wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 02:32 AM EDT

PDB ID	:	4V4P
Title	:	Crystal structure of 70S ribosome with thrS operator and tRNAs.
Authors	:	Jenner, L.; Romby, P.; Rees, B.; Schulze-Briese, C.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.; Yusupova, G.; Yusupov, M.
Deposited on	:	2005-01-19
Resolution	:	5.50 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:

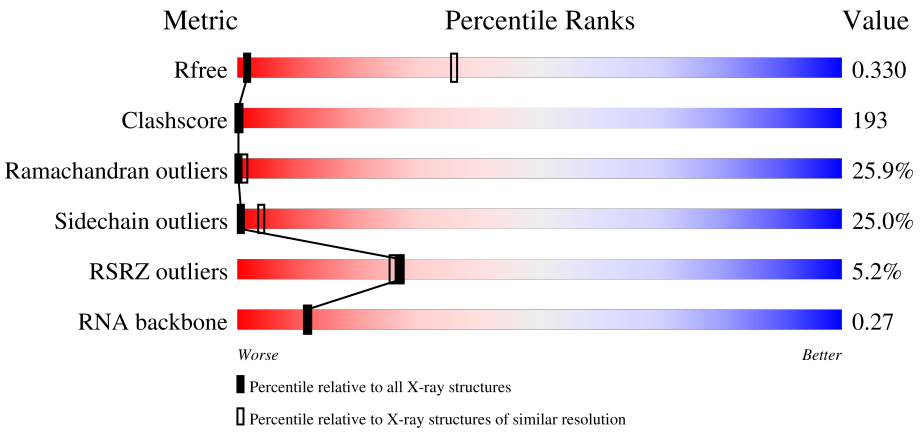
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 5.50 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	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)
RNA backbone	3102	1074 (7.80-3.00)

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	AB	123	52% 41% 7%
2	AA	2915	% 41% 39% 18%
3	AC	228	2% 9% 64% 19%
4	AD	178	6% 39% 40% 16%

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Mol	Chain	Length	Quality of chain
5	AE	338	11% 28% 22% 6% 43%
6	AF	246	% 42% 26% 8% 23%
7	AG	176	% 34% 28% 31%
8	AH	177	% 56% 31% 7%
9	AI	128	23% 10% 74% 14%
9	AJ	128	38% 9% 75% 15%
10	AK	149	3% 63% 30% 5%
11	AL	141	5% 6% 59% 26% 6%
12	AM	145	8% 43% 30% 7% 19%
13	AN	122	8% 52% 37% 9%
14	AO	164	3% 23% 21% 5% 49%
15	AP	138	7% 42% 43% 12%
16	AQ	186	26% 28% 6% 39%
17	AR	66	11% 35% 20% 24% 21%
18	AS	113	2% 61% 24% 6%
19	AT	84	5% 52% 25% 13% 10%
20	AU	119	6% 61% 24% 7% 8%
21	AV	253	3% 35% 24% 9% 30%
22	AW	70	% 47% 36% 9%
23	AX	60	47% 42% 10%
24	A0	118	2% 48% 35% 5% 11%
25	A1	118	% 55% 36% 8%
26	A2	100	16% 57% 32% 9%
27	A3	91	12% 7% 35% 44% 9% 5%
28	A4	73	8% 40% 48% 11%

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Mol	Chain	Length	Quality of chain
29	A5	60	3% 5% 45% 35% 12%
30	A6	82	5% 32% 28% 35%
31	A7	47	2% 49% 43% 6%
32	A8	64	2% 39% 47% 12%
33	A9	36	64% 28%
34	BA	1522	55% 34% 10%
35	BB	76	79% 9% 30% 59%
35	BC	76	42% 38% 18%
36	B1	78	55% 50% 26% 6% 15%
37	BE	256	8% 50% 33% 6% 9%
38	BF	239	16% 5% 54% 23% 5% 14%
39	BG	209	3% 56% 35% 5%
40	BH	162	12% 54% 31% 7%
41	BI	101	28% 55% 41%
42	BJ	156	4% 6% 62% 26% 6%
43	BK	138	7% 49% 41% 9%
44	BL	128	64% 31%
45	BM	105	10% 5% 53% 31% 7%
46	BN	129	7% 5% 53% 31% 8%
47	BO	135	3% 5% 54% 30% 8%
48	BP	126	10% 49% 39%
49	BQ	61	3% 48% 36% 11%
50	BR	89	3% 57% 37%
51	BS	88	% 51% 34% 8% 6%
52	BT	105	3% 61% 35%

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Mol	Chain	Length	Quality of chain
53	BU	88	10%, 49%, 20%, 10%, 17%
54	BV	93	5%, 48%, 28%, 5%, 14%
55	BW	106	56%, 32%, 6%, 7%
56	BX	27	56%, 30%, 11%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 148539 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 5S ribosomal RNA.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	-1	A	-	insertion	GB 48271
AB	120	U	-	insertion	GB 48271

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AA	2872	61847	27526	11556	19893	2872	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	494	G	-	insertion	GB 48268

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	221	1687	1066	306	312	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AI	128	945	599	152	193	1	0	0	0
9	AJ	128	945	599	152	193	1	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L11.

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

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S general stress protein CTC (L25).

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
24	A0	105	855	536	174	145	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	A1	117	978	608	210	159	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	A2	100	787	495	146	145	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	A3	86	641	402	124	114	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	A4	73	604	382	110	108	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	A5	58	457	281	94	77	5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	A6	53	431	274	80	76	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	A7	46	383	230	91	60	2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	A8	63	496	312	101	78	5	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	A9	35	285	172	64	45	4	0	0	0

- Molecule 34 is a RNA chain called 16S rRNA.

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

- Molecule 35 is a RNA chain called tRNA Phe (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	BB	76	1626	725	293	532	76	0	0	0
			Total	C	N	O	P			
35	BC	76	1626	725	293	532	76	0	0	0

- Molecule 36 is a RNA chain called thrS mRNA operator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	B1	66	1405	629	247	463	66	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S2.

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

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	25	ASP	GLU	conflict	UNP Q5SHQ2
BK	37	ARG	LYS	conflict	UNP Q5SHQ2
BK	52	ASP	GLU	conflict	UNP Q5SHQ2
BK	61	VAL	ILE	conflict	UNP Q5SHQ2
BK	62	TYR	HIS	conflict	UNP Q5SHQ2
BK	81	HIS	LYS	conflict	UNP Q5SHQ2
BK	88	LYS	ARG	conflict	UNP Q5SHQ2
BK	115	SER	PRO	conflict	UNP Q5SHQ2

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

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

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 53 is a protein called 30S ribosomal protein S18.

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

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	41	VAL	ILE	conflict	UNP Q5SIH2

- Molecule 56 is a protein called 30S ribosomal protein Thx.

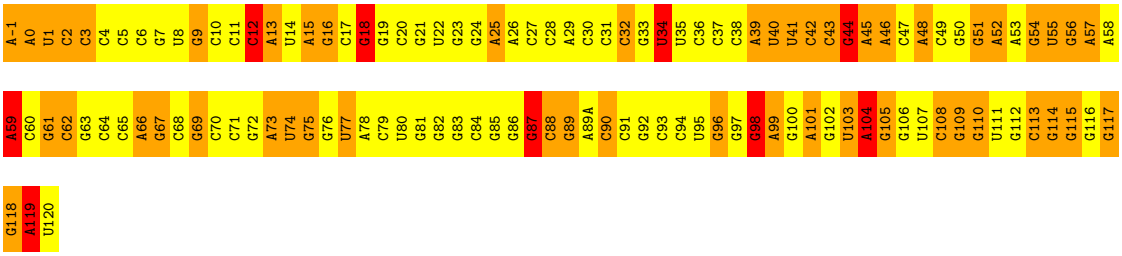
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	BX	24	208	128	50	30	0	0	0

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.

