	0
15	O	917	0	965	78	0
16	P	947	0	1022	94	0
17	Q	816	0	839	90	0
18	R	857	0	922	52	0
19	S	738	0	807	55	0
20	T	779	0	834	79	0
21	U	753	0	780	71	0
22	V	575	0	592	29	0
23	W	625	0	655	45	0
24	X	509	0	543	60	0
25	Y	449	0	491	41	0
26	Z	522	0	521	52	0
27	1	444	0	461	52	0
28	2	409	0	440	20	0
29	3	377	0	418	33	0
30	4	504	0	574	33	0
31	5	302	0	343	30	0
32	6	1704	0	1732	124	0
33	7	1624	0	1699	111	0
34	8	1643	0	1710	168	0
35	9	1156	0	1199	110	0
36	10	817	0	808	98	0
37	11	1181	0	1240	97	0
38	12	979	0	1034	84	0
39	13	1022	0	1070	130	0
40	14	786	0	828	92	0
41	15	869	0	878	89	0
42	16	955	0	1019	118	0
43	17	883	0	944	97	0
44	18	805	0	847	95	0
45	19	714	0	737	54	0
46	20	649	0	666	87	0
47	21	648	0	691	52	0
48	22	535	0	552	54	0
49	23	637	0	665	71	0
50	24	665	0	714	67	0
51	25	544	0	579	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	26	33016	0	16617	1573	0
53	27	62322	0	31345	2882	0
54	28	2572	0	1302	116	0
55	29	432	0	218	14	0
56	30	1623	0	821	75	0
57	31	1644	0	836	46	0
58	32	1643	0	836	66	0
59	33	4911	0	4550	655	0
All	All	154603	0	105189	8829	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 34.

The worst 5 of 8829 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)
53:27:45:G:H5"	53:27:46:G:H5'	1.22	1.18
59:33:17:PRO:HB3	59:33:39:TRP:NE1	1.57	1.17
7:G:55:VAL:HA	53:27:1084:A:H5'	1.26	1.15
53:27:1702:G:H2'	53:27:1703:G:H5"	1.15	1.14
59:33:24:LEU:HD21	59:33:70:SER:HA	1.19	1.12

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
1	A	269/273 (98%)	218 (81%)	41 (15%)	10 (4%)	2 23
2	B	207/209 (99%)	172 (83%)	28 (14%)	7 (3%)	3 24
3	C	199/201 (99%)	147 (74%)	32 (16%)	20 (10%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	175/179 (98%)	143 (82%)	27 (15%)	5 (3%)	3 27
5	E	174/177 (98%)	149 (86%)	20 (12%)	5 (3%)	3 27
6	F	147/149 (99%)	108 (74%)	20 (14%)	19 (13%)	0 4
7	G	129/165 (78%)	93 (72%)	25 (19%)	11 (8%)	0 10
8	H	139/142 (98%)	104 (75%)	25 (18%)	10 (7%)	1 13
9	I	140/142 (99%)	120 (86%)	14 (10%)	6 (4%)	2 21
10	J	120/123 (98%)	97 (81%)	16 (13%)	7 (6%)	1 17
11	K	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1 12
12	L	134/136 (98%)	113 (84%)	15 (11%)	6 (4%)	2 20
13	M	118/127 (93%)	91 (77%)	22 (19%)	5 (4%)	2 21
14	N	114/117 (97%)	98 (86%)	15 (13%)	1 (1%)	14 50
15	O	112/115 (97%)	93 (83%)	15 (13%)	4 (4%)	3 23
16	P	115/118 (98%)	103 (90%)	7 (6%)	5 (4%)	2 21
17	Q	101/103 (98%)	77 (76%)	16 (16%)	8 (8%)	1 12
18	R	108/110 (98%)	87 (81%)	15 (14%)	6 (6%)	1 17
19	S	91/100 (91%)	71 (78%)	16 (18%)	4 (4%)	2 20
20	T	100/104 (96%)	79 (79%)	14 (14%)	7 (7%)	1 13
21	U	92/94 (98%)	76 (83%)	11 (12%)	5 (5%)	1 18
22	V	73/85 (86%)	65 (89%)	7 (10%)	1 (1%)	9 40
23	W	75/78 (96%)	67 (89%)	6 (8%)	2 (3%)	4 28
24	X	61/63 (97%)	49 (80%)	7 (12%)	5 (8%)	1 11
25	Y	56/59 (95%)	52 (93%)	4 (7%)	0	100 100
26	Z	64/70 (91%)	47 (73%)	7 (11%)	10 (16%)	0 3
27	1	54/57 (95%)	43 (80%)	6 (11%)	5 (9%)	0 10
28	2	48/55 (87%)	41 (85%)	7 (15%)	0	100 100
29	3	44/46 (96%)	32 (73%)	11 (25%)	1 (2%)	5 31
30	4	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2 19
31	5	36/38 (95%)	26 (72%)	5 (14%)	5 (14%)	0 3
32	6	216/241 (90%)	170 (79%)	32 (15%)	14 (6%)	1 15
33	7	204/233 (88%)	175 (86%)	22 (11%)	7 (3%)	3 24
34	8	203/206 (98%)	157 (77%)	30 (15%)	16 (8%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	9	155/167 (93%)	109 (70%)	33 (21%)	13 (8%)	0	10
36	10	98/135 (73%)	77 (79%)	14 (14%)	7 (7%)	1	13
37	11	149/179 (83%)	123 (83%)	14 (9%)	12 (8%)	1	11
38	12	127/130 (98%)	110 (87%)	8 (6%)	9 (7%)	1	13
39	13	125/130 (96%)	93 (74%)	19 (15%)	13 (10%)	0	7
40	14	96/103 (93%)	76 (79%)	15 (16%)	5 (5%)	1	18
41	15	114/129 (88%)	90 (79%)	13 (11%)	11 (10%)	0	9
42	16	121/124 (98%)	95 (78%)	13 (11%)	13 (11%)	0	6
43	17	112/118 (95%)	88 (79%)	14 (12%)	10 (9%)	0	10
44	18	98/101 (97%)	72 (74%)	21 (21%)	5 (5%)	1	18
45	19	86/89 (97%)	70 (81%)	11 (13%)	5 (6%)	1	17
46	20	80/82 (98%)	59 (74%)	18 (22%)	3 (4%)	2	22
47	21	78/84 (93%)	54 (69%)	19 (24%)	5 (6%)	1	15
48	22	63/75 (84%)	50 (79%)	5 (8%)	8 (13%)	0	4
49	23	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	4	29
50	24	83/87 (95%)	75 (90%)	6 (7%)	2 (2%)	5	30
51	25	63/71 (89%)	40 (64%)	19 (30%)	4 (6%)	1	16
59	33	663/750 (88%)	557 (84%)	60 (9%)	46 (7%)	1	14
All	All	6509/6970 (93%)	5226 (80%)	879 (14%)	404 (6%)	2	16

