wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 12:48 PM EDT

PDB ID	:	4KZZ
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 (i) 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 (1)) were used in the production of this report:

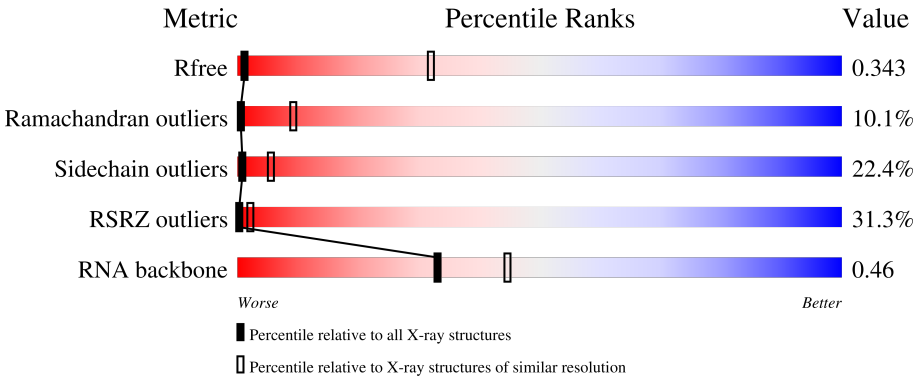
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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}	130704	1004 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)
RNA backbone	3102	1078 (10.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	14% 46% 20% • • 29%
2	B	264	28% 55% 23% • 19%
3	C	278	39% 58% 20% • • 19%
4	D	243	68% 63% 26% 5% 7%
5	E	263	51% 66% 29% •

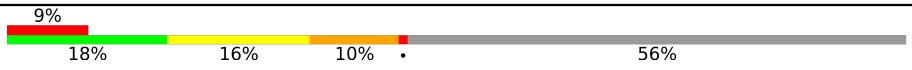
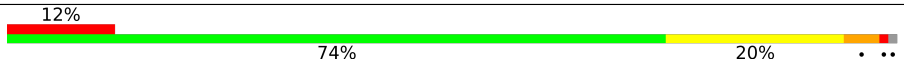
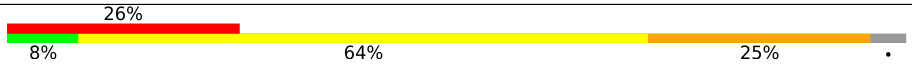
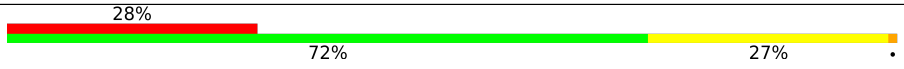
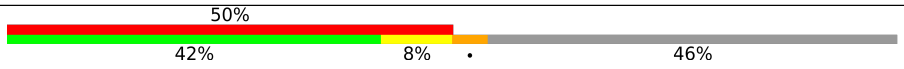
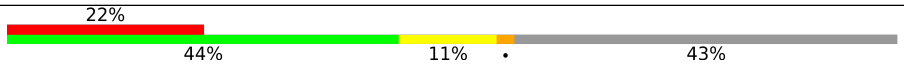
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	204	75% 66% 21% 6%
7	G	249	29% 65% 26% 5%
8	H	194	11% 61% 26% 7%
9	I	208	57% 70% 20% 8%
10	J	194	18% 58% 26% 8% 6%
11	K	165	18% 31% 15% 8% 5% 41%
12	L	158	39% 66% 26%
13	M	132	4% 62% 25% 7% 6%
14	N	151	15% 68% 30%
15	O	151	34% 60% 27% 10%
16	P	145	49% 50% 27% 8% 12%
17	Q	146	34% 68% 23% 5%
18	R	135	10% 66% 17% 7% 7%
19	S	152	16% 59% 20% 9% 10%
20	T	145	5% 70% 21% 5%
21	U	119	54% 48% 30% 5% 13%
22	V	83	14% 54% 30% 13%
23	W	130	36% 81% 16%
24	X	143	43% 68% 26% 6%
25	Y	133	7% 59% 26% 8% 5%
26	Z	125	10% 38% 16% 5% 40%
27	a	115	23% 63% 22% 7% 7%
28	b	84	7% 65% 25% 10%
29	c	69	52% 65% 20% 7% 7%
30	d	56	38% 66% 27% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
			Total	C	N	O	S			
1	A	208	1642	1045	289	300	8	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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.

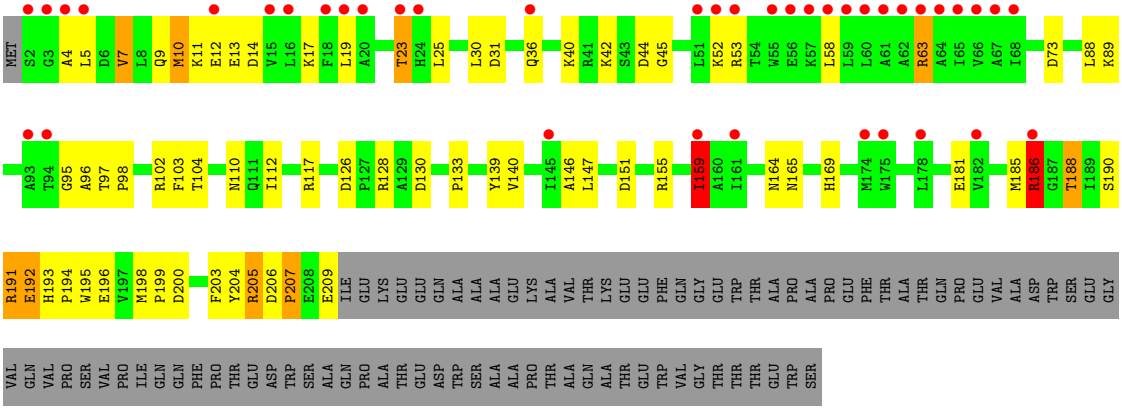
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	n	82	Total	C	N	O	S	0	0	0
			648	407	119	118	4			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

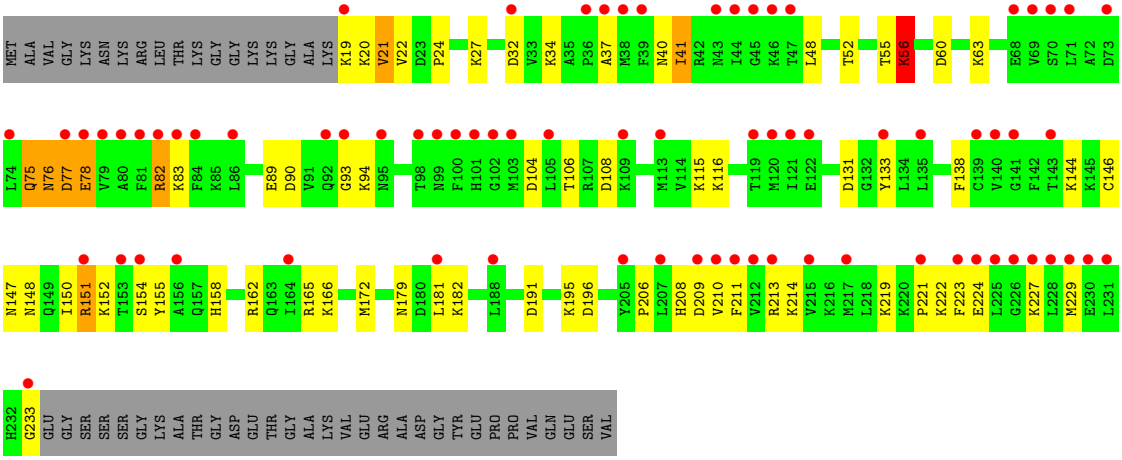
• Molecule 1: 40S Ribosomal Protein SA

Chain A:



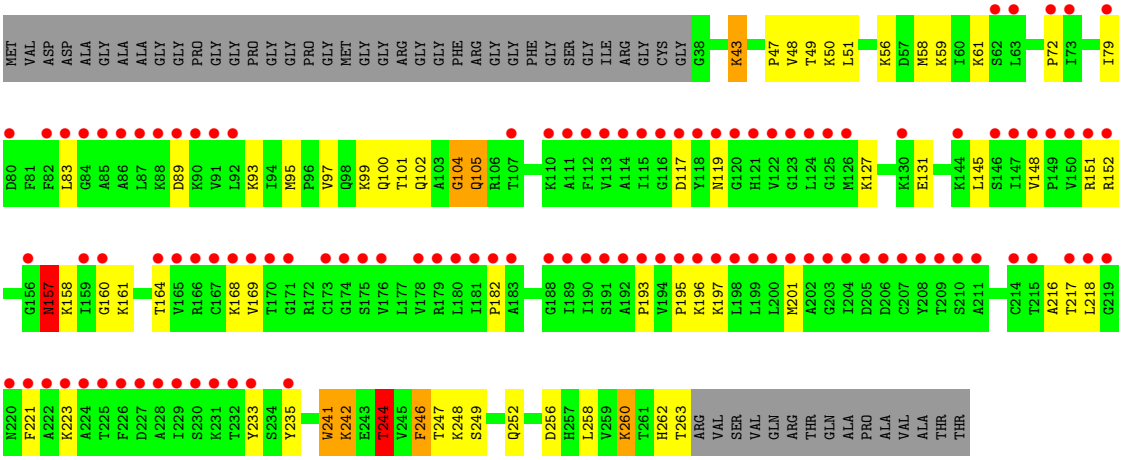
• Molecule 2: 40S Ribosomal Protein S3A

Chain B:



