wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2023 – 10:01 PM EDT

PDB ID : 4V4R
Title : Crystal structure of the whole ribosomal complex.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-09-30
Resolution : 5.90 Å(reported)

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

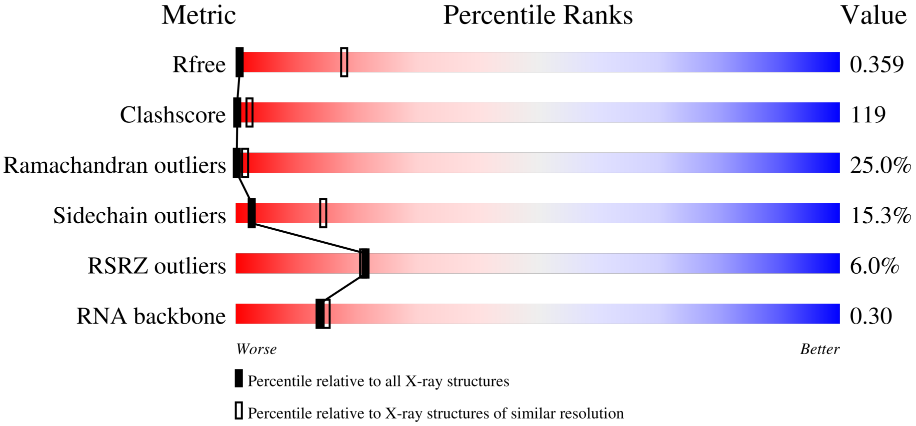
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

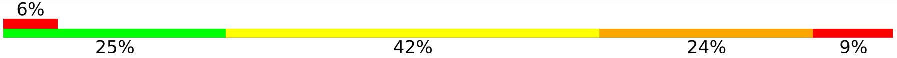
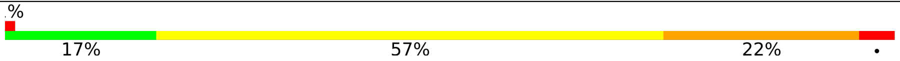
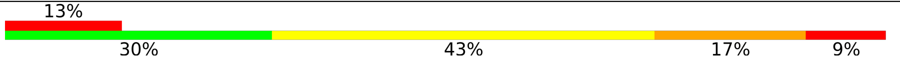
The reported resolution of this entry is 5.90 Å.

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.



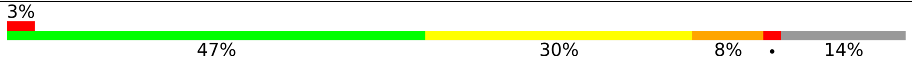
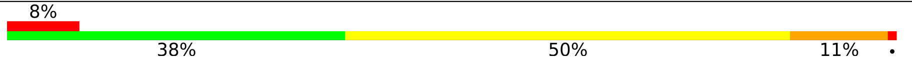
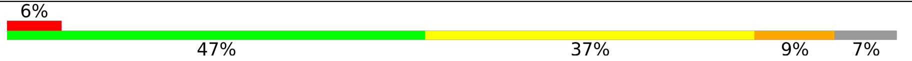
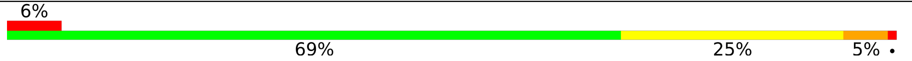
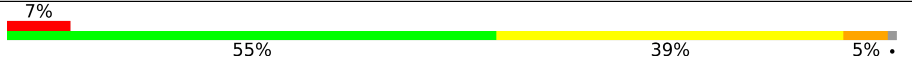
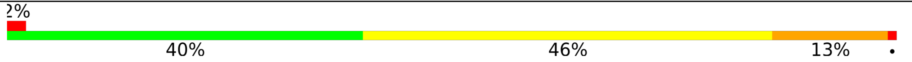
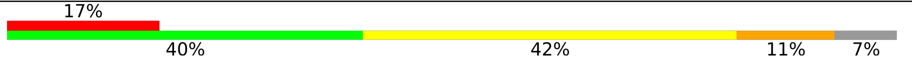
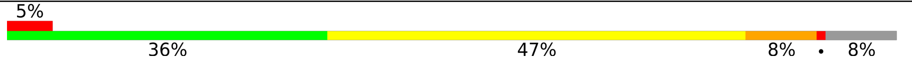
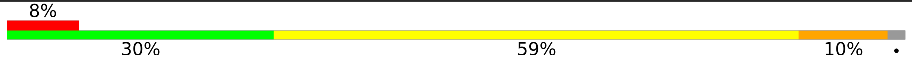
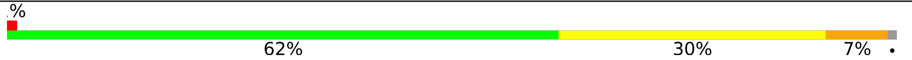
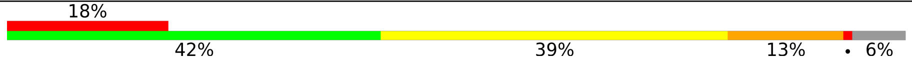
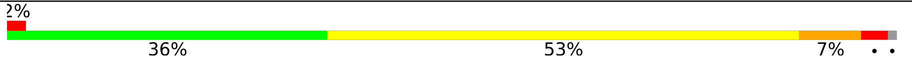
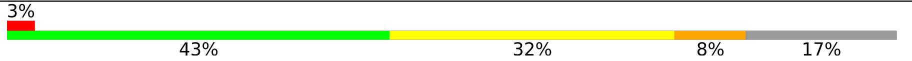
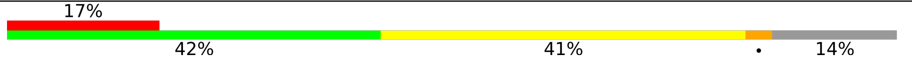
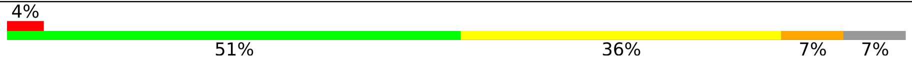
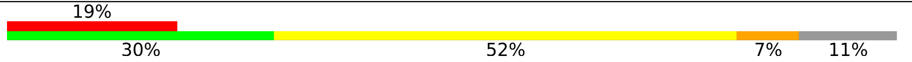
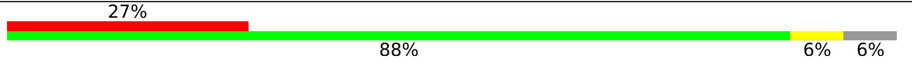
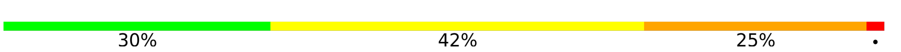
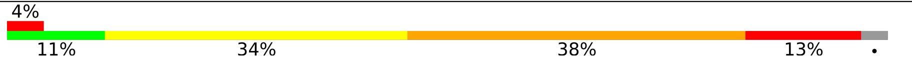
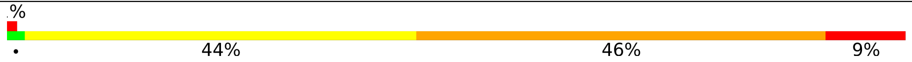
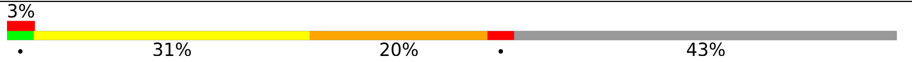
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1016 (7.94-3.86)
Clashscore	141614	1042 (7.88-3.90)
Ramachandran outliers	138981	1011 (7.94-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)
RSRZ outliers	127900	1014 (8.00-3.78)
RNA backbone	3102	1076 (8.70-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	AV	76	
3	AW	76	
4	AX	18	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	AB	256	
6	AC	239	
7	AD	209	
8	AE	162	
9	AF	101	
10	AG	156	
11	AH	138	
12	AI	128	
13	AJ	105	
14	AK	129	
15	AL	135	
16	AM	126	
17	AN	61	
18	AO	89	
19	AP	88	
20	AQ	105	
21	AR	88	
22	AS	93	
23	AT	106	
24	AU	27	
25	AY	354	
26	BB	123	
27	BA	2916	
28	BD	173	
29	BE	338	

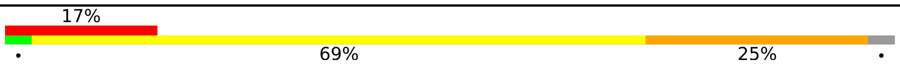
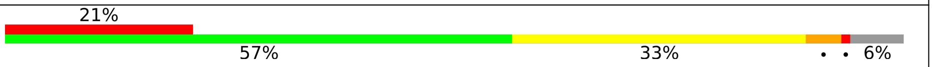
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	BF	246	2% • 37% 32% 7% 23%
31	BG	176	5% 8% 38% 21% • 31%
32	BH	177	5% 5% 51% 32% 5% 7%
33	BI	149	2% 6% 55% 34% 5% •
34	BN	145	% • 36% 38% 5% 19%
35	BO	122	2% • 61% 33% •
36	BP	164	% 5% 21% 23% • 49%
37	BQ	138	7% • 45% 46% 7%
38	BS	186	2% • 29% 25% 5% 39%
39	BT	66	6% 35% 29% 9% 21%
40	BW	113	% • 41% 49% • •
41	BX	84	• 40% 31% 15% 10%
42	BY	119	10% • 49% 31% 8% 8%
43	BZ	253	4% • 35% 29% • 30%
44	BR	118	% • 37% 46% 5% 11%
45	BU	118	3% 32% 50% 17% •
46	BV	100	% 9% 54% 33% •
47	B2	70	• 23% 49% 19% 9%
48	B3	60	2% 5% 57% 33% 5%
49	B0	91	4% 10% 41% 41% • 5%
50	B4	73	3% • 41% 49% 8%
51	B5	60	7% • 48% 38% 7% •
52	B6	82	% • 34% 27% • 35%
53	B7	47	2% 21% 68% 9% •
54	B8	64	9% 36% 44% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	B9	36	
56	BK	141	

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
3	YYG	AW	37	X	-	X	X
3	PSU	AW	39	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142780 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1515	32551	14490	6022	10525	1514	0	0	0

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AV	76	1622	725	293	529	75	0	0	0

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AW	76	1638	736	294	533	75	0	0	0

- Molecule 4 is a RNA chain called 5'-R(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	AX	17	136	56	19	44	17	0	0	11

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AB	234	1900	1213	341	341	5	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AC	206	1612	1016	314	281	1	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AD	208	1703	1066	339	291	7	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	AE	150	1146	724	217	201	4	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AF	101	843	531	155	154	3	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AG	155	1257	781	252	218	6	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AH	138	1116	705	215	193	3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	AI	127	1011	639	198	174	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AQ	104	857	547	161	147	2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	AR	73	597	380	118	99	0	0	0

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	AS	80	647	414	119	112	2	0	0	0

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	AT	99	762	469	162	129	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
24	AU	24	208	128	50	30	0	0	0

- Molecule 25 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
25	AY	333	333	333	0	0	333

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	BB	123	2637	1175	488	852	122	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	BA	2814	60600	26974	11331	19482	2813	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	INSERTION	GB 48268

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BD	173	1308	820	246	236	6	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BE	191	1507	940	290	273	4	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BF	189	1430	872	255	302	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	BG	122	957	597	176	180	4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BH	164	1251	787	225	237	2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BI	148	1145	727	205	212	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	BN	117	917	570	164	180	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BO	122	937	585	180	169	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
36	BP	84	639	391	109	139	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	BQ	138	1081	678	208	192	3	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	BS	113	866	536	165	164	1	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	BT	52	406	242	74	85	5	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	BW	108	860	542	169	149	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BX	76	602	366	102	131	3	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	BY	110	879	531	166	182	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BZ	177	1360	859	238	257	6	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
44	BR	105	855	536	174	145	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BU	117	978	608	210	159	1	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BV	100	787	495	146	145	1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	B8	63	496	312	101	78	5	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B9	35	285	172	64	45	4	0	0	0

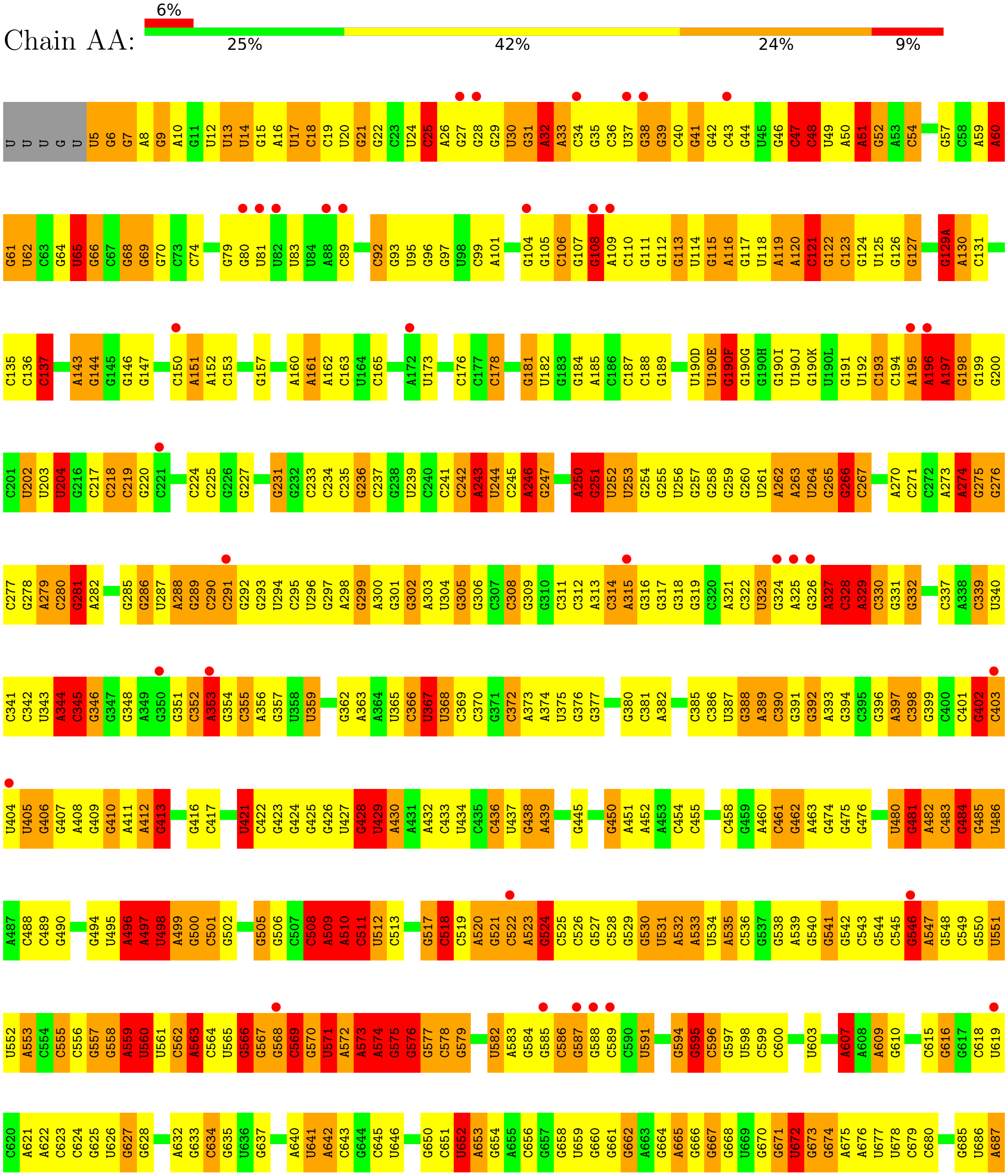
- Molecule 56 is a protein called 50S ribosomal protein L11.