5 of 404 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	GLU
2	B	102	ALA
3	C	6	LYS
3	C	11	ALA
3	C	57	LYS

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	A	216/218 (99%)	215 (100%)	1 (0%)	86 90
2	B	164/164 (100%)	164 (100%)	0	100 100
3	C	165/165 (100%)	165 (100%)	0	100 100
4	D	148/150 (99%)	146 (99%)	2 (1%)	62 76
5	E	137/138 (99%)	137 (100%)	0	100 100
6	F	114/114 (100%)	114 (100%)	0	100 100
7	G	100/123 (81%)	100 (100%)	0	100 100
8	H	109/110 (99%)	107 (98%)	2 (2%)	54 71
9	I	116/116 (100%)	116 (100%)	0	100 100
10	J	103/104 (99%)	102 (99%)	1 (1%)	73 81
11	K	102/103 (99%)	102 (100%)	0	100 100
12	L	109/109 (100%)	109 (100%)	0	100 100
13	M	100/103 (97%)	99 (99%)	1 (1%)	73 81
14	N	86/87 (99%)	86 (100%)	0	100 100
15	O	99/100 (99%)	99 (100%)	0	100 100
16	P	89/90 (99%)	89 (100%)	0	100 100
17	Q	84/84 (100%)	83 (99%)	1 (1%)	67 79
18	R	93/93 (100%)	93 (100%)	0	100 100
19	S	80/84 (95%)	80 (100%)	0	100 100
20	T	83/85 (98%)	82 (99%)	1 (1%)	67 79
21	U	78/78 (100%)	78 (100%)	0	100 100
22	V	57/63 (90%)	57 (100%)	0	100 100
23	W	67/68 (98%)	67 (100%)	0	100 100
24	X	55/55 (100%)	55 (100%)	0	100 100
25	Y	48/49 (98%)	48 (100%)	0	100 100
26	Z	59/62 (95%)	58 (98%)	1 (2%)	56 72
27	1	47/48 (98%)	47 (100%)	0	100 100
28	2	45/49 (92%)	45 (100%)	0	100 100
29	3	38/38 (100%)	38 (100%)	0	100 100
30	4	51/52 (98%)	50 (98%)	1 (2%)	50 68
31	5	34/34 (100%)	34 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	6	180/199 (90%)	178 (99%)	2 (1%)	70 80
33	7	170/190 (90%)	169 (99%)	1 (1%)	84 88
34	8	172/173 (99%)	172 (100%)	0	100 100
35	9	119/126 (94%)	117 (98%)	2 (2%)	56 72
36	10	87/116 (75%)	85 (98%)	2 (2%)	45 64
37	11	124/147 (84%)	123 (99%)	1 (1%)	79 84
38	12	104/105 (99%)	103 (99%)	1 (1%)	73 81
39	13	105/107 (98%)	104 (99%)	1 (1%)	73 81
40	14	86/90 (96%)	86 (100%)	0	100 100
41	15	89/99 (90%)	89 (100%)	0	100 100
42	16	103/104 (99%)	103 (100%)	0	100 100
43	17	92/96 (96%)	92 (100%)	0	100 100
44	18	83/84 (99%)	80 (96%)	3 (4%)	30 53
45	19	76/77 (99%)	75 (99%)	1 (1%)	65 77
46	20	65/65 (100%)	65 (100%)	0	100 100
47	21	74/78 (95%)	73 (99%)	1 (1%)	62 76
48	22	56/65 (86%)	55 (98%)	1 (2%)	54 71
49	23	70/79 (89%)	70 (100%)	0	100 100
50	24	65/66 (98%)	65 (100%)	0	100 100
51	25	55/61 (90%)	54 (98%)	1 (2%)	54 71
59	33	452/635 (71%)	449 (99%)	3 (1%)	81 86
All	All	5303/5698 (93%)	5272 (99%)	31 (1%)	82 88

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	9	80	LEU
51	25	36	PHE
36	10	47	LEU
59	33	338	ILE
45	19	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
50	24	47	GLN
59	33	88	ASN
16	P	58	GLN
16	P	55	GLN
59	33	264	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	26	1538/1539 (99%)	205 (13%)	9 (0%)
53	27	2902/2903 (99%)	447 (15%)	24 (0%)
54	28	119/120 (99%)	14 (11%)	1 (0%)
55	29	19/20 (95%)	5 (26%)	1 (5%)
56	30	75/76 (98%)	19 (25%)	0
57	31	76/77 (98%)	8 (10%)	0
58	32	76/77 (98%)	19 (25%)	1 (1%)
All	All	4805/4812 (99%)	717 (14%)	36 (0%)

5 of 717 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	26	4	U
52	26	6	G
52	26	9	G
52	26	19	A
52	26	22	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	27	2406	A
58	32	20	U
53	27	2655	G
53	27	2867	G
53	27	490	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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.

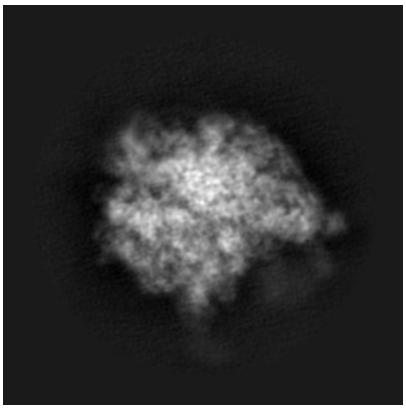
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8280. These allow visual inspection of the internal detail of the map and identification of artifacts.