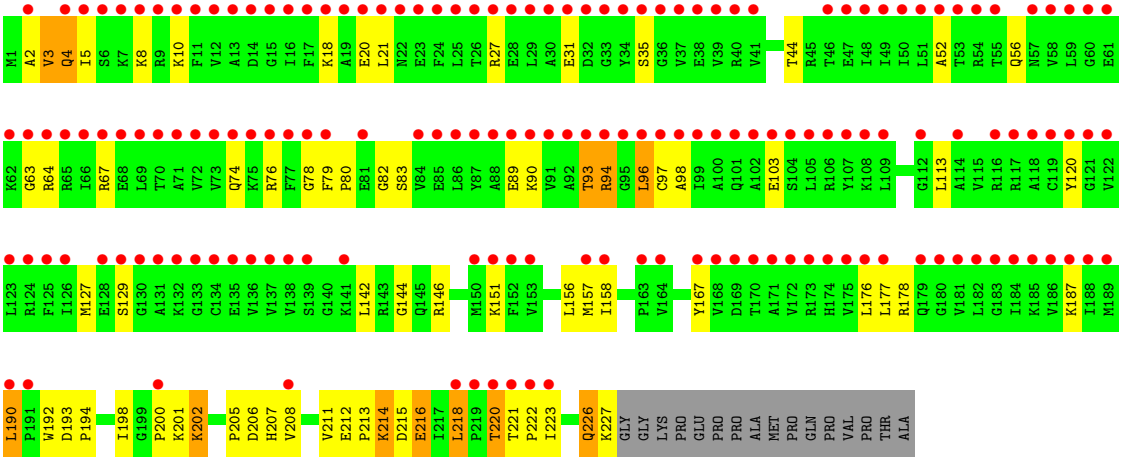
• Molecule 3: 40S Ribosomal Protein S2

Chain C:



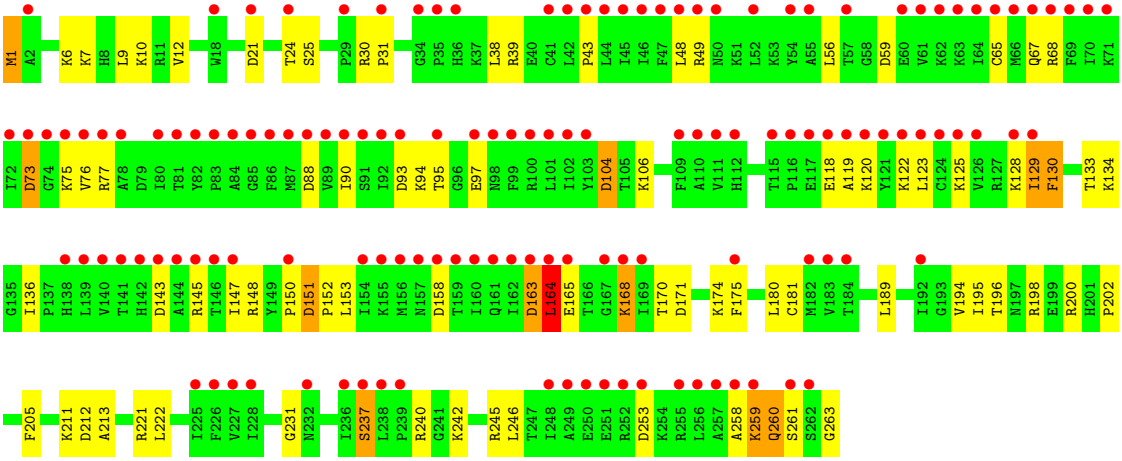
• Molecule 4: 40S Ribosomal Protein S3

Chain D:



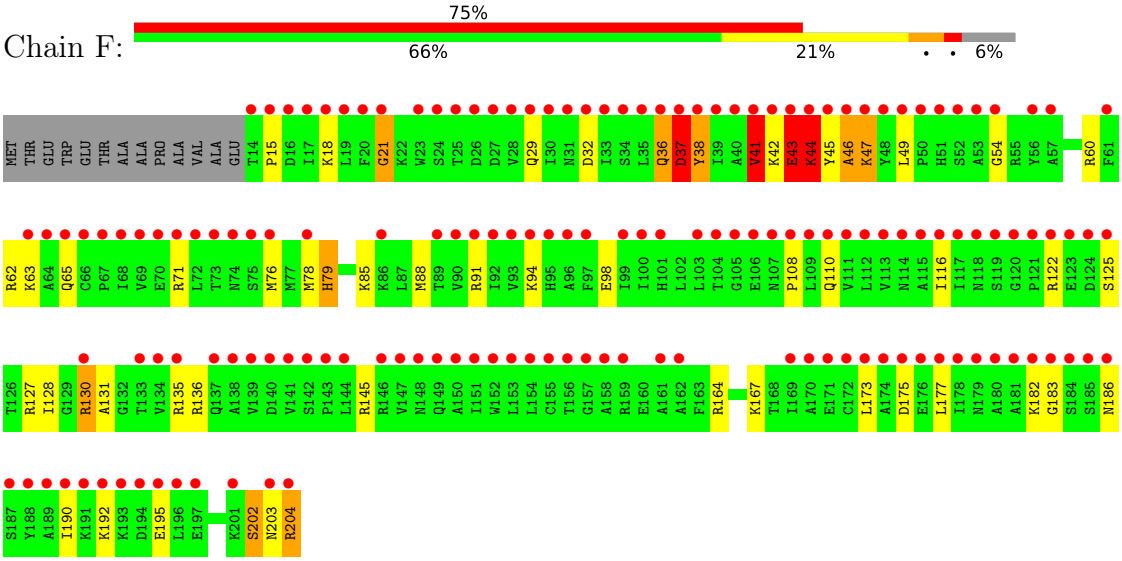
• Molecule 5: 40S Ribosomal Protein S4X

Chain E:



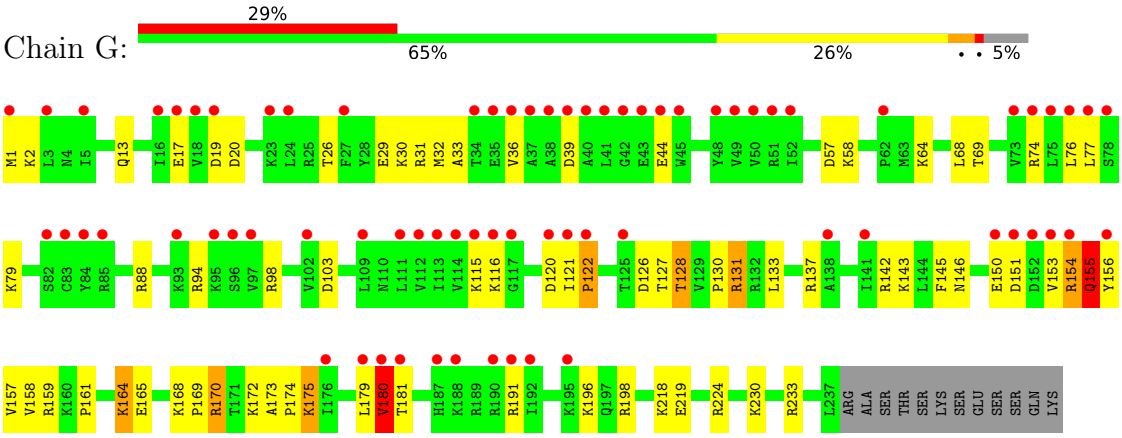
• Molecule 6: 40S Ribosomal Protein S5

Chain F:



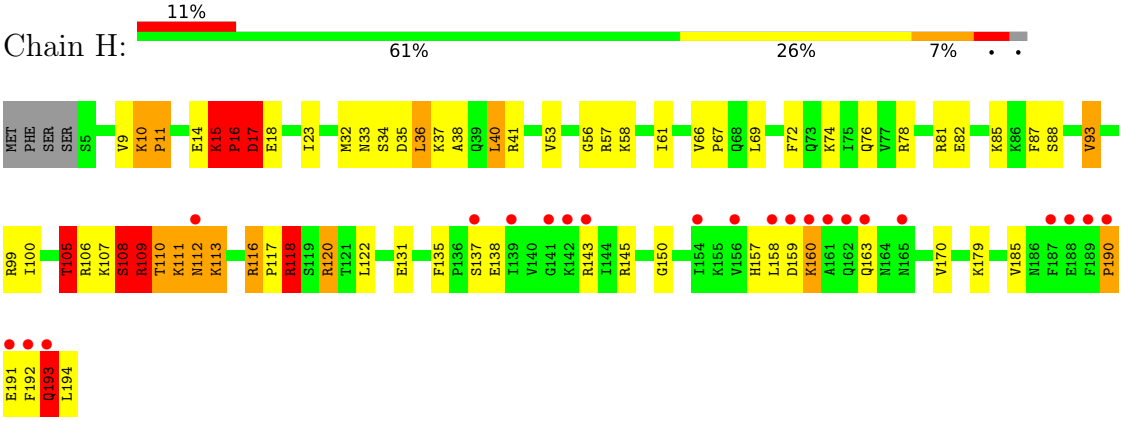
• Molecule 7: 40S Ribosomal Protein S6

Chain G:



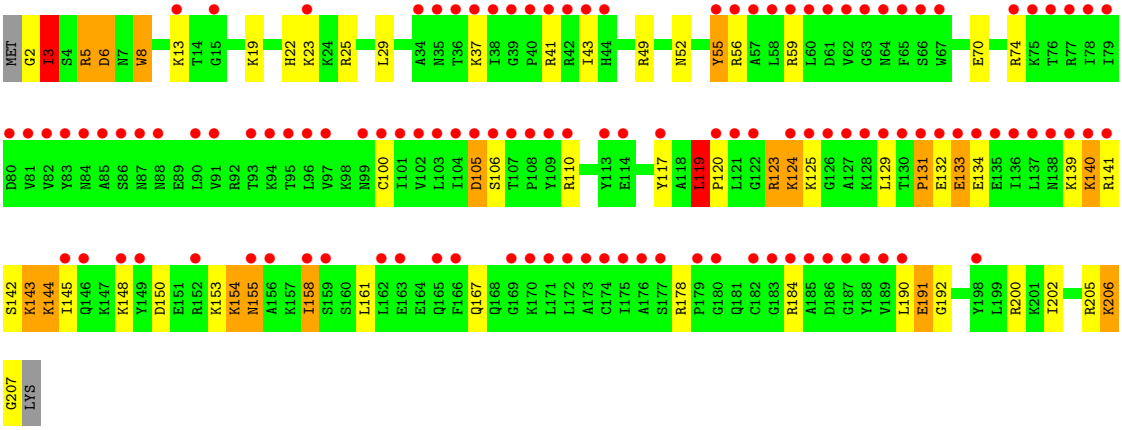
• Molecule 8: 40S Ribosomal Protein S7

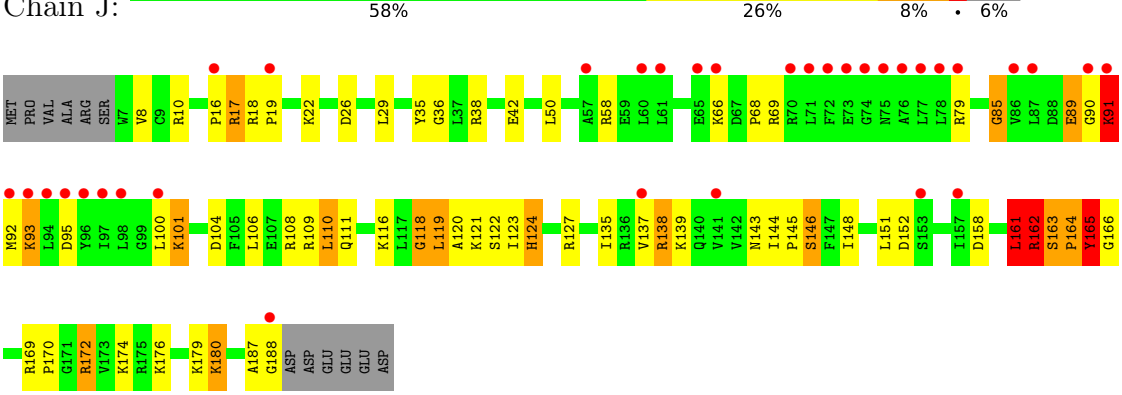
Chain H:



• Molecule 9: 40S Ribosomal Protein S8

Chain I:



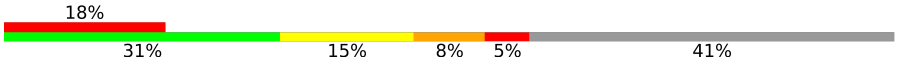


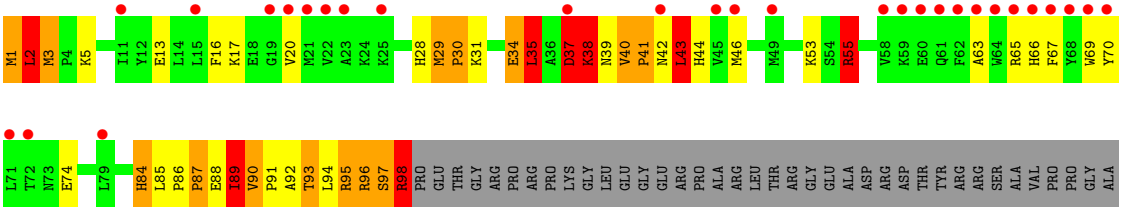
• Molecule 10: 40S Ribosomal Protein S9

Chain J:

• Molecule 11: 40S Ribosomal Protein S10

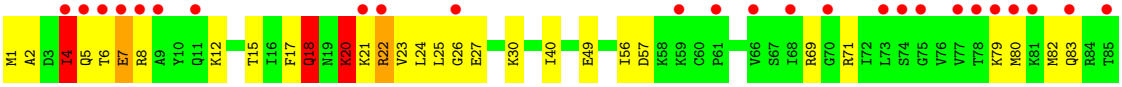
Chain K:

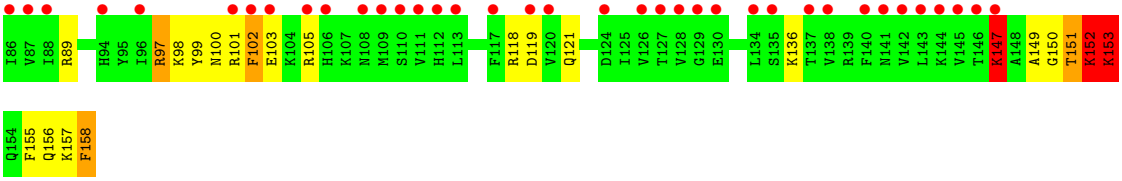




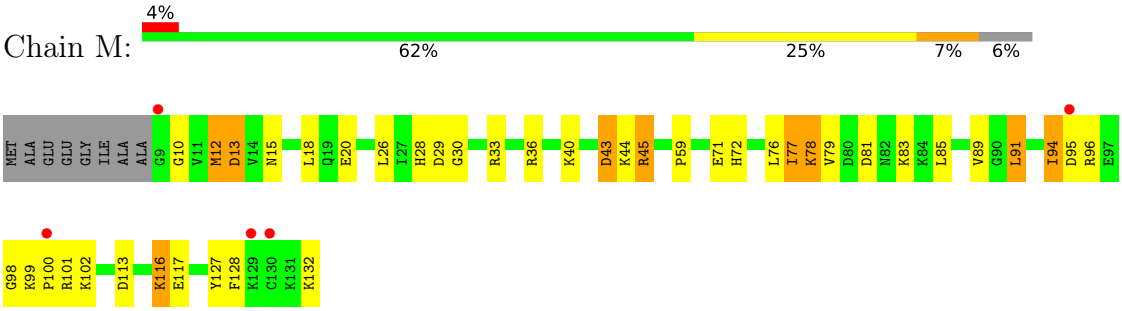
• Molecule 12: 40S Ribosomal Protein S11

Chain L:

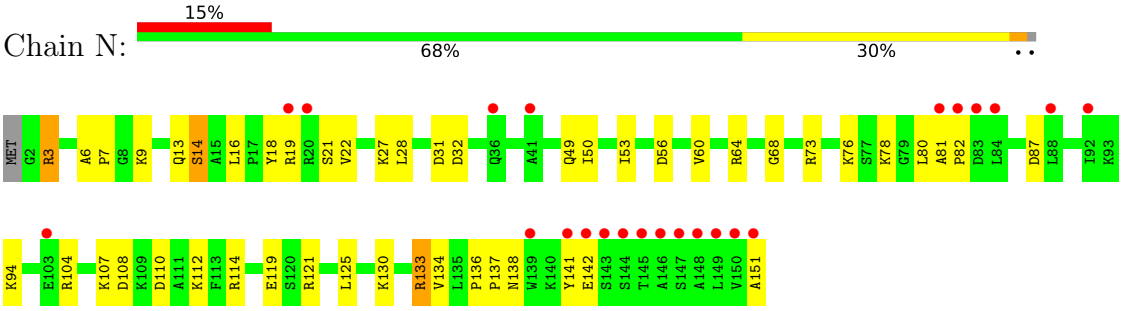




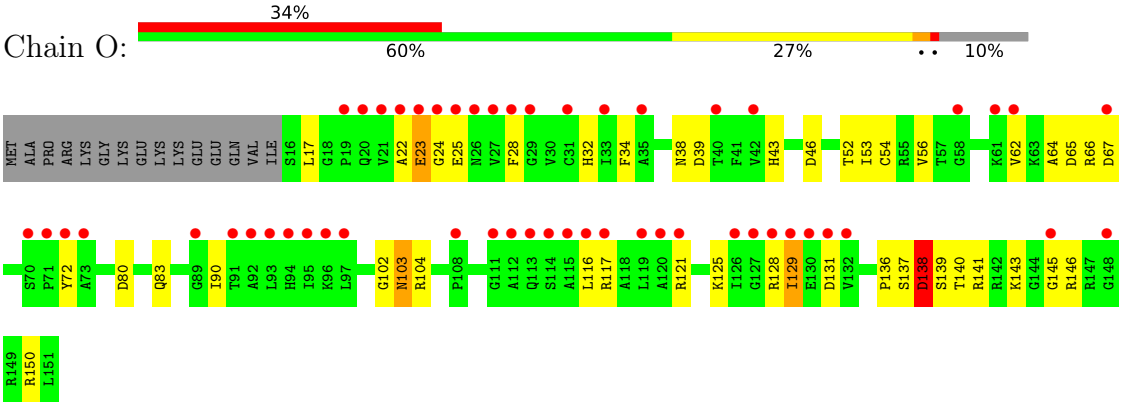
• Molecule 13: 40S Ribosomal Protein S12



