



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 4KZZ / pdb_00004kzz
Title : Rabbit 40S ribosomal subunit in complex with mRNA, initiator tRNA and eIF1A
Authors : Lomakin, I.B.; Steitz, T.A.
Deposited on : 2013-05-30
Resolution : 7.03 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

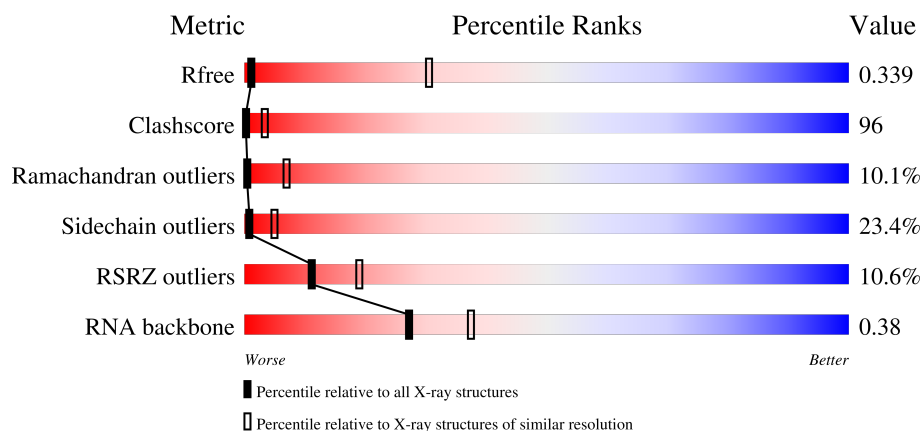
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.03 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}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)
RNA backbone	3983	1056 (10.00-3.10)

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 $\leq 5\%$. 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	A	295	
2	B	264	
3	C	278	
4	D	243	

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Mol	Chain	Length	Quality of chain
5	E	263	
6	F	204	
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	K	165	
12	L	158	
13	M	132	
14	N	151	
15	O	151	
16	P	145	
17	Q	146	
18	R	135	
19	S	152	
20	T	145	
21	U	119	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	Z	125	
27	a	115	
28	b	84	
29	c	69	

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Mol	Chain	Length	Quality of chain
30	d	56	
31	e	133	
32	f	156	
33	g	317	
34	i	1863	
35	j	75	
36	k	24	
37	n	144	

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 79048 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 protein called 40S Ribosomal Protein SA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1642	1045	289	300	8			

- Molecule 2 is a protein called 40S Ribosomal Protein S3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1741	1107	309	310	15			

- Molecule 3 is a protein called 40S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1742	1127	300	306	9			

- Molecule 4 is a protein called 40S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	0	0	0
			1764	1124	317	315	8			

- Molecule 5 is a protein called 40S Ribosomal Protein S4X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	263	Total	C	N	O	S	0	0	0
			2083	1329	385	359	10			

- Molecule 6 is a protein called 40S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			

- Molecule 7 is a protein called 40S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

- Molecule 8 is a protein called 40S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	190	Total	C	N	O	S	0	0	0
			1530	975	281	273	1			

- Molecule 9 is a protein called 40S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	206	Total	C	N	O	S	0	0	0
			1679	1054	329	291	5			

- Molecule 10 is a protein called 40S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	182	Total	C	N	O	S	0	0	0
			1498	952	300	244	2			

- Molecule 11 is a protein called 40S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			

- Molecule 12 is a protein called 40S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	158	Total	C	N	O	S	0	0	0
			1296	827	241	221	7			

- Molecule 13 is a protein called 40S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	124	Total	C	N	O	S	0	0	0
			950	594	169	179	8			

- Molecule 14 is a protein called 40S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			

- Molecule 15 is a protein called 40S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	136	Total	C	N	O	S	0	0	0
			1016	621	199	190	6			

- Molecule 16 is a protein called 40S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	127	Total	C	N	O	S	0	0	0
			1060	673	201	179	7			

- Molecule 17 is a protein called 40S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	141	Total	C	N	O	S	0	0	0
			1124	715	212	194	3			

- Molecule 18 is a protein called 40S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	126	Total	C	N	O	S	0	0	0
			1019	639	188	187	5			

- Molecule 19 is a protein called 40S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	137	Total	C	N	O	S	0	0	0
			1139	714	231	193	1			

- Molecule 20 is a protein called 40S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	141	Total	C	N	O	S	0	0	0
			1112	701	213	195	3			

- Molecule 21 is a protein called 40S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	104	Total	C	N	O	S	0	0	0
			822	514	156	148	4			

- Molecule 22 is a protein called 40S Ribosomal Protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	82	Total	C	N	O	S	0	0	0
			619	378	117	119	5			

- Molecule 23 is a protein called 40S Ribosomal Protein S15A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			

- Molecule 24 is a protein called 40S Ribosomal Protein S23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	142	Total	C	N	O	S	0	0	0
			1106	698	220	184	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	ALA	SEE REMARK 999	UNP G1SZ47

- Molecule 25 is a protein called 40S Ribosomal Protein S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	126	Total	C	N	O	S	0	0	0
			1021	645	198	173	5			

- Molecule 26 is a protein called 40S Ribosomal Protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			

- Molecule 27 is a protein called 40S Ribosomal Protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	a	107	Total	C	N	O	S	0	0	0
			844	527	173	138	6			

- Molecule 28 is a protein called 40S Ribosomal Protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	b	84	Total	C	N	O	S	0	0	0
			659	413	122	116	8			

- Molecule 29 is a protein called 40S Ribosomal Protein S28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	c	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			

- Molecule 30 is a protein called 40S Ribosomal Protein S29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	d	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			

- Molecule 31 is a protein called 40S Ribosomal Protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	e	59	Total	C	N	O	S	0	0	0
			473	293	104	75	1			

- Molecule 32 is a protein called 40S Ribosomal Protein S27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	f	71	Total	C	N	O	S	0	0	0
			581	367	109	98	7			

- Molecule 33 is a protein called 40S Ribosomal Protein RACK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	g	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			

- Molecule 34 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	i	1797	Total	C	N	O	P	0	0	0
			37514	16712	6634	12372	1796			

- Molecule 35 is a RNA chain called initiator Met-RNA-i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	j	75	Total	C	N	O	P	0	0	0
			1607	717	298	517	75			

- Molecule 36 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	k	13	Total	C	N	O	P	0	0	0
			273	123	47	90	13			

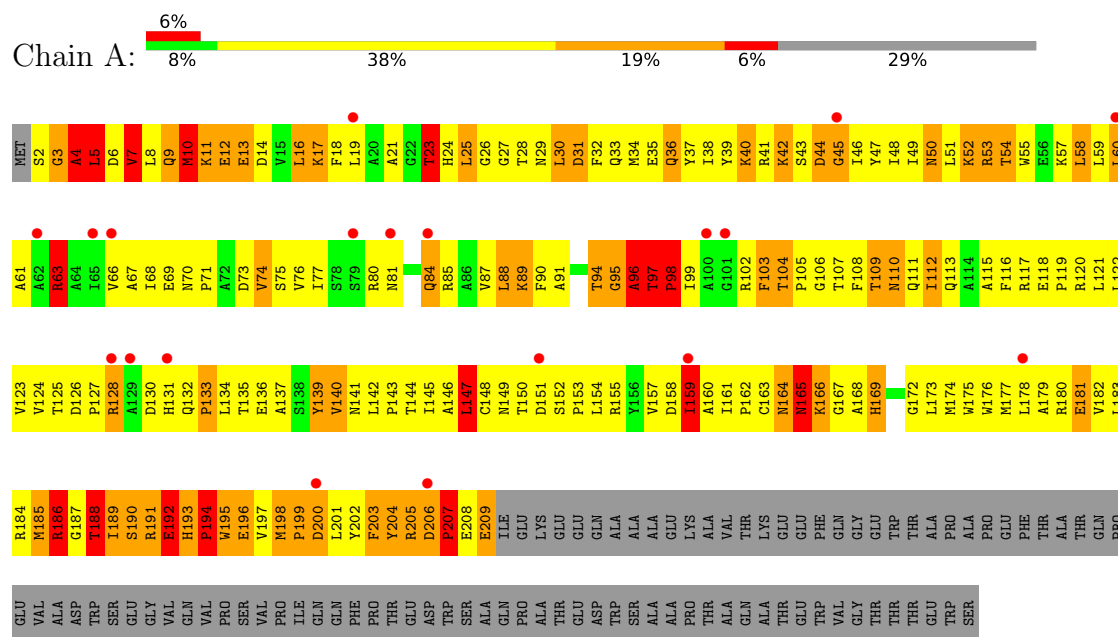
- Molecule 37 is a protein called human initiation factor eIF1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	n	82	Total	C	N	O	S	0	0	0
			648	407	119	118	4			

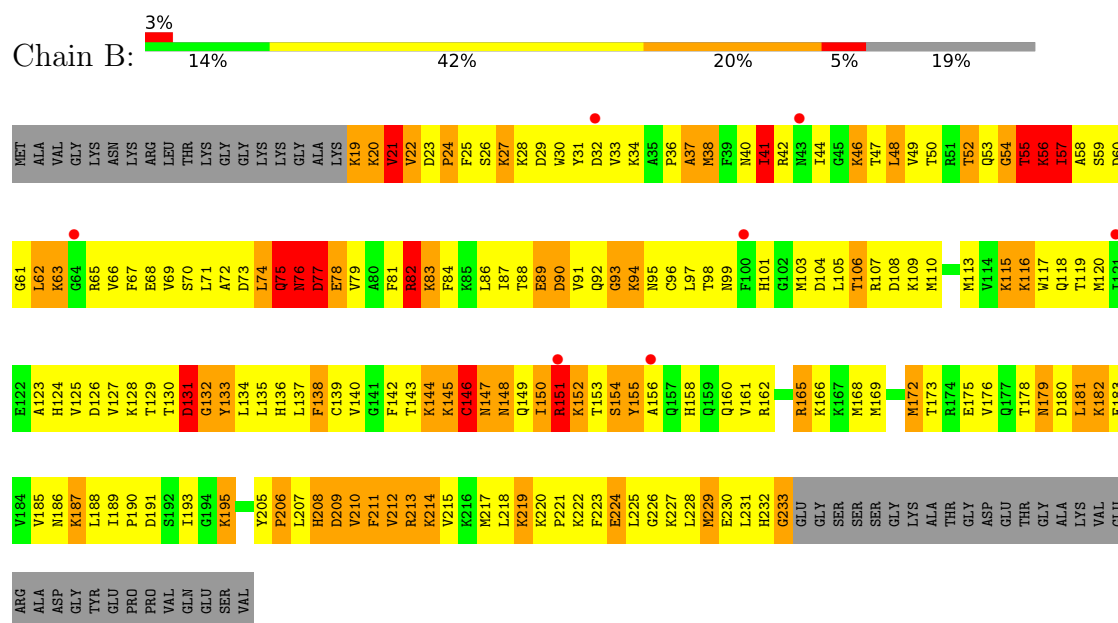
3 Residue-property plots

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.

