wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 02:59 PM EST

PDB ID	:	4V4T
Title	:	Crystal structure of the whole ribosomal complex with a stop codon in the A-site.
Authors	:	Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2005-10-12
Resolution	:	6.46 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:

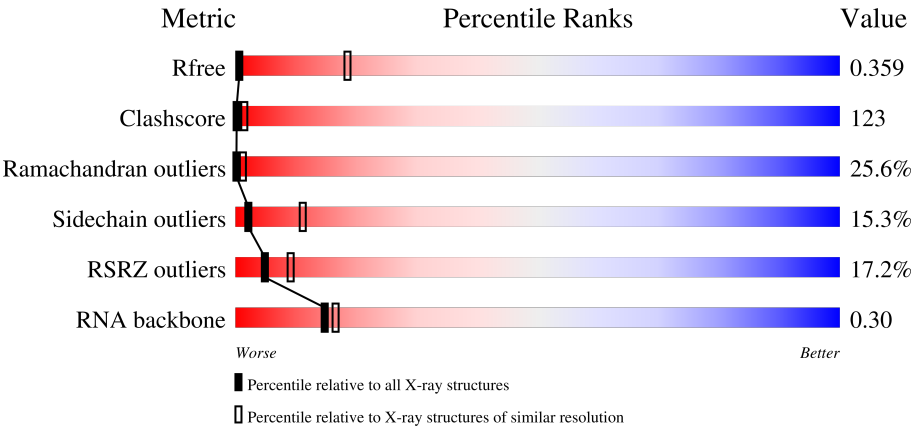
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 6.46 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}	164625	1095 (8.90-4.00)
Clashscore	180529	1136 (8.90-4.00)
Ramachandran outliers	177936	1005 (8.90-4.00)
Sidechain outliers	177891	1028 (8.90-3.96)
RSRZ outliers	164620	1090 (8.90-4.00)
RNA backbone	3690	1000 (9.50-3.02)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	3% 24% 42% 24% 9%
2	AV	76	11% 17% 61% 22%
3	AW	76	4% 28% 41% 21% 11%
4	AX	18	67% 61% 33% 6%

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Mol	Chain	Length	Quality of chain
5	AB	256	10% 44% 38% 7% • 9%
6	AC	239	6% 48% 30% 8% • 14%
7	AD	209	31% 35% 54% 10% •
8	AE	162	12% 47% 36% 10% 7%
9	AF	101	12% 67% 27% 5% •
10	AG	156	22% 58% 36% 5% •
11	AH	138	20% 39% 45% 15% •
12	AI	128	12% 55% 38% 5% ••
13	AJ	105	28% 41% 42% 10% 7%
14	AK	129	11% 49% 40% • • 8%
15	AL	135	27% 37% 44% 10% • 8%
16	AM	126	29% 52% 38% 9% ••
17	AN	61	30% 31% 59% 8% •
18	AO	89	30% 63% 29% 7% •
19	AP	88	35% 42% 40% 11% • 6%
20	AQ	105	29% 36% 55% 7% ••
21	AR	88	16% 41% 31% 11% 17%
22	AS	93	29% 41% 42% • 14%
23	AT	106	37% 50% 37% 7% 7%
24	AU	27	70% 26% 56% 7% 11%
25	BB	123	2% 31% 39% 28% •
26	BA	2916	5% 11% 34% 38% 13% •
27	BD	173	28% • 44% 46% 9%
28	BE	338	26% • 30% 21% • 43%
29	BF	246	27% • 37% 31% 7% 23%

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Mol	Chain	Length	Quality of chain
30	BG	176	21% 7% 39% 21% 31%
31	BH	177	14% 5% 50% 32% 6% 7%
32	BI	149	21% 6% 55% 34% 5%
33	BN	145	30% 36% 38% 5% 19%
34	BO	122	25% 61% 33%
35	BP	164	10% 5% 21% 23% 49%
36	BQ	138	38% 45% 46% 7%
37	BS	186	16% 28% 25% 5% 39%
38	BT	66	45% 6% 35% 29% 9% 21%
39	BW	113	19% 40% 50%
40	BX	84	54% 40% 31% 15% 10%
41	BY	119	34% 49% 31% 8% 8%
42	BZ	253	17% 35% 28% 30%
43	BR	118	25% 37% 46% 5% 11%
44	BU	118	32% 32% 50% 17%
45	BV	100	18% 9% 54% 33%
46	B2	70	31% 23% 49% 19% 9%
47	B3	60	30% 5% 57% 33% 5%
48	B0	91	23% 9% 42% 41% 5%
49	B4	73	45% 41% 49% 8%
50	B5	60	28% 48% 40% 5%
51	B6	82	16% 34% 27% 35%
52	B7	47	53% 21% 68% 9%
53	B8	64	47% 8% 38% 45% 8%
54	B9	36	67% 69% 25%

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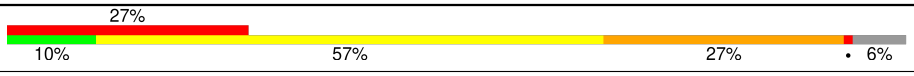
Mol	Chain	Length	Quality of chain
55	BK	141	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	YYG	AW	37	X	-	X	-

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 142447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	416	G	-	insertion	GB 155076
AA	905	U	-	insertion	GB 155076
AA	1395	C	-	insertion	GB 155076

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein 24.

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

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

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is a protein called 50S ribosomal protein L11.

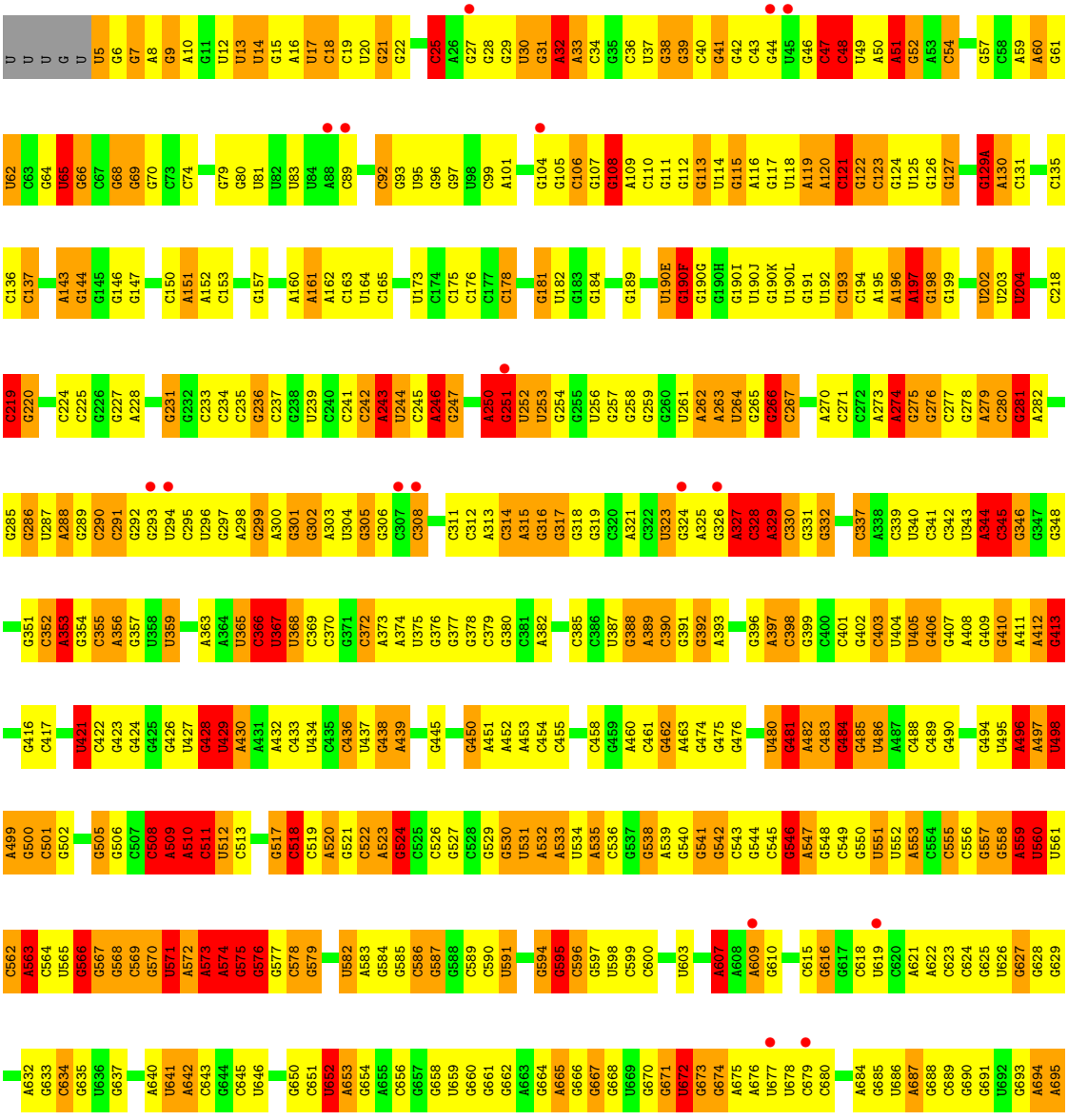
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BK	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

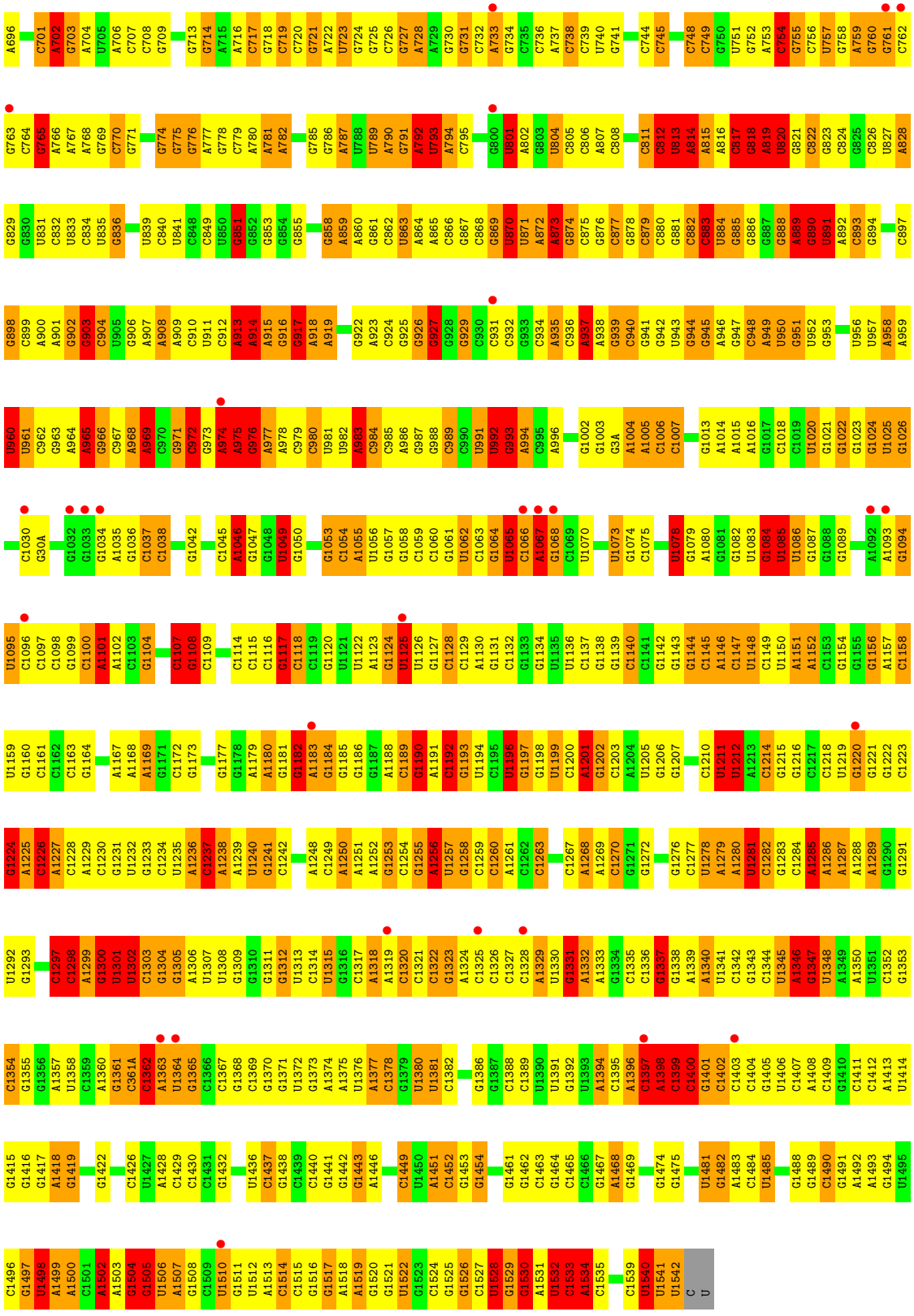
3 Residue-property plots (i)

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.

