wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 08:42 am GMT

PDB ID	:	6S0X
EMDB ID	:	EMD-10076
Title	:	Erythromycin Resistant Staphylococcus aureus 70S ribosome (delta R88 A89 uL22) in complex with erythromycin.
Authors	:	Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on	:	2019-06-18
Resolution	:	2.42 Å(reported)

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

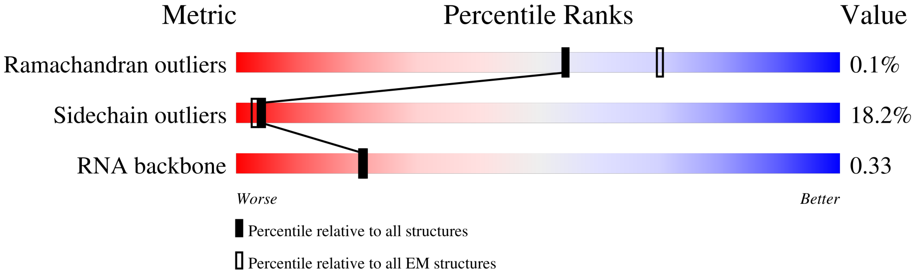
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

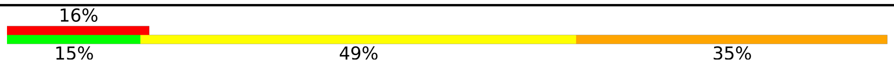
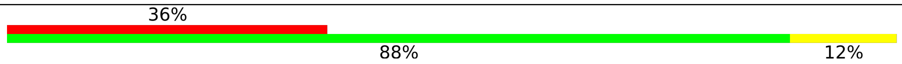
The reported resolution of this entry is 2.42 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2905	
2	B	115	
3	C	274	
4	D	215	
5	E	206	
6	F	173	
7	G	173	
8	H	145	

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Mol	Chain	Length	Quality of chain
9	I	122	85% 14% •
10	J	146	84% 15% •
11	K	137	90% 10%
12	L	120	• 86% 14%
13	M	118	7% 87% 11% •
14	N	114	• 90% 9% •
15	O	116	90% 10%
16	P	102	79% 21%
17	Q	110	5% 94% 6%
18	R	89	• 82% 18%
19	S	103	8% 83% 17%
20	T	94	• 88% 12%
21	U	77	• 83% 17%
22	V	49	8% 94% • •
23	W	67	• 84% 16%
24	X	58	84% 16%
25	Y	59	98% 95% 5%
26	Z	48	33% 77% 23%
27	1	47	21% 87% 13%
28	2	43	93% 5% •
29	3	64	84% 12% •
30	4	37	89% 11%
31	a	1539	78% 46% 46% 8%
32	b	226	99% 81% 19%
33	c	202	99% 83% 17%

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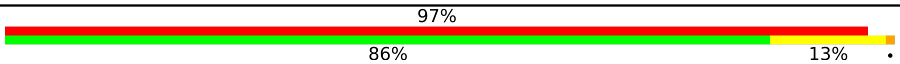
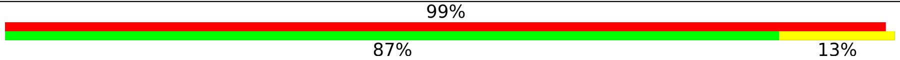
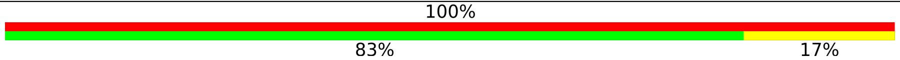
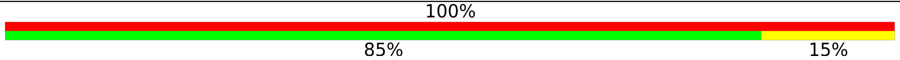
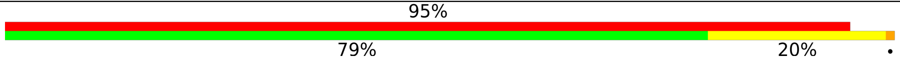
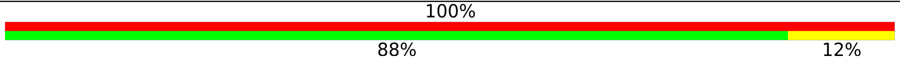
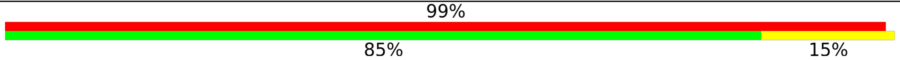
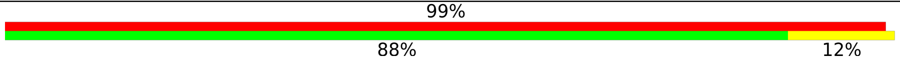
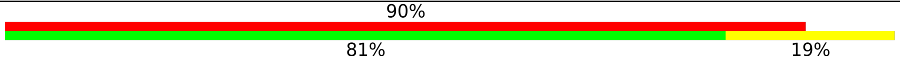
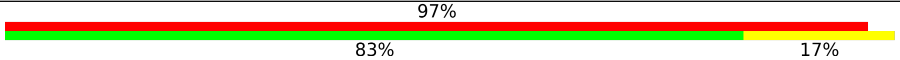
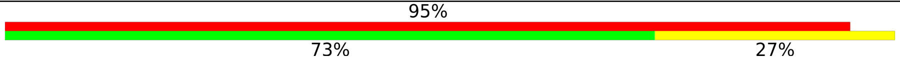
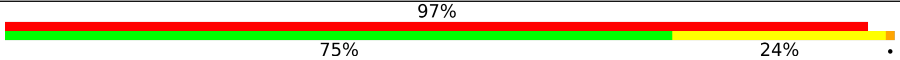
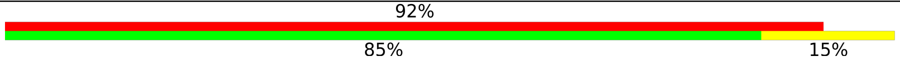
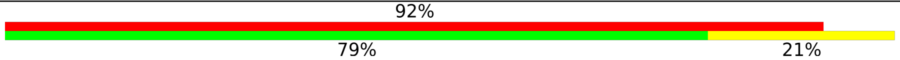
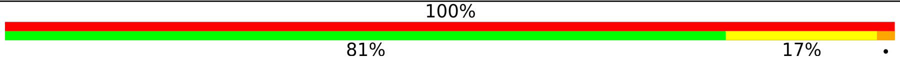
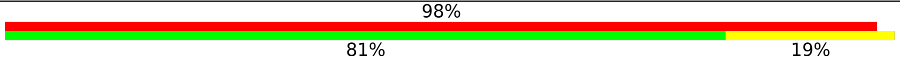
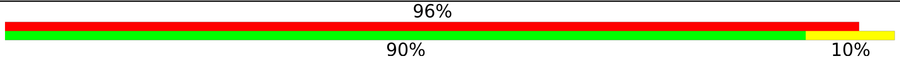
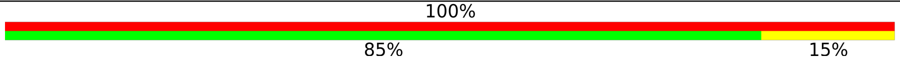
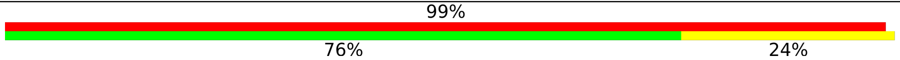
Mol	Chain	Length	Quality of chain
34	d	198	
35	e	156	
36	f	95	
37	g	152	
38	h	131	
39	i	127	
40	j	97	
41	k	114	
42	l	135	
43	m	104	
44	n	60	
45	o	88	
46	p	89	
47	q	80	
48	r	54	
49	s	80	
50	t	81	
51	u	52	
52	v	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	ERY	A	3001	X	-	-	-

2 Entry composition ⓘ

There are 53 unique types of molecules in this entry. The entry contains 140672 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2905	62277	27803	11387	20182	2905	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	115	2445	1094	436	801	114	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	274	2090	1301	415	369	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	215	1627	1018	299	305	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	206	1572	986	288	296	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	173	1315	831	225	253	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	173	1248	780	236	229	3	0	0

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	145	1149	717	211	218	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	122	918	572	174	168	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	146	1086	674	214	197	1	0	0

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	137	1079	694	204	177	4	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	120	932	576	182	173	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	118	883	552	173	158	0	0

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	N	114	889	563	175	151	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	116	943	593	189	157	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	102	790	503	142	144	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	110	838	525	159	151	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	89	715	453	127	131	4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	103	770	486	142	141	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	T	94	722	463	130	129	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	77	587	363	115	109	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	V	49	379	234	82	63	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	W	67	541	333	102	106	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	X	58	449	280	85	84	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	59	370	225	68	76	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	48	360	222	77	59	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	1	47	390	238	78	70	4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	2	43	367	225	89	52	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	3	64	521	324	113	82	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	4	37	295	186	60	44	5	0	0

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	a	1539	32969	14719	6017	10694	1539	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	226	1819	1159	317	335	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	202	1501	945	284	271	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	198	1497	952	275	268	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	156	1145	723	211	209	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	95	778	493	138	145	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	152	1161	722	218	217	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	131	1026	650	183	189	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	127	922	576	179	166	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	97	752	475	140	136	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total 810	C 498	N 151	O 159	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total 1037	C 646	N 211	O 178	S 2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
43	m	104	Total 727	C 453	N 139	O 135	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total 487	C 307	N 98	O 77	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total 723	C 448	N 150	O 124	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	89	Total 694	C 436	N 128	O 129	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
47	q	80	Total 621	C 392	N 112	O 117	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	54	Total 445	C 284	N 86	O 73	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	80	Total 636	C 410	N 113	O 111	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total 591	C 358	N 117	O 115	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
51	u	52	Total 400	C 249	N 79	O 72	0	0

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	162	Total 1333	C 835	N 242	O 254	S 2	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	PHE	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	LEU	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	MET	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

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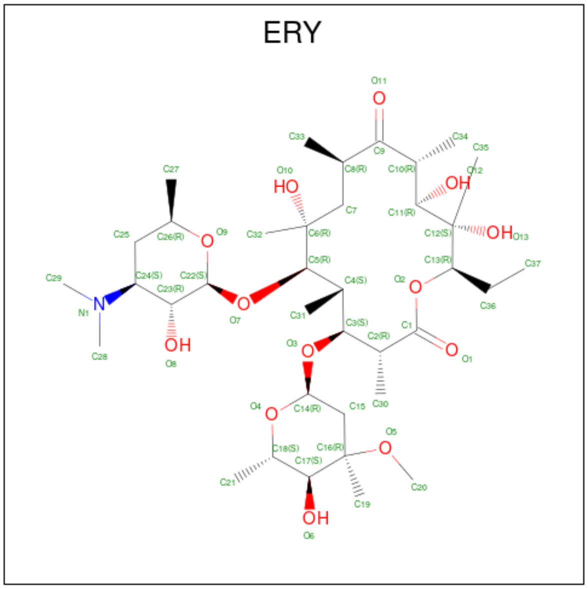
Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	THR	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	TYR	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

- Molecule 53 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



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<tr><th>Mol</th><th>Chain</th><th>Residues</th><th colspan="4">Atoms</th><th>AltConf</th></tr>
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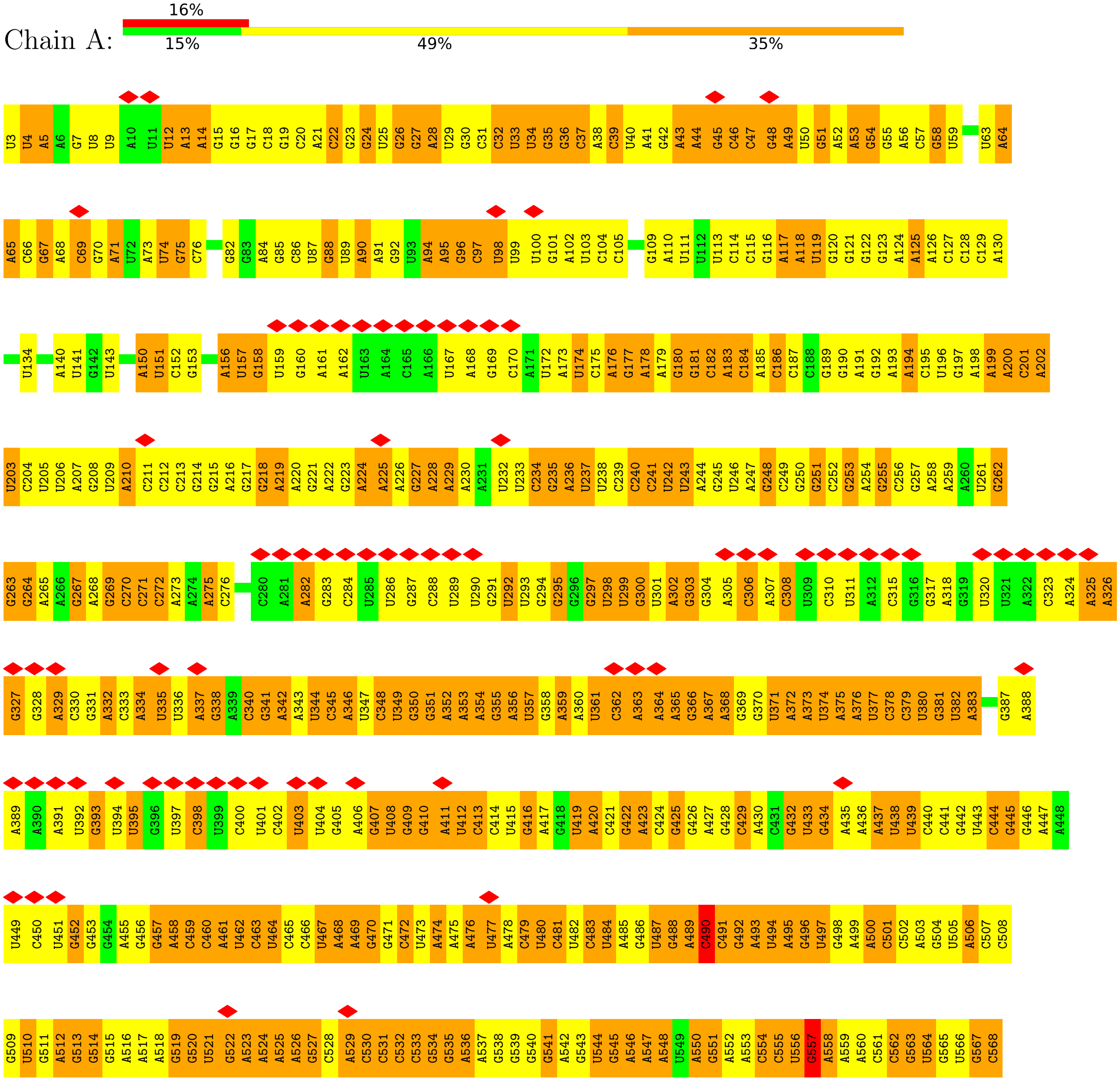
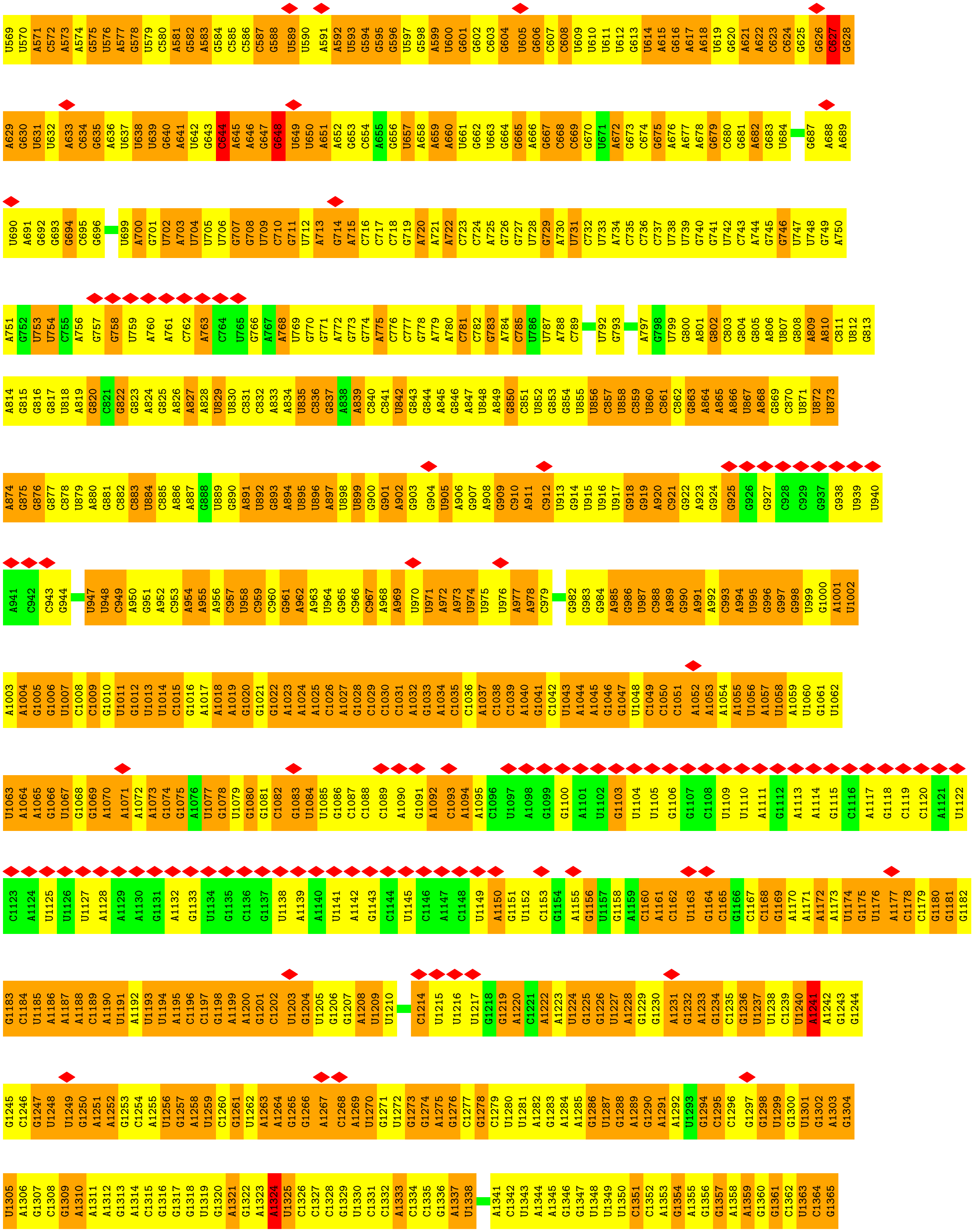
3 Residue-property plots ⓘ