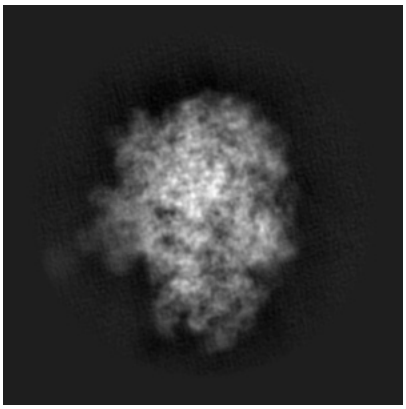
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

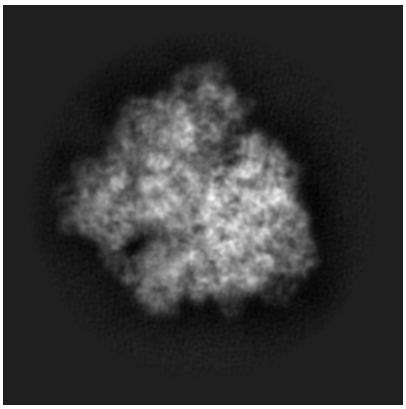
6.1.1 Primary map



X

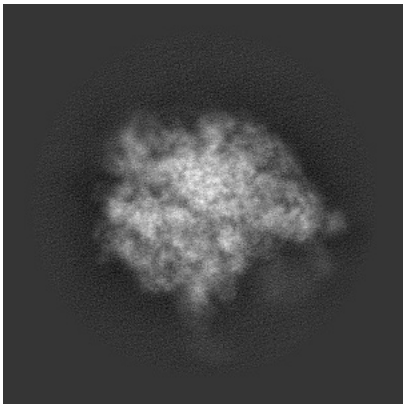


Y

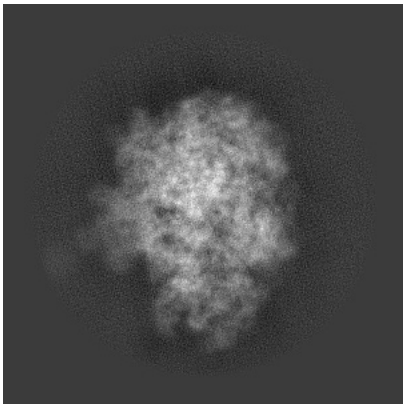


Z

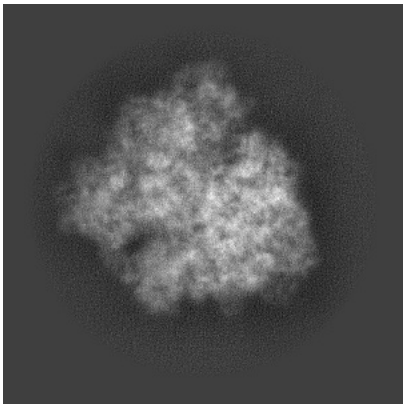
6.1.2 Raw map



X



Y

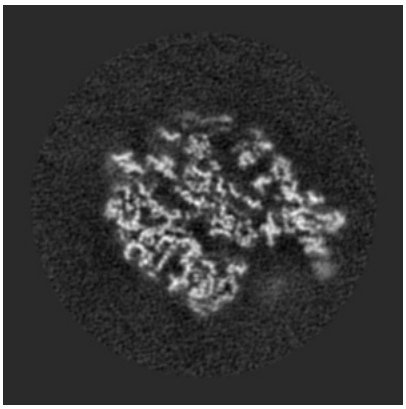


Z

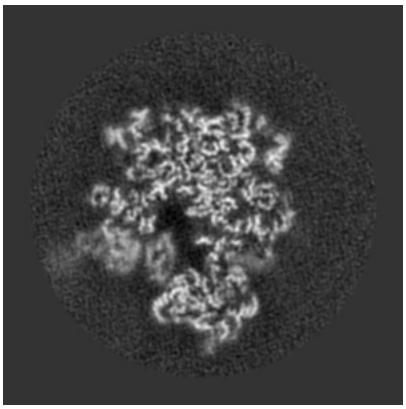
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

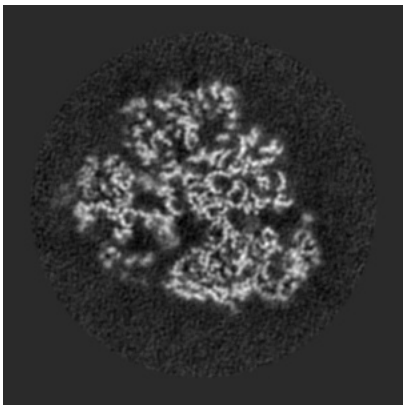
6.2.1 Primary map



X Index: 240

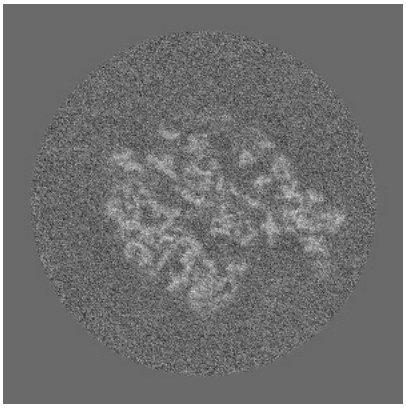


Y Index: 240

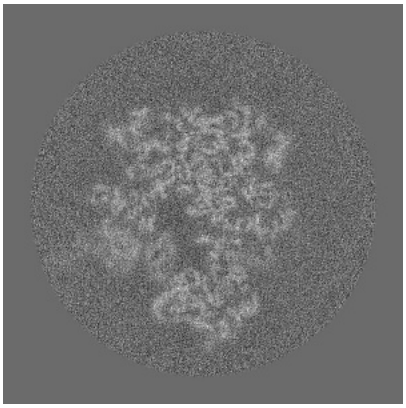


Z Index: 240

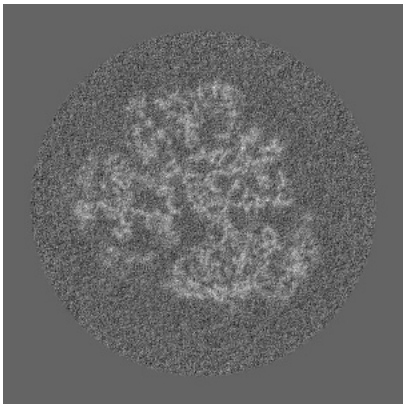
6.2.2 Raw map



X Index: 240



Y Index: 240

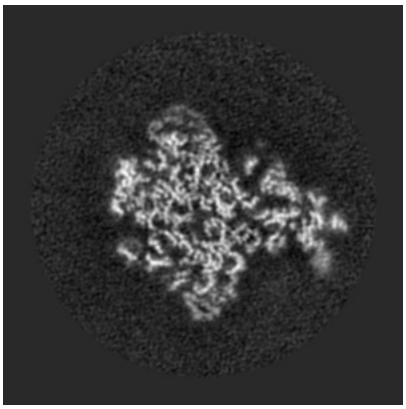


Z Index: 240

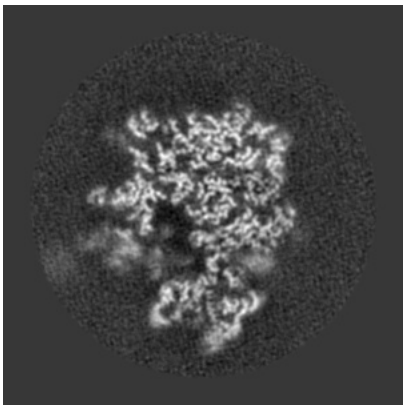
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

