wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 07:59 am BST

PDB ID	:	4V4X
Title	:	Crystal structure of the 70S Thermus thermophilus ribosome showing how the 16S 3'-end mimicks mRNA E and P codons.
Authors	:	Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on	:	2006-06-27
Resolution	:	5.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

The following versions of software and data (see references (1)) were used in the production of this report:

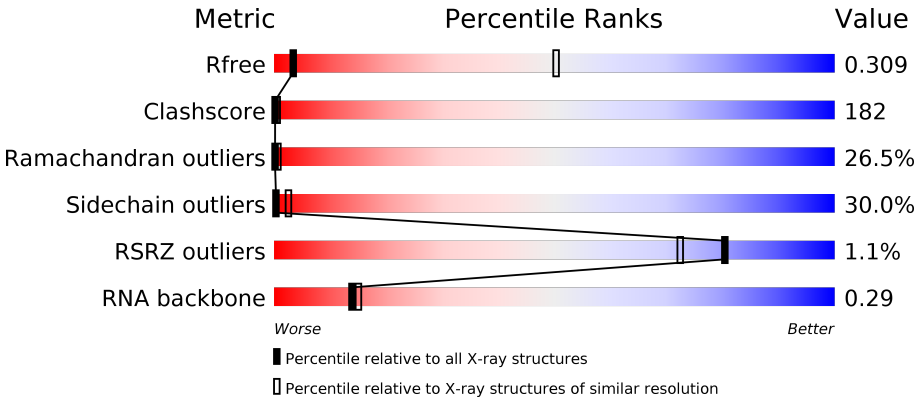
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.00 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	1140 (6.20-3.80)
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)
RNA backbone	3102	1068 (7.00-3.00)

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 on 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	55% 34% 9%
2	AC	77	45% 42% 10%
3	AD	76	54% 42%
4	AE	256	4% 48% 34% 7% 9%

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Mol	Chain	Length	Quality of chain
5	AF	239	2% 52% 28% 14%
6	AG	209	52% 39% 6%
7	AH	162	50% 31% 8% 7%
8	AI	101	2% 51% 40% 7%
9	AJ	156	58% 31% 7%
10	AK	138	46% 43% 9%
11	AL	128	5% 59% 30% 5%
12	AM	105	13% 49% 35% 6% 7%
13	AN	129	57% 29% 5% 8%
14	AO	132	6% 51% 30% 8% 6%
15	AP	126	60% 31% 6%
16	AQ	61	7% 49% 33% 10%
17	AR	89	57% 35%
18	AS	88	5% 48% 36% 6% 6%
19	AT	105	56% 38%
20	AU	88	5% 5% 45% 26% 7% 17%
21	AV	93	52% 25% 6% 14%
22	AW	106	7% 49% 36% 7%
23	AX	27	7% 52% 22% 7% 11%
24	BA	2916	43% 40% 15%
25	BB	123	46% 46% 7%
26	BC	229	7% 6% 61% 28% 5%
27	BD	276	43% 44% 10%
28	BE	206	45% 38% 15%
29	BF	210	50% 38% 9%

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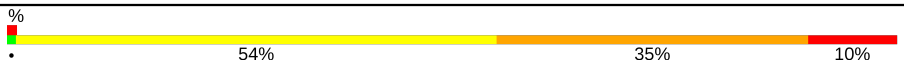
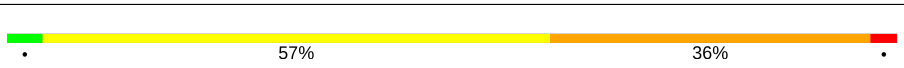
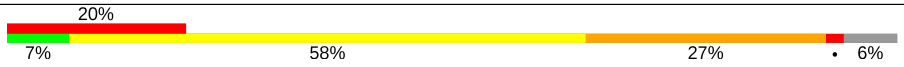
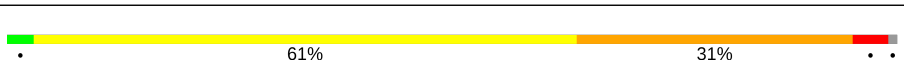
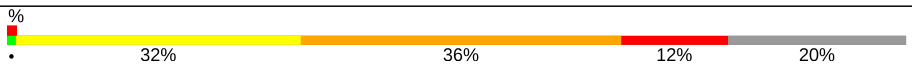
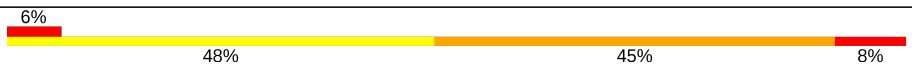
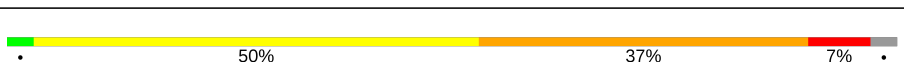
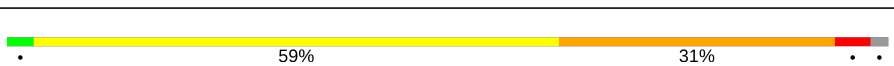
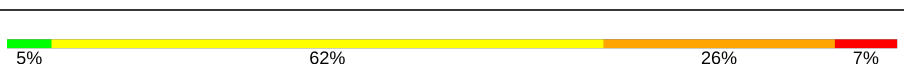
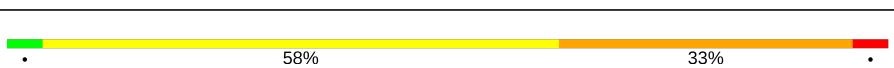
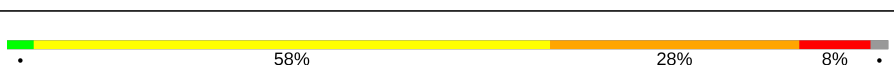
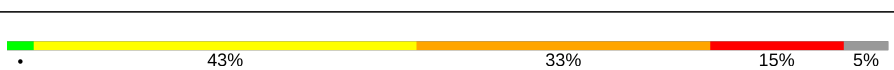
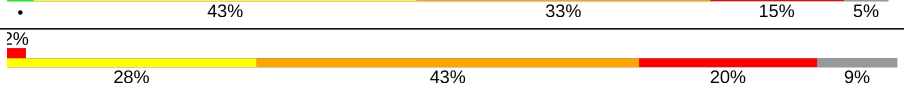
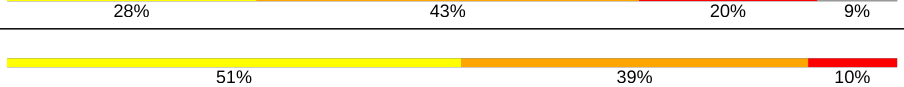
Mol	Chain	Length	Quality of chain
30	BG	182	
31	BH	180	
32	BK	148	
33	BL	147	
34	BM	140	
35	BN	122	
36	BO	150	
37	BP	141	
38	BQ	118	
39	BR	112	
40	BS	146	
41	BT	118	
42	BU	101	
43	BV	113	
44	BW	96	
45	BX	110	
46	BY	206	
47	BZ	85	
48	B1	67	
49	B2	60	
50	B3	71	
51	B4	60	
52	B5	54	
53	B6	49	
54	B7	65	

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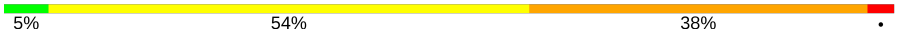
Mol	Chain	Length	Quality of chain
55	B8	37	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 149044 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1515	32554	14490	6022	10527	1515	0	0	0

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AC	76	1624	723	295	530	76	0	0	0

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AD	76	1623	723	290	534	76	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

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

- Molecule 5 is a protein called 30S ribosomal protein S3.

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

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

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

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AL	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 12 is a protein called 30S ribosomal protein S10.

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

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

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

- Molecule 15 is a protein called 30S ribosomal protein S13.

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

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

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

- Molecule 19 is a protein called 30S ribosomal protein S17.

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

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

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

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	496	G	-	INSERTION	GB 48268

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271
BB	120	U	-	INSERTION	GB 48271

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BR	110	Total	C	N	O	0	0	0
			877	553	175	149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	117	Total	C	N	O	S	0	0	0
			976	614	197	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	94	Total	C	N	O	0	0	0
			742	483	133	126			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	110	Total	C	N	O	S	0	0	0
			844	539	158	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B2	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

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

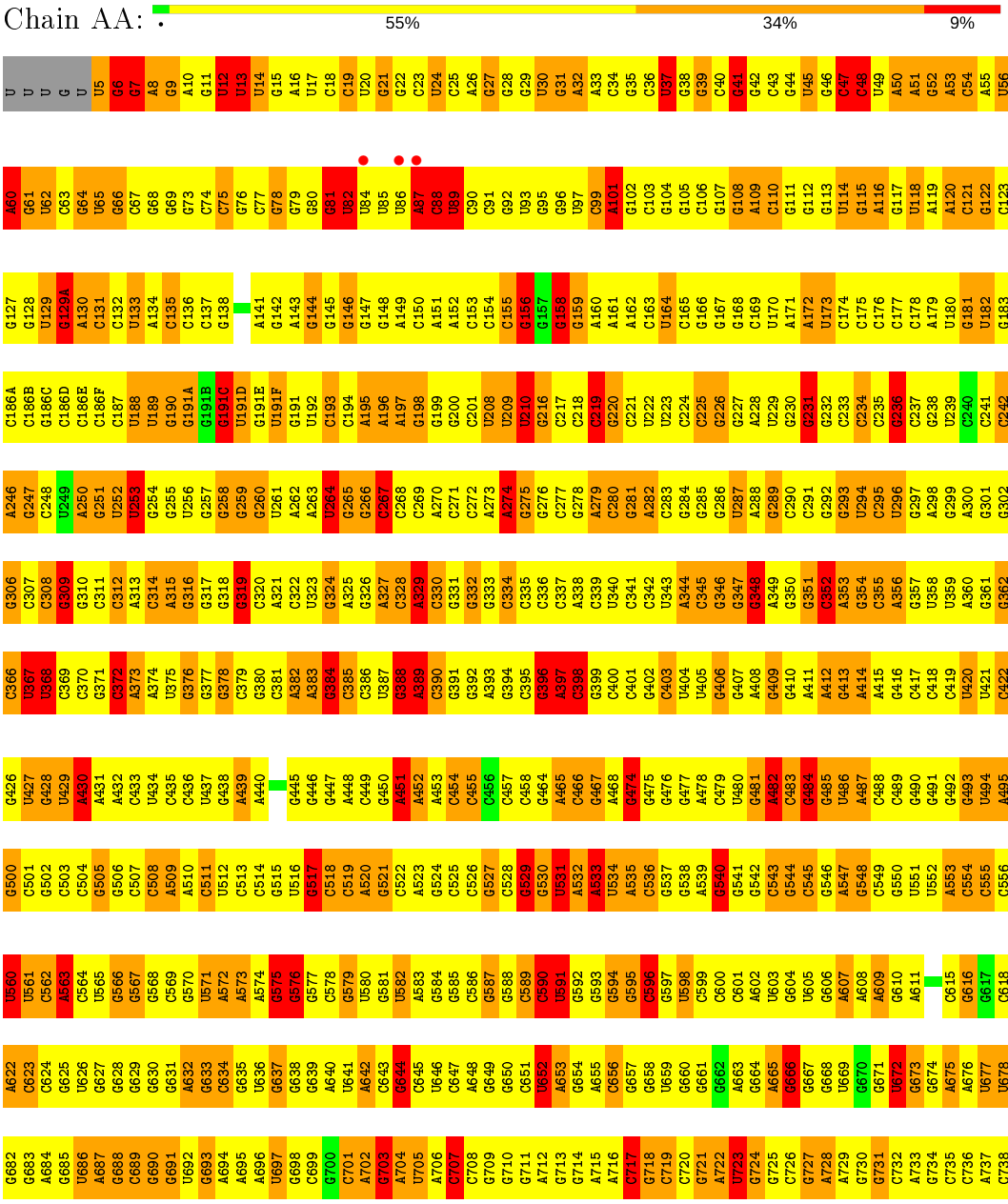
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