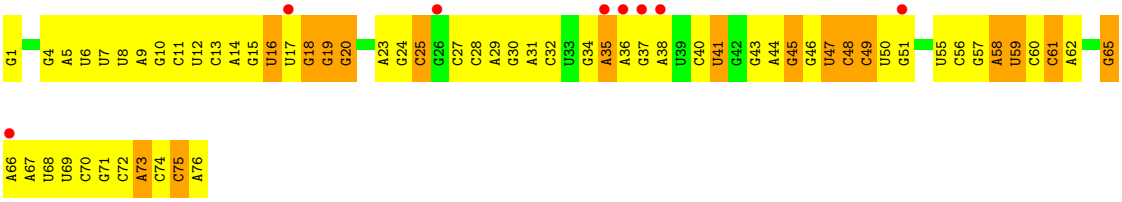
• Molecule 1: 16S ribosomal RNA

Chain AA: 3% 24% 42% 24% 9%



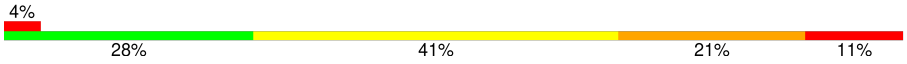


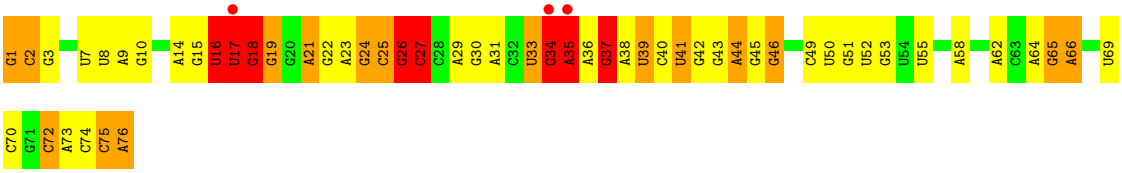
• Molecule 2: P-site tRNA (Phe)



• Molecule 3: E-site tRNA (Phe)

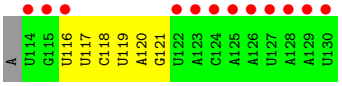
Chain AW:





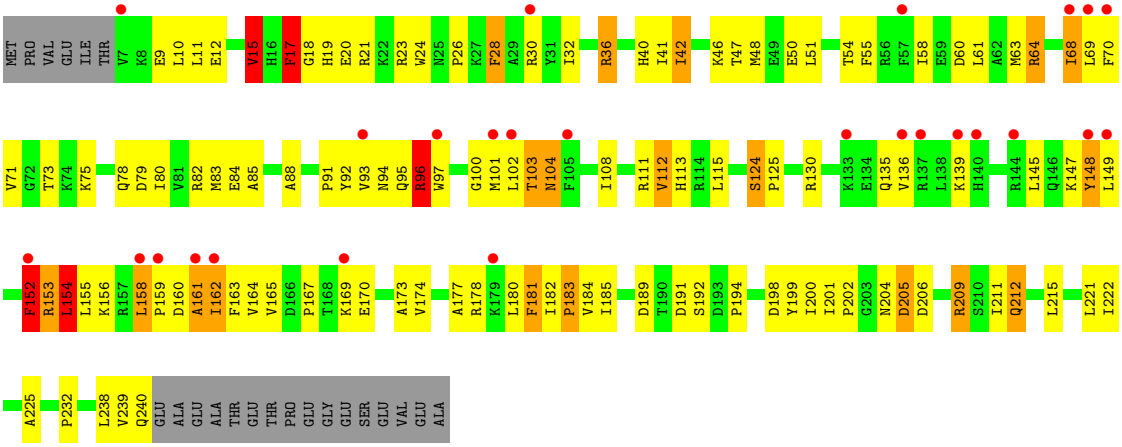
• Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

Chain AX:



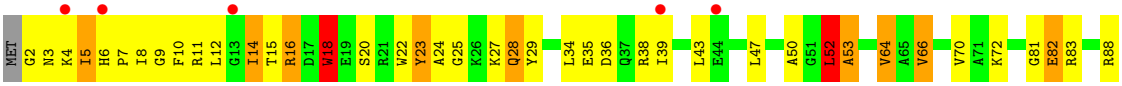
• Molecule 5: 30S ribosomal protein S2

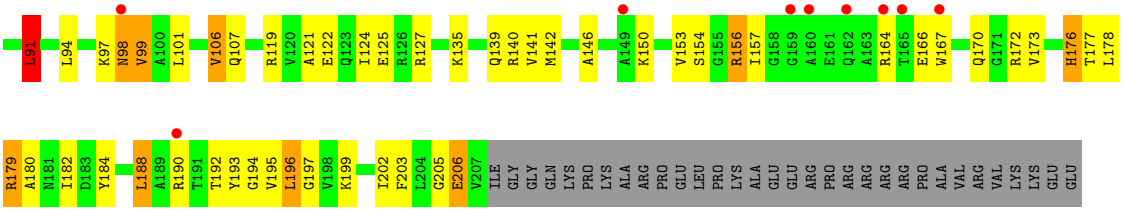
Chain AB:



• Molecule 6: 30S ribosomal protein S3

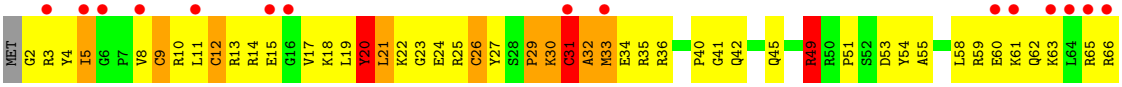
Chain AC:

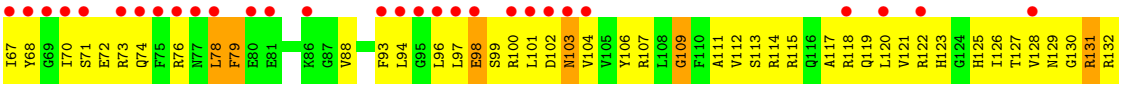


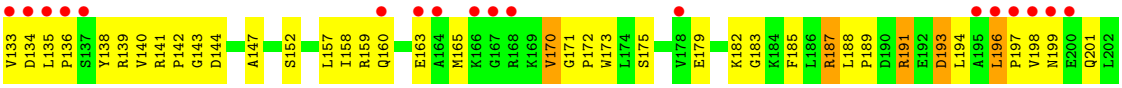


• Molecule 7: 30S ribosomal protein S4

Chain AD:

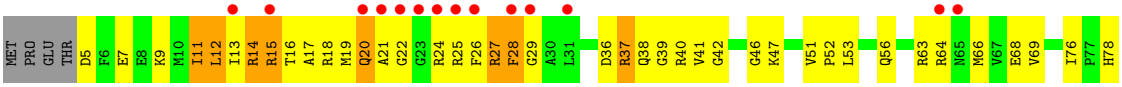


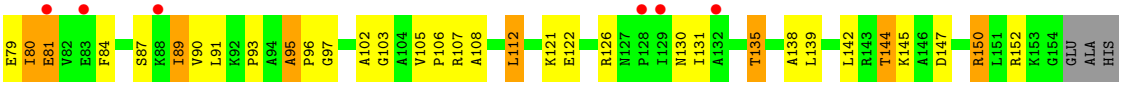




• Molecule 8: 30S ribosomal protein S5

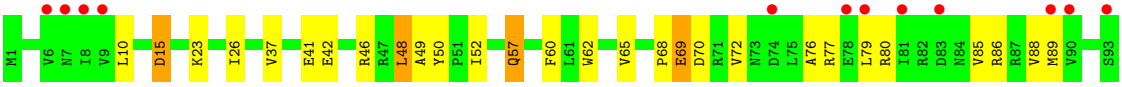
Chain AE:





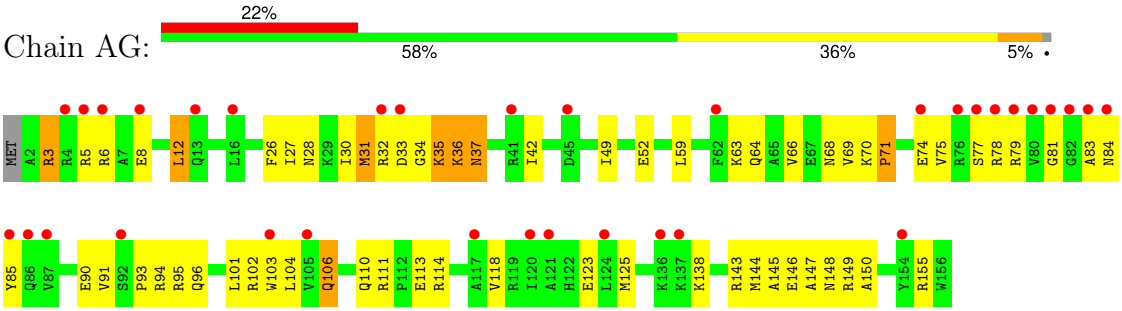
• Molecule 9: 30S ribosomal protein S6

Chain AF:



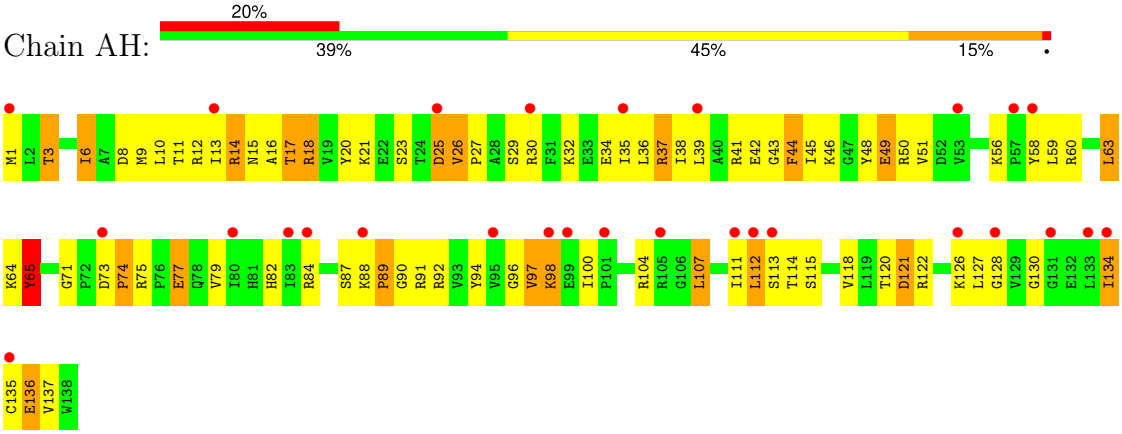
• Molecule 10: 30S ribosomal protein S7

Chain AG:



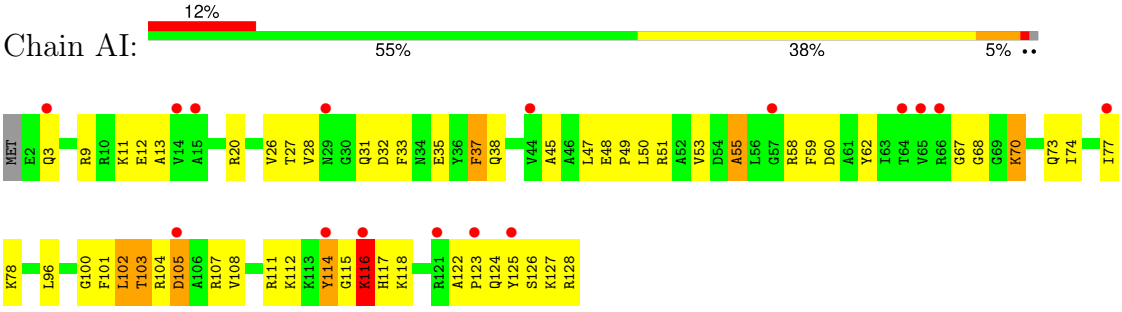
• Molecule 11: 30S ribosomal protein S8

Chain AH:



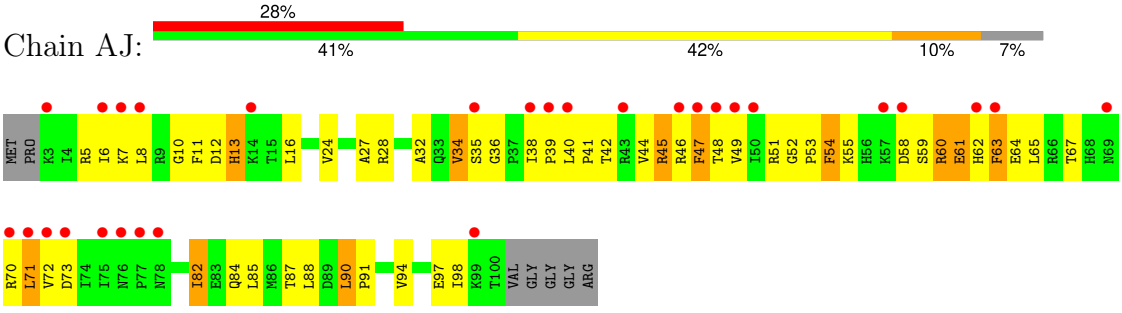
• Molecule 12: 30S ribosomal protein S9

Chain AI:



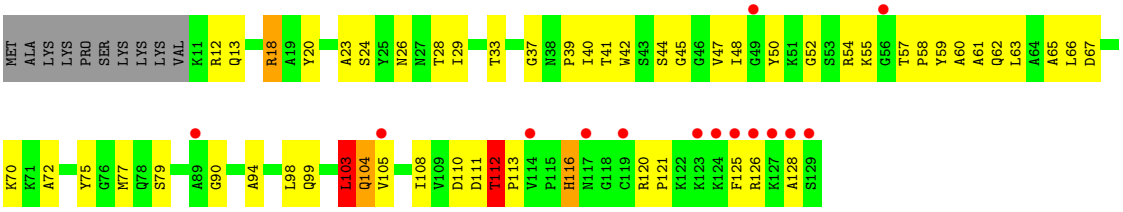
• Molecule 13: 30S ribosomal protein S10

Chain AJ:



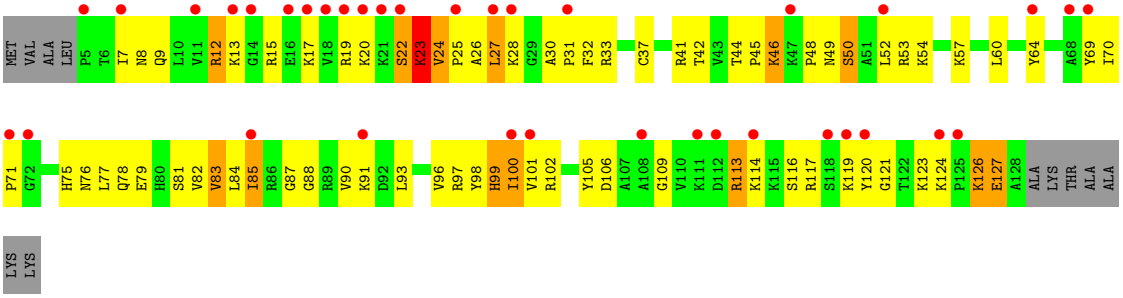
• Molecule 14: 30S ribosomal protein S11

Chain AK:



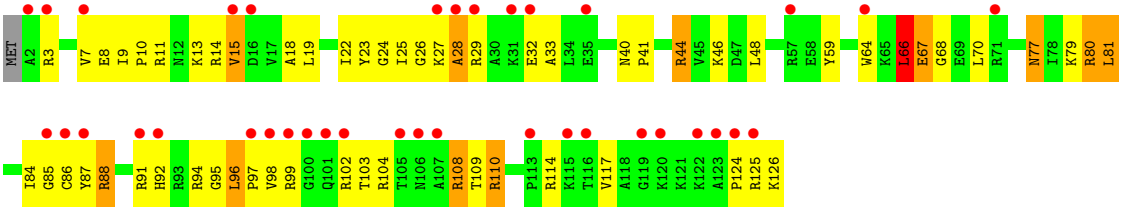
• Molecule 15: 30S ribosomal protein S12

Chain AL:



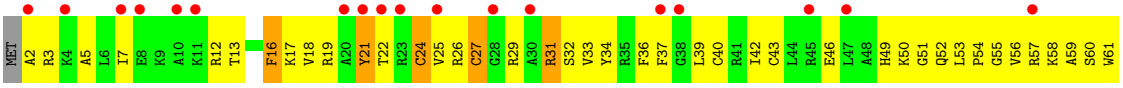
• Molecule 16: 30S ribosomal protein S13

Chain AM:



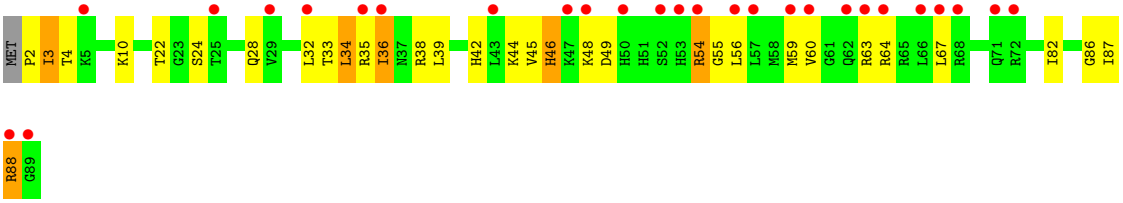
• Molecule 17: 30S ribosomal protein S14

Chain AN:



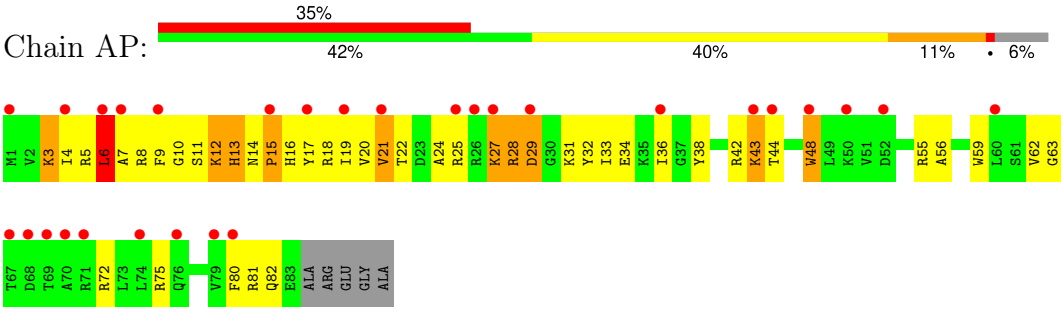
• Molecule 18: 30S ribosomal protein S15

Chain AO:



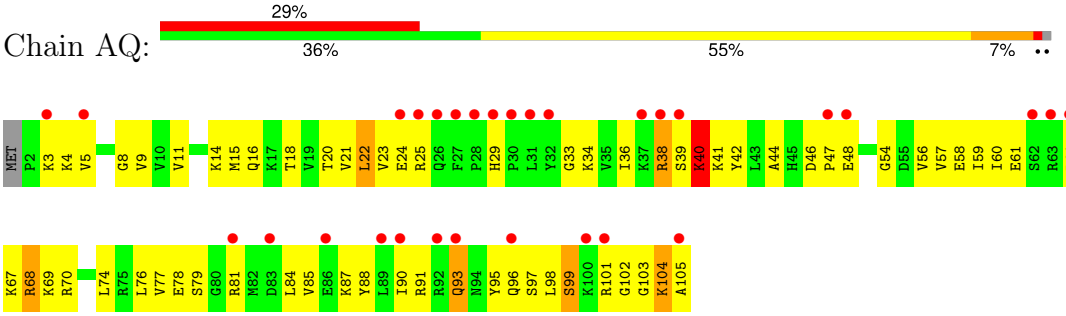
• Molecule 19: 30S ribosomal protein S16

Chain AP:



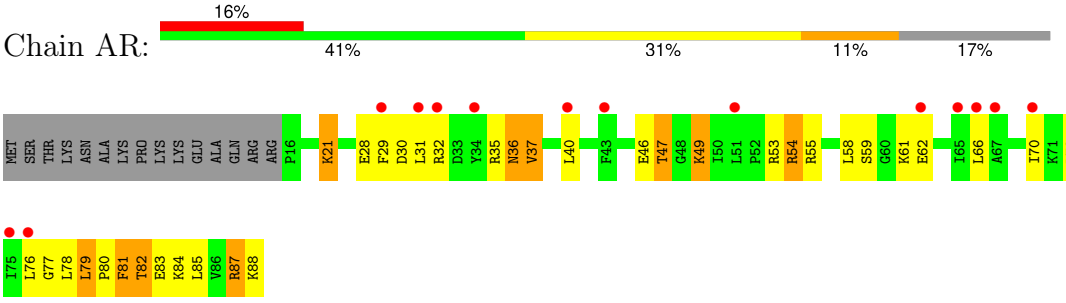
• Molecule 20: 30S ribosomal protein S17

Chain AQ:



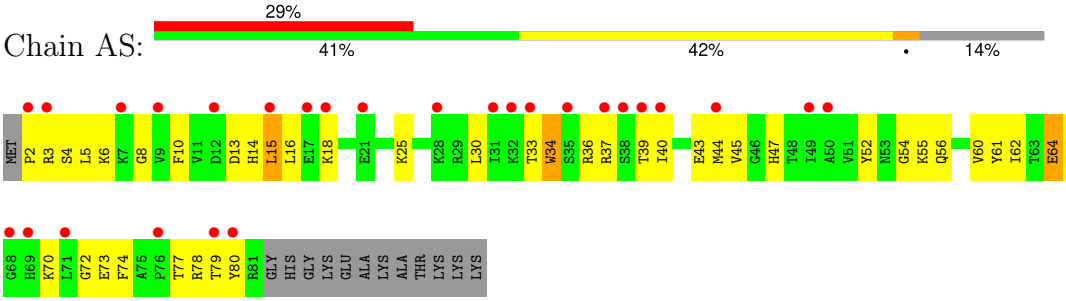
• Molecule 21: 30S ribosomal protein S18

Chain AR:



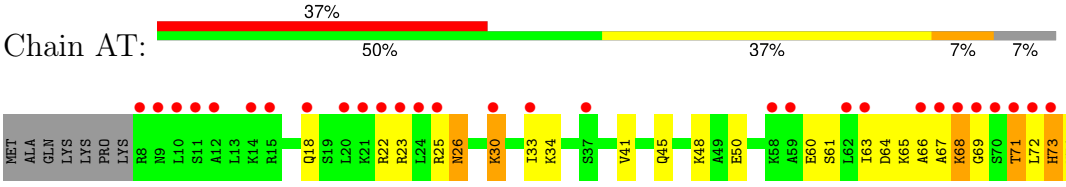
• Molecule 22: 30S ribosomal protein S19

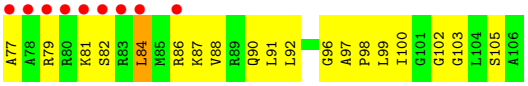
Chain AS:



• Molecule 23: 30S ribosomal protein S20

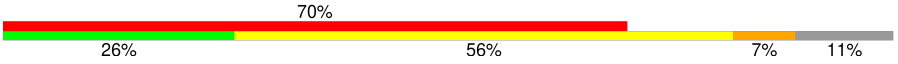
Chain AT:

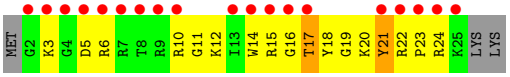




• Molecule 24: 30S ribosomal protein Thx

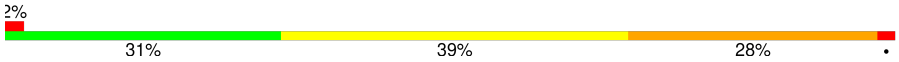
Chain AU:

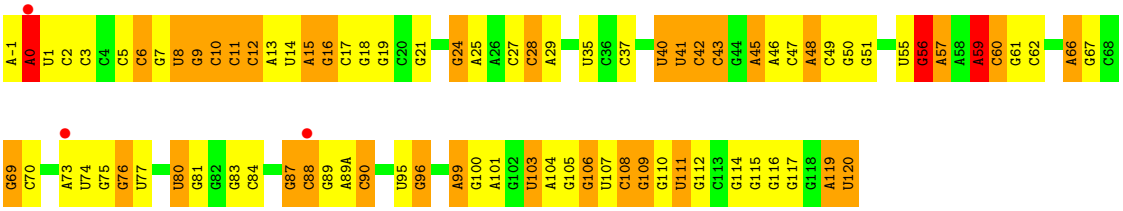




• Molecule 25: 5S ribosomal RNA

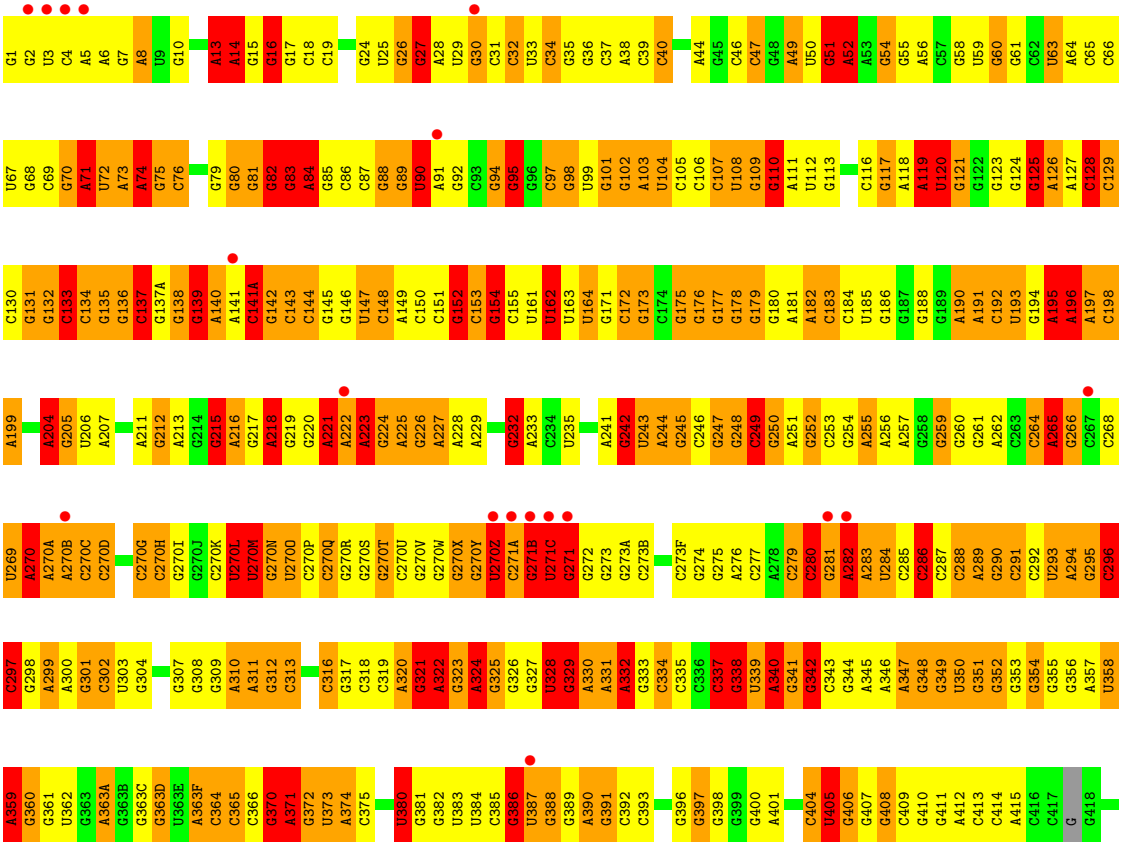
Chain BB:

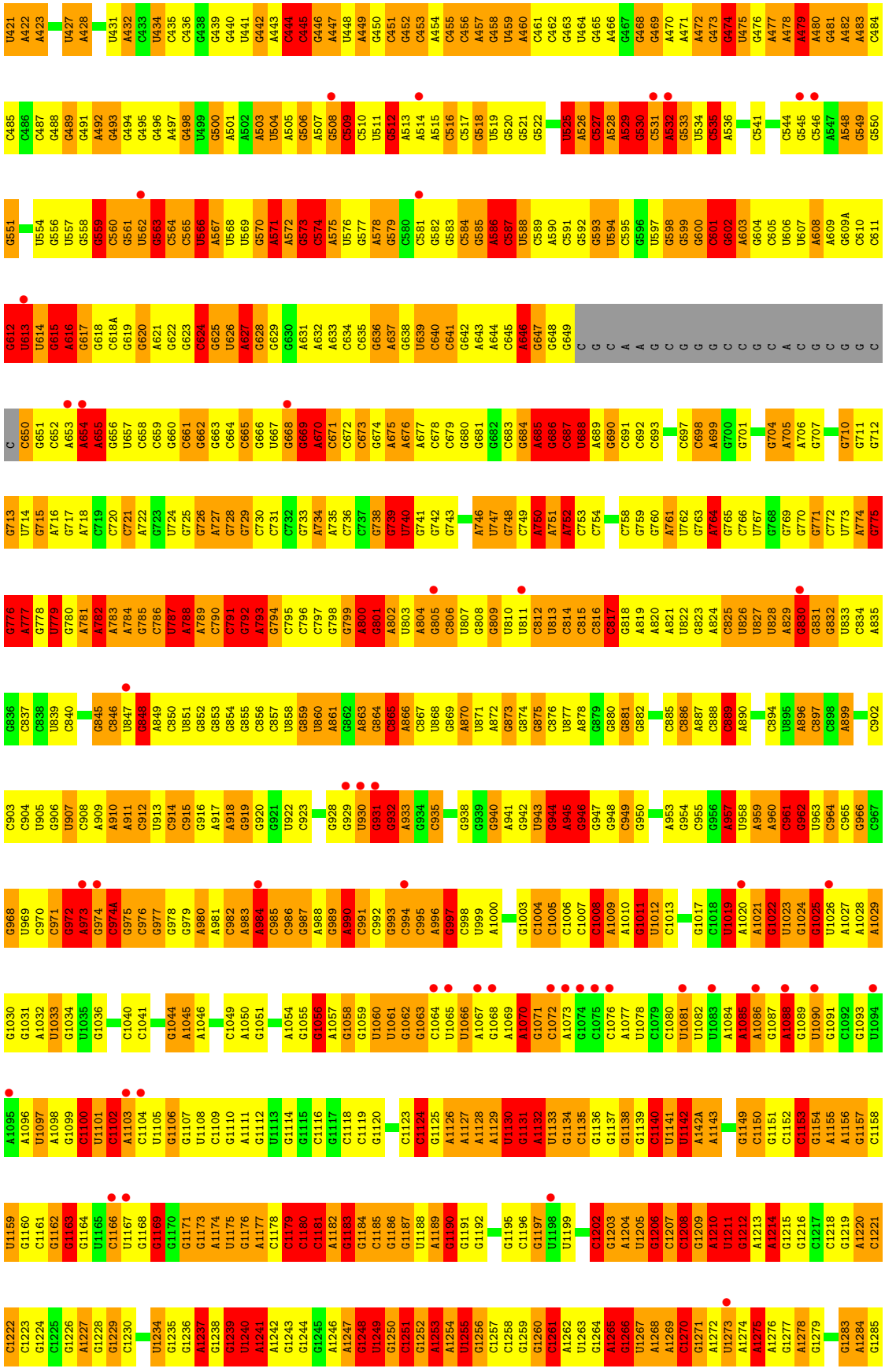


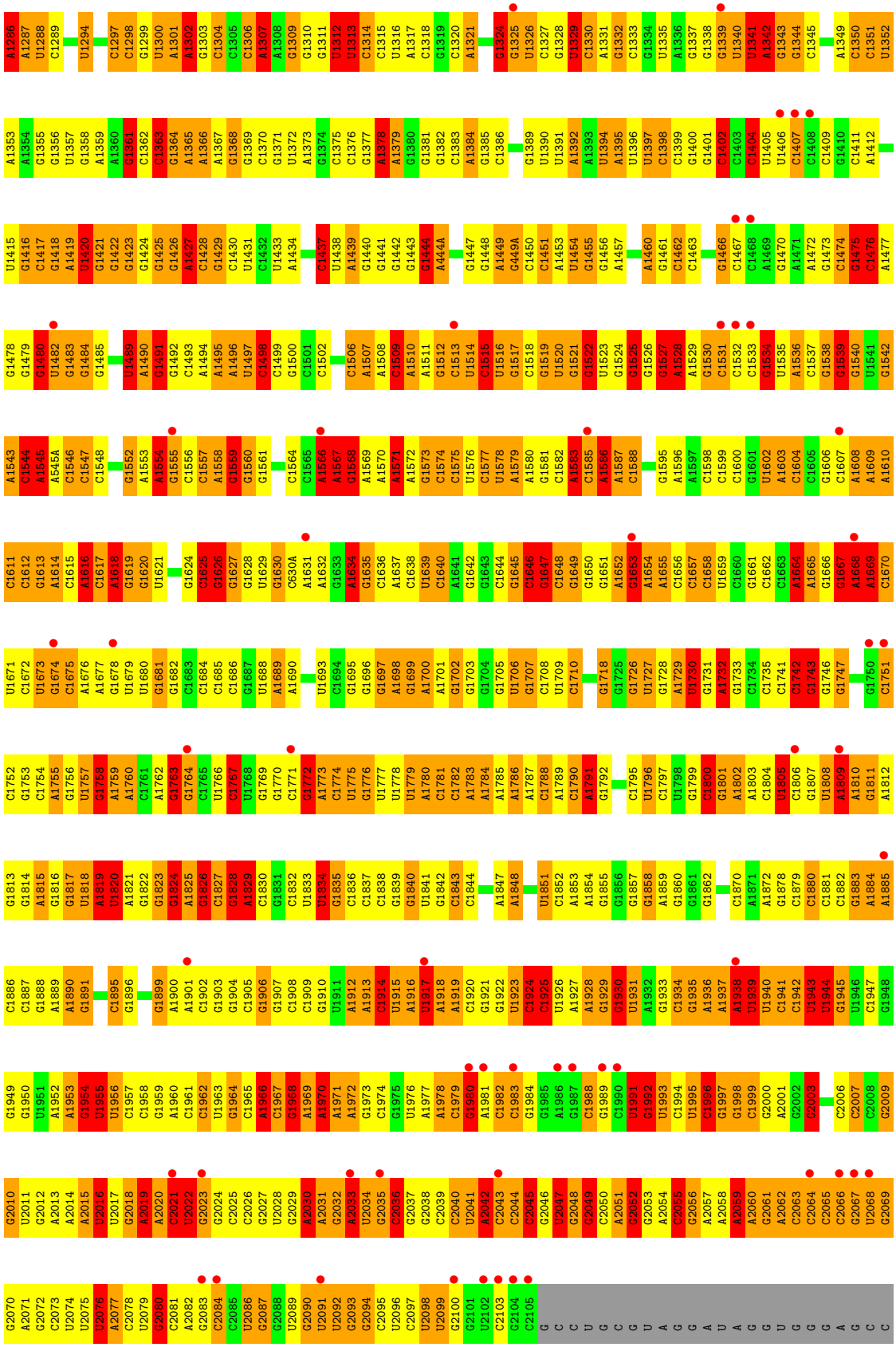


• Molecule 26: 23S ribosomal RNA

Chain BA:



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A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 G1377 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 C1399 G1400 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412
U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 C1437 U1438 A1439 G1440 G1441 G1442 G1443 G1444 A444A G1447 G1448 A1449 G449A C1450 C1451 A1453 U1454 G1455 G1456 A1457 A1460 G1461 C1462 C1463 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474 G1475 C1476 A1477
G1478 G1479 G1480 U1482 G1483 G1484 G1485 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 C1501 C1502 C1506 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 C1515 U1516 G1517 C1518 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 G1527 A1528 A1529 G1530 C1531 C1532 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542
A1543 C1544 A1545 A545A C1546 C1547 C1548 G1552 A1553 A1554 G1555 C1556 C1557 A1558 G1559 G1560 G1561 C1564 C1565 A1566 A1567 G1568 A1569 A1570 A1571 A1572 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1587 C1588 G1595 A1596 A1597 C1598 C1599 C1600 G1601 U1602 A1603 C1604 C1605 G1606 C1607 A1608 A1609 A1610
C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1620 U1621 G1624 C1625 G1626 G1627 G1628 U1629 G1630 C630A A1631 A1632 G1633 A1634 G1635 C1636 A1637 C1638 U1639 C1640 A1641 G1642 G1643 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1661 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670
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C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1759 A1760 C1761 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 U1808 A1809 A1810 G1811 A1812
G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 U1841 G1842 C1843 C1844 A1847 A1848 U1851 C1852 A1853 A1854 G1855 G1856 G1857 G1858 A1859 G1860 G1861 G1862 C1870 A1871 A1872 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885
C1886 C1887 G1888 A1889 A1890 G1891 C1895 G1896 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 U1946 C1947 G1948
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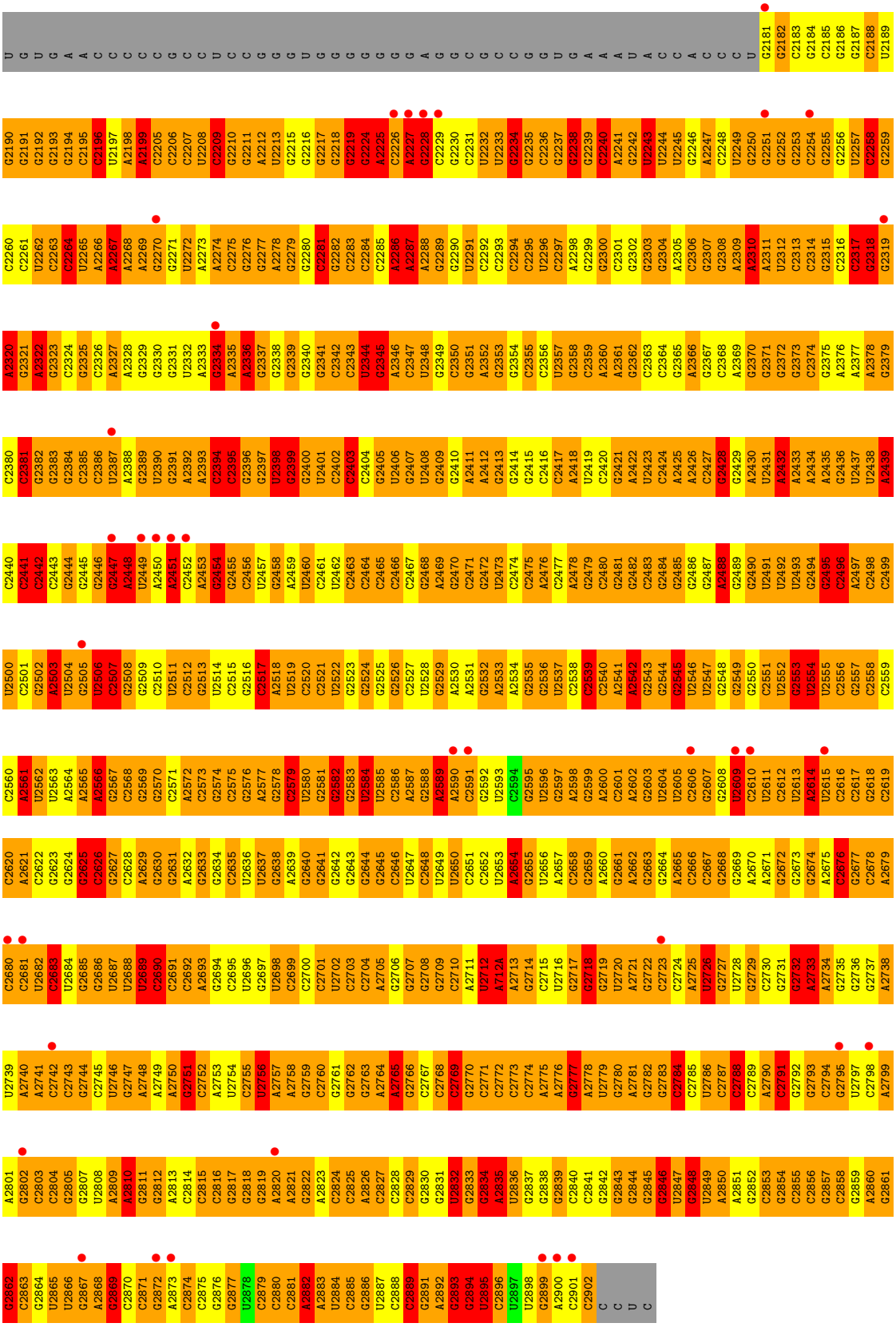
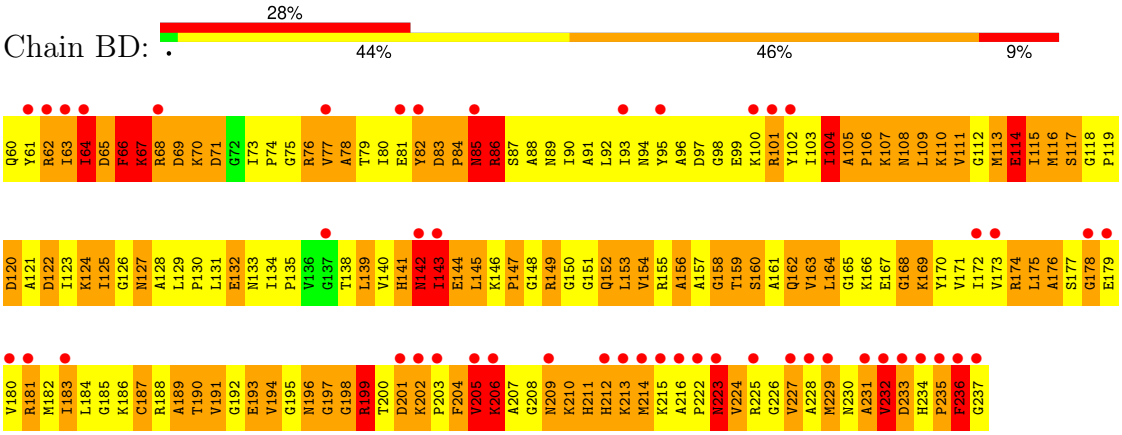
G2010 U2011 G2012 A2013 A2014 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 C2044 C2045 G2046 U2047 G2048 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069
G2070 A2071 G2072 C2073 U2074 U2075 U2076 A2077 C2078 U2079 G2080 C2081 A2082 G2083 C2084 C2085 U2086 G2087 G2088 U2089 G2090 U2091 U2092 G2093 G2094 C2095 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G C C U G C G U A G G A U A G C G U G G A G C