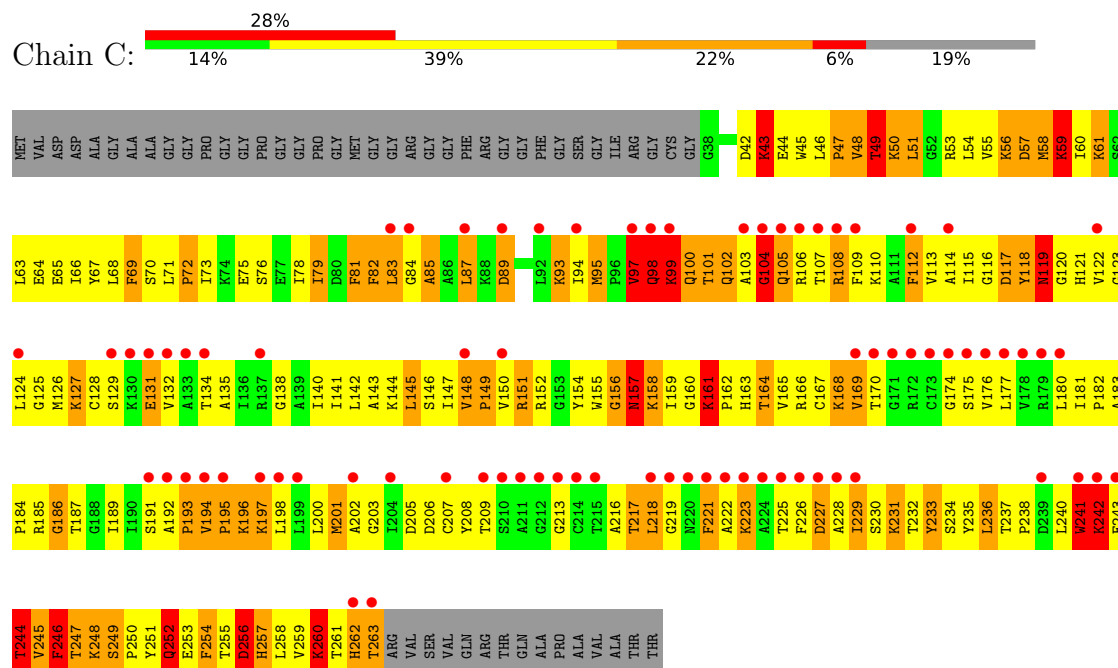
• Molecule 1: 40S Ribosomal Protein SA



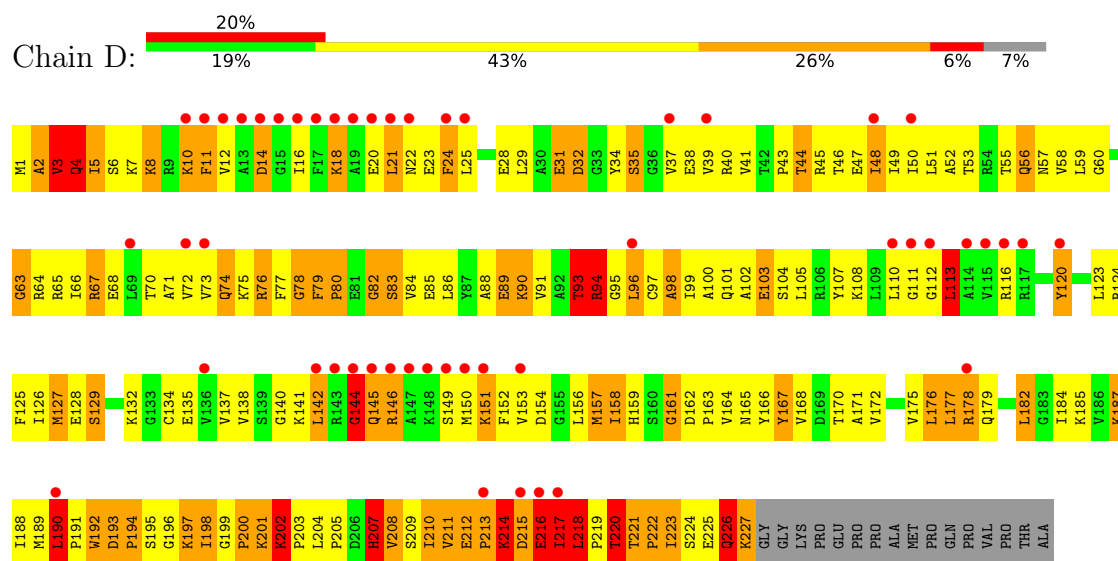
• Molecule 2: 40S Ribosomal Protein S3A



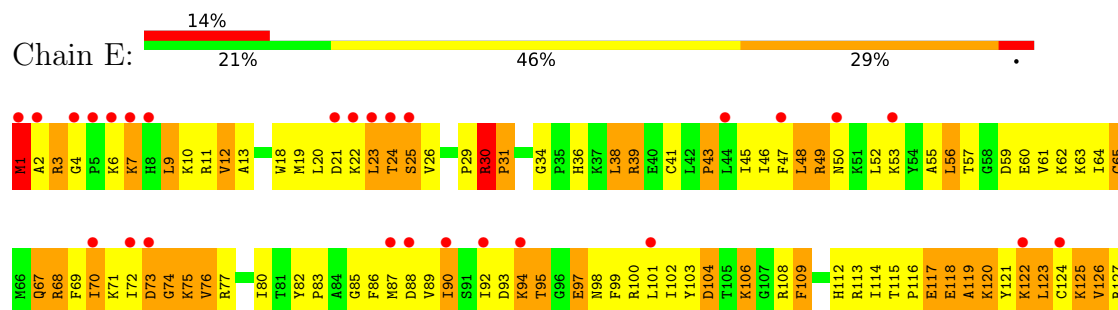
• Molecule 3: 40S Ribosomal Protein S2

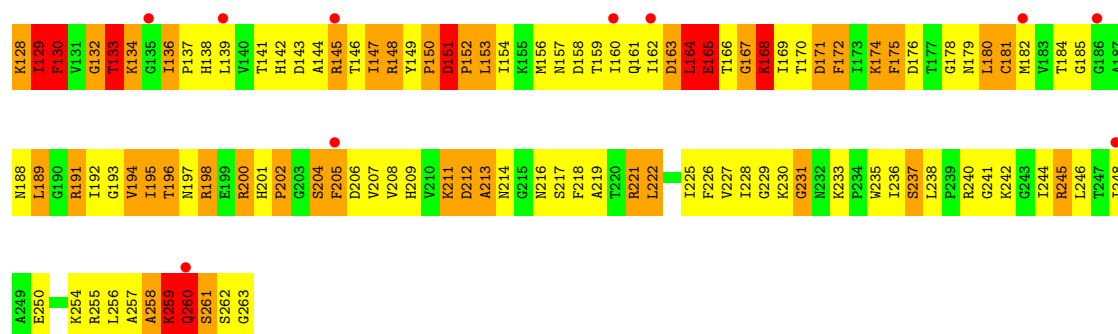


• Molecule 4: 40S Ribosomal Protein S3

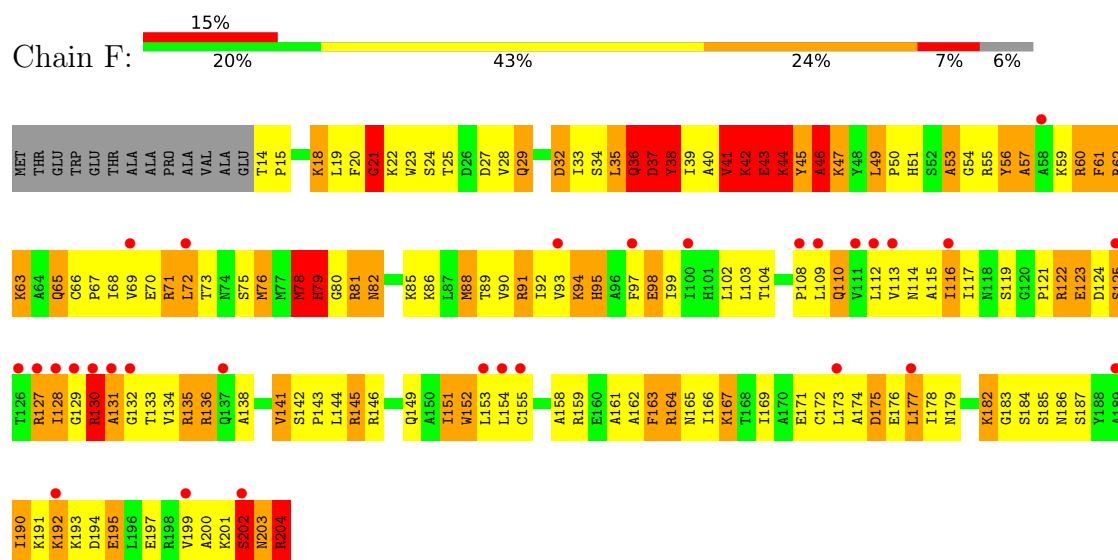


• Molecule 5: 40S Ribosomal Protein S4X

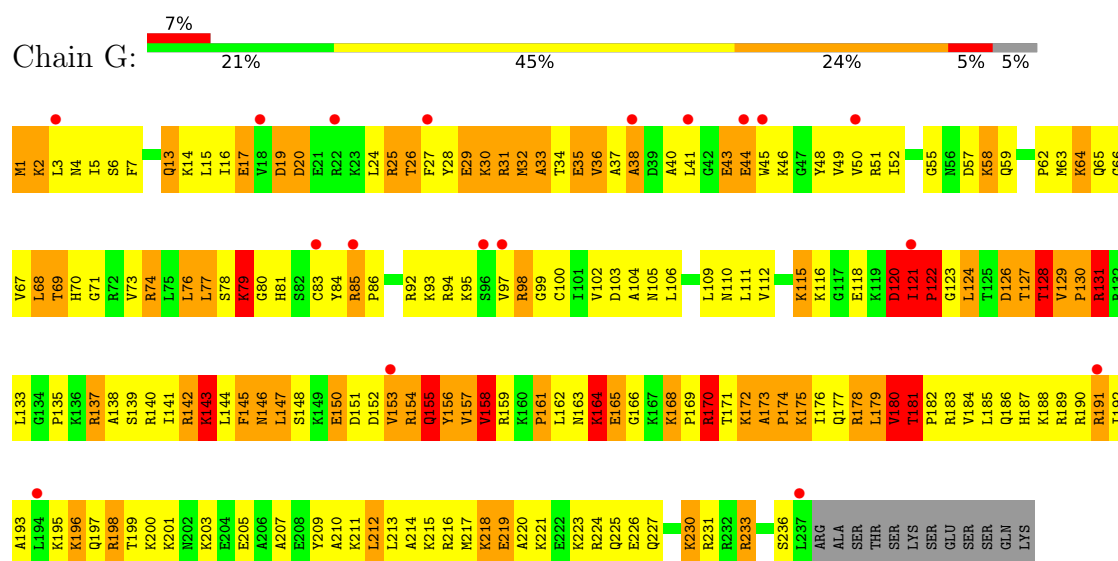