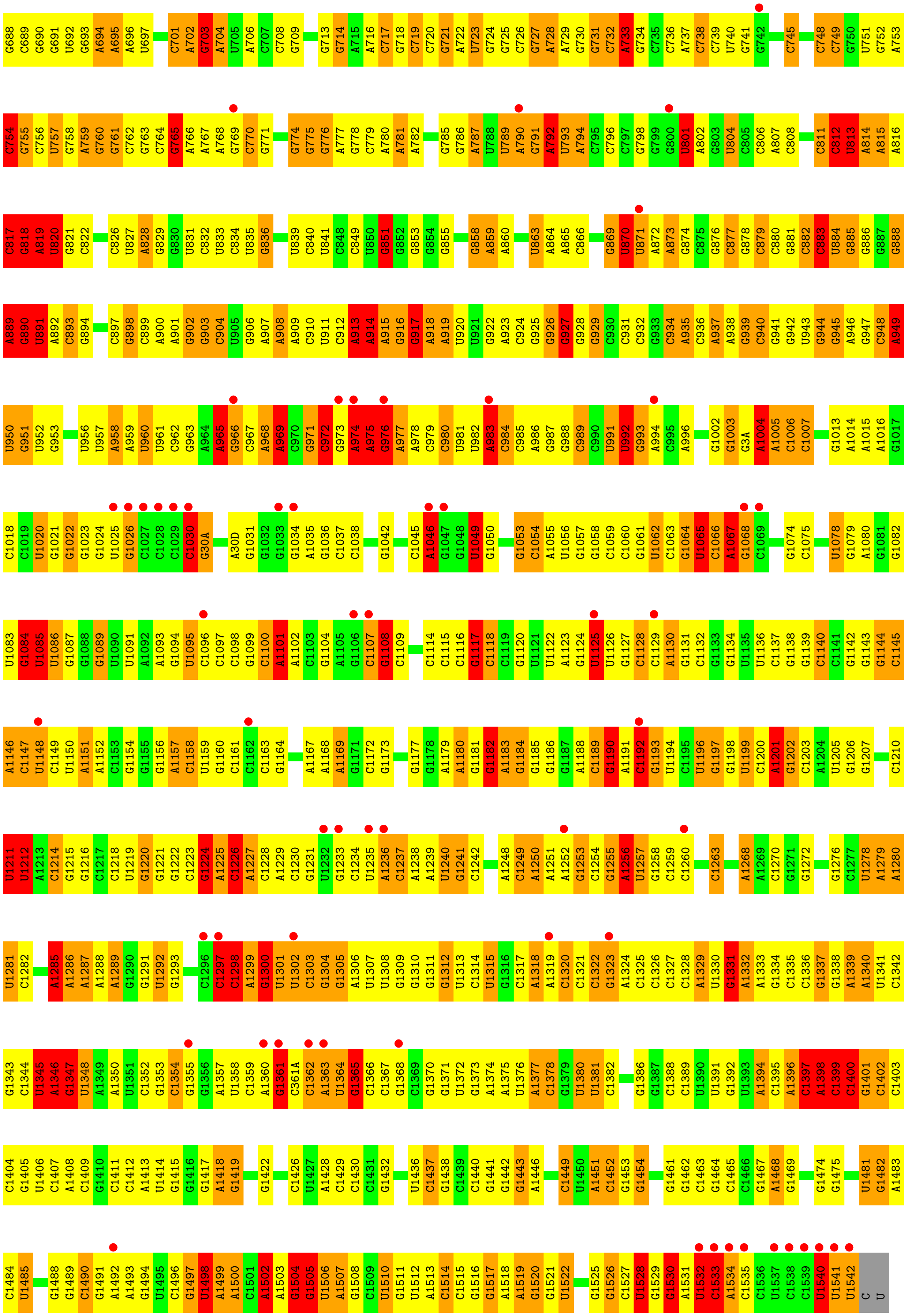
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	BK	133	999	642	169	182	6	0	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

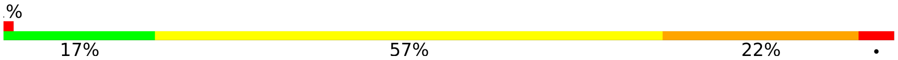
- Molecule 1: 16S ribosomal RNA

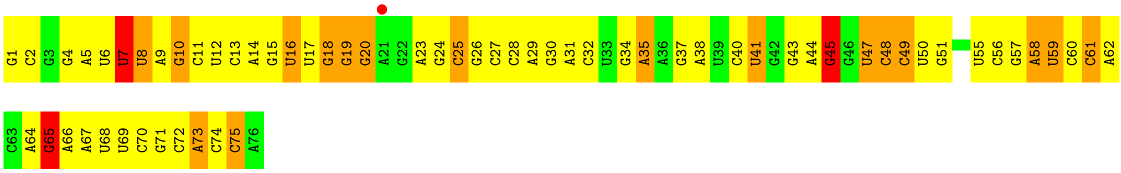




- Molecule 2: P-site tRNA (Phe)

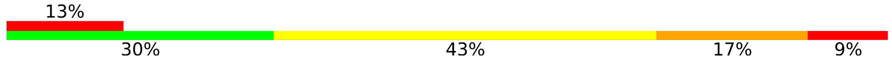
Chain AV:

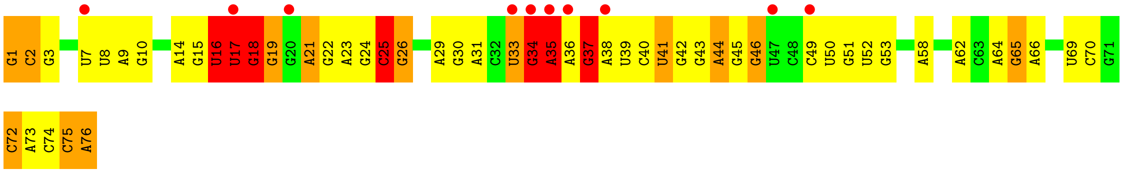




- Molecule 3: E-site tRNA (Phe)

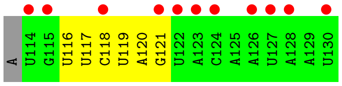
Chain AW:





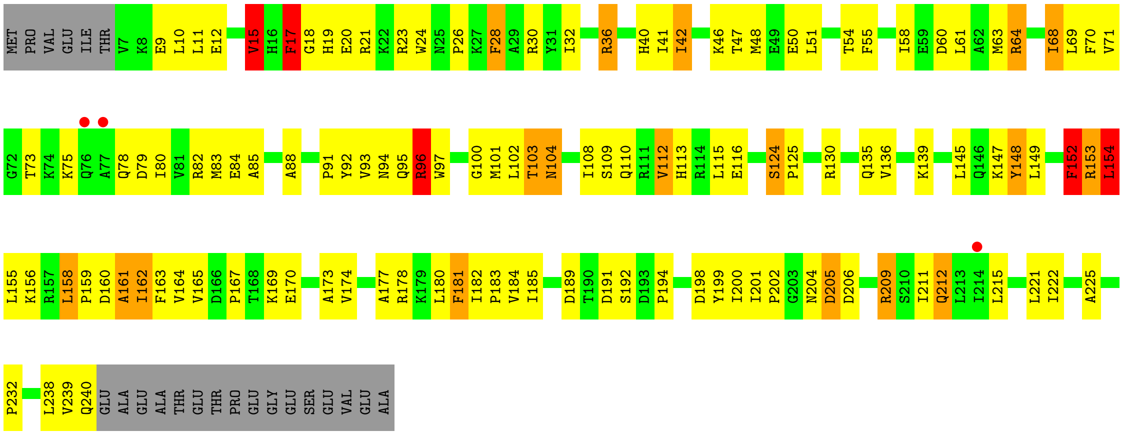
- Molecule 4: 5’-R(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3’

Chain AX:



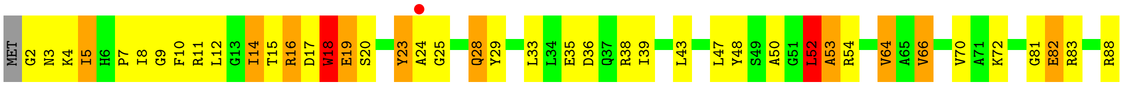
- Molecule 5: 30S ribosomal protein S2

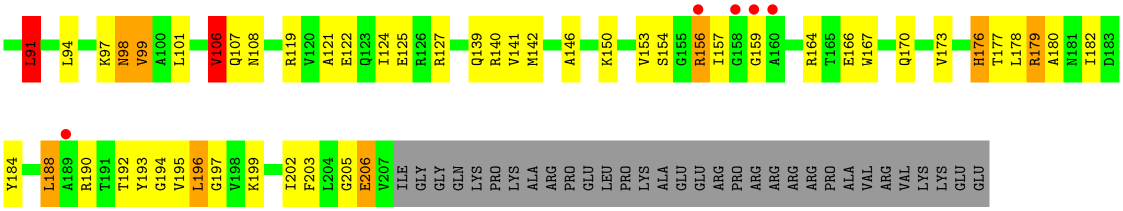
Chain AB:



- Molecule 6: 30S ribosomal protein S3

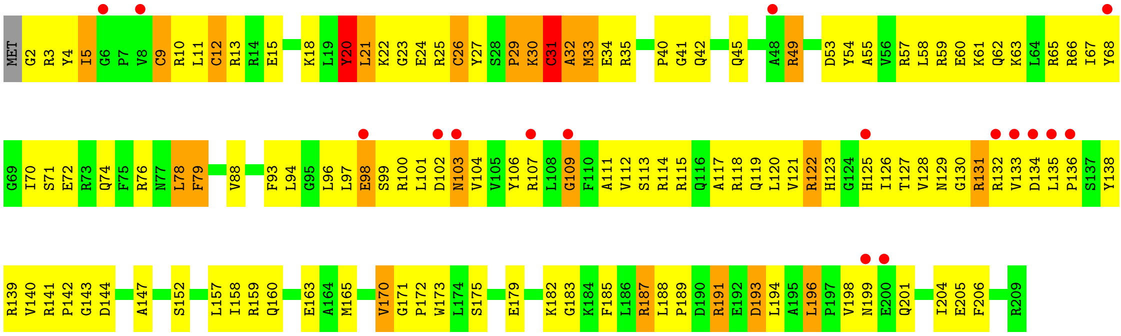
Chain AC:





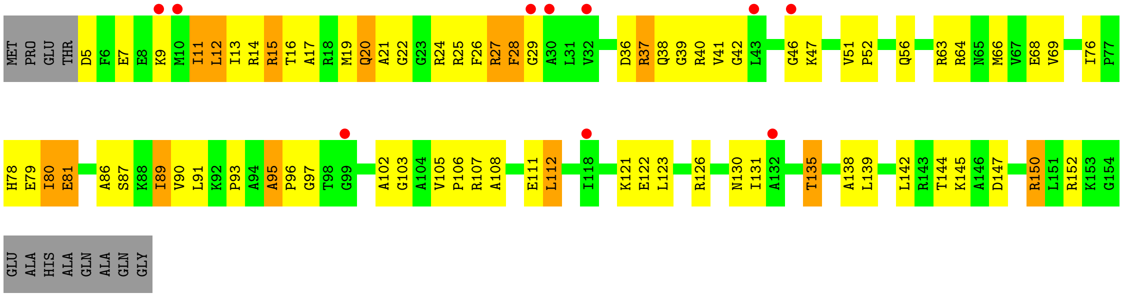
- Molecule 7: 30S ribosomal protein S4

Chain AD:



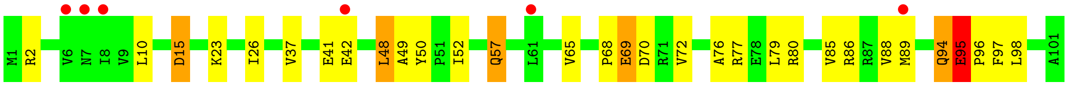
- Molecule 8: 30S ribosomal protein S5

Chain AE:



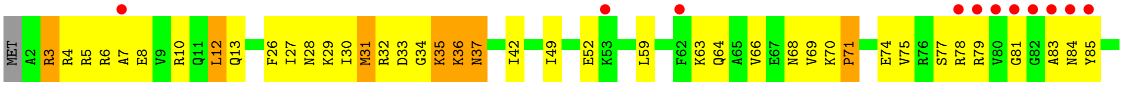
- Molecule 9: 30S ribosomal protein S6

Chain AF:

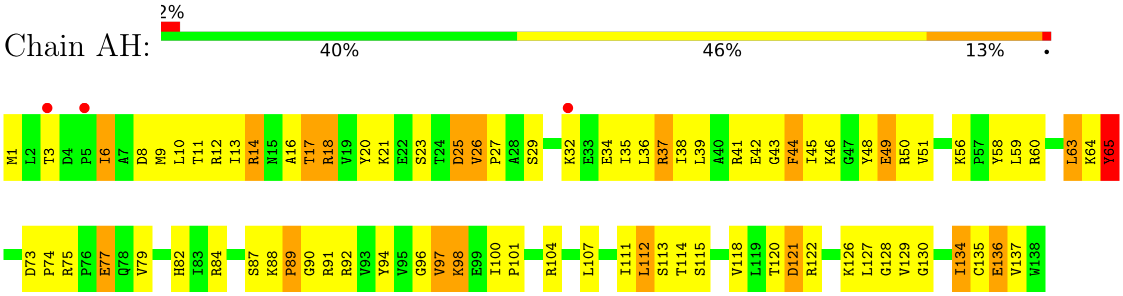


- Molecule 10: 30S ribosomal protein S7

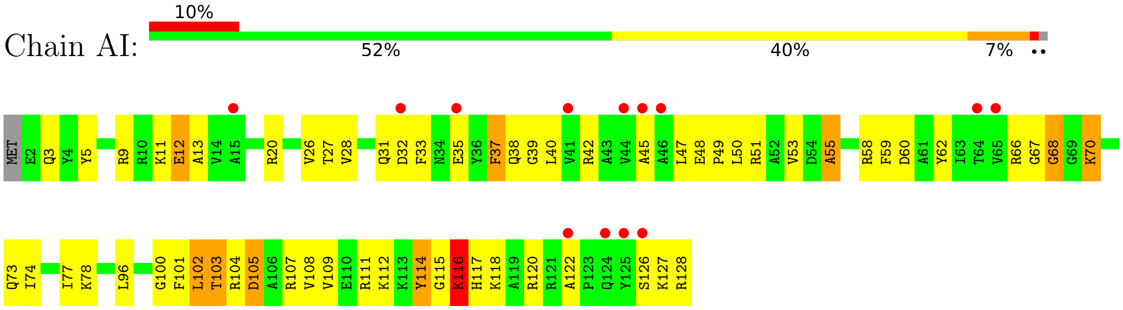
Chain AG:



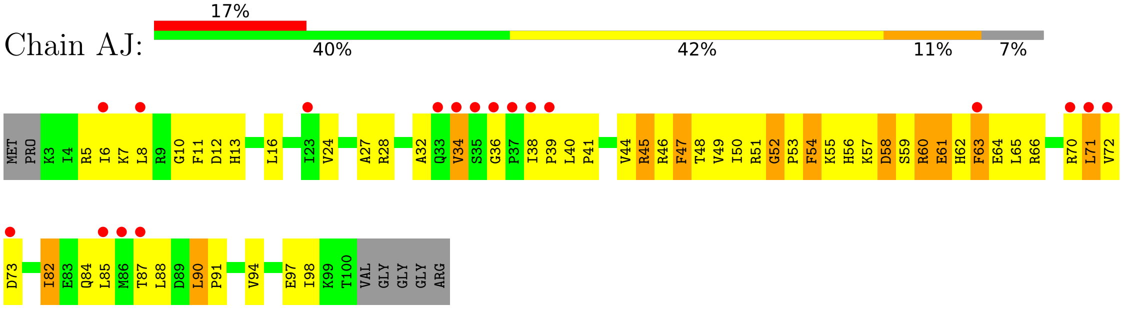
- Molecule 11: 30S ribosomal protein S8



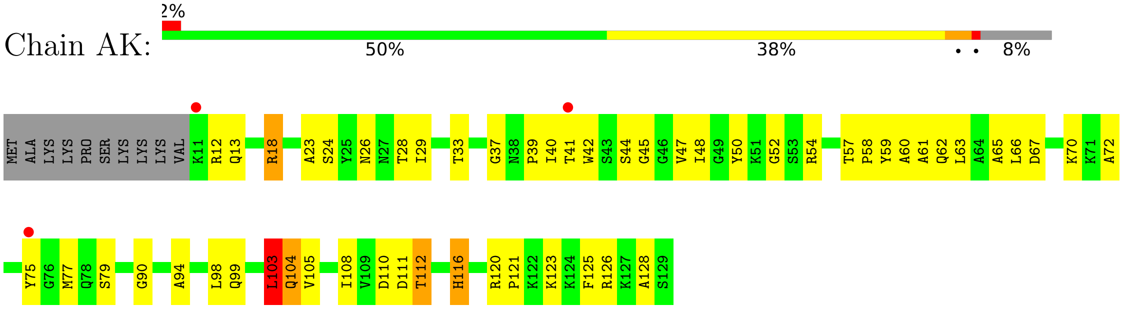
- Molecule 12: 30S ribosomal protein S9



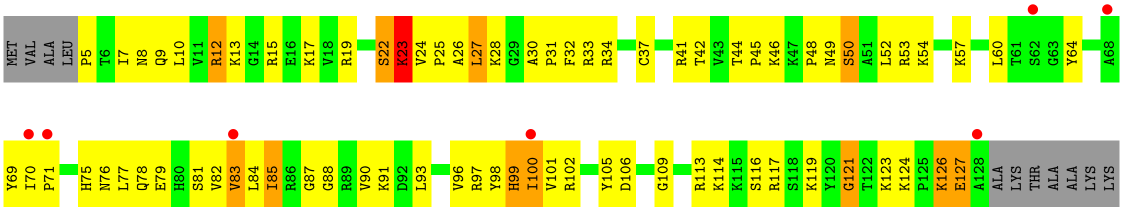
- Molecule 13: 30S ribosomal protein S10



- Molecule 14: 30S ribosomal protein S11

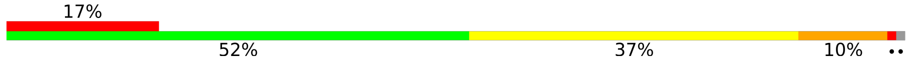


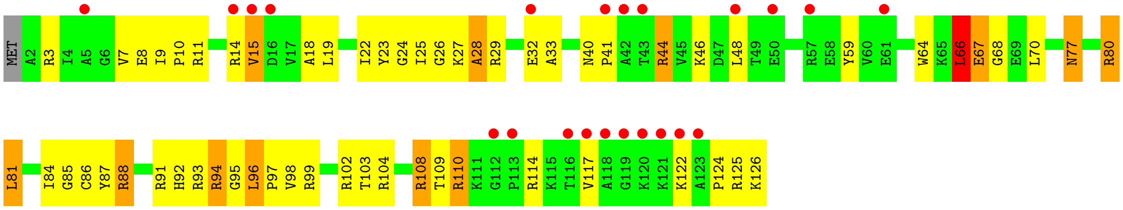
- Molecule 15: 30S ribosomal protein S12



- Molecule 16: 30S ribosomal protein S13

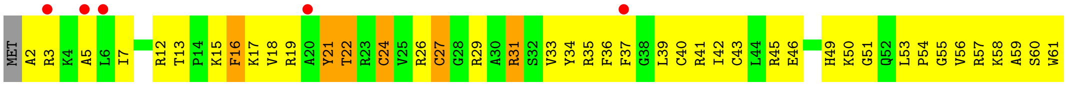
Chain AM:





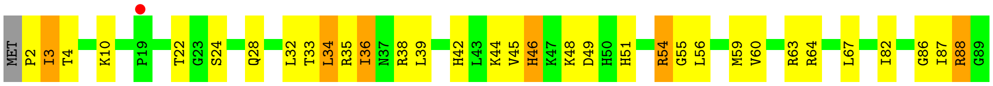
- Molecule 17: 30S ribosomal protein S14

Chain AN:



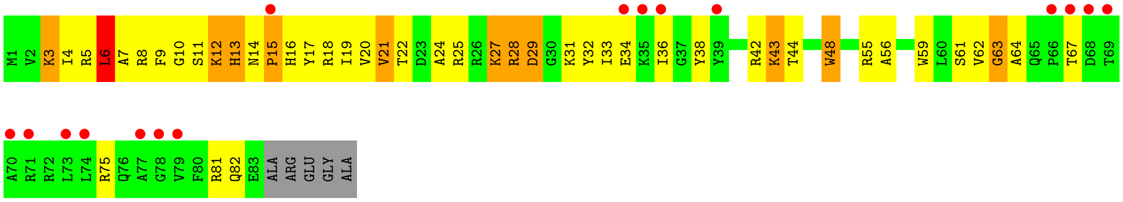
- Molecule 18: 30S ribosomal protein S15

Chain AO:



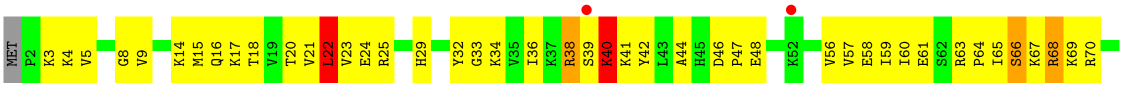
- Molecule 19: 30S ribosomal protein S16

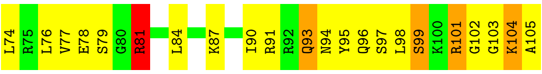
Chain AP:



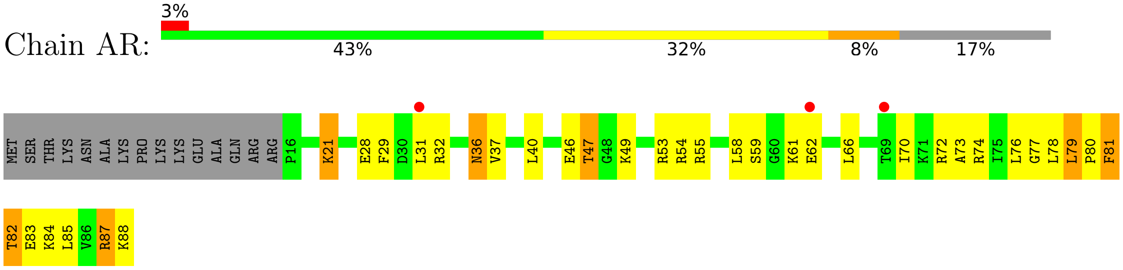
- Molecule 20: 30S ribosomal protein S17

Chain AQ:

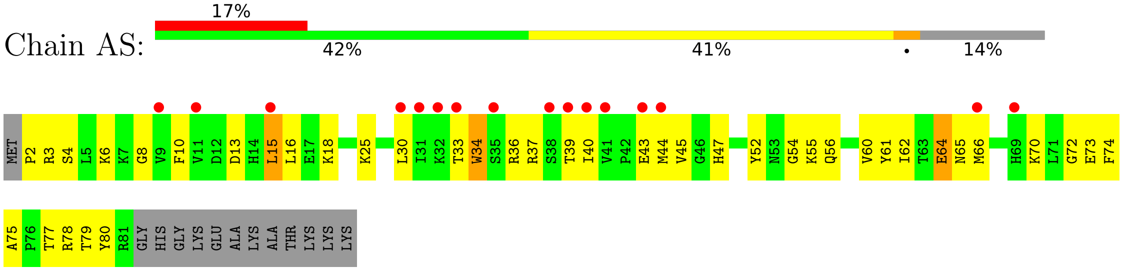




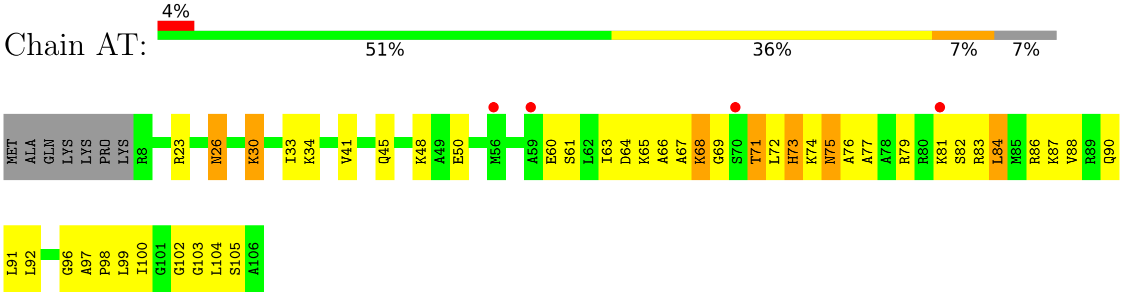
- Molecule 21: 30S ribosomal protein S18



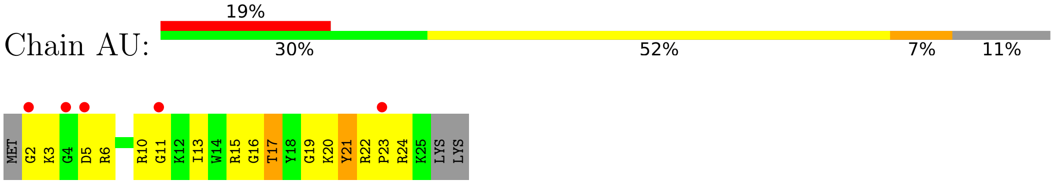
- Molecule 22: 30S ribosomal protein S19



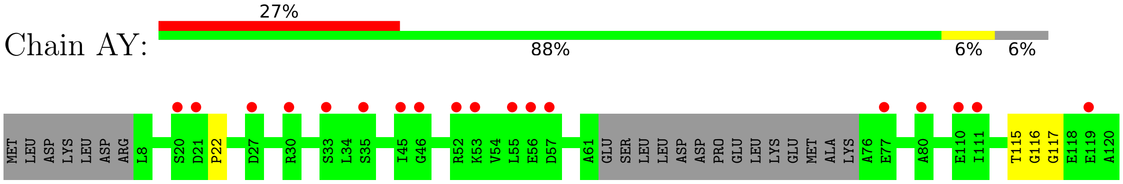
- Molecule 23: 30S ribosomal protein S20

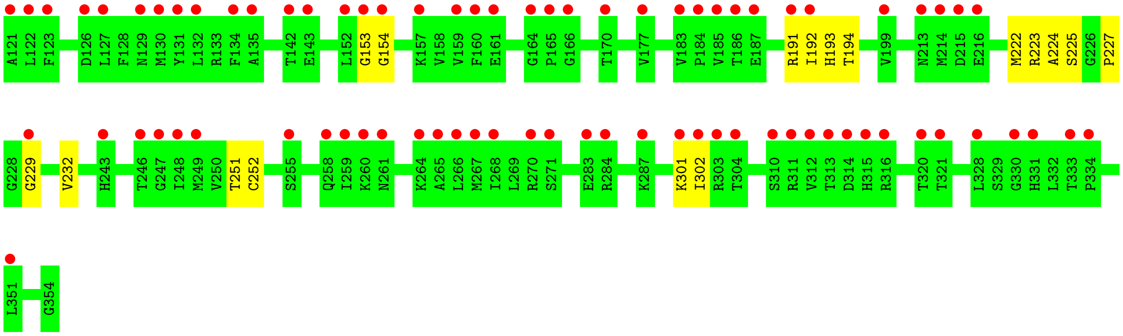


- Molecule 24: 30S ribosomal protein Thx



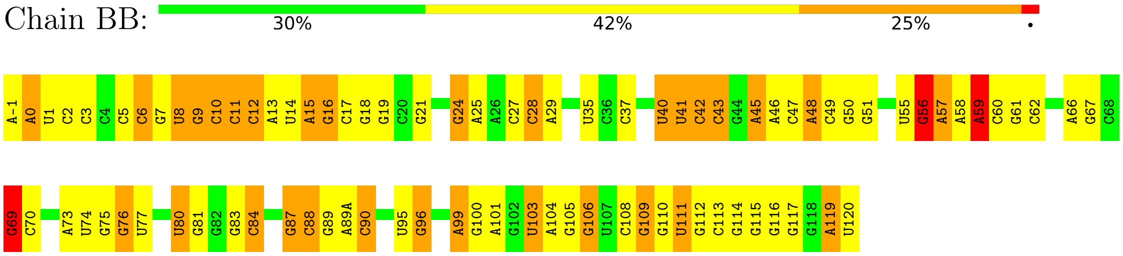
- Molecule 25: Peptide chain release factor 1