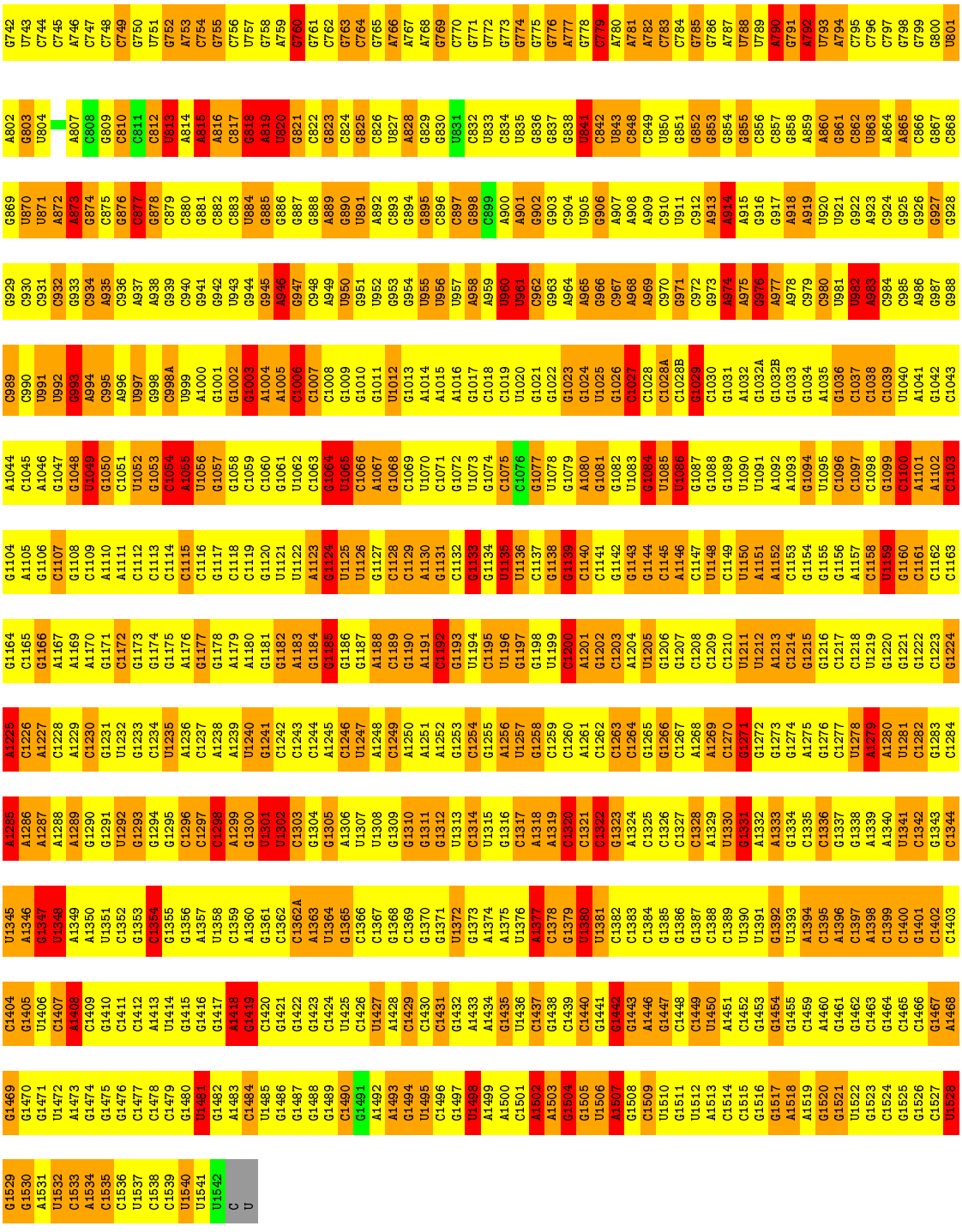
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 rRNA

Chain AA:





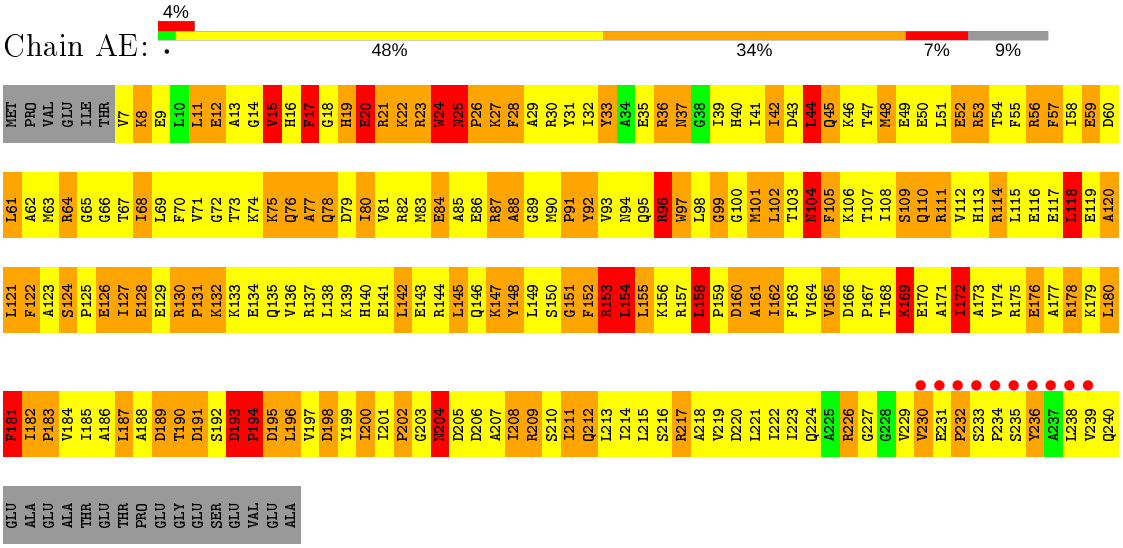
• Molecule 2: tRNA fMET (unmodified bases)

- Molecule 3: tRNA PHE (unmodified bases)

Chain AD:

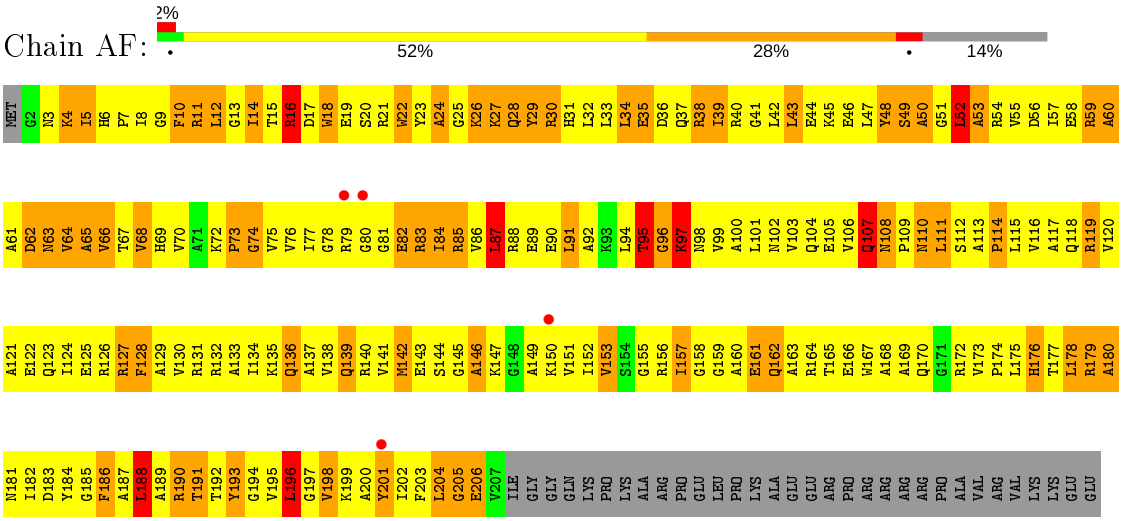
- Molecule 4: 30S ribosomal protein S2

Chain AE:



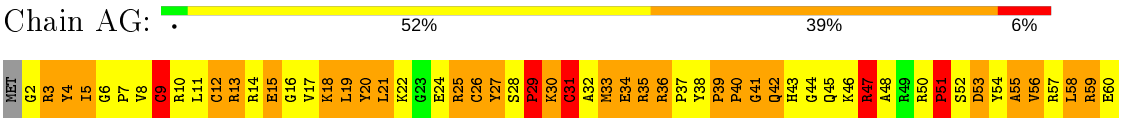
- Molecule 5: 30S ribosomal protein S3

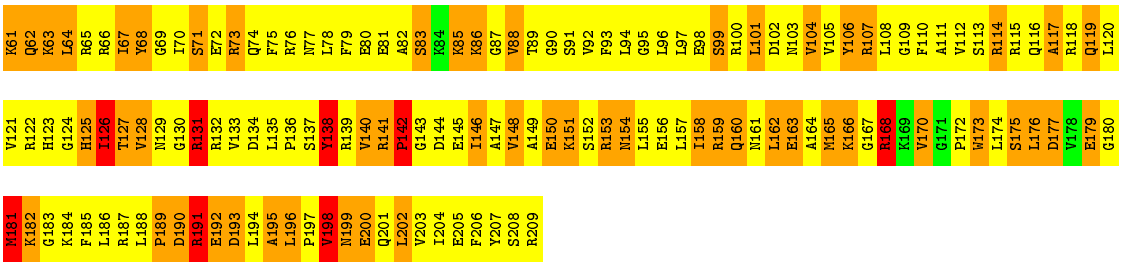
Chain AF:

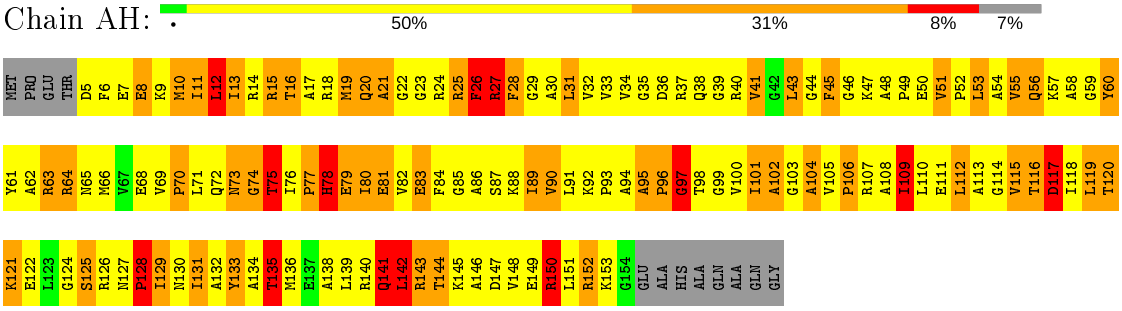


- Molecule 6: 30S ribosomal protein S4

Chain AG:





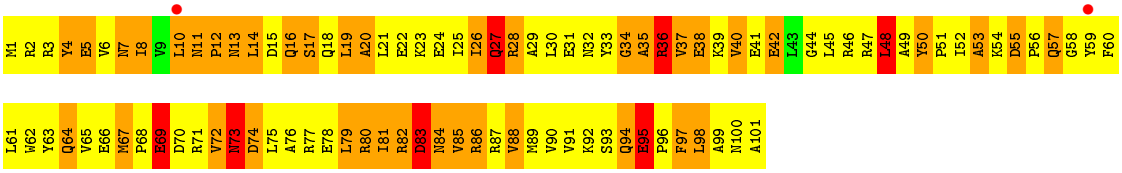


- Molecule 7: 30S ribosomal protein S5

Chain AH:

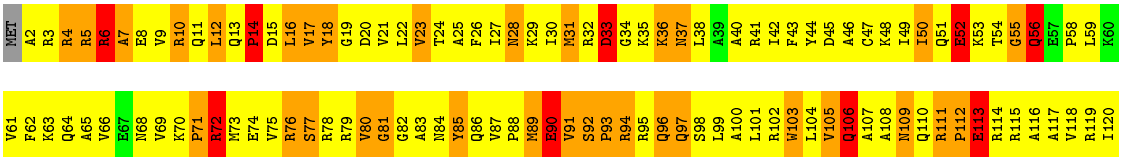
- Molecule 8: 30S ribosomal protein S6

Chain AI:



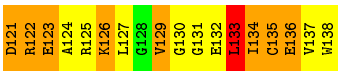
- Molecule 9: 30S ribosomal protein S7

Chain AJ:



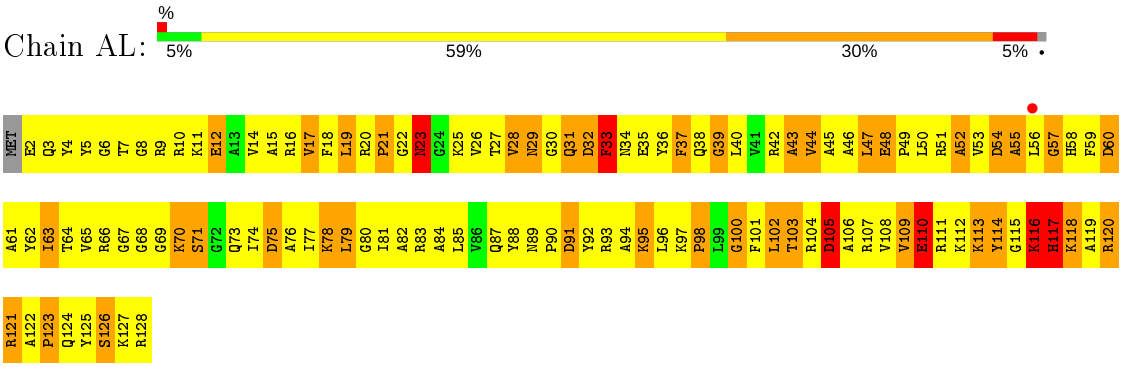
- Molecule 10: 30S ribosomal protein S8

Chain AK:



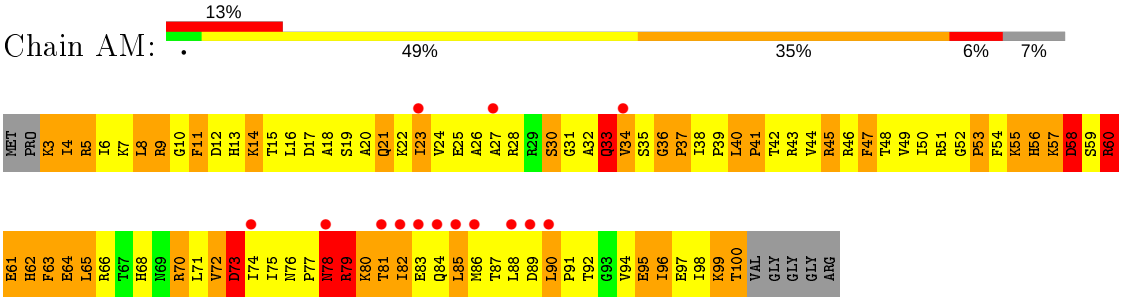
- Molecule 11: 30S ribosomal protein S9

Chain AL:



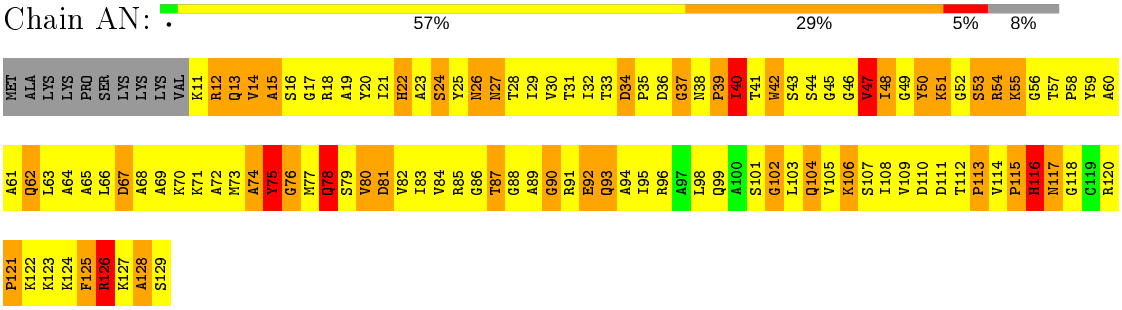
- Molecule 12: 30S ribosomal protein S10

Chain AM:



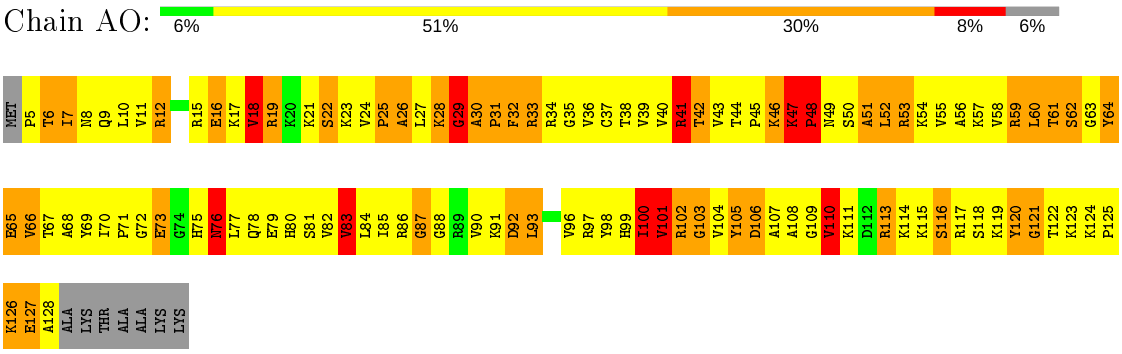
- Molecule 13: 30S ribosomal protein S11

Chain AN:



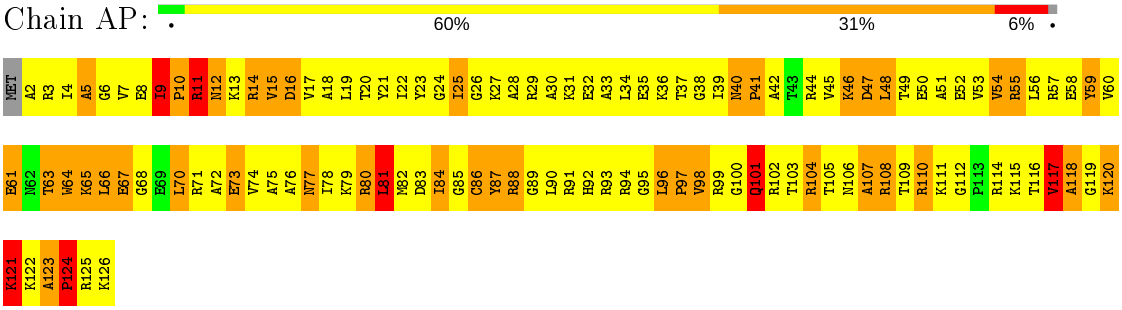
- Molecule 14: 30S ribosomal protein S12

Chain AO:



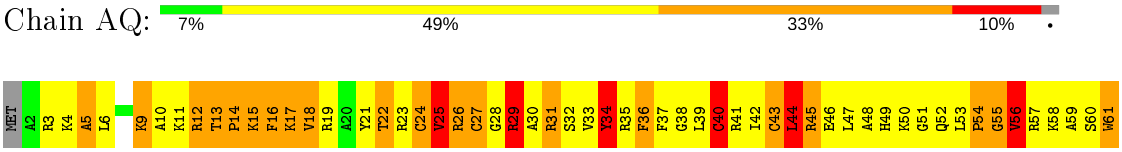
- Molecule 15: 30S ribosomal protein S13

Chain AP:



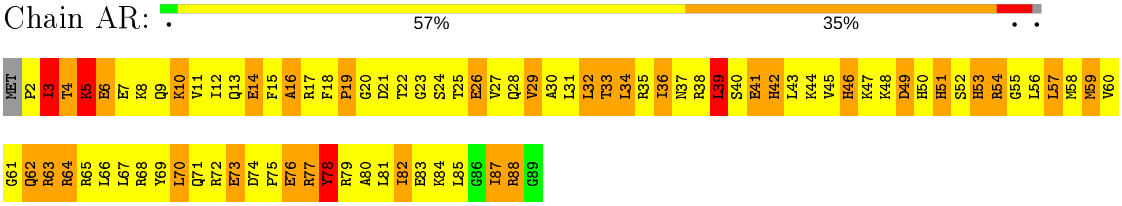
- Molecule 16: 30S ribosomal protein S14

Chain AQ:



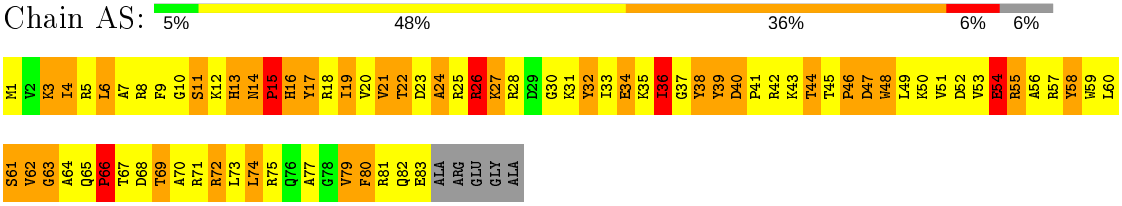
- Molecule 17: 30S ribosomal protein S15

Chain AR:



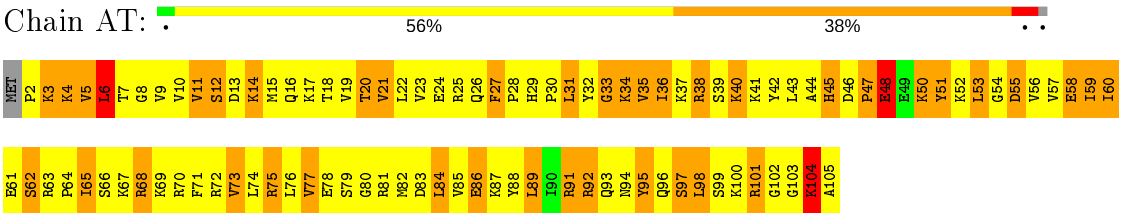
- Molecule 18: 30S ribosomal protein S16

Chain AS:



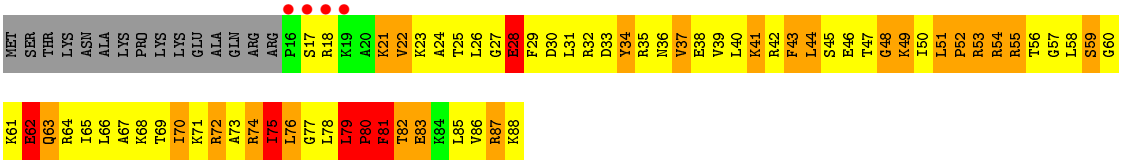
- Molecule 19: 30S ribosomal protein S17

Chain AT:

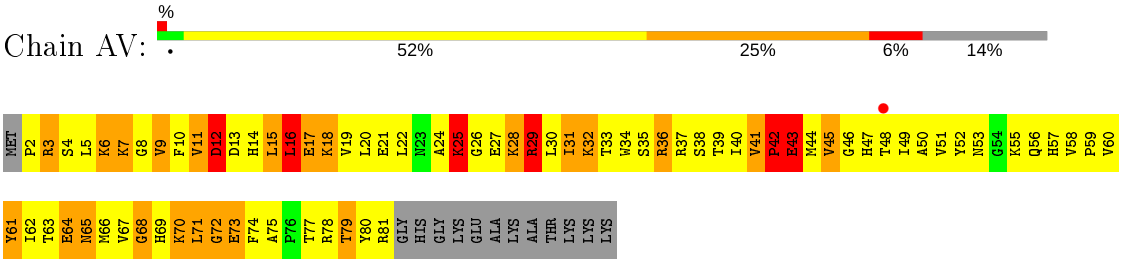


- Molecule 20: 30S ribosomal protein S18

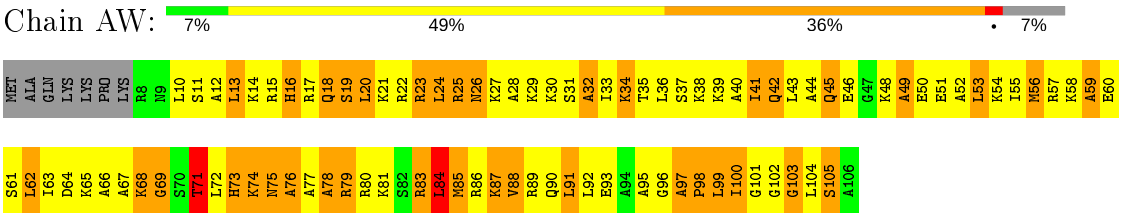
Chain AU:



- Molecule 21: 30S ribosomal protein S19

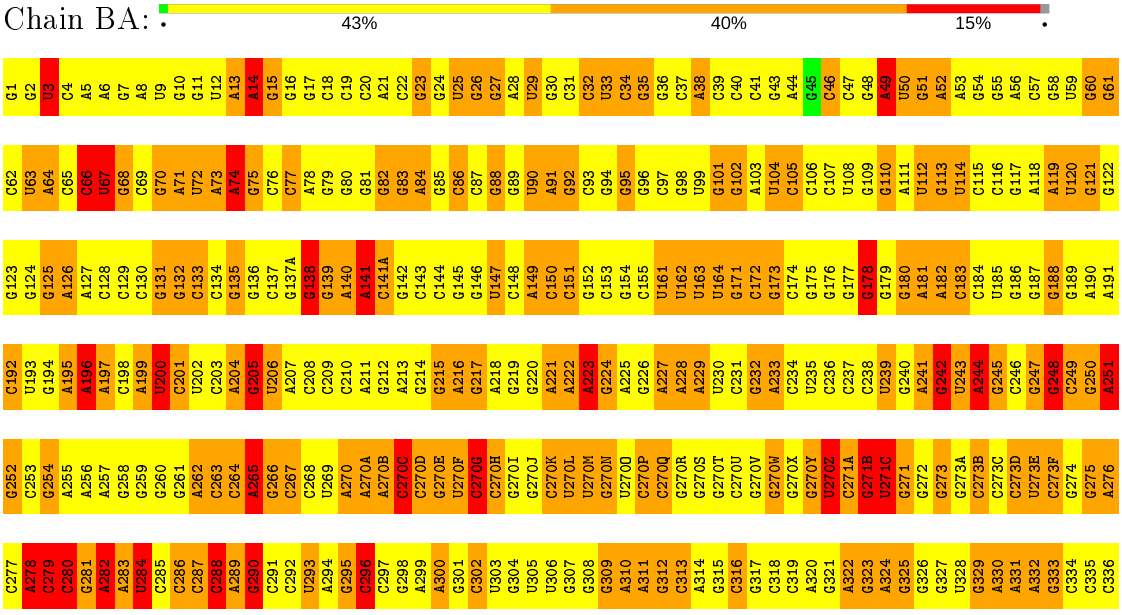


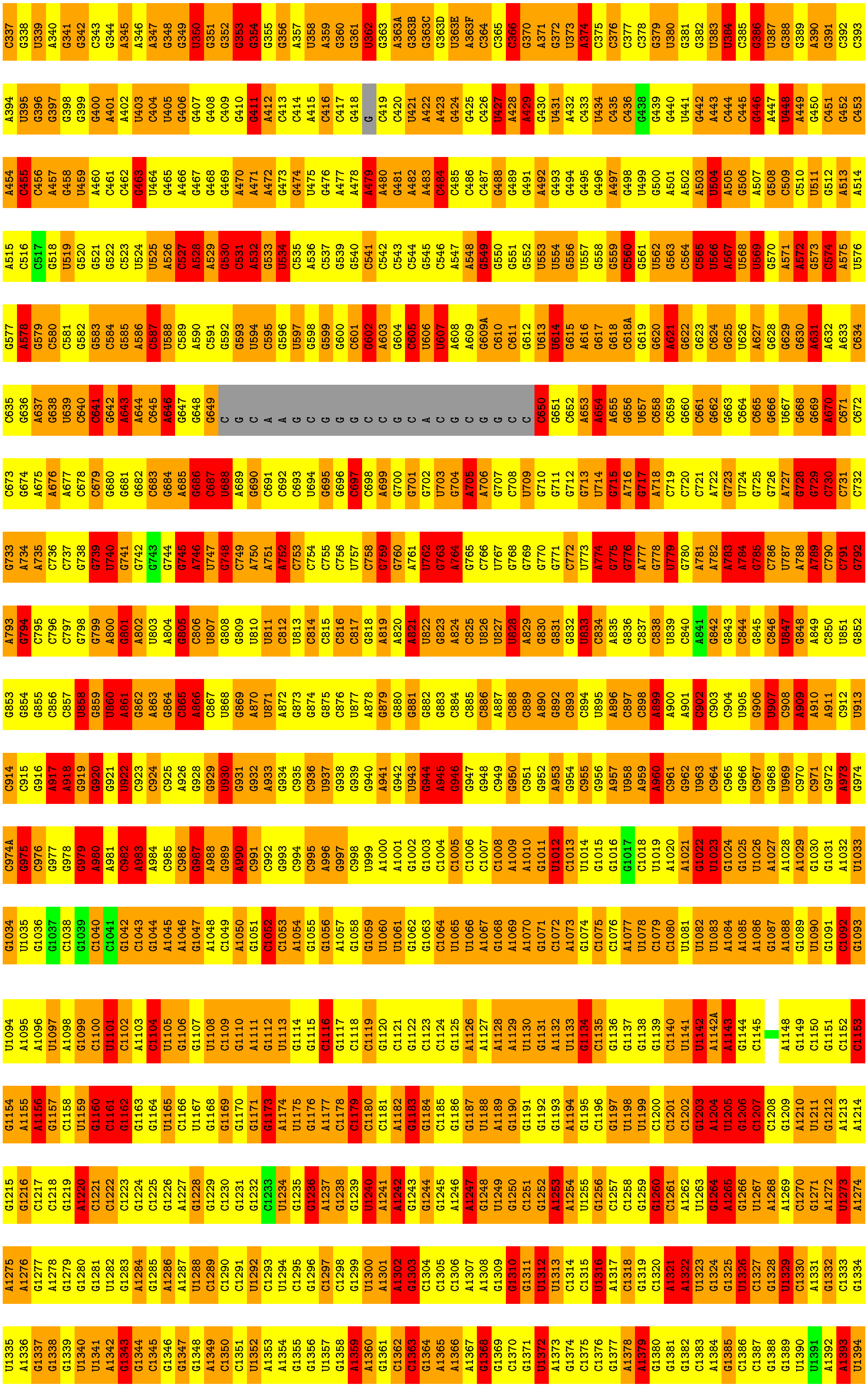
- Molecule 22: 30S ribosomal protein S20

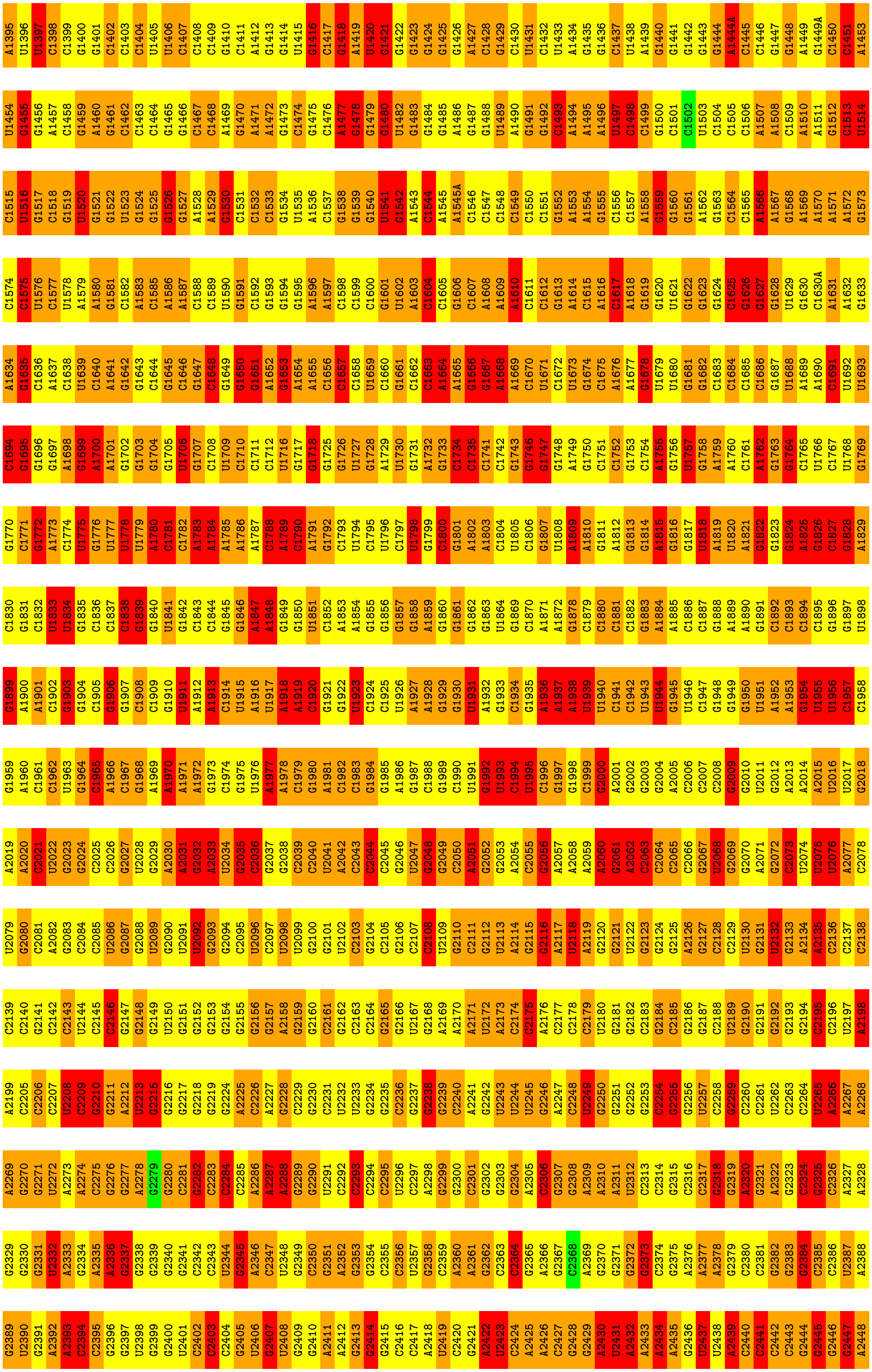


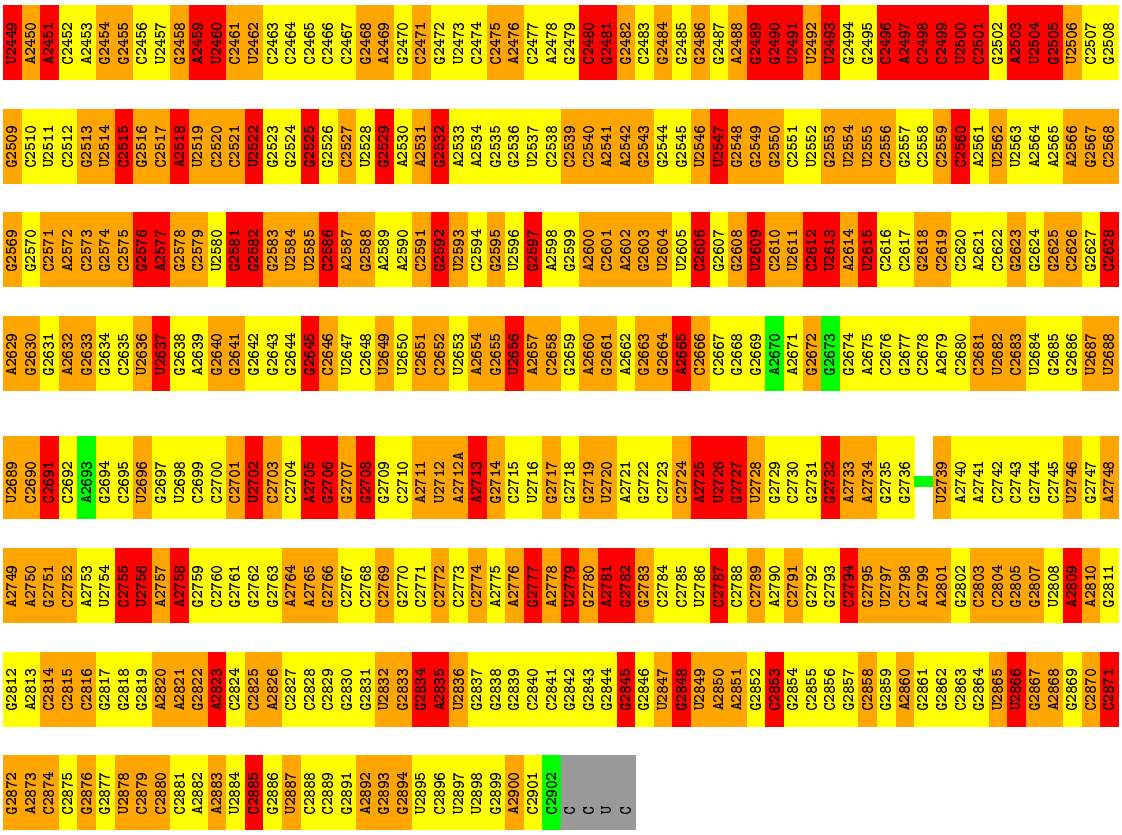
- Molecule 23: 30S ribosomal protein Thx

- Molecule 24: 23S ribosomal RNA



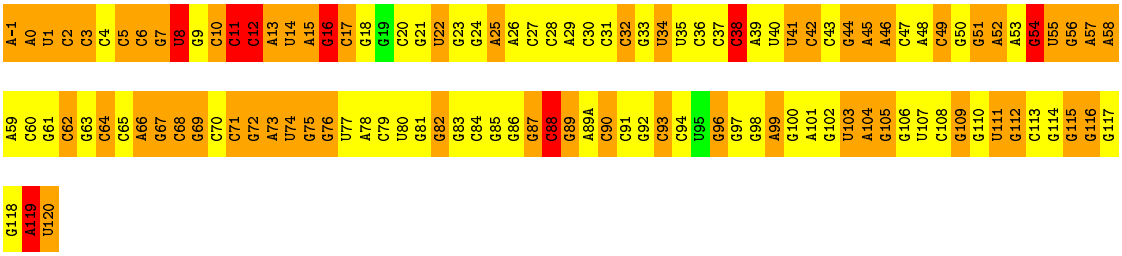

C337 G338 U339 A340 G341 G342 C343 G344 A345 A346 A347 G348 G349 U350 G351 G352 G353 G354 G355 G356 A357 U358 A359 G360 G361 U362 G363 A363A G363B G363C G363D U363E A363F C364 C365 C366 G370 A371 G372 U373 A374 C375 C376 C377 C378 G379 U380 G381 G382 U383 U384 C385 G386 U387 G388 G389 A390 G391 C392 C393
A394 U395 G396 G397 G398 G399 G400 A401 A402 U403 C404 U405 G406 G407 G408 C409 G410 G411 A412 C413 C414 A415 C416 C417 G418 G C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 A429 G430 U431 A432 C433 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 U476 A477 A478 A479 A480 G481 A482 A483 C484 C485 C486 C487 G488 G489 G490 G491 A492 G493 G494 G495 G496 A497 G498 U499 G500 A501 A502 A503 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514
A515 C516 C517 G518 U519 G520 G521 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 G540 C541 C542 C543 C544 G545 C546 A547 A548 G549 G550 G551 G552 U553 U554 G555 G556 U557 G558 G559 C560 G561 U562 G563 C564 C565 U566 A567 U568 U569 G570 A571 A572 G573 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 G611 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 G658 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 U694 G695 G696 C697 C698 A699 G700 G701 G702 U703 G704 A705 A706 G707 C708 U709 G710 G711 G712 G713 U714 G715 A716 G717 A718 C719 C720 C721 A722 G723 U724 G725 C726 A727 G728 G729 C730 C731 C732
G733 A734 A735 C736 C737 G738 G739 U740 G741 C742 G743 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C754 C755 C756 U757 C758 G759 G760 A761 U762 G763 A764 G765 C766 U767 G768 G769 G770 C771 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 A841 G842 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852
G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 U871 A872 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913
C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 C924 C925 A926 G928 G929 U930 G931 G932 A933 G934 C935 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951 G952 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 G994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033
G1034 U1035 G1036 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 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 G1091 C1092 G1093
U1094 A1095 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 G1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 G1134 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1145 A1148 G1149 C1150 G1151 C1152 C1153
G1154 A1155 A1156 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 G1193 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1212 A1213 A1214
G1215 G1216 C1217 C1218 G1219 A1220 C1221 C1222 C1223 G1224 C1225 G1226 A1227 G1228 G1229 C1230 G1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245 A1246 A1247 G1248 U1249 G1250 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 A1276 G1277 A1278 G1279 G1280 G1281 U1282 G1283 A1284 G1285 A1286 A1287 U1288 C1289 C1290 C1291 U1292 C1293 U1294 G1295 G1296 C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1304 C1305 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 G1320 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334
U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 G1346 G1347 G1348 A1349 C1350 C1351 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 G1373 G1374 C1375 C1376 G1377 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 C1387 G1388 G1389 U1390 U1391 A1392 A1393 U1394





