wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:54 PM BST

PDB ID	:	4V68
EMDB ID:	:	EMD-5030
Title	:	T. thermophilus 70S ribosome in complex with mRNA, tRNAs and EF-Tu.GDP.kirromycin ternary complex, fitted to a 6.4 A Cryo-EM map.
Authors	:	Schuette, J.-C.; Spahn, C.M.T.
Deposited on	:	2008-12-11
Resolution	:	6.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

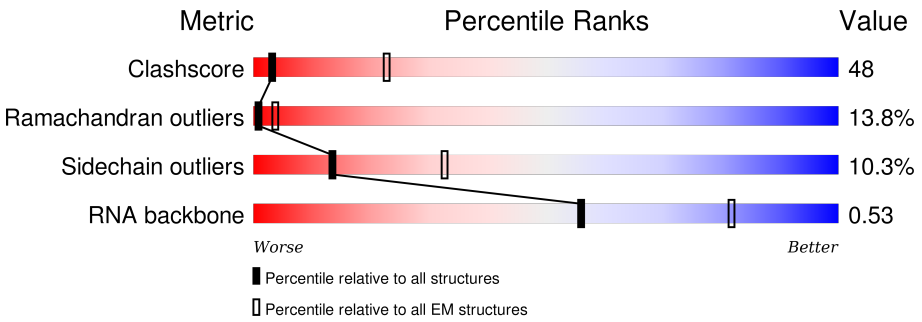
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.40 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	AA	1504	24% 63% 12% •
2	AB	235	21% 60% 17% •
3	AD	208	27% 55% 16% •
4	AE	151	21% 64% 15%
5	AF	101	32% 59% 8% •
6	AH	138	38% 57% 5%
7	AK	119	31% 63% 5% •
8	AL	125	35% 49% 15% •

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Mol	Chain	Length	Quality of chain
9	AO	88	33% 57% 10%
10	AP	84	25% 64% 11%
11	AQ	100	35% 55% 10%
12	AR	70	19% 63% 19%
13	AT	99	20% 62% 18%
14	AC	207	32% 57% 10% •
15	AG	155	32% 60% 8%
16	AI	127	21% 65% 13% •
17	AJ	99	27% 60% 13%
18	AM	125	19% 64% 17%
19	AN	60	27% 62% 12%
20	AS	79	22% 63% 15%
21	AU	25	36% 56% 8%
22	AV	77	21% 55% 23% •
23	AX	6	17% 50% 33%
24	AW	76	22% 57% 17% •
25	AY	72	31% 51% 14% •
26	A0	3	33% 67%
27	AZ	405	76% 17% 7%
28	B0	85	46% 46% 7% •
29	B1	89	20% 51% 25% •
30	B2	51	8% 41% 43% 8%
31	B3	60	25% 67% 8%
32	B4	50	40% 44% 12% •
33	B5	59	22% 58% 15% 5%

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Mol	Chain	Length	Quality of chain
34	B6	45	18% 53% 27% •
35	B7	49	43% 47% 10%
36	B8	64	17% 61% 22%
37	B9	35	11% 66% 23%
38	BA	2852	27% 54% 18% •
39	BB	119	31% 59% 10%
40	BC	191	47% 36% 16% •
41	BD	272	29% 51% 19% •
42	BE	205	23% 52% 23% •
43	BF	208	26% 60% 13%
44	BG	181	19% 60% 18% •
45	BH	160	24% 55% 18% •
46	BI	146	21% 68% 10% •
47	BL	138	• 62% 30% •
48	BN	139	19% 56% 21% •
49	BO	122	32% 56% 10% •
50	BP	146	14% 55% 26% 5%
51	BQ	136	19% 59% 21% •
52	BR	117	21% 58% 19% •
53	BS	99	12% 51% 35% •
54	BT	138	19% 54% 22% 5%
55	BU	117	29% 58% 12% •
56	BV	101	14% 48% 36% •
57	BW	113	25% 61% 13% •
58	BX	93	14% 56% 23% 8%

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Mol	Chain	Length	Quality of chain
59	BY	101	10% 51% 31% 8%
60	BZ	177	20% 62% 18%

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
25	M2G	AY	26	-	-	X	-
25	OMG	AY	34	-	-	X	-

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 152000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1504	32329	14390	5992	10444	1503	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	235	1901	1213	342	341	5	0	1

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AE	151	1147	724	218	201	4	0	1

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S8.

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

- Molecule 7 is a protein called 30S ribosomal protein S11.

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

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AL	125	971	611	196	163	1	0	1

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AP	84	701	443	140	117	1	0	1

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AQ	100	824	528	152	142	2	0	1

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	AR	70	574	367	112	95	0	0

- Molecule 13 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AT	99	763	470	162	129	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AC	207	1613	1016	315	281	1	0	1

- Molecule 15 is a protein called 30S ribosomal protein S7.

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

- Molecule 16 is a protein called 30S ribosomal protein S9.

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

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AJ	99	795	499	157	138	1	0	1

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	AM	125	988	611	206	169	2	0	1

- Molecule 19 is a protein called 30S ribosomal protein S14.

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

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AS	79	630	403	115	110	2	0	1

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	AU	25	209	128	51	30	0	1

- Molecule 22 is a RNA chain called P-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	AV	77	1645	733	297	538	77	0	0

- Molecule 23 is a RNA chain called SYNTHETIC MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	AX	6	132	59	27	40	6	0	0

- Molecule 24 is a RNA chain called E-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	AW	76	1623	723	290	534	76	0	0

- Molecule 25 is a RNA chain called AT-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	AY	72	1546	698	275	501	72	0	0

- Molecule 26 is a RNA chain called MRNA CODON.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	A0	3	60	27	6	24	3	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A0	100	U	A	CONFLICT	UNP Q5SHN6
A0	101	U	K	CONFLICT	UNP Q5SHN6
A0	102	U	G	CONFLICT	UNP Q5SHN6

- Molecule 27 is a protein called Elongation factor Tu-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	AZ	378	2962	1879	513	557	13	8	0

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	B0	85	650	401	137	111	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	B1	89	693	435	140	118	0	1

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	B2	51	421	263	85	72	1	0	1

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	B3	60	468	298	91	78	1	0	1

- Molecule 32 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	B4	50	242	143	50	49	0	1

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	B5	59	459	288	90	76	5	0	0

- Molecule 34 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	B6	45	381	235	78	64	4	0	1

- Molecule 35 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	B7	49	419	257	105	55	2	0	1

- Molecule 36 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B8	64	508	326	102	78	2	0	1

- Molecule 37 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	B9	35	294	181	66	44	3	0	0

- Molecule 38 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	BA	2852	61426	27338	11485	19752	2851	0	0

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	BB	119	2551	1136	471	826	118	0	0

- Molecule 40 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	BC	191	1142	691	221	230	0	1

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	?	-	LEU	DELETION	UNP Q5SLP7
BC	?	-	VAL	DELETION	UNP Q5SLP7
BC	?	-	LYS	DELETION	UNP Q5SLP7
BC	?	-	GLU	DELETION	UNP Q5SLP7
BC	?	-	LEU	DELETION	UNP Q5SLP7
BC	?	-	ALA	DELETION	UNP Q5SLP7
BC	?	-	ASP	DELETION	UNP Q5SLP7
BC	?	-	ALA	DELETION	UNP Q5SLP7
BC	?	-	VAL	DELETION	UNP Q5SLP7
BC	?	-	VAL	DELETION	UNP Q5SLP7
BC	?	-	ALA	DELETION	UNP Q5SLP7
BC	?	-	THR	DELETION	UNP Q5SLP7
BC	?	-	PRO	DELETION	UNP Q5SLP7
BC	?	-	ASP	DELETION	UNP Q5SLP7
BC	?	-	LEU	DELETION	UNP Q5SLP7
BC	?	-	PRO	DELETION	UNP Q5SLP7

- Molecule 41 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BD	272	2105	1329	417	356	3	0	1

- Molecule 42 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BE	205	1564	988	300	270	6	0	1

- Molecule 43 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BF	208	1624	1035	304	282	3	0	1

- Molecule 44 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BG	181	1474	942	268	260	4	0	0

- Molecule 45 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BH	160	1223	773	229	220	1	0	1

- Molecule 46 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BI	146	1132	723	201	207	1	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	146	VAL	ALA	CONFLICT	UNP Q5SLQ1

- Molecule 47 is a protein called 50S ribosomal protein L11.