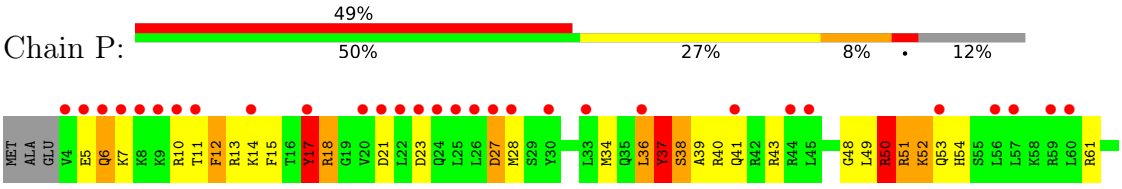
• Molecule 14: 40S Ribosomal Protein S13

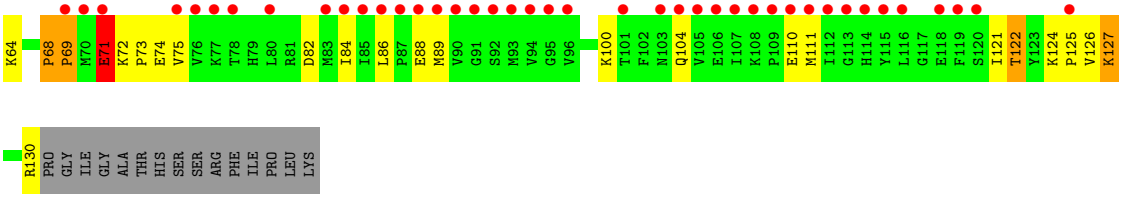


• Molecule 15: 40S Ribosomal Protein S14



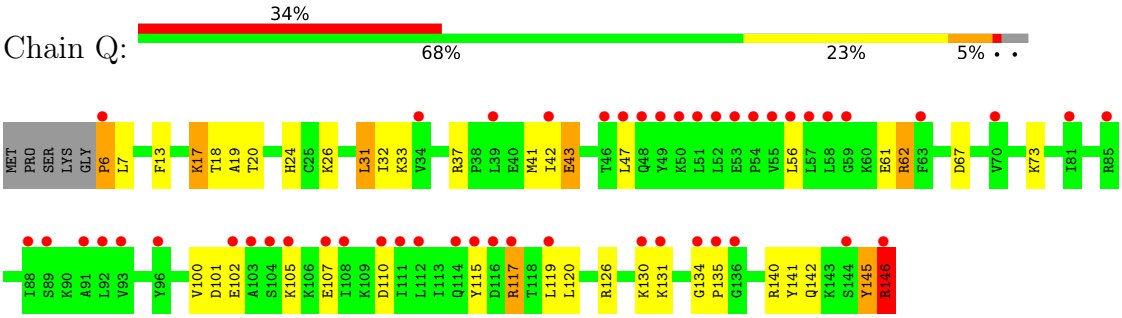
• Molecule 16: 40S Ribosomal Protein S15





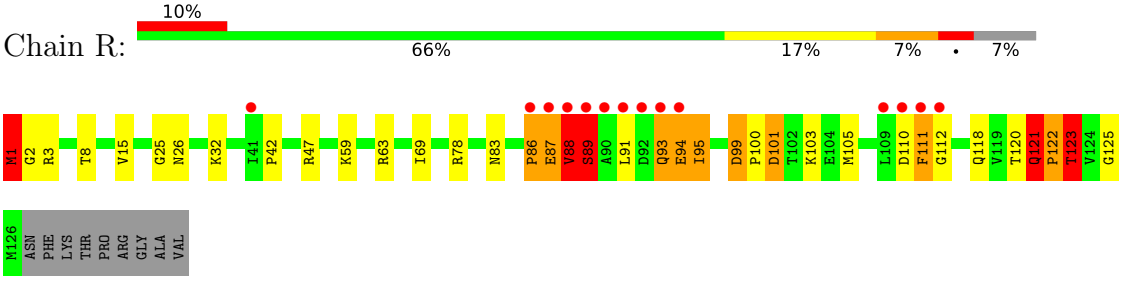
• Molecule 17: 40S Ribosomal Protein S16

Chain Q:



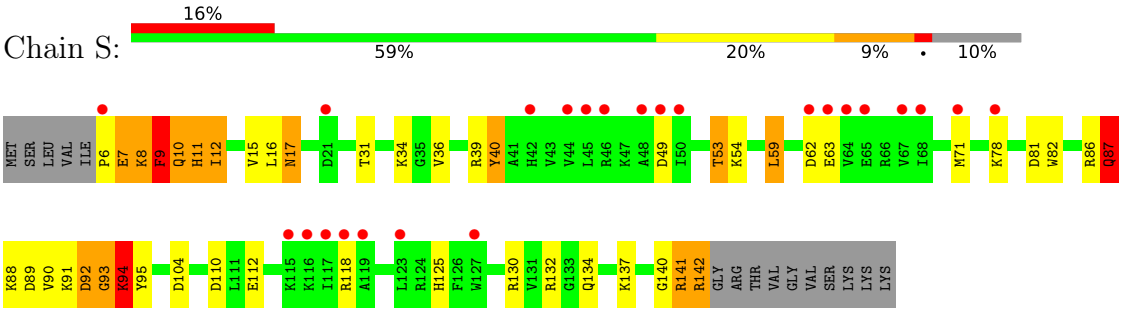
• Molecule 18: 40S Ribosomal Protein S17

Chain R:



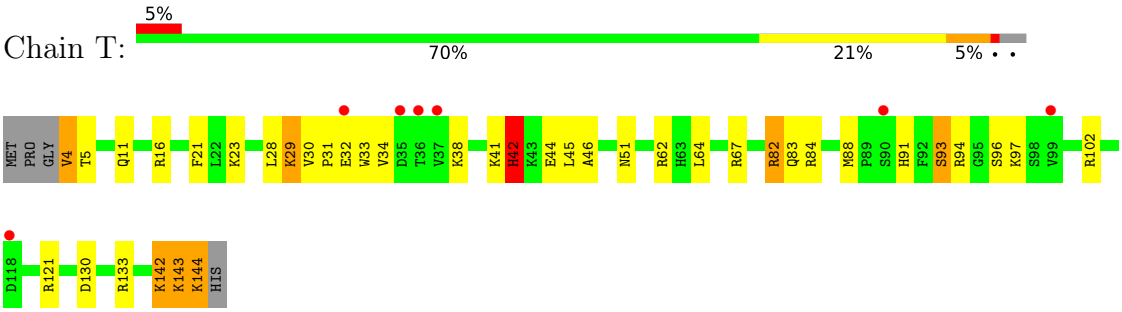
• Molecule 19: 40S Ribosomal Protein S18

Chain S:

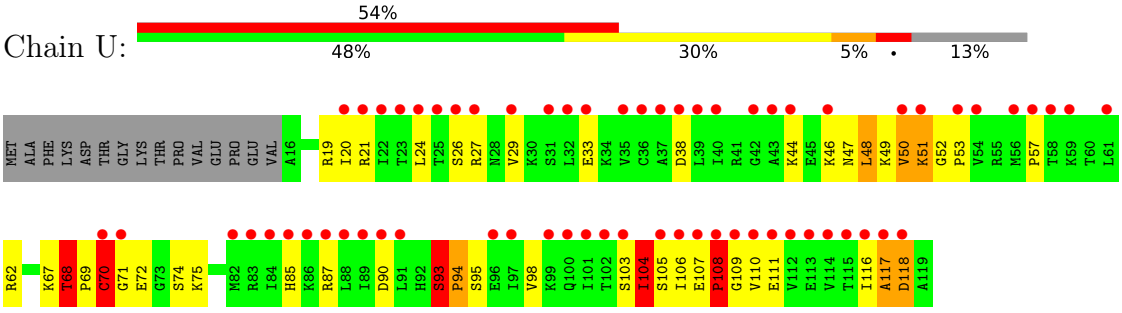


• Molecule 20: 40S Ribosomal Protein S19

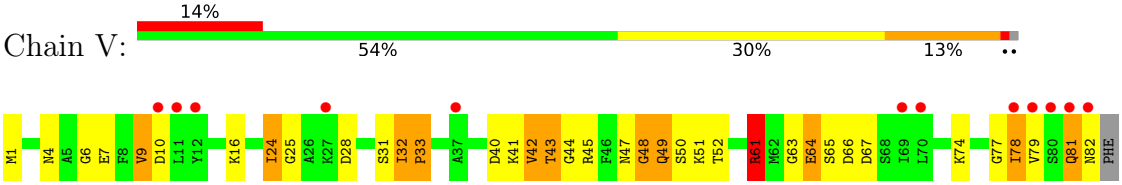
Chain T:



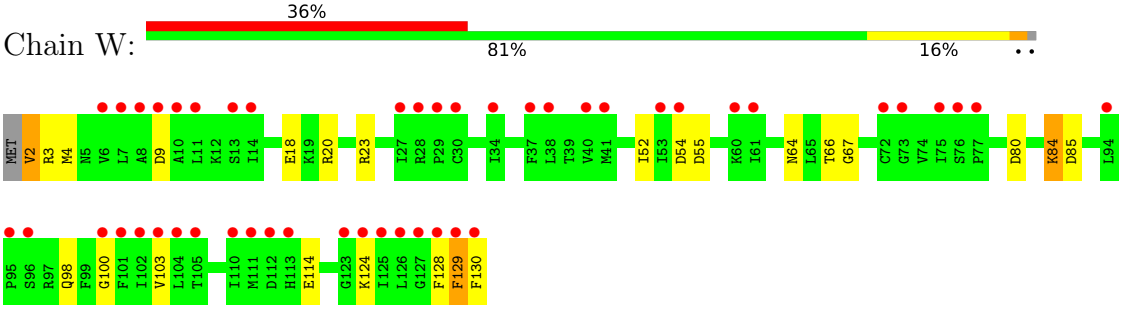
• Molecule 21: 40S Ribosomal Protein S20