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: 23S ribosomal RNA

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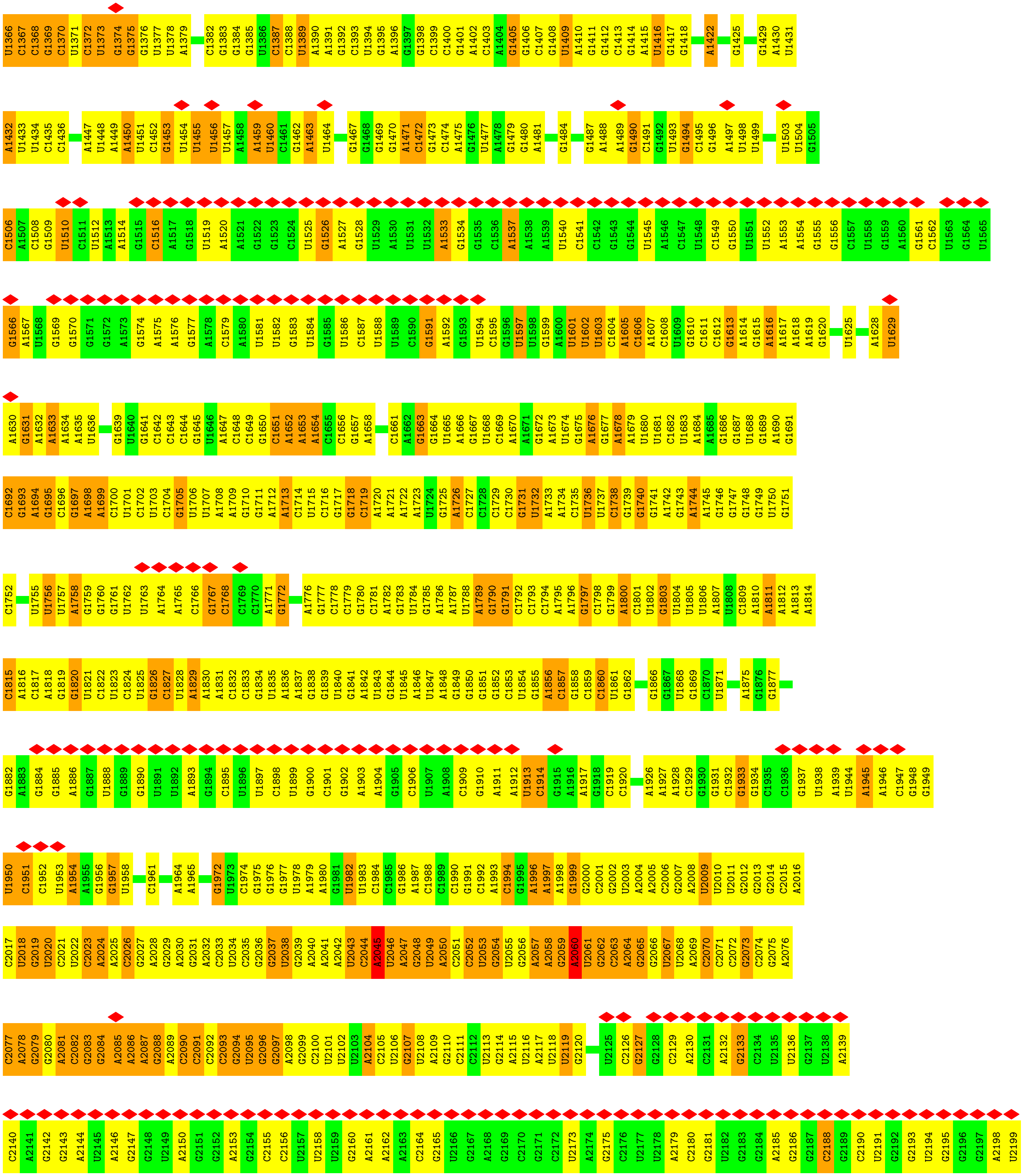
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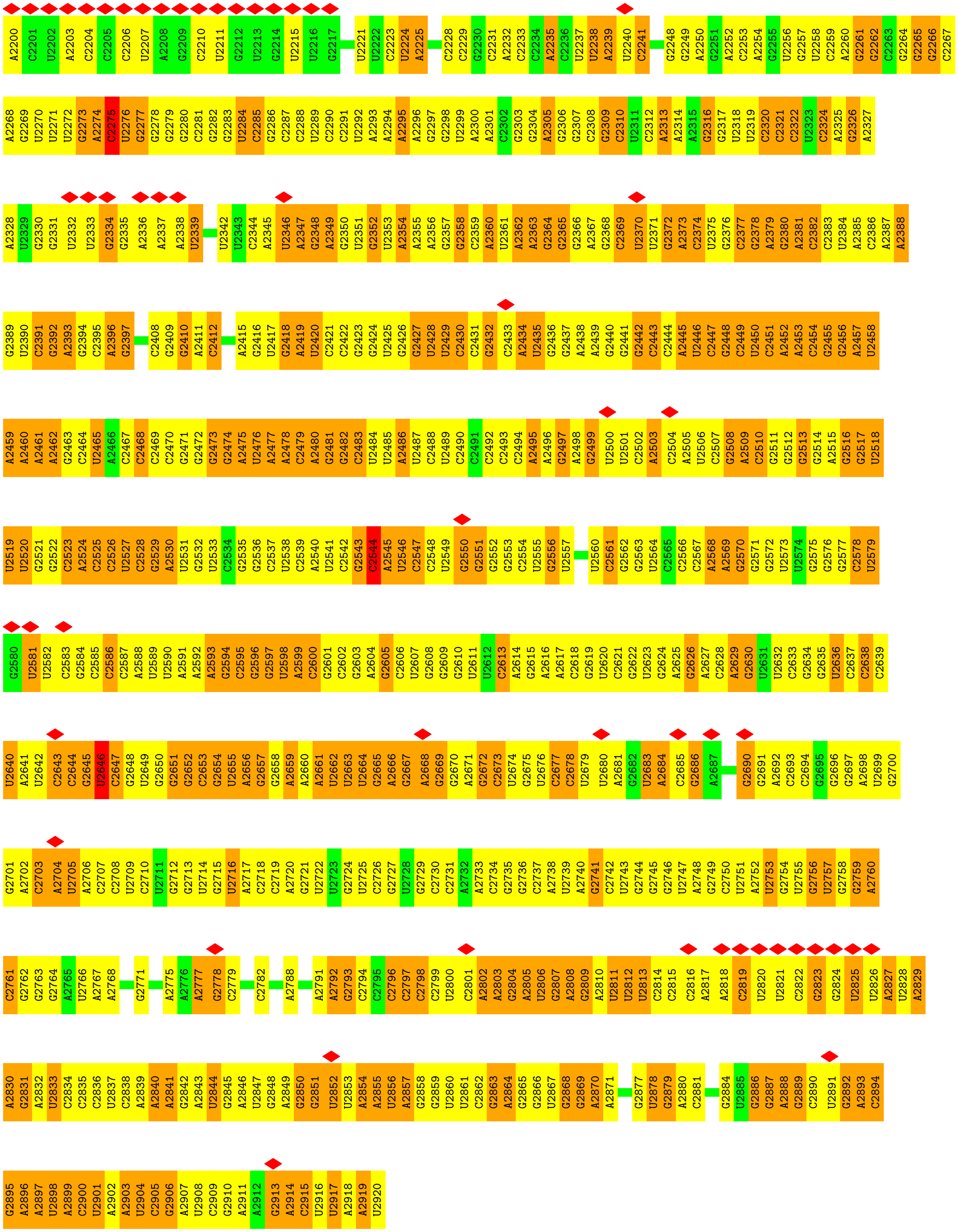

- Molecule 2: 5S ribosomal RNA

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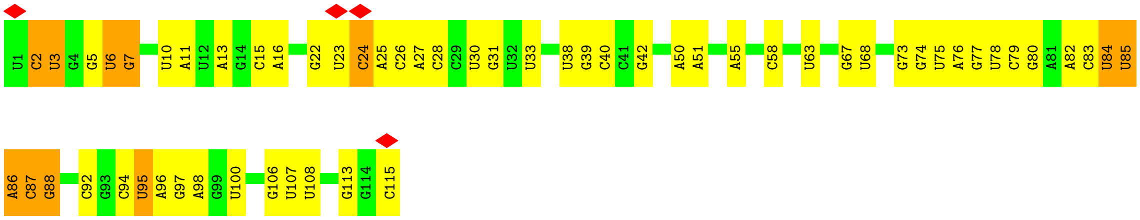
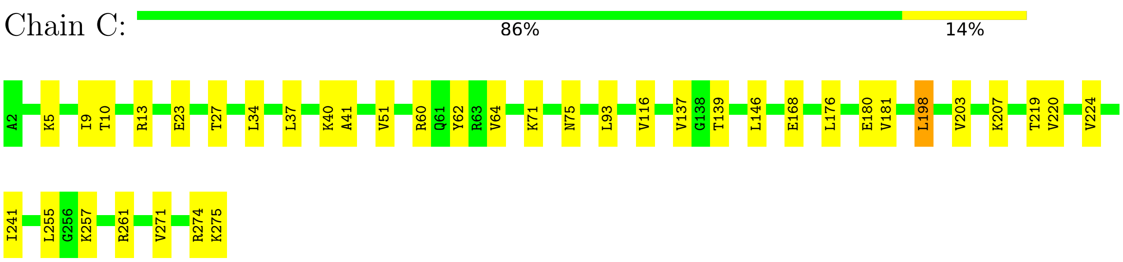
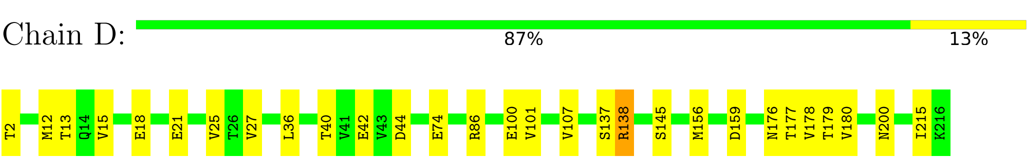


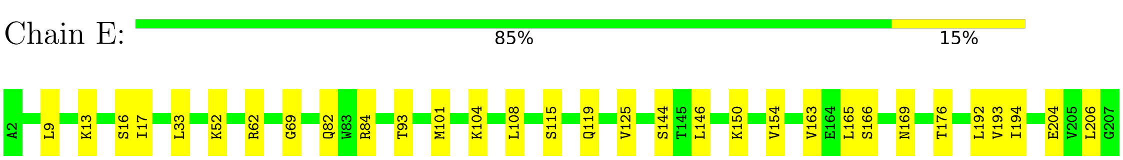
- Molecule 3: 50S ribosomal protein L2



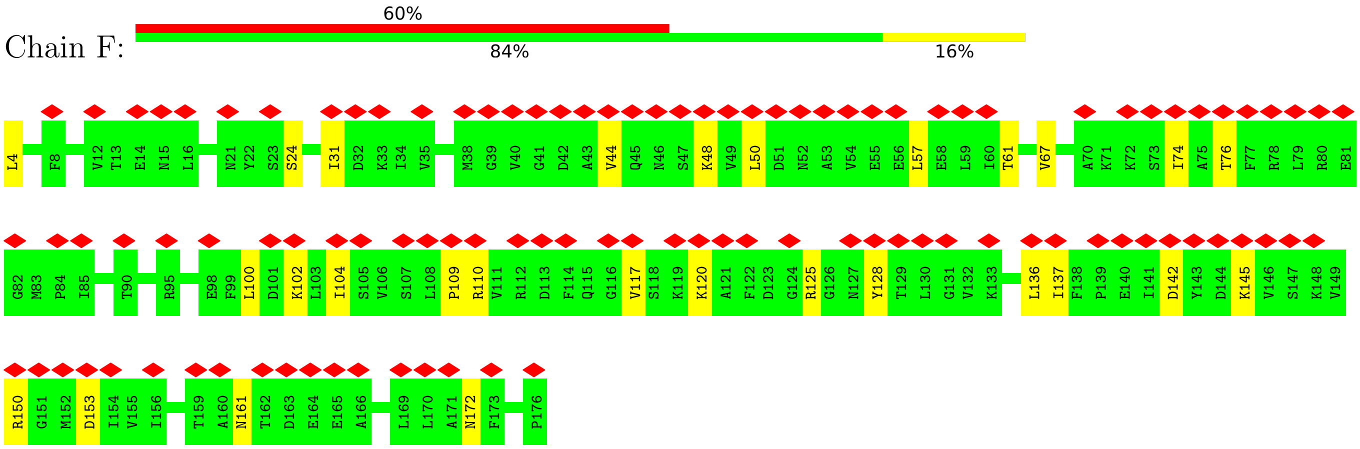
- Molecule 4: 50S ribosomal protein L3



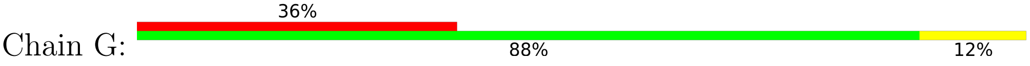
- Molecule 5: 50S ribosomal protein L4

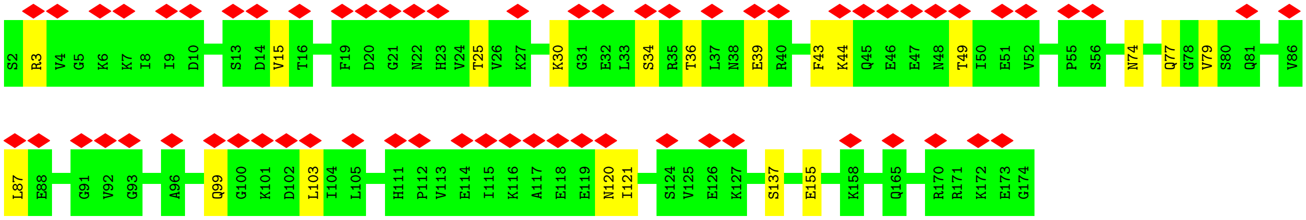


- Molecule 6: 50S ribosomal protein L5

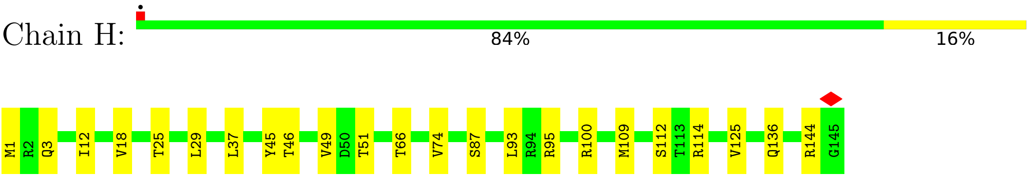


- Molecule 7: 50S ribosomal protein L6

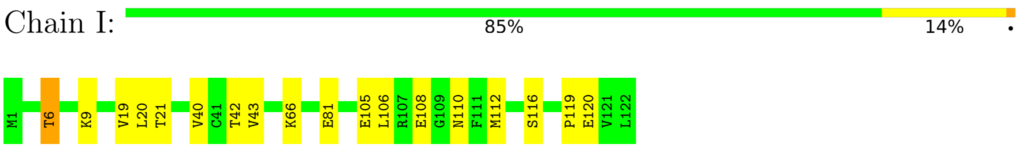




- Molecule 8: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L14



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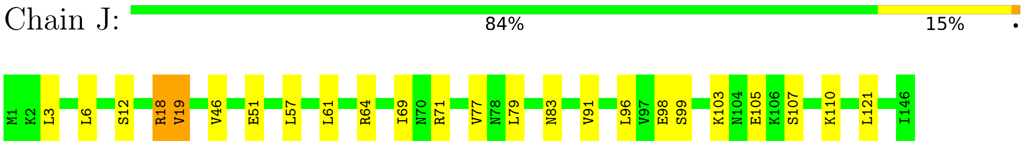
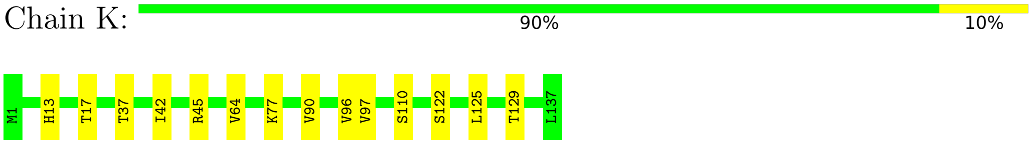