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

- Molecule 48 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BN	139	1105	712	207	182	4	0	1

- Molecule 49 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BO	122	933	588	171	170	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BP	146	1114	692	227	193	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BQ	136	1080	688	204	183	5	0	0

- Molecule 52 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	BR	117	960	599	202	159	0	0

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	BS	99	771	486	155	130	0	1

- Molecule 54 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BT	138	1142	710	235	196	1	0	1

- Molecule 55 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	BU	117	958	604	202	151	1	0	0

- Molecule 56 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	BV	101	779	501	142	135	1	0	0

- Molecule 57 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BW	113	896	563	176	155	2	0	0

- Molecule 58 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	BX	93	726	471	132	123	0	1

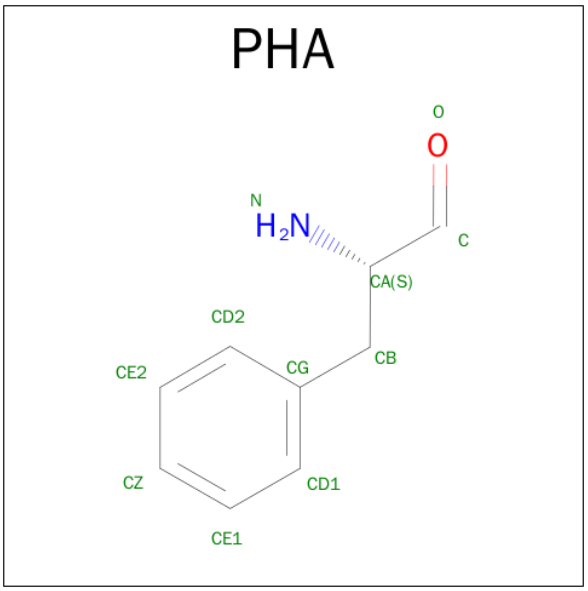
- Molecule 59 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	BY	101	776	500	149	123	4	0	1

- Molecule 60 is a protein called 50S ribosomal protein L25.

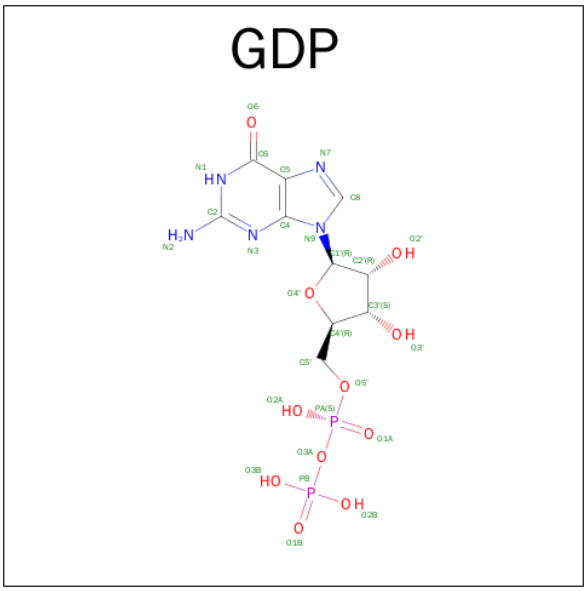
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	BZ	177	1404	897	253	252	2	0	1

- Molecule 61 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



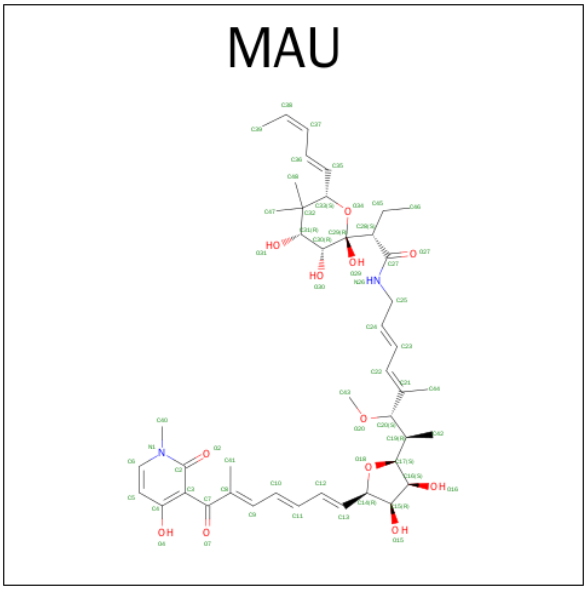
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
61	AY	1	11	9	1	1	0

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



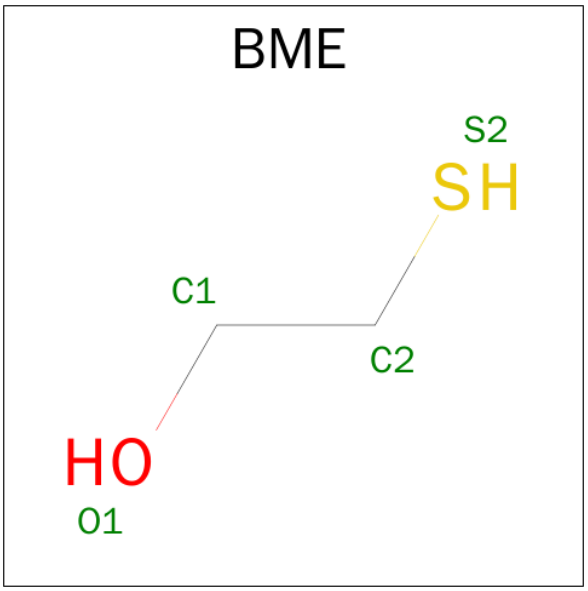
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
62	AZ	1	28	10	5	11	2	0

- Molecule 63 is N-METHYL KIRROMYCIN (three-letter code: MAU) (formula: $C_{44}H_{62}N_2O_{12}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
63	AZ	1	58	44	2	12	0