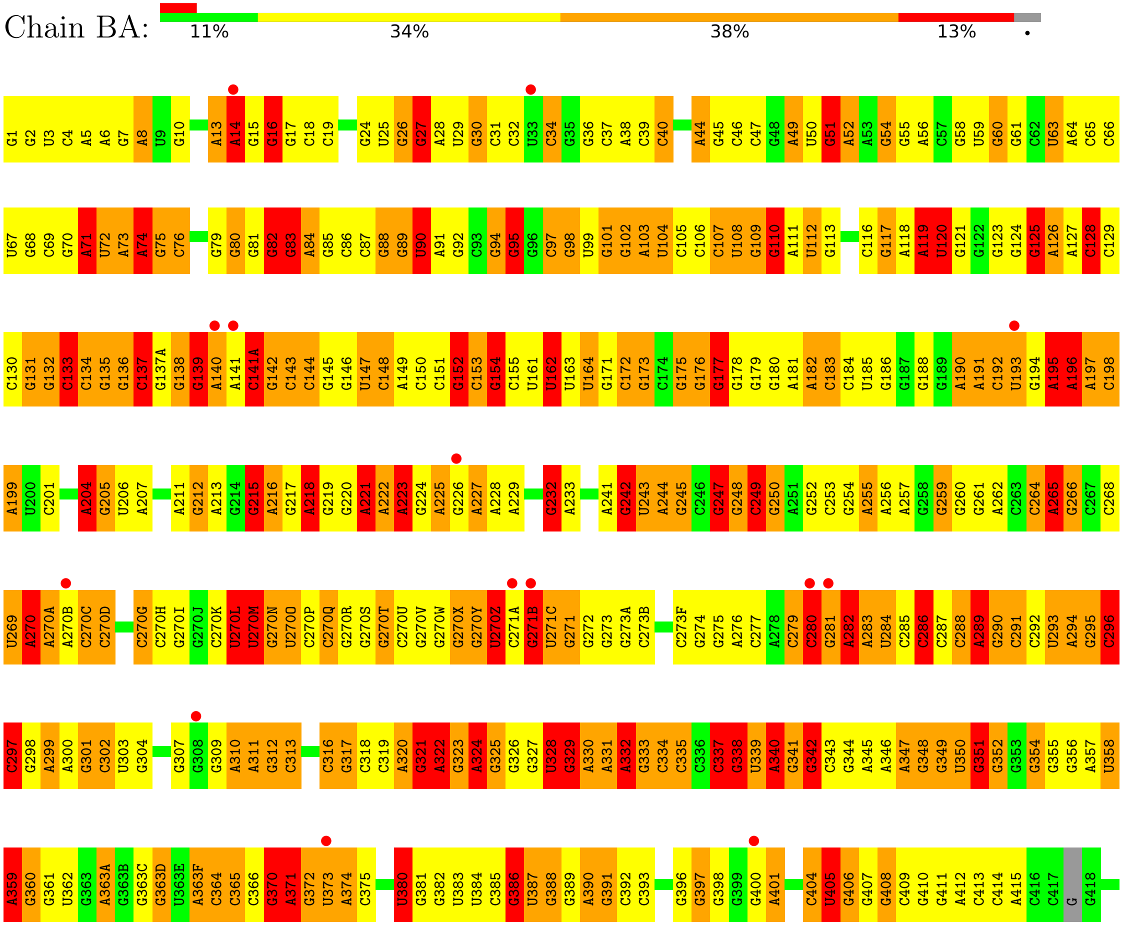
- Molecule 26: 5S ribosomal RNA

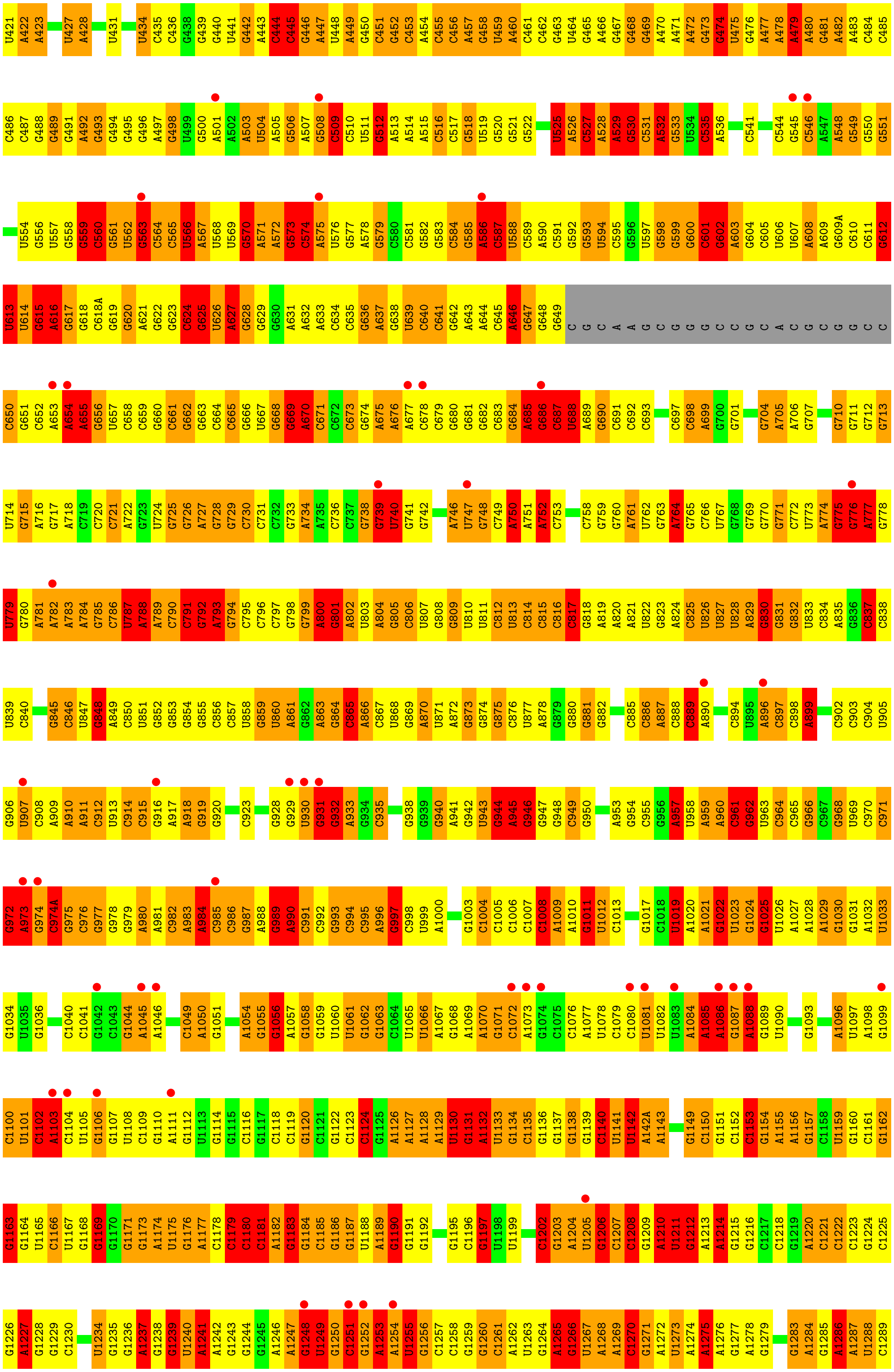
Chain BB:

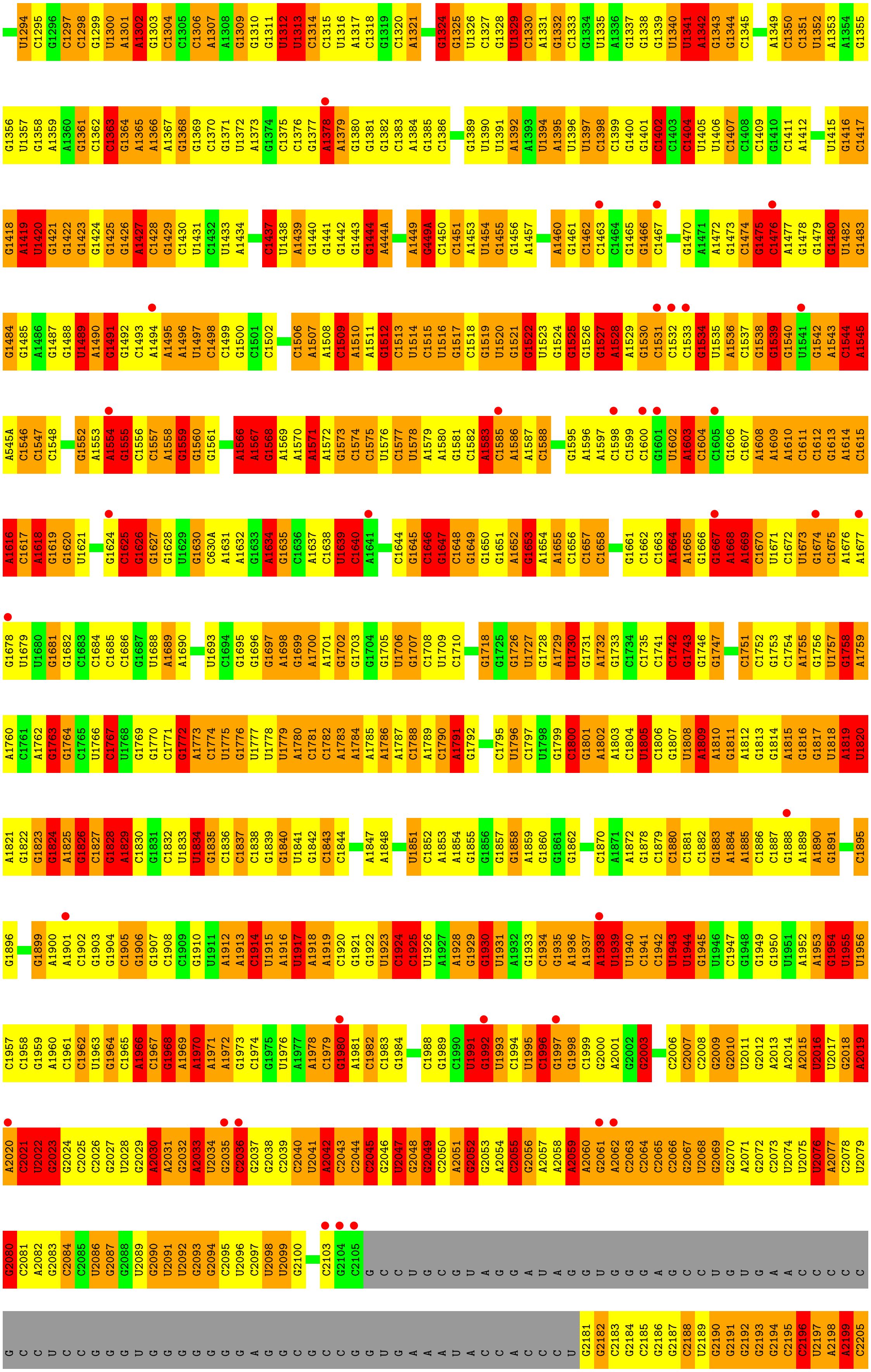


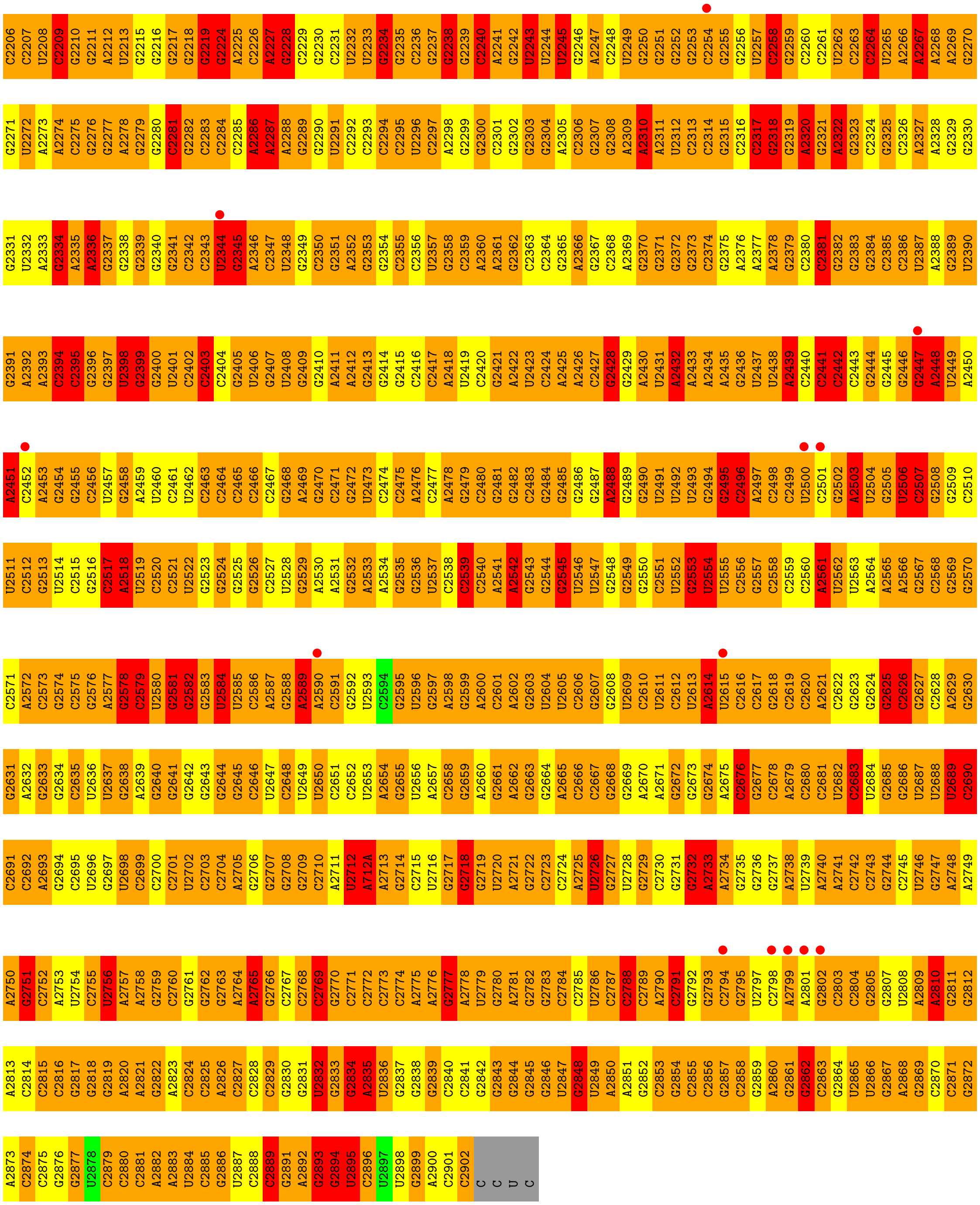
- Molecule 27: 23S ribosomal RNA

Chain BA:



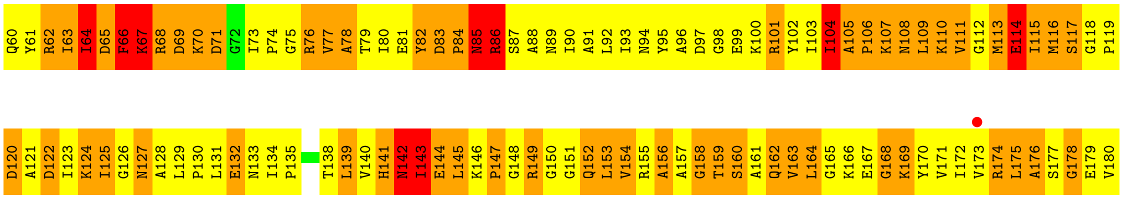

U421 A422 A423 U427 A428 U431 U434 C435 C436 G438 G439 G440 U441 G442 A443 C444 C445 G446 A447 U448 A449 G450 C451 G452 C453 A454 C455 C456 A457 G458 U459 A460 C461 C462 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 G473 G474 U475 G476 A477 A478 A479 A480 G481 A482 A483 C484 C485
C486 C487 G488 G489 G491 A492 G493 G494 G495 G496 A497 G498 U499 G500 A501 A502 A503 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 U515 C516 C517 G518 U519 G520 G521 G522 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C541 C544 G545 C546 A547 A548 G549 G550 G551
U554 G556 U557 G558 G559 C560 G561 U562 G563 C564 C565 U566 A567 U568 U569 G570 A571 A572 C573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 A590 C591 G592 G593 U594 C595 G596 U597 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 G609A C610 C611 G612
U613 U614 G615 A616 G617 G618 C618A G619 G620 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647 G648 G649 C G C A A G C G G G C C G C A C G C G G C C
C650 G651 C652 A653 A654 A655 G656 U657 C658 C659 G660 C661 G662 G663 C664 C665 G666 U667 G668 G669 A670 C671 C672 C673 G674 A675 A676 A677 C678 C679 G680 G681 G682 C683 G684 A685 G686 C687 U688 A689 G690 C691 C692 C693 C697 C698 A699 G700 G701 G704 A705 A706 G707 G710 G711 G712 G713
U714 G715 A716 G717 A718 C719 C720 C721 A722 G723 U724 G725 G726 A727 G728 G729 C730 C731 C732 G733 A734 A735 C736 C737 G738 G739 U740 G741 G742 A746 U747 G748 C749 A750 A751 A752 C753 C758 G759 G760 A761 U762 G763 A764 G765 C766 U767 G768 G769 G770 G771 C772 U773 A774 G775 G776 A777 G778
U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U822 G823 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 G836 C837 C838
U839 C840 G845 C846 U847 G848 A849 C850 U851 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 C864 C865 A866 C867 G868 G869 A870 U871 A872 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 C885 C886 A887 C888 C889 A890 C894 U895 A896 C897 C898 A899 C902 C903 C904 U905
G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 C923 G928 G929 U930 G931 G932 A933 G934 C935 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966 C967 G968 U969 C970 C971
G972 A973 G974 C974A G975 C976 G977 G978 G979 A980 A981 C982 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033
G1034 U1035 G1036 C1040 C1041 G1042 C1043 G1044 A1045 A1046 C1049 A1050 G1051 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1093 A1096 U1097 A1098 G1099
C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1120 C1121 G1122 C1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 G1134 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1149 C1150 G1151 C1152 G1153 G1154 A1155 G1156 G1157 C1158 U1159 G1160 C1161 G1162
G1163 G1164 U1165 C1166 U1167 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1195 C1196 G1197 U1198 U1199 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1212 A1213 A1214 G1215 G1216 C1217 C1218 G1219 A1220 C1221 C1222 G1223 G1224 C1225
G1226 A1227 G1228 G1229 C1230 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245 A1246 A1247 G1248 U1249 C1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 G1276 G1277 A1278 G1279 G1283 A1284 G1285 A1286 A1287 U1288 C1289

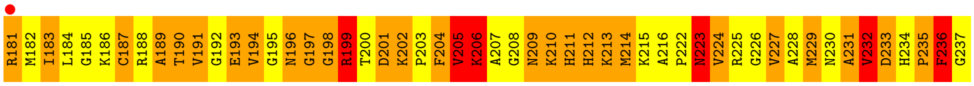

U1294 C1295 G1296 C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1304 C1305 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 G1324 G1325 U1326 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 A1349 C1350 C1351 U1352 A1353 A1354 G1355
G1356 U1357 G1358 A1359 A1360 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 G1377 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 C1399 G1400 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 U1415 G1416 C1417
G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 C1437 U1438 A1439 G1440 G1441 G1442 G1443 G1444 A444A A1449 G449A C1450 C1451 A1453 U1454 G1455 G1456 A1457 A1460 G1461 C1462 C1463 C1464 G1465 G1466 C1467 G1470 A1471 A1472 G1473 C1474 G1475 C1476 A1477 G1478 G1479 G1480 U1482 G1483
G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 G1501 C1502 C1506 A1507 U1508 C1509 A1510 A1511 G1512 C1513 U1514 C1515 U1516 G1517 C1518 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 G1527 A1528 A1529 G1530 C1531 C1532 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545
A545A C1546 C1547 C1548 G1552 A1553 A1554 G1555 C1556 C1557 A1558 G1559 G1560 G1561 A1566 A1567 G1568 A1569 A1570 A1571 A1572 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1587 C1588 G1595 A1596 A1597 C1598 C1599 C1600 G1601 U1602 A1603 C1604 C1605 G1606 C1607 A1608 A1609 A1610 C1611 G1612 G1613 A1614 C1615
A1616 C1617 A1618 G1619 G1620 U1621 G1624 C1625 G1626 G1627 C1628 U1629 G1630 C630A A1631 A1632 G1633 A1634 G1635 C1636 A1637 C1638 U1639 C1640 A1641 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 G1661 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 C1675 A1676 A1677
G1678 U1679 U1680 G1681 G1682 C1683 C1684 C1685 C1686 G1687 U1688 A1689 A1690 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 G1704 G1705 U1706 G1707 C1708 U1709 C1710 G1718 G1725 U1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1735 C1741 C1742 G1743 G1746 G1747 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1759
A1760 C1761 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 U1808 A1809 A1810 G1811 A1812 G1813 A1814 A1815 G1816 G1817 U1818 A1819 U1820
A1821 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 U1841 G1842 C1843 C1844 A1847 A1848 U1851 C1852 A1853 A1854 G1855 G1856 G1857 G1858 A1859 G1860 G1861 G1862 C1870 A1871 A1872 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 G1891 C1895
G1896 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956
C1957 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 U1976 A1977 A1978 C1979 G1980 A1981 C1982 C1983 G1984 C1988 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 A2001 G2002 G2003 C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2013 A2014 A2015 U2016 U2017 G2018 A2019
A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 C2044 C2045 G2046 U2047 G2048 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 U2076 A2077 C2078 U2079
G2080 C2081 A2082 G2083 C2084 C2085 U2086 G2087 G2088 U2089 G2090 U2091 U2092 G2093 G2094 C2095 U2096 C2097 U2098 U2099 G2100 C2103 G2104 C2105 G C C U G C G U A G G A U A G G U G G G A G C C U G U G A A C C C C C
G C C U C C G G G U G G G G G G A G G C C C C G G U G A A U A C C A C C C U G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2194 C2195 C2196 U2197 A2198 A2199 C2205



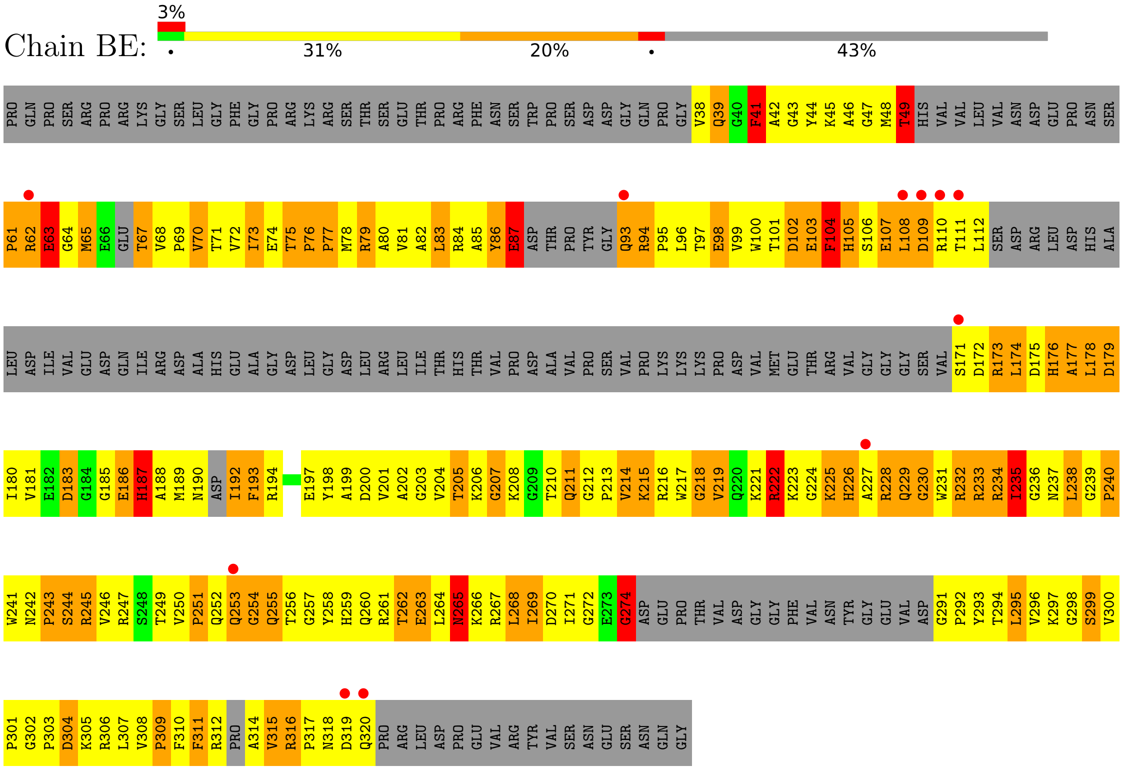
- Molecule 28: 50S ribosomal protein L2

Chain BD:

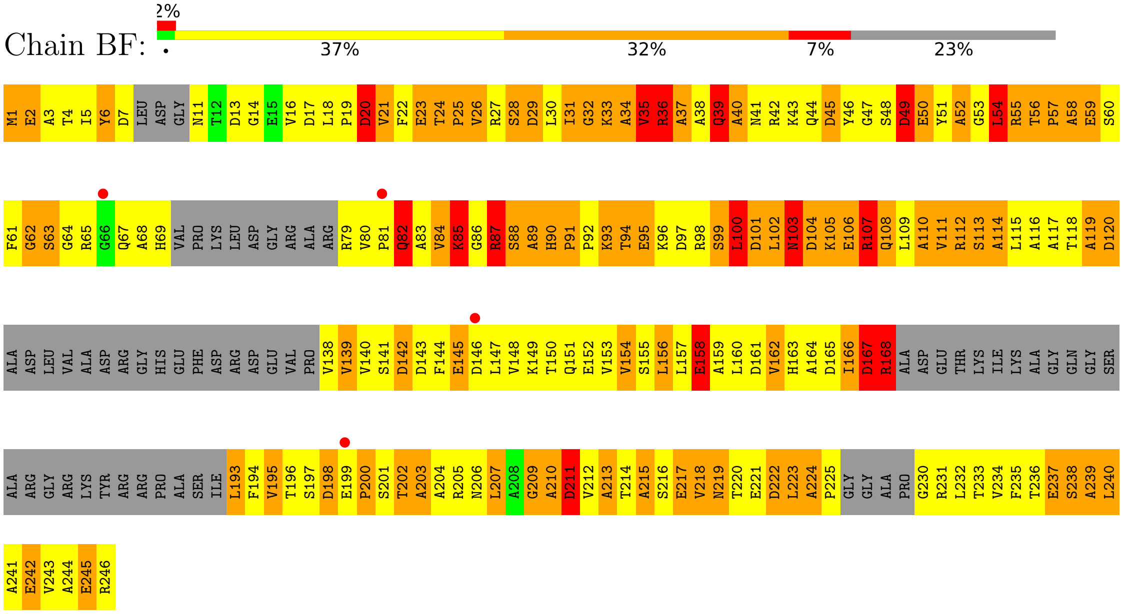




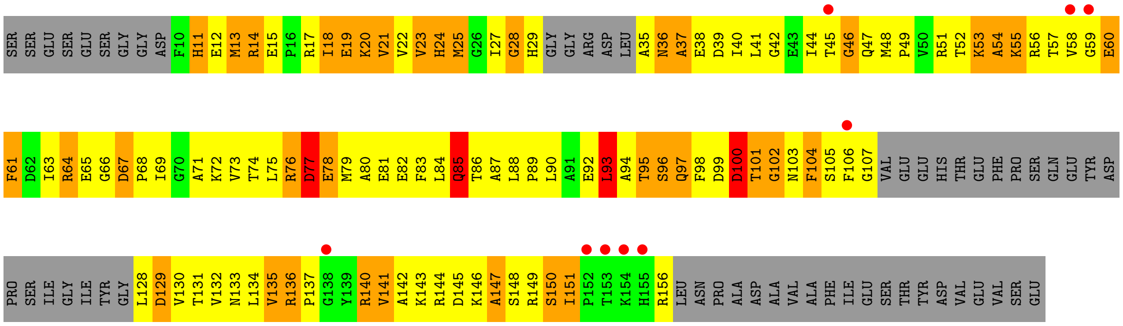
- Molecule 29: 50S ribosomal protein L3



- Molecule 30: 50S ribosomal protein L4

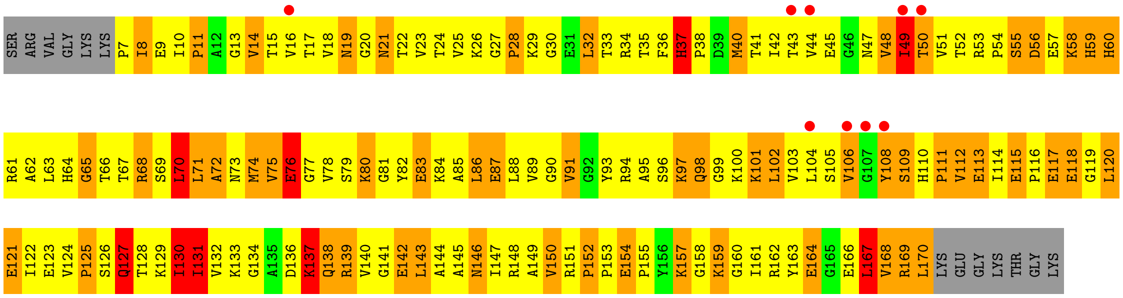


- Molecule 31: 50S ribosomal protein L5



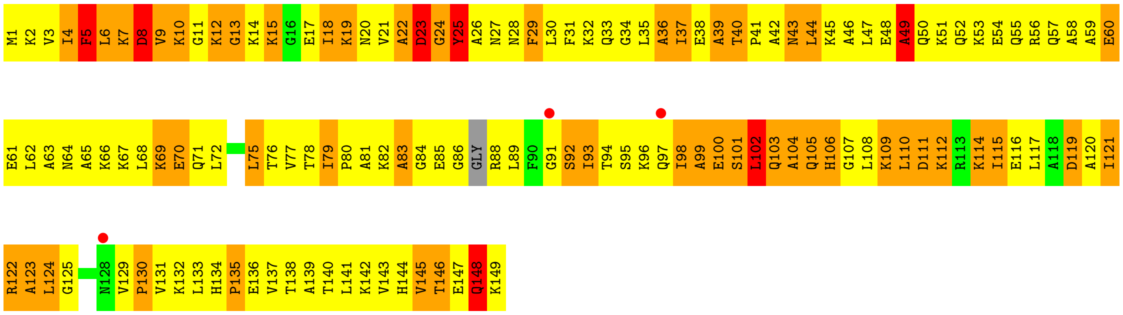
- Molecule 32: 50S ribosomal protein L6

Chain BH:



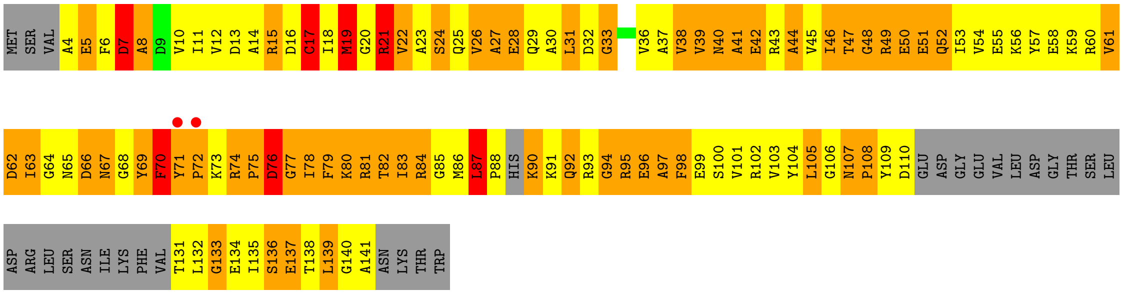
- Molecule 33: 50S ribosomal protein L9

Chain BI:

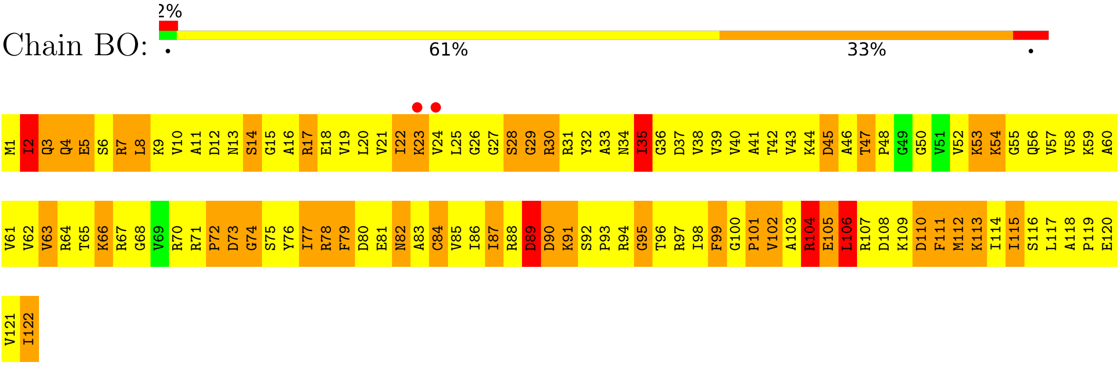


- Molecule 34: 50S ribosomal protein L13

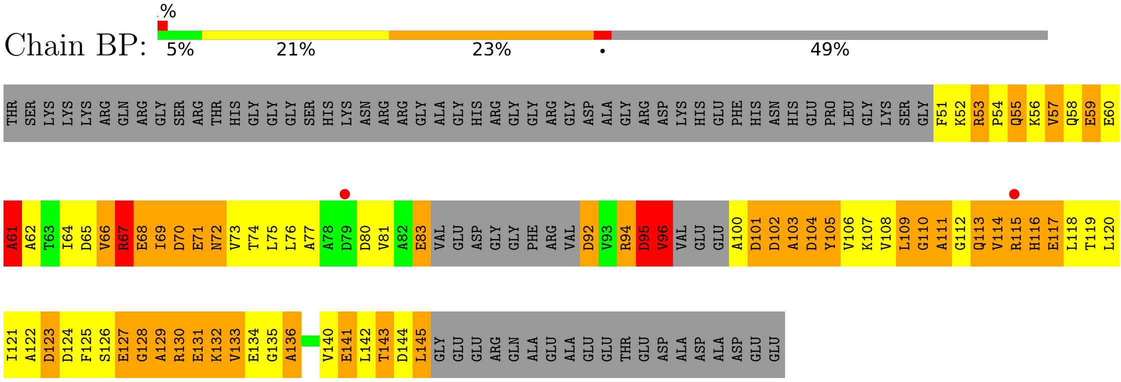
Chain BN:



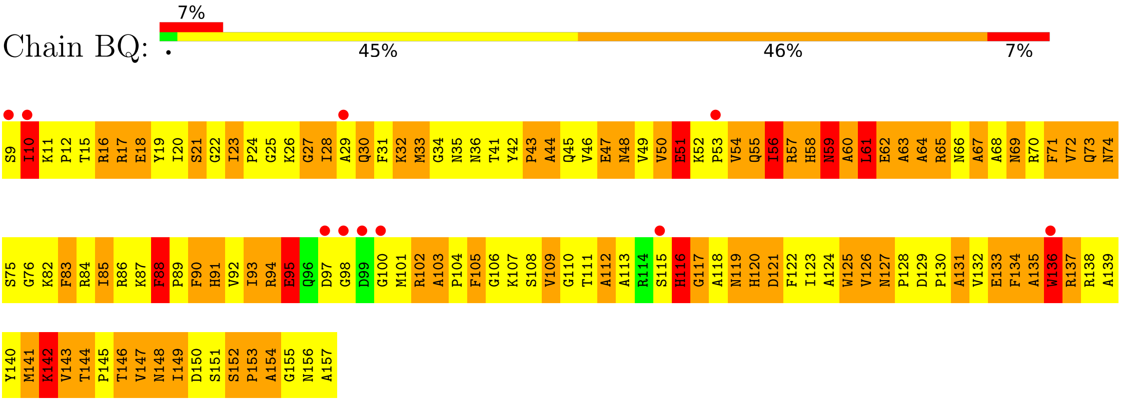
- Molecule 35: 50S ribosomal protein L14



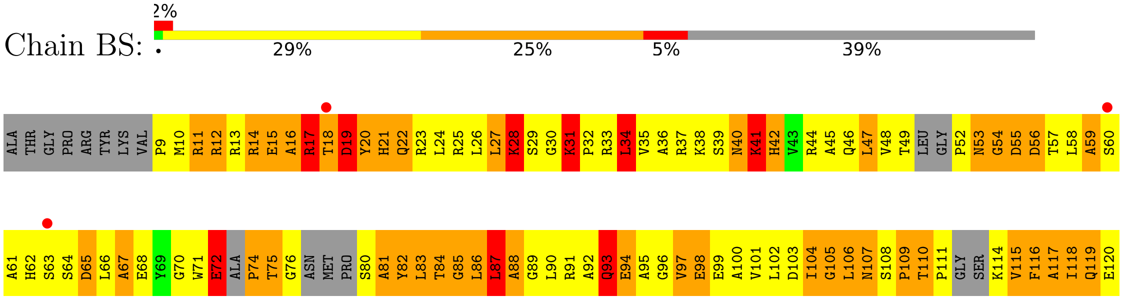
- Molecule 36: 50S ribosomal protein L15

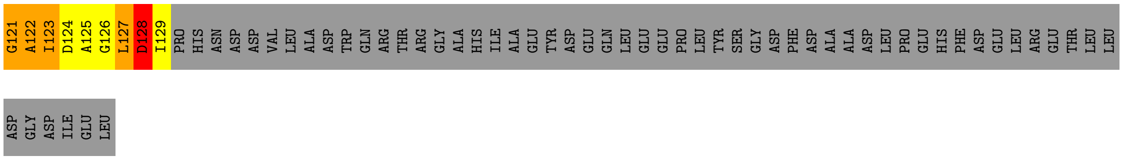


- Molecule 37: 50S ribosomal protein L16



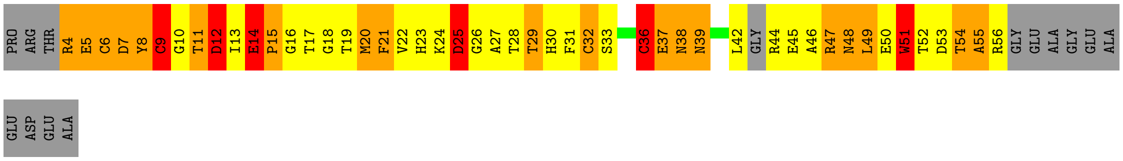
- Molecule 38: 50S ribosomal protein L18





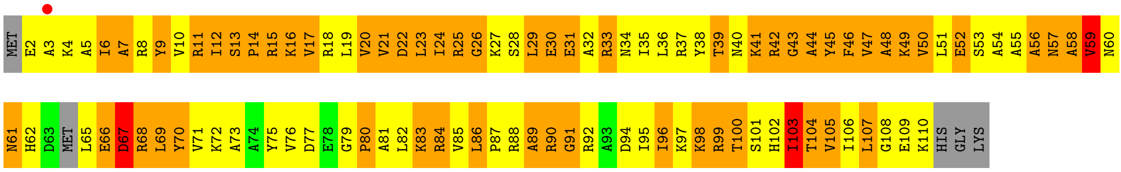
- Molecule 39: 50S ribosomal protein L19

Chain BT:



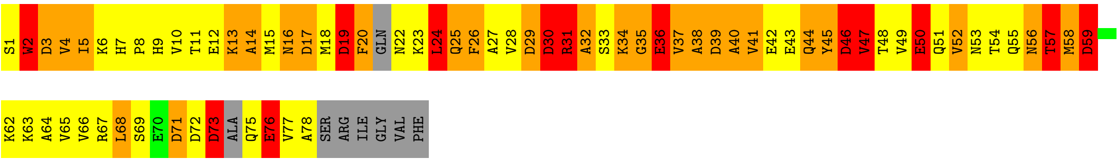
- Molecule 40: 50S ribosomal protein L22

Chain BW:



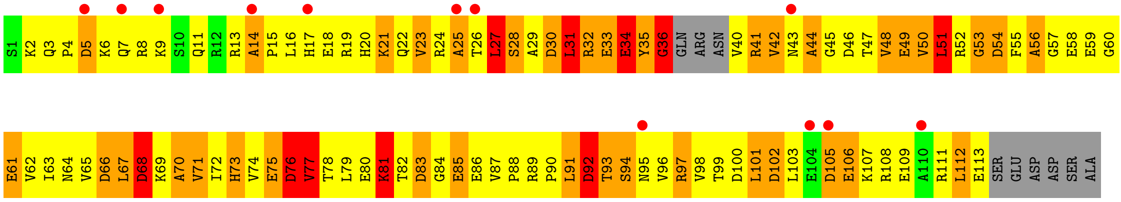
- Molecule 41: 50S ribosomal protein L23

Chain BX:



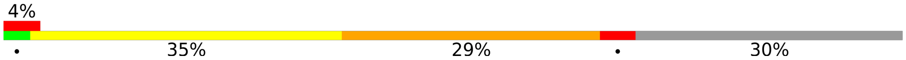
- Molecule 42: 50S ribosomal protein 24

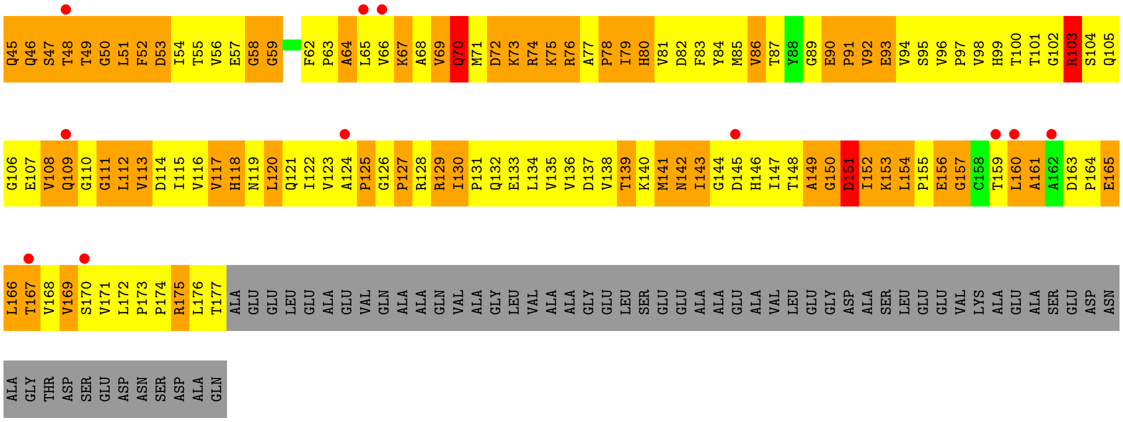
Chain BY:



- Molecule 43: 50S ribosomal protein CTC

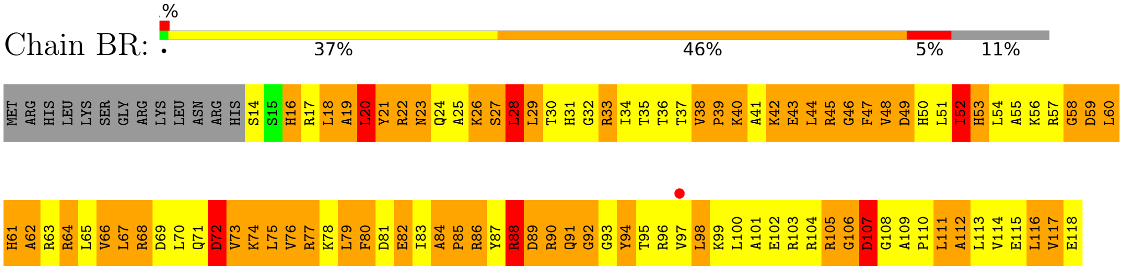
Chain BZ:





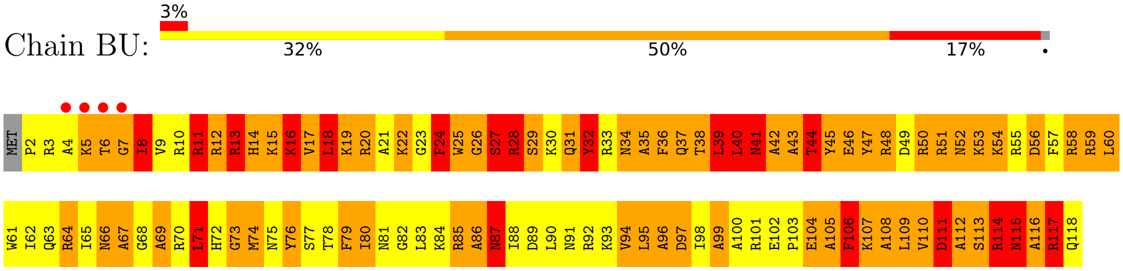
- Molecule 44: 50S ribosomal protein L17

Chain BR:



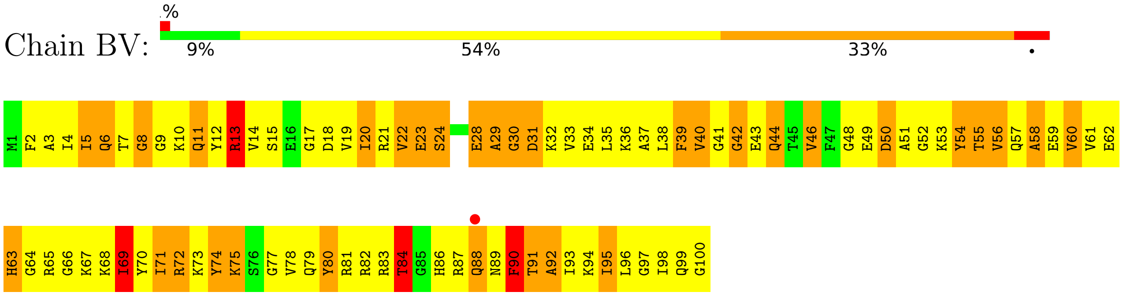
- Molecule 45: 50S ribosomal protein L20