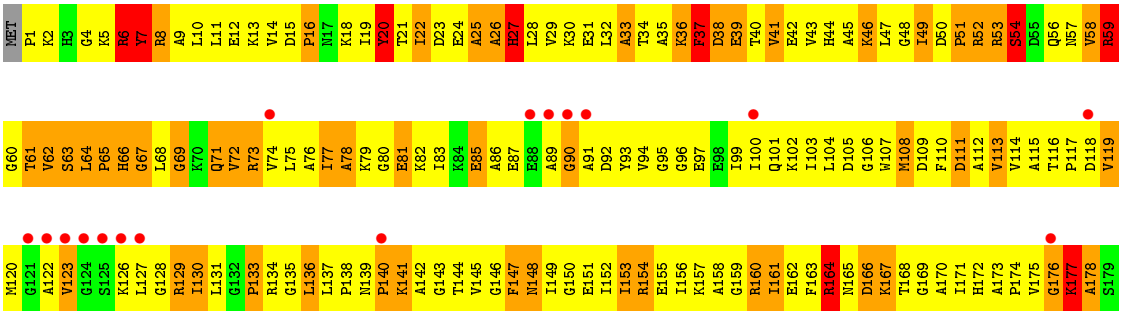
- Molecule 25: 5S ribosomal RNA

Chain BB:



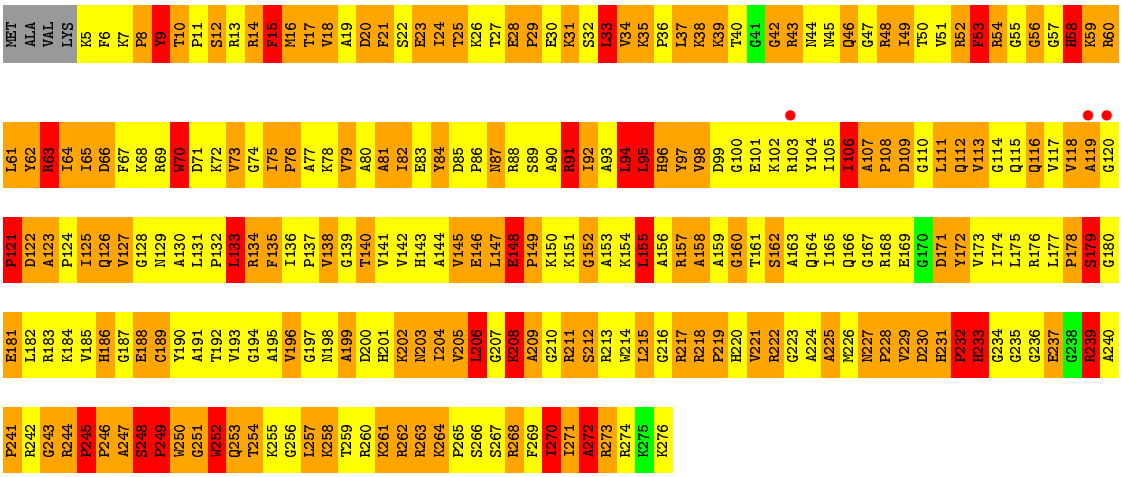
- Molecule 26: 50S ribosomal protein L1

Chain BC:



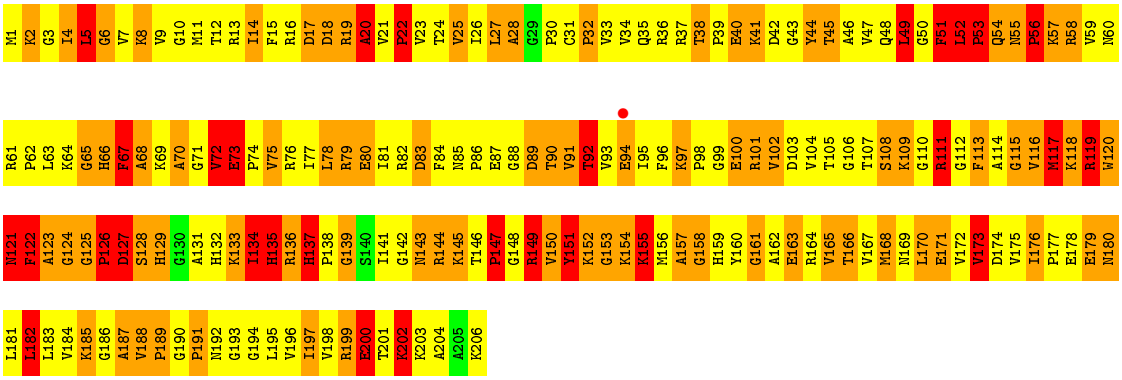
- Molecule 27: 50S ribosomal protein L2

Chain BD:



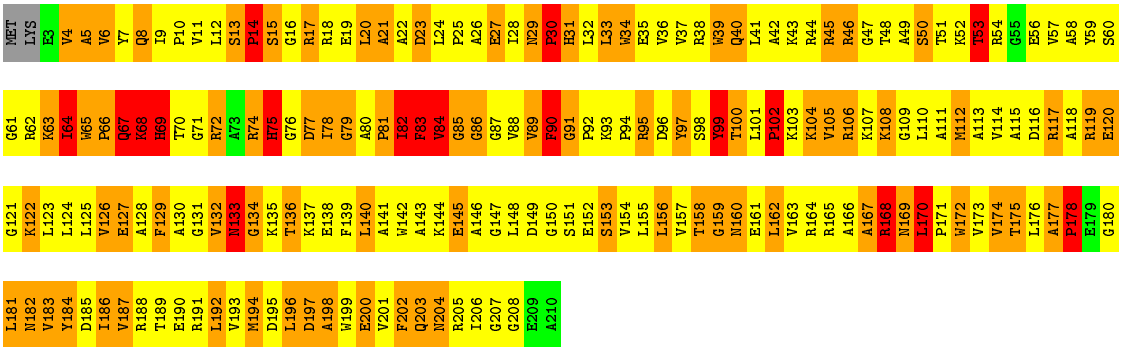
- Molecule 28: 50S ribosomal protein L3

Chain BE:



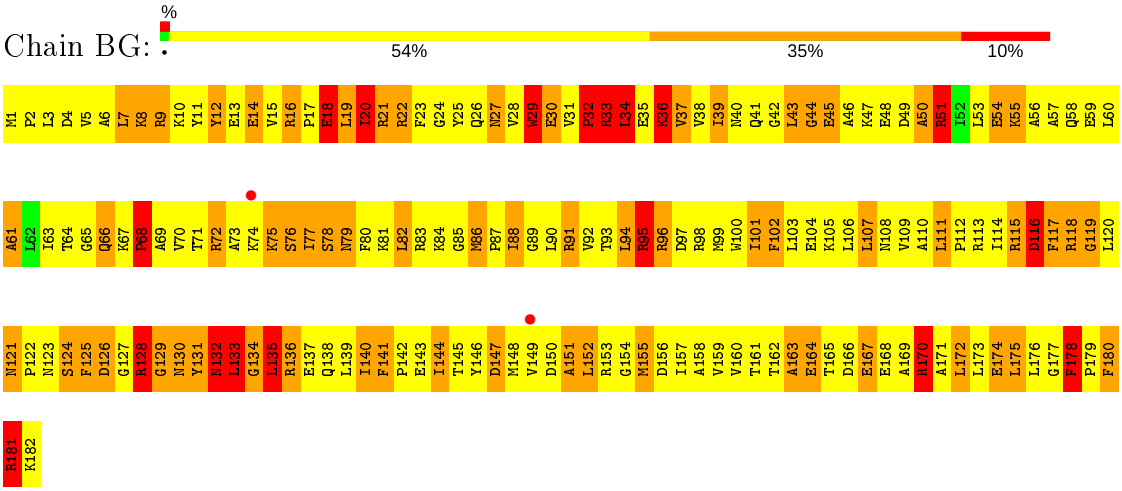
- Molecule 29: 50S ribosomal protein L4

Chain BF:



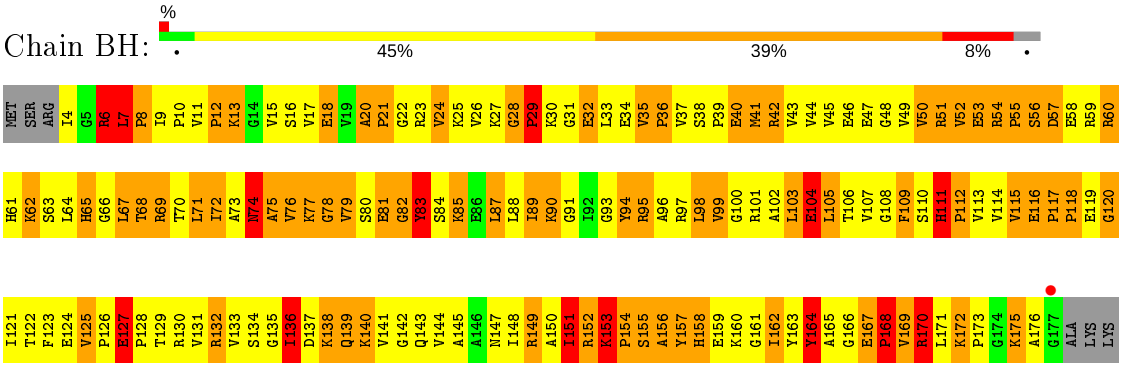
- Molecule 30: 50S ribosomal protein L5

Chain BG:



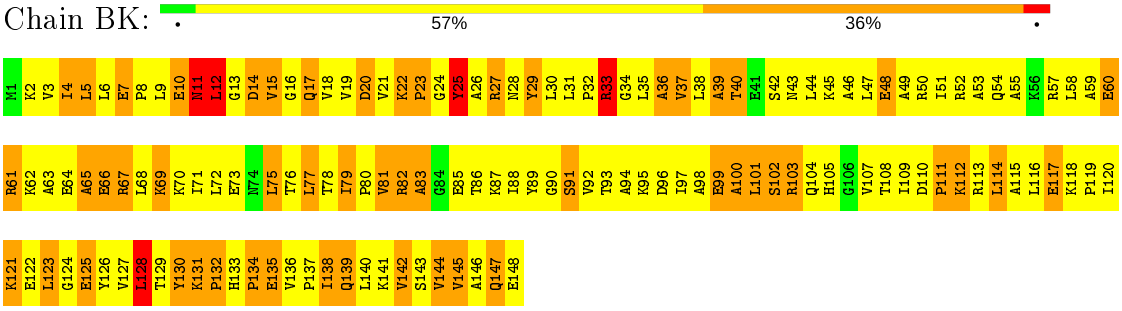
- Molecule 31: 50S ribosomal protein L6

Chain BH:



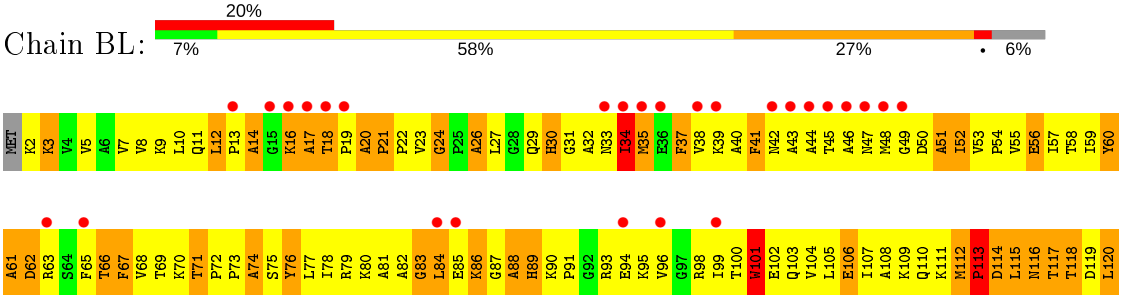
- Molecule 32: 50S ribosomal protein L9

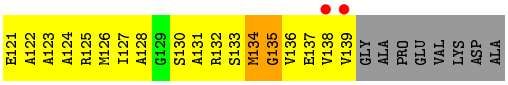
Chain BK:



- Molecule 33: 50S ribosomal protein L11

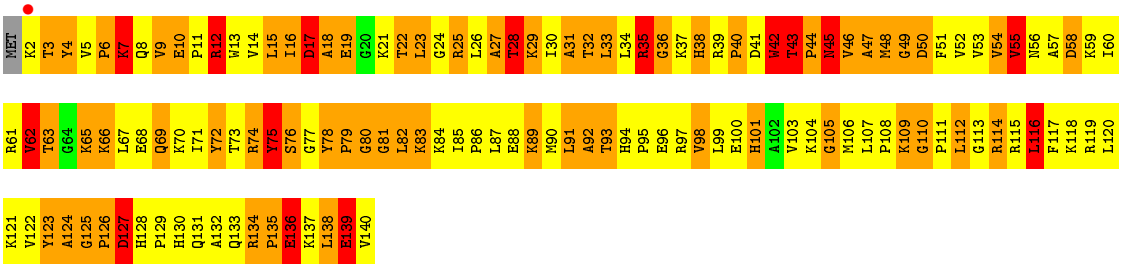
Chain BL:





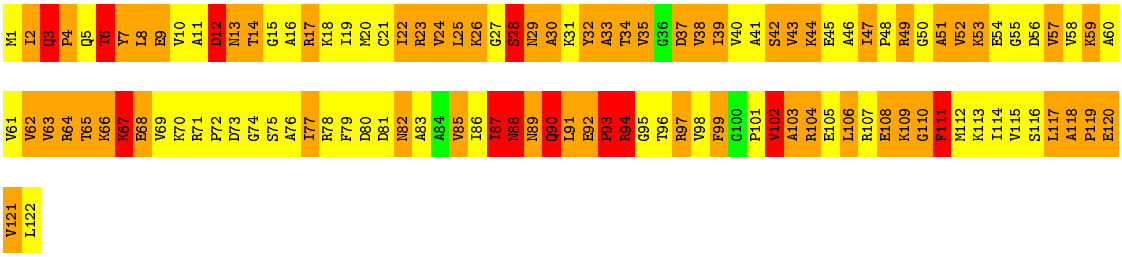
• Molecule 34: 50S ribosomal protein L13

Chain BM:



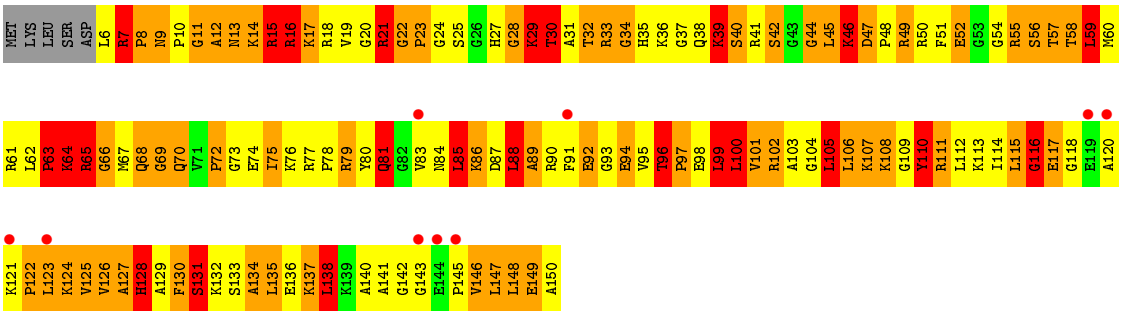
• Molecule 35: 50S ribosomal protein L14

Chain BN:



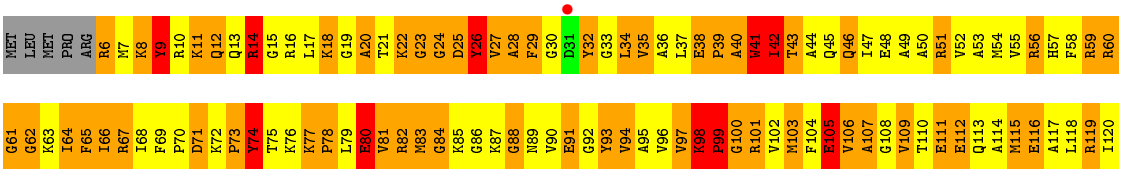
• Molecule 36: 50S ribosomal protein L15

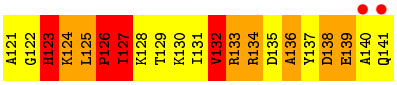
Chain BO:



• Molecule 37: 50S ribosomal protein L16

Chain BP:



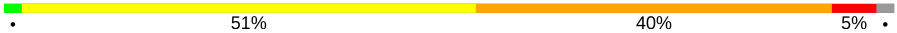


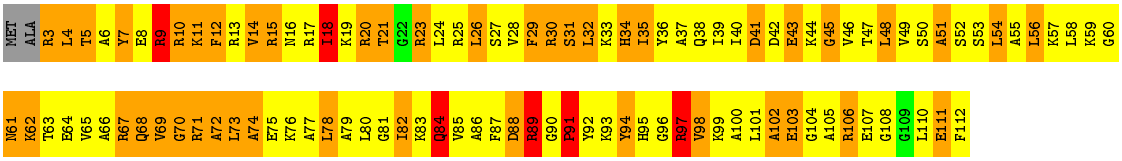
- Molecule 38: 50S ribosomal protein L17

Chain BQ:

- Molecule 39: 50S ribosomal protein L18

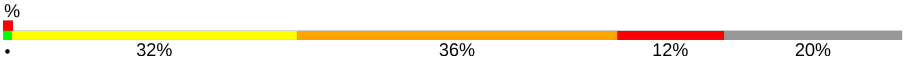
Chain BR:

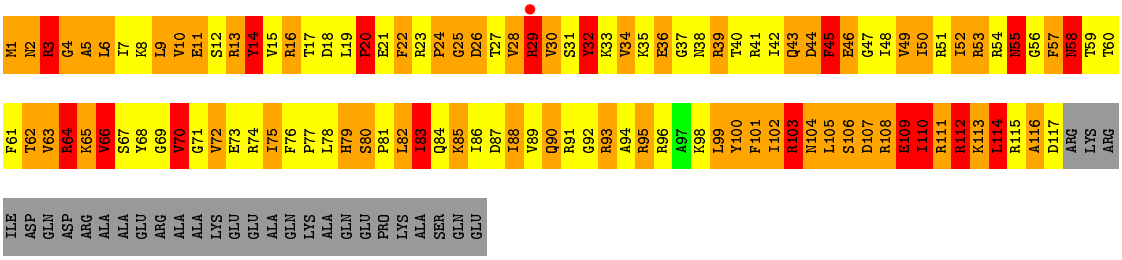




- Molecule 40: 50S ribosomal protein L19

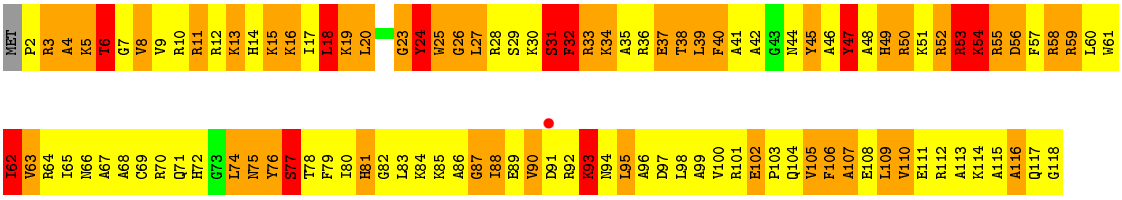
Chain BS:





- Molecule 41: 50S ribosomal protein L20

Chain BT:

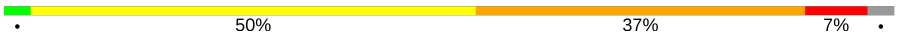


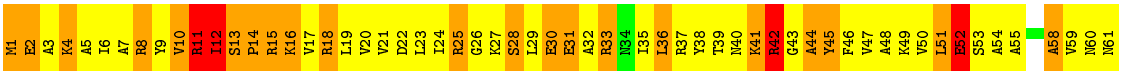
- Molecule 42: 50S ribosomal protein L21

Chain BU:

• Molecule 43: 50S ribosomal protein L22

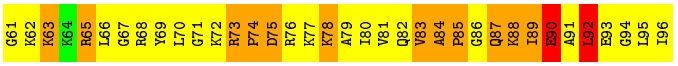
Chain BV:





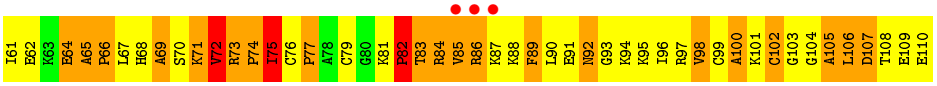
• Molecule 44: 50S ribosomal protein L23

Chain BW:



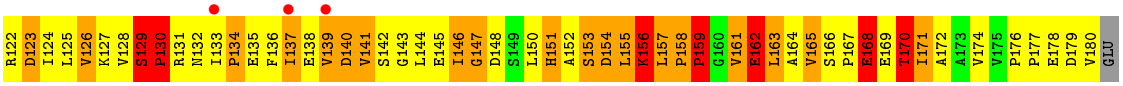
• Molecule 45: 50S ribosomal protein L24

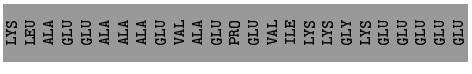
Chain BX:



• Molecule 46: 50S ribosomal protein L25

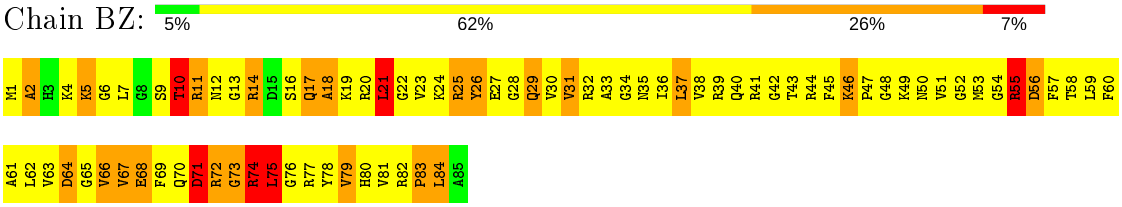
Chain BY:





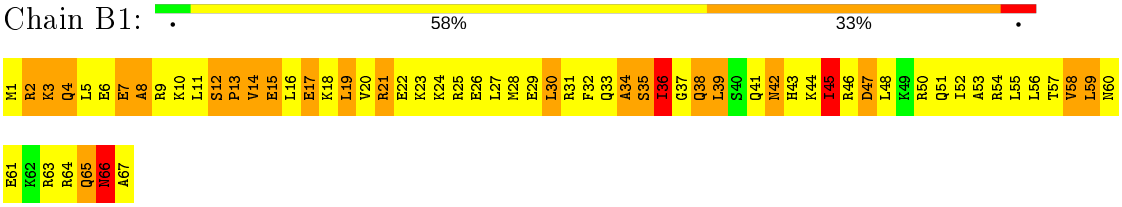
- Molecule 47: 50S ribosomal protein L27

Chain BZ:



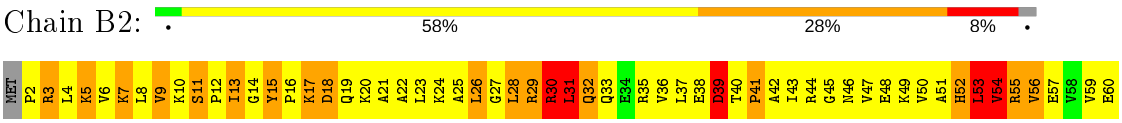
- Molecule 48: 50S ribosomal protein L29

Chain B1:



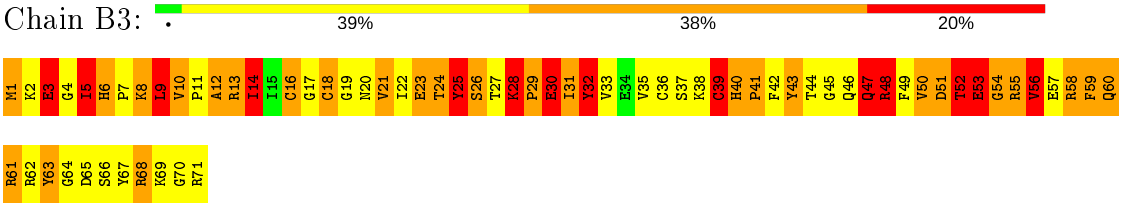
- Molecule 49: 50S ribosomal protein L30