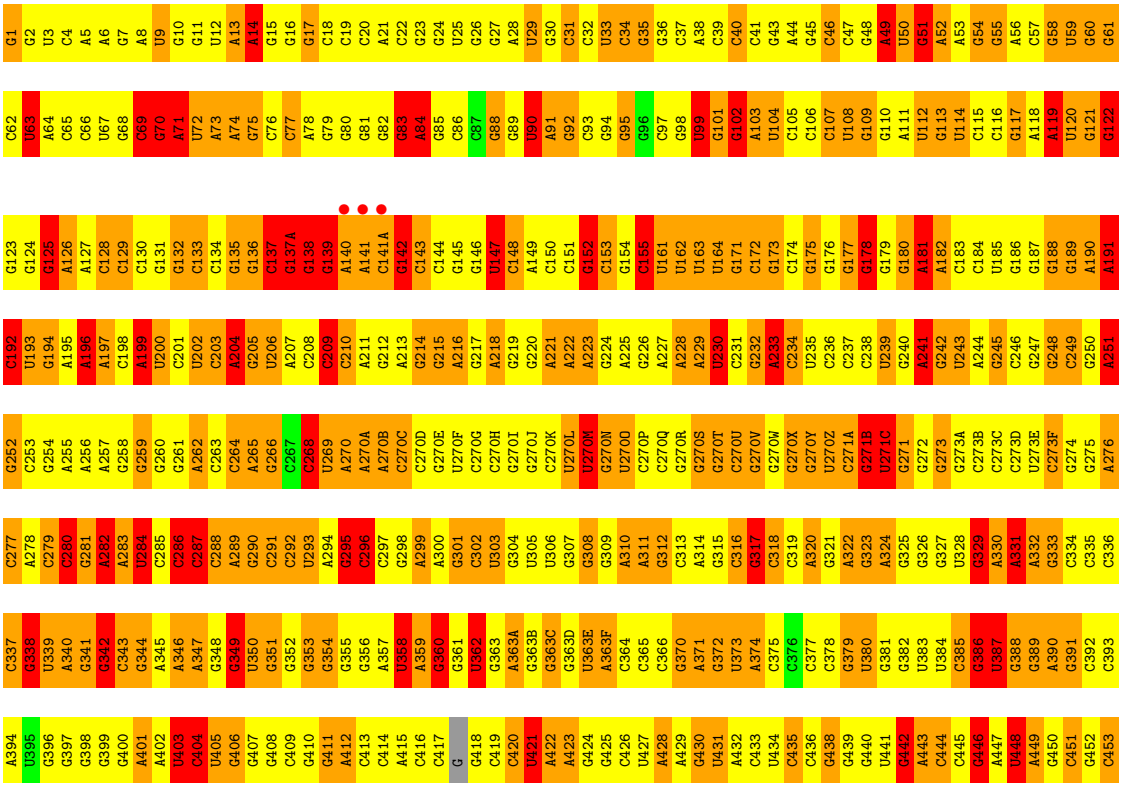
- Molecule 1: 5S ribosomal RNA

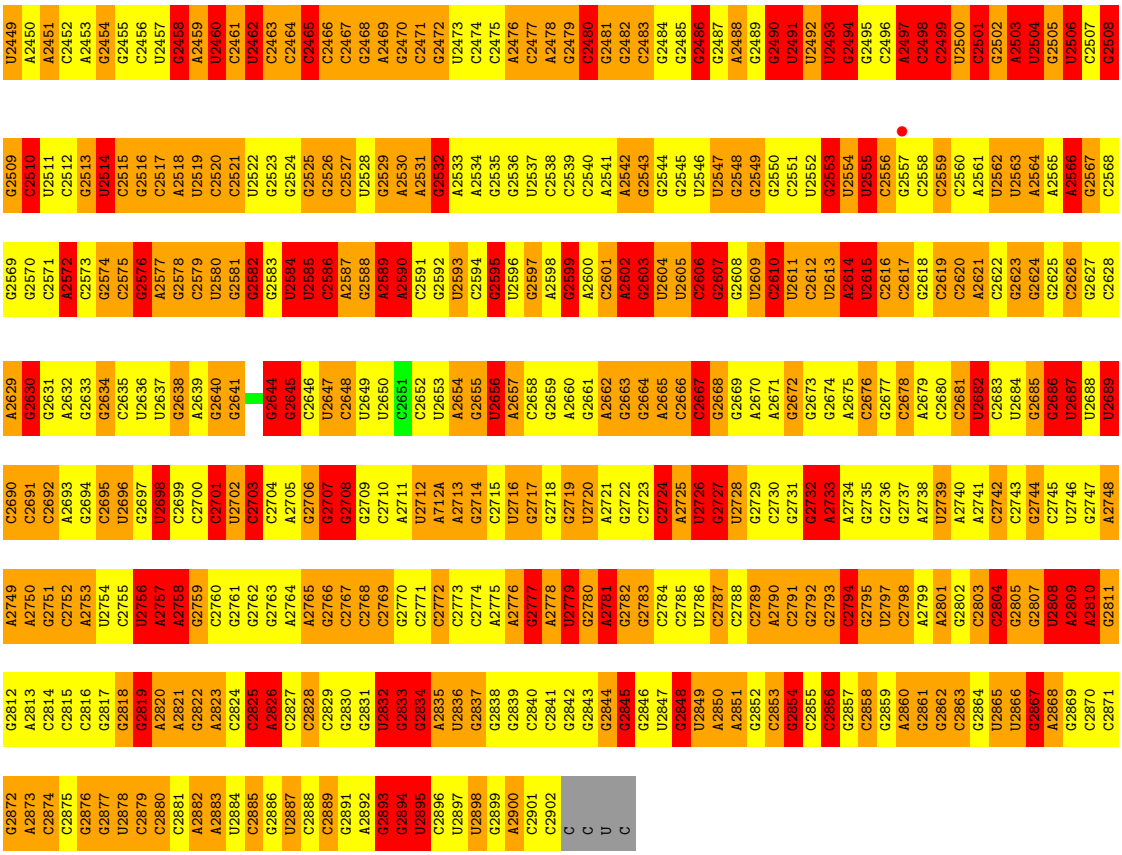
Chain AB: 52% 41% 7%



- Molecule 2: 23S ribosomal RNA

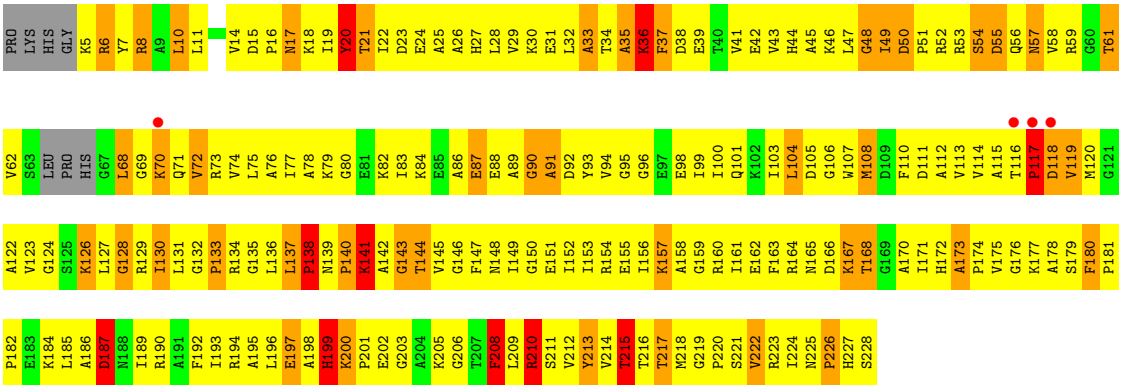
Chain AA: % 41% 39% 18%





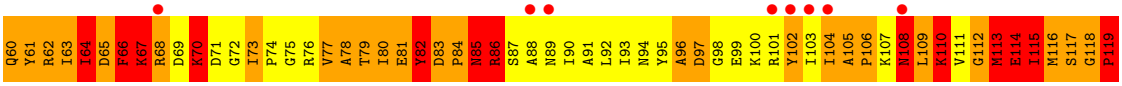
• Molecule 3: 50S ribosomal protein L1

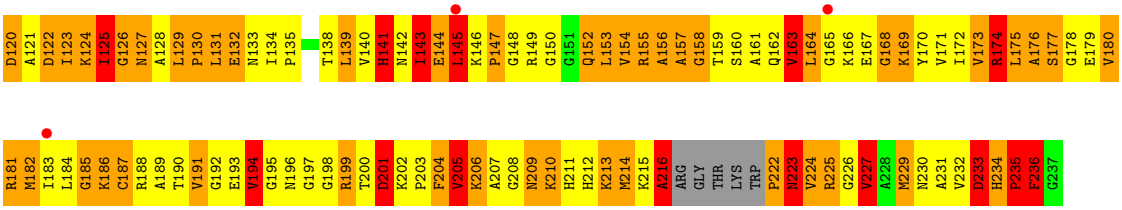
Chain AC:



• Molecule 4: 50S ribosomal protein L2

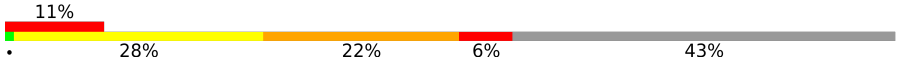
Chain AD:

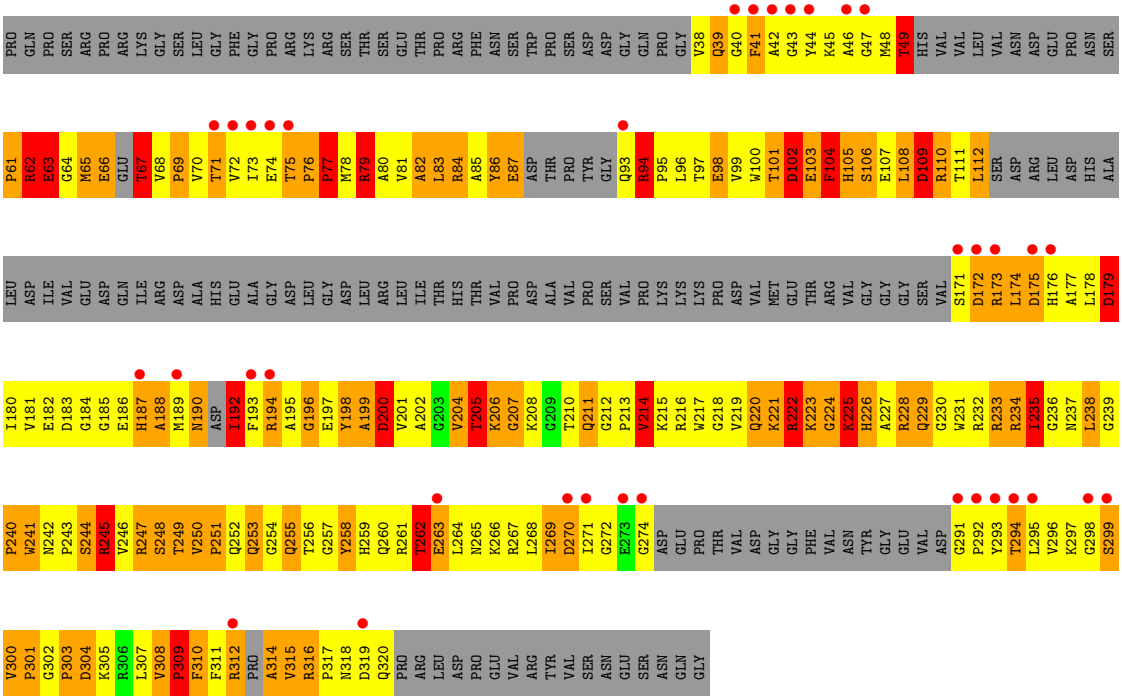




• Molecule 5: 50S ribosomal protein L3

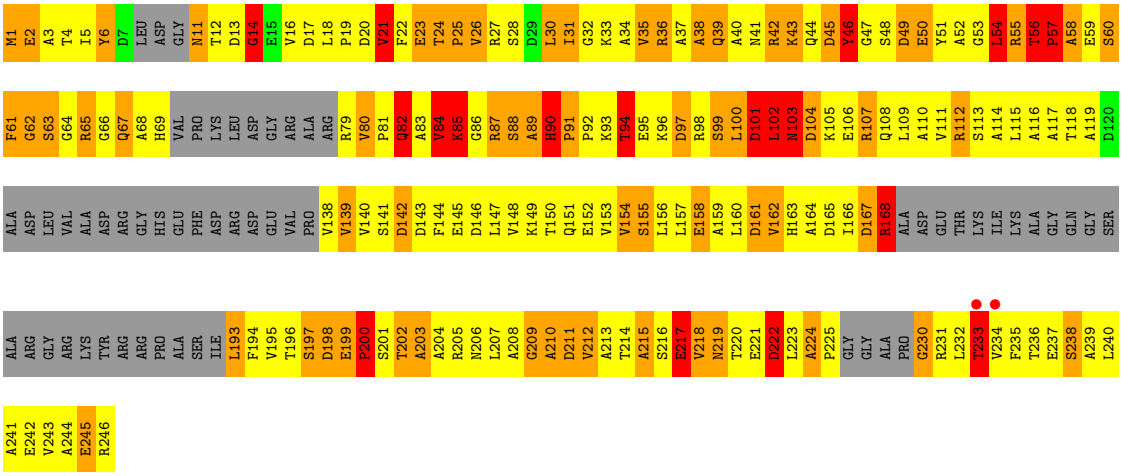
Chain AE:





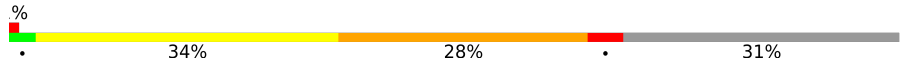
• Molecule 6: 50S ribosomal protein L4

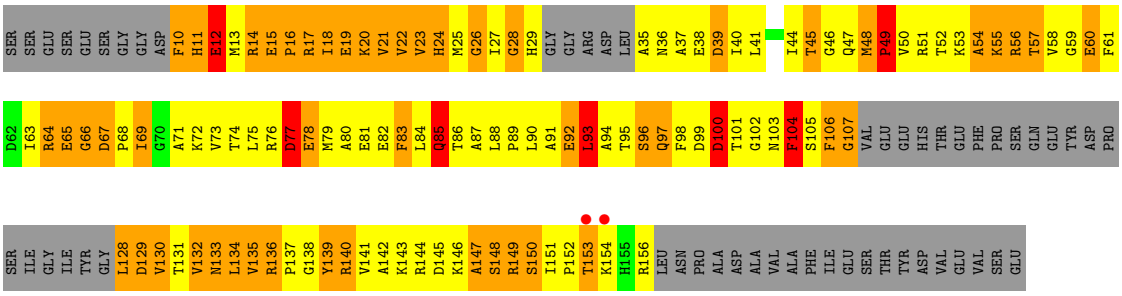
Chain AF:



• Molecule 7: 50S ribosomal protein L5

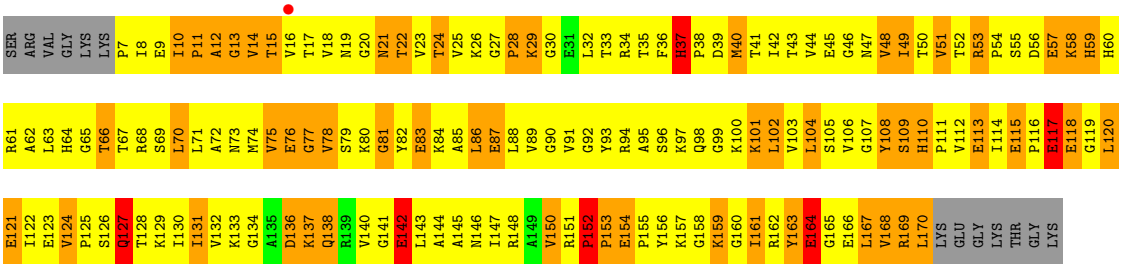
Chain AG:





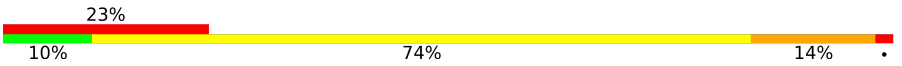
- Molecule 8: 50S ribosomal protein L6

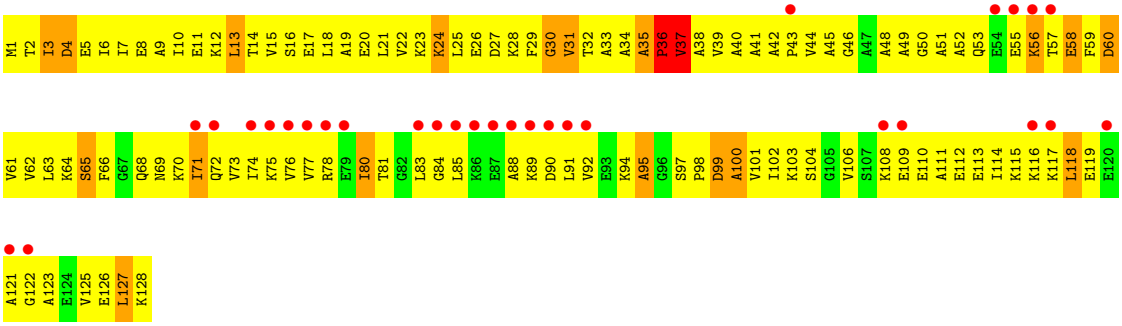
Chain AH:



- Molecule 9: 50S ribosomal protein L7/L12

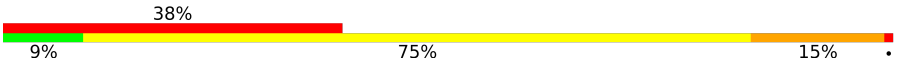
Chain AI:

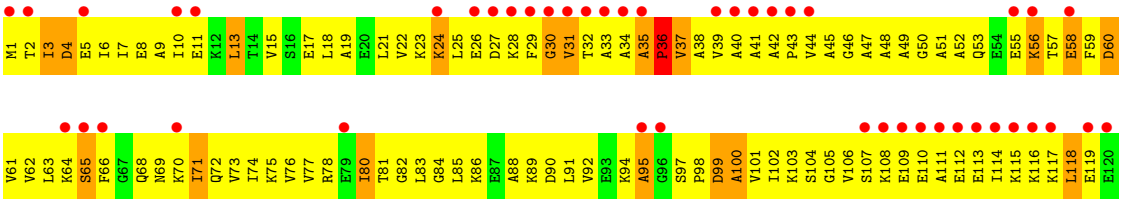




- Molecule 9: 50S ribosomal protein L7/L12

Chain AJ:





A121 G122 A123 E124 V125 E126 L127 K128

- Molecule 10: 50S ribosomal protein L9

Chain AK: 3% 63% 30% 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 E73 K74 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 R122 A123 L124 G125 Y126 T127 N128 V129 P130 V131 K132 L133 H134 P135 E136 V137 T138 A139 T140 L141 K142 V143 H144 V145 T146 E147 Q148 K149

- Molecule 11: 50S ribosomal protein L11

Chain AL: 5% 6% 59% 26% 6%

MET ALA LYS LYS VAL ALA ALA Q8 I9 K10 L11 Q12 L13 P14 A15 G16 K17 A18 T19 P20 A21 P22 P23 V24 G25 P26 A27 L28 G29 Q30 H31 G32 V33 N34 I35 M36 E37 F38 C39 K40 R41 F42 N43 A44 E45 T46 A47 D48 K49 A50 G51 M52 I53 L54 P55 V56 V57 I58 T59 V60

Y61 E62 D63 K64 S65 F66 T67 F68 I69 I70 K71 T72 P73 P74 A75 S76 F77 L78 L79 K80 K81 A82 I85 E86 K87 G88 S89 S90 E91 P92 K93 R94 K95 I96 V97 G98 K99 V100 T101 R102 K103 Q104 I105 E106 E107 I108 A109 K110 T111 K112 M113 P114 D115 L116 N117 A118 N119 S120 L121

E122 A123 A124 M125 K126 I127 I128 E129 G130 T131 A132 K133 S134 M135 G136 I137 E138 V139 V140 ASP

- Molecule 12: 50S ribosomal protein L13

Chain AM: 8% 43% 30% 7% 19%

MET SER VAL A4 E5 F6 D7 A8 D9 V10 I11 V12 D13 A14 R15 D16 C17 I18 M19 G20 R21 V22 A23 S24 Q25 V26 A27 E28 Q29 A30 L31 D32 G33 E34 T35 V36 A37 V38 V39 N40 A41 E42 R43 A44 V45 I46 T47 G48 R49 E50 E51 Q52 I53 V54 E55 K56 Y57 E58 K59 R60

V61 D62 I63 G64 N65 D66 N67 G68 Y69 F70 Y71 P72 K73 R74 P75 D76 G77 I78 F79 K80 R81 T82 I83 R84 G85 M86 L87 P88 HIS K90 K91 Q92 R93 G94 R95 E96 A97 F98 E99 S100 V101 R102 V103 Y104 L105 G106 N107 P108 Y109 D110 GLU ASP GLY GLU VAL LEU ASP GLY THR SER

LEU ASP ARG LEU SER ASN ILE LYS PHE VAL T131 L132 G133 E134 I135 S136 E137 T138 L139 G140 A141 ASN LYS THR TRP

- Molecule 13: 50S ribosomal protein L14

Chain AN: 8% 52% 37% 9%

M1 I2 Q3 Q4 E5 S6 R7 L8 K9 V10 A11 D12 N13 S14 G15 A16 R17 E18 V19 L20 V21 I22 K23 V24 L25 G26 G27 S28 G29 R30 R31 Y32 A33 N34 I35 G36 D37 V38 V39 V40 A41 T42 V43 K44 D45 A46 T47 P48 G49 G50 V51 V52 K53 K54 G55 Q56 V57 V58 K59 A60

V61 V62 V63 R64 T65 K66 R67 G68 V69 R70 R71 P72 D73 G74 S75 Y76 I77 R78 F79 D80 E81 N82 A83 C84 V85 I86 I87 R88 D89 D90 K91 S92 P93 R94 G95 T96 R97 I98 F99 G100 P101 V102 A103 R104 E105 L106 R107 D108 K109 D110 F111 M112 K113 I114 I115 S116 L117 A118 P119 E120

V121 I122

- Molecule 14: 50S ribosomal protein L15

Chain AO: 3% · 23% 21% 5% 49%

THR SER LYS LYS LYS ARG GLN ARG GLY SER ARG THR HIS GLY GLY GLY SER HIS LYS ASN ARG ARG GLY ALA GLY HIS ARG GLY GLY GLY ARG GLY ASP ALA GLY ARG ASP LYS HIS GLU PHE HIS ASN HIS GLU PRO LEU GLY LYS SER GLY F51 K52 R53 P54 Q55 K56 V57 Q58 E59 E60

A61 A62 T63 I64 D65 V66 R67 E68 I69 D70 E71 N72 V73 T74 L75 L76 A77 A78 D79 D80 V81 A82 E83 VAL GLU ASP GLY GLY PHE ARG VAL D92 V93 R94 D95 V96 VAL GLU GLU A100 D101 D102 A103 D104 Y105 V106 K107 V108 L109 G110 A111 G112 Q113 V114 R115 H116 E117 L118 T119 L120

I121 A122 D123 D124 F125 S126 E127 G128 A129 R130 E131 K132 V133 E134 G135 A136 G137 G138 S139 V140 E141 L142 T143 D144 L145 GLY GLU GLU ARG GLN ALA GLU ALA GLU GLU THR GLU ASP ALA ASP ALA ASP GLU GLU

- Molecule 15: 50S ribosomal protein L16

Chain AP: 7% · 42% 43% 12%

S9 I10 K11 P12 T15 R16 R17 E18 Y19 I20 S21 G22 I23 P24 G25 K26 G27 I28 A29 Q30 F31 K32 M33 G34 N35 N36 T41 Y42 P43 A44 Q45 V46 E47 N48 V49 V50 E51 K52 P53 V54 Q55 I56 R57 H58 N59 A60 L61 E62 A63 A64 R65 N66 A67 A68 N69 R70 F71 V72 Q73 N74

S75 G76 K82 F83 R84 I85 R86 K87 F88 P89 F90 H91 V92 I93 R94 E95 Q96 D97 G98 D99 G100 M101 R102 A103 P104 F105 G106 K107 S108 V109 G110 T111 A112 A113 R114 S115 H116 G117 A118 N119 H120 D121 F122 I123 A124 W125 V126 N127 P128 D129 P130 A131 V132 E133 F134 A135 W136 R137 R138 A139

Y140 M141 K142 V143 T144 P145 T146 V147 N148 I149 D150 S151 S152 P153 A154 G155 N156 A157

- Molecule 16: 50S ribosomal protein L18

Chain AQ: · 26% 28% 6% 39%

ALA THR GLY PRO ARG TYR LYS VAL P9 M10 R11 R12 R13 R14 E15 A16 R17 T18 D19 Y20 H21 Q22 R23 L24 R25 L26 L27 K28 S29 G30 K31 P32 R33 L34 V35 A36 R37 K38 S39 N40 K41 H42 V43 R44 A45 Q46 L47 V48 T49 LEU GLY P52 N53 G54 D55 D56 T57 L58 A59 S60

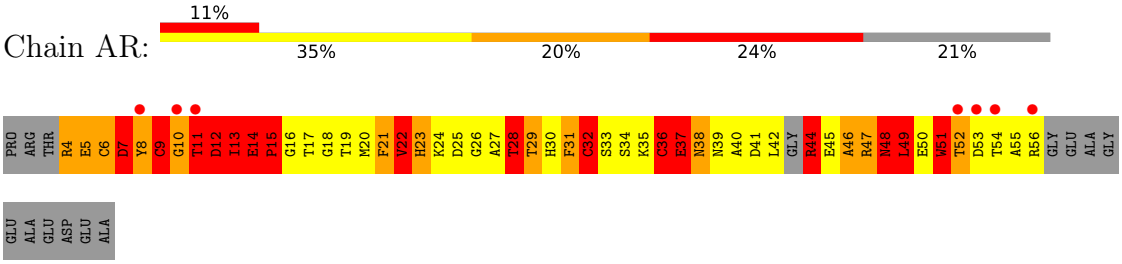
A61 H62 S63 S64 D65 L66 A67 E68 Y69 G70 W71 E72 ALA P74 T75 G76 ASN MET PRO S80 A81 Y82 L83 T84 G85 L86 L87 A88 G89 L90 R91 A92 Q93 E94 A95 G96 V97 E98 E99 A100 V101 L102 D103 I104 G105 L106 N107 S108 P109 T110 P111 GLY SER K114 V115 F116 A117 I118 Q119 E120

G121 A122 I123 D124 A125 G126 L127 D128 I129 PRO HIS ASN ASP ASP VAL LEU ALA ASP TRP GLN ARG THR ARG GLY ALA HIS ILE ALA GLU TYR ASP GLU GLN LEU GLU GLU PRO LEU TYR SER GLY ASP PHE ASP ALA ALA ASP LEU PRO GLU HIS PHE ASP GLU LEU ARG GLU THR LEU LEU

ASP GLY ASP ILE GLU LEU

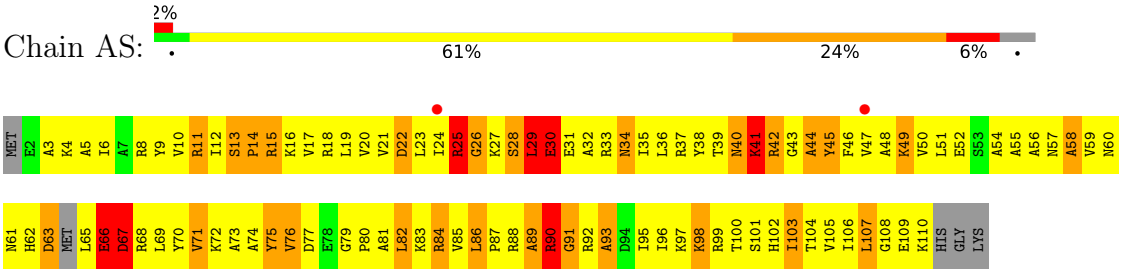
- Molecule 17: 50S ribosomal protein L19

Chain AR:



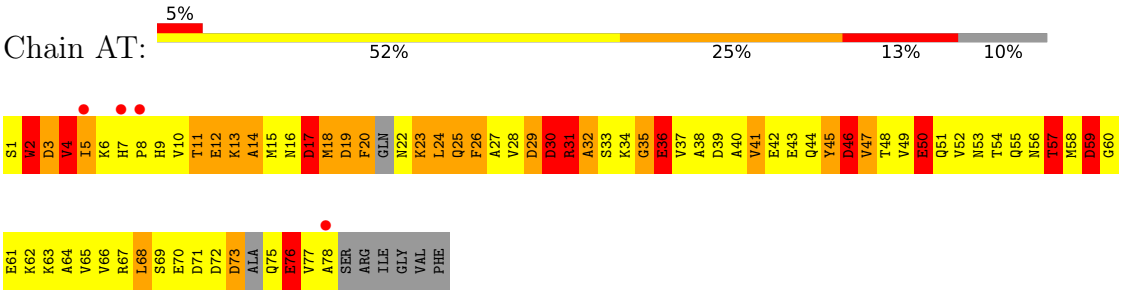
- Molecule 18: 50S ribosomal protein L22

Chain AS:



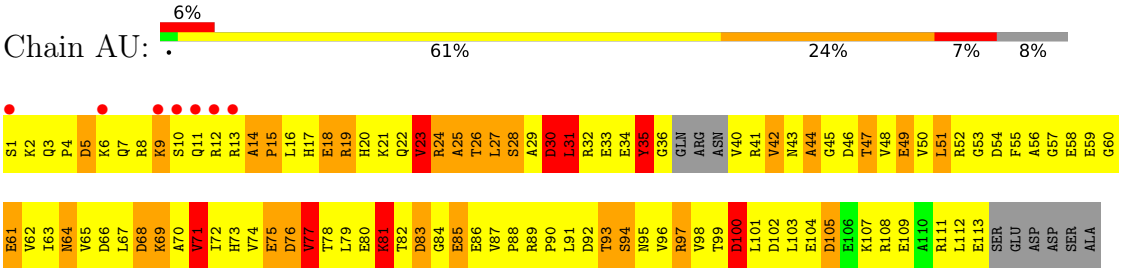
- Molecule 19: 50S ribosomal protein L23