- Molecule 64 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



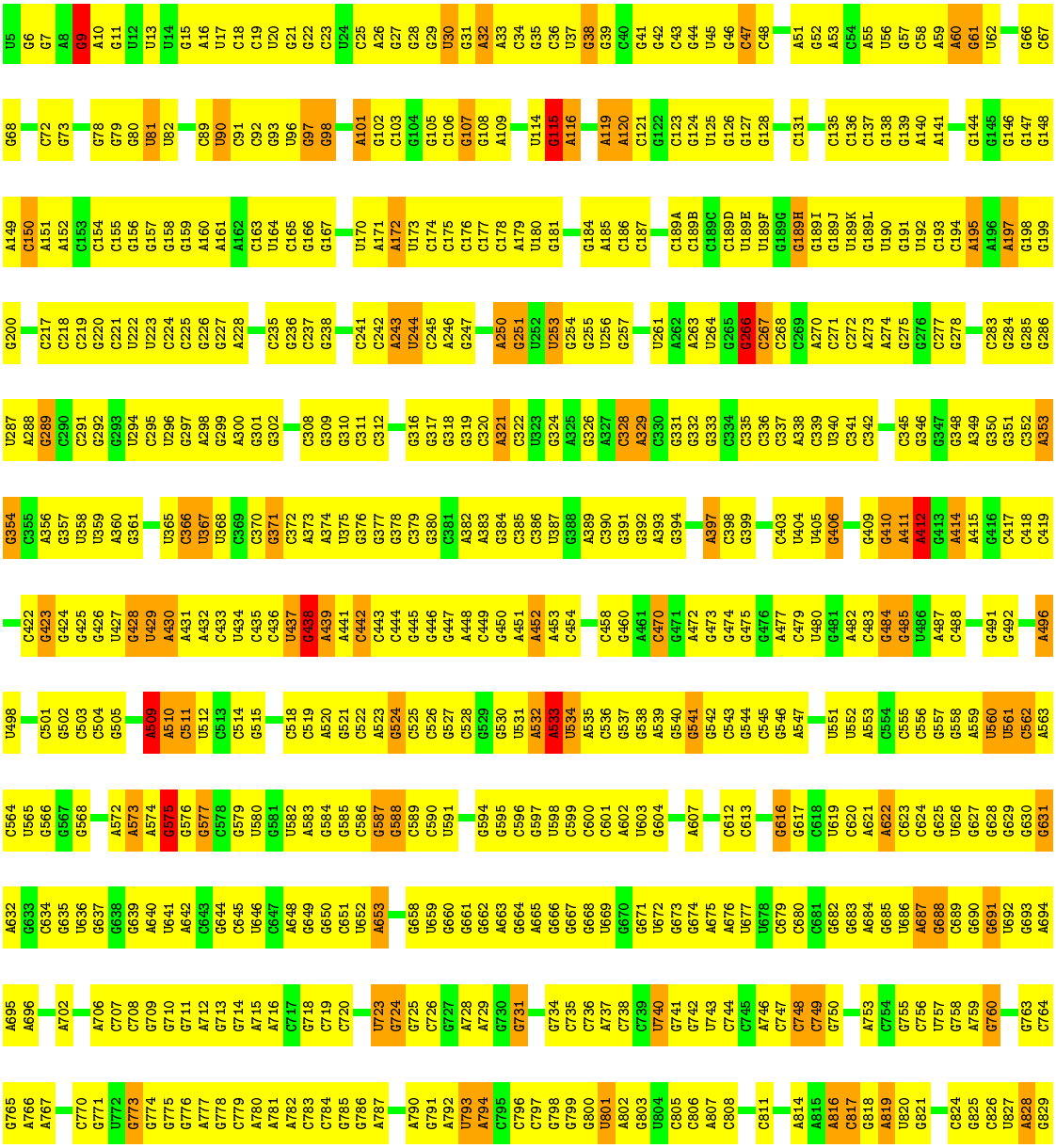
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
64	AZ	1	4	2	1	1	0

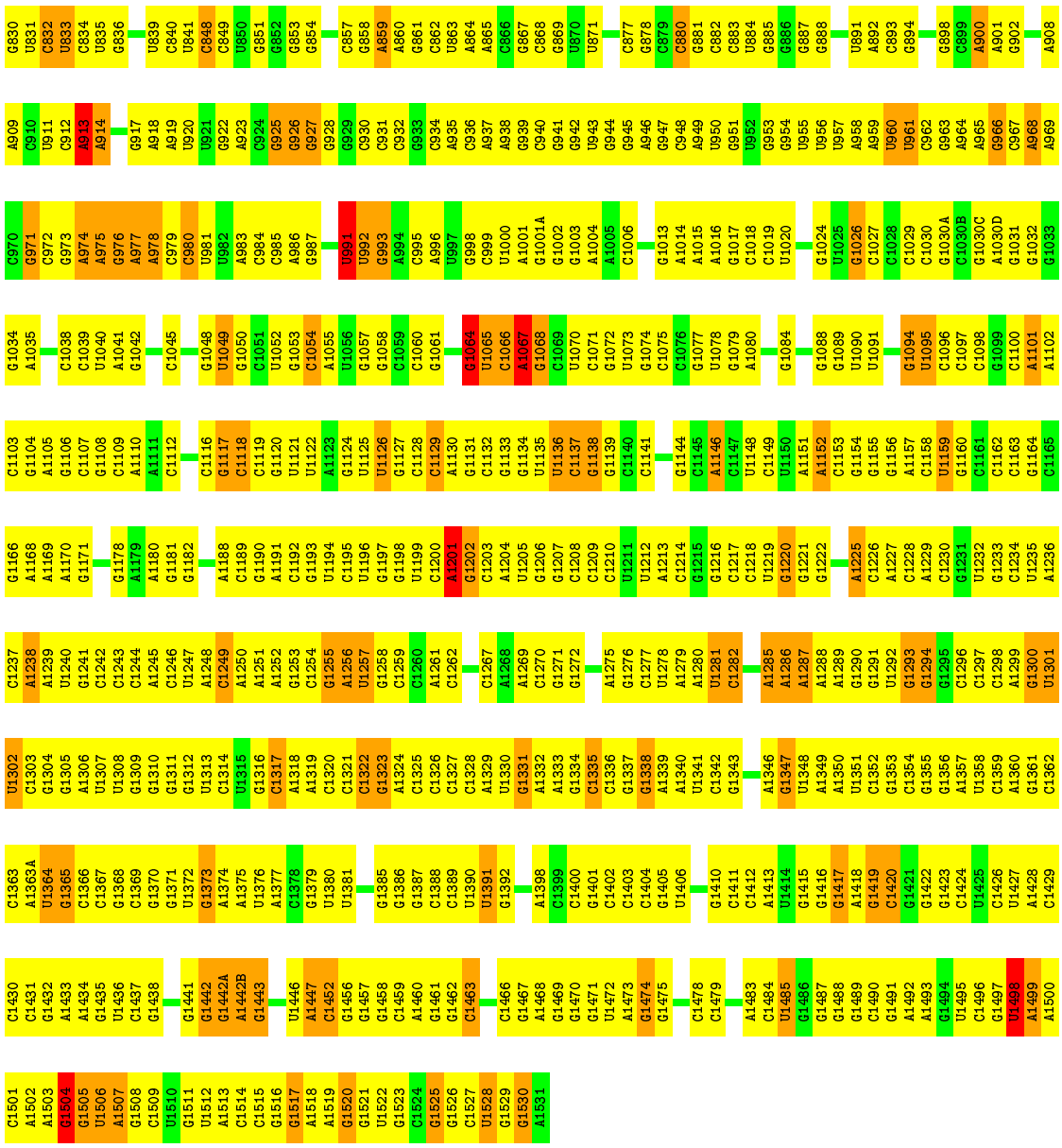
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S rRNA

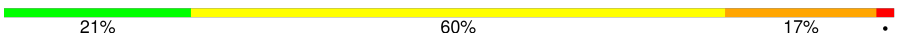
Chain AA: 24% 63% 12%

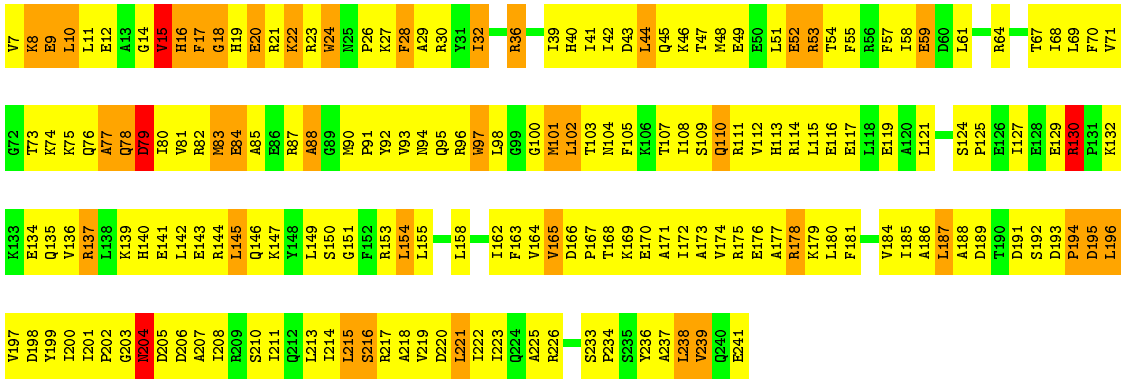




- Molecule 2: 30S ribosomal protein S2

Chain AB:





- Molecule 3: 30S ribosomal protein S4

Chain AD: 27% 55% 16%

G2 R3 Y4 I5 G6 F7 V8 C9 R10 L11 C12 R13 R14 E15 G16 V17 K18 L19 Y20 R25 C26 Y27 S28 P29 K30 C31 A32 M33 E34 R35 R36 P37 Y38 H43 G44 Q45 K46 R49 R50 P51 S52 D53 Y54 A55 V56 R57 L58 R59 E60 K61 Q62 K63 L64 R65 R66 I67 Y68

G69 I70 R73 Q74 F75 R76 N77 L78 F79 E80 E81 A82 S83 V88 S91 V92 F93 L94 G95 L96 L97 E98 S99 R100 L101 D102 N103 V104 V105 Y106 R107 L108 G109 F110 A111 V112 S113 R114 R115 Q116 A117 R118 Q119 L120 V121 R122 H123 G124 H125 I126 T127 V128 R131 R132 V133 D134

L135 P136 S137 Y138 R139 V140 R141 P142 G143 D144 E145 I146 A147 V148 A149 E150 K151 S152 R153 N154 L157 I158 R159 Q160 N161 L162 E163 R168 K169 V170 G171 P172 W173 L174 S175 L176 D177 V178 E179 G180 M181 K182 G183 K184 F185 L186 R187 L188 P189 D193 L194 A195 L196 P197 V198 N199 E200

Q201 L202 V203 I204 E205 F206 Y207 S208 R209

- Molecule 4: 30S ribosomal protein S5

Chain AE: 21% 64% 15%

D5 F6 E7 E8 K9 M10 I11 L12 I13 R14 R15 T16 A17 R18 M19 Q20 A21 G22 G23 R24 R25 F26 R27 F28 G29 A30 L31 V32 V33 V34 G35 D36 R37 Q38 G39 R40 V41 G42 L43 G46 K47 A48 P49 E50 V51 P52 L53 A54 V55 Q56 K57 A58 G59 Y60 Y61 A62 R63 R64 N65

M66 V67 E68 V69 P70 L71 Q72 N73 G74 T75 I76 F77 H78 E79 I80 E81 V82 A86 S87 V90 L91 K92 P93 A94 A95 T98 G99 V100 I101 A102 G103 A104 V105 P106 R107 A108 I109 L110 E111 L112 A113 G114 V115 T116 D117 I118 L119 T120 K121 E122 L123 R126 N127 P128 I129 N130

I131 A132 Y133 A134 T135 M136 E137 A138 L139 R140 Q141 L142 R143 T144 K145 A146 D147 V148 E149 R150 L151 E155

- Molecule 5: 30S ribosomal protein S6

Chain AF: 32% 59% 8%

M1 R2 E5 V6 N7 I8 V9 L10 N11 P12 N13 L14 D15 Q16 S17 Q18 L19 A20 L21 E22 K23 E24 I25 I26 Q27 R28 A29 L30 Y33 V40 E41 E42 L43 G44 L45 R46 Y50 P51 I52 A53 K54 D55 P56 Q57 G58 Y59 F60 L61 W62 Y63 Q64 V65 E66 M67 P68 E69

D70 R71 V72 N73 D74 L75 A76 R77 E78 I81 R82 R86 R87 V88 M89 V90 V91 K92 P96 F97 I98 A99 N100 A101

- Molecule 6: 30S ribosomal protein S8

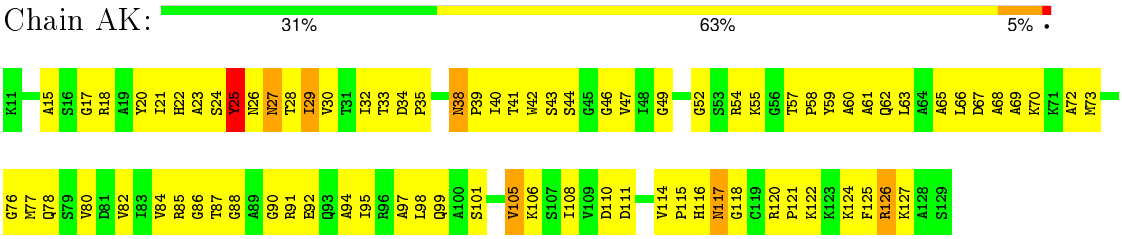
Chain AH: 38% 57% 5%

M1 L2 T3 D4 P5 I6 A7 D8 N9 L10 T11 R12 I13 R14 N15 A16 T17 R18 V19 Y20 S23 T24 A28 S29 R30 F31 K32 E33 E34 I35 L36 R37 I38 L39 A40 R41 E42 G43 F44 I45 Y48 V51 D52 V53 D54 Y58 L59 R60 V61 Y62 L63 K64 Y65 R68

R69 Q70 G71 P72 D73 F74 R75 V79 I80 H81 R85 I86 S87 K88 P89 R92 V93 V97 I100 P101 R102 V103 R104 R105 G108 I109 A110 I111 L112 S113 T114 S115 V118 L119 T120 D121 R122 E123 A124 R125 V129 L133 I134 C135 E136 V137 W138

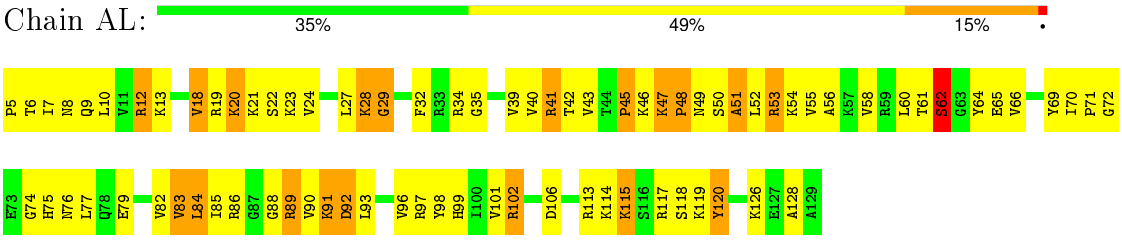
- Molecule 7: 30S ribosomal protein S11

Chain AK:



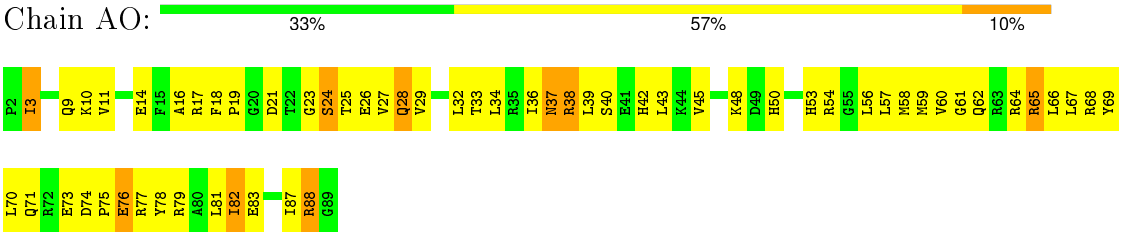
- Molecule 8: 30S ribosomal protein S12

Chain AL:



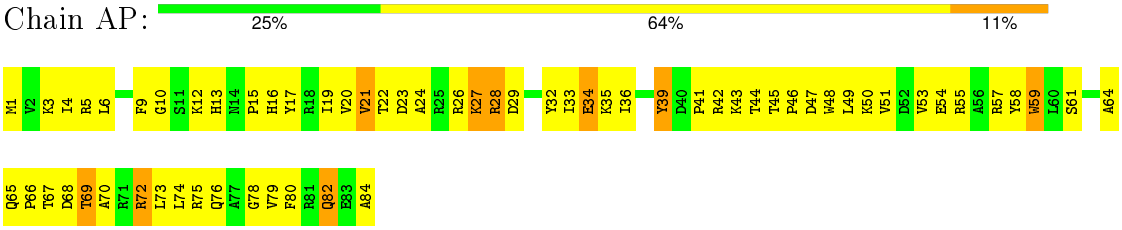
- Molecule 9: 30S ribosomal protein S15

Chain AO:



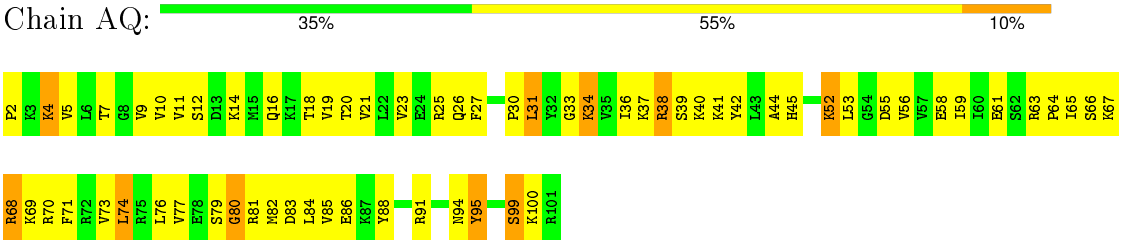
- Molecule 10: 30S ribosomal protein S16

Chain AP:



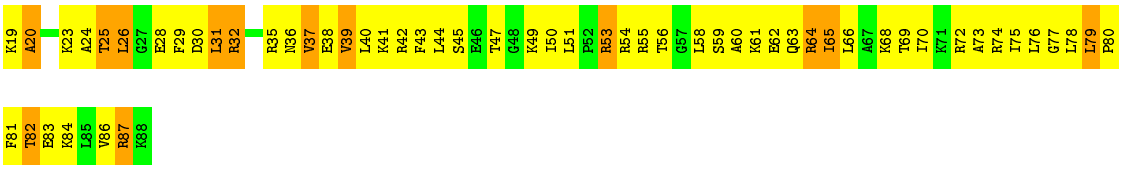
- Molecule 11: 30S ribosomal protein S17

Chain AQ:



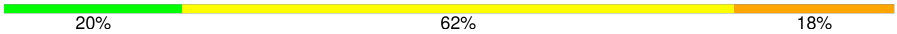
- Molecule 12: 30S ribosomal protein S18

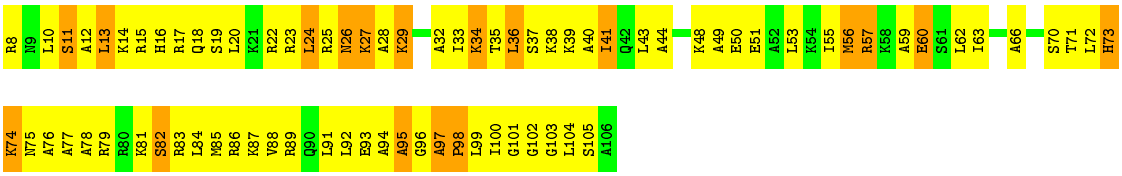
Chain AR:



- Molecule 13: 30S ribosomal protein S20

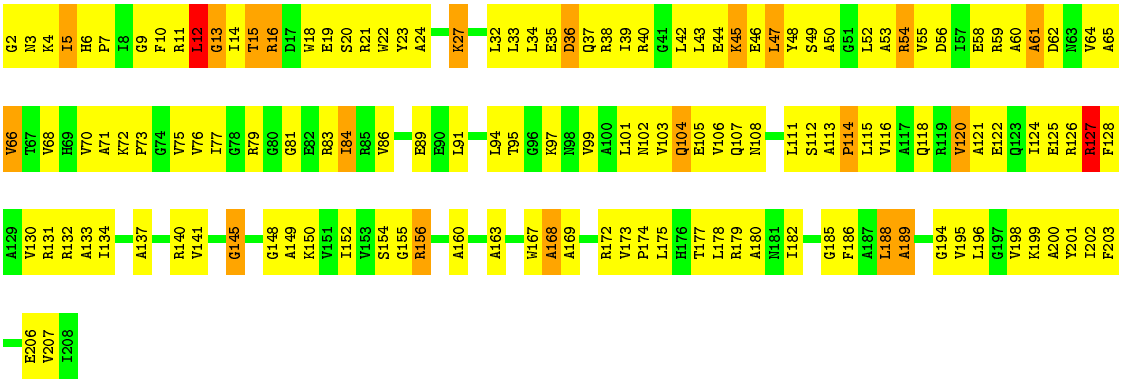
Chain AT:





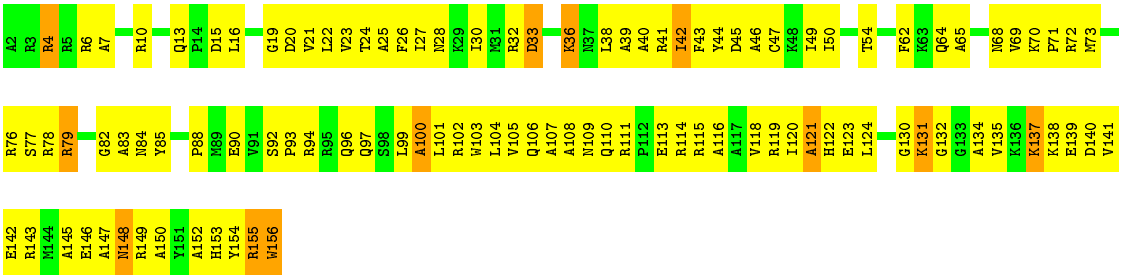
- Molecule 14: 30S ribosomal protein S3

Chain AC:



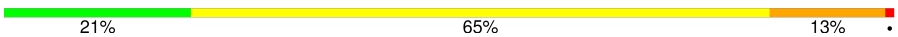
- Molecule 15: 30S ribosomal protein S7

Chain AG:



- Molecule 16: 30S ribosomal protein S9

Chain AI:



R66 G67 G68 G69 K70 S71 G72 Q73 I74 D75 A76 I77 K78 L79 G80 I81 A82 R83 A84 L85 V86 Q87 Y88 N89 Y92 R93 A94 K95 L96 K97 P98 L99 G100 F101 L102 T103 R104 D105 A106 R107 R111 K112 K113 Y114 G115 K116 H117 K118 A119 R120 R121 A122 P123 Q124 Y125 S126 K127 R128

- Molecule 17: 30S ribosomal protein S10

Chain AJ: 27% 60% 13%

K3 I4 R5 I6 K7 L8 R9 H13 K14 T15 L16 D17 A18 S19 A20 Q21 K22 I23 V24 R28 R29 S30 G31 A32 Q33 V34 S35 G36 P37 I38 P39 L40 P41 T42 R43 V44 R45 R46 F47 T48 V49 I50 R51 G52 P53 F54 K55 H56 K57 D58 S59 R60 E61 H62 F63 E64 L65 R66

T67 H68 N69 R70 L71 V72 D73 I74 I75 N76 P77 N78 R79 K80 T81 I82 E83 Q84 L88 D89 L90 P91 T92 G93 V94 E95 I96 E97 I98 K99 T100 V101

- Molecule 18: 30S ribosomal protein S13

Chain AM: 19% 64% 17%

A2 R3 I4 A5 G6 V7 E8 I9 P10 R11 N12 K13 R14 V15 D16 V17 A18 L19 T20 Y21 I22 Y23 G24 I25 G26 K27 A28 R29 A30 K31 E32 A33 L34 E35 K36 T37 G38 I39 N40 P41 A42 T43 R44 V45 K46 D47 L48 T49 E50 A51 E52 V53 V54 R55 L56 R57 E58 Y59 V60

T63 W64 K65 L66 E67 G68 E69 L70 R71 A72 A75 A76 N77 I78 K79 R80 L81 M82 D83 I84 G85 C86 Y87 R88 G89 L90 R91 H92 R93 R94 G95 L96 P97 V98 R99 G100 Q101 R102 T103 R104 T105 N106 A107 R108 T109 R110 K111 G112 P113 R114 K115 T116 V117 A118 G119 K120 P124 R125

K126

- Molecule 19: 30S ribosomal protein S14

Chain AN: 27% 62% 12%

A2 R3 K4 A5 L6 I7 E8 K9 T13 P14 K15 F16 K17 V18 Y21 T22 R23 C24 V25 R26 C27 G28 R29 A30 R31 S32 V33 Y34 R35 F36 F37 G38 L39 C40 R41 I42 C43 L44 R45 E46 L47 A48 H49 K50 G51 Q52 L53 P54 G55 V56 R57 K58 A59 S60 W61