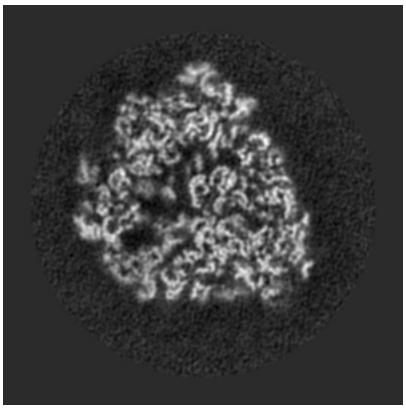
6.3.1 Primary map



X Index: 250

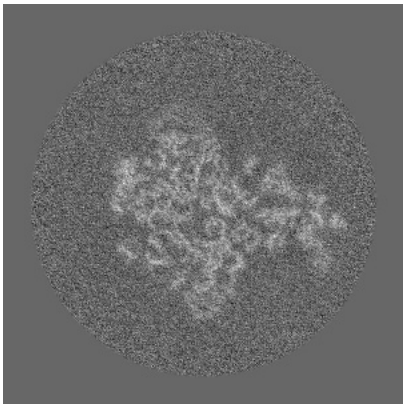


Y Index: 247

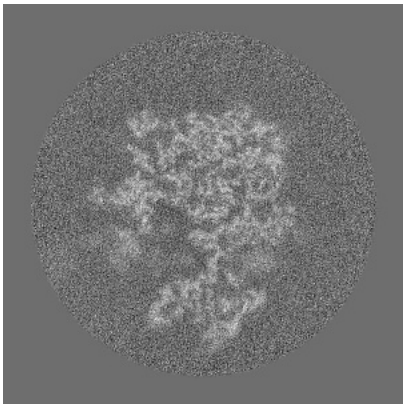


Z Index: 226

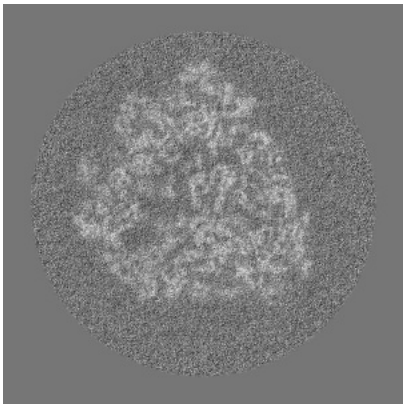
6.3.2 Raw map



X Index: 250



Y Index: 249

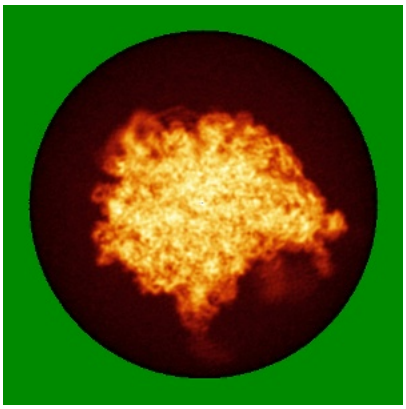


Z Index: 226

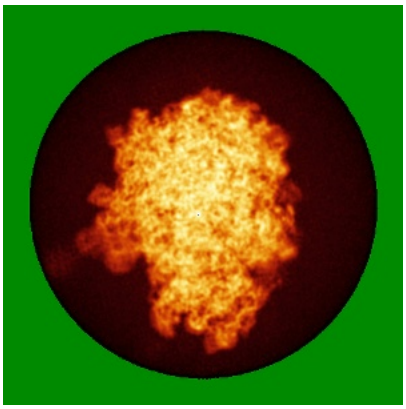
The images above show the largest variance slices of the map in three orthogonal directions.

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

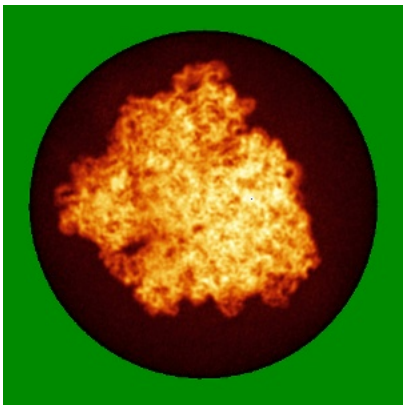
6.4.1 Primary map



X

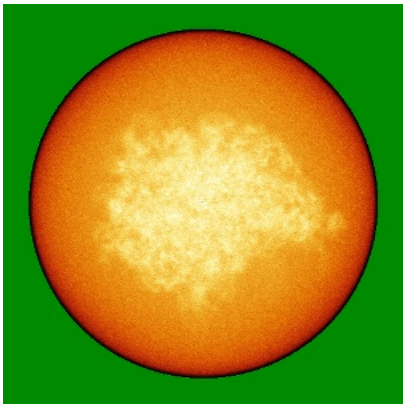


Y

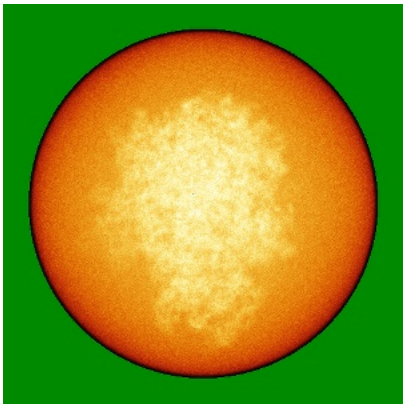


Z

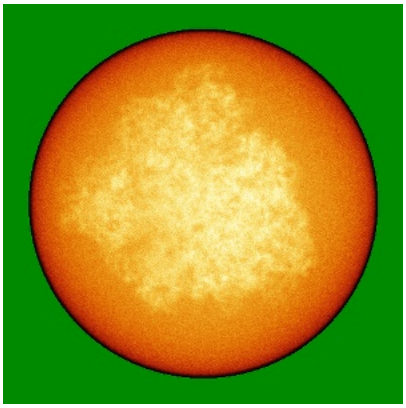
6.4.2 Raw map



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 0.1. 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.