- Molecule 11: 50S ribosomal protein L16



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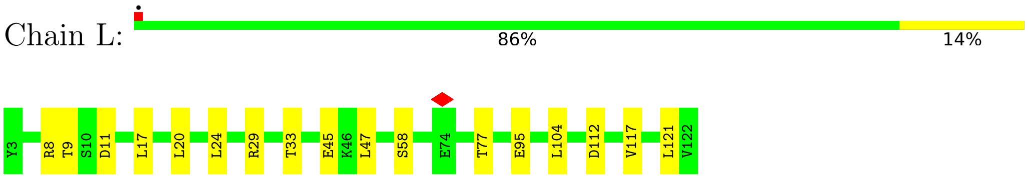
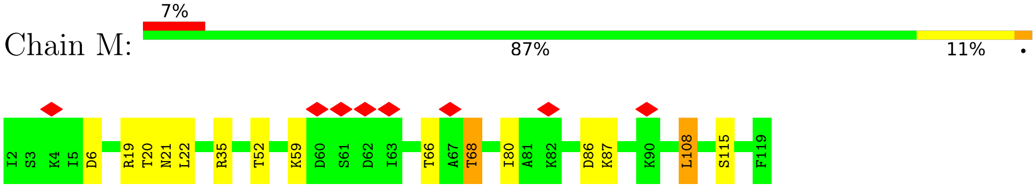
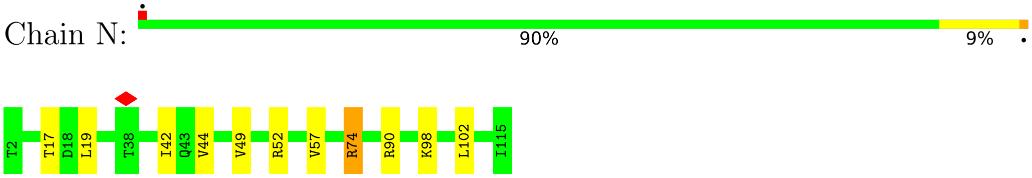


- Molecule 13: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L19



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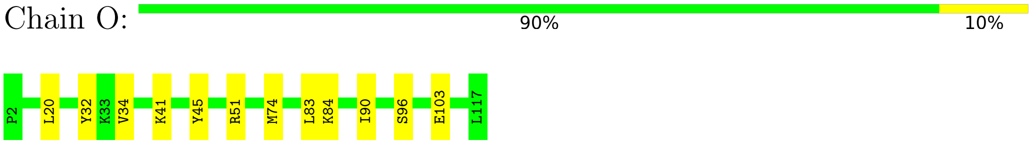

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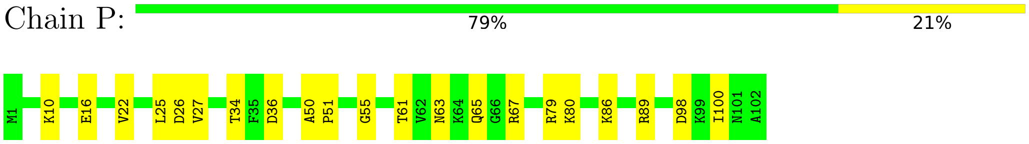

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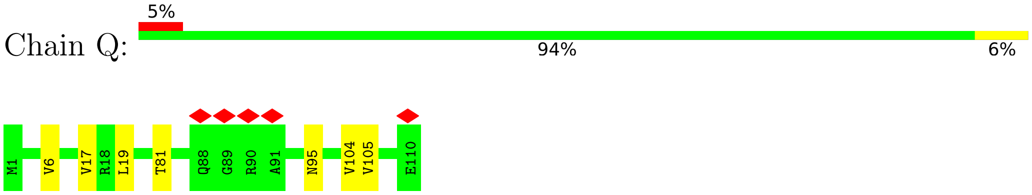

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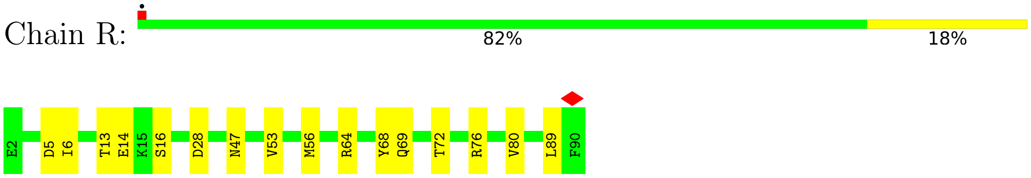

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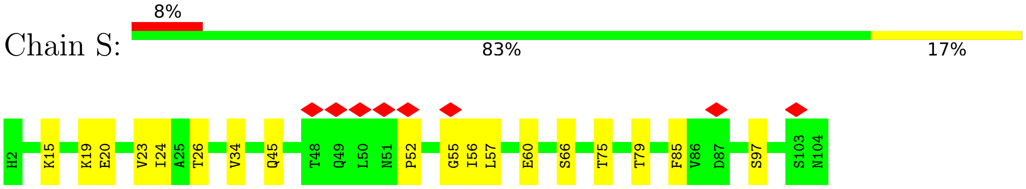

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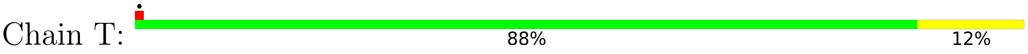

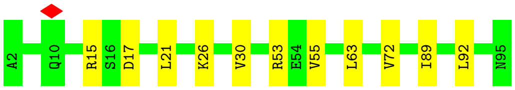

- Molecule 21: 50S ribosomal protein L27

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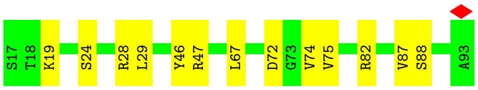

- Molecule 22: 50S ribosomal protein L28

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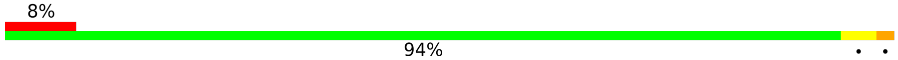

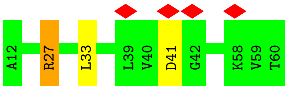

- Molecule 23: 50S ribosomal protein L29

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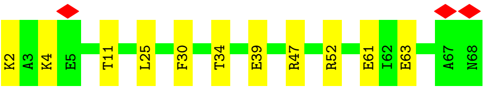

- Molecule 24: 50S ribosomal protein L30

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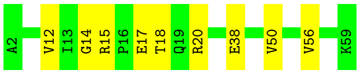
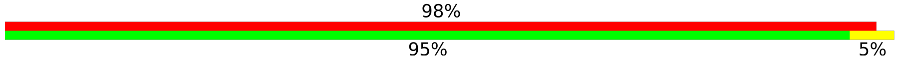
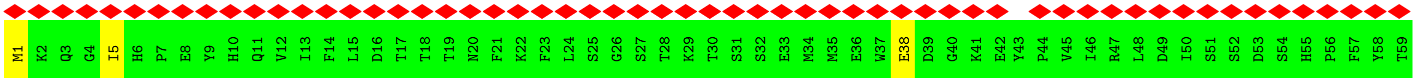


- Molecule 25: 50S ribosomal protein L31 type B

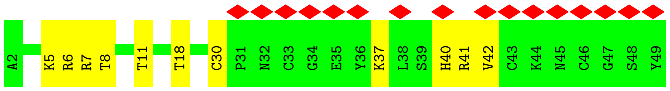
Chain Y:





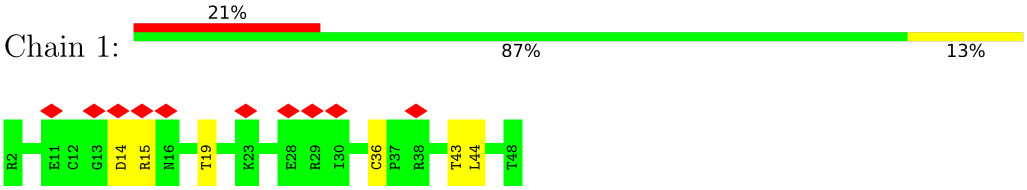
- Molecule 26: 50S ribosomal protein L32

Chain Z:



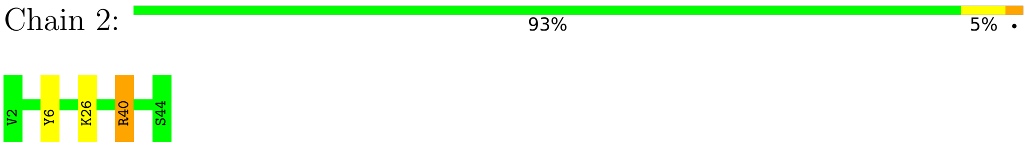
- Molecule 27: 50S ribosomal protein L33

Chain 1:



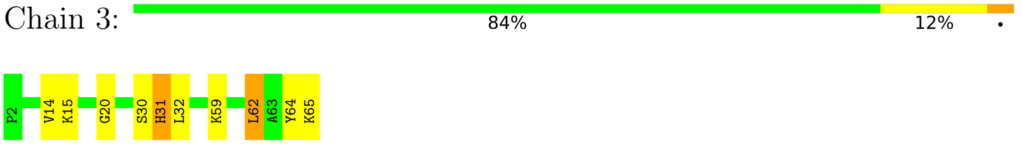
- Molecule 28: 50S ribosomal protein L34

Chain 2:



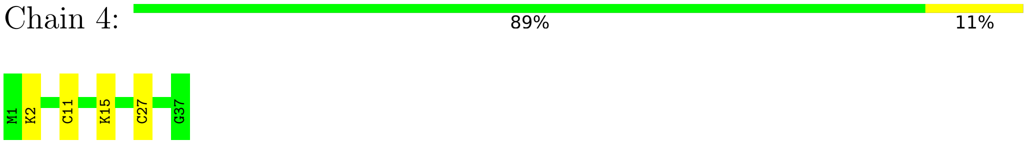
- Molecule 29: 50S ribosomal protein L35

Chain 3:



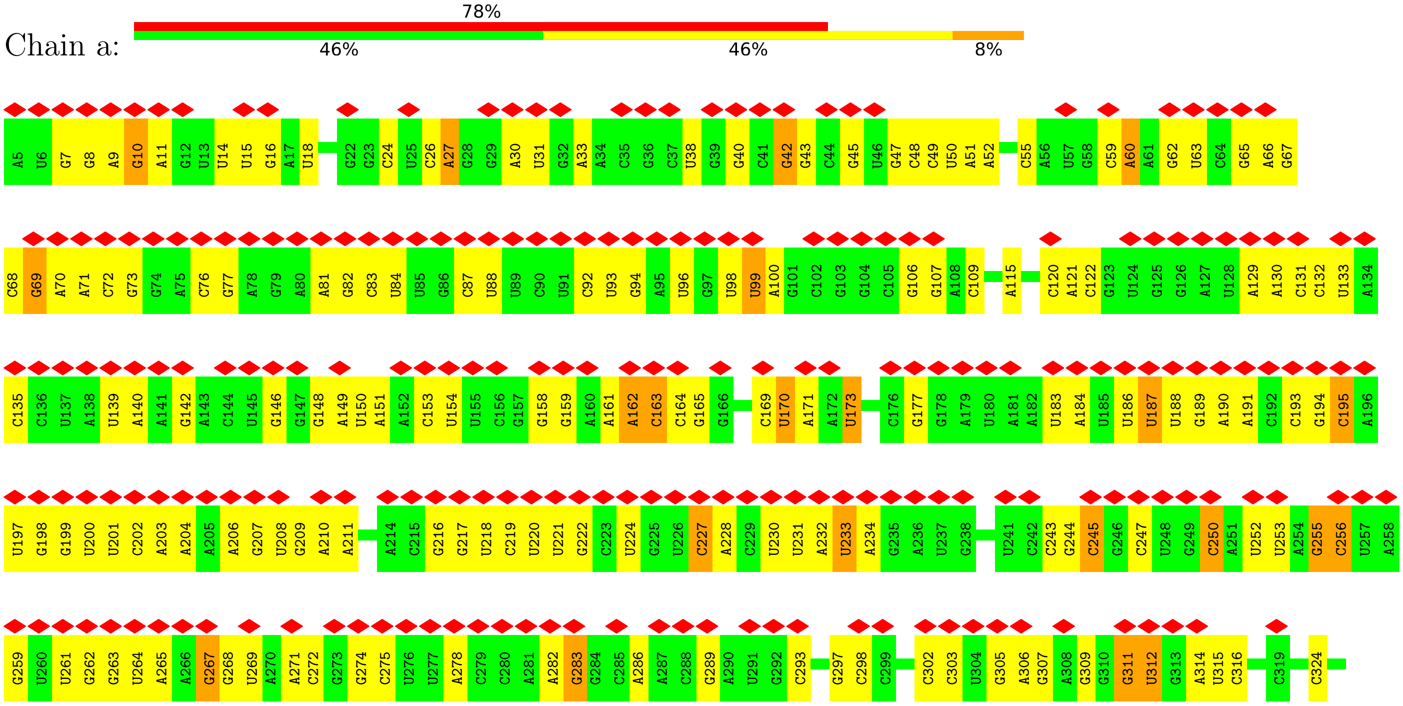
- Molecule 30: 50S ribosomal protein L36

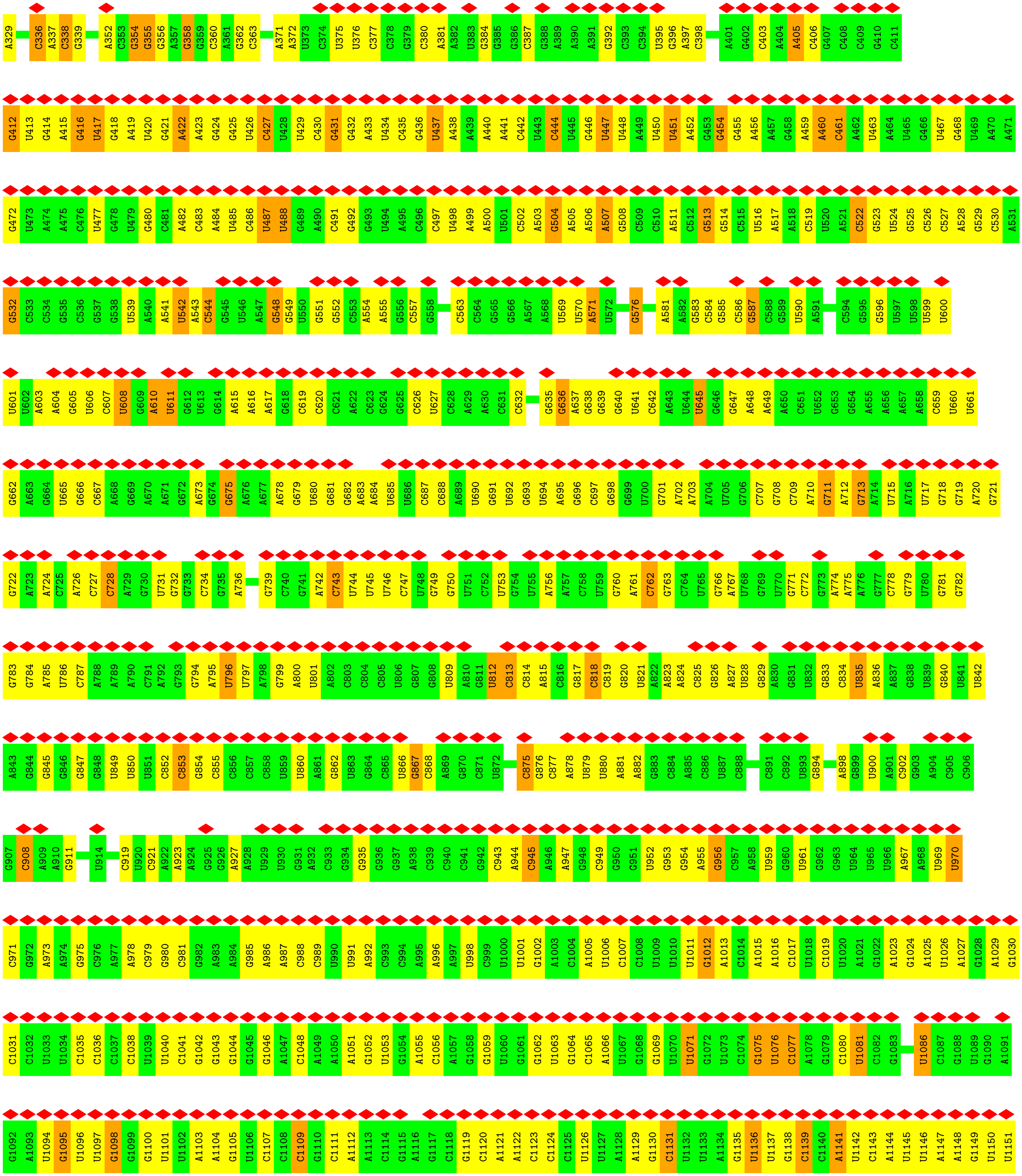
Chain 4:

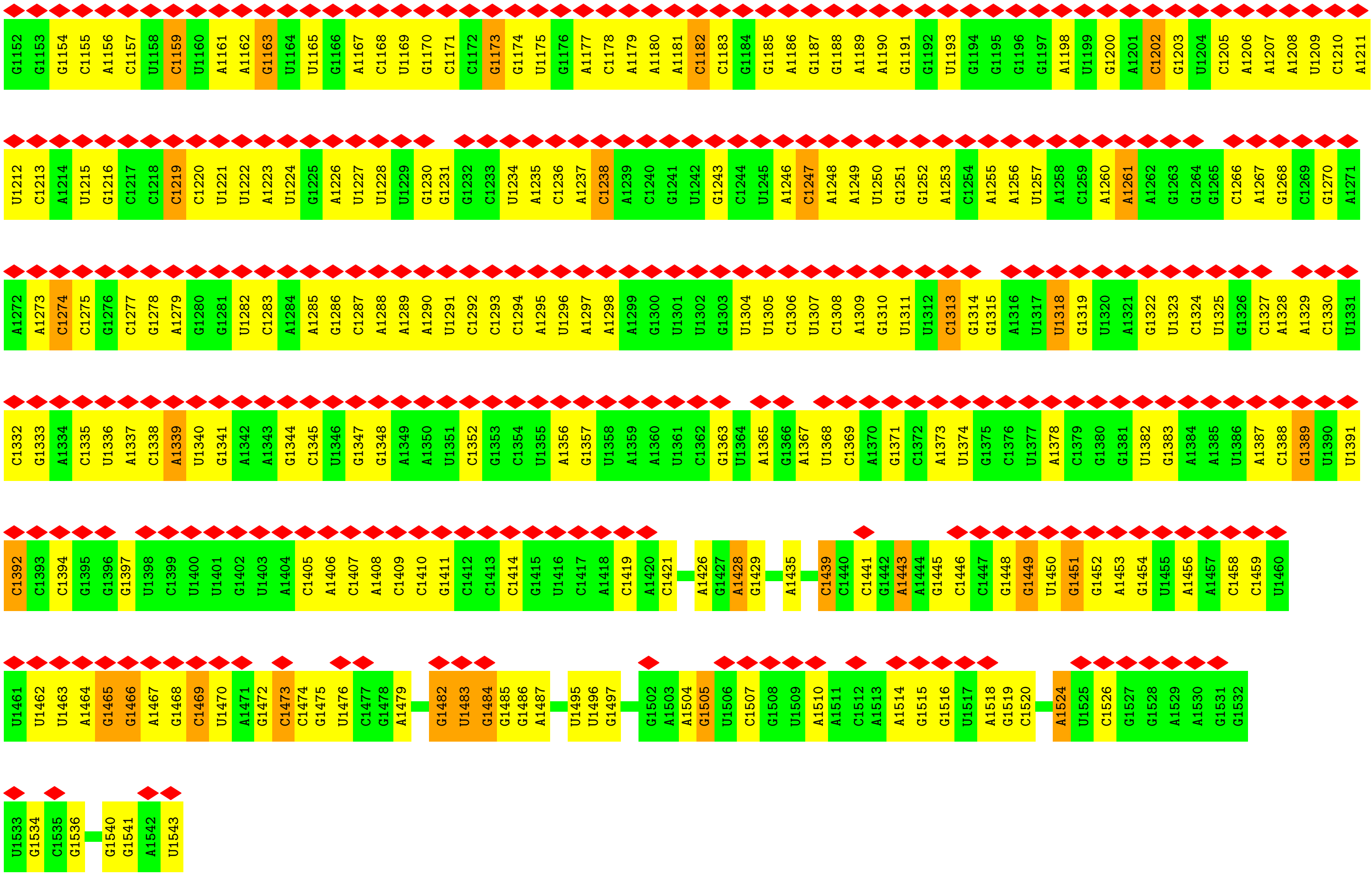


- Molecule 31: 16S ribosomal RNA

Chain a:

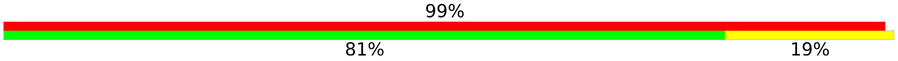


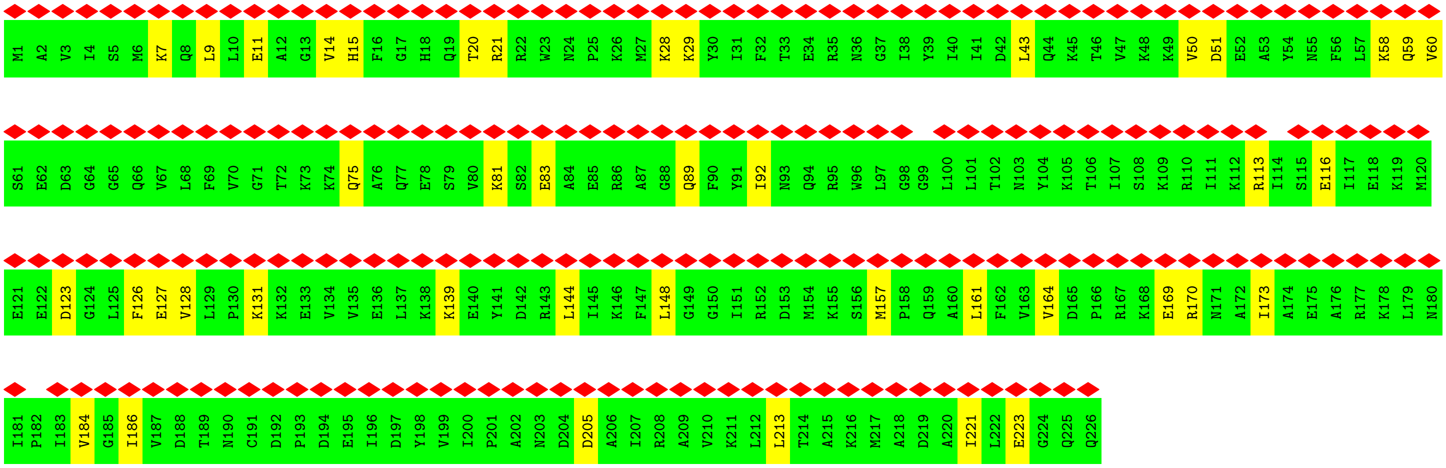

A329 C336 A337 C338 G339 A352 C353 G354 G355 G356 A357 G358 G359 C360 A361 G362 C363 A371 A372 U373 C374 U375 U376 C377 C378 G379 C380 A381 A382 U383 G384 G385 G386 C387 G388 A389 A390 U391 G392 C393 C394 U395 G396 A397 C398 A401 G402 C403 A404 A405 C406 G407 C408 C409 G410 C411
G412 U413 G414 A415 G416 U417 G418 A419 U420 G421 A422 A423 G424 G425 U426 C427 U428 U429 C430 G431 G432 A433 U434 C435 G436 U437 A438 A439 A440 A441 C442 U443 C444 U445 G446 U447 U448 A449 U450 U451 A452 G453 G454 G455 A456 A457 G458 A459 A460 C461 A462 U463 A464 U465 G466 U467 G468 U469 A470 A471
G472 U473 A474 A475 C476 U477 G478 U479 G480 C481 A482 C483 A484 U485 C486 U487 U488 G489 A490 C491 G492 G493 U494 A495 C496 C497 U498 A499 A500 U501 C502 A503 G504 A505 A506 A507 G508 C509 C510 A511 C512 G513 G514 C515 U516 A517 A518 C519 U520 A521 C522 G523 U524 G525 C526 C527 A528 G529 C530 A531
G532 C533 C534 G535 C536 G537 G538 U539 A540 A541 U542 A543 C544 G545 U546 A547 G548 C549 U550 G551 G552 C553 A554 A555 G556 C557 G558 C563 C564 G565 G566 A567 A568 U569 U570 A571 U572 G576 A581 A582 G583 C584 G585 C586 G587 C588 G589 U590 A591 C594 G595 G596 U597 U598 U599 U600
U601 U602 A603 A604 G605 U606 C607 U608 G609 A610 U611 G612 U613 G614 A615 A616 A617 G618 C619 C620 C621 A622 C623 G624 G625 C626 U627 C628 A629 A630 C631 C632 G635 G636 A637 G638 G639 G640 U641 C642 A643 U644 C645 G646 G647 A648 A649 A650 C651 U652 G653 G654 A655 A656 A657 A658 C659 U660 U661
G662 A663 G664 U665 G666 C667 A668 G669 A670 A671 G672 A673 G674 G675 A676 A677 A678 G679 U680 G681 G682 A683 A684 U685 U686 C687 G688 A689 U690 G691 U692 G693 U694 A695 G696 C697 G698 G699 U700 G701 A702 A703 A704 U705 G706 C707 G708 C709 A710 G711 A712 G713 A714 U715 A716 U717 G718 G719 A720 G721
G722 A723 A724 C725 A726 C727 C728 A729 G730 U731 G732 G733 C734 G735 A736 G739 C740 G741 A742 C743 U744 U745 U746 C747 U748 G749 G750 U751 C752 U753 G754 U755 A756 A757 C758 U759 G760 A761 C762 G763 C764 U765 G766 A767 U768 G769 U770 G771 C772 G773 A774 A775 A776 G777 C778 G779 U780 G781 G782
G783 G784 A785 U786 C787 A788 A789 U790 C791 A792 G793 G794 A795 U796 U797 A798 G799 A800 U801 A802 C803 C804 C805 U806 G807 G808 U809 A810 G811 U812 C813 C814 A815 C816 G817 C818 C819 G820 U821 A822 A823 A824 C825 G826 A827 U828 G829 A830 G831 U832 G833 C834 U835 A836 A837 G838 U839 G840 U841 U842
A843 G844 G845 G846 G847 G848 U849 U850 U851 C852 C853 G854 C855 C856 C857 C858 U859 U860 A861 G862 U863 G864 C865 U866 G867 C868 A869 G870 C871 U872 C875 G876 C877 A878 U879 U880 A881 A882 G883 C884 A885 C886 U887 C888 C891 C892 U893 G894 A898 G899 U900 A901 C902 G903 A904 C905 G906
G907 C908 A909 A910 G911 U914 C919 U920 C921 A922 A923 A924 G925 G926 A927 A928 U929 U930 G931 A932 C933 G934 G935 G936 G937 A938 C939 C940 C941 G942 C943 A944 C945 A946 A947 G948 C949 G950 G951 U952 G953 G954 A955 G956 C957 A958 U959 G960 U961 G962 G963 U964 U965 U966 A967 A968 U969 U970
C971 G972 A973 A974 G975 C976 A977 A978 C979 G980 C981 G982 A983 A984 G985 A986 A987 C988 C989 U990 U991 A992 C993 C994 A995 A996 A997 U998 C999 U1000 U1001 G1002 A1003 C1004 A1005 U1006 C1007 C1008 U1009 U1010 U1011 G1012 A1013 C1014 A1015 U1016 C1017 U1018 C1019 U1020 A1021 G1022 A1023 G1024 A1025 U1026 A1027 G1028 A1029 G1030
C1031 C1032 U1033 U1034 C1035 C1036 C1037 C1038 U1039 U1040 C1041 G1042 G1043 G1044 G1045 G1046 A1047 C1048 A1049 A1050 A1051 G1052 U1053 G1054 A1055 C1056 A1057 G1058 G1059 U1060 G1061 G1062 U1063 G1064 C1065 A1066 U1067 G1068 G1069 U1070 U1071 G1072 U1073 C1074 G1075 U1076 C1077 A1078 G1079 C1080 U1081 C1082 G1083 U1086 C1087 G1088 U1089 G1090 A1091
G1092 A1093 U1094 G1095 U1096 U1097 G1098 G1099 G1100 U1101 U1102 A1103 A1104 G1105 U1106 C1107 C1108 C1109 G1110 C1111 A1112 A1113 C1114 G1115 A1116 G1117 C1118 G1119 C1120 A1121 A1122 C1123 C1124 C1125 U1126 U1127 A1128 A1129 G1130 C1131 U1132 U1133 A1134 G1135 U1136 U1137 G1138 C1139 C1140 A1141 U1142 C1143 A1144 U1145 U1146 A1147 A1148 G1149 U1150 U1151



- Molecule 32: 30S ribosomal protein S2

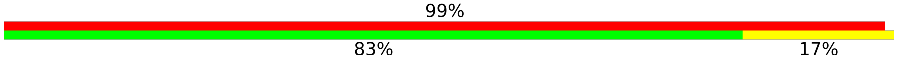
Chain b:





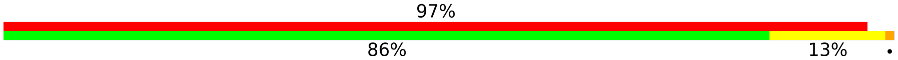
- Molecule 33: 30S ribosomal protein S3

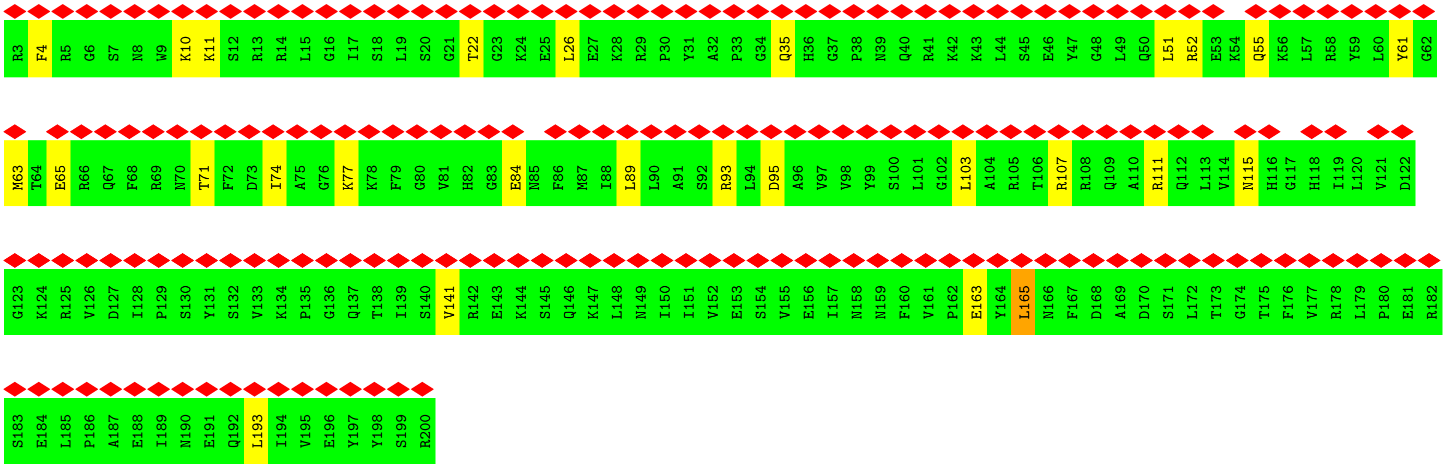
Chain c:



- Molecule 34: 30S ribosomal protein S4

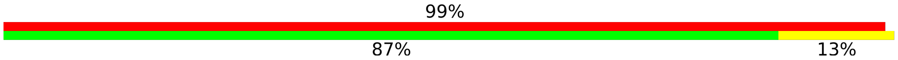
Chain d:

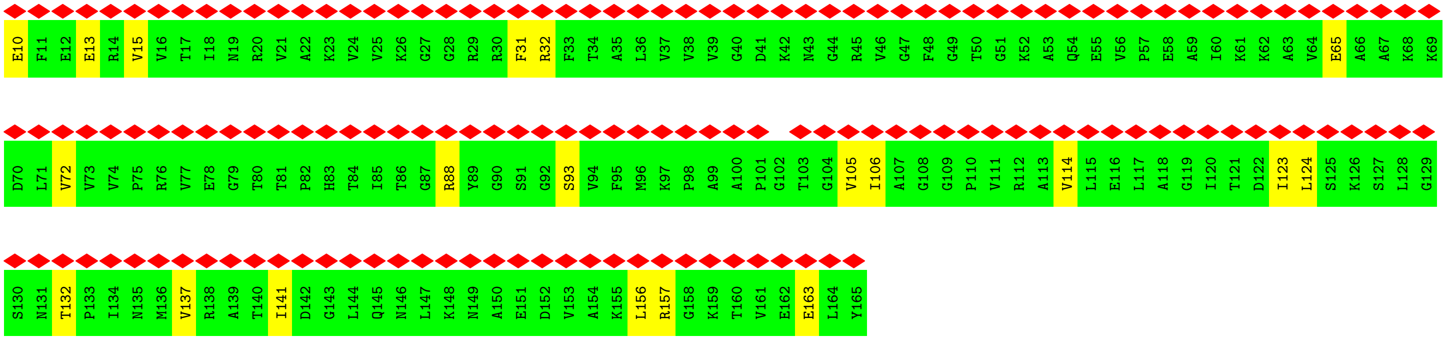




- Molecule 35: 30S ribosomal protein S5

Chain e:

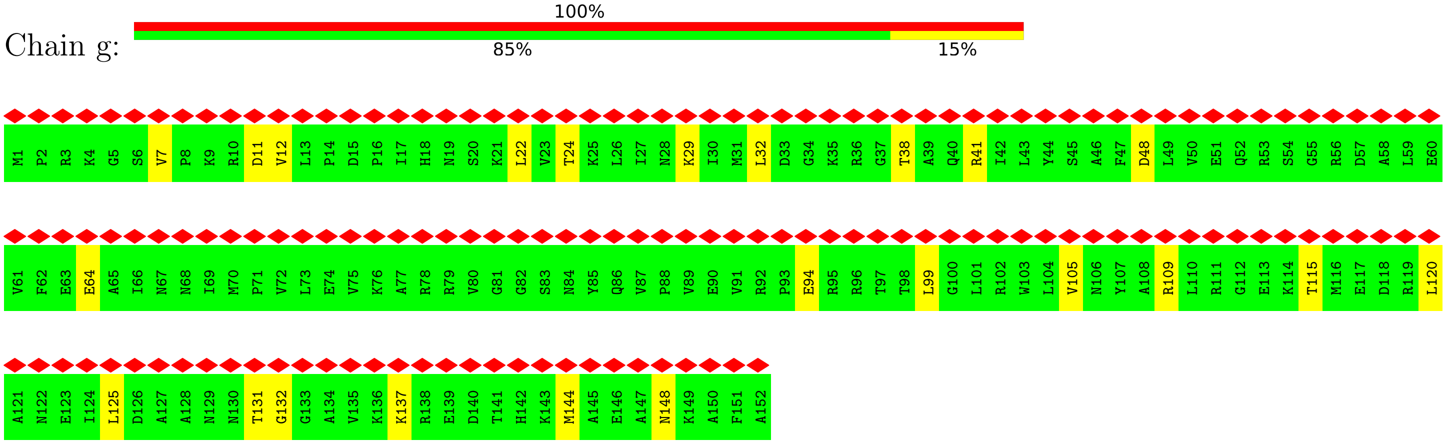




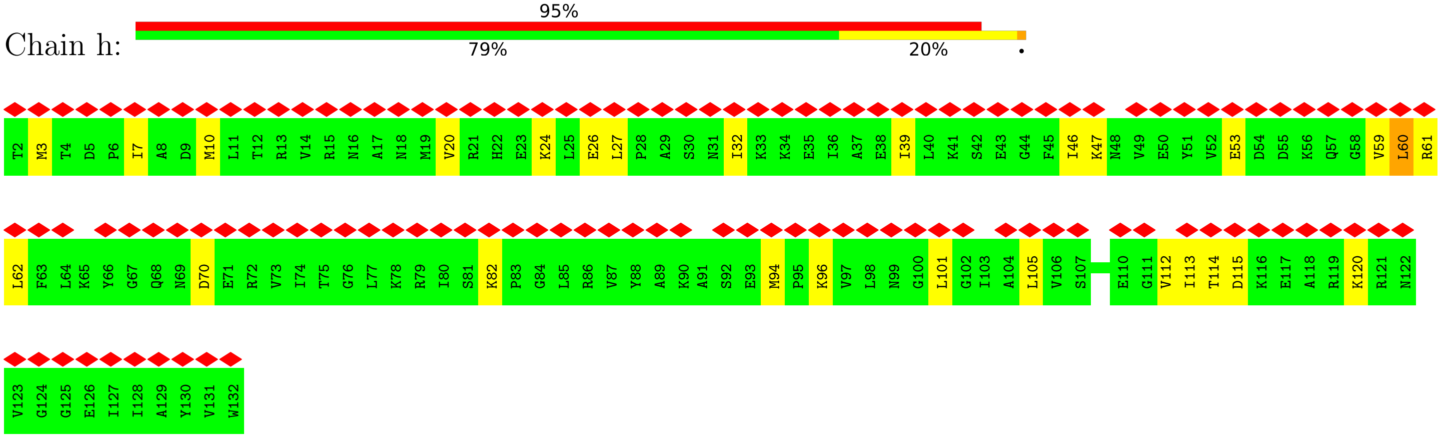
- Molecule 36: 30S ribosomal protein S6

Chain f:

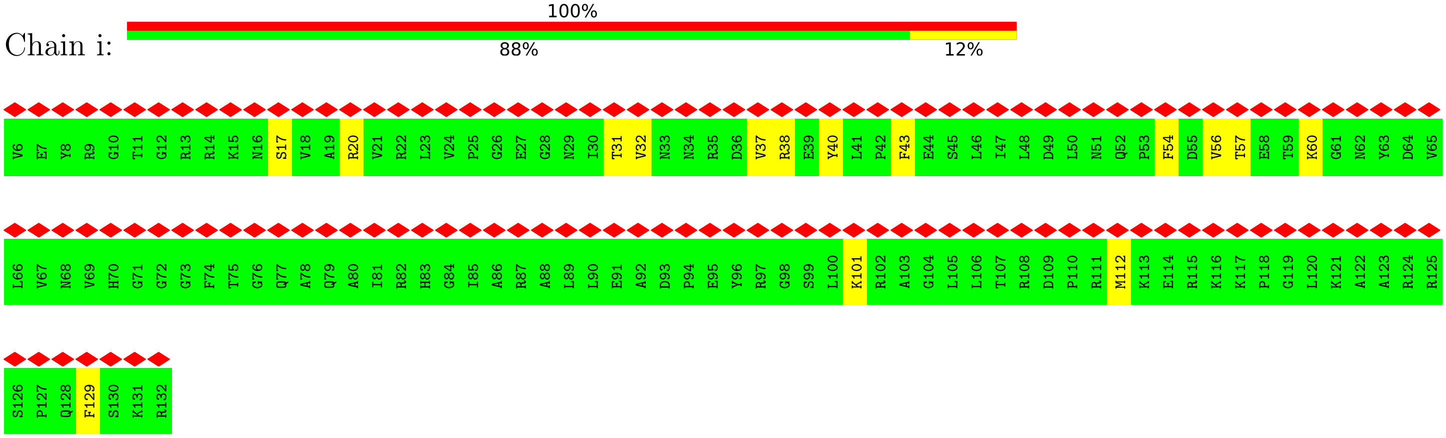
- Molecule 37: 30S ribosomal protein S7



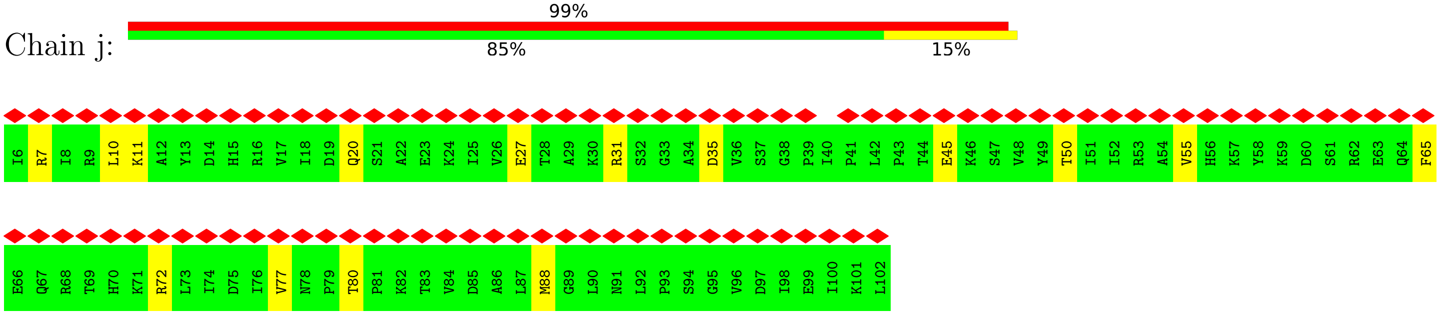
- Molecule 38: 30S ribosomal protein S8



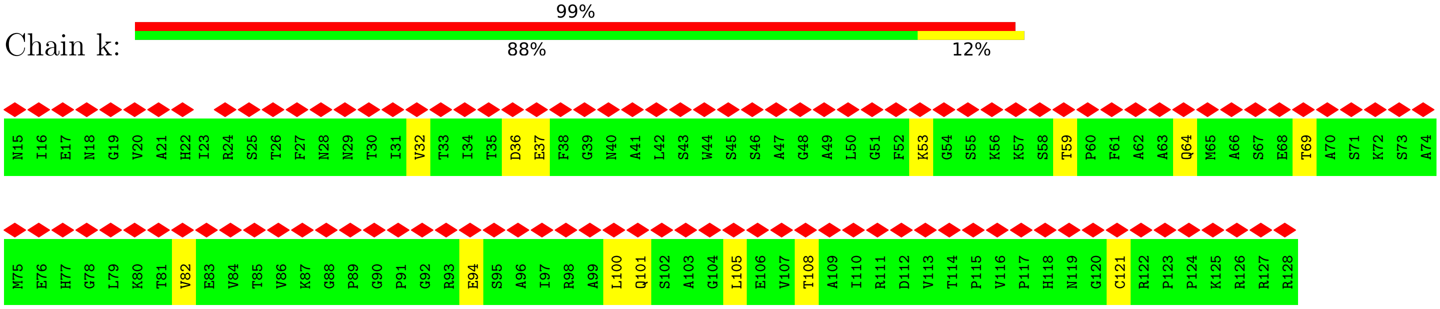
- Molecule 39: 30S ribosomal protein S9



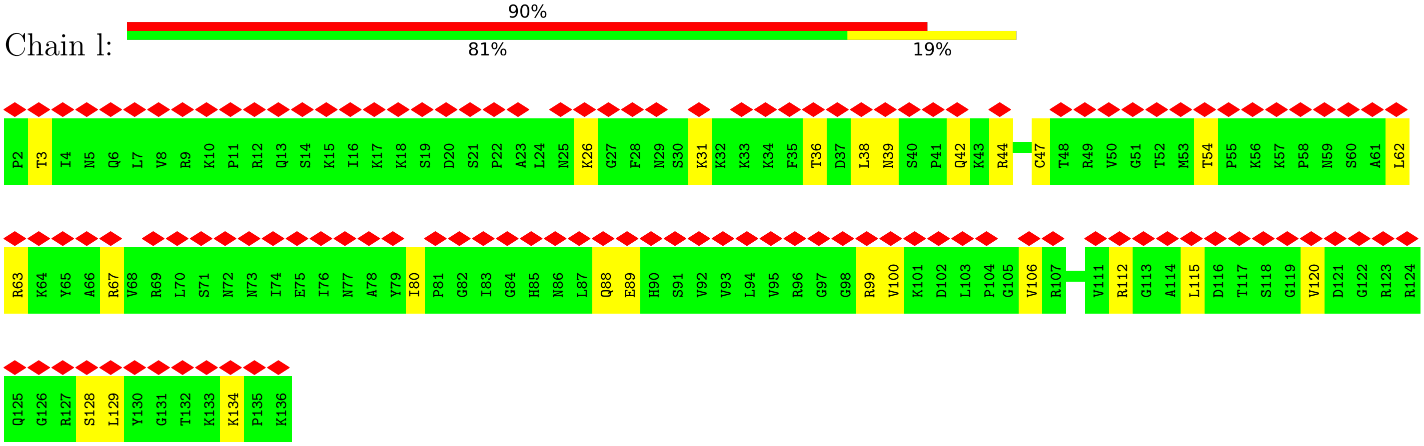
- Molecule 40: 30S ribosomal protein S10



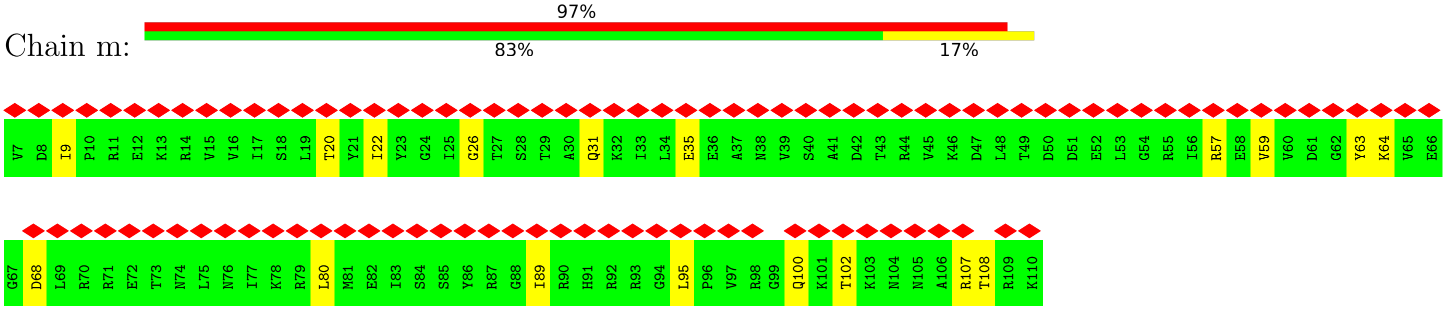
- Molecule 41: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S12

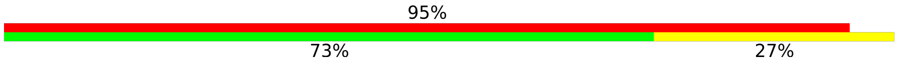


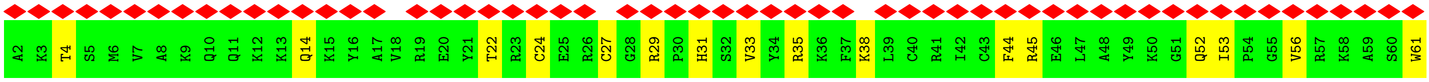
- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14 type Z

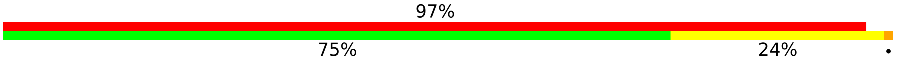
Chain n:

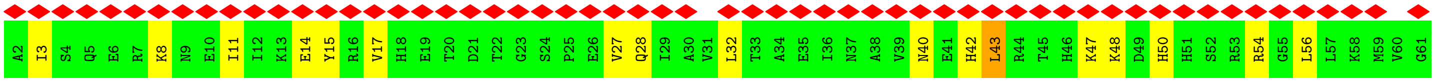


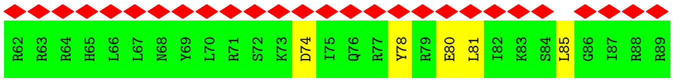


- Molecule 45: 30S ribosomal protein S15

Chain o:

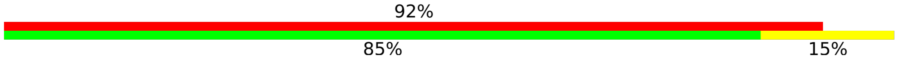


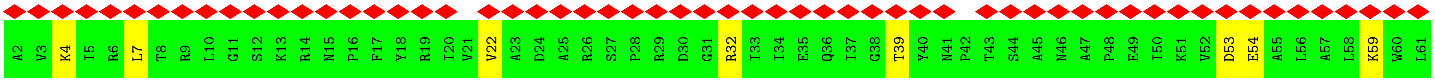


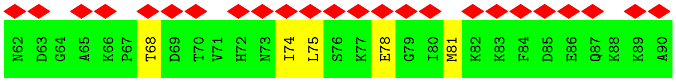


- Molecule 46: 30S ribosomal protein S16

Chain p:

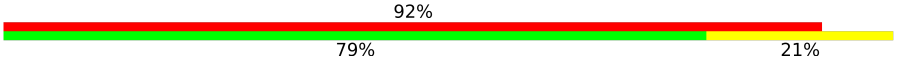


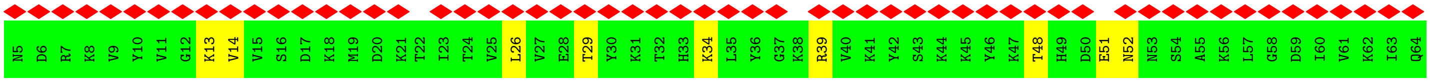


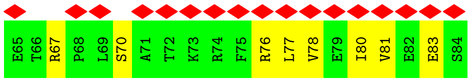


- Molecule 47: 30S ribosomal protein S17

Chain q:

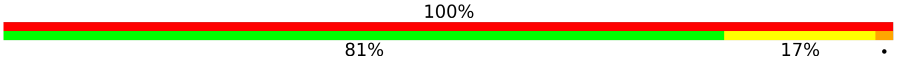


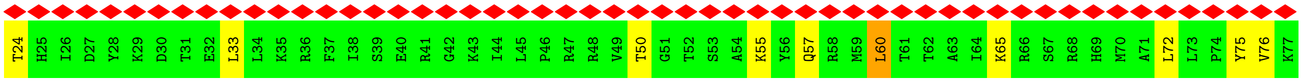




- Molecule 48: 30S ribosomal protein S18

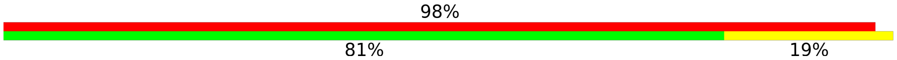
Chain r:

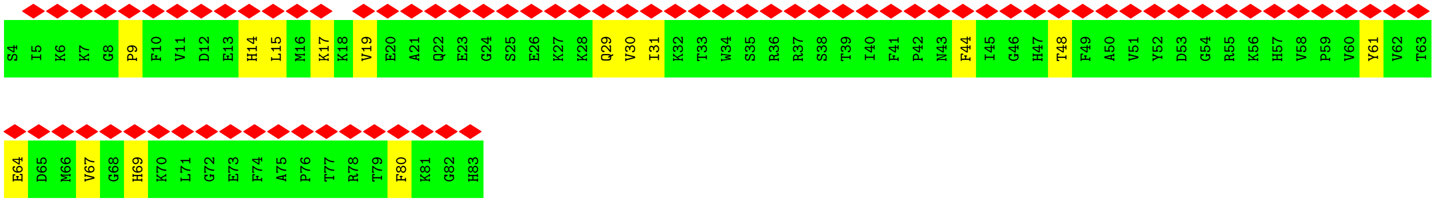




- Molecule 49: 30S ribosomal protein S19

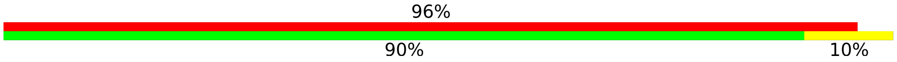
Chain s:

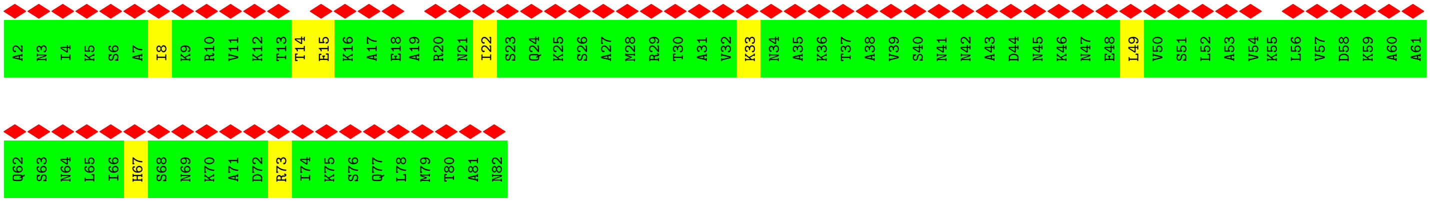




- Molecule 50: 30S ribosomal protein S20

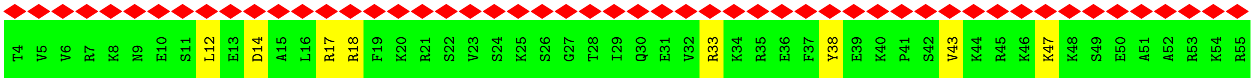
Chain t:





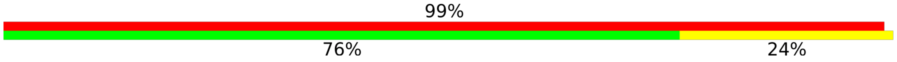
- Molecule 51: 30S ribosomal protein S21

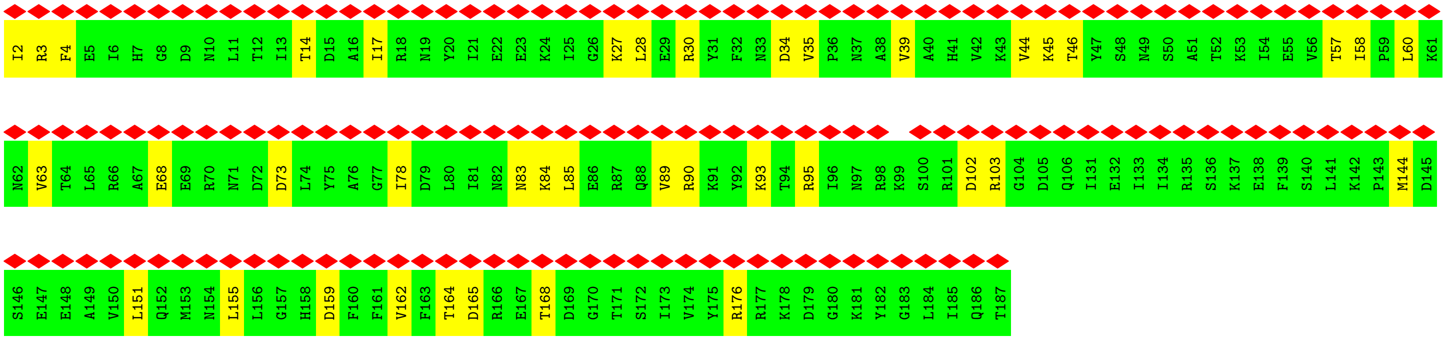
Chain u:



- Molecule 52: Ribosome hibernation promoting factor

Chain v:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	378309	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.076	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.320	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	426.80002, 426.80002, 426.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	3.16	6081/69740 (8.7%)	3.34	9273/108755 (8.5%)
2	B	1.67	25/2733 (0.9%)	1.75	88/4257 (2.1%)
3	C	1.14	3/2125 (0.1%)	0.81	1/2853 (0.0%)
4	D	1.22	1/1651 (0.1%)	0.83	1/2215 (0.0%)
5	E	1.14	1/1595 (0.1%)	0.85	1/2154 (0.0%)
6	F	0.39	0/1329	0.60	0/1791
7	G	0.39	0/1266	0.54	0/1717
8	H	1.23	3/1171 (0.3%)	0.85	0/1577
9	I	1.16	2/925 (0.2%)	0.84	0/1242
10	J	1.07	1/1100 (0.1%)	0.84	1/1467 (0.1%)
11	K	1.10	1/1103 (0.1%)	0.70	0/1481
12	L	1.12	0/936	0.79	0/1253
13	M	0.62	0/892	0.66	1/1195 (0.1%)
14	N	1.17	2/901 (0.2%)	0.78	0/1209
15	O	1.33	3/955 (0.3%)	0.86	0/1265
16	P	1.22	1/800 (0.1%)	0.88	0/1070
17	Q	1.09	2/846 (0.2%)	0.78	0/1140
18	R	0.98	0/723	0.70	0/966
19	S	0.82	0/779	0.72	0/1043
20	T	0.77	0/730	0.71	1/981 (0.1%)
21	U	1.25	1/593 (0.2%)	0.77	0/788
22	V	0.98	0/384	0.81	1/515 (0.2%)
23	W	0.75	0/542	0.67	0/722
24	X	1.17	1/451 (0.2%)	0.82	0/606
25	Y	0.34	0/378	0.56	0/521
26	Z	1.06	0/366	0.80	0/489
27	1	0.55	0/395	0.58	0/530
28	2	1.37	1/371 (0.3%)	0.90	1/484 (0.2%)
29	3	1.08	2/526 (0.4%)	0.75	0/690
30	4	0.76	0/298	0.61	0/392
31	a	0.62	3/36913 (0.0%)	1.38	509/57564 (0.9%)
32	b	0.30	0/1846	0.53	0/2477

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
33	c	0.27	0/1523	0.56	0/2062
34	d	0.31	0/1526	0.62	1/2063 (0.0%)
35	e	0.31	0/1159	0.58	0/1566
36	f	0.34	0/789	0.58	0/1060
37	g	0.38	1/1176 (0.1%)	0.53	0/1588
38	h	0.29	0/1038	0.55	1/1395 (0.1%)
39	i	0.28	0/937	0.59	0/1269
40	j	0.27	0/764	0.52	0/1034
41	k	0.32	0/824	0.60	0/1119
42	l	0.32	0/1054	0.54	0/1415
43	m	0.26	0/732	0.59	0/991
44	n	0.32	0/497	0.55	0/662
45	o	0.27	0/732	0.55	1/979 (0.1%)
46	p	0.28	0/705	0.56	1/952 (0.1%)
47	q	0.32	0/629	0.58	0/849
48	r	0.30	0/452	0.60	1/604 (0.2%)
49	s	0.34	0/654	0.56	0/879
50	t	0.25	0/591	0.47	0/793
51	u	0.29	0/403	0.48	0/535
52	v	0.27	0/1350	0.55	0/1812
All	All	2.21	6135/152898 (4.0%)	2.44	9883/229036 (4.3%)

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
1	A	3	15
5	E	0	3
9	I	0	1
11	K	0	1
13	M	0	1
16	P	0	2
19	S	0	1
23	W	0	1
26	Z	0	1
29	3	0	1
43	m	0	1
49	s	0	3
All	All	3	31

The worst 5 of 6135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	A	N7-C5	192.33	2.54	1.39
1	A	332	A	N9-C4	181.51	2.46	1.37
1	A	332	A	C8-N7	159.80	2.43	1.31
1	A	332	A	N9-C8	145.76	2.54	1.37
1	A	332	A	C5-C4	134.74	2.33	1.38

The worst 5 of 9883 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	393	G	C8-N9-C4	-165.41	40.24	106.40
1	A	393	G	C5-N7-C8	-101.22	53.69	104.30
1	A	650	U	N3-C2-O2	-47.45	88.98	122.20
1	A	1016	G	C8-N9-C4	-47.36	87.45	106.40
1	A	393	G	N7-C8-N9	46.20	136.20	113.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	990	G	C4’
1	A	1289	A	C1’
1	A	2077	C	C1’

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	C	Sidechain
1	A	557	G	Sidechain
1	A	627	C	Sidechain
1	A	644	C	Sidechain
1	A	648	G	Sidechain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
3	C	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	34	47
4	D	213/215 (99%)	194 (91%)	19 (9%)	0	100	100
5	E	204/206 (99%)	187 (92%)	17 (8%)	0	100	100
6	F	171/173 (99%)	142 (83%)	29 (17%)	0	100	100
7	G	171/173 (99%)	154 (90%)	17 (10%)	0	100	100
8	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
9	I	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	J	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
11	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
12	L	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
13	M	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
14	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
15	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	P	100/102 (98%)	92 (92%)	7 (7%)	1 (1%)	15	22
17	Q	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
18	R	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
19	S	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	15	22
20	T	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
21	U	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
22	V	47/49 (96%)	39 (83%)	8 (17%)	0	100	100
23	W	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
24	X	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
25	Y	57/59 (97%)	44 (77%)	13 (23%)	0	100	100
26	Z	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
27	1	45/47 (96%)	45 (100%)	0	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	9	12
30	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
32	b	224/226 (99%)	206 (92%)	18 (8%)	0	100	100
33	c	200/202 (99%)	174 (87%)	26 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	d	196/198 (99%)	166 (85%)	30 (15%)	0	100	100
35	e	154/156 (99%)	133 (86%)	21 (14%)	0	100	100
36	f	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
37	g	150/152 (99%)	142 (95%)	8 (5%)	0	100	100
38	h	129/131 (98%)	110 (85%)	19 (15%)	0	100	100
39	i	125/127 (98%)	99 (79%)	26 (21%)	0	100	100
40	j	95/97 (98%)	79 (83%)	16 (17%)	0	100	100
41	k	112/114 (98%)	94 (84%)	18 (16%)	0	100	100
42	l	133/135 (98%)	116 (87%)	17 (13%)	0	100	100
43	m	100/104 (96%)	84 (84%)	16 (16%)	0	100	100
44	n	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
45	o	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
46	p	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
47	q	78/80 (98%)	67 (86%)	11 (14%)	0	100	100
48	r	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
49	s	78/80 (98%)	63 (81%)	15 (19%)	0	100	100
50	t	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
51	u	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
52	v	158/162 (98%)	144 (91%)	14 (9%)	0	100	100
All	All	5487/5589 (98%)	4951 (90%)	532 (10%)	4 (0%)	54	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	41	ALA
16	P	51	PRO
19	S	52	PRO
29	3	20	GLY

5.3.2 Protein sidechains ⓘ

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	
3	C	220/221 (100%)	186 (84%)	34 (16%)	2	3
4	D	173/173 (100%)	145 (84%)	28 (16%)	2	2
5	E	168/168 (100%)	141 (84%)	27 (16%)	2	2
6	F	141/152 (93%)	113 (80%)	28 (20%)	1	1
7	G	122/151 (81%)	102 (84%)	20 (16%)	2	2
8	H	123/123 (100%)	103 (84%)	20 (16%)	2	2
9	I	100/100 (100%)	84 (84%)	16 (16%)	2	2
10	J	109/112 (97%)	85 (78%)	24 (22%)	1	1
11	K	110/114 (96%)	98 (89%)	12 (11%)	6	8
12	L	96/101 (95%)	79 (82%)	17 (18%)	2	2
13	M	85/94 (90%)	70 (82%)	15 (18%)	2	2
14	N	93/100 (93%)	83 (89%)	10 (11%)	6	8
15	O	96/96 (100%)	87 (91%)	9 (9%)	8	12
16	P	84/86 (98%)	67 (80%)	17 (20%)	1	1
17	Q	88/90 (98%)	82 (93%)	6 (7%)	16	24
18	R	78/80 (98%)	62 (80%)	16 (20%)	1	1
19	S	81/88 (92%)	65 (80%)	16 (20%)	1	1
20	T	78/82 (95%)	68 (87%)	10 (13%)	4	5
21	U	59/60 (98%)	47 (80%)	12 (20%)	1	1
22	V	39/41 (95%)	36 (92%)	3 (8%)	13	19
23	W	58/60 (97%)	48 (83%)	10 (17%)	2	2
24	X	52/52 (100%)	44 (85%)	8 (15%)	2	3
25	Y	23/56 (41%)	20 (87%)	3 (13%)	4	4
26	Z	35/44 (80%)	25 (71%)	10 (29%)	0	0
27	1	44/45 (98%)	38 (86%)	6 (14%)	3	4
28	2	39/39 (100%)	37 (95%)	2 (5%)	24	37
29	3	55/55 (100%)	47 (86%)	8 (14%)	3	3
30	4	35/35 (100%)	31 (89%)	4 (11%)	5	7
32	b	196/196 (100%)	154 (79%)	42 (21%)	1	1
33	c	138/164 (84%)	104 (75%)	34 (25%)	0	0
34	d	147/174 (84%)	120 (82%)	27 (18%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	e	118/122 (97%)	98 (83%)	20 (17%)	2	2
36	f	80/83 (96%)	64 (80%)	16 (20%)	1	1
37	g	118/128 (92%)	96 (81%)	22 (19%)	1	1
38	h	111/112 (99%)	84 (76%)	27 (24%)	0	0
39	i	86/105 (82%)	71 (83%)	15 (17%)	2	2
40	j	81/87 (93%)	66 (82%)	15 (18%)	1	1
41	k	82/90 (91%)	68 (83%)	14 (17%)	2	2
42	l	111/117 (95%)	86 (78%)	25 (22%)	1	1
43	m	62/92 (67%)	45 (73%)	17 (27%)	0	0
44	n	48/52 (92%)	32 (67%)	16 (33%)	0	0
45	o	77/80 (96%)	55 (71%)	22 (29%)	0	0
46	p	73/75 (97%)	61 (84%)	12 (16%)	2	2
47	q	65/75 (87%)	48 (74%)	17 (26%)	0	0
48	r	48/49 (98%)	38 (79%)	10 (21%)	1	1
49	s	67/70 (96%)	55 (82%)	12 (18%)	2	2
50	t	61/67 (91%)	53 (87%)	8 (13%)	4	4
51	u	40/48 (83%)	32 (80%)	8 (20%)	1	1
52	v	147/147 (100%)	108 (74%)	39 (26%)	0	0
All	All	4440/4751 (94%)	3631 (82%)	809 (18%)	4	1

5 of 809 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	c	191	THR
38	h	105	LEU
52	v	103	ARG
34	d	61	TYR
33	c	178	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
38	h	22	HIS
45	o	40	ASN
39	i	29	ASN

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Mol	Chain	Res	Type
41	k	64	GLN
49	s	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2905 (99%)	1345 (46%)	256 (8%)
2	B	114/115 (99%)	32 (28%)	2 (1%)
31	a	1537/1539 (99%)	710 (46%)	0
All	All	4548/4559 (99%)	2087 (45%)	258 (5%)

5 of 2087 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	A
1	A	12	U
1	A	13	A
1	A	14	A

5 of 258 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2578	C
1	A	2665	G
1	A	858	U
1	A	809	A
1	A	2760	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	ERY	A	3001	-	53,53,53	2.19	11 (20%)	82,82,82	4.95	38 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	ERY	A	3001	-	3/3/21/21	30/72/107/107	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3001	ERY	O2-C1	10.04	1.57	1.34
53	A	3001	ERY	O10-C6	-4.84	1.36	1.44
53	A	3001	ERY	O2-C13	-4.27	1.39	1.46
53	A	3001	ERY	C19-C16	3.73	1.60	1.52
53	A	3001	ERY	C10-C11	-3.66	1.49	1.54

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	3001	ERY	O5-C16-C15	-18.50	83.30	112.96
53	A	3001	ERY	O13-C12-C13	-14.57	83.86	107.28
53	A	3001	ERY	O10-C6-C32	-14.39	75.32	108.47
53	A	3001	ERY	O13-C12-C35	-12.64	81.67	107.78
53	A	3001	ERY	O13-C12-C11	-12.44	83.82	108.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	A	3001	ERY	C6
53	A	3001	ERY	C12
53	A	3001	ERY	C14

5 of 30 torsion outliers are listed below:

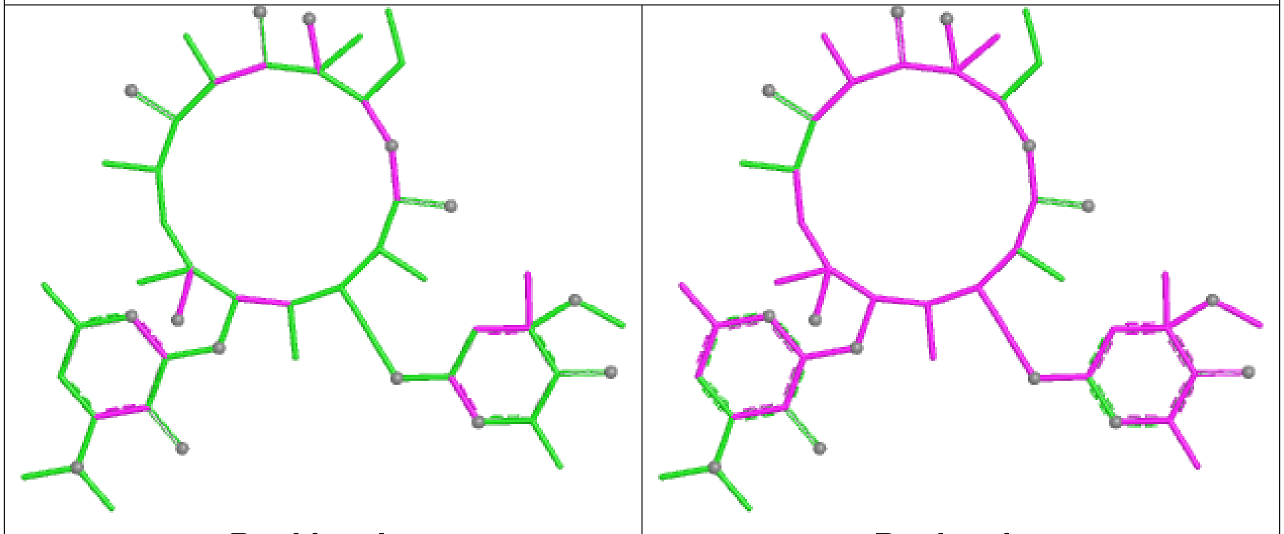
Mol	Chain	Res	Type	Atoms
53	A	3001	ERY	C10-C11-C12-C13
53	A	3001	ERY	C10-C11-C12-C35
53	A	3001	ERY	C10-C11-C12-O13
53	A	3001	ERY	O12-C11-C12-C13
53	A	3001	ERY	O12-C11-C12-C35

There are no ring outliers.