- Molecule 20: 30S ribosomal protein S19

Chain AS: 22% 63% 15%

S4 L5 K6 K7 G8 V9 F10 V11 D12 D13 H14 L15 L16 V19 L20 E21 L22 N23 A24 K25 G26 E27 K28 R29 L30 I31 K32 T33 W34 S35 R36 R37 S38 T39 I40 V41 P42 E43 M44 H47 T48 I49 A50 V51 Y52 N53 G54 K55 Q56 H57 V58 P59 V60 Y61 I62 T63 E64 N65

M66 V67 G68 H69 K70 L71 G72 E73 F74 A75 P76 T77 R78 T79 Y80 R81 G82

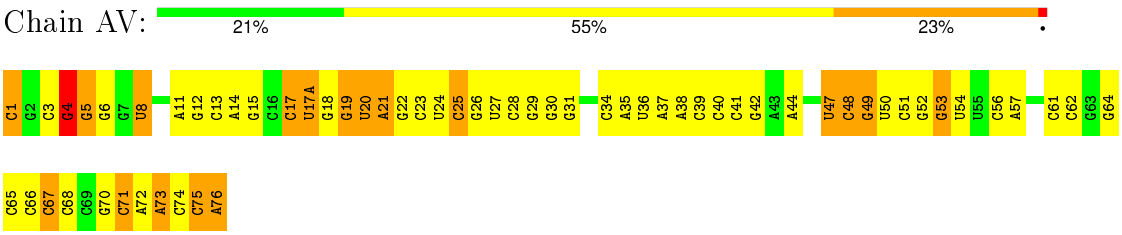
- Molecule 21: 30S ribosomal protein Thx

Chain AU: 36% 56% 8%

G2 K3 G4 D5 R6 R7 T8 R9 R10 G11 K12 I13 W14 R15 K20 Y21 R22 P23 R24 K25 K26

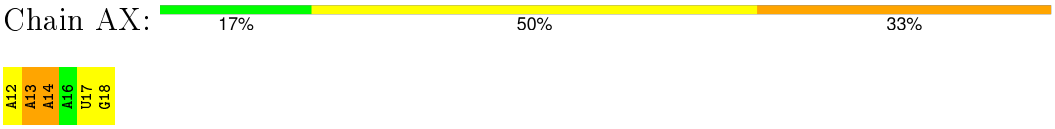
- Molecule 22: P-SITE TRNA

Chain AV:



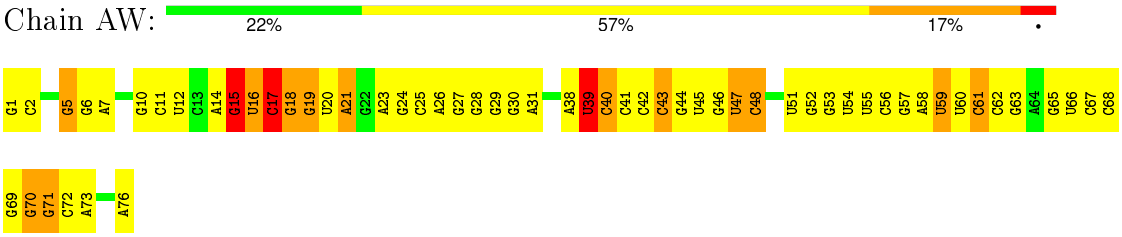
- Molecule 23: SYNTHETIC MRNA

Chain AX:



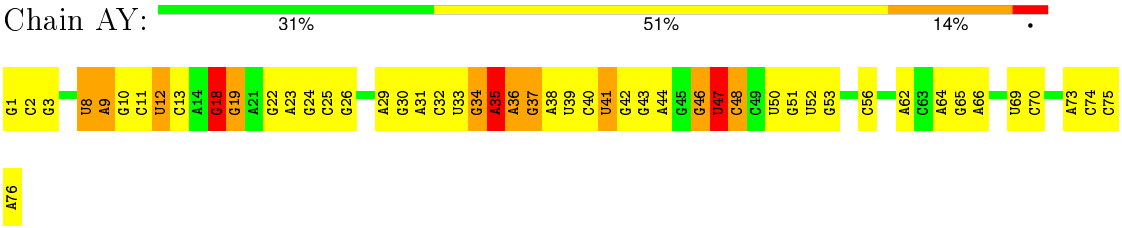
- Molecule 24: E-SITE TRNA

Chain AW:



- Molecule 25: AT-SITE TRNA

Chain AY:

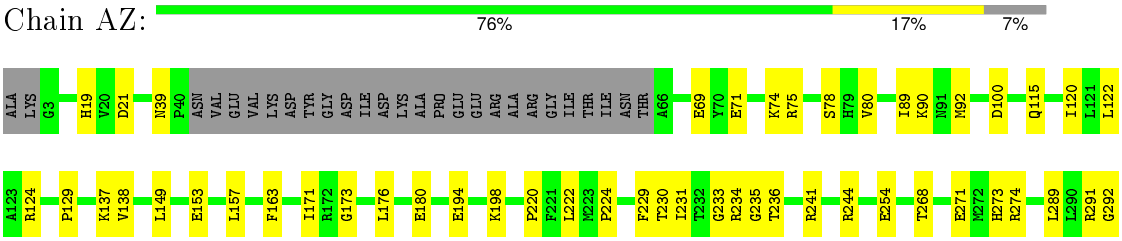


- Molecule 26: MRNA CODON

Chain A0:

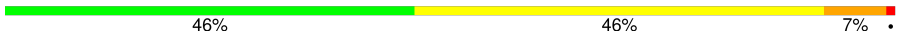
- Molecule 27: Elongation factor Tu-A

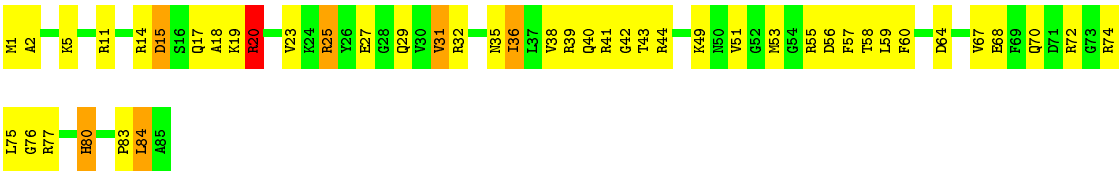
Chain AZ:



- Molecule 28: 50S ribosomal protein L27

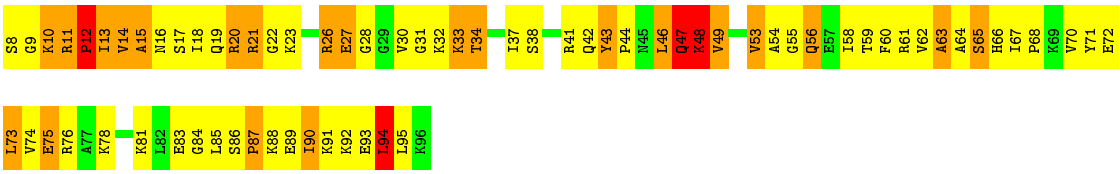
Chain B0:





- Molecule 29: 50S ribosomal protein L28

Chain B1:

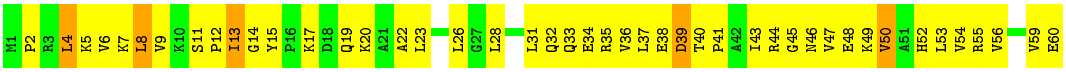


- Molecule 30: 50S ribosomal protein L29

Chain B2:

- Molecule 31: 50S ribosomal protein L30

Chain B3:

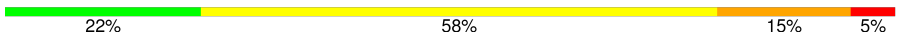


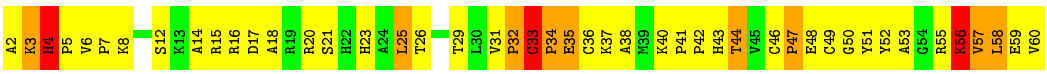
- Molecule 32: 50S ribosomal protein L31

Chain B4:

- Molecule 33: 50S ribosomal protein L32

Chain B5:



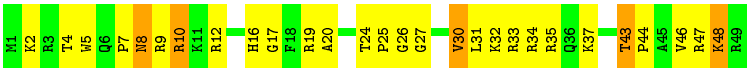


- Molecule 34: 50S ribosomal protein L33

Chain B6: 18% 53% 27%

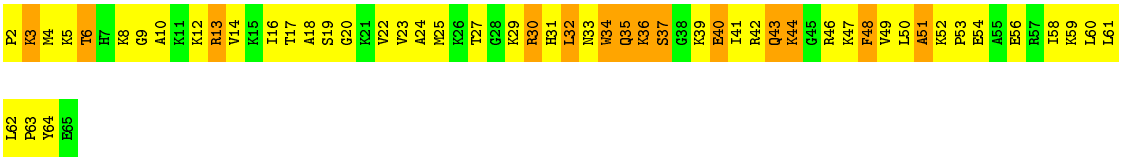
- Molecule 35: 50S ribosomal protein L34