Chain B2:



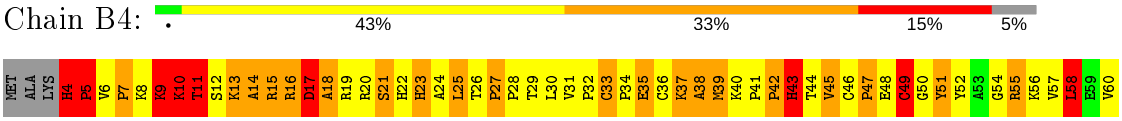
- Molecule 50: 50S ribosomal protein L31

Chain B3:



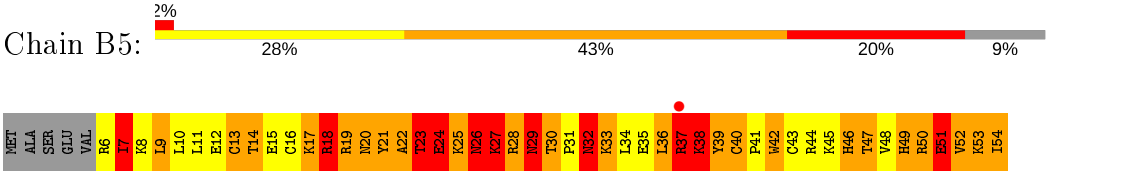
- Molecule 51: 50S ribosomal protein L32

Chain B4:



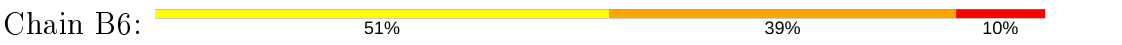
- Molecule 52: 50S ribosomal protein L33

Chain B5:



- Molecule 53: 50S ribosomal protein L34

Chain B6:

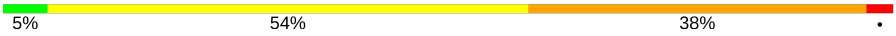


- Molecule 54: 50S ribosomal protein L35

Chain B7:

- Molecule 55: 50S ribosomal protein L36

Chain B8:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 430.52 – 4.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 96.7 (430.52-4.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.323 0.257 , 0.309	Depositor DCC
R_{free} test set	10840 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å^2)	99.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	149044	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.94	48/36438 (0.1%)	1.12	150/56869 (0.3%)
2	AC	1.00	1/1814 (0.1%)	0.92	3/2825 (0.1%)
3	AD	0.80	1/1813 (0.1%)	0.94	3/2823 (0.1%)
4	AE	0.65	0/1935	1.02	3/2609 (0.1%)
5	AF	0.55	0/1636	0.98	4/2205 (0.2%)
6	AG	0.68	1/1733 (0.1%)	1.07	5/2318 (0.2%)
7	AH	0.68	0/1162	1.06	2/1564 (0.1%)
8	AI	0.68	0/856	1.01	3/1154 (0.3%)
9	AJ	0.60	0/1276	0.90	0/1709
10	AK	0.68	0/1136	1.10	5/1527 (0.3%)
11	AL	0.54	0/1029	0.87	0/1379
12	AM	0.49	0/807	0.88	0/1085
13	AN	0.73	0/900	1.06	3/1213 (0.2%)
14	AO	0.67	0/986	1.12	6/1320 (0.5%)
15	AP	0.53	0/1008	0.90	2/1347 (0.1%)
16	AQ	0.57	0/501	1.01	1/664 (0.2%)
17	AR	0.71	0/745	1.00	1/992 (0.1%)
18	AS	0.72	0/716	1.05	3/963 (0.3%)
19	AT	0.73	0/870	1.07	2/1159 (0.2%)
20	AU	0.64	0/603	1.02	3/799 (0.4%)
21	AV	0.55	0/661	0.94	0/890
22	AW	0.77	0/765	1.03	1/1007 (0.1%)
23	AX	0.48	0/212	0.85	1/277 (0.4%)
24	BA	1.06	154/69685 (0.2%)	1.16	463/108786 (0.4%)
25	BB	0.86	4/2954 (0.1%)	1.01	8/4606 (0.2%)
26	BC	0.50	0/1775	0.89	2/2393 (0.1%)
27	BD	0.83	3/2174 (0.1%)	1.25	12/2927 (0.4%)
28	BE	0.86	2/1611 (0.1%)	1.29	13/2171 (0.6%)
29	BF	0.69	0/1660	1.11	8/2247 (0.4%)
30	BG	0.63	0/1507	1.05	4/2027 (0.2%)
31	BH	0.62	0/1354	1.06	5/1831 (0.3%)
32	BK	0.69	0/1170	1.08	2/1581 (0.1%)
33	BL	0.49	0/1044	0.90	1/1415 (0.1%)
34	BM	0.83	1/1140 (0.1%)	1.19	8/1537 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	BN	1.00	0/942	1.39	8/1268 (0.6%)
36	BO	0.79	0/1123	1.27	15/1493 (1.0%)
37	BP	0.85	1/1100 (0.1%)	1.27	6/1470 (0.4%)
38	BQ	0.69	0/974	1.08	2/1302 (0.2%)
39	BR	0.78	0/887	1.11	2/1180 (0.2%)
40	BS	0.95	0/990	1.44	13/1325 (1.0%)
41	BT	0.79	0/982	1.18	6/1306 (0.5%)
42	BU	0.90	1/790 (0.1%)	1.44	11/1057 (1.0%)
43	BV	0.78	0/886	1.11	2/1189 (0.2%)
44	BW	0.57	0/756	0.91	0/1015
45	BX	0.53	0/857	1.09	4/1142 (0.4%)
46	BY	0.66	0/1467	1.13	6/1992 (0.3%)
47	BZ	0.72	0/679	1.11	2/902 (0.2%)
48	B1	0.64	0/569	0.91	0/751
49	B2	0.63	0/474	1.08	1/635 (0.2%)
50	B3	1.00	2/594 (0.3%)	1.37	8/795 (1.0%)
51	B4	0.74	1/459 (0.2%)	1.12	2/621 (0.3%)
52	B5	0.91	0/433	1.61	7/576 (1.2%)
53	B6	0.81	0/438	1.03	1/575 (0.2%)
54	B7	0.70	0/523	1.23	3/690 (0.4%)
55	B8	0.69	0/310	1.19	2/407 (0.5%)
All	All	0.93	220/161909 (0.1%)	1.13	828/241910 (0.3%)

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	AA	0	217
2	AC	0	13
3	AD	0	7
5	AF	0	1
10	AK	0	1
13	AN	0	1
24	BA	0	546
25	BB	0	16
27	BD	0	2
28	BE	0	1
29	BF	0	1
31	BH	0	1
37	BP	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	BS	0	2
42	BU	0	2
43	BV	0	1
44	BW	0	1
50	B3	0	2
All	All	0	818

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1203	G	O3'-P	-34.70	1.19	1.61
24	BA	607	U	N3-C4	-31.59	1.10	1.38
24	BA	2501	C	O3'-P	24.61	1.90	1.61
24	BA	607	U	C2-N3	-22.10	1.22	1.37
1	AA	173	U	O3'-P	19.93	1.85	1.61

The worst 5 of 828 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1064	G	N1-C2-N2	-70.70	52.57	116.20
1	AA	1064	G	N3-C2-N2	58.69	160.98	119.90
24	BA	607	U	N3-C4-O4	-29.32	98.87	119.40
24	BA	1203	G	P-O3'-C3'	27.75	153.00	119.70
1	AA	1064	G	N1-C2-N3	-25.80	108.42	123.90

There are no chirality outliers.

5 of 818 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	21	G	Sidechain
1	AA	24	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32554	0	16429	6468	0
2	AC	1624	0	826	363	0
3	AD	1623	0	821	385	0
4	AE	1900	0	1951	934	0
5	AF	1612	0	1677	695	0
6	AG	1703	0	1763	800	0
7	AH	1146	0	1207	493	0
8	AI	843	0	857	370	0
9	AJ	1257	0	1296	561	0
10	AK	1116	0	1177	644	0
11	AL	1010	0	1037	460	0
12	AM	794	0	840	363	0
13	AN	885	0	904	407	0
14	AO	970	0	1057	440	0
15	AP	997	0	1072	511	0
16	AQ	492	0	529	255	0
17	AR	734	0	771	300	0
18	AS	700	0	720	308	0
19	AT	857	0	930	415	0
20	AU	597	0	668	331	0
21	AV	647	0	673	300	0
22	AW	763	0	861	356	0
23	AX	208	0	221	83	0
24	BA	62218	0	31353	15020	0
25	BB	2641	0	1337	589	1
26	BC	1742	0	1796	854	0
27	BD	2124	0	2207	1514	0
28	BE	1578	0	1647	1071	0
29	BF	1625	0	1666	891	0
30	BG	1482	0	1546	966	0
31	BH	1328	0	1408	737	0
32	BK	1155	0	1244	550	0
33	BL	1025	0	1074	489	0
34	BM	1113	0	1183	765	0
35	BN	932	0	994	688	0
36	BO	1106	0	1183	834	0
37	BP	1080	0	1127	704	0
38	BQ	960	0	1021	511	0
39	BR	877	0	938	586	0
40	BS	976	0	1033	667	0
41	BT	964	0	1022	665	0
42	BU	779	0	852	580	0
43	BV	876	0	941	448	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BW	742	0	800	376	0
45	BX	844	0	930	504	0
46	BY	1435	0	1463	735	0
47	BZ	670	0	700	371	0
48	B1	567	0	621	314	0
49	B2	469	0	518	304	0
50	B3	581	0	577	360	0
51	B4	445	0	459	296	0
52	B5	426	0	452	291	0
53	B6	430	0	480	261	0
54	B7	515	0	587	388	0
55	B8	307	0	335	148	0
All	All	149044	0	101781	45453	1

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 182.

The worst 5 of 45453 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)
46:BY:27:VAL:HG23	46:BY:85:HIS:CE1	1.45	1.50
46:BY:27:VAL:CG2	46:BY:85:HIS:CE1	1.95	1.45
35:BN:64:ARG:HH11	35:BN:68:GLU:N	1.15	1.44
24:BA:775:G:H2'	24:BA:794:G:C8	1.54	1.42
24:BA:1201:C:N4	24:BA:1241:A:H61	1.15	1.39

All (1) 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)
25:BB:-1:A:O2'	25:BB:-1:A:O2'[15_545]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	AE	232/256 (91%)	119 (51%)	48 (21%)	65 (28%)	0	0
5	AF	204/239 (85%)	117 (57%)	41 (20%)	46 (22%)	0	1
6	AG	206/209 (99%)	99 (48%)	52 (25%)	55 (27%)	0	0
7	AH	148/162 (91%)	89 (60%)	26 (18%)	33 (22%)	0	1
8	AI	99/101 (98%)	62 (63%)	14 (14%)	23 (23%)	0	1
9	AJ	153/156 (98%)	65 (42%)	45 (29%)	43 (28%)	0	0
10	AK	136/138 (99%)	71 (52%)	28 (21%)	37 (27%)	0	0
11	AL	125/128 (98%)	57 (46%)	38 (30%)	30 (24%)	0	1
12	AM	96/105 (91%)	53 (55%)	21 (22%)	22 (23%)	0	1
13	AN	117/129 (91%)	63 (54%)	28 (24%)	26 (22%)	0	1
14	AO	122/132 (92%)	60 (49%)	29 (24%)	33 (27%)	0	0
15	AP	123/126 (98%)	64 (52%)	33 (27%)	26 (21%)	0	2
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	43 (50%)	26 (30%)	17 (20%)	0	2
18	AS	81/88 (92%)	46 (57%)	22 (27%)	13 (16%)	0	3
19	AT	102/105 (97%)	63 (62%)	20 (20%)	19 (19%)	0	2
20	AU	71/88 (81%)	29 (41%)	23 (32%)	19 (27%)	0	0
21	AV	78/93 (84%)	32 (41%)	24 (31%)	22 (28%)	0	0
22	AW	97/106 (92%)	31 (32%)	43 (44%)	23 (24%)	0	1
23	AX	22/27 (82%)	11 (50%)	5 (23%)	6 (27%)	0	0
26	BC	226/229 (99%)	110 (49%)	62 (27%)	54 (24%)	0	1
27	BD	270/276 (98%)	110 (41%)	66 (24%)	94 (35%)	0	0
28	BE	204/206 (99%)	108 (53%)	40 (20%)	56 (28%)	0	0
29	BF	206/210 (98%)	106 (52%)	45 (22%)	55 (27%)	0	0
30	BG	180/182 (99%)	71 (39%)	52 (29%)	57 (32%)	0	0
31	BH	172/180 (96%)	75 (44%)	50 (29%)	47 (27%)	0	0
32	BK	146/148 (99%)	85 (58%)	36 (25%)	25 (17%)	0	3
33	BL	136/147 (92%)	68 (50%)	38 (28%)	30 (22%)	0	1
34	BM	137/140 (98%)	63 (46%)	28 (20%)	46 (34%)	0	0
35	BN	120/122 (98%)	60 (50%)	24 (20%)	36 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	143/150 (95%)	52 (36%)	40 (28%)	51 (36%)	0	0
37	BP	134/141 (95%)	53 (40%)	36 (27%)	45 (34%)	0	0
38	BQ	115/118 (98%)	60 (52%)	37 (32%)	18 (16%)	0	4
39	BR	108/112 (96%)	43 (40%)	35 (32%)	30 (28%)	0	0
40	BS	115/146 (79%)	55 (48%)	27 (24%)	33 (29%)	0	0
41	BT	115/118 (98%)	46 (40%)	40 (35%)	29 (25%)	0	1
42	BU	99/101 (98%)	53 (54%)	19 (19%)	27 (27%)	0	0
43	BV	108/113 (96%)	64 (59%)	20 (18%)	24 (22%)	0	1
44	BW	92/96 (96%)	53 (58%)	18 (20%)	21 (23%)	0	1
45	BX	108/110 (98%)	39 (36%)	34 (32%)	35 (32%)	0	0
46	BY	178/206 (86%)	85 (48%)	50 (28%)	43 (24%)	0	1
47	BZ	83/85 (98%)	48 (58%)	20 (24%)	15 (18%)	0	2
48	B1	65/67 (97%)	30 (46%)	20 (31%)	15 (23%)	0	1
49	B2	57/60 (95%)	33 (58%)	12 (21%)	12 (21%)	0	2
50	B3	69/71 (97%)	20 (29%)	23 (33%)	26 (38%)	0	0
51	B4	55/60 (92%)	14 (26%)	22 (40%)	19 (34%)	0	0
52	B5	47/54 (87%)	15 (32%)	8 (17%)	24 (51%)	0	0
53	B6	47/49 (96%)	18 (38%)	14 (30%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	21 (60%)	6 (17%)	8 (23%)	0	1
All	All	5988/6337 (94%)	2879 (48%)	1522 (25%)	1587 (26%)	0	1