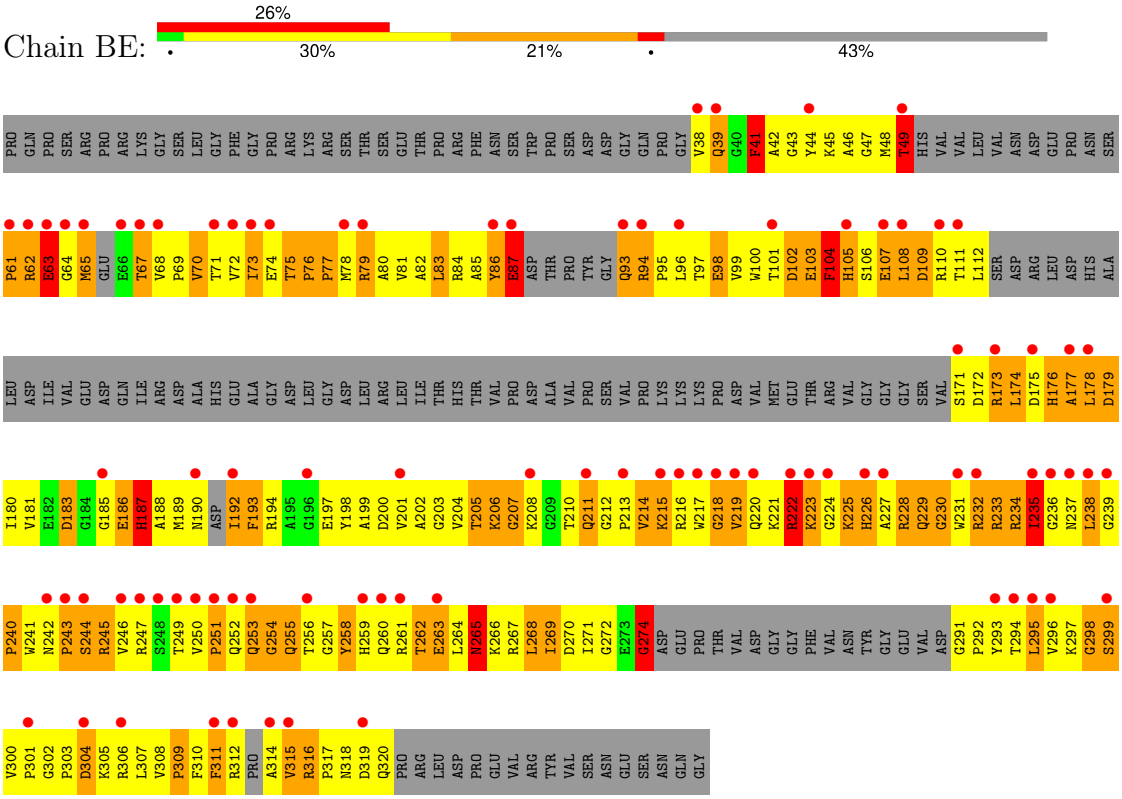
• Molecule 27: 50S ribosomal protein L2

Chain BD:



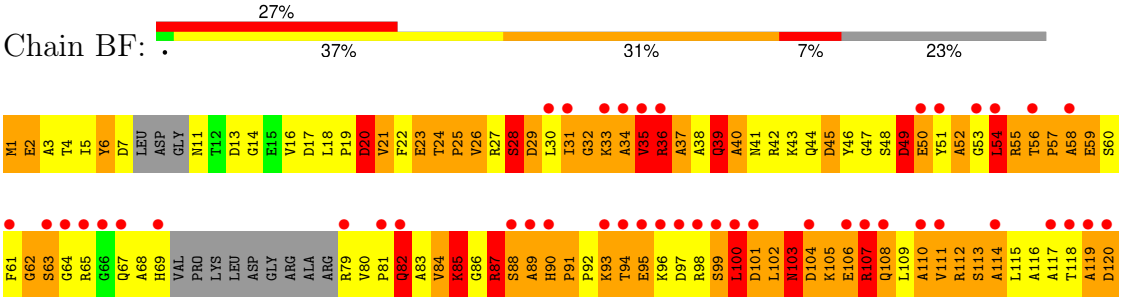
• Molecule 28: 50S ribosomal protein L3

Chain BE:



• Molecule 29: 50S ribosomal protein L4

Chain BF:



ALA ASP LEU VAL ALA ASP ARG GLY HIS GLU PHE ASP ARG ASP GLU VAL PRO V138 V139 V140 S141 D142 D143 F144 E145 D146 L147 V148 K149 T150 Q151 E152 V153 V154 S155 L156 L157 E158 A159 L160 D161 V162 H163 A164 D165 I166 D167 R168 ALA ASP GLU THR LYS ILE LYS ALA GLY GLN GLY SER

ALA ARG GLY ARG LYS TYR ARG ARG PRO ALA SER ILE L193 F194 V195 T196 S197 D198 E199 P200 S201 T202 A203 A204 R205 N206 L207 A208 G209 A210 D211 V212 A213 T214 A215 S216 E217 V218 N219 T220 E221 D222 L223 A224 P225 GLY GLY ALA PRO G230 R231 L232 T233 V234 F235 T236 E237 S238 A239 L240

A241 E242 V243 A244 E245 R246

- Molecule 30: 50S ribosomal protein L5

Chain BG: 21% | 7% | 39% | 21% | • | 31%

SER SER GLU SER GLU SER GLY GLY ASP F10 H11 E12 M13 R14 E15 P16 R17 I18 E19 K20 V21 V22 V23 H24 M25 G26 I27 G28 H29 GLY GLY ARG ASP LEU A35 N36 A37 E38 D39 I40 L41 G42 E43 I44 T45 G46 Q47 M48 P49 V50 R51 T52 K53 A54 K55 R56 T57 V58 G59 E60

F61 D62 I63 R64 E65 G66 D67 P68 I69 G70 A71 K72 V73 T74 L75 R76 D77 E78 M79 A80 E81 E82 F83 L84 Q85 T86 A87 L88 P89 L90 A91 E92 L93 A94 T95 S96 Q97 F98 D99 D100 T101 G102 N103 F104 S105 F106 G107 VAL GLU GLU HIS THR GLU PHE PRO SER GLN GLU TYR ASP

PRO SER ILE GLY ILE TYR GLY L128 D129 V130 T131 V132 N133 L134 V135 R136 P137 R140 V141 A142 K143 R144 D145 K146 A147 S148 R149 S150 I151 P152 R156 LEU ASN PRO ALA ASP ALA VAL ALA PHE ILE GLU SER THR TYR ASP VAL GLU VAL SER GLU

- Molecule 31: 50S ribosomal protein L6

Chain BH: 14% | 5% | 50% | 32% | 6% | 7%

SER ARG VAL GLY LYS LYS P7 I8 E9 I10 P11 A12 G13 V14 T15 V16 T17 V18 N19 G20 N21 T22 V23 T24 V25 K26 G27 P28 K29 G30 E31 L32 T33 R34 T35 F36 H37 P38 D39 M40 T41 I42 T43 V44 E45 G46 N47 V48 T49 T50 V51 T52 R53 P54 S55 D56 E57 K58 H59 H60

R61 A62 L63 H64 G65 T66 T67 R68 S69 L70 L71 A72 N73 M74 V75 E76 G77 V78 S79 K80 G81 Y82 E83 K84 A85 L86 E87 L88 V89 G90 V91 G92 Y93 R94 A95 S96 K97 Q98 G99 K100 K101 L102 V103 L104 S105 V106 G107 Y108 S109 H110 P111 V112 E113 I114 E115 P116 E117 E118 G119 L120

E121 I122 E123 V124 P125 S126 Q127 T128 K129 I130 I131 V132 K133 G134 A135 D136 K137 Q138 R139 V140 G141 E142 L143 A144 A145 N146 I147 R148 A149 V150 R151 P152 P153 E154 P155 Y156 K157 G158 K159 G160 I161 R162 Y163 E164 G165 E166 L167 V168 R169 L170 LYS GLU GLY LYS THR GLY LYS

- Molecule 32: 50S ribosomal protein L9

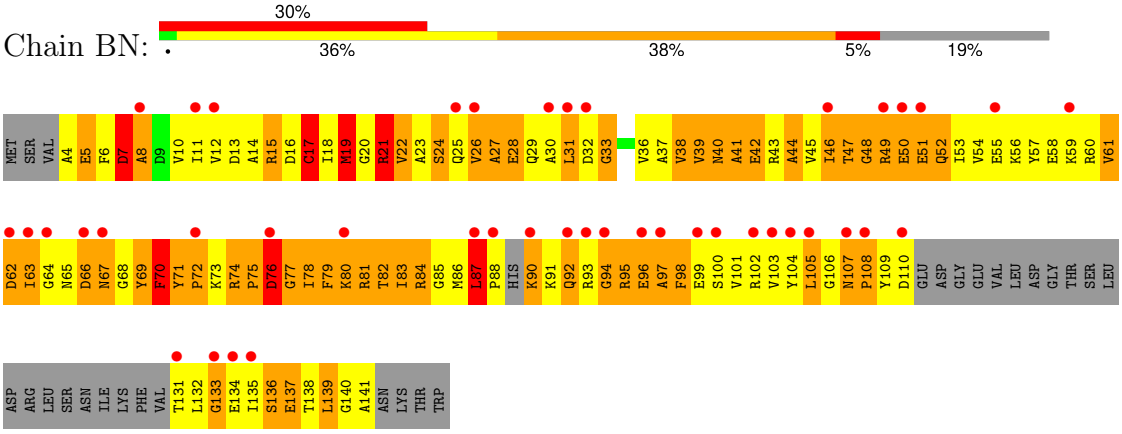
Chain BI: 21% | 6% | 55% | 34% | 5% | •

M1 K2 V3 I4 F5 L6 K7 D8 V9 K10 G11 K12 G13 K14 K15 G16 E17 I18 K19 N20 V21 A22 D23 G24 Y25 A26 N27 N28 F29 L30 F31 K32 Q33 G34 L35 A36 I37 E38 A39 T40 P41 A42 N43 L44 K45 A46 L47 E48 A49 Q50 K51 Q52 K53 E54 Q55 R56 Q57 A58 A59 E60

E61 L62 A63 N64 A65 K66 K67 L68 K69 E70 Q71 L72 L75 T76 V77 T78 I79 P80 A81 K82 A83 G84 E85 G86 GLY R88 L89 F90 G91 S92 I93 T94 S95 K96 Q97 I98 A99 E100 S101 L102 Q103 A104 Q105 H106 G107 L108 K109 L110 D111 K112 R113 K114 I115 E116 L117 A118 D119 A120 I121

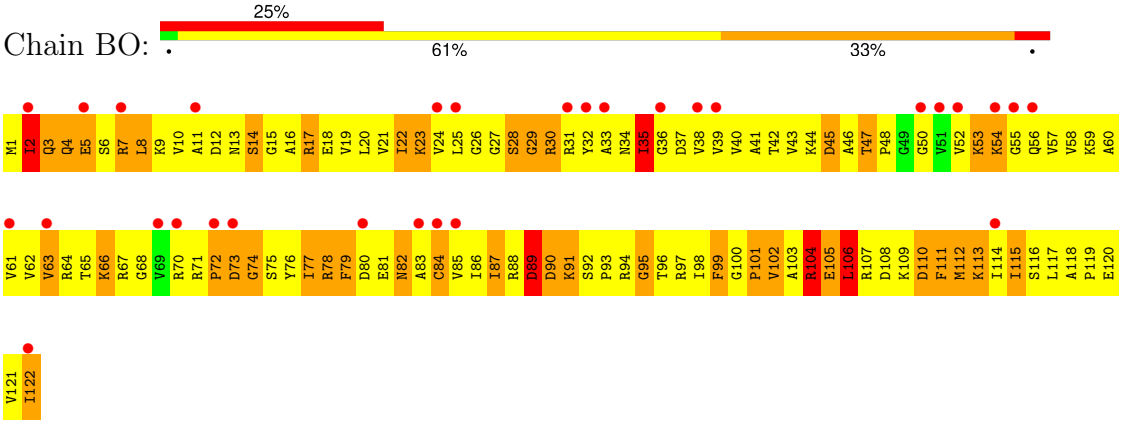
• Molecule 33: 50S ribosomal protein L13

Chain BN:



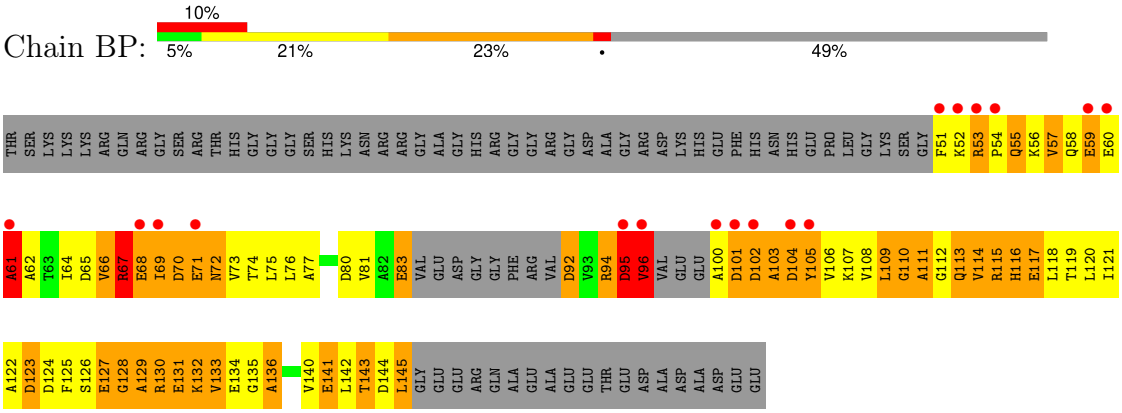
• Molecule 34: 50S ribosomal protein L14

Chain BO:



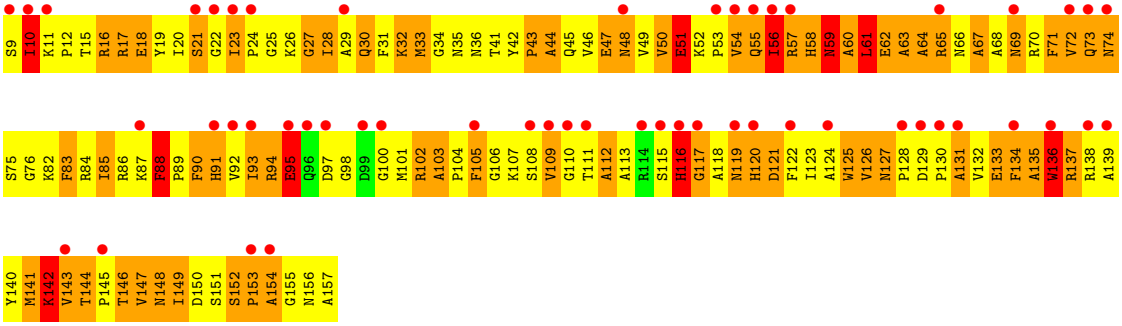
• Molecule 35: 50S ribosomal protein L15

Chain BP:



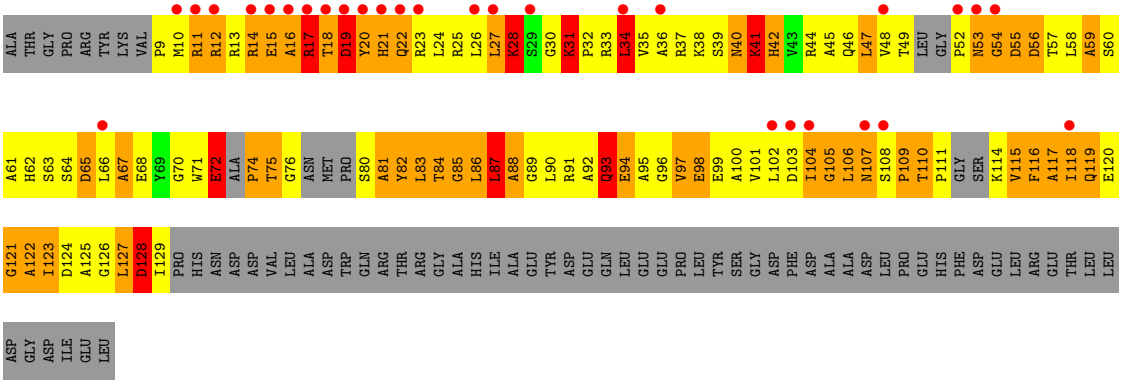
• Molecule 36: 50S ribosomal protein L16

Chain BQ:



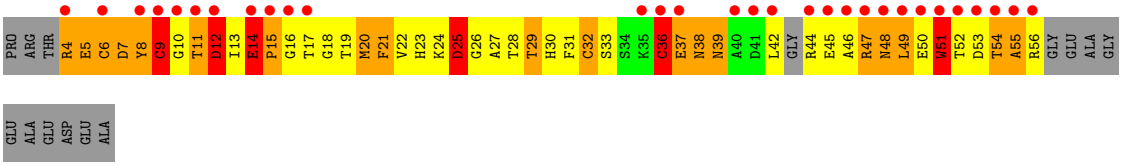
• Molecule 37: 50S ribosomal protein L18

Chain BS:



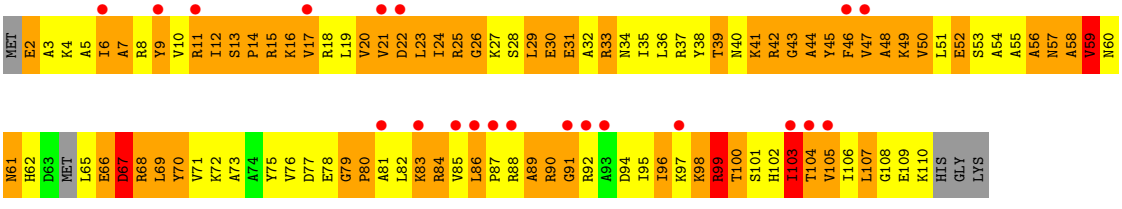
• Molecule 38: 50S ribosomal protein L19

Chain BT:



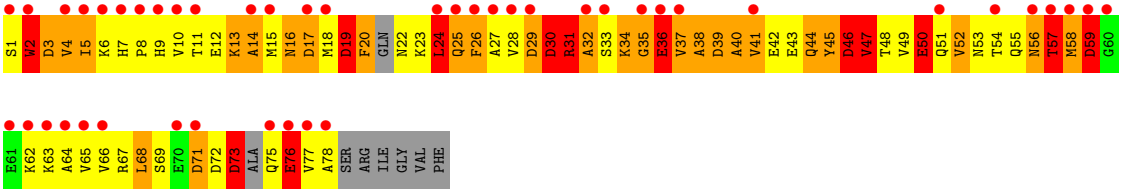
• Molecule 39: 50S ribosomal protein L22

Chain BW:



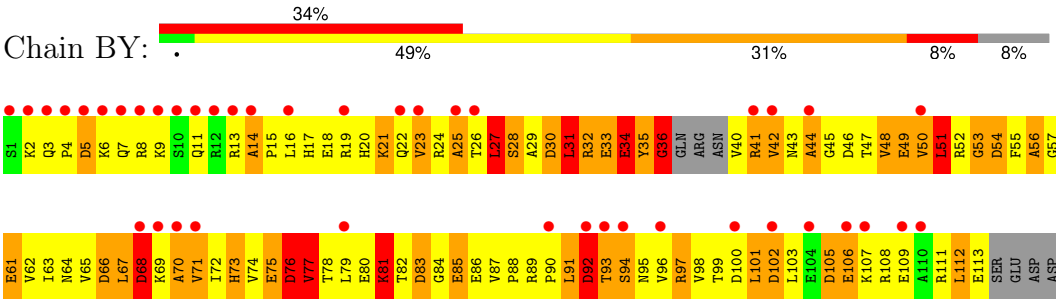
• Molecule 40: 50S ribosomal protein L23

Chain BX:



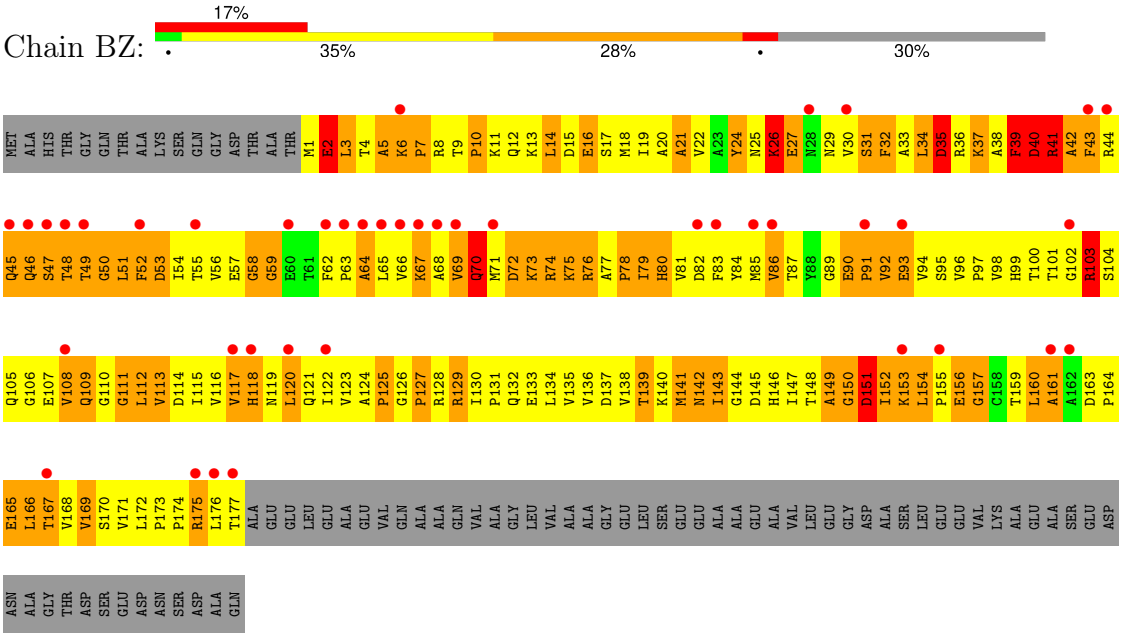
• Molecule 41: 50S ribosomal protein 24

Chain BY:



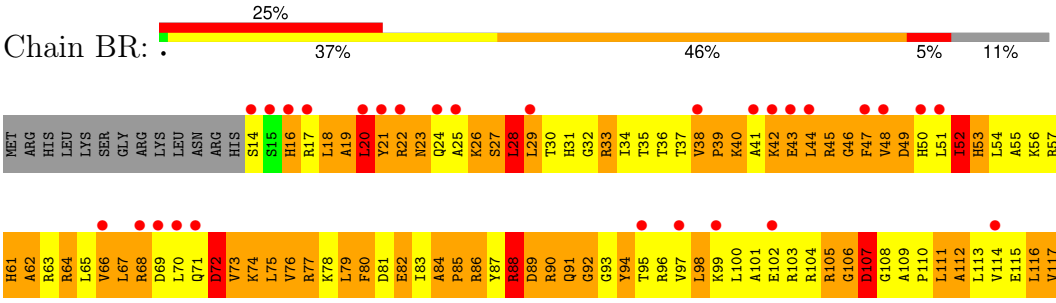
• Molecule 42: 50S ribosomal protein CTC

Chain BZ:



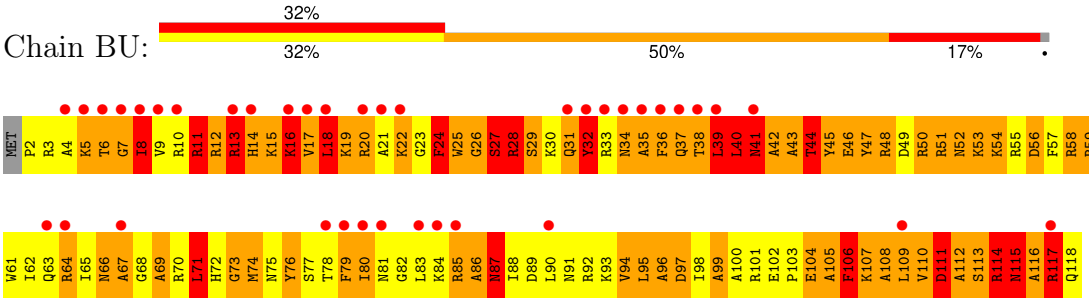
• Molecule 43: 50S ribosomal protein L17

Chain BR:



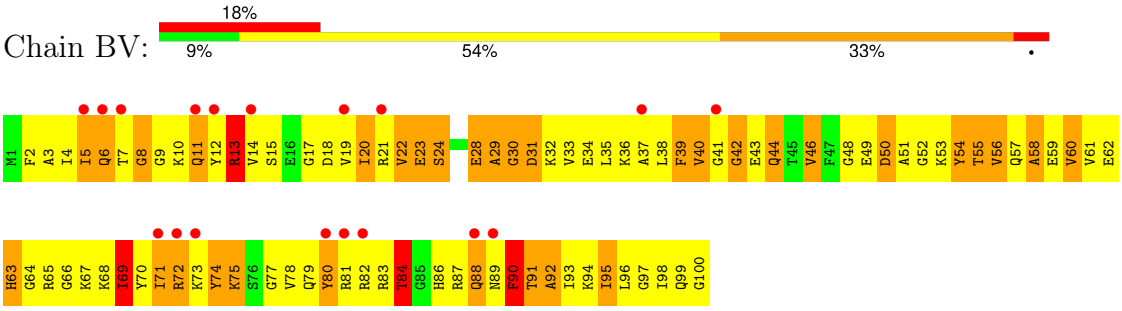
• Molecule 44: 50S ribosomal protein L20

Chain BU:



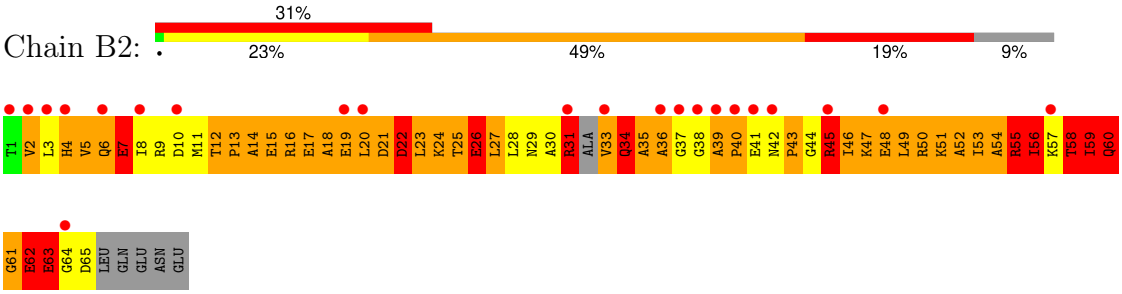
• Molecule 45: 50S ribosomal protein L21

Chain BV:



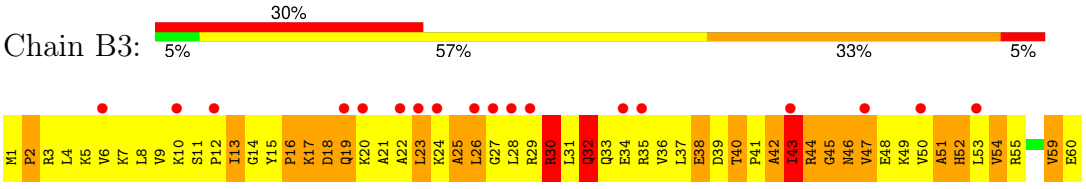
• Molecule 46: 50S ribosomal protein L29

Chain B2:



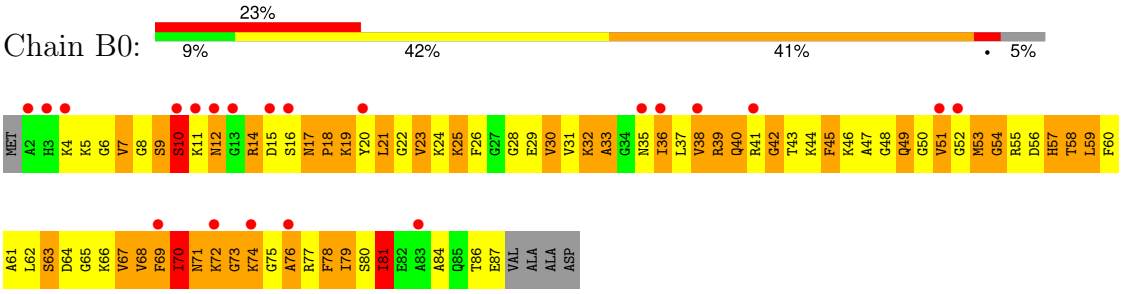
• Molecule 47: 50S ribosomal protein L30

Chain B3:



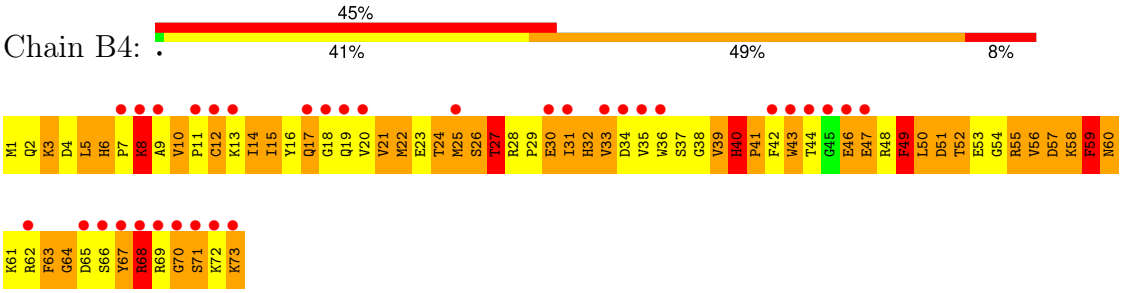
• Molecule 48: 50S ribosomal protein L27