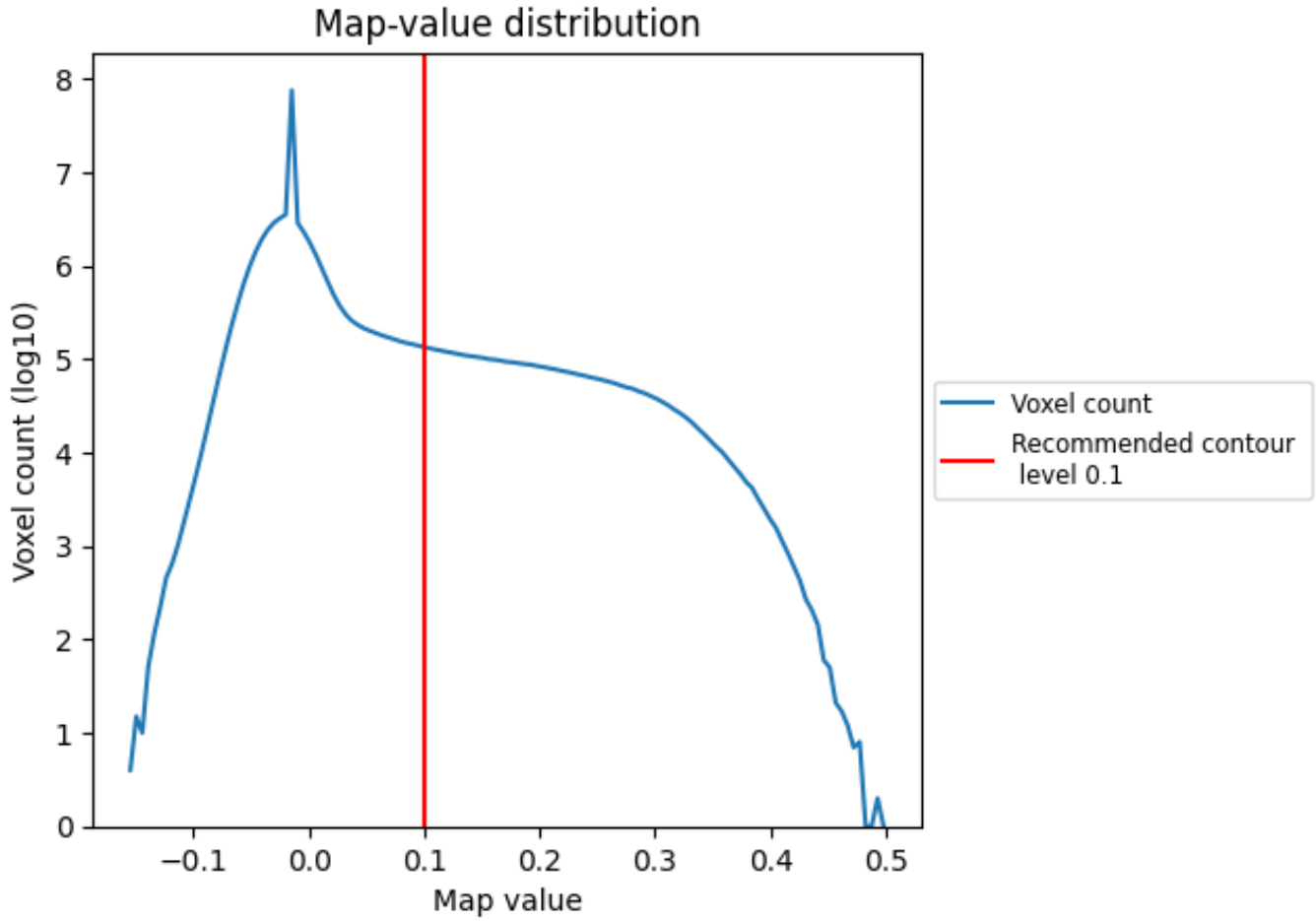
6.6 Mask visualisation (i)

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

7 Map analysis

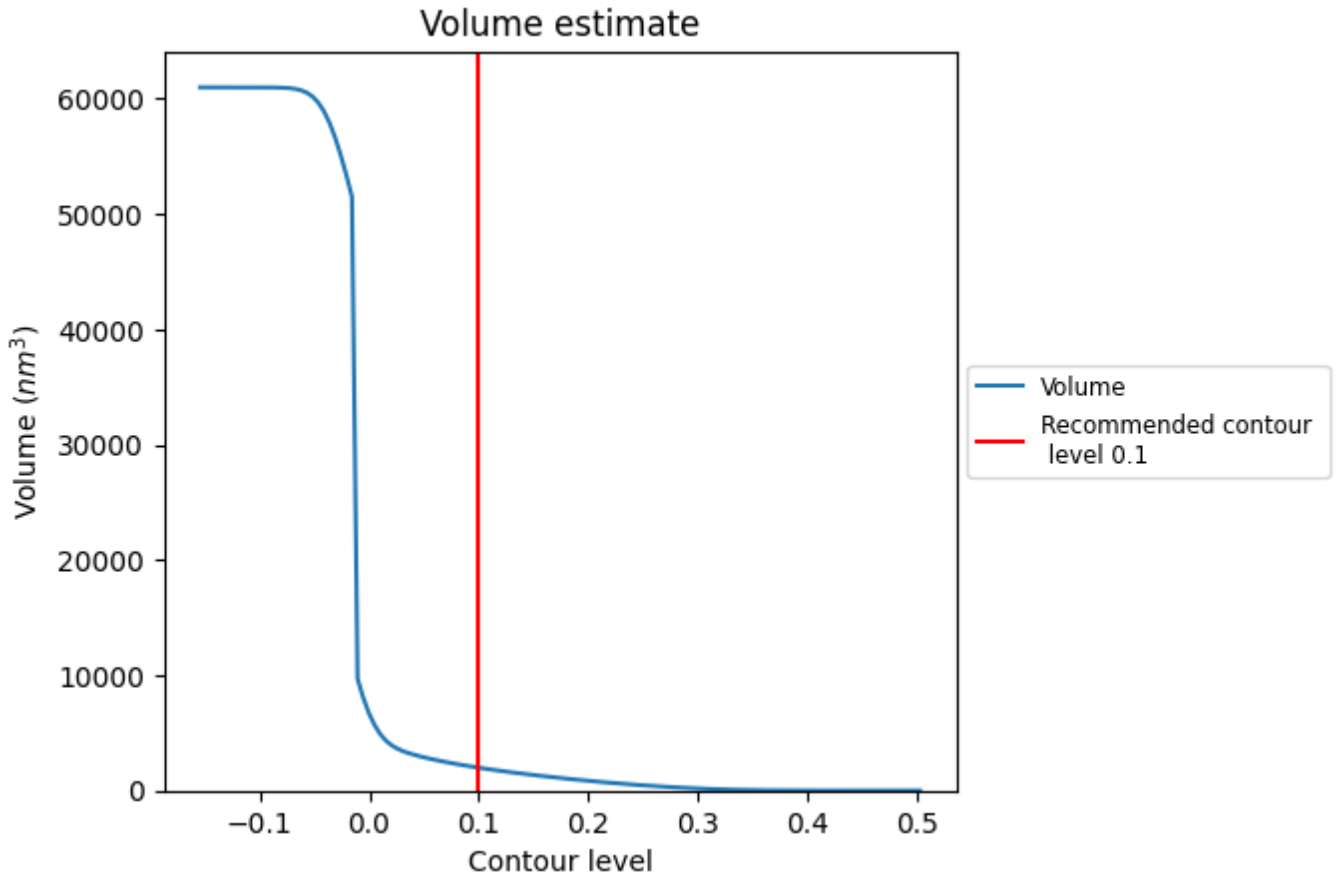
This section contains the results of statistical analysis of the map.