5 of 1587 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	13	ALA
4	AE	15	VAL
4	AE	17	PHE
4	AE	20	GLU
4	AE	42	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
4	AE	202/220 (92%)	142 (70%)	60 (30%)	0 2
5	AF	160/188 (85%)	122 (76%)	38 (24%)	0 5
6	AG	180/181 (99%)	130 (72%)	50 (28%)	0 3
7	AH	115/123 (94%)	70 (61%)	45 (39%)	0 0
8	AI	90/90 (100%)	59 (66%)	31 (34%)	0 1
9	AJ	126/127 (99%)	97 (77%)	29 (23%)	1 5
10	AK	119/119 (100%)	76 (64%)	43 (36%)	0 1
11	AL	98/99 (99%)	74 (76%)	24 (24%)	0 4
12	AM	88/92 (96%)	61 (69%)	27 (31%)	0 2
13	AN	90/99 (91%)	70 (78%)	20 (22%)	1 6
14	AO	104/109 (95%)	79 (76%)	25 (24%)	0 5
15	AP	100/101 (99%)	73 (73%)	27 (27%)	0 3
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	0 4
17	AR	79/80 (99%)	56 (71%)	23 (29%)	0 3
18	AS	72/74 (97%)	45 (62%)	27 (38%)	0 1
19	AT	96/97 (99%)	69 (72%)	27 (28%)	0 3
20	AU	64/77 (83%)	50 (78%)	14 (22%)	1 6
21	AV	71/80 (89%)	57 (80%)	14 (20%)	1 8
22	AW	76/82 (93%)	57 (75%)	19 (25%)	0 4
23	AX	19/22 (86%)	16 (84%)	3 (16%)	2 15
26	BC	180/181 (99%)	145 (81%)	35 (19%)	1 9
27	BD	215/218 (99%)	146 (68%)	69 (32%)	0 2
28	BE	166/166 (100%)	95 (57%)	71 (43%)	0 0
29	BF	164/166 (99%)	106 (65%)	58 (35%)	0 1
30	BG	156/156 (100%)	113 (72%)	43 (28%)	0 3
31	BH	143/148 (97%)	91 (64%)	52 (36%)	0 1
32	BK	124/124 (100%)	88 (71%)	36 (29%)	0 3
33	BL	105/111 (95%)	86 (82%)	19 (18%)	1 11
34	BM	118/119 (99%)	82 (70%)	36 (30%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BN	100/100 (100%)	60 (60%)	40 (40%)	0	0
36	BO	111/116 (96%)	66 (60%)	45 (40%)	0	0
37	BP	106/111 (96%)	68 (64%)	38 (36%)	0	1
38	BQ	100/101 (99%)	73 (73%)	27 (27%)	0	3
39	BR	87/88 (99%)	61 (70%)	26 (30%)	0	2
40	BS	105/127 (83%)	65 (62%)	40 (38%)	0	1
41	BT	93/94 (99%)	61 (66%)	32 (34%)	0	1
42	BU	82/82 (100%)	55 (67%)	27 (33%)	0	2
43	BV	90/92 (98%)	56 (62%)	34 (38%)	0	1
44	BW	76/78 (97%)	59 (78%)	17 (22%)	1	6
45	BX	91/91 (100%)	71 (78%)	20 (22%)	1	6
46	BY	159/179 (89%)	107 (67%)	52 (33%)	0	2
47	BZ	67/67 (100%)	49 (73%)	18 (27%)	0	3
48	B1	62/62 (100%)	49 (79%)	13 (21%)	1	7
49	B2	51/52 (98%)	37 (72%)	14 (28%)	0	3
50	B3	63/63 (100%)	42 (67%)	21 (33%)	0	2
51	B4	50/52 (96%)	33 (66%)	17 (34%)	0	1
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	2
54	B7	54/55 (98%)	39 (72%)	15 (28%)	0	3
55	B8	34/34 (100%)	25 (74%)	9 (26%)	0	4
All	All	5040/5237 (96%)	3528 (70%)	1512 (30%)	0	2

5 of 1512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BE	57	LYS
31	BH	52	VAL
48	B1	7	GLU
28	BE	119	ARG
29	BF	119	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 190 such sidechains are listed below:

Mol	Chain	Res	Type
26	BC	56	GLN
29	BF	169	ASN
50	B3	20	ASN
26	BC	225	ASN
28	BE	54	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	430 (28%)	157 (10%)
2	AC	75/77 (97%)	29 (38%)	6 (8%)
24	BA	2888/2916 (99%)	1218 (42%)	265 (9%)
25	BB	122/123 (99%)	49 (40%)	4 (3%)
3	AD	75/76 (98%)	27 (36%)	4 (5%)
All	All	4675/4714 (99%)	1753 (37%)	436 (9%)

5 of 1753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 436 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	350	U
24	BA	776	G
24	BA	2491	U
24	BA	442	G
24	BA	620	G

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	BA	4
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2501:C	O3'	2502:G	P	1.90
1	AA	173:U	O3'	174:C	P	1.85
1	BA	2446:G	O3'	2447:G	P	1.40
1	BA	2499:C	O3'	2500:U	P	1.38
1	BA	1203:G	O3'	1204:A	P	1.19

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, 95^{th} 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%)	-0.53	3 (0%) 95 93	88, 158, 260, 350	0
2	AC	76/77 (98%)	-0.55	0 100 100	133, 166, 216, 249	0
3	AD	76/76 (100%)	-0.37	0 100 100	219, 265, 316, 334	0
4	AE	234/256 (91%)	-0.08	10 (4%) 35 30	122, 163, 221, 265	0
5	AF	206/239 (86%)	-0.08	4 (1%) 66 58	143, 182, 210, 228	0
6	AG	208/209 (99%)	-0.76	0 100 100	106, 148, 170, 187	0
7	AH	150/162 (92%)	-0.39	0 100 100	114, 139, 171, 200	0
8	AI	101/101 (100%)	0.17	2 (1%) 65 56	121, 150, 168, 203	0
9	AJ	155/156 (99%)	-0.08	0 100 100	155, 180, 208, 214	0
10	AK	138/138 (100%)	-0.67	0 100 100	113, 133, 153, 160	0
11	AL	127/128 (99%)	-0.26	1 (0%) 86 79	161, 225, 247, 255	0
12	AM	98/105 (93%)	0.51	14 (14%) 2 3	146, 208, 237, 240	0
13	AN	119/129 (92%)	-0.30	0 100 100	114, 142, 176, 206	0
14	AO	124/132 (93%)	-0.17	0 100 100	96, 129, 162, 184	0
15	AP	125/126 (99%)	-0.52	0 100 100	167, 194, 223, 230	0
16	AQ	60/61 (98%)	-0.46	0 100 100	163, 188, 203, 206	0
17	AR	88/89 (98%)	-0.73	0 100 100	113, 131, 168, 183	0
18	AS	83/88 (94%)	-0.93	0 100 100	104, 128, 155, 185	0
19	AT	104/105 (99%)	-0.75	0 100 100	98, 126, 169, 215	0
20	AU	73/88 (82%)	-0.39	4 (5%) 25 22	109, 136, 190, 224	0
21	AV	80/93 (86%)	0.16	1 (1%) 77 68	175, 198, 217, 222	0
22	AW	99/106 (93%)	-0.63	0 100 100	105, 134, 163, 166	0
23	AX	24/27 (88%)	-0.85	0 100 100	168, 210, 224, 229	0
24	BA	2889/2916 (99%)	-0.53	0 100 100	63, 155, 266, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	BB	123/123 (100%)	-0.46	0 100 100	146, 209, 257, 291	0
26	BC	228/229 (99%)	0.19	16 (7%) 16 13	220, 256, 308, 312	0
27	BD	272/276 (98%)	-0.04	3 (1%) 80 72	80, 125, 153, 198	0
28	BE	206/206 (100%)	-0.39	1 (0%) 91 85	69, 117, 172, 224	0
29	BF	208/210 (99%)	-0.45	0 100 100	111, 179, 215, 231	0
30	BG	182/182 (100%)	-0.34	2 (1%) 80 72	160, 198, 226, 240	0
31	BH	174/180 (96%)	-0.33	1 (0%) 89 83	146, 186, 216, 238	0
32	BK	148/148 (100%)	-0.47	0 100 100	135, 161, 188, 190	0
33	BL	138/147 (93%)	0.90	29 (21%) 1 1	277, 307, 330, 334	0
34	BM	139/140 (99%)	-0.46	1 (0%) 87 82	107, 133, 167, 183	0
35	BN	122/122 (100%)	-0.33	0 100 100	78, 106, 140, 154	0
36	BO	145/150 (96%)	-0.02	9 (6%) 20 17	106, 190, 227, 239	0
37	BP	136/141 (96%)	-0.17	3 (2%) 62 52	109, 141, 173, 186	0
38	BQ	117/118 (99%)	-0.50	0 100 100	91, 124, 157, 173	0
39	BR	110/112 (98%)	-0.70	0 100 100	152, 183, 210, 248	0
40	BS	117/146 (80%)	-0.17	1 (0%) 84 77	83, 127, 165, 184	0
41	BT	117/118 (99%)	-0.42	1 (0%) 84 77	100, 138, 152, 158	0
42	BU	101/101 (100%)	0.27	6 (5%) 22 19	104, 160, 186, 197	0
43	BV	110/113 (97%)	-0.42	0 100 100	110, 143, 179, 195	0
44	BW	94/96 (97%)	-0.34	0 100 100	153, 170, 232, 237	0
45	BX	110/110 (100%)	-0.25	3 (2%) 54 45	157, 199, 247, 273	0
46	BY	180/206 (87%)	0.31	4 (2%) 62 52	142, 190, 211, 226	0
47	BZ	85/85 (100%)	-0.67	0 100 100	139, 166, 181, 197	0
48	B1	67/67 (100%)	-0.21	0 100 100	172, 186, 199, 209	0
49	B2	59/60 (98%)	-0.38	0 100 100	127, 163, 188, 202	0
50	B3	71/71 (100%)	-0.71	0 100 100	127, 160, 176, 185	0
51	B4	57/60 (95%)	-0.49	0 100 100	96, 147, 217, 241	0
52	B5	49/54 (90%)	-0.22	1 (2%) 65 56	141, 163, 183, 198	0
53	B6	49/49 (100%)	-0.42	0 100 100	87, 145, 164, 188	0
54	B7	64/65 (98%)	-0.47	0 100 100	113, 131, 153, 165	0
55	B8	37/37 (100%)	-0.82	0 100 100	146, 157, 169, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	10767/11051 (97%)	-0.38	120 (1%)	80	72	63, 160, 260, 350	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	BH	177	GLY	6.3
33	BL	17	ALA	5.5
4	AE	231	GLU	4.8
12	AM	81	THR	4.3
26	BC	126	LYS	4.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.