Chain AT:



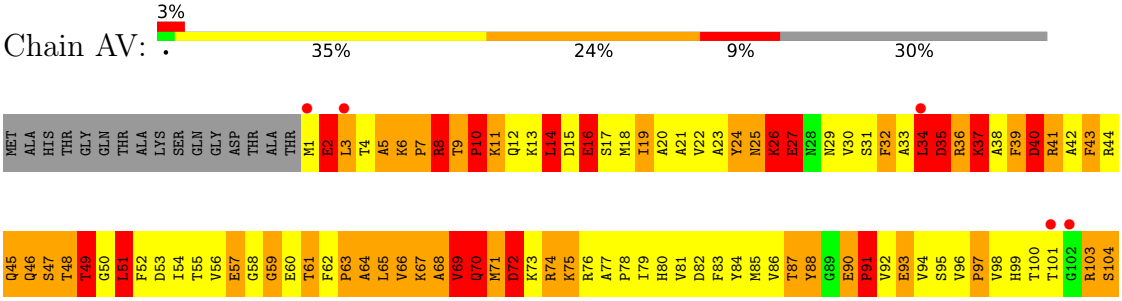
- Molecule 20: 50S ribosomal protein L24

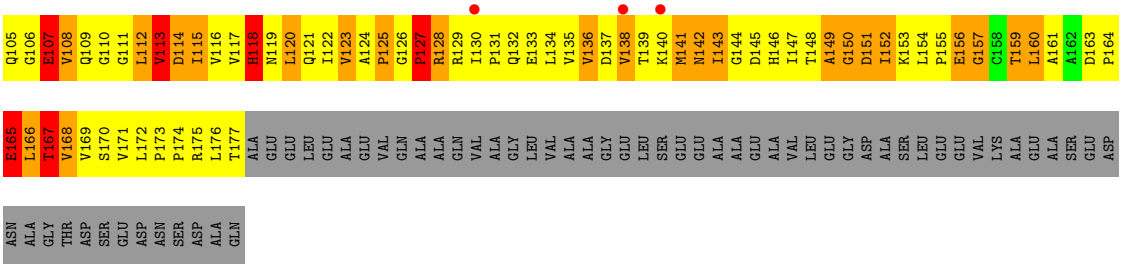
Chain AU:



- Molecule 21: 50S general stress protein CTC (L25)

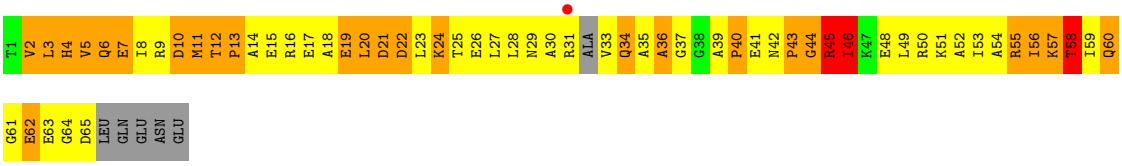
Chain AV:





- Molecule 22: 50S ribosomal protein L29

Chain AW:

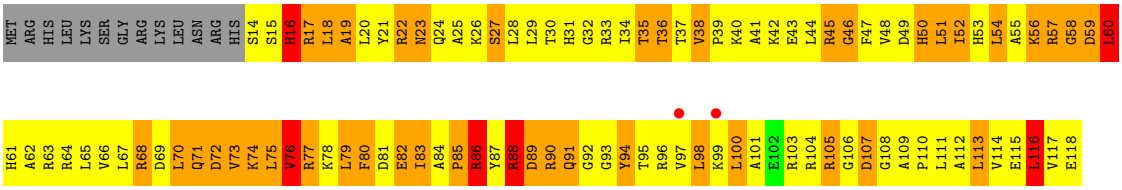


- Molecule 23: 50S ribosomal protein L30

Chain AX:

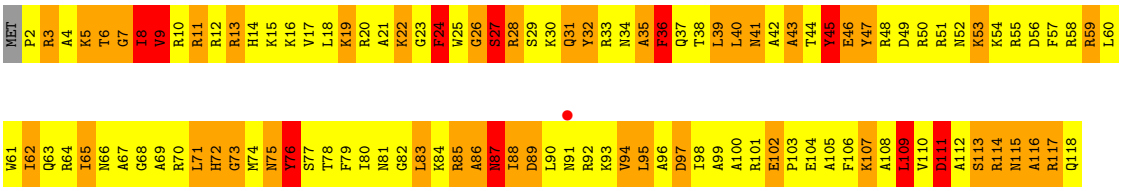
- Molecule 24: 50S ribosomal protein L17

Chain A0:



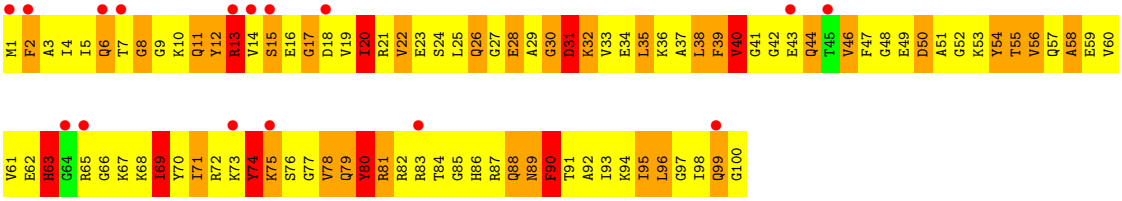
- Molecule 25: 50S ribosomal protein L20

Chain A1:



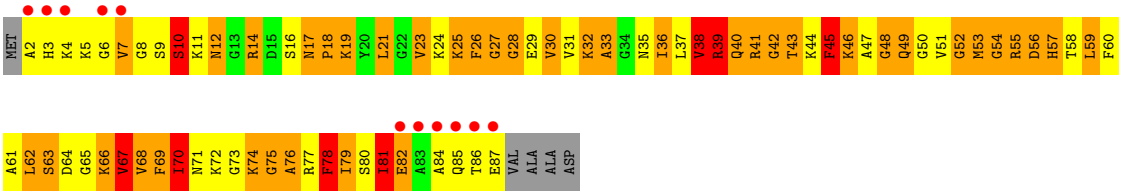
- Molecule 26: 50S ribosomal protein L21

Chain A2:



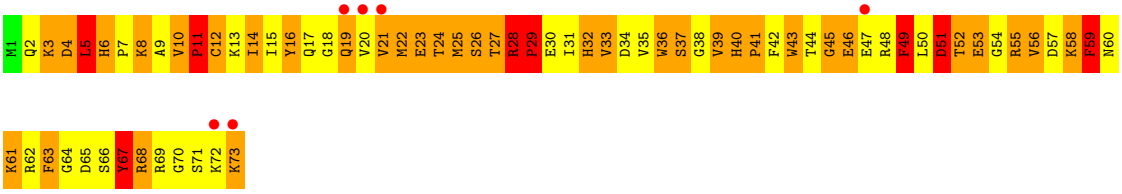
- Molecule 27: 50S ribosomal protein L27

Chain A3:



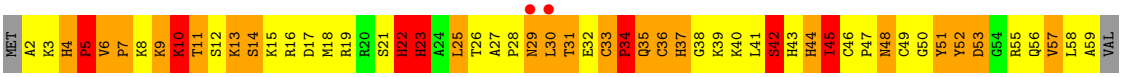
- Molecule 28: 50S ribosomal protein L31

Chain A4:



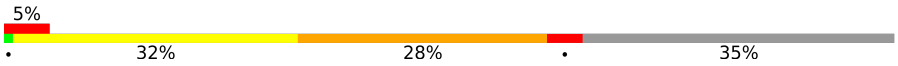
- Molecule 29: 50S ribosomal protein L32

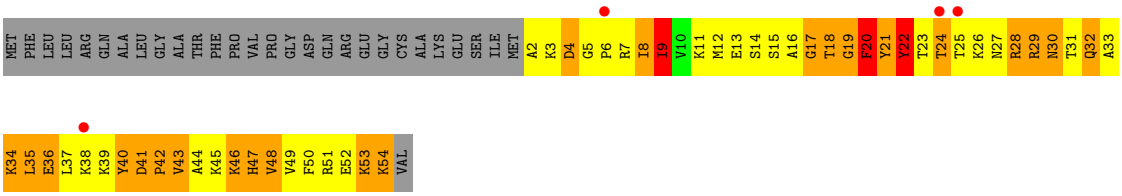
Chain A5:



- Molecule 30: 50S ribosomal protein L33

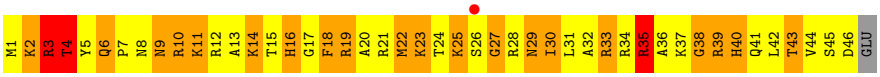
Chain A6:





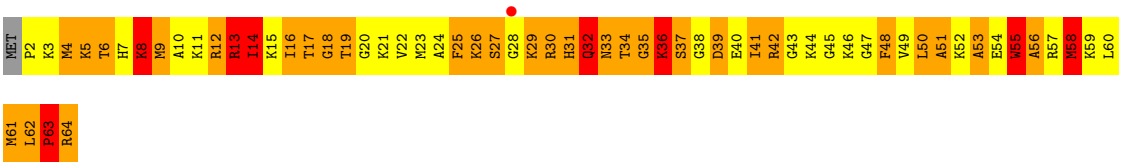
- Molecule 31: 50S ribosomal protein L34

Chain A7:



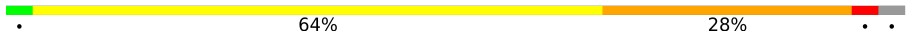
• Molecule 32: 50S ribosomal protein L35

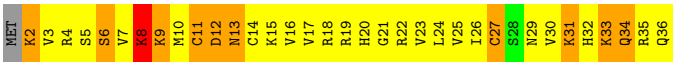
Chain A8:



• Molecule 33: 50S ribosomal protein L36

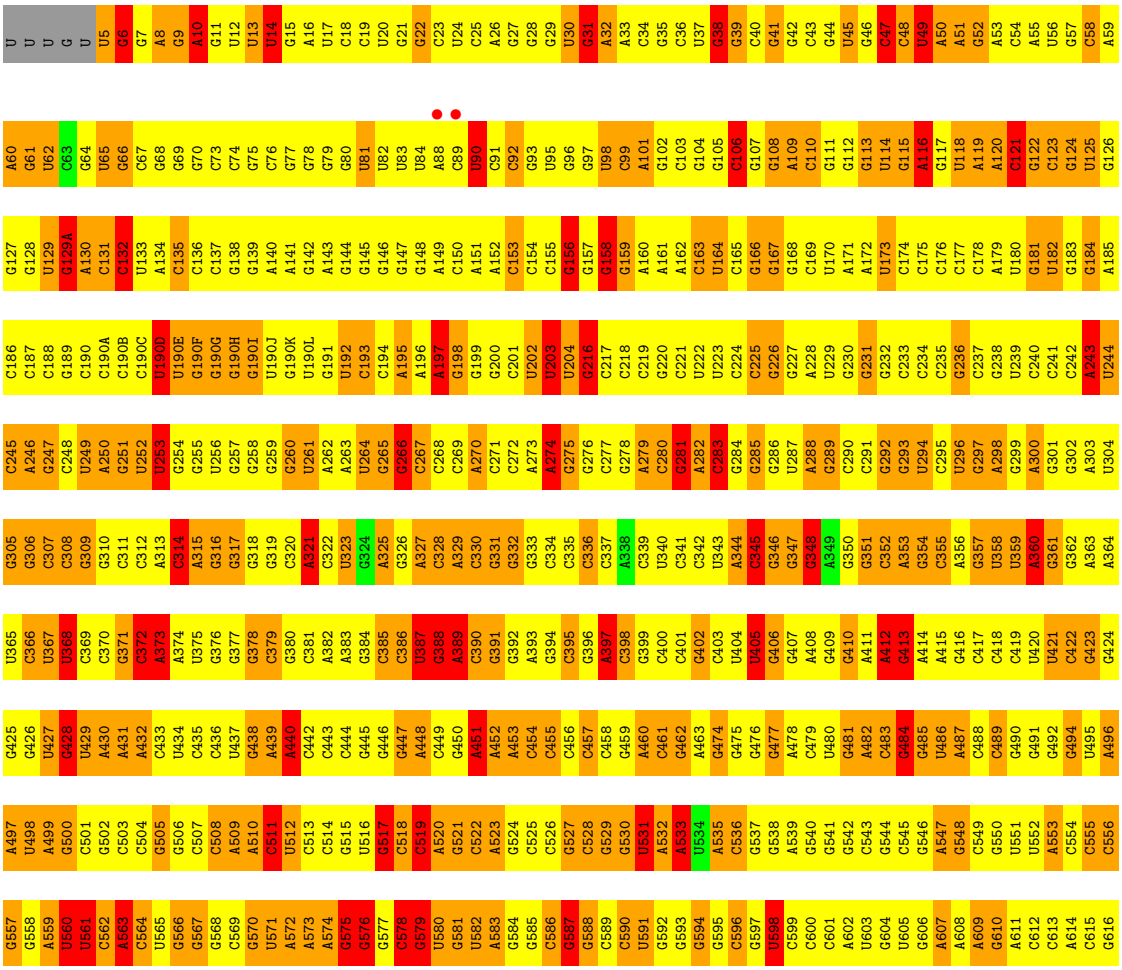
Chain A9:

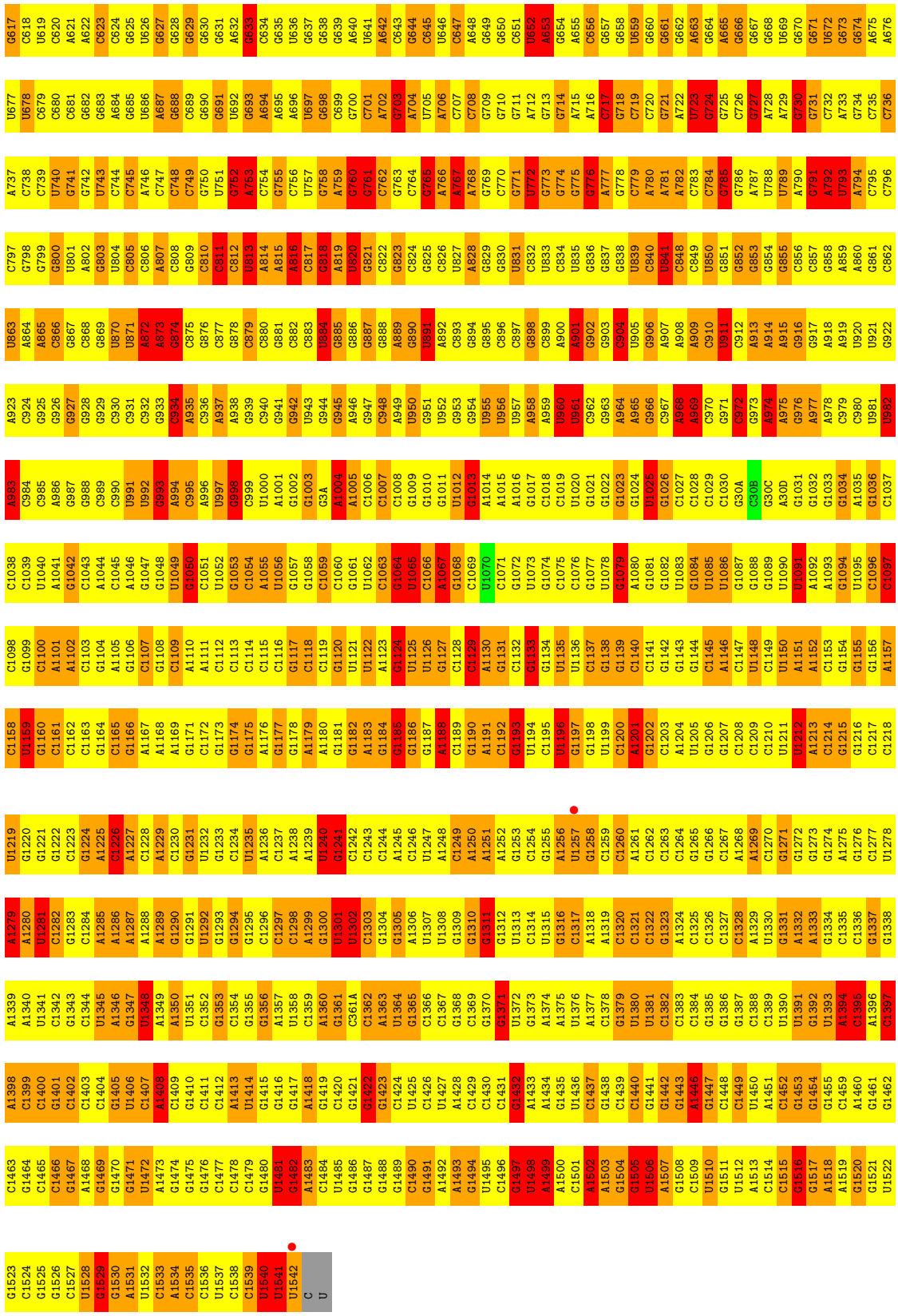




• Molecule 34: 16S rRNA

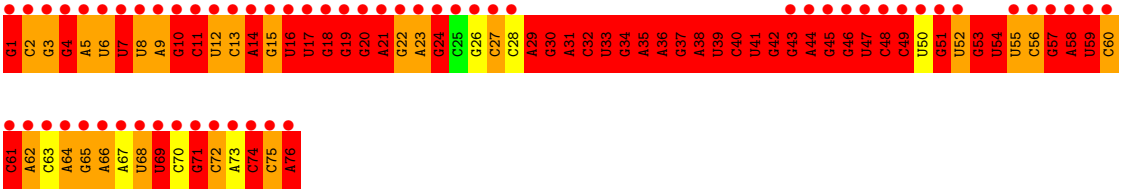
Chain BA:





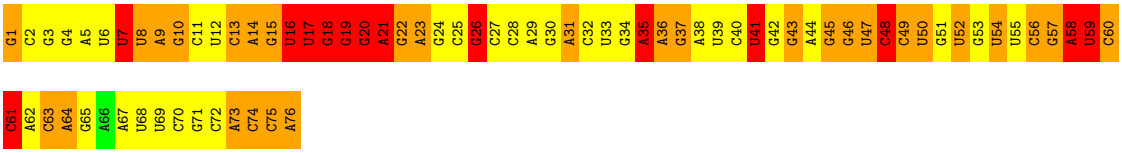
- Molecule 35: tRNA Phe (unmodified bases)

Chain BB:



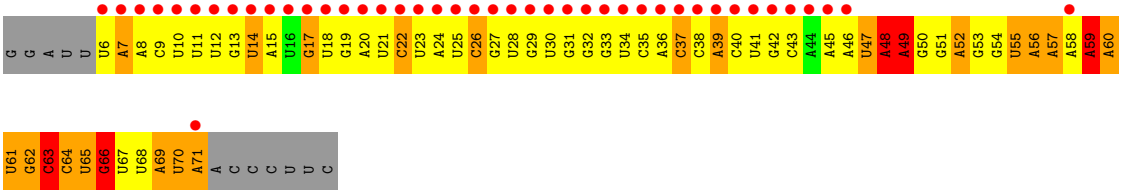
• Molecule 35: tRNA Phe (unmodified bases)

Chain BC:



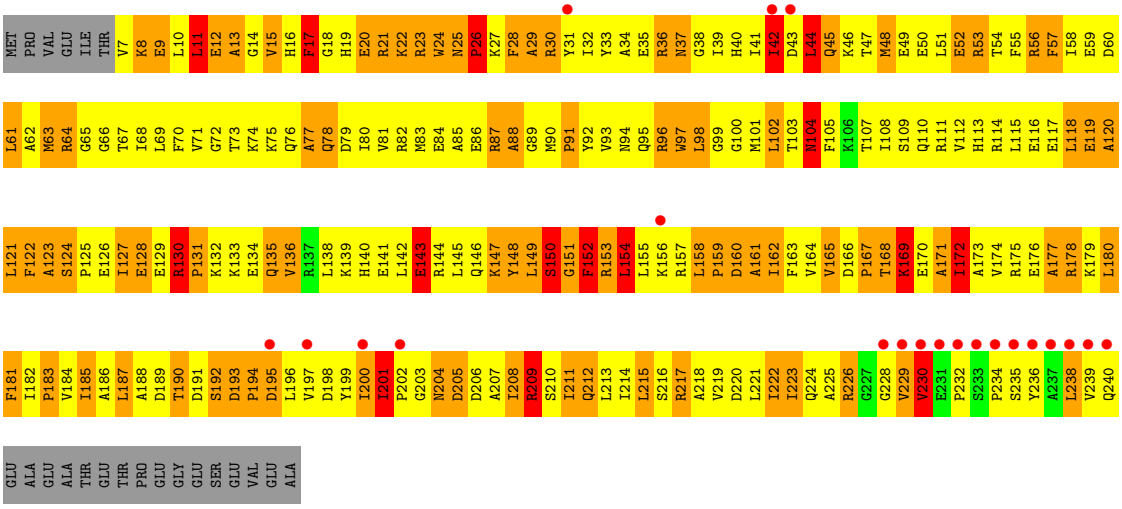
• Molecule 36: thrS mRNA operator

Chain B1:



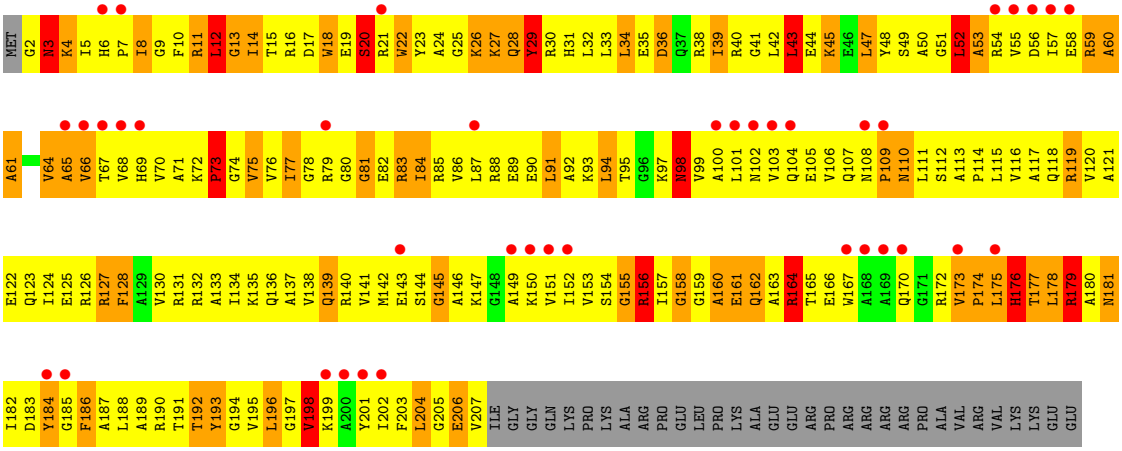
• Molecule 37: 30S ribosomal protein S2

Chain BE:



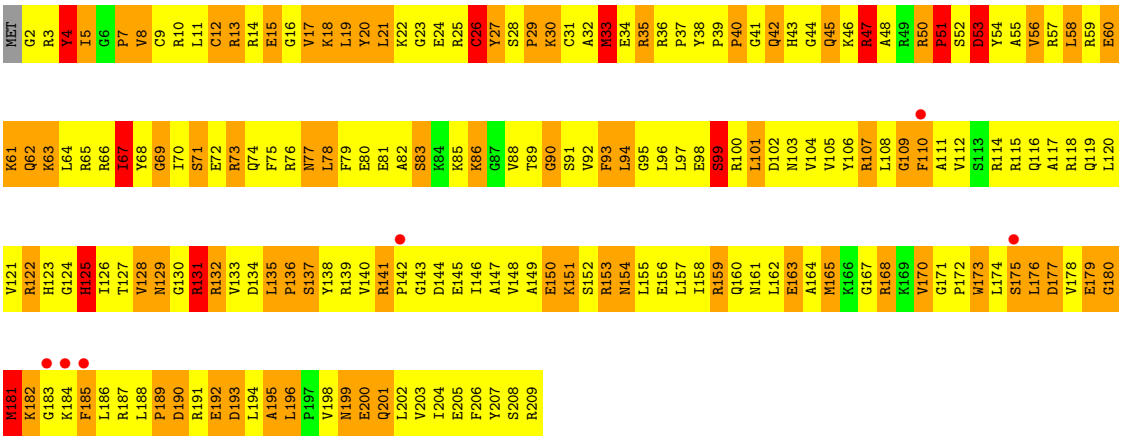
• Molecule 38: 30S ribosomal protein S3

Chain BF:



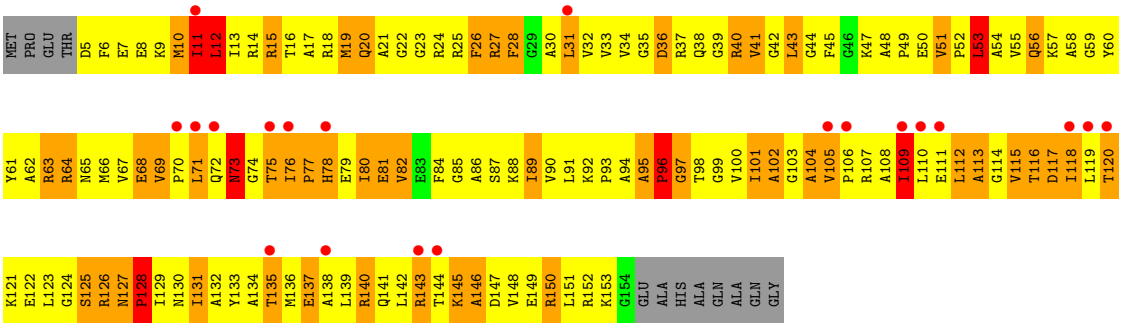
- Molecule 39: 30S ribosomal protein S4

Chain BG: 3% 56% 35% 5%



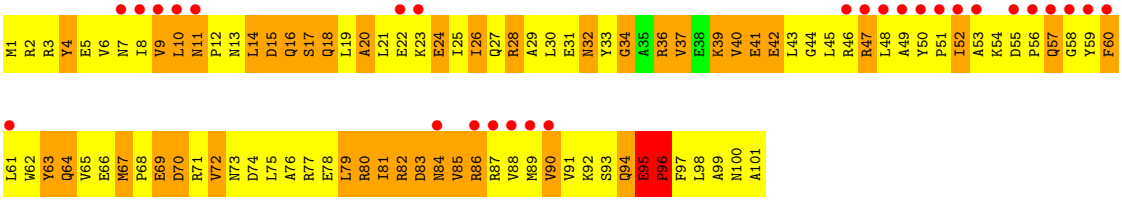
- Molecule 40: 30S ribosomal protein S5

Chain BH: 12% 54% 31% 7%



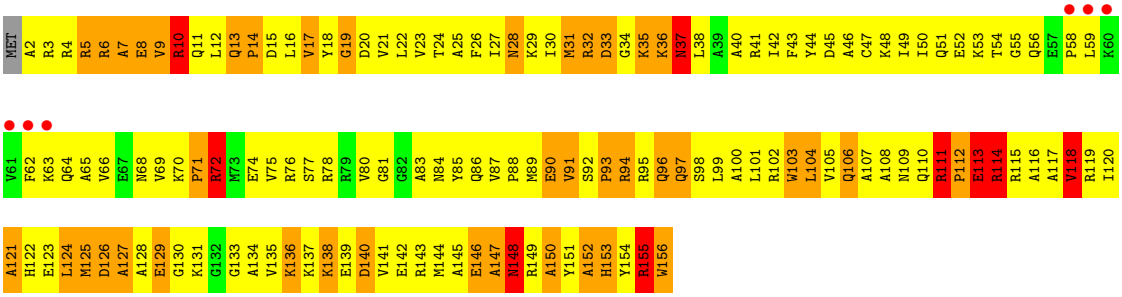
- Molecule 41: 30S ribosomal protein S6

Chain BI: 28% 55% 41%



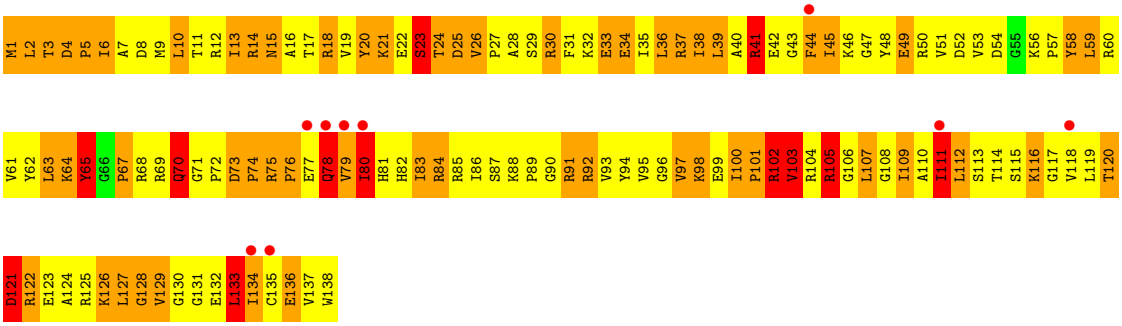
- Molecule 42: 30S ribosomal protein S7

Chain BJ:



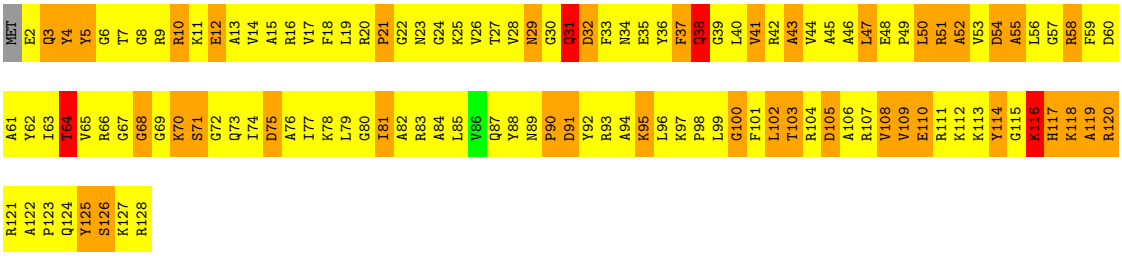
- Molecule 43: 30S ribosomal protein S8

Chain BK:



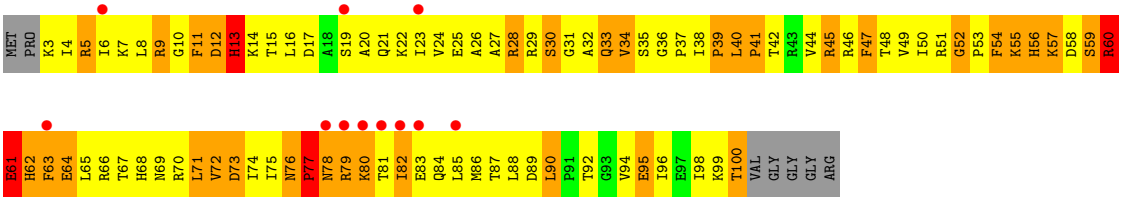
- Molecule 44: 30S ribosomal protein S9

Chain BL:



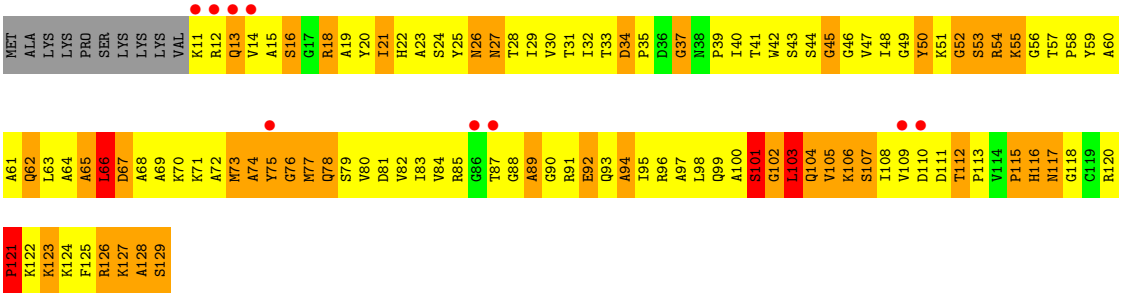
- Molecule 45: 30S ribosomal protein S10

Chain BM:



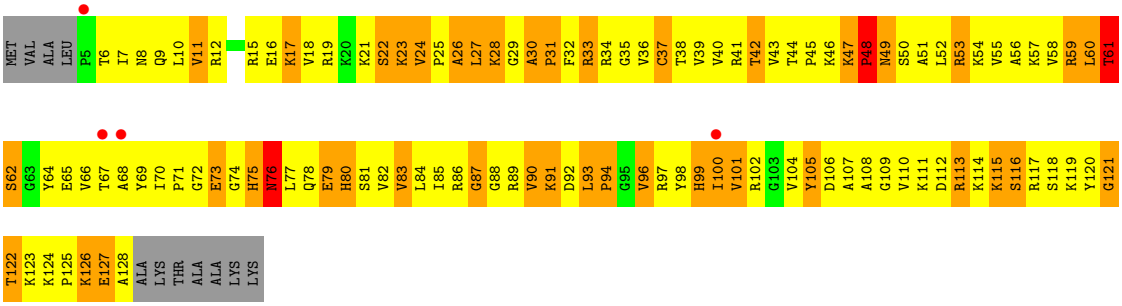
- Molecule 46: 30S ribosomal protein S11

Chain BN:



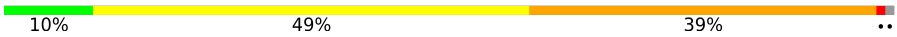
- Molecule 47: 30S ribosomal protein S12

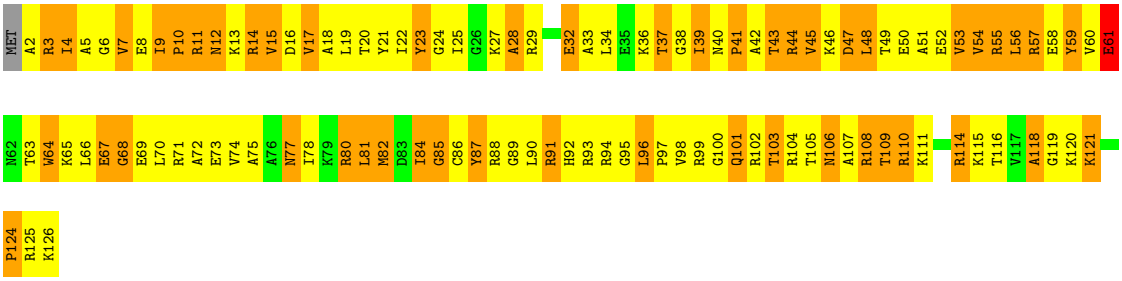
Chain BO:



- Molecule 48: 30S ribosomal protein S13

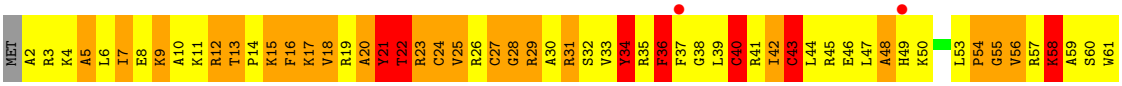
Chain BP:



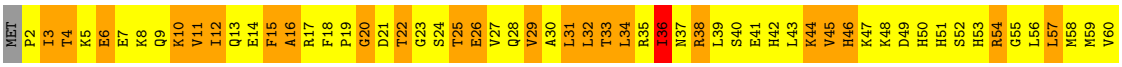


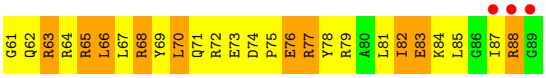
- Molecule 49: 30S ribosomal protein S14

Chain BQ:



• Molecule 50: 30S ribosomal protein S15

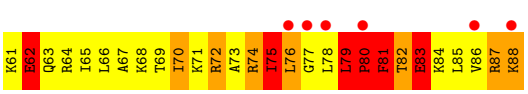




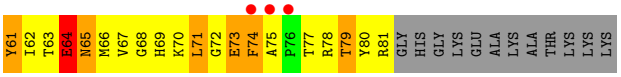
• Molecule 51: 30S ribosomal protein S16

• Molecule 52: 30S ribosomal protein S17

• Molecule 53: 30S ribosomal protein S18

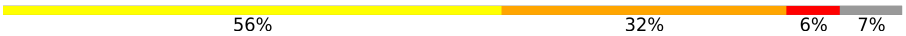


• Molecule 54: 30S ribosomal protein S19



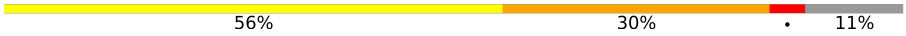
- Molecule 55: 30S ribosomal protein S20

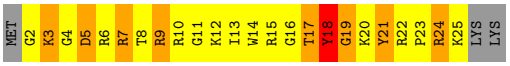
Chain BW:



- Molecule 56: 30S ribosomal protein Thx

Chain BX:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	508.64Å 508.64Å 806.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 268.38 – 5.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (300.00-5.50) 97.5 (268.38-5.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 5.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.307 , 0.356 0.288 , 0.330	Depositor DCC
R_{free} test set	7724 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	206.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.11 , 178.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	148539	wwPDB-VP
Average B, all atoms (Å^2)	338.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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	AB	0.95	1/2954 (0.0%)	1.06	7/4606 (0.2%)
2	AA	1.16	181/69267 (0.3%)	1.22	549/108130 (0.5%)
3	AC	0.62	0/1715	0.94	2/2310 (0.1%)
4	AD	1.11	6/1329 (0.5%)	1.52	22/1787 (1.2%)
5	AE	1.04	3/1542 (0.2%)	1.41	21/2084 (1.0%)
6	AF	0.82	0/1446	1.26	14/1960 (0.7%)
7	AG	0.83	0/972	1.20	6/1307 (0.5%)
8	AH	0.76	0/1272	1.13	1/1721 (0.1%)
9	AI	0.48	0/950	0.72	0/1275
9	AJ	0.43	0/950	0.68	0/1275
10	AK	0.73	0/1157	1.17	8/1547 (0.5%)
11	AL	0.48	0/1015	0.91	4/1366 (0.3%)
12	AM	1.04	2/928 (0.2%)	1.23	2/1248 (0.2%)
13	AN	1.06	2/946 (0.2%)	1.43	14/1269 (1.1%)
14	AO	0.67	0/643	1.30	9/870 (1.0%)
15	AP	1.04	1/1109 (0.1%)	1.43	16/1499 (1.1%)
16	AQ	0.71	0/880	1.23	5/1189 (0.4%)
17	AR	1.37	4/413 (1.0%)	2.01	18/557 (3.2%)
18	AS	0.81	0/869	1.19	3/1166 (0.3%)
19	AT	0.76	0/609	1.05	0/823
20	AU	0.46	0/887	0.89	0/1195
21	AV	0.71	0/1385	1.10	7/1883 (0.4%)
22	AW	0.73	0/497	1.05	1/668 (0.1%)
23	AX	0.81	0/482	1.18	2/646 (0.3%)
24	A0	0.86	0/867	1.24	3/1162 (0.3%)
25	A1	1.03	0/994	1.33	6/1323 (0.5%)
26	A2	0.71	0/797	1.14	4/1061 (0.4%)
27	A3	0.72	0/649	1.14	3/860 (0.3%)
28	A4	0.97	1/620 (0.2%)	1.18	4/831 (0.5%)
29	A5	0.79	0/469	1.41	5/629 (0.8%)
30	A6	0.93	0/438	1.25	4/583 (0.7%)
31	A7	0.78	0/387	1.05	0/509
32	A8	0.98	2/503 (0.4%)	1.48	8/657 (1.2%)
33	A9	1.36	1/286 (0.3%)	1.44	4/375 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BA	1.03	30/36438 (0.1%)	1.17	167/56869 (0.3%)
35	BB	2.33	76/1818 (4.2%)	2.48	157/2831 (5.5%)
35	BC	1.09	5/1818 (0.3%)	1.11	7/2831 (0.2%)
36	B1	1.14	7/1571 (0.4%)	0.96	7/2445 (0.3%)
37	BE	0.75	0/1935	1.06	3/2609 (0.1%)
38	BF	0.62	0/1636	0.99	5/2205 (0.2%)
39	BG	0.86	2/1733 (0.1%)	1.16	4/2318 (0.2%)
40	BH	0.85	0/1162	1.12	1/1564 (0.1%)
41	BI	0.78	0/856	1.06	1/1154 (0.1%)
42	BJ	0.70	1/1276 (0.1%)	1.00	6/1709 (0.4%)
43	BK	0.81	0/1136	1.18	5/1527 (0.3%)
44	BL	0.52	0/1029	0.86	1/1378 (0.1%)
45	BM	0.58	0/807	0.94	2/1085 (0.2%)
46	BN	0.75	0/900	1.04	0/1213
47	BO	0.78	0/986	1.22	3/1320 (0.2%)
48	BP	0.59	0/1008	0.98	0/1347
49	BQ	0.83	1/501 (0.2%)	1.09	2/664 (0.3%)
50	BR	0.74	0/745	1.05	2/992 (0.2%)
51	BS	0.81	0/716	1.10	3/963 (0.3%)
52	BT	0.82	0/870	1.11	2/1159 (0.2%)
53	BU	0.72	0/603	1.18	2/799 (0.3%)
54	BV	0.59	0/661	0.98	1/890 (0.1%)
55	BW	0.84	0/764	1.12	2/1006 (0.2%)
56	BX	0.45	0/212	0.81	0/277
All	All	1.05	326/161408 (0.2%)	1.21	1135/241526 (0.5%)

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	AB	0	14
2	AA	0	527
4	AD	0	1
5	AE	0	1
6	AF	0	1
7	AG	0	2
12	AM	0	2
13	AN	0	2
14	AO	0	2
16	AQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	AX	0	1
25	A1	0	3
26	A2	0	1
28	A4	0	1
30	A6	0	1
34	BA	0	220
35	BB	0	35
35	BC	0	12
36	B1	0	4
38	BF	0	1
39	BG	0	1
41	BI	0	1
43	BK	0	1
48	BP	0	1
51	BS	0	2
All	All	0	838

The worst 5 of 326 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	142	G	C5-C6	27.73	1.70	1.42
36	B1	48	A	C5-C6	27.45	1.65	1.41
35	BB	37	G	C2-N2	18.34	1.52	1.34
34	BA	1541	U	C4-C5	17.23	1.59	1.43
2	AA	142	G	C2-N3	16.69	1.46	1.32

The worst 5 of 1135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	1064	G	N1-C2-N2	-65.61	57.15	116.20
34	BA	1064	G	N3-C2-N2	63.69	164.48	119.90
34	BA	1064	G	N1-C2-N3	-27.38	107.47	123.90
2	AA	1084	A	O5'-P-OP2	-26.59	78.79	110.70
35	BB	36	A	OP1-P-O3'	-18.47	64.57	105.20

There are no chirality outliers.

5 of 838 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	12	C	Sidechain
1	AB	18	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AB	34	U	Sidechain
1	AB	39	A	Sidechain
1	AB	44	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2641	0	1337	635	1
2	AA	61847	0	31165	17729	1
3	AC	1687	0	1737	723	0
4	AD	1308	0	1355	898	0
5	AE	1507	0	1494	986	0
6	AF	1430	0	1386	832	0
7	AG	957	0	959	519	0
8	AH	1251	0	1298	612	0
9	AI	945	0	999	497	0
9	AJ	945	0	999	362	0
10	AK	1145	0	1227	630	0
11	AL	999	0	1071	497	0
12	AM	917	0	904	616	0
13	AN	937	0	1000	549	0
14	AO	639	0	615	373	0
15	AP	1081	0	1062	743	0
16	AQ	866	0	875	512	0
17	AR	406	0	361	160	0
18	AS	860	0	919	442	0
19	AT	602	0	563	332	0
20	AU	879	0	868	477	0
21	AV	1360	0	1390	788	0
22	AW	494	0	506	240	0
23	AX	477	0	529	309	0
24	A0	855	0	906	492	0
25	A1	978	0	1020	685	0
26	A2	787	0	804	571	0
27	A3	641	0	668	421	0
28	A4	604	0	595	365	0
29	A5	457	0	462	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A6	431	0	456	224	0
31	A7	383	0	414	260	0
32	A8	496	0	549	296	0
33	A9	285	0	312	125	0
34	BA	32554	0	16429	7563	1
35	BB	1626	0	817	629	0
35	BC	1626	0	820	429	0
36	B1	1405	0	706	258	1
37	BE	1900	0	1951	930	0
38	BF	1612	0	1677	662	0
39	BG	1703	0	1763	719	0
40	BH	1146	0	1207	489	1
41	BI	843	0	857	398	0
42	BJ	1257	0	1296	527	0
43	BK	1116	0	1177	677	0
44	BL	1011	0	1043	442	0
45	BM	794	0	840	332	0
46	BN	885	0	904	409	0
47	BO	970	0	1057	459	0
48	BP	997	0	1072	493	0
49	BQ	492	0	529	258	0
50	BR	734	0	771	330	0
51	BS	700	0	720	318	0
52	BT	857	0	930	423	0
53	BU	597	0	668	334	0
54	BV	647	0	673	254	0
55	BW	762	0	859	366	0
56	BX	208	0	221	103	0
All	All	148539	0	99792	47710	3

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 193.

The worst 5 of 47710 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)
2:AA:2515:C:N4	2:AA:2569:G:H1	1.08	1.45
34:BA:144:G:H1	34:BA:178:C:N4	1.13	1.45
34:BA:292:G:H1	34:BA:308:C:N4	1.08	1.45
2:AA:447:A:H1'	2:AA:449:A:N6	1.28	1.44
33:A9:11:CYS:SG	33:A9:11:CYS:CB	2.06	1.44

All (3) 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)
1:AB:-1:A:O2'	1:AB:-1:A:O2'[15_545]	1.59	0.61
2:AA:2153:G:O2'	34:BA:423:G:OP2[3_655]	2.16	0.04
36:B1:29:G:O3'	40:BH:5:ASP:OD2[3_655]	2.17	0.03

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	
3	AC	217/228 (95%)	143 (66%)	36 (17%)	38 (18%)	0	3
4	AD	171/178 (96%)	71 (42%)	38 (22%)	62 (36%)	0	0
5	AE	187/338 (55%)	89 (48%)	41 (22%)	57 (30%)	0	0
6	AF	183/246 (74%)	83 (45%)	40 (22%)	60 (33%)	0	0
7	AG	118/176 (67%)	57 (48%)	29 (25%)	32 (27%)	0	0
8	AH	162/177 (92%)	89 (55%)	39 (24%)	34 (21%)	0	2
9	AI	126/128 (98%)	87 (69%)	24 (19%)	15 (12%)	0	6
9	AJ	126/128 (98%)	86 (68%)	25 (20%)	15 (12%)	0	6
10	AK	146/149 (98%)	83 (57%)	34 (23%)	29 (20%)	0	2
11	AL	131/141 (93%)	66 (50%)	33 (25%)	32 (24%)	0	1
12	AM	113/145 (78%)	48 (42%)	26 (23%)	39 (34%)	0	0
13	AN	120/122 (98%)	60 (50%)	33 (28%)	27 (22%)	0	1
14	AO	82/164 (50%)	40 (49%)	17 (21%)	25 (30%)	0	0
15	AP	136/138 (99%)	50 (37%)	43 (32%)	43 (32%)	0	0
16	AQ	111/186 (60%)	41 (37%)	32 (29%)	38 (34%)	0	0
17	AR	50/66 (76%)	19 (38%)	17 (34%)	14 (28%)	0	0
18	AS	104/113 (92%)	70 (67%)	18 (17%)	16 (15%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	74/84 (88%)	33 (45%)	17 (23%)	24 (32%)	0	0
20	AU	108/119 (91%)	60 (56%)	25 (23%)	23 (21%)	0	2
21	AV	175/253 (69%)	69 (39%)	46 (26%)	60 (34%)	0	0
22	AW	62/70 (89%)	21 (34%)	25 (40%)	16 (26%)	0	1
23	AX	58/60 (97%)	29 (50%)	13 (22%)	16 (28%)	0	0
24	A0	103/118 (87%)	50 (48%)	33 (32%)	20 (19%)	0	2
25	A1	115/118 (98%)	48 (42%)	40 (35%)	27 (24%)	0	1
26	A2	98/100 (98%)	54 (55%)	18 (18%)	26 (26%)	0	0
27	A3	84/91 (92%)	32 (38%)	16 (19%)	36 (43%)	0	0
28	A4	71/73 (97%)	21 (30%)	19 (27%)	31 (44%)	0	0
29	A5	56/60 (93%)	25 (45%)	11 (20%)	20 (36%)	0	0
30	A6	51/82 (62%)	26 (51%)	8 (16%)	17 (33%)	0	0
31	A7	44/47 (94%)	14 (32%)	12 (27%)	18 (41%)	0	0
32	A8	61/64 (95%)	24 (39%)	16 (26%)	21 (34%)	0	0
33	A9	33/36 (92%)	19 (58%)	8 (24%)	6 (18%)	0	3
37	BE	232/256 (91%)	107 (46%)	58 (25%)	67 (29%)	0	0
38	BF	204/239 (85%)	113 (55%)	46 (22%)	45 (22%)	0	1
39	BG	206/209 (99%)	97 (47%)	63 (31%)	46 (22%)	0	1
40	BH	148/162 (91%)	90 (61%)	38 (26%)	20 (14%)	0	4
41	BI	99/101 (98%)	55 (56%)	24 (24%)	20 (20%)	0	2
42	BJ	153/156 (98%)	63 (41%)	49 (32%)	41 (27%)	0	0
43	BK	136/138 (99%)	67 (49%)	39 (29%)	30 (22%)	0	1
44	BL	125/128 (98%)	64 (51%)	27 (22%)	34 (27%)	0	0
45	BM	96/105 (91%)	54 (56%)	19 (20%)	23 (24%)	0	1
46	BN	117/129 (91%)	54 (46%)	33 (28%)	30 (26%)	0	1
47	BO	122/135 (90%)	65 (53%)	28 (23%)	29 (24%)	0	1
48	BP	123/126 (98%)	59 (48%)	30 (24%)	34 (28%)	0	0
49	BQ	58/61 (95%)	22 (38%)	10 (17%)	26 (45%)	0	0
50	BR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	3
51	BS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	2
52	BT	102/105 (97%)	62 (61%)	20 (20%)	20 (20%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	BU	71/88 (81%)	29 (41%)	24 (34%)	18 (25%)	0 1
54	BV	78/93 (84%)	35 (45%)	17 (22%)	26 (33%)	0 0
55	BW	97/106 (92%)	27 (28%)	46 (47%)	24 (25%)	0 1
56	BX	22/27 (82%)	9 (41%)	5 (23%)	8 (36%)	0 0
All	All	5832/6739 (86%)	2857 (49%)	1467 (25%)	1508 (26%)	0 1