Chain B0:



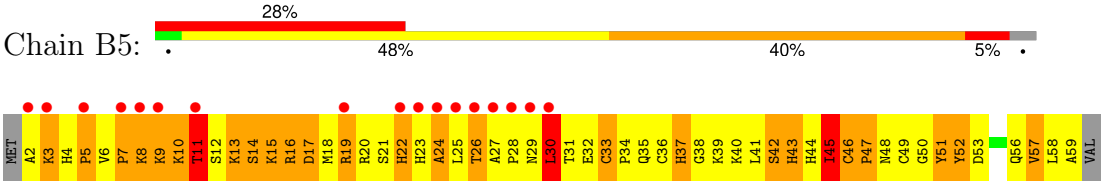
• Molecule 49: 50S ribosomal protein L31

Chain B4:



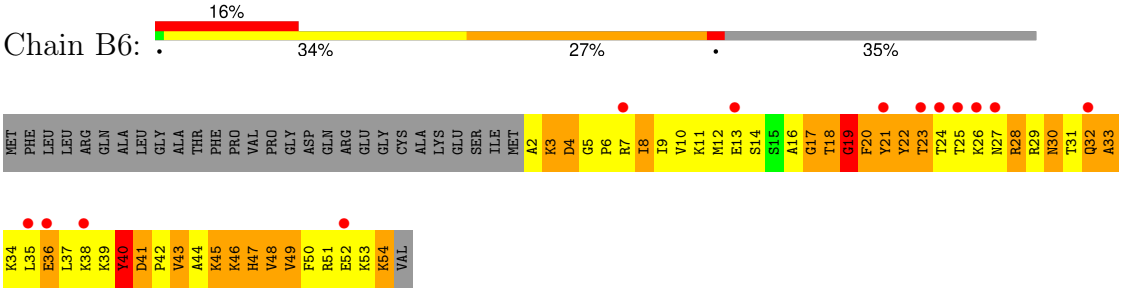
• Molecule 50: 50S ribosomal protein L32

Chain B5:



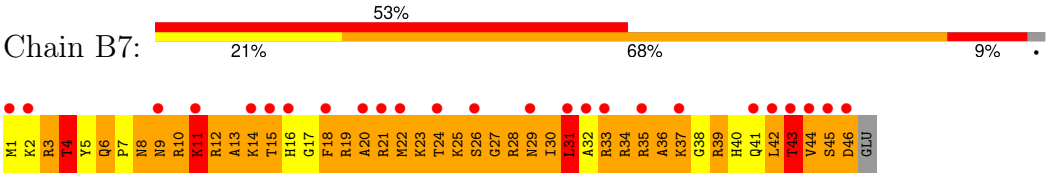
• Molecule 51: 50S ribosomal protein L33

Chain B6:



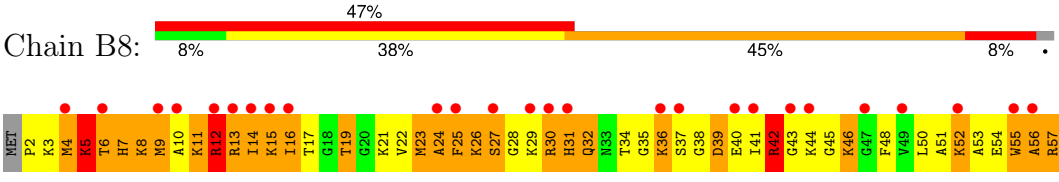
• Molecule 52: 50S ribosomal protein L34

Chain B7:



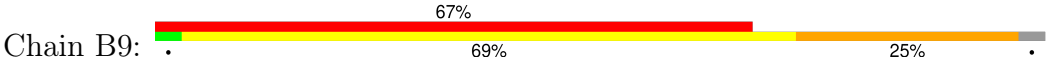
• Molecule 53: 50S ribosomal protein L35

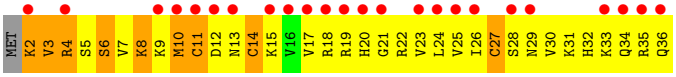
Chain B8:



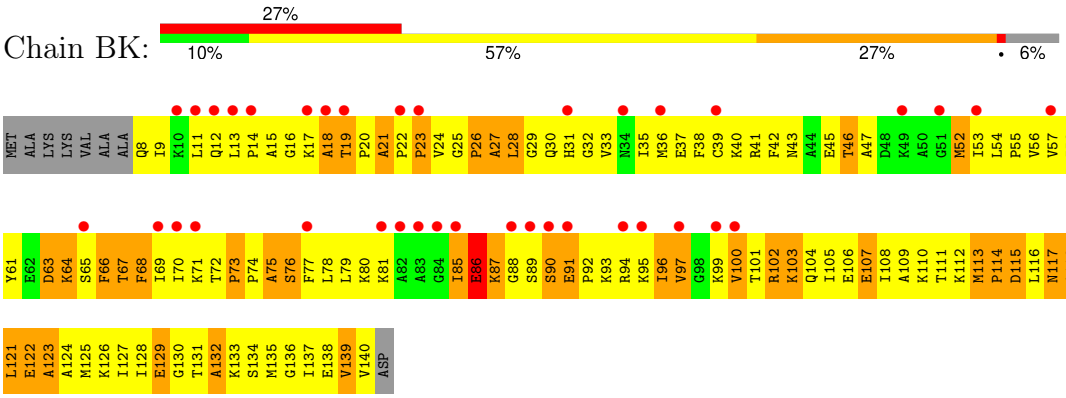
• Molecule 54: 50S ribosomal protein L36

Chain B9:





• Molecule 55: 50S ribosomal protein L11



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	517.41Å 517.41Å 365.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 6.46 40.00 – 6.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-6.46) 99.4 (40.00-6.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 6.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.354 , 0.361 0.346 , 0.359	Depositor DCC
R_{free} test set	4886 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	240.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 103.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	142447	wwPDB-VP
Average B, all atoms (Å^2)	314.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	1.32	68/36413 (0.2%)	1.49	439/56777 (0.8%)
2	AV	0.74	3/1812 (0.2%)	1.20	8/2819 (0.3%)
3	AW	1.81	19/1739 (1.1%)	2.15	47/2698 (1.7%)
4	AX	0.18	0/139	0.67	0/213
5	AB	0.60	2/1935 (0.1%)	0.61	0/2609
6	AC	0.73	2/1636 (0.1%)	0.61	4/2205 (0.2%)
7	AD	0.70	4/1733 (0.2%)	1.03	11/2318 (0.5%)
8	AE	0.83	1/1162 (0.1%)	0.63	1/1564 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.34	0/1276	0.59	3/1709 (0.2%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.59	1/900 (0.1%)	0.54	0/1213
15	AL	1.33	1/986 (0.1%)	1.11	3/1320 (0.2%)
16	AM	0.92	1/1007 (0.1%)	0.59	1/1344 (0.1%)
17	AN	0.49	1/501 (0.2%)	0.65	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.23	2/870 (0.2%)	1.38	6/1159 (0.5%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.49	0/277
25	BB	1.25	6/2950 (0.2%)	1.44	25/4602 (0.5%)
26	BA	1.17	153/67839 (0.2%)	1.46	906/105818 (0.9%)
27	BD	0.38	0/1328	0.60	0/1783
28	BE	0.65	4/1540 (0.3%)	1.07	7/2078 (0.3%)
29	BF	0.76	3/1444 (0.2%)	0.83	1/1954 (0.1%)
30	BG	0.25	0/971	0.46	0/1304
31	BH	0.54	1/1272 (0.1%)	0.80	3/1721 (0.2%)
32	BI	0.32	0/1156	0.71	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BN	0.35	0/927	0.55	0/1245
34	BO	0.32	0/946	0.57	0/1269
35	BP	1.59	3/643 (0.5%)	1.31	5/870 (0.6%)
36	BQ	0.32	0/1106	0.53	0/1490
37	BS	1.13	3/877 (0.3%)	0.69	1/1179 (0.1%)
38	BT	0.39	0/412	0.70	0/554
39	BW	0.75	3/869 (0.3%)	0.75	4/1166 (0.3%)
40	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
41	BY	0.26	0/887	0.83	3/1195 (0.3%)
42	BZ	0.32	1/1385 (0.1%)	0.62	3/1883 (0.2%)
43	BR	0.30	0/867	0.50	0/1162
44	BU	0.64	1/994 (0.1%)	0.74	3/1323 (0.2%)
45	BV	0.82	1/796 (0.1%)	0.91	3/1058 (0.3%)
46	B2	0.37	0/497	1.00	2/668 (0.3%)
47	B3	0.31	0/482	0.50	0/646
48	B0	0.38	1/649 (0.2%)	0.87	3/860 (0.3%)
49	B4	0.89	2/620 (0.3%)	0.54	0/831
50	B5	0.36	0/469	0.90	3/629 (0.5%)
51	B6	0.32	0/438	0.55	1/583 (0.2%)
52	B7	0.38	0/387	0.64	0/509
53	B8	0.91	2/503 (0.4%)	0.92	3/657 (0.5%)
54	B9	0.33	0/286	0.59	0/375
55	BK	0.27	1/1014 (0.1%)	0.44	0/1363
All	All	1.09	291/154800 (0.2%)	1.33	1508/231822 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AW	1	5
5	AB	0	1
6	AC	0	1
7	AD	0	1
14	AK	0	1
15	AL	0	1
20	AQ	0	1
27	BD	0	1
28	BE	0	3
29	BF	0	4
31	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	BI	0	1
35	BP	0	1
37	BS	0	1
40	BX	0	1
41	BY	0	1
46	B2	0	1
50	B5	0	1
55	BK	0	1
All	All	1	28

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2199	A	O3'-P	-71.04	0.75	1.61
1	AA	1278	U	O3'-P	-56.53	0.93	1.61
1	AA	1337	G	O3'-P	-53.91	0.96	1.61
26	BA	1546	C	O3'-P	-51.62	0.99	1.61
1	AA	1004	A	O3'-P	48.18	2.19	1.61

The worst 5 of 1508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AW	65	G	P-O3'-C3'	-50.68	58.88	119.70
26	BA	712(A)	A	P-O3'-C3'	-43.62	67.36	119.70
26	BA	2199	A	O3'-P-O5'	-43.07	22.17	104.00
2	AV	65	G	P-O3'-C3'	39.88	167.56	119.70
1	AA	1255	G	P-O3'-C3'	-38.36	73.67	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 28 planarity outliers are listed below:

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

5.2 Too-close contacts (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	32551	0	16459	2042	3
2	AV	1622	0	821	231	0
3	AW	1638	0	836	245	0
4	AX	136	0	63	26	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	99	0
7	AD	1703	0	1761	289	0
8	AE	1146	0	1206	68	0
9	AF	843	0	857	30	0
10	AG	1257	0	1295	103	0
11	AH	1116	0	1177	100	0
12	AI	1011	0	1040	80	0
13	AJ	794	0	840	81	0
14	AK	885	0	904	53	0
15	AL	970	0	1056	72	0
16	AM	997	0	1070	149	0
17	AN	492	0	529	82	0
18	AO	734	0	771	28	0
19	AP	700	0	720	70	0
20	AQ	857	0	928	80	0
21	AR	597	0	668	40	0
22	AS	647	0	673	155	0
23	AT	762	0	859	37	0
24	AU	208	0	221	84	0
25	BB	2637	0	1339	219	1
26	BA	60600	0	30514	11064	138
27	BD	1308	0	1346	1086	0
28	BE	1507	0	1478	1144	3
29	BF	1430	0	1357	1085	0
30	BG	957	0	952	692	0
31	BH	1251	0	1291	754	0
32	BI	1145	0	1225	625	3
33	BN	917	0	896	771	2
34	BO	937	0	992	613	0
35	BP	639	0	605	482	0
36	BQ	1081	0	1047	932	0
37	BS	866	0	866	677	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BT	406	0	359	167	0
39	BW	860	0	909	557	0
40	BX	602	0	558	460	0
41	BY	879	0	860	755	0
42	BZ	1360	0	1378	902	0
43	BR	855	0	904	579	0
44	BU	978	0	996	895	0
45	BV	787	0	782	635	0
46	B2	494	0	504	393	0
47	B3	477	0	527	460	0
48	B0	641	0	661	531	0
49	B4	604	0	587	489	0
50	B5	457	0	456	279	0
51	B6	431	0	454	289	0
52	B7	383	0	409	382	0
53	B8	496	0	539	349	0
54	B9	285	0	312	195	0
55	BK	999	0	1064	573	0
All	All	142447	0	94546	28975	145

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 123.