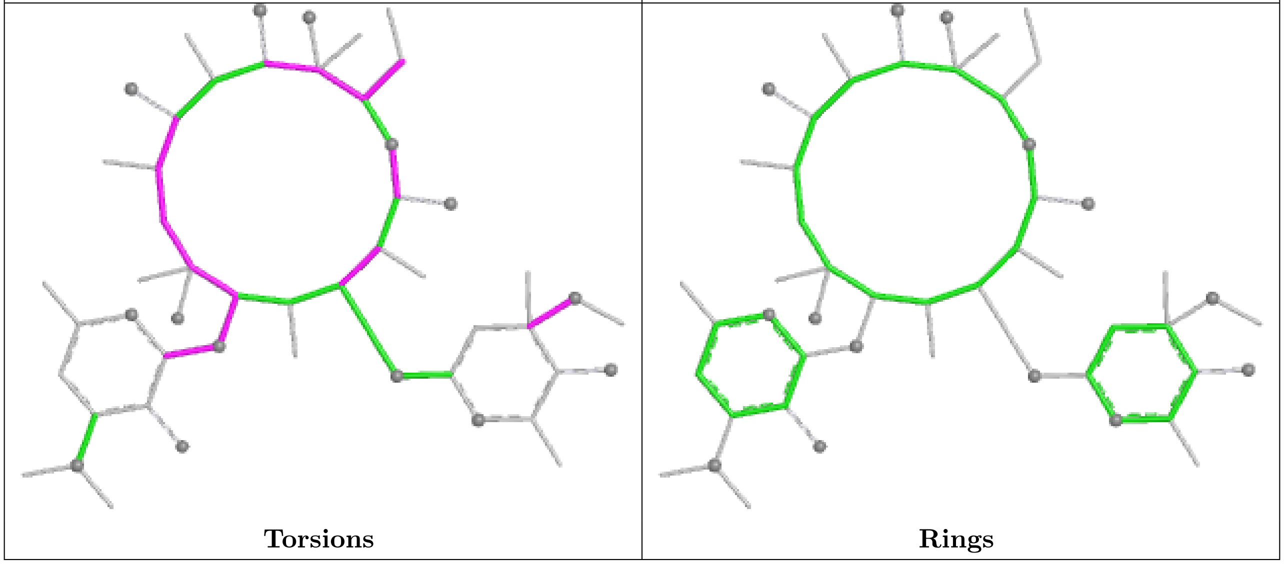
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ERY A 3001



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7
52	v	1
31	a	1
43	m	1

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Mol	Chain	Number of breaks
8	H	1
24	X	1
11	K	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	106:GLN	C	131:ILE	N	27.31
1	A	2207:U	O3'	2208:A	P	12.57
1	A	1939:A	O3'	1944:U	P	12.49
1	A	929:C	O3'	937:G	P	11.52
1	a	465:U	O3'	466:G	P	9.63

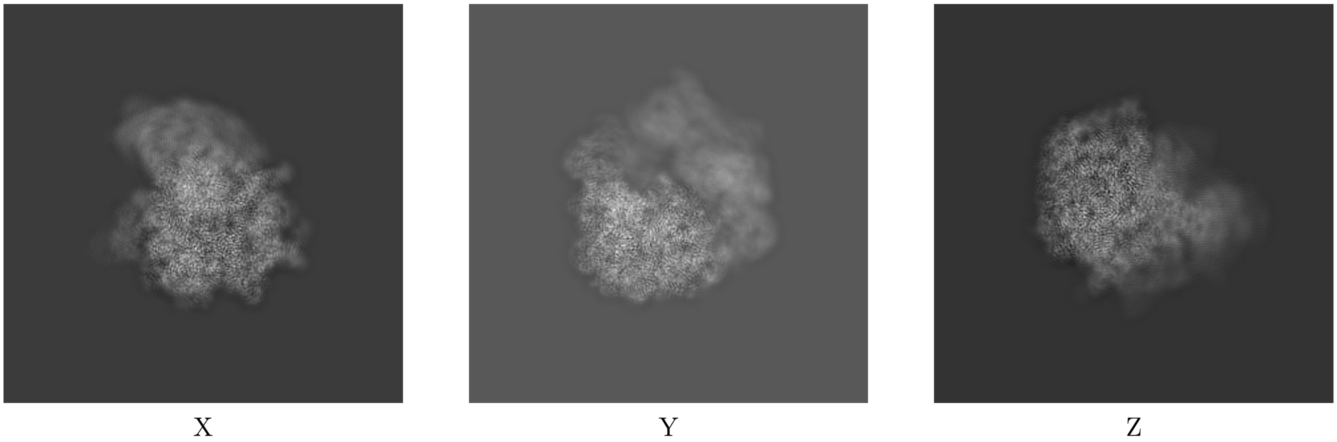
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10076. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

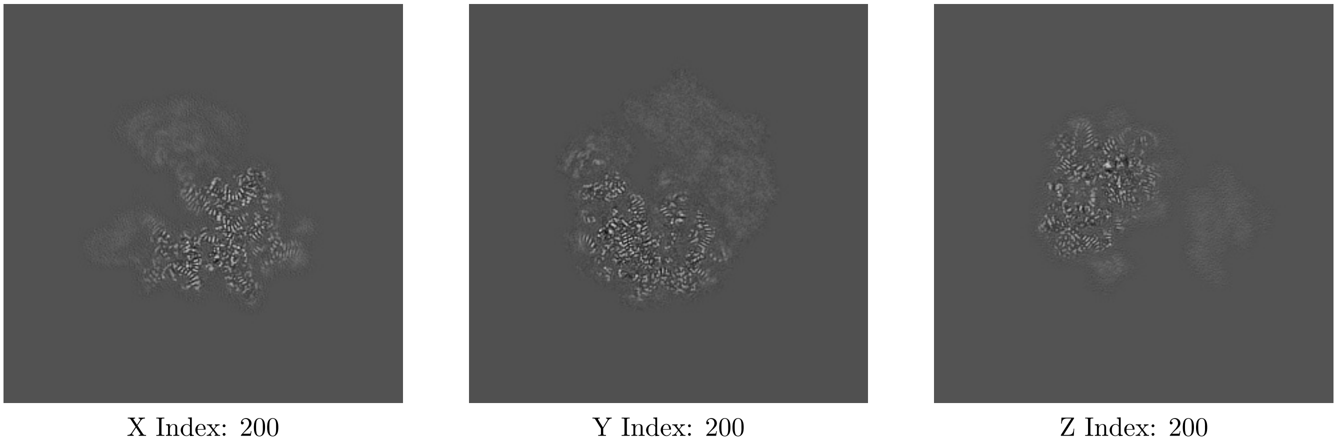
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

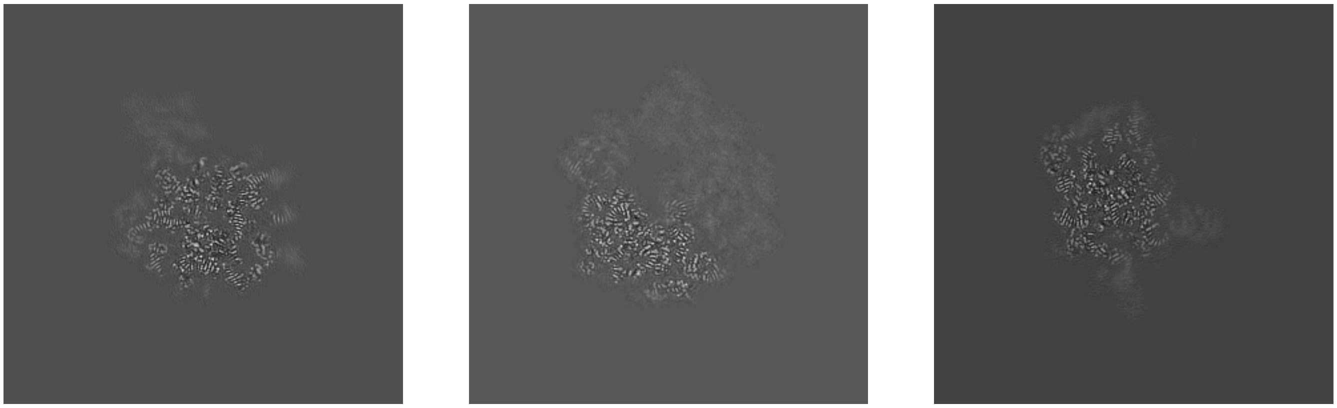
6.2.1 Primary map


X Index: 200 Y Index: 200 Z Index: 200

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

6.3 Largest variance slices

6.3.1 Primary map

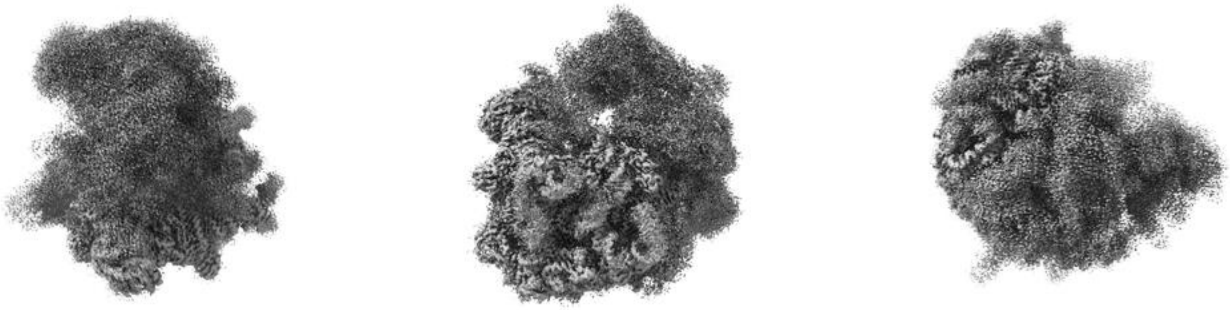


X Index: 171 Y Index: 185 Z Index: 147

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

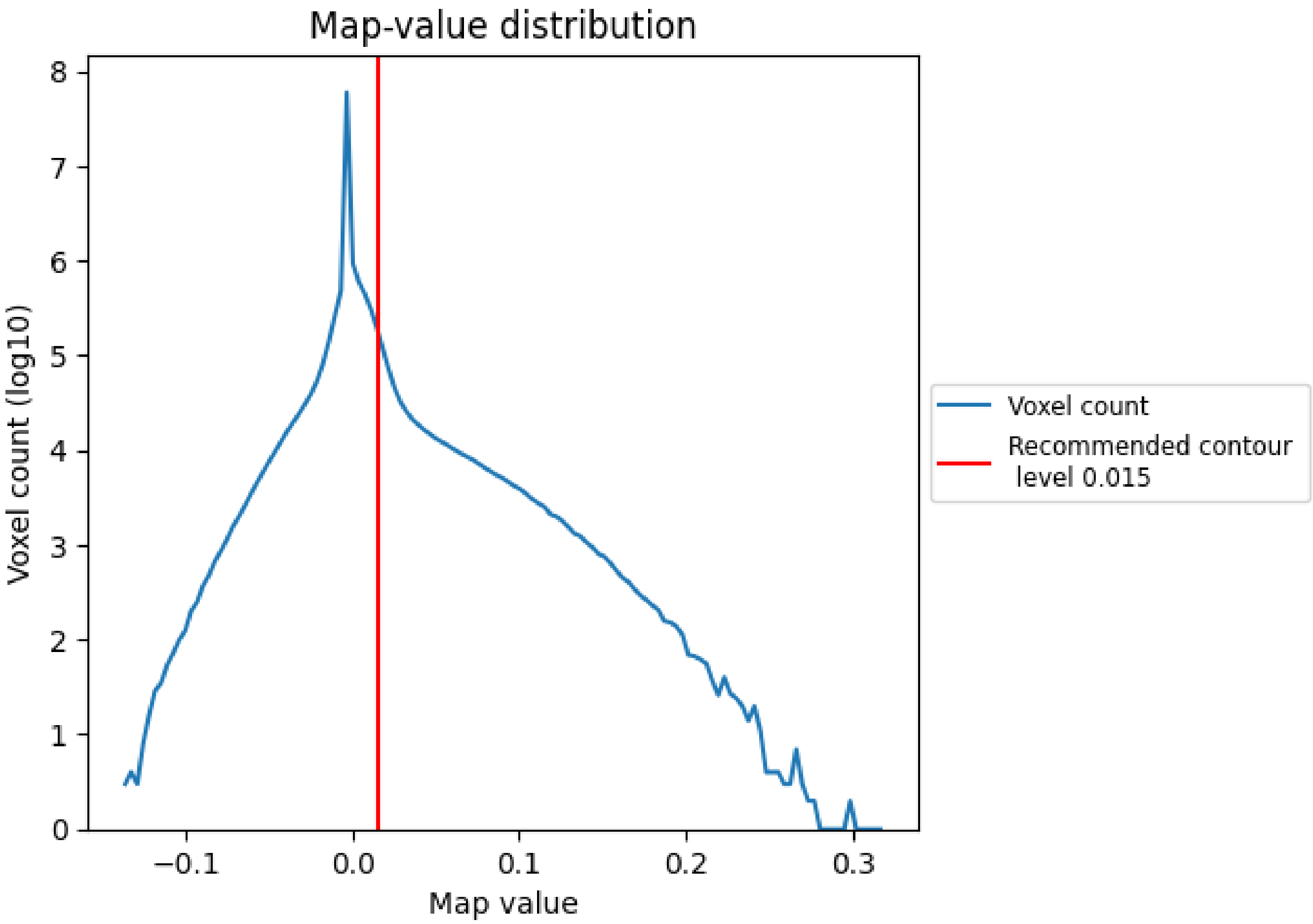
6.5 Mask visualisation ⓘ

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

7 Map analysis (i)

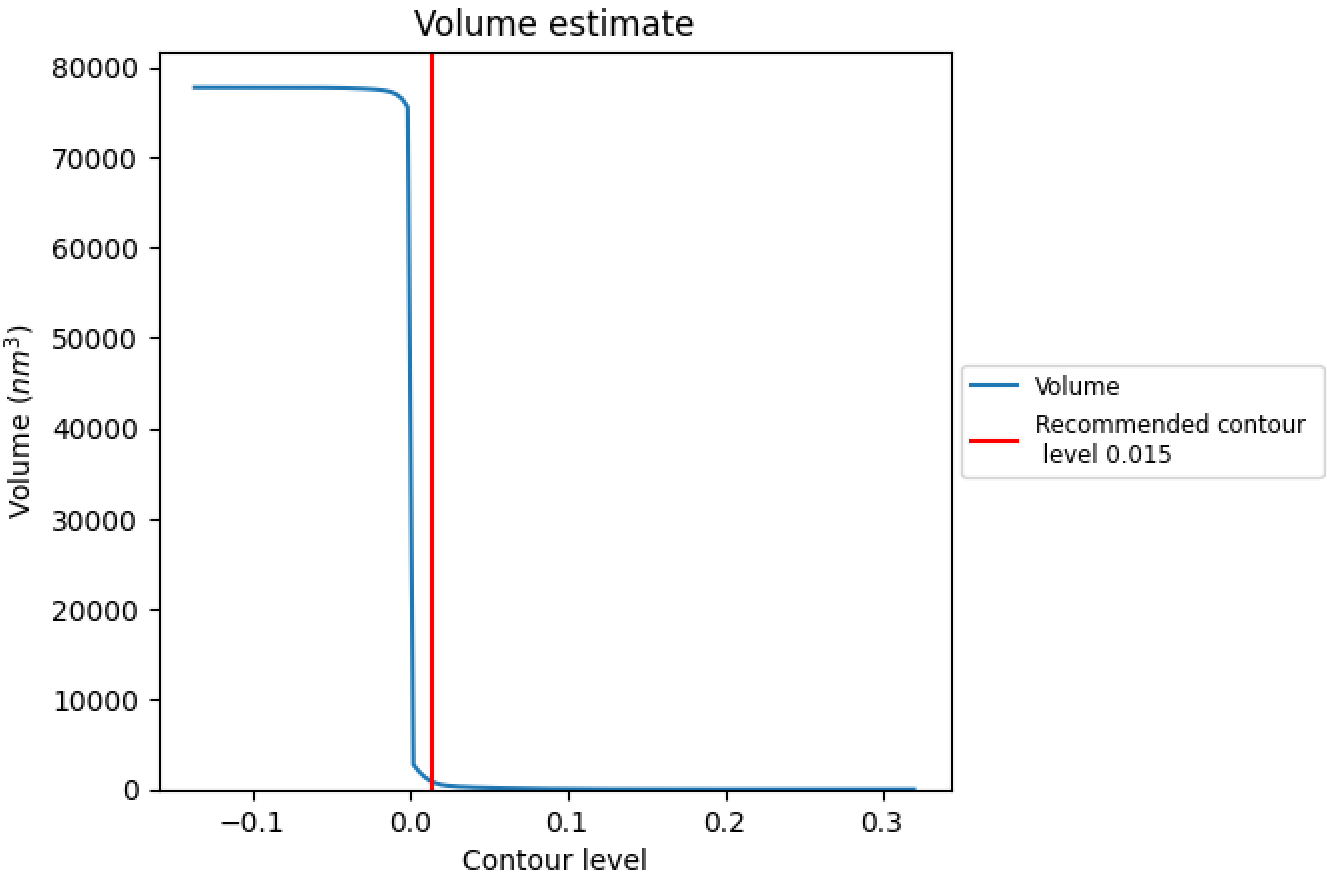
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