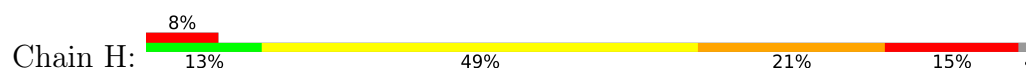
• Molecule 6: 40S Ribosomal Protein S5

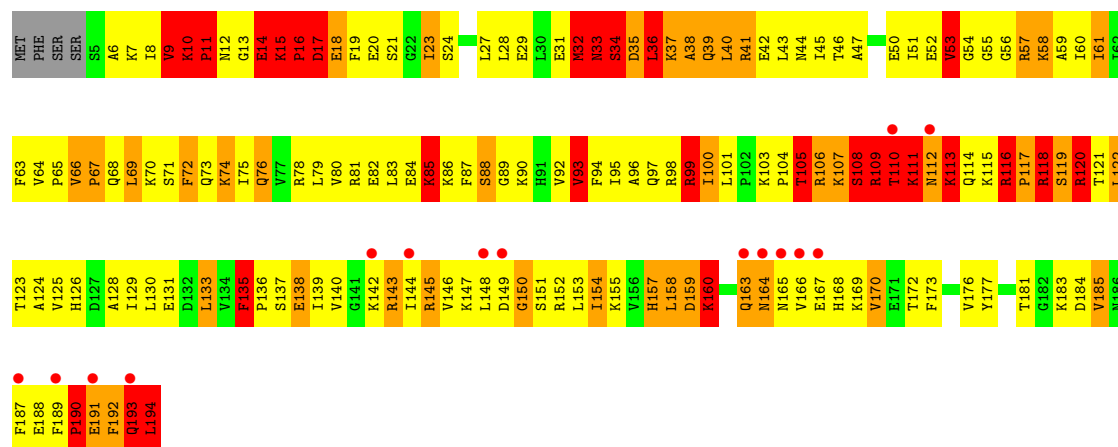


• Molecule 7: 40S Ribosomal Protein S6

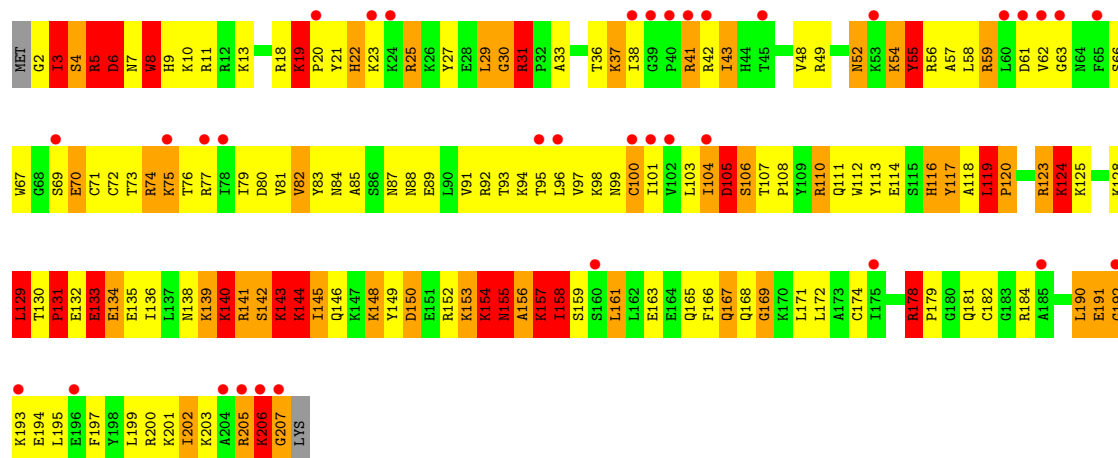
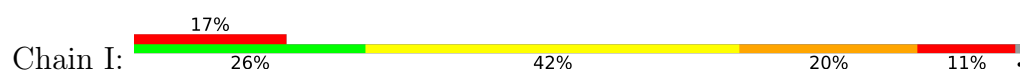


• Molecule 8: 40S Ribosomal Protein S7

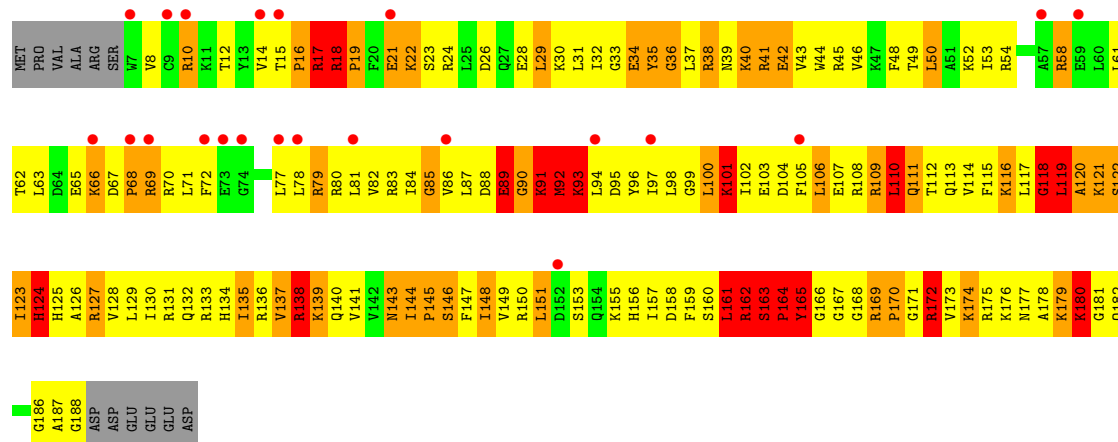
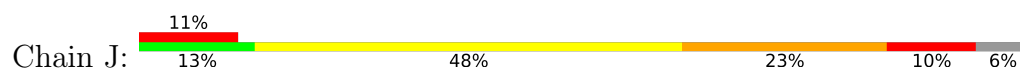




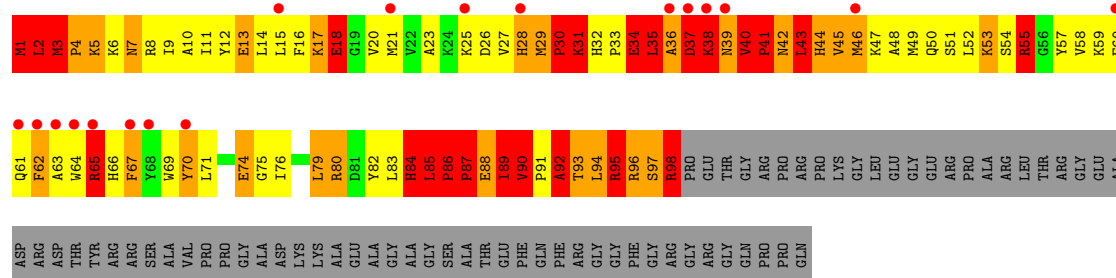
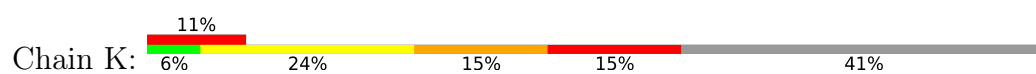
• Molecule 9: 40S Ribosomal Protein S8