Chain BU:



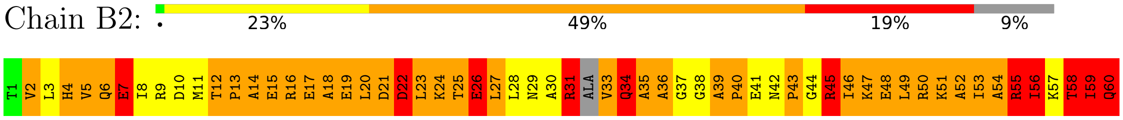
- Molecule 46: 50S ribosomal protein L21

Chain BV:



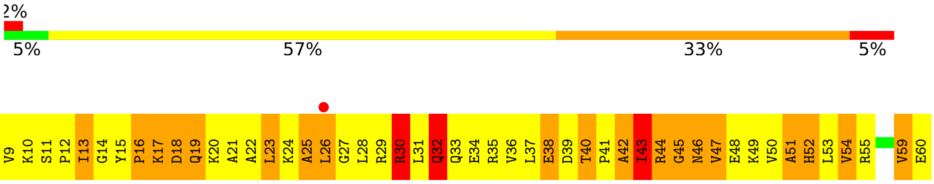
- Molecule 47: 50S ribosomal protein L29

Chain B2:



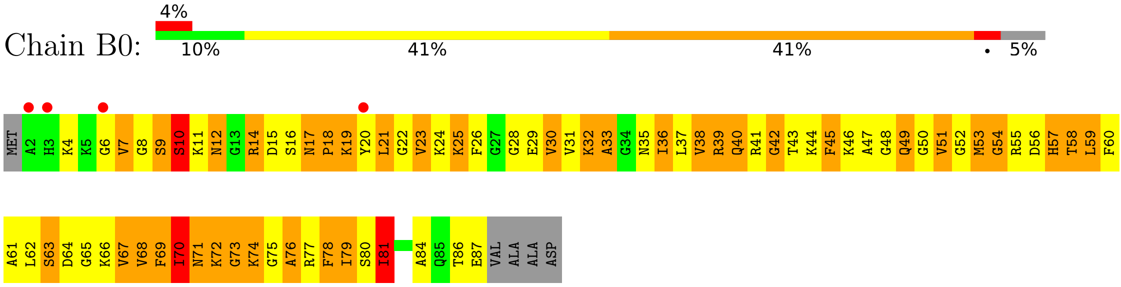
- Molecule 48: 50S ribosomal protein L30

Chain B3:



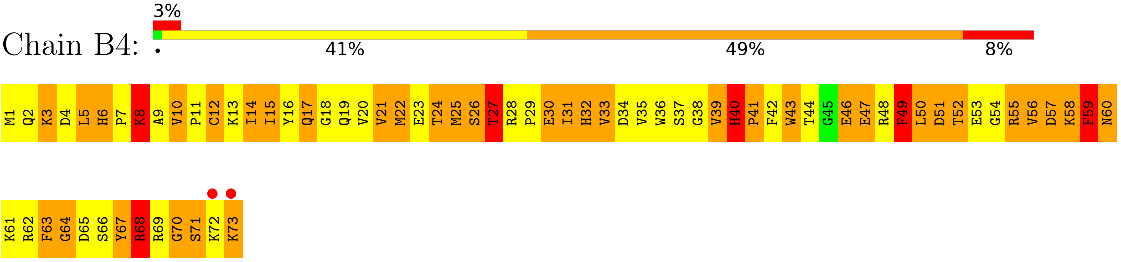
- Molecule 49: 50S ribosomal protein L27

Chain B0:



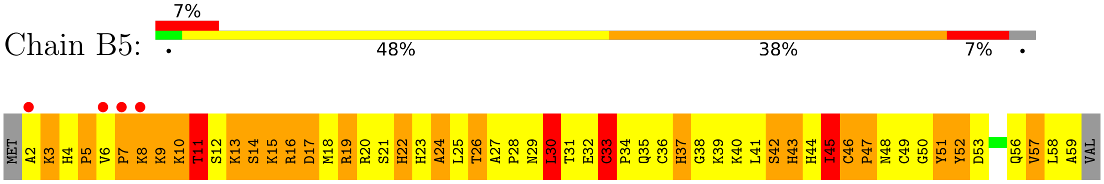
- Molecule 50: 50S ribosomal protein L31

Chain B4:



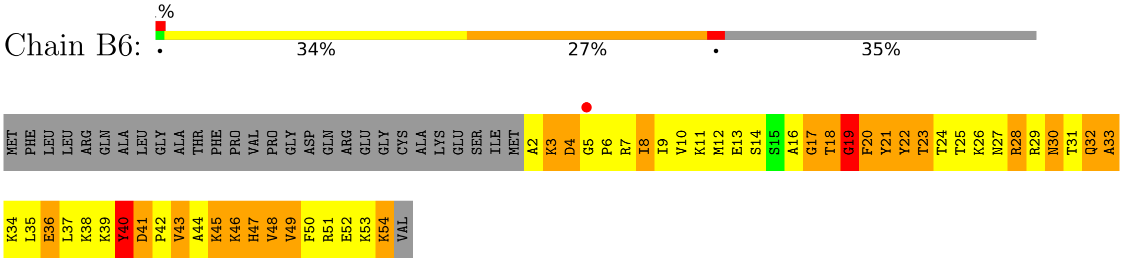
- Molecule 51: 50S ribosomal protein L32

Chain B5:



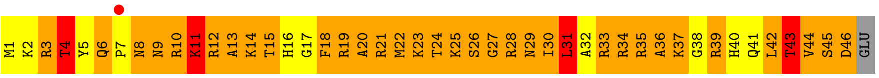
- Molecule 52: 50S ribosomal protein L33

Chain B6:



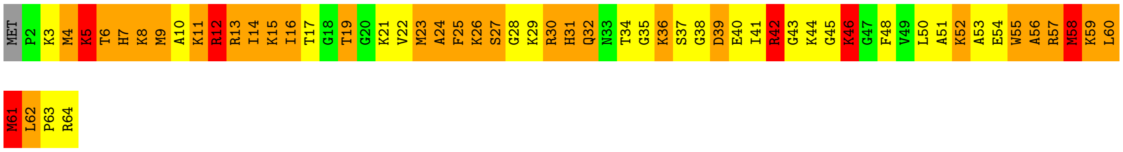
- Molecule 53: 50S ribosomal protein L34

Chain B7:



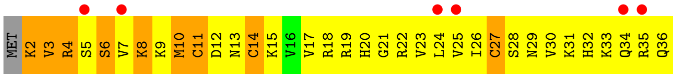
- Molecule 54: 50S ribosomal protein L35

Chain B8:



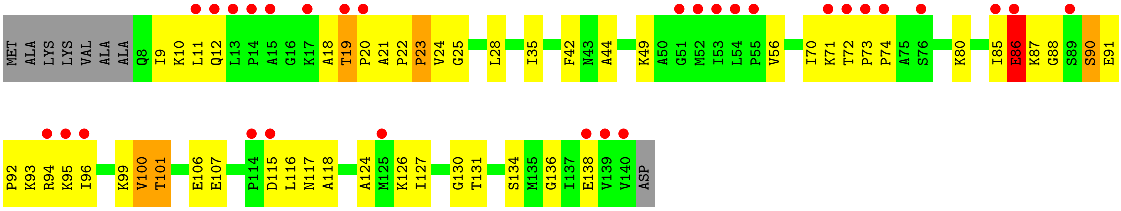
- Molecule 55: 50S ribosomal protein L36

Chain B9:



- Molecule 56: 50S ribosomal protein L11

Chain BK:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	518.99Å 518.99Å 365.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 5.90 49.92 – 5.54	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-5.90) 94.5 (49.92-5.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 5.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.351 , 0.371 0.339 , 0.359	Depositor DCC
R_{free} test set	7425 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	223.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.11 , 78.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	142780	wwPDB-VP
Average B, all atoms (Å^2)	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AA	1.25	68/36411 (0.2%)	1.47	415/56769 (0.7%)
2	AV	2.34	3/1813 (0.2%)	1.16	11/2823 (0.4%)
3	AW	1.82	17/1739 (1.0%)	1.97	36/2698 (1.3%)
4	AX	0.18	0/139	0.66	0/213
5	AB	0.63	1/1935 (0.1%)	0.66	4/2609 (0.2%)
6	AC	0.60	2/1636 (0.1%)	1.10	6/2205 (0.3%)
7	AD	0.65	4/1733 (0.2%)	0.97	9/2318 (0.4%)
8	AE	0.46	0/1161	0.61	1/1561 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.60	1/1276 (0.1%)	0.59	2/1709 (0.1%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.87	1/900 (0.1%)	0.56	0/1213
15	AL	0.49	1/986 (0.1%)	0.70	1/1320 (0.1%)
16	AM	1.15	2/1008 (0.2%)	1.16	3/1347 (0.2%)
17	AN	0.49	1/501 (0.2%)	0.64	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.15	2/870 (0.2%)	1.38	5/1159 (0.4%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.48	0/277
26	BB	1.11	5/2950 (0.2%)	1.43	23/4602 (0.5%)
27	BA	1.21	152/67844 (0.2%)	1.45	897/105838 (0.8%)
28	BD	0.37	0/1328	0.61	0/1783
29	BE	0.64	3/1540 (0.2%)	1.07	7/2078 (0.3%)
30	BF	0.69	3/1444 (0.2%)	0.82	1/1954 (0.1%)
31	BG	0.25	0/971	0.46	0/1304
32	BH	0.58	1/1272 (0.1%)	0.48	0/1721
33	BI	0.39	1/1156 (0.1%)	0.64	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BN	0.35	0/927	0.55	0/1245
35	BO	0.32	0/946	0.57	0/1269
36	BP	1.55	3/643 (0.5%)	1.32	5/870 (0.6%)
37	BQ	0.32	0/1106	0.53	0/1490
38	BS	0.79	2/877 (0.2%)	0.87	5/1179 (0.4%)
39	BT	0.39	0/412	0.70	0/554
40	BW	0.37	0/869	0.59	0/1166
41	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
42	BY	0.25	0/887	0.83	3/1195 (0.3%)
43	BZ	0.32	1/1385 (0.1%)	0.55	3/1883 (0.2%)
44	BR	0.31	0/867	0.49	0/1162
45	BU	0.70	1/994 (0.1%)	0.65	3/1323 (0.2%)
46	BV	0.75	1/796 (0.1%)	0.89	3/1058 (0.3%)
47	B2	0.37	0/497	1.00	2/668 (0.3%)
48	B3	0.31	0/482	0.50	0/646
49	B0	0.29	0/649	1.15	3/860 (0.3%)
50	B4	0.77	2/620 (0.3%)	0.57	0/831
51	B5	0.36	0/469	0.79	3/629 (0.5%)
52	B6	0.32	0/438	0.55	1/583 (0.2%)
53	B7	0.38	0/387	0.64	0/509
54	B8	0.73	2/503 (0.4%)	1.23	5/657 (0.8%)
55	B9	0.33	0/286	0.59	0/375
56	BK	0.30	0/1010	0.60	3/1349 (0.2%)
All	All	1.11	281/154800 (0.2%)	1.32	1469/231824 (0.6%)

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
3	AW	1	5
5	AB	0	1
6	AC	0	2
7	AD	0	1
15	AL	0	1
16	AM	0	1
20	AQ	0	2
28	BD	0	1
29	BE	0	3
30	BF	0	3
32	BH	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	BI	0	1
36	BP	0	1
38	BS	0	1
41	BX	0	1
42	BY	0	1
47	B2	0	1
54	B8	0	1
56	BK	0	1
All	All	1	29

The worst 5 of 281 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2199	A	O3'-P	-71.12	0.75	1.61
2	AV	45	G	O3'-P	-70.03	0.77	1.61
2	AV	65	G	O3'-P	-62.91	0.85	1.61
27	BA	2196	C	O3'-P	-59.20	0.90	1.61
1	AA	1211	U	O3'-P	-53.33	0.97	1.61

The worst 5 of 1469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	712(A)	A	P-O3'-C3'	-48.47	61.54	119.70
1	AA	196	A	P-O3'-C3'	44.40	172.99	119.70
3	AW	25	C	O3'-P-O5'	-43.47	21.42	104.00
27	BA	2199	A	O3'-P-O5'	-43.09	22.13	104.00
26	BB	24	G	P-O3'-C3'	29.89	155.56	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	Sidechain

5.2 Too-close contacts

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	AA	32551	0	16464	1922	4
2	AV	1622	0	823	187	0
3	AW	1638	0	835	231	0
4	AX	136	0	63	35	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	104	0
7	AD	1703	0	1762	190	0
8	AE	1146	0	1206	57	0
9	AF	843	0	857	27	0
10	AG	1257	0	1294	138	0
11	AH	1116	0	1177	79	0
12	AI	1011	0	1041	80	0
13	AJ	794	0	840	118	0
14	AK	885	0	904	50	0
15	AL	970	0	1056	79	0
16	AM	997	0	1071	129	0
17	AN	492	0	529	111	0
18	AO	734	0	771	31	0
19	AP	700	0	720	68	0
20	AQ	857	0	929	96	0
21	AR	597	0	668	31	0
22	AS	647	0	672	146	0
23	AT	762	0	859	43	0
24	AU	208	0	221	22	0
25	AY	333	0	0	47	0
26	BB	2637	0	1338	198	0
27	BA	60600	0	30513	10823	139
28	BD	1308	0	1345	1087	0
29	BE	1507	0	1474	1127	3
30	BF	1430	0	1359	1069	0
31	BG	957	0	950	685	0
32	BH	1251	0	1289	743	0
33	BI	1145	0	1225	635	4
34	BN	917	0	896	775	1
35	BO	937	0	993	614	0
36	BP	639	0	605	490	0
37	BQ	1081	0	1048	916	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BS	866	0	867	686	0
39	BT	406	0	360	166	0
40	BW	860	0	911	559	0
41	BX	602	0	558	457	0
42	BY	879	0	860	748	0
43	BZ	1360	0	1377	887	0
44	BR	855	0	904	580	0
45	BU	978	0	995	924	0
46	BV	787	0	783	652	0
47	B2	494	0	504	385	0
48	B3	477	0	528	446	0
49	B0	641	0	657	501	0
50	B4	604	0	587	493	0
51	B5	457	0	457	293	0
52	B6	431	0	454	288	0
53	B7	383	0	409	396	0
54	B8	496	0	541	358	0
55	B9	285	0	312	203	0
56	BK	999	0	1068	144	0
All	All	142780	0	94554	28108	146

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 119.