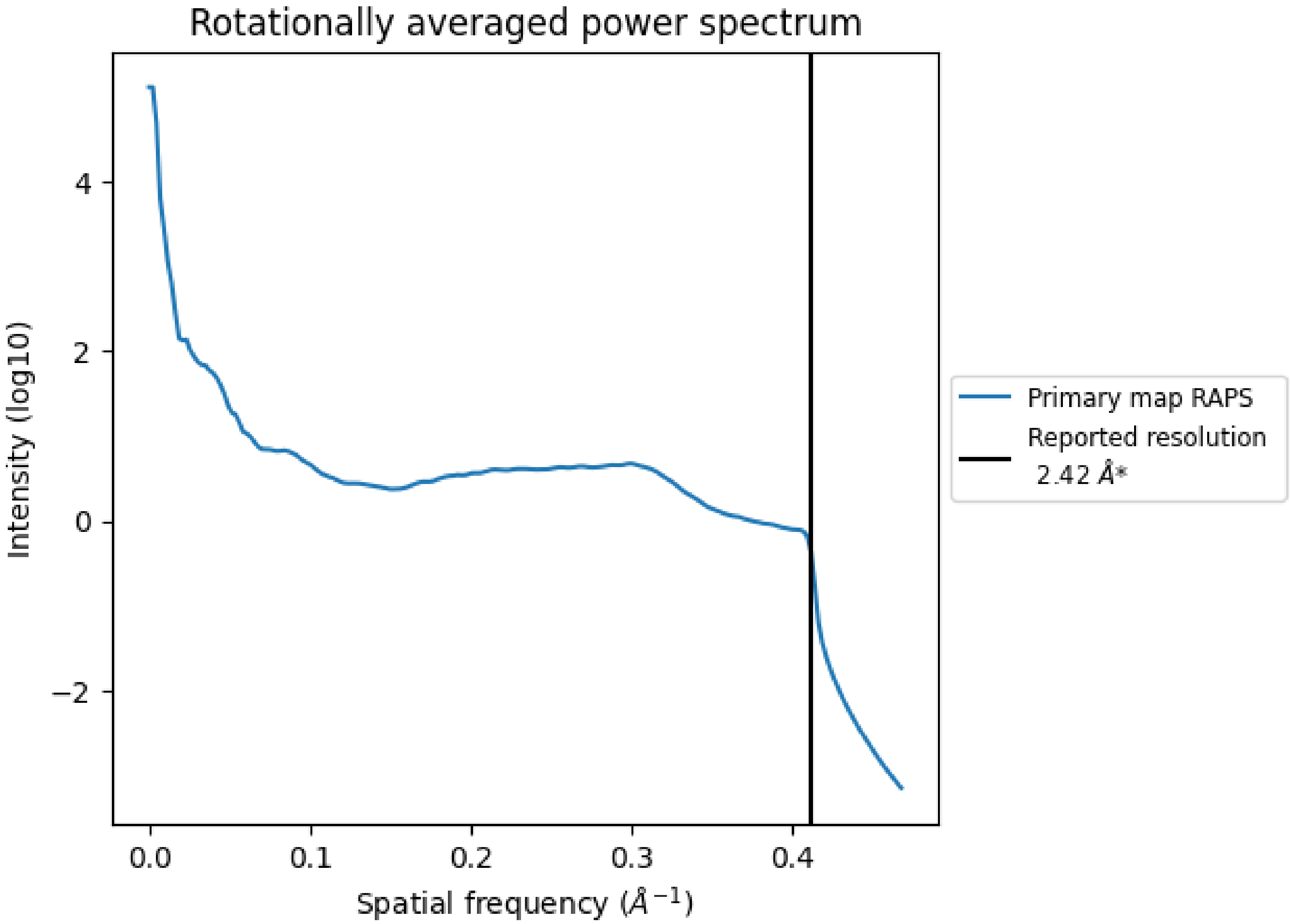
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 827 nm^3; this corresponds to an approximate mass of 747 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.412 $Å^{-1}$

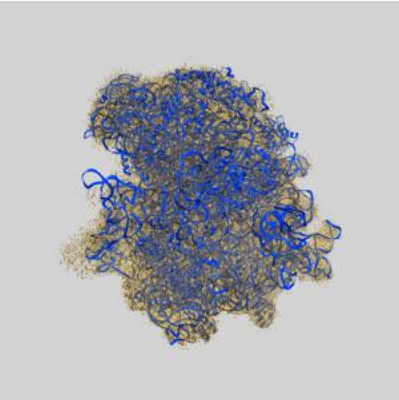
8 Fourier-Shell correlation ⓘ

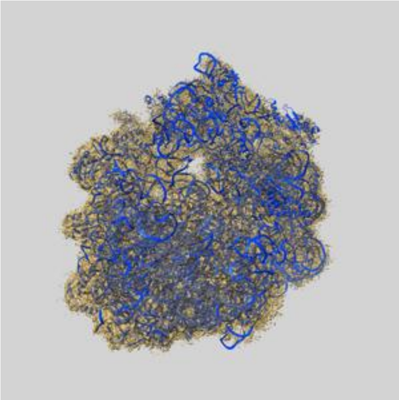
This section was not generated. No FSC curve or half-maps provided.

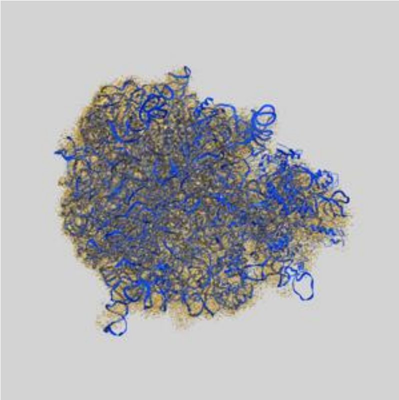
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10076 and PDB model 6S0X. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay

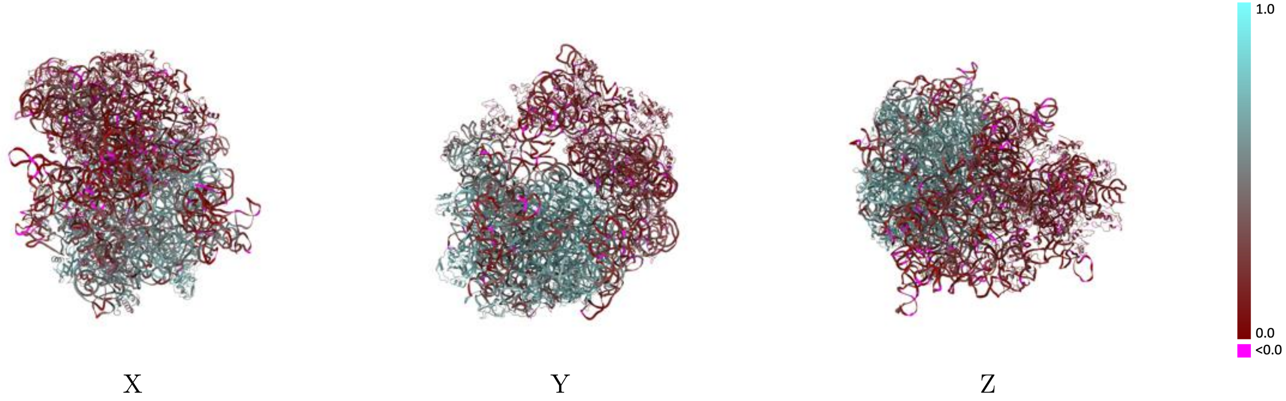

X


Y


Z

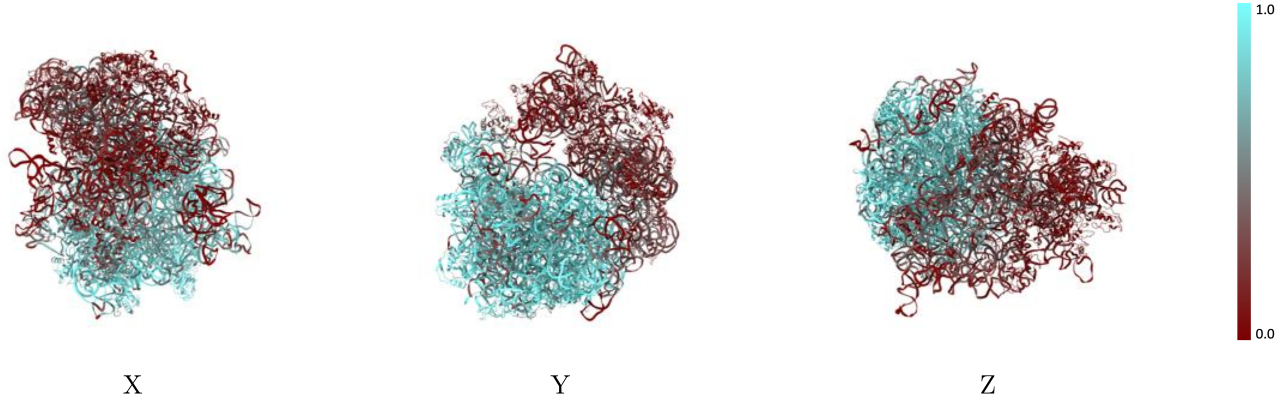
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



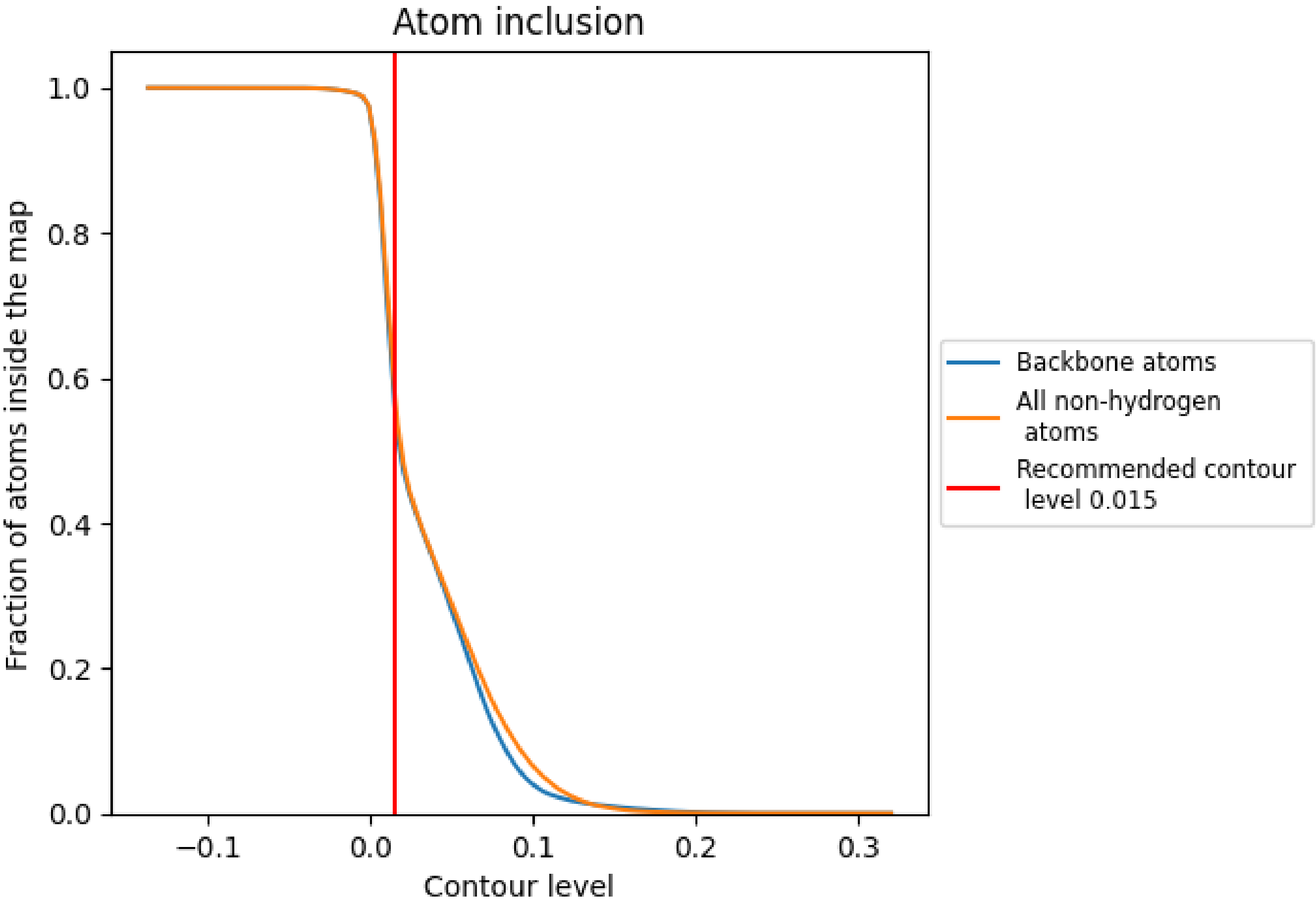
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 56% of all backbone atoms, 58% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5781	0.3950
1	0.6107	0.5660
2	0.9769	0.7030
3	0.9482	0.6780
4	0.8858	0.6120
A	0.7699	0.4870
B	0.8920	0.5200
C	0.9592	0.6800
D	0.9601	0.6750
E	0.9364	0.6600
F	0.3568	0.2880
G	0.5074	0.4070
H	0.9536	0.6750
I	0.9508	0.6720
J	0.9398	0.6480
K	0.9532	0.6590
L	0.9499	0.6770
M	0.7991	0.5230
N	0.9406	0.6600
O	0.9725	0.6950
P	0.9550	0.6720
Q	0.9108	0.6470
R	0.9099	0.6290
S	0.8165	0.5610
T	0.8420	0.5900
U	0.9525	0.6660
V	0.8877	0.6150
W	0.8343	0.5500
X	0.9456	0.6750
Y	0.1549	0.2060
Z	0.7233	0.5340
a	0.2676	0.1630
b	0.0628	0.2110
c	0.0758	0.2020
d	0.1301	0.2350

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Chain	Atom inclusion	Q-score
e	🟥 0.0972	🟥 0.2040
f	🟥 0.0782	🟥 0.2010
g	🟥 0.0389	🟥 0.1850
h	🟥 0.1505	🟥 0.2220
i	🟥 0.0535	🟥 0.1810
j	🟥 0.0982	🟥 0.2040
k	🟥 0.1205	🟥 0.2060
l	🟥 0.1701	🟥 0.2810
m	🟥 0.0919	🟥 0.1990
n	🟥 0.1245	🟥 0.2100
o	🟥 0.1207	🟥 0.2160
p	🟥 0.1994	🟥 0.2480
q	🟥 0.1881	🟥 0.2290
r	🟥 0.1379	🟥 0.2430
s	🟥 0.1148	🟥 0.1900
t	🟥 0.1286	🟥 0.2400
u	🟥 0.0543	🟥 0.2300
v	🟥 0.0239	🟥 0.1830