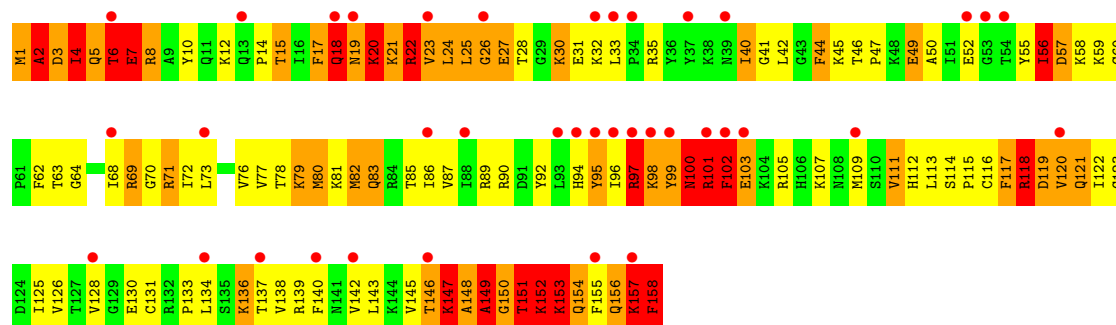
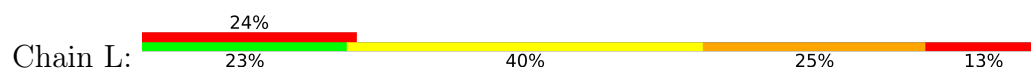
• Molecule 10: 40S Ribosomal Protein S9



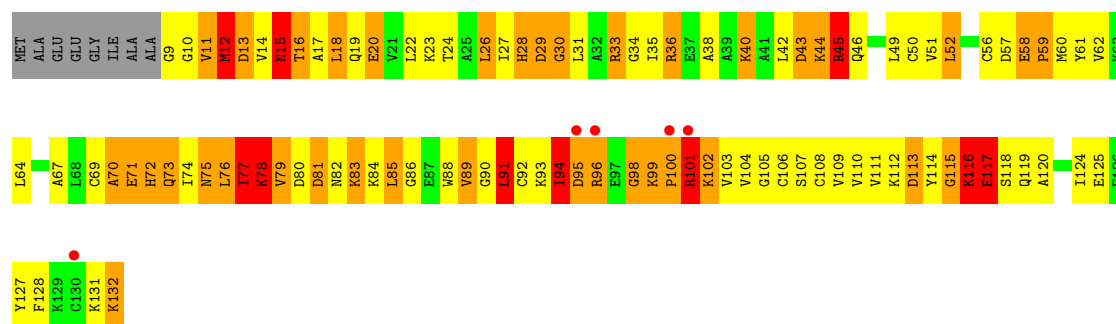
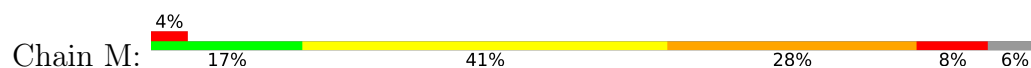
• Molecule 11: 40S Ribosomal Protein S10



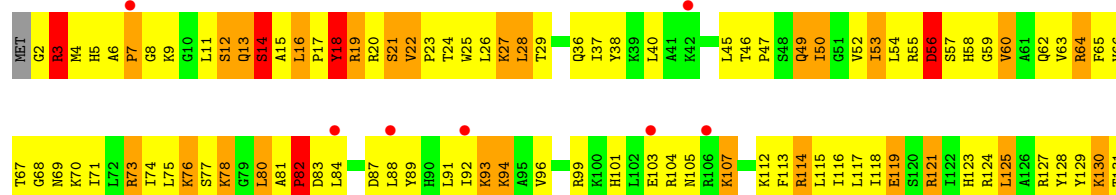
• Molecule 12: 40S Ribosomal Protein S11

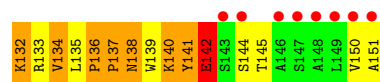


• Molecule 13: 40S Ribosomal Protein S12

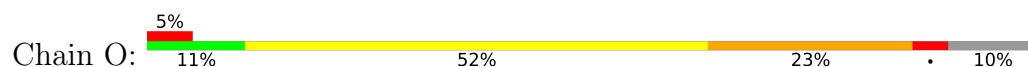


• Molecule 14: 40S Ribosomal Protein S13

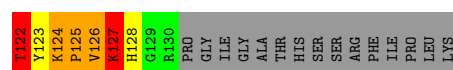
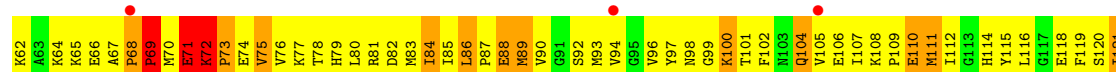
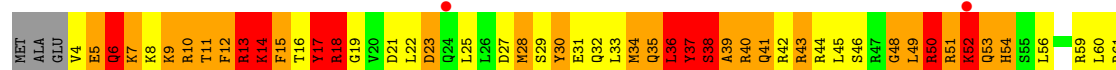




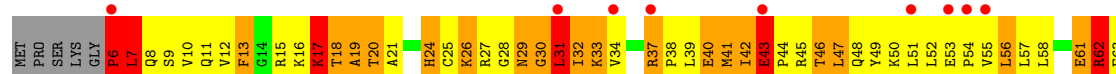
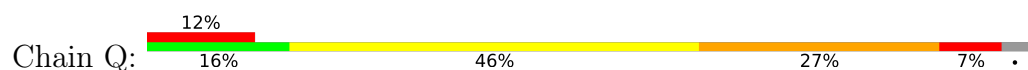
• Molecule 15: 40S Ribosomal Protein S14



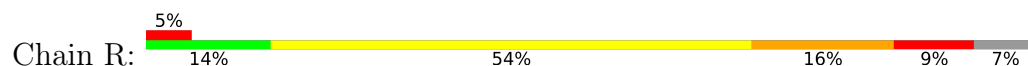
• Molecule 16: 40S Ribosomal Protein S15

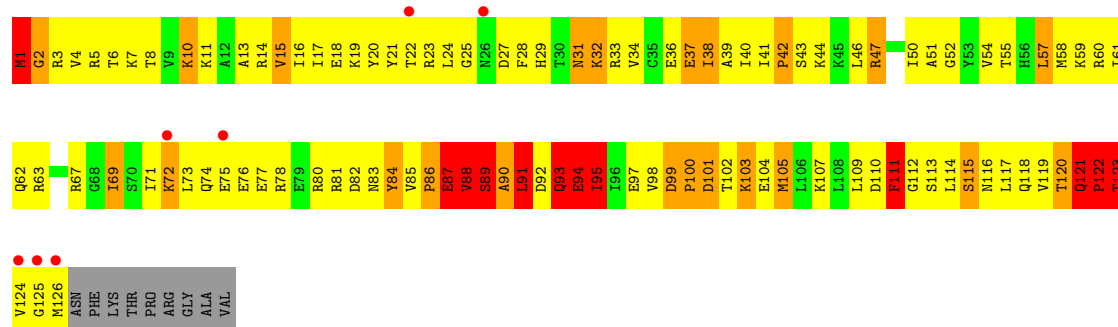


• Molecule 17: 40S Ribosomal Protein S16



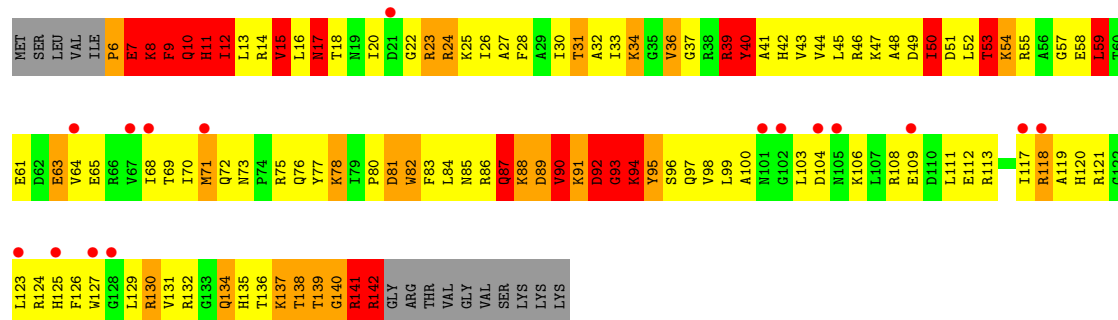
• Molecule 18: 40S Ribosomal Protein S17





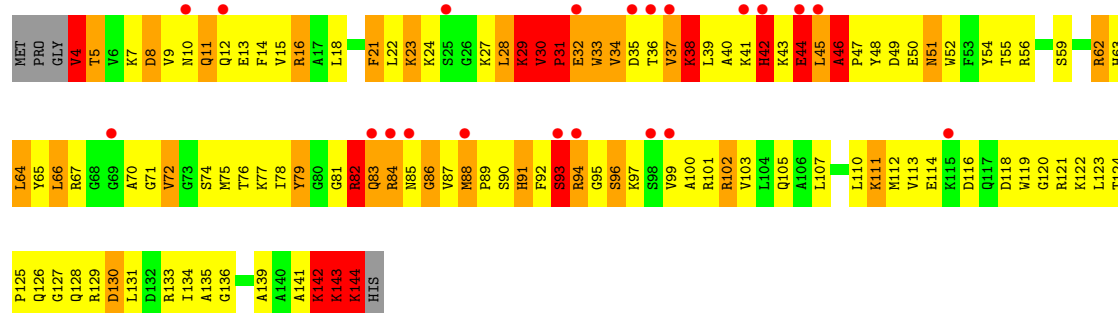
• Molecule 19: 40S Ribosomal Protein S18

Chain S: 11% 15% 47% 15% 13% 10%



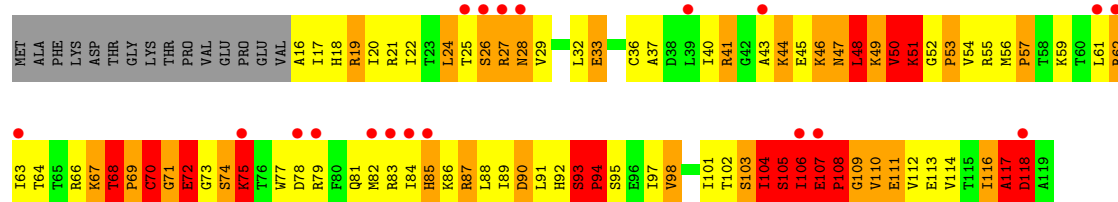
• Molecule 20: 40S Ribosomal Protein S19