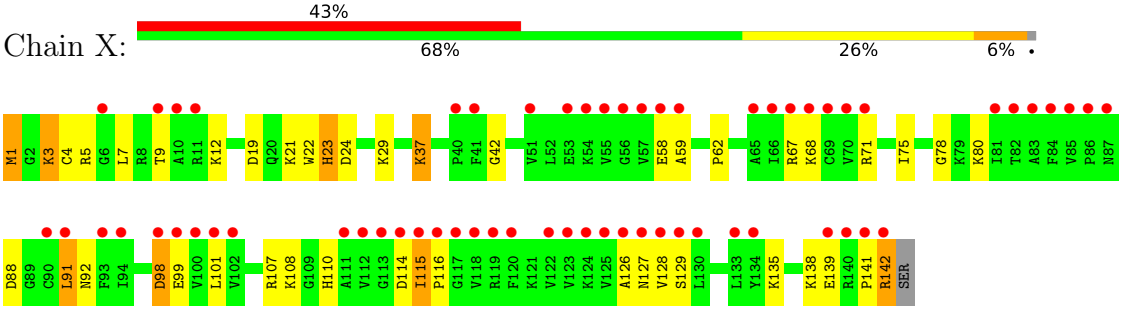
• Molecule 22: 40S Ribosomal Protein S21



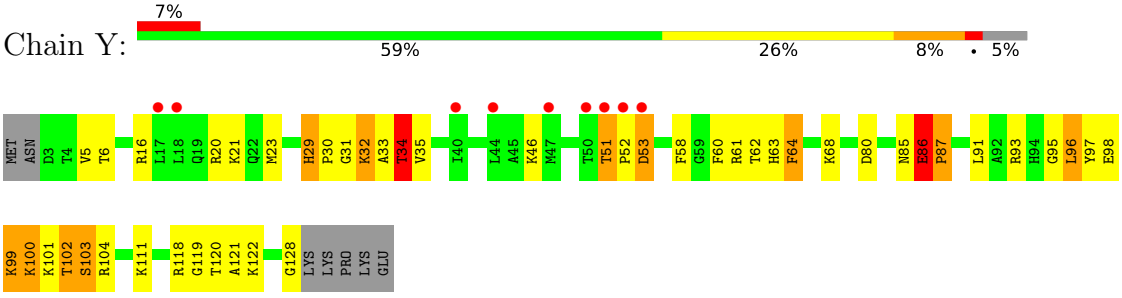
• Molecule 23: 40S Ribosomal Protein S15A



• Molecule 24: 40S Ribosomal Protein S23

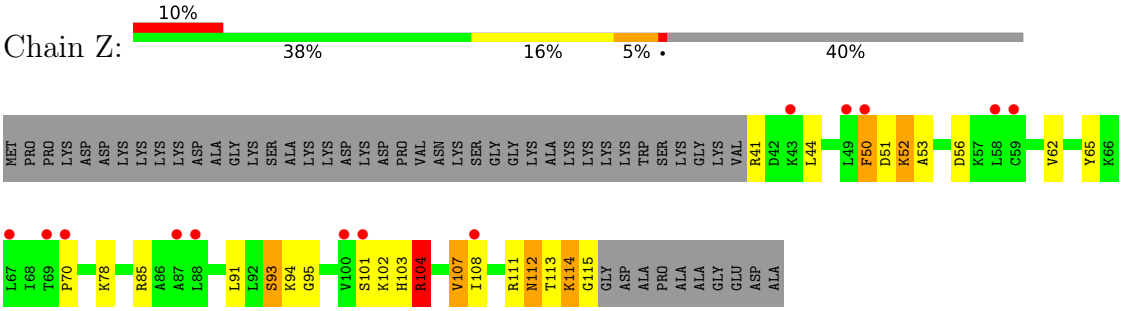


• Molecule 25: 40S Ribosomal Protein S24



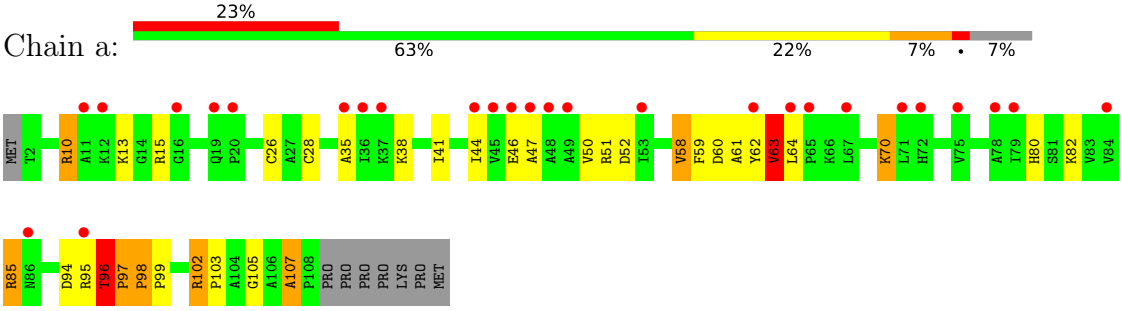
• Molecule 26: 40S Ribosomal Protein S25

Chain Z:



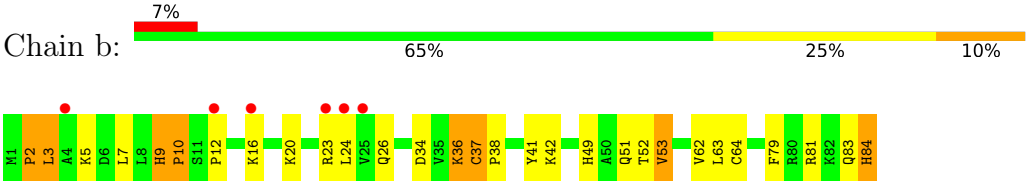
• Molecule 27: 40S Ribosomal Protein S26

Chain a:



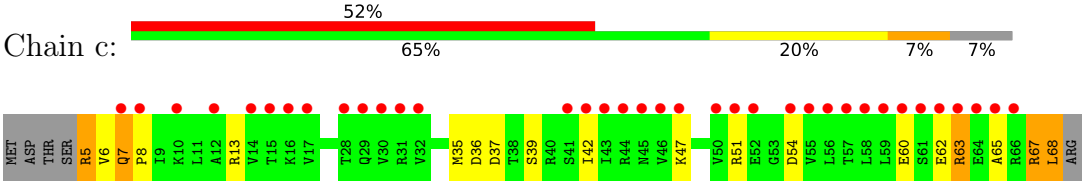
• Molecule 28: 40S Ribosomal Protein S27

Chain b:



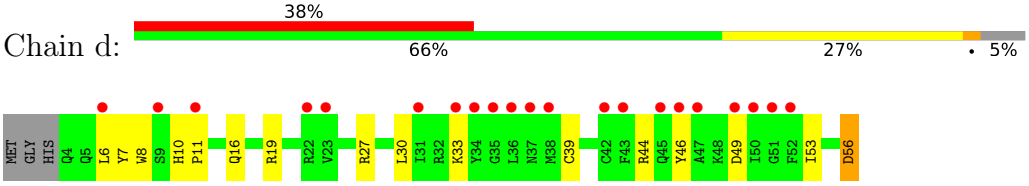
• Molecule 29: 40S Ribosomal Protein S28

Chain c:



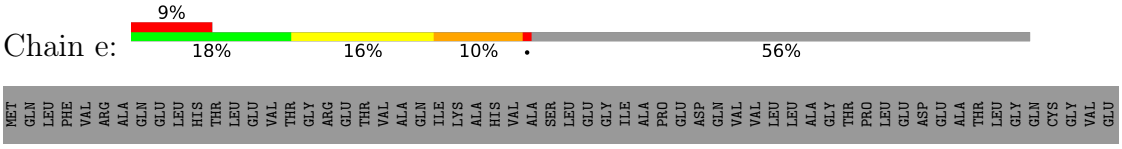
• Molecule 30: 40S Ribosomal Protein S29

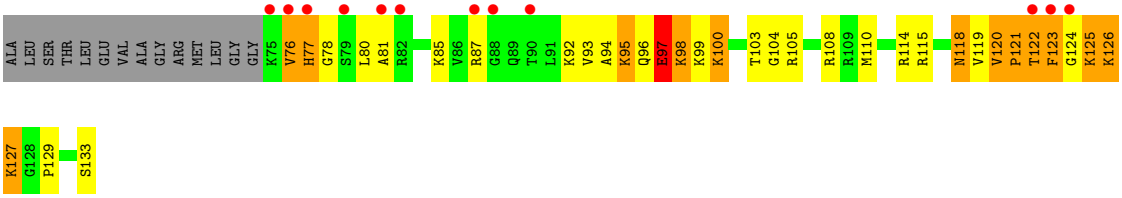
Chain d:



• Molecule 31: 40S Ribosomal Protein S30

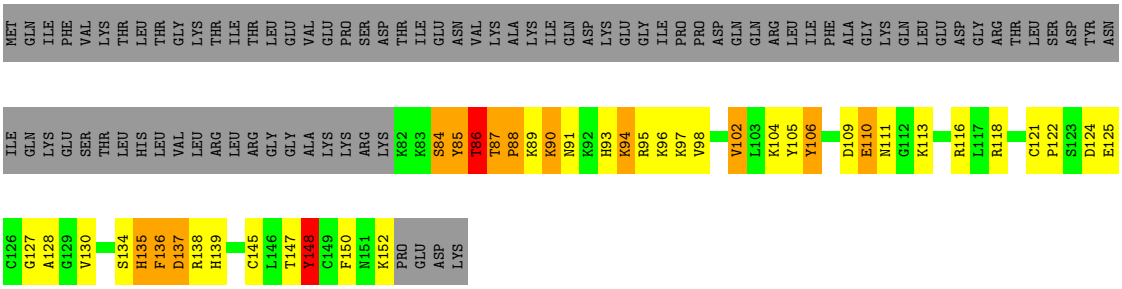
Chain e:





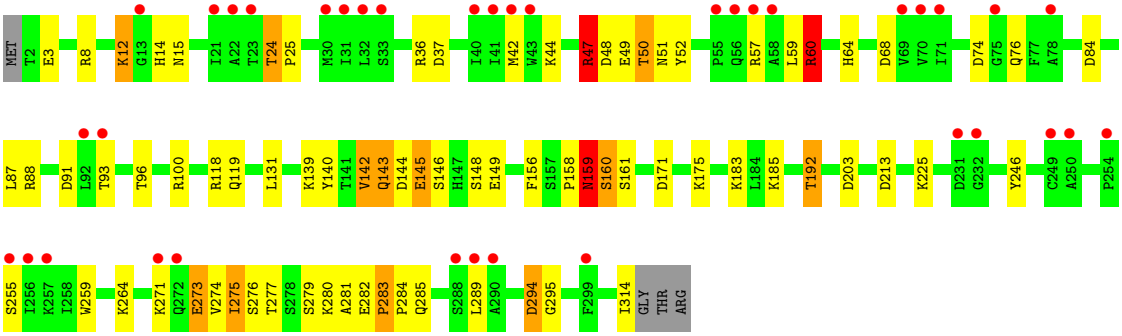
• Molecule 32: 40S Ribosomal Protein S27A

Chain f:



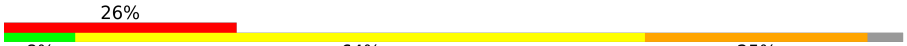
• Molecule 33: 40S Ribosomal Protein RACK1

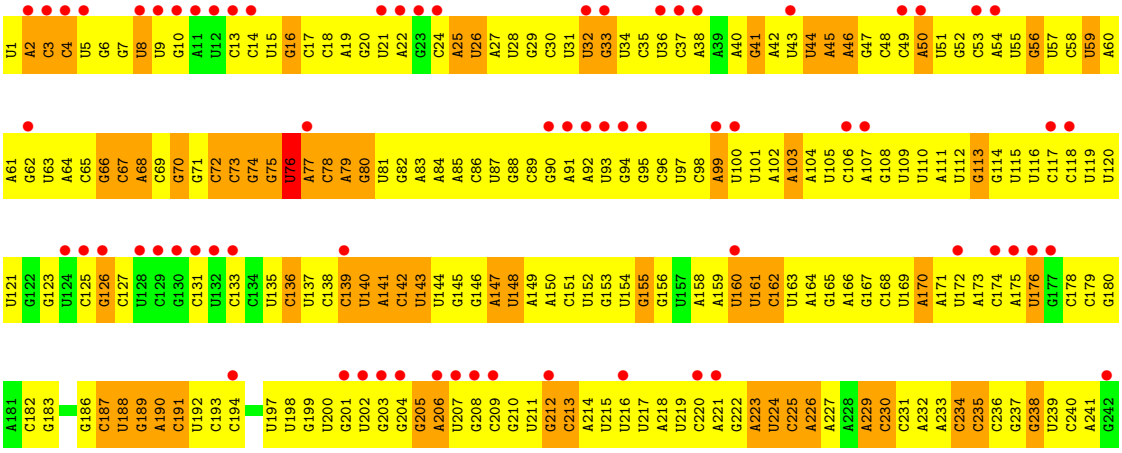
Chain g:

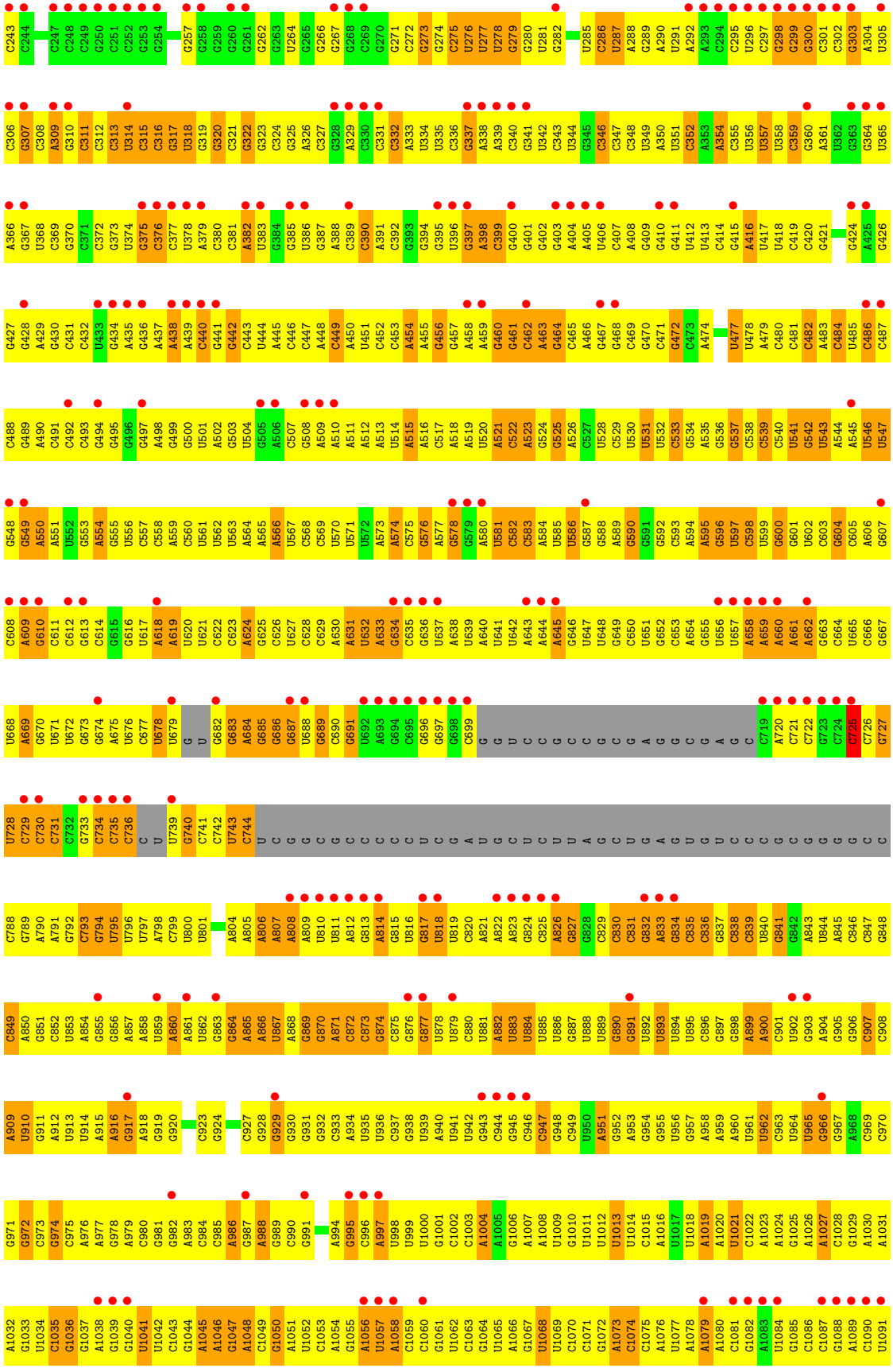


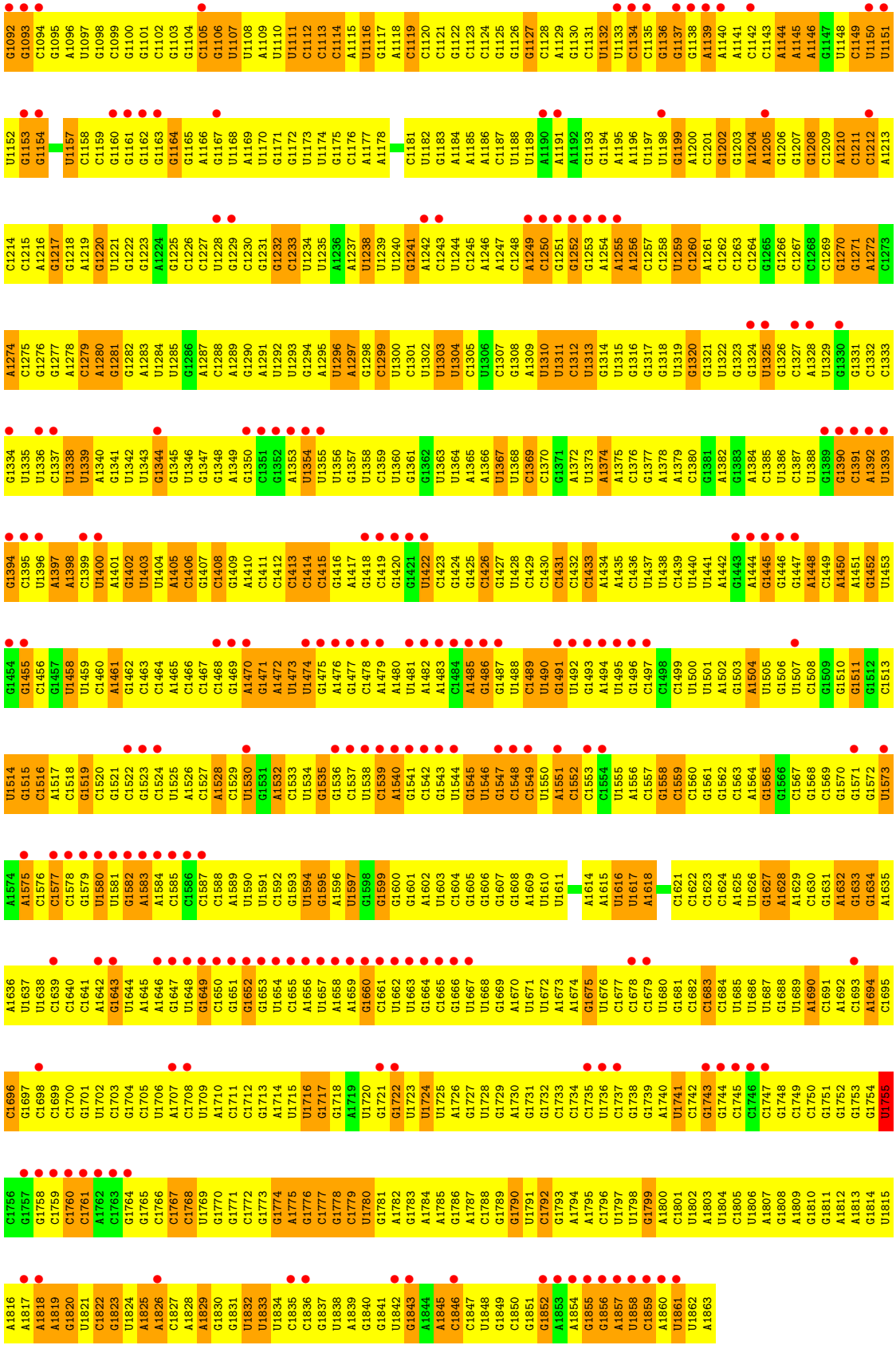
• Molecule 34: 18S Ribosomal RNA

Chain i:



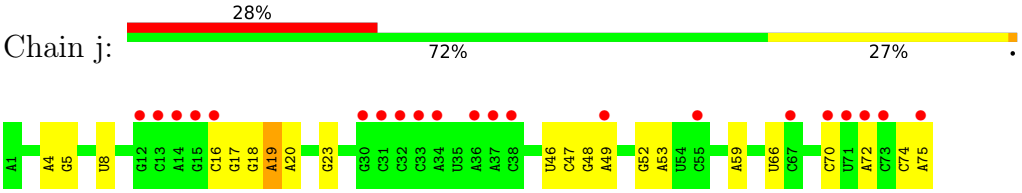






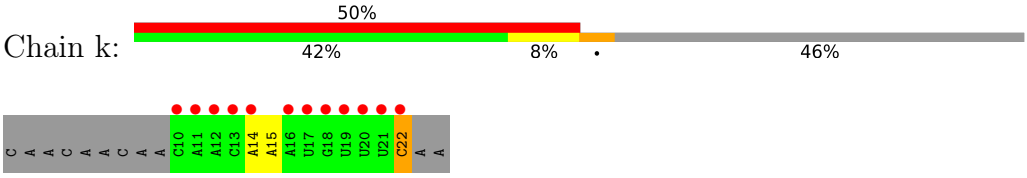
• Molecule 35: initiator Met-RNA-i

Chain j:



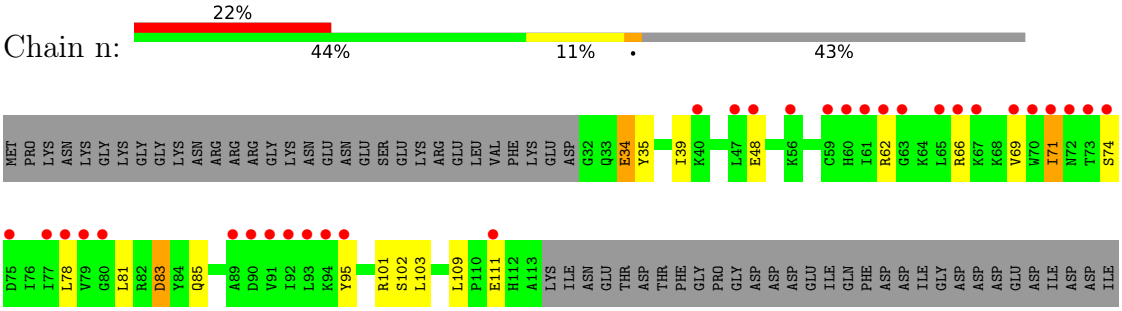
• Molecule 36: mRNA

Chain k:



• Molecule 37: human initiation factor eIF1A

Chain n:



4 Data and refinement statistics (i)

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) 98.7 (77.53-7.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 6.72Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.345 , 0.359 0.339 , 0.343	Depositor DCC
R_{free} test set	1946 reflections (5.01%)	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)	0.22 , 125.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	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.*

[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	A	0.76	2/1679 (0.1%)	1.06	17/2283 (0.7%)
2	B	0.79	7/1769 (0.4%)	1.08	22/2367 (0.9%)
3	C	0.97	7/1778 (0.4%)	1.19	18/2399 (0.8%)
4	D	1.03	6/1792 (0.3%)	1.30	22/2412 (0.9%)
5	E	0.76	5/2125 (0.2%)	0.98	23/2856 (0.8%)
6	F	0.99	5/1531 (0.3%)	1.21	17/2059 (0.8%)
7	G	0.97	15/1946 (0.8%)	1.23	25/2590 (1.0%)
8	H	1.09	7/1553 (0.5%)	2.19	29/2079 (1.4%)
9	I	1.11	7/1708 (0.4%)	1.51	33/2278 (1.4%)
10	J	1.27	19/1522 (1.2%)	1.51	42/2031 (2.1%)
11	K	1.21	6/851 (0.7%)	1.78	31/1147 (2.7%)
12	L	1.10	6/1319 (0.5%)	1.40	17/1761 (1.0%)
13	M	1.00	3/960 (0.3%)	1.23	7/1287 (0.5%)
14	N	0.83	4/1232 (0.3%)	1.01	12/1656 (0.7%)
15	O	0.61	0/1029	1.05	12/1380 (0.9%)
16	P	0.75	1/1079 (0.1%)	1.43	32/1437 (2.2%)
17	Q	0.71	3/1142 (0.3%)	1.11	15/1528 (1.0%)
18	R	1.23	10/1031 (1.0%)	1.64	30/1383 (2.2%)
19	S	1.21	10/1157 (0.9%)	1.61	36/1548 (2.3%)
20	T	0.95	3/1132 (0.3%)	1.26	13/1517 (0.9%)
21	U	0.96	1/832 (0.1%)	1.59	29/1117 (2.6%)
22	V	0.75	1/626 (0.2%)	1.39	15/839 (1.8%)
23	W	0.85	4/1051 (0.4%)	0.86	9/1406 (0.6%)
24	X	1.00	8/1124 (0.7%)	1.24	21/1500 (1.4%)
25	Y	0.93	3/1038 (0.3%)	1.42	21/1380 (1.5%)
26	Z	1.04	5/604 (0.8%)	1.35	17/810 (2.1%)
27	a	0.89	4/860 (0.5%)	1.60	21/1156 (1.8%)
28	b	1.02	2/673 (0.3%)	1.36	12/902 (1.3%)
29	c	0.80	1/508 (0.2%)	1.18	8/680 (1.2%)
30	d	0.90	2/455 (0.4%)	0.79	3/603 (0.5%)
31	e	1.47	5/478 (1.0%)	1.43	11/628 (1.8%)
32	f	1.10	4/593 (0.7%)	1.49	16/786 (2.0%)
33	g	0.91	1/2493 (0.0%)	1.29	27/3394 (0.8%)
34	i	2.41	1848/41879 (4.4%)	2.21	2565/65157 (3.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	j	0.67	5/1798 (0.3%)	0.82	0/2802
36	k	1.64	1/304 (0.3%)	1.35	3/470 (0.6%)
37	n	0.40	0/657	0.38	0/881
All	All	1.83	2021/84308 (2.4%)	1.84	3231/122509 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 2021 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	22	C	C1'-N1	28.08	1.90	1.48
34	i	1322	U	C2'-C1'	-25.56	1.25	1.53
34	i	66	G	C2'-C1'	-24.65	1.26	1.53
34	i	652	G	C2'-C1'	-23.81	1.27	1.53
34	i	858	A	C2'-C1'	-23.76	1.27	1.53

The worst 5 of 3231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	109	ARG	NE-CZ-NH2	-53.45	93.58	120.30
8	H	109	ARG	NE-CZ-NH1	42.58	141.59	120.30
34	i	1774	G	P-O3'-C3'	38.31	165.68	119.70
34	i	1114	C	O4'-C1'-N1	35.28	136.42	108.20
34	i	582	C	O4'-C1'-N1	32.53	134.22	108.20