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.

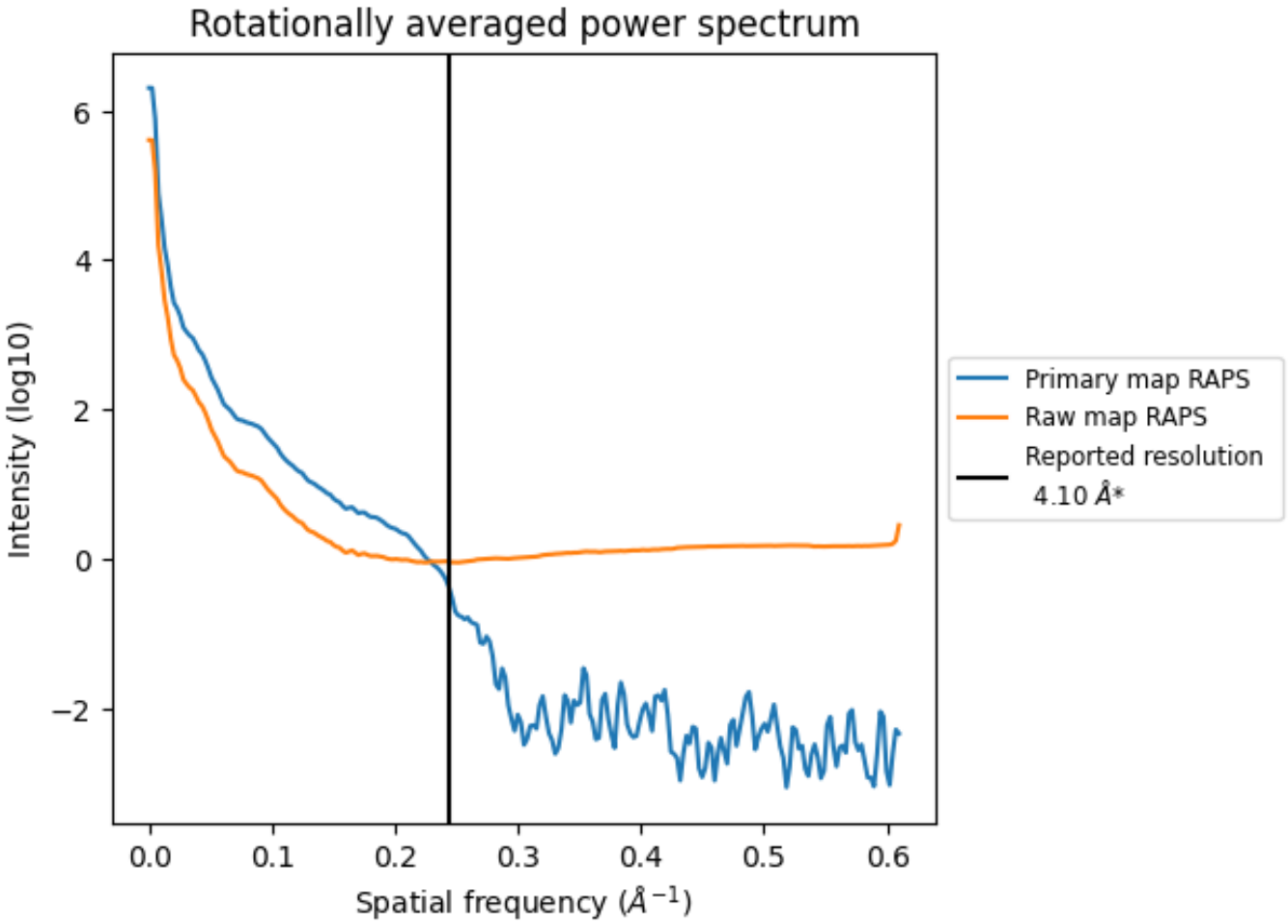
7.2 Volume estimate (i)



The volume at the recommended contour level is 1983 nm^3; this corresponds to an approximate mass of 1791 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)