Chain T: 14% 18% 51% 19% 9%



• Molecule 21: 40S Ribosomal Protein S20

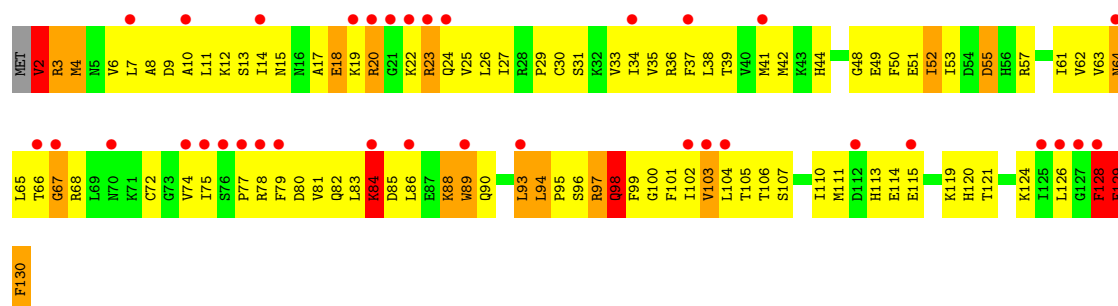
Chain U: 16% 15% 36% 23% 13% 13%



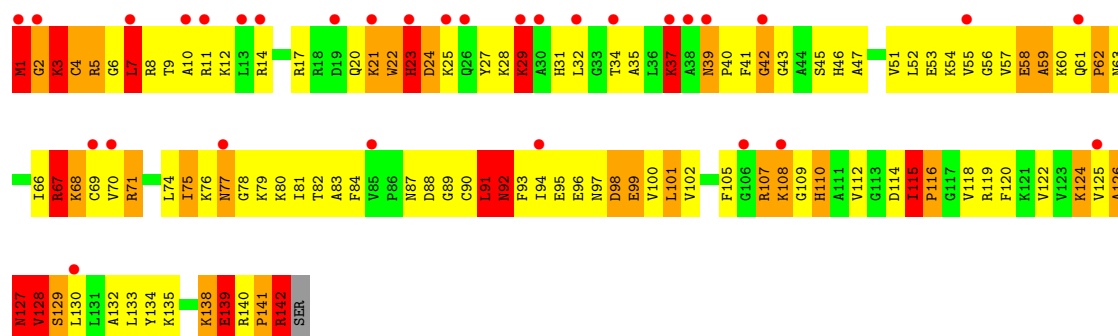
• Molecule 22: 40S Ribosomal Protein S21



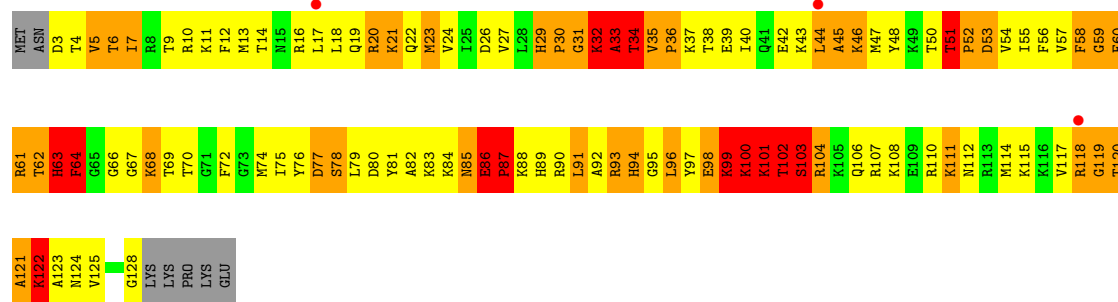
Chain W: 27% 25% 58% 12%



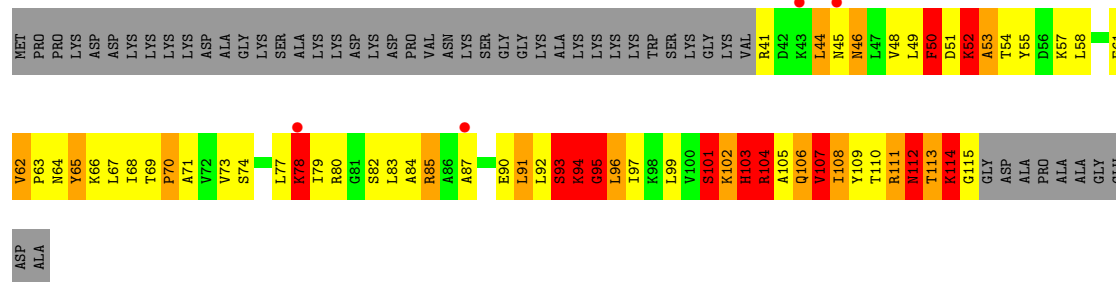
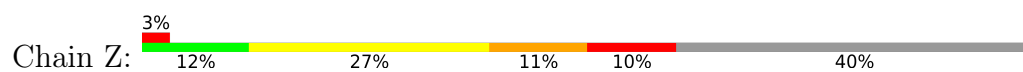
Chain X:



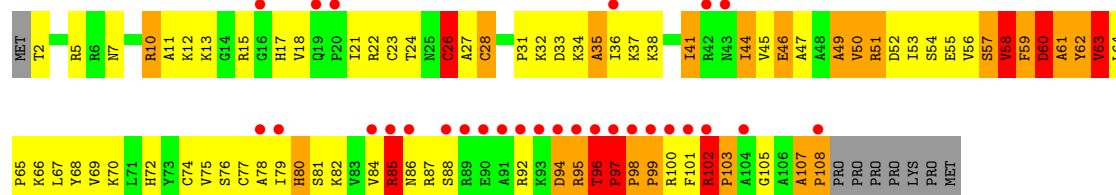
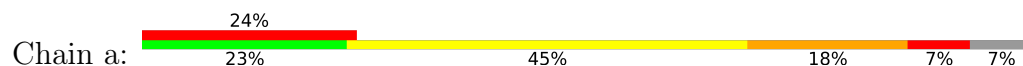
Chain Y:



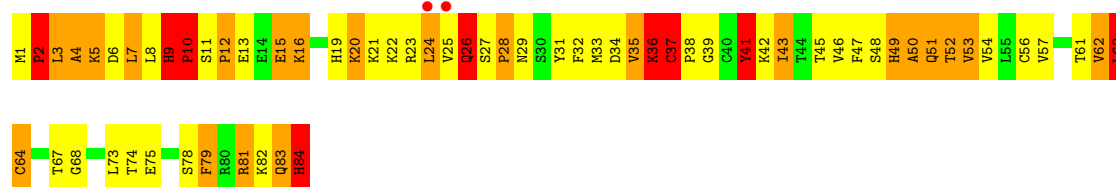
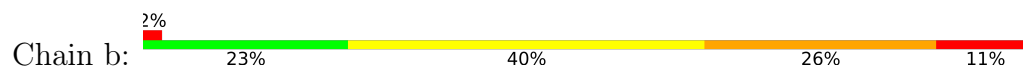
- Molecule 26: 40S Ribosomal Protein S25



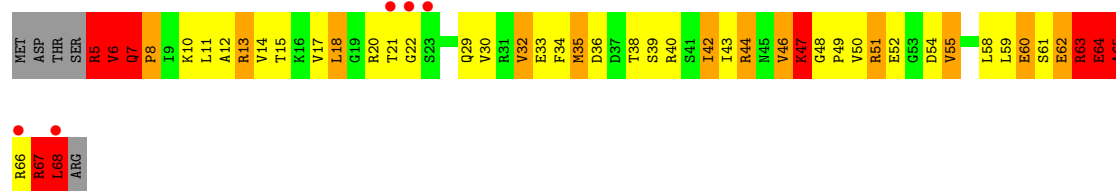
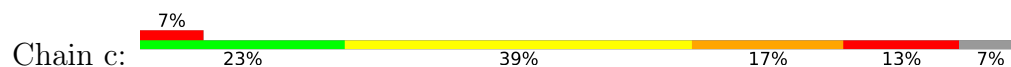
• Molecule 27: 40S Ribosomal Protein S26



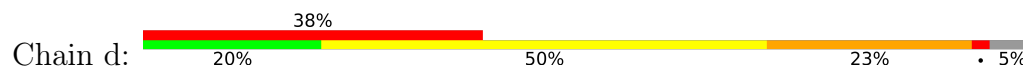
• Molecule 28: 40S Ribosomal Protein S27



• Molecule 29: 40S Ribosomal Protein S28



• Molecule 30: 40S Ribosomal Protein S29



[illegible]

Chain f:

Amino Acid	Percentage
ILE	2%
GLN	6%
LYS	15%
THR	14%
LEU	10%
GLY	54%

2% 6% 15% 14% 10% 54%

ILE GLN LYS THR LEU GLY ARG LEU PHE ASP GLN ALA VAL GLU PRO SER ASP THR ILE GLN ASP LYS GLY ILE PRO PRO ASP GLN ARG LEU PHE GLY LYS GLN LEU ASP THR GLY TYR ASN

ILE GLN LYS THR LEU VAL GLY ALA LYS LYS ARG LYS K82 K83 S84 Y85 T86 T87 P88 P89 K90 K91 K92 K93 K94 K95 K96 K97 Y98 Y99 K99 L100 L101 Y102 L103 Y104 Y105 Y106 K107 Y108 D109 E110 N111 G112 K113 L114 S115 R116 L117 R118 R119 E120 C121 P122 S123 E124 E125 C126 G127 A128 A129 G129 V130 F131 S134 H135 F136 D137 R138 H139 Y140 K143 K144 C145 L146 T147 Y148 C149 F150 M151 M152 PRO GLU ASP LYS

Chain g:

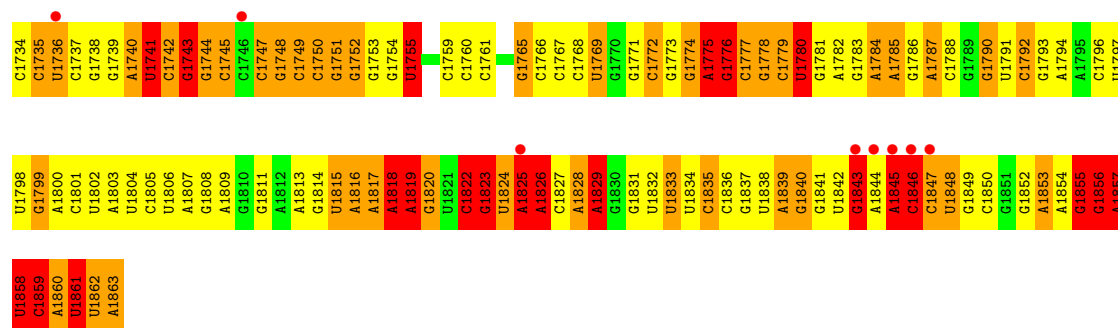
7% 18% 52% 21% 8%

MET T2 T3 T4 T5 T6 T7 T8 T9 T10 T11 T12 T13 T14 T15 T16 T17 T18 T19 T20 T21 T22 T23 T24 T25 T26 T27 T28 T29 T30 T31 T32 T33 T34 T35 T36 T37 T38 T39 T40 T41 T42 T43 T44 T45 T46 T47 T48 T49 T50 T51 T52 T53 T54 T55 T56 T57 T58 T59 T60 T61 T62 T63 T64 T65 T66 T67 T68 T69 T70 T71 T72 T73 T74 T75 T76 T77 T78 T79 T80 T81 T82 T83 T84 T85 T86 T87 T88 T89 T90 T91 T92 T93 T94 T95 T96 T97 T98 T99 T100 T101 T102 T103 T104 T105 T106 T107 T108 T109 T110 T111 T112 T113 T114 T115 T116 T117 T118 T119 T120 T121 T122 T123 T124 T125 T126 T127 T128 T129 T130 T131 T132 T133 T134 T135 T136 T137 T138 T139 T140 T141 T142 T143 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T195 T196 T197 T198 T199 T200 T201 T202 T203 T204 T205 T206 T207 T208 T209 T210 T211 T212 T213 T214 T215 T216 T217 T218 T219 T220 T221 T222 T223 T224 T225 T226 T227 T228 T229 T230 T231 T232 T233 T234 T235 T236 T237 T238 T239 T240 T241 T242 T243 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255 T256 T257 T258 T259 T260 T261 T262 T263 T264 T265 T266 T267 T268 T269 T270 T271 T272 T273 T274 T275 T276 T277 T278 T279 T280 T281 T282 T283 T284 T285 T286 T287 T288 T289 T290 T291 T292 T293 T294 T295 T296 T297 T298 T299 T300 T301 T302 T303 T304 T305 T306 T307 T308 T309 T310 T311 T312 T313 T314 T315 T316 T317 T318 T319 T320 T321 T322 T323 T324 T325 T326 T327 T328 T329 T330 T331 T332 T333 T334 T335 T336 T337 T338 T339 T340 T341 T342 T343 T344 T345 T346 T347 T348 T349 T350 T351 T352 T353 T354 T355 T356 T357 T358 T359 T360 T361 T362 T363 T364 T365 T366 T367 T368 T369 T370 T371 T372 T373 T374 T375 T376 T377 T378 T379 T380 T381 T382 T383 T384 T385 T386 T387 T388 T389 T390 T391 T392 T393 T394 T395 T396 T397 T398 T399 T400 T401 T402 T403 T404 T405 T406 T407 T408 T409 T410 T411 T412 T413 T414 T415 T416 T417 T418 T419 T420 T421 T422 T423 T424 T425 T426 T427 T428 T429 T430 T431 T432 T433 T434 T435 T436 T437 T438 T439 T440 T441 T442 T443 T444 T445 T446 T447 T448 T449 T450 T451 T452 T453 T454 T455 T456 T457 T458 T459 T460 T461 T462 T463 T464 T465 T466 T467 T468 T469 T470 T471 T472 T473 T474 T475 T476 T477 T478 T479 T480 T481 T482 T483 T484 T485 T486 T487 T488 T489 T490 T491 T492 T493 T494 T495 T496 T497 T498 T499 T500 T501 T502 T503 T504 T505 T506 T507 T508 T509 T510 T511 T512 T513 T514 T515 T516 T517 T518 T519 T520 T521 T522 T523 T524 T525 T526 T527 T528 T529 T530 T531 T532 T533 T534 T535 T536 T537 T538 T539 T540 T541 T542 T543 T544 T545 T546 T547 T548 T549 T550 T551 T552 T553 T554 T555 T556 T557 T558 T559 T560 T561 T562 T563 T564 T565 T566 T567 T568 T569 T570 T571 T572 T573 T574 T575 T576 T577 T578 T579 T580 T581 T582 T583 T584 T585 T586 T587 T588 T589 T590 T591 T592 T593 T594 T595 T596 T597 T598 T599 T600 T601 T602 T603 T604 T605 T606 T607 T608 T609 T610 T611 T612 T613 T614 T615 T616 T617 T618 T619 T620 T621 T622 T623 T624 T625 T626 T627 T628 T629 T630 T631 T632 T633 T634 T635 T636 T637 T638 T639 T640 T641 T642 T643 T644 T645 T646 T647 T648 T649 T650 T651 T652 T653 T654 T655 T656 T657 T658 T659 T660 T661 T662 T663 T664 T665 T666 T667 T668 T669 T670 T671 T672 T673 T674 T675 T676 T677 T678 T679 T680 T681 T682 T683 T684 T685 T686 T687 T688 T689 T690 T691 T692 T693 T694 T695 T696 T697 T698 T699 T700 T701 T702 T703 T704 T705 T706 T707 T708 T709 T710 T711 T712 T713 T714 T715 T716 T717 T718 T719 T720 T721 T722 T723 T724 T725 T726 T727 T728 T729 T730 T731 T732 T733 T734 T735 T736 T737 T738 T739 T740 T741 T742 T743 T744 T745 T746 T747 T748 T749 T750 T751 T752 T753 T754 T755 T756 T757 T758 T759 T760 T761 T762 T763 T764 T765 T766 T767 T768 T769 T770 T771 T772 T773 T774 T775 T776 T777 T778 T779 T780 T781 T782 T783 T784 T785 T786 T787 T788 T789 T790 T791 T792 T793 T794 T795 T796 T797 T798 T799 T800 T801 T802 T803 T804 T805 T806 T807 T808 T809 T810 T811 T812 T813 T814 T815 T816 T817 T818 T819 T820 T821 T822 T823 T824 T825 T826 T827 T828 T829 T830 T831 T832 T833 T834 T835 T836 T837 T838 T839 T840 T841 T842 T843 T844 T845 T846 T847 T848 T849 T850 T851 T852 T853 T854 T855 T856 T857 T858 T859 T860 T861 T862 T863 T864 T865 T866 T867 T868 T869 T870 T871 T872 T873 T874 T875 T876 T877 T878 T879 T880 T881 T882 T883 T884 T885 T886 T887 T888 T889 T890 T891 T892 T893 T894 T895 T896 T897 T898 T899 T900 T901 T902 T903 T904 T905 T906 T907 T908 T909 T910 T911 T912 T913 T914 T915 T916 T917 T918 T919 T920 T921 T922 T923 T924 T925 T926 T927 T928 T929 T930 T931 T932 T933 T934 T935 T936 T937 T938 T939 T940 T941 T942 T943 T944 T945 T946 T947 T948 T949 T95

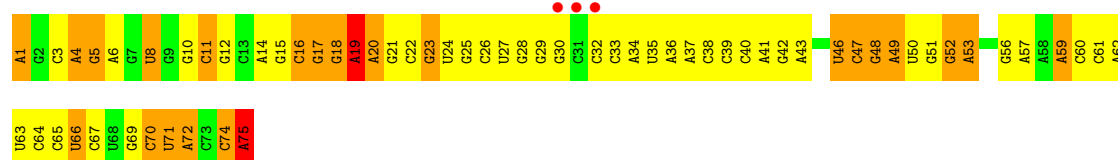
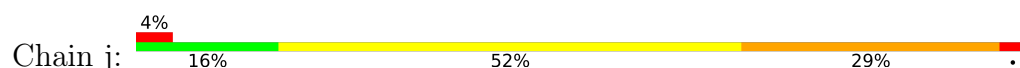
Chain i:

Category	Sub-category	Value	Color
U	U	6966	Red
	C	6967	Red
	C	6968	Red
	C	6969	Red
	A	6970	Green
	A	6971	Green
	A	6972	Green
	G	6973	Green
	G	6974	Green
	G	6975	Green
C	C	6976	Red
	C	6977	Red
	C	6978	Red
	C	6979	Red
	C	6980	Red
	C	6981	Red
	C	6982	Red
	C	6983	Red
	C	6984	Red
	C	6985	Red
A	A	6986	Green
	A	6987	Green
	A	6988	Green
	A	6989	Green
	A	6990	Green
	A	6991	Green
	A	6992	Green
	A	6993	Green
	A	6994	Green
	A	6995	Green
G	G	6996	Green
	G	6997	Green
	G	6998	Green
	G	6999	Green
	G	7000	Green
	G	7001	Green
	G	7002	Green
	G	7003	Green
	G	7004	Green
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	G	7011	Green
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	G	7107	Green
	G	7108	Green
	G	7109	Green
	G	7110	Green
	G	7111	Green
	G	7112	Green
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	G	7114	Green
	G	7115	Green
G	G	7116	Green
	G	7117	Green
	G		