5 of 1508 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	ASN
3	AC	35	ALA
3	AC	54	SER
3	AC	68	LEU
3	AC	87	GLU

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
3	AC	174/180 (97%)	144 (83%)	30 (17%)	2 12
4	AD	135/139 (97%)	90 (67%)	45 (33%)	0 2
5	AE	156/284 (55%)	114 (73%)	42 (27%)	0 3
6	AF	152/193 (79%)	121 (80%)	31 (20%)	1 7
7	AG	102/147 (69%)	74 (72%)	28 (28%)	0 3
8	AH	137/147 (93%)	99 (72%)	38 (28%)	0 3
9	AI	98/98 (100%)	89 (91%)	9 (9%)	9 30
9	AJ	98/98 (100%)	89 (91%)	9 (9%)	9 30
10	AK	119/119 (100%)	96 (81%)	23 (19%)	1 9
11	AL	108/113 (96%)	91 (84%)	17 (16%)	2 14
12	AM	95/121 (78%)	71 (75%)	24 (25%)	0 4
13	AN	101/101 (100%)	74 (73%)	27 (27%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	67/126 (53%)	51 (76%)	16 (24%)	0	4
15	AP	110/110 (100%)	73 (66%)	37 (34%)	0	2
16	AQ	89/149 (60%)	58 (65%)	31 (35%)	0	1
17	AR	44/52 (85%)	24 (54%)	20 (46%)	0	0
18	AS	88/92 (96%)	65 (74%)	23 (26%)	0	3
19	AT	67/73 (92%)	48 (72%)	19 (28%)	0	2
20	AU	97/105 (92%)	75 (77%)	22 (23%)	1	5
21	AV	151/203 (74%)	109 (72%)	42 (28%)	0	3
22	AW	51/56 (91%)	36 (71%)	15 (29%)	0	2
23	AX	52/52 (100%)	34 (65%)	18 (35%)	0	1
24	A0	89/101 (88%)	59 (66%)	30 (34%)	0	2
25	A1	96/97 (99%)	67 (70%)	29 (30%)	0	2
26	A2	79/79 (100%)	60 (76%)	19 (24%)	0	4
27	A3	64/67 (96%)	46 (72%)	18 (28%)	0	3
28	A4	66/66 (100%)	50 (76%)	16 (24%)	0	4
29	A5	51/53 (96%)	38 (74%)	13 (26%)	0	4
30	A6	46/69 (67%)	35 (76%)	11 (24%)	0	4
31	A7	39/40 (98%)	30 (77%)	9 (23%)	1	5
32	A8	50/51 (98%)	33 (66%)	17 (34%)	0	1
33	A9	34/35 (97%)	30 (88%)	4 (12%)	5	21
37	BE	202/220 (92%)	152 (75%)	50 (25%)	0	4
38	BF	160/188 (85%)	127 (79%)	33 (21%)	1	7
39	BG	180/181 (99%)	136 (76%)	44 (24%)	0	4
40	BH	115/123 (94%)	66 (57%)	49 (43%)	0	0
41	BI	90/90 (100%)	64 (71%)	26 (29%)	0	2
42	BJ	126/127 (99%)	106 (84%)	20 (16%)	2	14
43	BK	119/119 (100%)	73 (61%)	46 (39%)	0	0
44	BL	98/99 (99%)	81 (83%)	17 (17%)	2	12
45	BM	88/92 (96%)	70 (80%)	18 (20%)	1	7
46	BN	90/99 (91%)	70 (78%)	20 (22%)	1	6
47	BO	104/111 (94%)	85 (82%)	19 (18%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	BP	100/101 (99%)	80 (80%)	20 (20%)	1 8
49	BQ	49/50 (98%)	41 (84%)	8 (16%)	2 13
50	BR	79/80 (99%)	59 (75%)	20 (25%)	0 4
51	BS	72/74 (97%)	44 (61%)	28 (39%)	0 0
52	BT	96/97 (99%)	74 (77%)	22 (23%)	1 5
53	BU	64/77 (83%)	47 (73%)	17 (27%)	0 3
54	BV	71/80 (89%)	59 (83%)	12 (17%)	2 12
55	BW	76/82 (93%)	53 (70%)	23 (30%)	0 2
56	BX	19/22 (86%)	17 (90%)	2 (10%)	7 26
All	All	4903/5528 (89%)	3677 (75%)	1226 (25%)	0 4

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BI	70	ASP
51	BS	69	THR
42	BJ	155	ARG
41	BI	67	MET
46	BN	50	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
37	BE	240	GLN
42	BJ	68	ASN
38	BF	107	GLN
40	BH	65	ASN
44	BL	3	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	122/123 (99%)	47 (38%)	5 (4%)
2	AA	2870/2915 (98%)	1226 (42%)	290 (10%)
34	BA	1515/1522 (99%)	452 (29%)	161 (10%)
35	BB	76/76 (100%)	34 (44%)	16 (21%)
35	BC	75/76 (98%)	31 (41%)	9 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	B1	65/78 (83%)	24 (36%)	4 (6%)
All	All	4723/4790 (98%)	1814 (38%)	485 (10%)

5 of 1814 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	0	A
1	AB	1	U
1	AB	2	C
1	AB	3	C
1	AB	9	G

5 of 485 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AA	2067	G
34	BA	1399	C
2	AA	2781	A
34	BA	1362	C
35	BC	9	A

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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AB	123/123 (100%)	-0.47	0 100 100	308, 357, 402, 412	0
2	AA	2872/2915 (98%)	-0.48	15 (0%) 91 85	232, 307, 404, 474	0
3	AC	221/228 (96%)	-0.06	4 (1%) 68 60	384, 428, 464, 467	0
4	AD	173/178 (97%)	0.47	11 (6%) 19 17	243, 279, 292, 298	0
5	AE	191/338 (56%)	0.54	36 (18%) 1 3	258, 311, 397, 403	0
6	AF	189/246 (76%)	-0.37	2 (1%) 80 73	233, 399, 427, 434	0
7	AG	122/176 (69%)	-0.35	2 (1%) 72 63	350, 366, 443, 447	0
8	AH	164/177 (92%)	-0.37	1 (0%) 89 84	320, 351, 366, 370	0
9	AI	128/128 (100%)	1.33	30 (23%) 0 2	580, 591, 602, 603	0
9	AJ	128/128 (100%)	1.93	49 (38%) 0 1	569, 582, 594, 596	0
10	AK	148/149 (99%)	-0.12	4 (2%) 54 46	305, 329, 353, 361	0
11	AL	133/141 (94%)	0.11	7 (5%) 26 25	455, 504, 541, 543	0
12	AM	117/145 (80%)	0.25	12 (10%) 6 8	286, 310, 364, 368	0
13	AN	122/122 (100%)	0.29	10 (8%) 11 12	245, 262, 277, 293	0
14	AO	84/164 (51%)	0.22	5 (5%) 21 20	330, 452, 471, 473	0
15	AP	138/138 (100%)	0.42	9 (6%) 18 17	283, 324, 364, 379	0
16	AQ	113/186 (60%)	-0.77	0 100 100	317, 367, 386, 390	0
17	AR	52/66 (78%)	0.62	7 (13%) 3 5	251, 267, 285, 288	0
18	AS	108/113 (95%)	0.15	2 (1%) 66 58	280, 311, 324, 332	0
19	AT	76/84 (90%)	-0.09	4 (5%) 26 25	329, 344, 360, 363	0
20	AU	110/119 (92%)	-0.08	7 (6%) 19 17	647, 661, 722, 724	0
21	AV	177/253 (69%)	-0.07	8 (4%) 33 29	295, 365, 416, 424	0
22	AW	64/70 (91%)	0.11	1 (1%) 72 63	346, 364, 373, 375	0
23	AX	60/60 (100%)	-0.22	0 100 100	291, 306, 315, 316	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
24	A0	105/118 (88%)	-0.16	2 (1%) 66 58	263, 281, 304, 308	0
25	A1	117/118 (99%)	-0.52	1 (0%) 84 77	267, 297, 311, 317	0
26	A2	100/100 (100%)	0.72	16 (16%) 1 4	416, 430, 462, 470	0
27	A3	86/91 (94%)	0.53	11 (12%) 3 6	359, 389, 475, 486	0
28	A4	73/73 (100%)	-0.00	6 (8%) 11 12	319, 354, 373, 378	0
29	A5	58/60 (96%)	0.04	2 (3%) 45 38	259, 314, 361, 373	0
30	A6	53/82 (64%)	0.17	4 (7%) 14 14	287, 316, 332, 340	0
31	A7	46/47 (97%)	0.19	1 (2%) 62 53	316, 339, 352, 357	0
32	A8	63/64 (98%)	-0.02	1 (1%) 72 63	262, 282, 294, 306	0
33	A9	35/36 (97%)	-0.58	0 100 100	281, 303, 316, 319	0
34	BA	1515/1522 (99%)	-0.49	4 (0%) 94 90	251, 312, 419, 609	0
35	BB	76/76 (100%)	7.38	60 (78%) 0 0	631, 651, 667, 669	0
35	BC	76/76 (100%)	-0.66	0 100 100	273, 310, 328, 337	0
36	B1	66/78 (84%)	5.89	43 (65%) 0 0	337, 829, 918, 922	0
37	BE	234/256 (91%)	0.16	21 (8%) 9 10	293, 321, 364, 385	0
38	BF	206/239 (86%)	0.73	39 (18%) 1 3	301, 349, 377, 382	0
39	BG	208/209 (99%)	0.05	6 (2%) 51 43	276, 299, 318, 329	0
40	BH	150/162 (92%)	0.64	20 (13%) 3 5	277, 295, 315, 324	0
41	BI	101/101 (100%)	1.10	28 (27%) 0 2	299, 318, 330, 336	0
42	BJ	155/156 (99%)	0.02	6 (3%) 39 33	326, 357, 370, 373	0
43	BK	138/138 (100%)	0.17	9 (6%) 18 17	266, 284, 297, 306	0
44	BL	127/128 (99%)	-0.37	0 100 100	385, 487, 499, 500	0
45	BM	98/105 (93%)	0.83	11 (11%) 5 8	337, 394, 423, 424	0
46	BN	119/129 (92%)	0.20	9 (7%) 13 14	288, 307, 330, 334	0
47	BO	124/135 (91%)	0.20	4 (3%) 47 39	265, 282, 319, 328	0
48	BP	125/126 (99%)	-0.90	0 100 100	350, 370, 412, 415	0
49	BQ	60/61 (98%)	-0.09	2 (3%) 46 39	322, 352, 360, 365	0
50	BR	88/89 (98%)	-0.39	3 (3%) 45 38	277, 288, 315, 318	0
51	BS	83/88 (94%)	-0.41	1 (1%) 79 70	271, 284, 303, 316	0
52	BT	104/105 (99%)	-0.21	3 (2%) 51 43	249, 268, 323, 344	0
53	BU	73/88 (82%)	0.27	9 (12%) 4 7	259, 296, 323, 348	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
54	BV	80/93 (86%)	0.17	5 (6%) 20 17	353, 369, 395, 399	0
55	BW	99/106 (93%)	-0.54	0 100 100	264, 281, 292, 300	0
56	BX	24/27 (88%)	-1.09	0 100 100	475, 489, 493, 496	0
All	All	10678/11529 (92%)	-0.05	553 (5%) 27 26	232, 322, 533, 922	0

The worst 5 of 553 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	B1	15	A	20.7
35	BB	4	G	18.9
36	B1	42	G	18.3
36	B1	17	G	17.4
35	BB	5	A	17.2

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

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

6.3 Carbohydrates (i)

There are no 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.