The worst 5 of 28108 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)
51:B5:33:CYS:SG	51:B5:36:CYS:HB2	1.24	1.69
27:BA:2470:G:C2	27:BA:2471:C:C5	1.81	1.68
27:BA:994:C:C2	45:BU:53:LYS:HD3	1.16	1.68
53:B7:30:ILE:HA	53:B7:33:ARG:CD	1.21	1.67
27:BA:2580:U:C6	27:BA:2581:G:C8	1.82	1.66

The worst 5 of 146 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:6:A:C4’	27:BA:2902:C:O2’[8_554]	0.49	1.71
1:AA:359:U:OP1	33:BI:82:LYS:NZ[3_454]	0.68	1.52
27:BA:6:A:N9	27:BA:2902:C:C6[8_554]	0.88	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1:G:O6	27:BA:2898:U:C2[8_554]	0.92	1.28
27:BA:6:A:O4'	27:BA:2902:C:C2'[8_554]	0.97	1.23

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
5	AB	232/256 (91%)	183 (79%)	34 (15%)	15 (6%)	1	16
6	AC	204/239 (85%)	165 (81%)	23 (11%)	16 (8%)	1	12
7	AD	206/209 (99%)	156 (76%)	34 (16%)	16 (8%)	1	12
8	AE	146/162 (90%)	114 (78%)	29 (20%)	3 (2%)	7	36
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	3	23
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	5	31
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1	13
12	AI	125/128 (98%)	87 (70%)	30 (24%)	8 (6%)	1	16
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	0	10
14	AK	117/129 (91%)	89 (76%)	23 (20%)	5 (4%)	2	22
15	AL	122/135 (90%)	91 (75%)	14 (12%)	17 (14%)	0	4
16	AM	123/126 (98%)	96 (78%)	21 (17%)	6 (5%)	2	20
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1	14
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	13	50
19	AP	81/88 (92%)	64 (79%)	10 (12%)	7 (9%)	1	11
20	AQ	102/105 (97%)	78 (76%)	17 (17%)	7 (7%)	1	14
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	11
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	3	24
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	10
28	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
29	BE	183/338 (54%)	89 (49%)	35 (19%)	59 (32%)	0	0
30	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
31	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
32	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	0
33	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	0
34	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
35	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	0
36	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
37	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
38	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
39	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
40	BW	104/113 (92%)	42 (40%)	15 (14%)	47 (45%)	0	0
41	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
42	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
43	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
44	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
45	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
46	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
47	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
48	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
49	B0	84/91 (92%)	33 (39%)	16 (19%)	35 (42%)	0	0
50	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
51	B5	56/60 (93%)	16 (29%)	17 (30%)	23 (41%)	0	0
52	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
53	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
54	B8	61/64 (95%)	23 (38%)	9 (15%)	29 (48%)	0	0
55	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	0
56	BK	124/141 (88%)	93 (75%)	26 (21%)	5 (4%)	3	23
All	All	5320/6250 (85%)	2968 (56%)	1021 (19%)	1331 (25%)	0	1

5 of 1331 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	ALA

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
5	AB	202/220 (92%)	173 (86%)	29 (14%)	3	16
6	AC	160/188 (85%)	146 (91%)	14 (9%)	10	31
7	AD	180/181 (99%)	162 (90%)	18 (10%)	7	26
8	AE	115/123 (94%)	94 (82%)	21 (18%)	1	10
9	AF	90/90 (100%)	83 (92%)	7 (8%)	12	36
10	AG	126/127 (99%)	116 (92%)	10 (8%)	12	36
11	AH	119/119 (100%)	91 (76%)	28 (24%)	1	4
12	AI	98/99 (99%)	90 (92%)	8 (8%)	11	34
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	19
14	AK	90/99 (91%)	85 (94%)	5 (6%)	21	46
15	AL	104/111 (94%)	93 (89%)	11 (11%)	6	24
16	AM	100/101 (99%)	87 (87%)	13 (13%)	4	18
17	AN	49/50 (98%)	43 (88%)	6 (12%)	5	20
18	AO	79/80 (99%)	70 (89%)	9 (11%)	5	21
19	AP	72/74 (97%)	62 (86%)	10 (14%)	3	17
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	8	28
21	AR	64/77 (83%)	57 (89%)	7 (11%)	6	23
22	AS	71/80 (89%)	64 (90%)	7 (10%)	8	26
23	AT	76/82 (93%)	68 (90%)	8 (10%)	7	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AU	19/22 (86%)	19 (100%)	0	100	100
28	BD	135/135 (100%)	99 (73%)	36 (27%)	0	3
29	BE	156/284 (55%)	128 (82%)	28 (18%)	2	10
30	BF	152/193 (79%)	124 (82%)	28 (18%)	1	10
31	BG	102/147 (69%)	93 (91%)	9 (9%)	10	31
32	BH	137/147 (93%)	111 (81%)	26 (19%)	1	8
33	BI	119/119 (100%)	98 (82%)	21 (18%)	2	11
34	BN	95/121 (78%)	80 (84%)	15 (16%)	2	14
35	BO	101/101 (100%)	81 (80%)	20 (20%)	1	8
36	BP	67/126 (53%)	56 (84%)	11 (16%)	2	13
37	BQ	110/110 (100%)	83 (76%)	27 (24%)	0	4
38	BS	89/149 (60%)	73 (82%)	16 (18%)	1	10
39	BT	44/52 (85%)	30 (68%)	14 (32%)	0	2
40	BW	88/92 (96%)	74 (84%)	14 (16%)	2	14
41	BX	67/73 (92%)	44 (66%)	23 (34%)	0	1
42	BY	97/105 (92%)	80 (82%)	17 (18%)	2	11
43	BZ	151/203 (74%)	129 (85%)	22 (15%)	3	15
44	BR	89/101 (88%)	71 (80%)	18 (20%)	1	7
45	BU	96/97 (99%)	68 (71%)	28 (29%)	0	2
46	BV	79/79 (100%)	69 (87%)	10 (13%)	4	19
47	B2	51/56 (91%)	37 (72%)	14 (28%)	0	3
48	B3	52/52 (100%)	47 (90%)	5 (10%)	8	27
49	B0	64/67 (96%)	57 (89%)	7 (11%)	6	23
50	B4	66/66 (100%)	54 (82%)	12 (18%)	1	10
51	B5	51/53 (96%)	43 (84%)	8 (16%)	2	14
52	B6	46/69 (67%)	39 (85%)	7 (15%)	3	15
53	B7	39/40 (98%)	31 (80%)	8 (20%)	1	7
54	B8	50/51 (98%)	39 (78%)	11 (22%)	1	6
55	B9	34/35 (97%)	30 (88%)	4 (12%)	5	21
56	BK	108/113 (96%)	105 (97%)	3 (3%)	43	65
All	All	4533/5148 (88%)	3840 (85%)	693 (15%)	2	14

5 of 693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BS	87	LEU
44	BR	105	ARG
39	BT	25	ASP
38	BS	83	LEU
42	BY	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
29	BE	318	ASN
47	B2	42	ASN
34	BN	92	GLN
47	B2	29	ASN
52	B6	27	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1498/1522 (98%)	518 (34%)	166 (11%)
2	AV	74/76 (97%)	16 (21%)	4 (5%)
26	BB	122/123 (99%)	44 (36%)	3 (2%)
27	BA	2785/2916 (95%)	1488 (53%)	360 (12%)
3	AW	70/76 (92%)	14 (20%)	4 (5%)
4	AX	5/18 (27%)	0	0
All	All	4554/4731 (96%)	2080 (45%)	537 (11%)

5 of 2080 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 537 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2426	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	BA	2493	U
27	BA	2425	A
27	BA	2777	G
27	BA	197	A

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

3 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
3	YYG	AW	37	10,3	31,42,43	0.92	1 (3%)	33,62,65	2.60	10 (30%)
3	PSU	AW	55	3	18,21,22	0.72	0	22,30,33	0.86	0
3	PSU	AW	39	3	18,21,22	0.73	0	22,30,33	0.69	0

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
3	YYG	AW	37	10,3	1/1/8/9	7/20/42/43	0/3/4/4
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	37	YYG	C8-N7	-2.19	1.31	1.35

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AW	37	YYG	C11-C12-N1	8.60	111.38	106.53
3	AW	37	YYG	C24-O23-C21	6.32	123.12	115.66
3	AW	37	YYG	C3-N3-C4	4.97	125.54	116.71
3	AW	37	YYG	O23-C21-N20	4.37	118.47	110.80
3	AW	37	YYG	C4-N3-C2	-3.40	111.82	122.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AW	37	YYG	C12-C13-C14-C15
3	AW	37	YYG	C15-C16-O18-C19
3	AW	37	YYG	O17-C16-O18-C19
3	AW	37	YYG	C13-C14-C15-C16
3	AW	37	YYG	C14-C15-C16-O18

There are no ring outliers.

2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	37	YYG	37	0
3	AW	39	PSU	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	BA	104
1	AA	67
3	AW	8
56	BK	5
2	AV	4
37	BQ	3
26	BB	3
46	BV	2
6	AC	2
28	BD	1
8	AE	1
16	AM	1
5	AB	1
36	BP	1
10	AG	1
38	BS	1
30	BF	1
15	AL	1
43	BZ	1
33	BI	1
7	AD	1
32	BH	1
45	BU	1
14	AK	1
20	AQ	1

The worst 5 of 214 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	70:ILE	C	71:LYS	N	5.81
1	BK	73:PRO	C	74:PRO	N	5.30
1	BK	72:THR	C	73:PRO	N	5.11
1	AA	30(D):A	O3'	1031:G	P	4.82
1	BA	142(A):A	O3'	1143:A	P	4.82

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1515/1522 (99%)	0.50	95 (6%)	20	19	236, 236, 236, 236	0
2	AV	76/76 (100%)	0.36	1 (1%)	77	68	236, 236, 236, 236	0
3	AW	73/76 (96%)	0.96	10 (13%)	3	6	236, 236, 236, 236	0
4	AX	17/18 (94%)	3.82	11 (64%)	0	0	236, 236, 236, 236	0
5	AB	234/256 (91%)	-0.06	3 (1%)	77	68	236, 236, 236, 236	0
6	AC	206/239 (86%)	-0.02	6 (2%)	51	44	236, 236, 236, 236	0
7	AD	208/209 (99%)	0.28	17 (8%)	11	13	236, 236, 236, 236	0
8	AE	150/162 (92%)	0.16	10 (6%)	17	17	236, 236, 236, 236	0
9	AF	101/101 (100%)	0.05	6 (5%)	22	22	236, 236, 236, 236	0
10	AG	155/156 (99%)	0.14	11 (7%)	16	16	236, 236, 236, 236	0
11	AH	138/138 (100%)	-0.19	3 (2%)	62	54	236, 236, 236, 236	0
12	AI	127/128 (99%)	0.28	13 (10%)	6	9	236, 236, 236, 236	0
13	AJ	98/105 (93%)	0.91	18 (18%)	1	3	236, 236, 236, 236	0
14	AK	119/129 (92%)	-0.11	3 (2%)	57	50	236, 236, 236, 236	0
15	AL	124/135 (91%)	0.12	7 (5%)	24	24	236, 236, 236, 236	0
16	AM	125/126 (99%)	0.66	22 (17%)	1	4	236, 236, 236, 236	0
17	AN	60/61 (98%)	0.30	5 (8%)	11	13	236, 236, 236, 236	0
18	AO	88/89 (98%)	0.16	1 (1%)	80	73	236, 236, 236, 236	0
19	AP	83/88 (94%)	0.86	16 (19%)	1	3	236, 236, 236, 236	0
20	AQ	104/105 (99%)	-0.05	2 (1%)	66	59	236, 236, 236, 236	0
21	AR	73/88 (82%)	0.08	3 (4%)	37	34	236, 236, 236, 236	0
22	AS	80/93 (86%)	0.86	16 (20%)	1	3	236, 236, 236, 236	0
23	AT	99/106 (93%)	-0.07	4 (4%)	38	34	236, 236, 236, 236	0
24	AU	24/27 (88%)	1.04	5 (20%)	1	3	236, 236, 236, 236	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	AY	333/354 (94%)	1.37	95 (28%) 0 2	236, 236, 236, 236	0
26	BB	123/123 (100%)	0.22	0 100 100	236, 236, 236, 236	0
27	BA	2814/2916 (96%)	0.35	110 (3%) 39 34	236, 236, 236, 236	0
28	BD	173/173 (100%)	-0.31	2 (1%) 79 71	236, 236, 236, 236	0
29	BE	191/338 (56%)	0.17	11 (5%) 23 23	236, 236, 236, 236	0
30	BF	189/246 (76%)	-0.14	4 (2%) 63 56	236, 236, 236, 236	0
31	BG	122/176 (69%)	0.46	9 (7%) 14 15	236, 236, 236, 236	0
32	BH	164/177 (92%)	-0.04	9 (5%) 25 25	236, 236, 236, 236	0
33	BI	148/149 (99%)	0.06	3 (2%) 65 58	236, 236, 236, 236	0
34	BN	117/145 (80%)	-0.28	2 (1%) 70 62	236, 236, 236, 236	0
35	BO	122/122 (100%)	-0.09	2 (1%) 72 64	236, 236, 236, 236	0
36	BP	84/164 (51%)	0.13	2 (2%) 59 52	236, 236, 236, 236	0
37	BQ	138/138 (100%)	0.21	10 (7%) 15 16	236, 236, 236, 236	0
38	BS	113/186 (60%)	-0.09	3 (2%) 54 47	236, 236, 236, 236	0
39	BT	52/66 (78%)	0.28	0 100 100	236, 236, 236, 236	0
40	BW	108/113 (95%)	-0.14	1 (0%) 84 77	236, 236, 236, 236	0
41	BX	76/84 (90%)	-0.12	0 100 100	236, 236, 236, 236	0
42	BY	110/119 (92%)	0.51	12 (10%) 5 8	236, 236, 236, 236	0
43	BZ	177/253 (69%)	0.11	11 (6%) 20 20	236, 236, 236, 236	0
44	BR	105/118 (88%)	-0.30	1 (0%) 82 75	236, 236, 236, 236	0
45	BU	117/118 (99%)	-0.35	4 (3%) 45 40	236, 236, 236, 236	0
46	BV	100/100 (100%)	-0.18	1 (1%) 82 75	236, 236, 236, 236	0
47	B2	64/70 (91%)	-0.64	0 100 100	236, 236, 236, 236	0
48	B3	60/60 (100%)	-0.37	1 (1%) 70 62	236, 236, 236, 236	0
49	B0	86/91 (94%)	0.10	4 (4%) 31 30	236, 236, 236, 236	0
50	B4	73/73 (100%)	-0.02	2 (2%) 54 47	236, 236, 236, 236	0
51	B5	58/60 (96%)	0.09	4 (6%) 16 16	236, 236, 236, 236	0
52	B6	53/82 (64%)	-0.29	1 (1%) 66 59	236, 236, 236, 236	0
53	B7	46/47 (97%)	-0.03	1 (2%) 62 54	236, 236, 236, 236	0
54	B8	63/64 (98%)	-0.29	0 100 100	236, 236, 236, 236	0
55	B9	35/36 (97%)	0.87	6 (17%) 1 4	236, 236, 236, 236	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
56	BK	133/141 (94%)	1.24	30 (22%)	0	2	236, 236, 236, 236	0
All	All	10424/11335 (91%)	0.28	629 (6%)	21	21	236, 236, 236, 236	0

The worst 5 of 629 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	AY	260	LYS	13.0
4	AX	123	A	11.5
56	BK	52	MET	9.9
4	AX	122	U	8.6
27	BA	1532	C	8.4

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	YYG	AW	37	39/40	0.52	0.68	236,236,236,236	0
3	PSU	AW	39	20/21	0.72	0.43	236,236,236,236	0
3	PSU	AW	55	20/21	0.85	0.17	236,236,236,236	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.