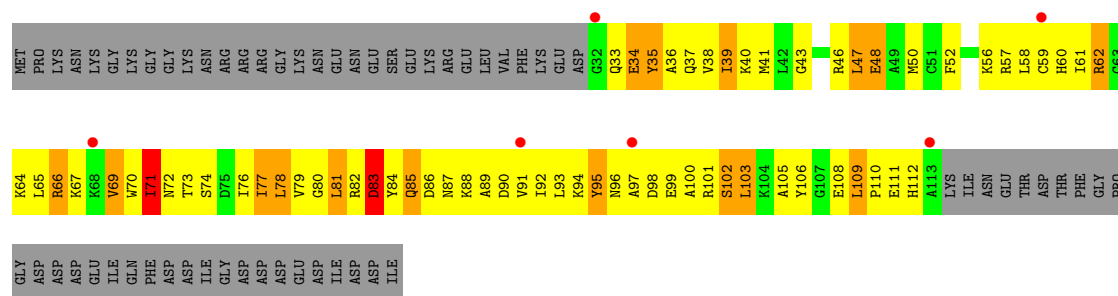
• Molecule 35: initiator Met-RNA-i



• Molecule 36: mRNA



• Molecule 37: human initiation factor eIF1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	297.75Å 297.75Å 485.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.53 – 7.03 77.53 – 7.03	Depositor EDS
% Data completeness (in resolution range)	98.3 (77.53-7.03) 98.6 (77.53-7.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 6.72Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.345 , 0.359 0.335 , 0.339	Depositor DCC
R_{free} test set	1946 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	566.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 84.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	79048	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	14/1679 (0.8%)	1.61	47/2283 (2.1%)
2	B	0.94	9/1769 (0.5%)	1.64	47/2367 (2.0%)
3	C	1.38	22/1778 (1.2%)	1.88	55/2399 (2.3%)
4	D	1.57	9/1792 (0.5%)	1.97	55/2412 (2.3%)
5	E	0.90	8/2125 (0.4%)	1.48	48/2856 (1.7%)
6	F	1.29	10/1531 (0.7%)	1.77	40/2059 (1.9%)
7	G	1.30	27/1946 (1.4%)	1.76	48/2590 (1.9%)
8	H	1.47	20/1553 (1.3%)	2.04	62/2079 (3.0%)
9	I	1.58	21/1708 (1.2%)	1.98	51/2278 (2.2%)
10	J	1.87	27/1522 (1.8%)	2.13	75/2031 (3.7%)
11	K	1.72	18/851 (2.1%)	2.31	62/1147 (5.4%)
12	L	1.45	13/1319 (1.0%)	1.99	56/1761 (3.2%)
13	M	1.38	6/960 (0.6%)	1.79	27/1287 (2.1%)
14	N	1.01	8/1232 (0.6%)	1.27	14/1656 (0.8%)
15	O	0.89	7/1029 (0.7%)	1.55	26/1380 (1.9%)
16	P	1.03	8/1079 (0.7%)	1.84	52/1437 (3.6%)
17	Q	0.84	1/1142 (0.1%)	1.67	40/1528 (2.6%)
18	R	1.61	17/1031 (1.6%)	1.99	47/1383 (3.4%)
19	S	1.76	25/1157 (2.2%)	2.17	62/1548 (4.0%)
20	T	1.30	10/1132 (0.9%)	1.70	28/1517 (1.8%)
21	U	1.22	7/832 (0.8%)	2.34	53/1117 (4.7%)
22	V	1.13	5/626 (0.8%)	1.82	29/839 (3.5%)
23	W	1.10	4/1051 (0.4%)	1.38	15/1406 (1.1%)
24	X	1.49	17/1124 (1.5%)	1.97	37/1500 (2.5%)
25	Y	1.15	6/1038 (0.6%)	1.82	37/1380 (2.7%)
26	Z	1.17	6/604 (1.0%)	1.89	30/810 (3.7%)
27	a	1.32	11/860 (1.3%)	2.24	31/1156 (2.7%)
28	b	1.26	7/673 (1.0%)	2.20	33/902 (3.7%)
29	c	1.06	4/508 (0.8%)	1.76	20/680 (2.9%)
30	d	0.98	2/455 (0.4%)	1.24	3/603 (0.5%)
31	e	2.07	10/478 (2.1%)	2.14	20/628 (3.2%)
32	f	1.21	3/593 (0.5%)	2.01	34/786 (4.3%)
33	g	1.29	12/2493 (0.5%)	1.86	81/3394 (2.4%)
34	i	1.91	1346/41879 (3.2%)	1.93	2099/65157 (3.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
35	j	0.60	8/1798 (0.4%)	0.64	1/2802 (0.0%)
36	k	1.67	1/304 (0.3%)	0.89	3/470 (0.6%)
37	n	0.52	0/657	0.64	0/881
All	All	1.63	1729/84308 (2.1%)	1.87	3468/122509 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
2	B	0	4
3	C	1	5
4	D	0	5
5	E	1	2
6	F	0	3
7	G	0	1
8	H	0	10
9	I	0	8
10	J	1	11
11	K	0	11
12	L	0	7
13	M	0	1
14	N	0	4
15	O	0	1
16	P	0	10
17	Q	0	4
18	R	1	5
19	S	1	10
20	T	1	6
21	U	0	8
22	V	0	9
23	W	0	2
24	X	0	4
25	Y	1	6
26	Z	0	6
27	a	0	2
28	b	0	3
31	e	0	5
32	f	0	6
33	g	0	13

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
34	i	6	0
All	All	13	183

The worst 5 of 1729 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	ILE	C-N	37.67	1.82	1.33
31	e	95	LYS	C-N	30.65	1.76	1.33
10	J	85	GLY	C-N	-30.43	0.95	1.33
10	J	118	GLY	C-N	28.43	1.73	1.33
36	k	22	C	Cl'-N1	28.28	1.90	1.48

The worst 5 of 3468 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	97	PRO	N-CA-C	32.75	150.66	110.70
34	i	1774	G	P-O3'-C3'	30.32	165.68	120.20
4	D	5	ILE	O-C-N	-29.05	97.70	122.97
8	H	109	ARG	NE-CZ-NH2	-28.47	93.58	119.20
27	a	97	PRO	CB-CA-C	-26.13	79.04	110.92

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	157	ASN	CA
5	E	171	ASP	CA
10	J	138	ARG	CA
18	R	3	ARG	CA
19	S	92	ASP	CA

5 of 183 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ALA	Mainchain
1	A	23	THR	Mainchain
1	A	4	ALA	Peptide
1	A	63	ARG	Sidechain
1	A	97	THR	Mainchain

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	A	1642	0	1638	654	0
2	B	1741	0	1808	517	0
3	C	1742	0	1830	598	0
4	D	1764	0	1856	624	0
5	E	2083	0	2189	539	0
6	F	1509	0	1557	554	0
7	G	1923	0	2087	546	3
8	H	1530	0	1624	504	0
9	I	1679	0	1762	464	3
10	J	1498	0	1599	626	0
11	K	827	0	853	363	18
12	L	1296	0	1370	421	0
13	M	950	0	969	282	0
14	N	1208	0	1294	325	0
15	O	1016	0	1037	421	0
16	P	1060	0	1120	514	0
17	Q	1124	0	1189	507	0
18	R	1019	0	1067	390	0
19	S	1139	0	1188	460	1
20	T	1112	0	1149	432	0
21	U	822	0	887	232	0
22	V	619	0	620	282	0
23	W	1034	0	1079	301	0
24	X	1106	0	1177	345	0
25	Y	1021	0	1083	515	0
26	Z	598	0	652	217	0
27	a	844	0	895	201	0
28	b	659	0	681	265	0
29	c	506	0	534	212	0
30	d	445	0	441	139	0
31	e	473	0	519	287	31
32	f	581	0	598	191	0
33	g	2436	0	2388	708	0
34	i	37514	0	18808	1212	78
35	j	1607	0	811	157	0
36	k	273	0	139	104	0
37	n	648	0	642	307	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	79048	0	61140	13410	81

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 96.

The worst 5 of 13410 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)
33:g:5:MET:SD	33:g:312:VAL:HG22	1.20	1.74
32:f:135:HIS:HB3	32:f:138:ARG:CG	1.22	1.69
28:b:64:CYS:SG	28:b:73:LEU:HD23	1.11	1.69
3:C:197:LYS:HA	3:C:200:LEU:CD2	1.22	1.68
9:I:141:ARG:CB	9:I:144:LYS:HB2	1.24	1.68

The worst 5 of 81 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)
31:e:123:PHE:CD1	34:i:1759:C:C4'[3_564]	0.62	1.58
31:e:123:PHE:CE1	34:i:1759:C:C5'[3_564]	0.70	1.50
34:i:531:U:O2'	34:i:1767:C:O4'[3_564]	0.72	1.48
31:e:125:LYS:CE	34:i:1761:C:OP1[3_564]	0.73	1.47
11:K:97:SER:O	34:i:76:U:OP1[3_564]	0.95	1.25