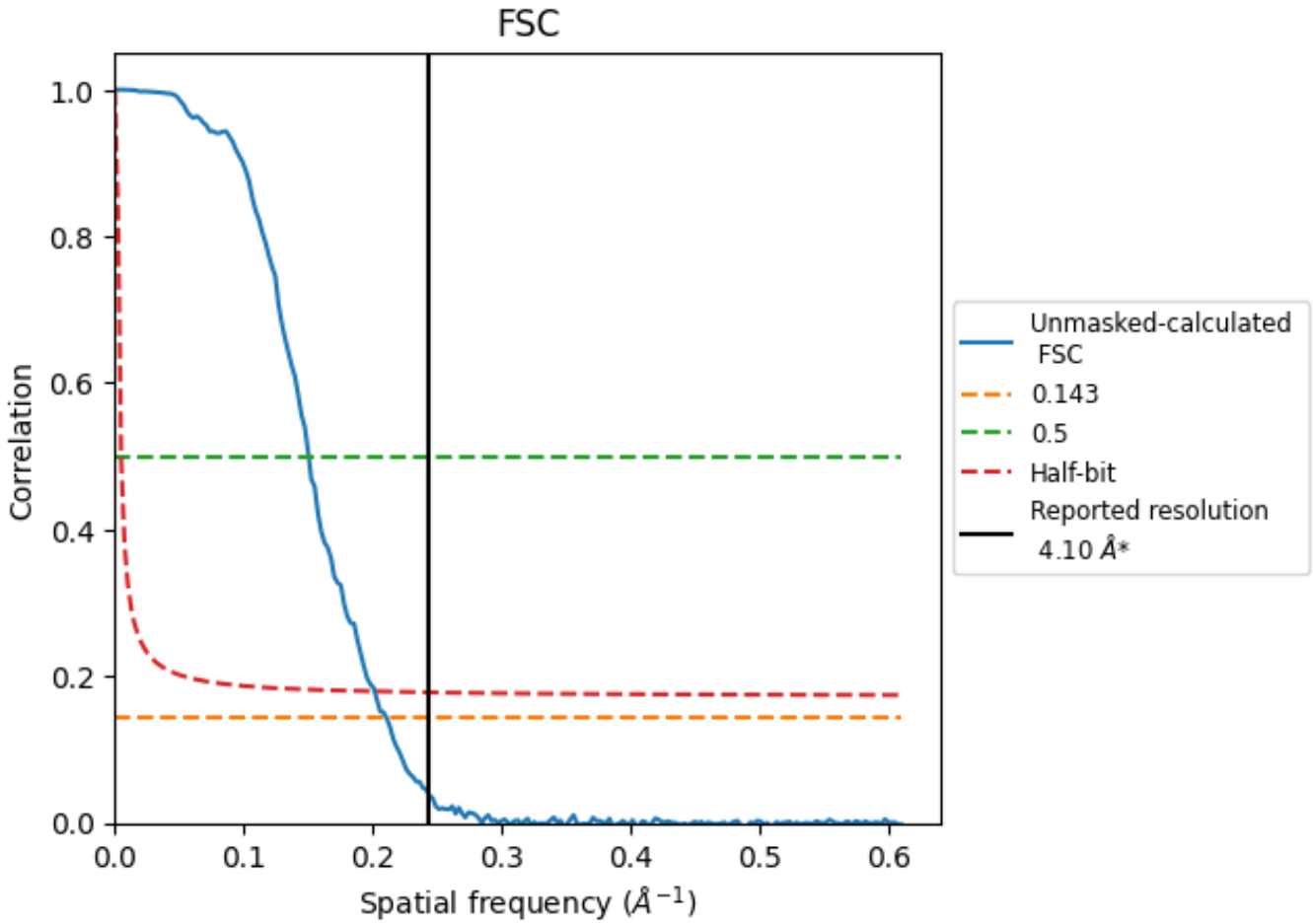


*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

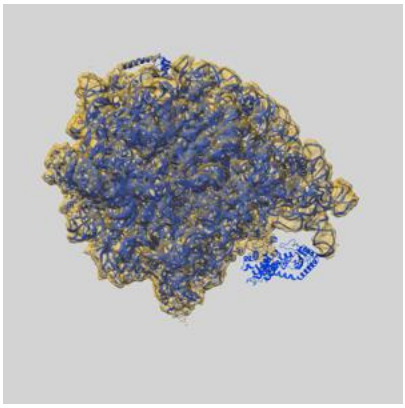
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.75	6.65	4.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.75 differs from the reported value 4.1 by more than 10 %

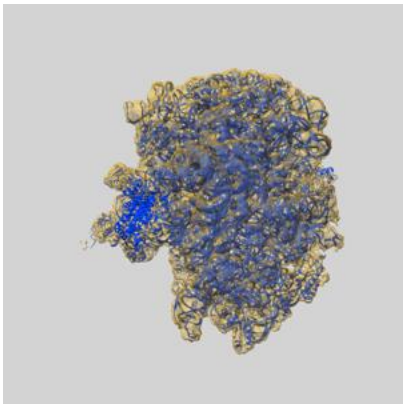
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8280 and PDB model 5KPV. Per-residue inclusion information can be found in section 3 on page 15.

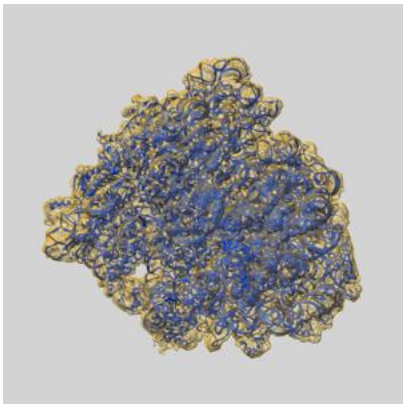
9.1 Map-model overlay



X



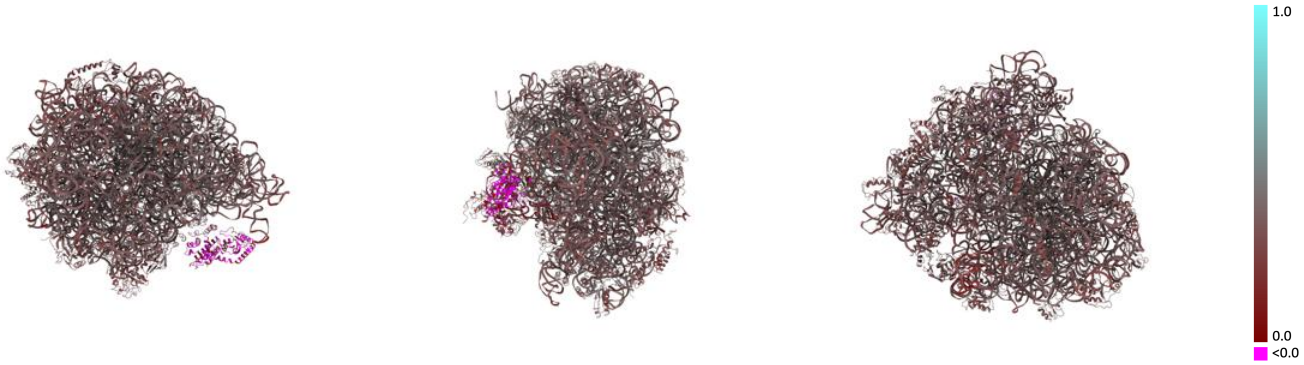
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

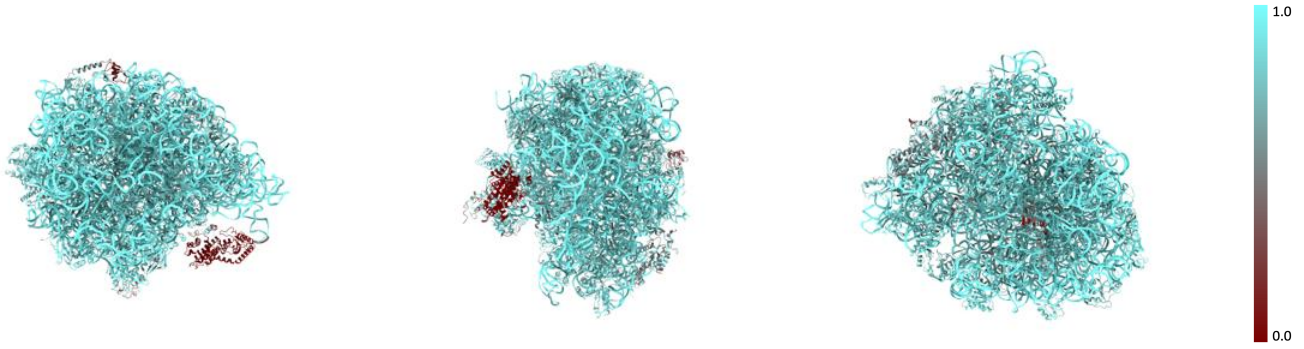
9.2 Q-score mapped to coordinate model



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.