The worst 5 of 28975 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)
50:B5:33:CYS:SG	50:B5:36:CYS:HB2	1.24	1.69
26:BA:2470:G:C2	26:BA:2471:C:C5	1.81	1.68
52:B7:30:ILE:HA	52:B7:33:ARG:CD	1.21	1.67
26:BA:2712:U:C6	26:BA:712(A):A:C8	1.77	1.67
26:BA:2580:U:C6	26:BA:2581:G:C8	1.82	1.66

The worst 5 of 145 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)
26:BA:6:A:O4'	26:BA:2902:C:C2'[8_554]	0.72	1.48
26:BA:2899:G:N1	26:BA:2901:C:C4[8_554]	0.79	1.41
26:BA:6:A:C4'	26:BA:2902:C:C2'[8_554]	0.97	1.23
26:BA:2900:A:N7	26:BA:2900:A:N6[8_554]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:3:U:O4	26:BA:2899:G:O2'[8_554]	1.09	1.11

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
5	AB	232/256 (91%)	183 (79%)	33 (14%)	16 (7%)	1 11
6	AC	204/239 (85%)	166 (81%)	24 (12%)	14 (7%)	1 11
7	AD	206/209 (99%)	157 (76%)	33 (16%)	16 (8%)	1 10
8	AE	148/162 (91%)	116 (78%)	29 (20%)	3 (2%)	6 31
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2 18
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	4 25
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1 10
12	AI	125/128 (98%)	86 (69%)	31 (25%)	8 (6%)	1 12
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	0 8
14	AK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	1 13
15	AL	122/135 (90%)	90 (74%)	13 (11%)	19 (16%)	0 3
16	AM	121/126 (96%)	95 (78%)	20 (16%)	6 (5%)	1 16
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1 11
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	11 44
19	AP	81/88 (92%)	64 (79%)	11 (14%)	6 (7%)	1 10
20	AQ	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	1 13
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	0 9
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	2 19
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1 13
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
28	BE	183/338 (54%)	89 (49%)	34 (19%)	60 (33%)	0	0
29	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
30	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
31	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	0
32	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	0
33	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
34	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	0
35	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
36	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
37	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
38	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
39	BW	104/113 (92%)	41 (39%)	16 (15%)	47 (45%)	0	0
40	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
41	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
42	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
43	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
44	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
45	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
46	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
47	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
48	B0	84/91 (92%)	32 (38%)	17 (20%)	35 (42%)	0	0
49	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
50	B5	56/60 (93%)	16 (29%)	18 (32%)	22 (39%)	0	0
51	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
52	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
53	B8	61/64 (95%)	22 (36%)	10 (16%)	29 (48%)	0	0
54	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	0
55	BK	129/141 (92%)	73 (57%)	18 (14%)	38 (30%)	0	0
All	All	5325/6250 (85%)	2945 (55%)	1015 (19%)	1365 (26%)	0	1

5 of 1365 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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
5	AB	202/220 (92%)	173 (86%)	29 (14%)	2 12
6	AC	160/188 (85%)	146 (91%)	14 (9%)	8 25
7	AD	180/181 (99%)	162 (90%)	18 (10%)	6 20
8	AE	115/123 (94%)	94 (82%)	21 (18%)	1 8
9	AF	90/90 (100%)	83 (92%)	7 (8%)	10 29
10	AG	126/127 (99%)	116 (92%)	10 (8%)	10 29
11	AH	119/119 (100%)	92 (77%)	27 (23%)	0 4
12	AI	98/99 (99%)	90 (92%)	8 (8%)	9 28
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	3 15
14	AK	90/99 (91%)	85 (94%)	5 (6%)	17 38
15	AL	104/111 (94%)	93 (89%)	11 (11%)	5 19
16	AM	100/101 (99%)	87 (87%)	13 (13%)	3 14
17	AN	49/50 (98%)	43 (88%)	6 (12%)	4 15
18	AO	79/80 (99%)	70 (89%)	9 (11%)	4 16
19	AP	72/74 (97%)	62 (86%)	10 (14%)	3 13
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	7 23
21	AR	64/77 (83%)	57 (89%)	7 (11%)	5 18
22	AS	71/80 (89%)	64 (90%)	7 (10%)	6 21
23	AT	76/82 (93%)	68 (90%)	8 (10%)	5 19
24	AU	19/22 (86%)	19 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	BD	135/135 (100%)	99 (73%)	36 (27%)	0 3
28	BE	156/284 (55%)	128 (82%)	28 (18%)	1 8
29	BF	152/193 (79%)	124 (82%)	28 (18%)	1 8
30	BG	102/147 (69%)	93 (91%)	9 (9%)	8 25
31	BH	137/147 (93%)	111 (81%)	26 (19%)	1 7
32	BI	119/119 (100%)	98 (82%)	21 (18%)	1 8
33	BN	95/121 (78%)	80 (84%)	15 (16%)	2 10
34	BO	101/101 (100%)	81 (80%)	20 (20%)	1 7
35	BP	67/126 (53%)	56 (84%)	11 (16%)	2 10
36	BQ	110/110 (100%)	83 (76%)	27 (24%)	0 3
37	BS	89/149 (60%)	73 (82%)	16 (18%)	1 8
38	BT	44/52 (85%)	30 (68%)	14 (32%)	0 2
39	BW	88/92 (96%)	74 (84%)	14 (16%)	2 10
40	BX	67/73 (92%)	44 (66%)	23 (34%)	0 1
41	BY	97/105 (92%)	80 (82%)	17 (18%)	1 8
42	BZ	151/203 (74%)	130 (86%)	21 (14%)	3 13
43	BR	89/101 (88%)	71 (80%)	18 (20%)	1 6
44	BU	96/97 (99%)	68 (71%)	28 (29%)	0 2
45	BV	79/79 (100%)	69 (87%)	10 (13%)	3 14
46	B2	51/56 (91%)	37 (72%)	14 (28%)	0 2
47	B3	52/52 (100%)	47 (90%)	5 (10%)	7 22
48	B0	64/67 (96%)	57 (89%)	7 (11%)	5 18
49	B4	66/66 (100%)	54 (82%)	12 (18%)	1 8
50	B5	51/53 (96%)	43 (84%)	8 (16%)	2 11
51	B6	46/69 (67%)	39 (85%)	7 (15%)	2 11
52	B7	39/40 (98%)	31 (80%)	8 (20%)	1 6
53	B8	50/51 (98%)	39 (78%)	11 (22%)	1 5
54	B9	34/35 (97%)	30 (88%)	4 (12%)	4 16
55	BK	108/113 (96%)	104 (96%)	4 (4%)	29 49
All	All	4533/5148 (88%)	3841 (85%)	692 (15%)	2 11

5 of 692 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	BS	93	GLN
43	BR	116	LEU
38	BT	36	CYS
37	BS	87	LEU
41	BY	34	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
46	B2	42	ASN
48	B0	71	ASN
23	AT	73	HIS
23	AT	26	ASN
50	B5	29	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1497/1522 (98%)	520 (34%)	164 (10%)
2	AV	73/76 (96%)	16 (21%)	1 (1%)
25	BB	122/123 (99%)	45 (36%)	3 (2%)
26	BA	2780/2916 (95%)	1487 (53%)	360 (12%)
3	AW	70/76 (92%)	16 (22%)	3 (4%)
4	AX	5/18 (27%)	0	0
All	All	4547/4731 (96%)	2084 (45%)	531 (11%)

5 of 2084 RNA backbone outliers are listed below:

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

5 of 531 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2454	G
26	BA	2532	G
26	BA	2451	A

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Mol	Chain	Res	Type
26	BA	2820	A
26	BA	247	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PSU	AW	39	3	18,21,22	0.73	1 (5%)	21,30,33	0.71	0
3	YYG	AW	37	3	30,42,43	0.95	1 (3%)	32,62,65	2.77	10 (31%)
3	PSU	AW	55	3	18,21,22	0.72	0	21,30,33	0.91	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2
3	YYG	AW	37	3	1/1/8/9	7/20/42/43	0/3/4/4
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	37	YYG	C8-N7	-2.28	1.31	1.34
3	AW	39	PSU	C6-N1	-2.05	1.33	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AW	37	YYG	C11-C12-N1	8.65	111.41	106.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AW	37	YYG	C24-O23-C21	6.47	123.13	115.63
3	AW	37	YYG	C3-N3-C4	5.82	125.55	116.76
3	AW	37	YYG	O23-C21-N20	4.58	118.48	110.77
3	AW	37	YYG	C4-N3-C2	-3.89	111.80	122.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AW	37	YYG	C12-C13-C14-C15
3	AW	37	YYG	C15-C16-O18-C19
3	AW	37	YYG	O17-C16-O18-C19
3	AW	37	YYG	C13-C14-C15-C16
3	AW	37	YYG	C13-C14-C15-N20

There are no ring outliers.

2 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	39	PSU	4	0
3	AW	37	YYG	39	0

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BA	98
1	AA	68
3	AW	7
25	BB	4
36	BQ	3
2	AV	3
45	BV	2
16	AM	2
5	AB	2
49	B4	2
39	BW	2
20	AQ	2
6	AC	2
27	BD	1
55	BK	1
37	BS	1
8	AE	1
35	BP	1
53	B8	1
48	B0	1
14	AK	1
31	BH	1
29	BF	1
44	BU	1
7	AD	1
15	AL	1

The worst 5 of 210 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	30(D):A	O3'	1031:G	P	5.01
1	BA	142(A):A	O3'	1143:A	P	4.98
1	AW	73:A	O3'	74:C	P	4.88
1	BA	1171:G	O3'	1173:G	P	4.41
1	AA	440:A	O3'	442:C	P	4.34

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%)	0.15	45 (2%) 52 42	188, 339, 400, 400	0
2	AV	76/76 (100%)	0.58	8 (10%) 13 16	242, 299, 394, 394	0
3	AW	73/76 (96%)	0.37	3 (4%) 42 35	253, 400, 400, 400	0
4	AX	17/18 (94%)	9.24	12 (70%) 0 1	400, 400, 400, 400	0
5	AB	234/256 (91%)	0.67	26 (11%) 12 15	395, 395, 400, 400	0
6	AC	206/239 (86%)	0.39	14 (6%) 25 24	393, 398, 398, 398	0
7	AD	208/209 (99%)	1.56	64 (30%) 1 5	257, 391, 400, 400	0
8	AE	150/162 (92%)	0.50	20 (13%) 8 13	371, 400, 400, 400	0
9	AF	101/101 (100%)	0.53	12 (11%) 10 14	400, 400, 400, 400	0
10	AG	155/156 (99%)	1.15	34 (21%) 3 7	358, 400, 400, 400	0
11	AH	138/138 (100%)	0.79	28 (20%) 3 8	396, 396, 396, 396	0
12	AI	127/128 (99%)	0.98	16 (12%) 9 13	395, 395, 395, 395	0
13	AJ	98/105 (93%)	1.47	29 (29%) 1 5	400, 400, 400, 400	0
14	AK	119/129 (92%)	0.50	14 (11%) 10 14	202, 202, 400, 400	0
15	AL	124/135 (91%)	1.50	36 (29%) 1 5	399, 399, 400, 400	0
16	AM	125/126 (99%)	1.81	37 (29%) 1 5	348, 400, 400, 400	0
17	AN	60/61 (98%)	1.66	18 (30%) 1 5	400, 400, 400, 400	0
18	AO	88/89 (98%)	1.96	27 (30%) 1 5	400, 400, 400, 400	0
19	AP	83/88 (94%)	2.14	31 (37%) 1 4	400, 400, 400, 400	0
20	AQ	104/105 (99%)	1.14	30 (28%) 1 5	400, 400, 400, 400	0
21	AR	73/88 (82%)	1.04	14 (19%) 4 8	400, 400, 400, 400	0
22	AS	80/93 (86%)	1.72	27 (33%) 1 4	400, 400, 400, 400	0
23	AT	99/106 (93%)	2.26	39 (39%) 1 3	400, 400, 400, 400	0
24	AU	24/27 (88%)	3.29	19 (79%) 0 1	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	BB	123/123 (100%)	0.11	3 (2%) 59 48	267, 323, 388, 388	0
26	BA	2814/2916 (96%)	0.22	157 (5%) 31 28	65, 238, 393, 400	0
27	BD	173/173 (100%)	1.72	48 (27%) 2 5	392, 392, 400, 400	0
28	BE	191/338 (56%)	2.01	89 (46%) 0 3	400, 400, 400, 400	0
29	BF	189/246 (76%)	1.88	66 (34%) 1 4	393, 396, 396, 396	0
30	BG	122/176 (69%)	1.32	37 (30%) 1 5	400, 400, 400, 400	0
31	BH	164/177 (92%)	0.85	25 (15%) 6 11	400, 400, 400, 400	0
32	BI	148/149 (99%)	1.13	31 (20%) 3 7	400, 400, 400, 400	0
33	BN	117/145 (80%)	1.97	43 (36%) 1 4	400, 400, 400, 400	0
34	BO	122/122 (100%)	1.26	30 (24%) 2 6	400, 400, 400, 400	0
35	BP	84/164 (51%)	1.08	17 (20%) 3 8	395, 395, 400, 400	0
36	BQ	138/138 (100%)	2.02	53 (38%) 1 3	393, 393, 393, 393	0
37	BS	113/186 (60%)	1.17	29 (25%) 2 6	278, 400, 400, 400	0
38	BT	52/66 (78%)	2.86	30 (57%) 0 2	400, 400, 400, 400	0
39	BW	108/113 (95%)	1.23	21 (19%) 4 8	278, 395, 400, 400	0
40	BX	76/84 (90%)	3.12	45 (59%) 0 2	400, 400, 400, 400	0
41	BY	110/119 (92%)	2.61	41 (37%) 1 4	400, 400, 400, 400	0
42	BZ	177/253 (69%)	1.23	42 (23%) 2 6	396, 398, 398, 398	0
43	BR	105/118 (88%)	1.58	29 (27%) 2 5	400, 400, 400, 400	0
44	BU	117/118 (99%)	1.80	38 (32%) 1 4	391, 391, 400, 400	0
45	BV	100/100 (100%)	1.02	18 (18%) 4 9	400, 400, 400, 400	0
46	B2	64/70 (91%)	1.70	22 (34%) 1 4	400, 400, 400, 400	0
47	B3	60/60 (100%)	1.54	18 (30%) 1 5	398, 398, 398, 398	0
48	B0	86/91 (94%)	1.47	21 (24%) 2 6	396, 400, 400, 400	0
49	B4	73/73 (100%)	2.11	33 (45%) 1 3	396, 397, 397, 397	0
50	B5	58/60 (96%)	1.39	17 (29%) 1 5	400, 400, 400, 400	0
51	B6	53/82 (64%)	1.22	13 (24%) 2 6	400, 400, 400, 400	0
52	B7	46/47 (97%)	2.06	25 (54%) 0 3	396, 396, 396, 396	0
53	B8	63/64 (98%)	2.46	30 (47%) 0 3	400, 400, 400, 400	0
54	B9	35/36 (97%)	3.59	24 (68%) 0 1	400, 400, 400, 400	0
55	BK	133/141 (94%)	1.52	38 (28%) 1 5	392, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	10091/10981 (91%)	0.89	1736 (17%)	5 9	65, 395, 400, 400	0

The worst 5 of 1736 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AX	126	A	34.4
4	AX	115	G	25.6
4	AX	124	C	23.1
16	AM	124	PRO	21.0
16	AM	123	ALA	20.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PSU	AW	39	20/21	0.47	0.15	399,399,399,399	0
3	PSU	AW	55	20/21	0.52	0.08	400,400,400,400	0
3	YYG	AW	37	39/40	0.62	0.23	399,399,399,399	0

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.