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

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 14
3	C	224/278 (81%)	199 (89%)	14 (6%)	11 (5%)	2 20
4	D	225/243 (93%)	180 (80%)	23 (10%)	22 (10%)	0 9
5	E	261/263 (99%)	210 (80%)	27 (10%)	24 (9%)	1 11
6	F	189/204 (93%)	162 (86%)	15 (8%)	12 (6%)	1 17
7	G	235/249 (94%)	201 (86%)	19 (8%)	15 (6%)	1 16
8	H	188/194 (97%)	146 (78%)	11 (6%)	31 (16%)	0 3
9	I	204/208 (98%)	169 (83%)	13 (6%)	22 (11%)	0 8
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%)	1 11
13	M	122/132 (92%)	85 (70%)	16 (13%)	21 (17%)	0 3
14	N	148/151 (98%)	123 (83%)	19 (13%)	6 (4%)	3 22
15	O	134/151 (89%)	101 (75%)	14 (10%)	19 (14%)	0 4
16	P	125/145 (86%)	92 (74%)	16 (13%)	17 (14%)	0 4
17	Q	139/146 (95%)	110 (79%)	19 (14%)	10 (7%)	1 14
18	R	124/135 (92%)	97 (78%)	13 (10%)	14 (11%)	0 7
19	S	135/152 (89%)	106 (78%)	20 (15%)	9 (7%)	1 15
20	T	139/145 (96%)	119 (86%)	10 (7%)	10 (7%)	1 14
21	U	102/119 (86%)	76 (74%)	10 (10%)	16 (16%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	V	80/83 (96%)	55 (69%)	11 (14%)	14 (18%)	0 2
23	W	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	9 44
24	X	140/143 (98%)	121 (86%)	11 (8%)	8 (6%)	1 18
25	Y	124/133 (93%)	91 (73%)	15 (12%)	18 (14%)	0 4
26	Z	73/125 (58%)	52 (71%)	12 (16%)	9 (12%)	0 5
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 12
30	d	51/56 (91%)	46 (90%)	3 (6%)	2 (4%)	3 23
31	e	57/133 (43%)	37 (65%)	7 (12%)	13 (23%)	0 2
32	f	69/156 (44%)	38 (55%)	13 (19%)	18 (26%)	0 1
33	g	311/317 (98%)	271 (87%)	23 (7%)	17 (6%)	2 19
37	n	80/144 (56%)	61 (76%)	15 (19%)	4 (5%)	2 20
All	All	4906/5679 (86%)	3899 (80%)	510 (10%)	497 (10%)	0 9

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 (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
1	A	174/244 (71%)	139 (80%)	35 (20%)	1 7
2	B	196/231 (85%)	155 (79%)	41 (21%)	1 6
3	C	187/215 (87%)	147 (79%)	40 (21%)	1 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	190/202 (94%)	144 (76%)	46 (24%)	0 4
5	E	225/225 (100%)	173 (77%)	52 (23%)	1 4
6	F	161/170 (95%)	116 (72%)	45 (28%)	0 3
7	G	207/218 (95%)	157 (76%)	50 (24%)	0 4
8	H	170/174 (98%)	124 (73%)	46 (27%)	0 3
9	I	177/179 (99%)	142 (80%)	35 (20%)	1 8
10	J	157/168 (94%)	128 (82%)	29 (18%)	1 9
11	K	89/136 (65%)	61 (68%)	28 (32%)	0 2
12	L	142/142 (100%)	105 (74%)	37 (26%)	0 3
13	M	101/108 (94%)	78 (77%)	23 (23%)	1 5
14	N	130/131 (99%)	103 (79%)	27 (21%)	1 6
15	O	106/119 (89%)	87 (82%)	19 (18%)	2 10
16	P	116/130 (89%)	84 (72%)	32 (28%)	0 3
17	Q	117/121 (97%)	89 (76%)	28 (24%)	0 4
18	R	114/121 (94%)	90 (79%)	24 (21%)	1 6
19	S	119/132 (90%)	95 (80%)	24 (20%)	1 7
20	T	113/116 (97%)	87 (77%)	26 (23%)	1 4
21	U	94/107 (88%)	74 (79%)	20 (21%)	1 6
22	V	67/68 (98%)	50 (75%)	17 (25%)	0 3
23	W	112/113 (99%)	98 (88%)	14 (12%)	4 19
24	X	114/115 (99%)	91 (80%)	23 (20%)	1 7
25	Y	108/115 (94%)	85 (79%)	23 (21%)	1 6
26	Z	66/103 (64%)	53 (80%)	13 (20%)	1 8
27	a	91/99 (92%)	76 (84%)	15 (16%)	2 12
28	b	76/76 (100%)	63 (83%)	13 (17%)	2 11
29	c	57/62 (92%)	46 (81%)	11 (19%)	1 8
30	d	47/49 (96%)	35 (74%)	12 (26%)	0 3
31	e	49/106 (46%)	26 (53%)	23 (47%)	0 0
32	f	64/140 (46%)	43 (67%)	21 (33%)	0 2
33	g	272/275 (99%)	224 (82%)	48 (18%)	2 11
37	n	66/123 (54%)	48 (73%)	18 (27%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4274/4833 (88%)	3316 (78%)	958 (22%)	1 5

5 of 958 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	79	LYS
32	f	121	CYS
16	P	74	GLU
32	f	96	LYS
37	n	69	VAL

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	28	HIS
33	g	76	GLN
17	Q	80	GLN
33	g	64	HIS
27	a	80	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	i	1720/1863 (92%)	496 (28%)	0
35	j	74/75 (98%)	17 (22%)	0
36	k	12/24 (50%)	3 (25%)	0
All	All	1806/1962 (92%)	516 (28%)	0

5 of 516 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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, 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	A	208/295 (70%)	0.77	40 (19%) 1 3	188, 273, 325, 347	0
2	B	215/264 (81%)	1.44	75 (34%) 0 2	140, 249, 309, 321	0
3	C	226/278 (81%)	2.76	109 (48%) 0 1	76, 163, 267, 284	0
4	D	227/243 (93%)	4.76	165 (72%) 0 0	110, 175, 253, 280	0
5	E	263/263 (100%)	2.66	135 (51%) 0 1	38, 138, 196, 225	0
6	F	191/204 (93%)	5.07	154 (80%) 0 0	133, 175, 212, 224	0
7	G	237/249 (95%)	1.41	73 (30%) 0 2	68, 198, 289, 311	0
8	H	190/194 (97%)	0.10	22 (11%) 4 8	129, 278, 329, 340	0
9	I	206/208 (99%)	3.73	119 (57%) 0 1	17, 164, 268, 289	0
10	J	182/194 (93%)	0.70	34 (18%) 1 4	73, 158, 221, 259	0
11	K	98/165 (59%)	1.83	29 (29%) 0 2	167, 238, 289, 308	0
12	L	158/158 (100%)	1.68	62 (39%) 0 1	22, 90, 224, 255	0
13	M	124/132 (93%)	-0.16	5 (4%) 38 34	280, 347, 384, 417	0
14	N	150/151 (99%)	0.74	23 (15%) 2 5	46, 118, 251, 261	0
15	O	136/151 (90%)	2.04	52 (38%) 0 1	45, 205, 320, 353	0
16	P	127/145 (87%)	3.24	71 (55%) 0 1	163, 254, 297, 310	0
17	Q	141/146 (96%)	1.87	49 (34%) 0 2	108, 200, 225, 231	0
18	R	126/135 (93%)	0.07	14 (11%) 5 9	130, 194, 302, 306	0
19	S	137/152 (90%)	0.95	24 (17%) 1 4	151, 218, 239, 249	0
20	T	141/145 (97%)	0.10	7 (4%) 28 28	161, 214, 230, 234	0
21	U	104/119 (87%)	3.99	64 (61%) 0 0	116, 213, 258, 269	0
22	V	82/83 (98%)	0.66	12 (14%) 2 6	175, 237, 316, 328	0
23	W	129/130 (99%)	1.72	47 (36%) 0 1	75, 141, 196, 216	0
24	X	142/143 (99%)	2.43	62 (43%) 0 1	22, 54, 84, 93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	126/133 (94%)	0.28	9 (7%) 16 16	85, 153, 198, 218	0
26	Z	75/125 (60%)	0.84	13 (17%) 1 4	197, 207, 217, 225	0
27	a	107/115 (93%)	1.57	27 (25%) 0 2	55, 111, 285, 317	0
28	b	84/84 (100%)	0.05	6 (7%) 16 16	156, 236, 276, 286	0
29	c	64/69 (92%)	2.52	36 (56%) 0 1	125, 173, 216, 221	0
30	d	53/56 (94%)	1.75	21 (39%) 0 1	136, 159, 235, 256	0
31	e	59/133 (44%)	0.73	12 (20%) 1 3	63, 136, 177, 192	0
32	f	71/156 (45%)	-0.55	0 100 100	145, 320, 392, 408	0
33	g	313/317 (98%)	0.39	37 (11%) 4 8	190, 248, 277, 291	0
34	i	1797/1863 (96%)	1.40	476 (26%) 0 2	13, 142, 348, 527	0
35	j	75/75 (100%)	1.24	21 (28%) 0 2	308, 379, 421, 436	0
36	k	13/24 (54%)	3.58	12 (92%) 0 0	186, 317, 324, 325	0
37	n	82/144 (56%)	1.71	31 (37%) 0 1	212, 216, 222, 224	0
All	All	6859/7641 (89%)	1.63	2148 (31%) 0 2	13, 190, 328, 527	0

The worst 5 of 2148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	i	697	G	34.6
34	i	698	G	32.3
4	D	95	GLY	24.0
34	i	696	G	22.1
34	i	695	C	22.1

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 monosaccharides 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.