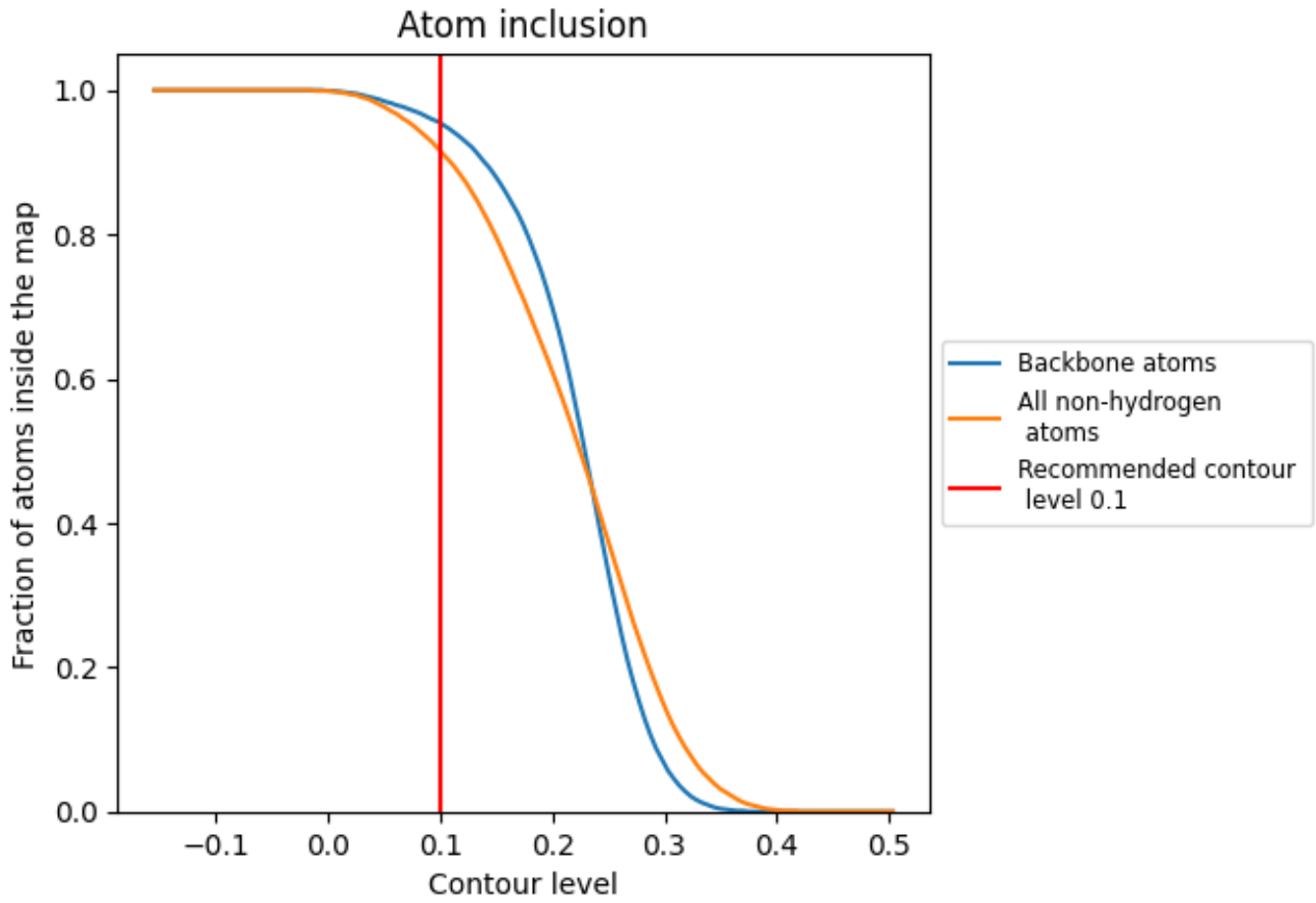
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9160	0.3500
1	0.8760	0.3710
10	0.8770	0.3530
11	0.8570	0.3250
12	0.8490	0.3570
13	0.8850	0.3410
14	0.7990	0.3440
15	0.8650	0.3510
16	0.7910	0.3770
17	0.8460	0.3370
18	0.8450	0.3360
19	0.8570	0.3220
2	0.7280	0.3520
20	0.8710	0.3510
21	0.8510	0.3640
22	0.8930	0.3520
23	0.8810	0.3430
24	0.8680	0.3230
25	0.7350	0.3160
26	0.9880	0.3630
27	0.9920	0.3650
28	0.9940	0.3590
29	0.7680	0.2970
3	0.8840	0.3610
30	0.8740	0.2400
31	0.9580	0.3470
32	0.7270	0.2370
33	0.4050	0.1560
4	0.8190	0.3740
5	0.8220	0.3680
6	0.5650	0.3130
7	0.8030	0.3620
8	0.8230	0.3300
9	0.8430	0.3680
A	0.8460	0.3840

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Chain	Atom inclusion	Q-score
B	0.8480	0.3850
C	0.7850	0.3360
D	0.8540	0.3440
E	0.8740	0.3680
F	0.4760	0.3210
G	0.5700	0.2520
H	0.7230	0.2430
I	0.8570	0.3670
J	0.8040	0.3940
K	0.8730	0.3700
L	0.8250	0.3810
M	0.8720	0.3580
N	0.8900	0.3430
O	0.8550	0.3900
P	0.8700	0.3390
Q	0.8810	0.3770
R	0.8110	0.3610
S	0.8660	0.3670
T	0.8810	0.3540
U	0.8790	0.3640
V	0.8610	0.3790
W	0.8590	0.3650
X	0.8550	0.3070
Y	0.8540	0.3640
Z	0.8360	0.3290