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
1	A	206/295 (70%)	156 (76%)	23 (11%)	27 (13%)	0 4
2	B	213/264 (81%)	174 (82%)	24 (11%)	15 (7%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	224/278 (81%)	199 (89%)	14 (6%)	11 (5%)	1	16
4	D	225/243 (93%)	180 (80%)	23 (10%)	22 (10%)	0	7
5	E	261/263 (99%)	210 (80%)	27 (10%)	24 (9%)	0	8
6	F	189/204 (93%)	162 (86%)	15 (8%)	12 (6%)	1	13
7	G	235/249 (94%)	201 (86%)	19 (8%)	15 (6%)	1	12
8	H	188/194 (97%)	146 (78%)	11 (6%)	31 (16%)	0	2
9	I	204/208 (98%)	169 (83%)	13 (6%)	22 (11%)	0	6
10	J	180/194 (93%)	138 (77%)	18 (10%)	24 (13%)	0	4
11	K	96/165 (58%)	67 (70%)	11 (12%)	18 (19%)	0	2
12	L	156/158 (99%)	132 (85%)	10 (6%)	14 (9%)	0	8
13	M	122/132 (92%)	85 (70%)	16 (13%)	21 (17%)	0	2
14	N	148/151 (98%)	123 (83%)	19 (13%)	6 (4%)	2	18
15	O	134/151 (89%)	101 (75%)	14 (10%)	19 (14%)	0	3
16	P	125/145 (86%)	92 (74%)	16 (13%)	17 (14%)	0	3
17	Q	139/146 (95%)	110 (79%)	19 (14%)	10 (7%)	1	11
18	R	124/135 (92%)	97 (78%)	13 (10%)	14 (11%)	0	5
19	S	135/152 (89%)	106 (78%)	20 (15%)	9 (7%)	1	12
20	T	139/145 (96%)	119 (86%)	10 (7%)	10 (7%)	1	11
21	U	102/119 (86%)	76 (74%)	10 (10%)	16 (16%)	0	2
22	V	80/83 (96%)	55 (69%)	11 (14%)	14 (18%)	0	2
23	W	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	7	38
24	X	140/143 (98%)	121 (86%)	11 (8%)	8 (6%)	1	14
25	Y	124/133 (93%)	91 (73%)	15 (12%)	18 (14%)	0	3
26	Z	73/125 (58%)	52 (71%)	12 (16%)	9 (12%)	0	4
27	a	105/115 (91%)	72 (69%)	14 (13%)	19 (18%)	0	2
28	b	82/84 (98%)	57 (70%)	14 (17%)	11 (13%)	0	4
29	c	62/69 (90%)	44 (71%)	13 (21%)	5 (8%)	1	9
30	d	51/56 (91%)	46 (90%)	3 (6%)	2 (4%)	2	19
31	e	57/133 (43%)	37 (65%)	7 (12%)	13 (23%)	0	1
32	f	69/156 (44%)	38 (55%)	13 (19%)	18 (26%)	0	1
33	g	311/317 (98%)	271 (87%)	23 (7%)	17 (6%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
37	n	80/144 (56%)	61 (76%)	15 (19%)	4 (5%)	1 16
All	All	4906/5679 (86%)	3899 (80%)	510 (10%)	497 (10%)	0 7

5 of 497 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	31	ASP
1	A	45	GLY
1	A	103	PHE
1	A	164	ASN

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
1	A	174/244 (71%)	141 (81%)	33 (19%)	1 8
2	B	196/231 (85%)	153 (78%)	43 (22%)	1 6
3	C	187/215 (87%)	142 (76%)	45 (24%)	1 4
4	D	190/202 (94%)	144 (76%)	46 (24%)	1 4
5	E	225/225 (100%)	170 (76%)	55 (24%)	1 4
6	F	161/170 (95%)	114 (71%)	47 (29%)	0 2
7	G	207/218 (95%)	157 (76%)	50 (24%)	1 4
8	H	170/174 (98%)	124 (73%)	46 (27%)	0 3
9	I	177/179 (99%)	137 (77%)	40 (23%)	1 6
10	J	157/168 (94%)	128 (82%)	29 (18%)	1 8
11	K	89/136 (65%)	63 (71%)	26 (29%)	0 2
12	L	142/142 (100%)	106 (75%)	36 (25%)	0 3
13	M	101/108 (94%)	78 (77%)	23 (23%)	1 6
14	N	130/131 (99%)	100 (77%)	30 (23%)	1 5
15	O	106/119 (89%)	88 (83%)	18 (17%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	116/130 (89%)	86 (74%)	30 (26%)	0	3
17	Q	117/121 (97%)	83 (71%)	34 (29%)	0	2
18	R	114/121 (94%)	87 (76%)	27 (24%)	1	4
19	S	119/132 (90%)	95 (80%)	24 (20%)	1	7
20	T	113/116 (97%)	84 (74%)	29 (26%)	0	3
21	U	94/107 (88%)	72 (77%)	22 (23%)	1	5
22	V	67/68 (98%)	47 (70%)	20 (30%)	0	2
23	W	112/113 (99%)	97 (87%)	15 (13%)	4	14
24	X	114/115 (99%)	90 (79%)	24 (21%)	1	6
25	Y	108/115 (94%)	85 (79%)	23 (21%)	1	6
26	Z	66/103 (64%)	53 (80%)	13 (20%)	1	7
27	a	91/99 (92%)	76 (84%)	15 (16%)	2	10
28	b	76/76 (100%)	64 (84%)	12 (16%)	2	12
29	c	57/62 (92%)	43 (75%)	14 (25%)	1	4
30	d	47/49 (96%)	35 (74%)	12 (26%)	0	3
31	e	49/106 (46%)	27 (55%)	22 (45%)	0	0
32	f	64/140 (46%)	42 (66%)	22 (34%)	0	1
33	g	272/275 (99%)	219 (80%)	53 (20%)	1	7
37	n	66/123 (54%)	44 (67%)	22 (33%)	0	2
All	All	4274/4833 (88%)	3274 (77%)	1000 (23%)	1	5

5 of 1000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	8	ARG
31	e	97	GLU
16	P	14	LYS
30	d	44	ARG
33	g	118	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	82	ASN

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Mol	Chain	Res	Type
33	g	119	GLN
18	R	74	GLN
33	g	76	GLN
27	a	80	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	i	1720/1863 (92%)	498 (28%)	0
35	j	74/75 (98%)	17 (22%)	0
36	k	12/24 (50%)	3 (25%)	0
All	All	1806/1962 (92%)	518 (28%)	0

5 of 518 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	i	2	A
34	i	3	C
34	i	4	C
34	i	8	U
34	i	16	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	i	11
10	J	3
19	S	2
4	D	1
31	e	1
9	I	1
21	U	1
3	C	1
7	G	1
18	R	1

The worst 5 of 23 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	326:A	O3'	327:C	P	9.94
1	i	309:A	O3'	310:G	P	7.21
1	i	209:C	O3'	210:G	P	6.66
1	i	1826:A	O3'	1827:C	P	5.44
1	i	304:A	O3'	305:U	P	4.93

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	A	208/295 (70%)	0.14	19 (9%) 15 22	188, 273, 325, 347	0
2	B	215/264 (81%)	-0.08	7 (3%) 49 45	140, 249, 309, 321	0
3	C	226/278 (81%)	2.23	77 (34%) 1 6	76, 163, 267, 284	0
4	D	227/243 (93%)	1.04	49 (21%) 2 9	110, 175, 253, 280	0
5	E	263/263 (100%)	0.57	37 (14%) 6 15	38, 138, 196, 225	0
6	F	191/204 (93%)	0.60	30 (15%) 5 13	133, 175, 212, 224	0
7	G	237/249 (95%)	0.26	18 (7%) 20 26	68, 198, 289, 311	0
8	H	190/194 (97%)	-0.04	15 (7%) 18 25	129, 278, 329, 340	0
9	I	206/208 (99%)	0.80	35 (16%) 4 12	17, 164, 268, 289	0
10	J	182/194 (93%)	0.44	22 (12%) 8 17	73, 158, 221, 258	0
11	K	98/165 (59%)	0.72	18 (18%) 3 11	167, 238, 289, 308	0
12	L	158/158 (100%)	1.06	38 (24%) 2 9	22, 90, 224, 255	0
13	M	124/132 (93%)	-0.30	5 (4%) 42 41	280, 347, 384, 417	0
14	N	150/151 (99%)	0.05	15 (10%) 12 20	46, 118, 251, 261	0
15	O	136/151 (90%)	-0.03	8 (5%) 28 32	45, 205, 320, 353	0
16	P	127/145 (87%)	0.15	5 (3%) 43 42	163, 254, 297, 310	0
17	Q	141/146 (96%)	0.43	18 (12%) 7 16	108, 200, 225, 231	0
18	R	126/135 (93%)	-0.12	7 (5%) 30 34	130, 194, 302, 306	0
19	S	137/152 (90%)	0.45	16 (11%) 9 17	151, 218, 239, 249	0
20	T	141/145 (97%)	0.48	21 (14%) 5 14	161, 214, 230, 234	0
21	U	104/119 (87%)	0.90	19 (18%) 3 11	116, 213, 258, 269	0
22	V	82/83 (98%)	0.01	4 (4%) 35 36	175, 237, 316, 328	0
23	W	129/130 (99%)	1.55	35 (27%) 1 8	75, 141, 196, 216	0
24	X	142/143 (99%)	1.07	31 (21%) 2 9	22, 54, 84, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	126/133 (94%)	-0.06	3 (2%) 59 52	85, 153, 198, 218	0
26	Z	75/125 (60%)	-0.25	4 (5%) 32 34	197, 207, 217, 225	0
27	a	107/115 (93%)	1.47	28 (26%) 1 8	55, 111, 285, 317	0
28	b	84/84 (100%)	-0.18	2 (2%) 59 52	156, 236, 276, 286	0
29	c	64/69 (92%)	0.03	5 (7%) 19 25	125, 173, 216, 221	0
30	d	53/56 (94%)	3.14	21 (39%) 1 5	136, 159, 235, 256	0
31	e	59/133 (44%)	-0.01	6 (10%) 12 20	63, 136, 177, 192	0
32	f	71/156 (45%)	-0.32	3 (4%) 40 40	145, 320, 392, 408	0
33	g	313/317 (98%)	0.01	23 (7%) 21 27	190, 248, 277, 291	0
34	i	1797/1863 (96%)	-0.02	72 (4%) 42 41	13, 142, 348, 527	0
35	j	75/75 (100%)	-0.10	3 (4%) 42 41	308, 379, 421, 436	0
36	k	13/24 (54%)	1.65	5 (38%) 1 5	186, 317, 324, 325	0
37	n	82/144 (56%)	0.16	6 (7%) 21 27	212, 216, 222, 224	0
All	All	6859/7641 (89%)	0.35	730 (10%) 11 19	13, 190, 328, 527	0

The worst 5 of 730 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	a	100	ARG	21.0
3	C	212	GLY	19.0
3	C	194	VAL	17.1
23	W	75	ILE	16.3
3	C	172	ARG	16.1

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 oligosaccharides 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.