Chain B7: 43% 47% 10%



- Molecule 36: 50S ribosomal protein L35

Chain B8: 17% 61% 22%

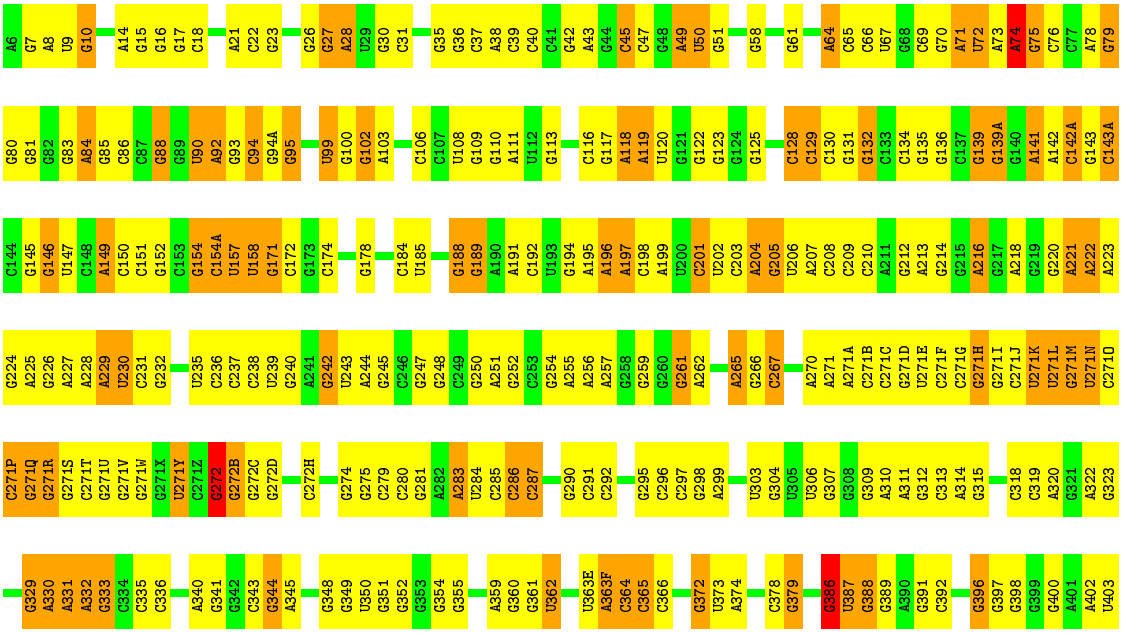


- Molecule 37: 50S ribosomal protein L36

Chain B9: 11% 66% 23%

- Molecule 38: 23S rRNA

Chain BA: 27% 54% 18%



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A1419	U1352	G1280	A1220	C1152	A1088	A1028	C964	C898	G818	A752	A676	C611	C542	G473	U405
U1420	A1353	G1281	C1221	C1153	G1089	A1029	C965	A899	A819	C753		C612	C543	G474	G406
G1421	A1354		C1221A	G1154	U1090	G1030		A900		C754	G680	G613	A547	U475	G407
	G1355	A1284	C1222	A1155	G1091	G1031	G968	A901	C825	C755	G681	U614	A548	G476	G408
G1424	G1356	G1285	G1223	A1156	C1092	A1032	U969	C902	U826	C756		U614A	G549		C409
G1425	U1357	A1286	C1224	G1157	G1093	U1033	C970	C903	U827	U757	G684	G614B	G551	A480	G410
G1426	G1358	A1287	G1225	G1158	U1094	G1034	C971		U828	C758	A685	A614C		G481	G411
A1427	A1359	U1288	A1226	U1159	A1095	U1035	G972	U907	A829	G759	G686	G615	U554	A482	A412
C1428	A1360	C1289	G1227	G1160	A1096	G1036	A973	C908	G830	G760	C687	G616	U555	A483	C413
G1429	G1361	C1290	G1228	C1161	U1097	G1037	G974	A909	G831	A761	U688	C618	G556	C484	C414
C1430	C1362	C1291	G1229	G1162	A1098	C1038	C975	A910	G832		A689	G619	U557	C485	A415
U1431	C1363	U1292	C1230	G1163	G1099	G1039		A911	U833	G765	G690	G620	G558	C486	
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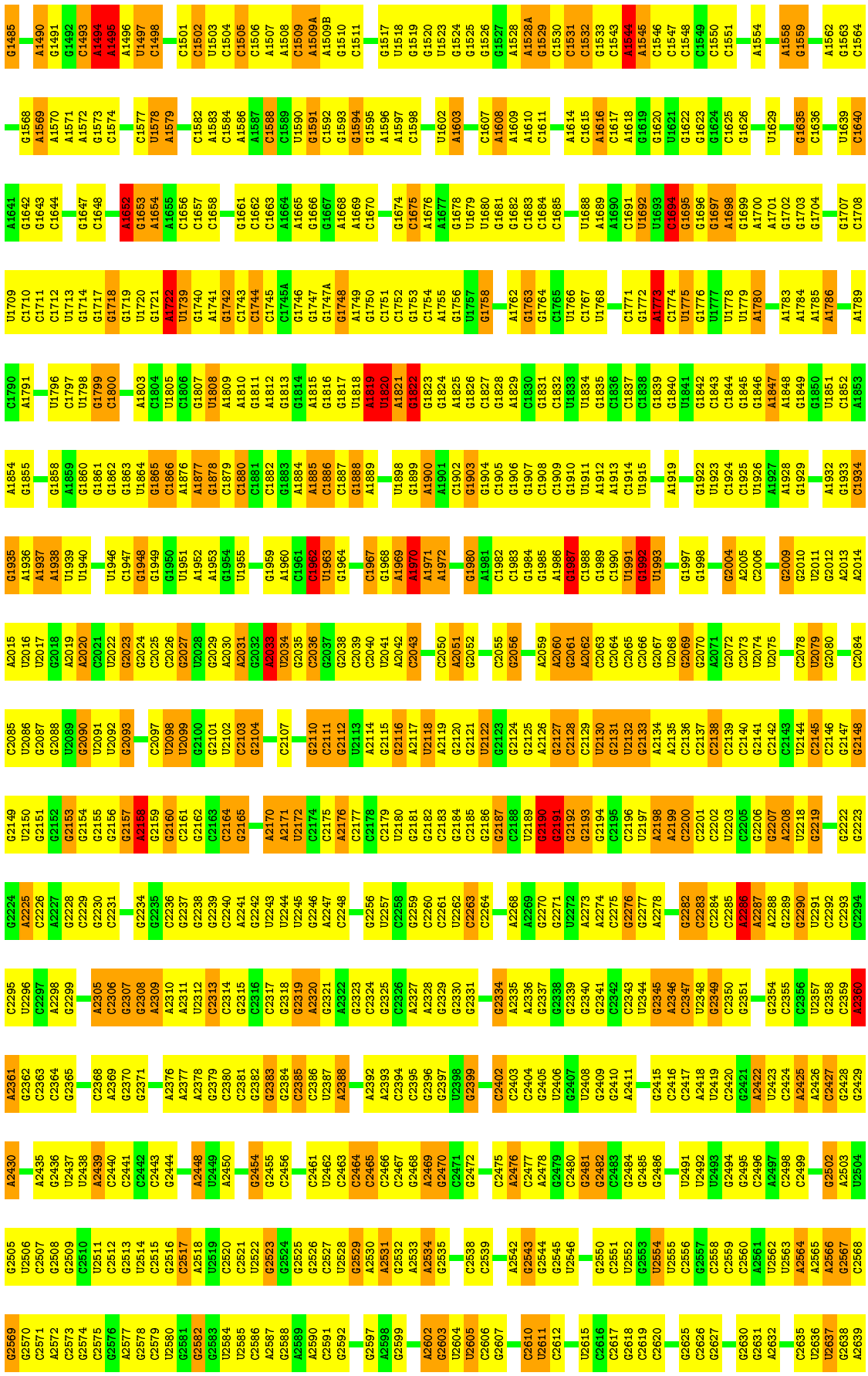
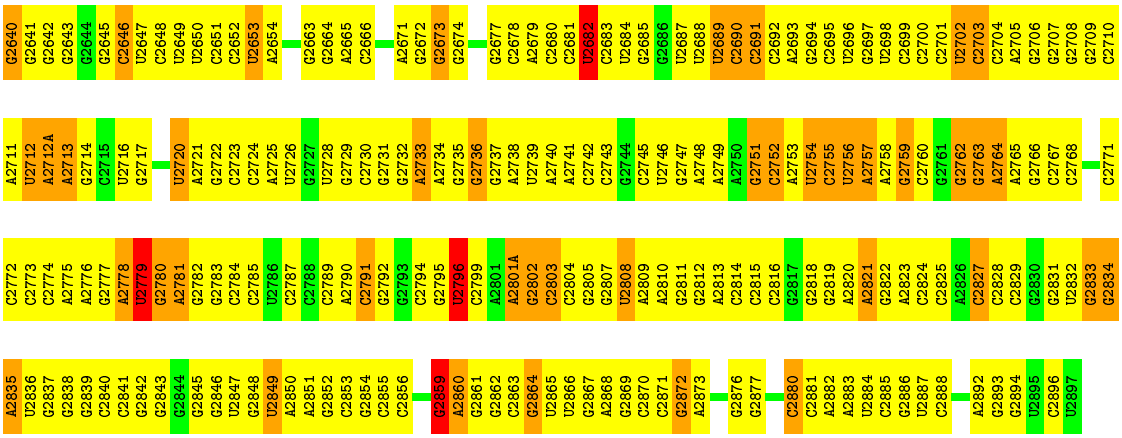
U1433	A1365		G1232	U1165	U1101	C1041	G978	U913	A835	U767	C692	G622	C560	G488	C419
A1434	A1366	C1298	C1233	C1166	C1102	G1042	G979	C914	G836	G768	C693	G623	G561	G489	C420
G1435	A1367	G1299	U1234	U1167	A1103	C1043	A980	C915	C837	G769		C624	U562	G491	U421
G1436	G1368	U1300	G1235	G1168	C1104	G1044	A981	G916	C838		A699	G625	G563	A492	A422
C1437	G1369	A1301		G1169	U1105	A1045	C982	A917	U839	A774	G700	U626	C564	G493	A423
U1438	C1370	A1302	G1238	G1170	G1106	A1046	A983	A918		G775		A627	C565	G494	G424
A1439			G1239	G1171	G1107	G1047	A984	G919	U847	G776	U703	G628		G495	G425
G1440	C1376	G1309	U1240	G1173	U1108	A1048	C985		G848	A777	G704	G629	G570	G496	C426
G1441	G1377	G1310	A1241	A1174	C1109	C1049	C986	U922	A849		A705	G630	A571		U427
G1442	A1378	G1311	A1242	U1175	G1110	A1050	G987	C923	C850	G780	A706	A631	A572	G500	A428
G1443	A1379	U1312	G1243	G1176	A1111	G1051	A988	C924	U851	A781	G707	A632	G573	A501	A429
G1444	G1380	U1313	G1244	A1177	G1112	C1052	G989	C925	G852	A782	C708	A633	C574	A502	G430
A1445	G1381	C1314	G1245	C1178	U1113	C1053	A990	A926	G853	A783	U709	C634	A575	A503	U431
C1445A	G1382	C1315	A1246	C1179	G1114	A1054	C991	G927	G854	A784	G710	C635	U576	U504	A432
C1446	C1383	U1316	A1247	C1180	G1115	G1055	C992	G928	G855	G785		G636	G577	A505	C433
G1447	A1384	A1317	G1248	C1181	C1116	G1056	G993		C856	C786	G715	A637	A578	G506	
G1448	G1385	C1318	U1249	A1182	G1117	A1057	C994	G932	C857	U787	A716	G638	G579	A507	G438
A1449	C1386	U1319	G1250	G1183	C1118	G1058	C995	A933	U858	A788	G717	U639	C580	G508	G440
G1450	C1387		C1251	G1184	C1119	G1059	A996	G934	G859	A789	A718	C640	C581	C509	U441
	G1388	A1322	G1252	C1185	G1120	U1060	G997	C935	U860	C790	C719		G582	C510	G442
U1453	G1389	U1323	A1253	G1186	C1121	U1061	C998	C936	A861	C791	C720	A643	G583	U511	A443
G1455		G1324	A1254	G1187	G1122	G1062	U999		G862	G792	C721	A644	C584	G512	C444
G1456	U1394	G1325	U1255	U1188	C1123	G1063	A1000	G939	A863	A793	A722	C645	G585	A513	C445
A1457	A1395	U1326	G1256	A1189	C1124	C1064	A1001	G940	G864	G794	G723	A646	A586		G446
C1458	U1396	C1327	C1257	G1190	G1125	U1065	G1002	A941	C865	C795	U724	G647	C587	C517	A447
G1459	U1397	G1328	C1258	G1191		U1066	G1003	G942	A866	C796	G725	G648	U588	G518	U448
A1460	C1398	U1329	G1259	G1192	A1129	A1067	C1004	U943	C867	C797	G726	G649	C589	U519	
G1461	C1399	C1330	G1260	G1193	U1130	G1068	C1005	G944	U868	G798		G650	A590	G520	C451
	G1400	A1331	C1261	A1194	G1131	A1069	C1006	A945	G869	G799	G729	G651	C591	G521	G452
C1464	G1401	G1332	A1262	G1195	A1132	A1070	C1007	G946	A870	A800	C730	C652	G592	G522	C453
G1465	C1402		U1263	C1196	U1133	G1071		G947	U871	G801		G656	G593	C523	
G1466	C1403	U1335	G1264		C1135	C1072	A1010	G948		A802	G733	U657	U594	U524	C456
C1467	C1404	A1336	A1265	C1201	G1136	A1073	G1011	G949	G874	U803	A734	C658	C595		A457
	U1405	G1337	G1266	C1202		G1074	U1012	G950	G875	A804		C659	G596	C527	G458
A1471	U1406	G1338	U1267	G1203	C1140	C1075	C1013	C951	C876	G805	C737	G660	U597	A528	U459
A1472	C1407	G1339	A1268	A1204	U1141	C1076	U1014	G952	U877	C806	G738	C661	G598		A460
G1473	C1408	U1340	A1269	U1205	U1142	A1077		A953	A878	U807	G739	G662		C531	C461
C1474	C1409	U1341	C1270	G1206	A1142A	U1078	C1018	G954	G879	G808	U740		C601	A532	C462
G1475	G1410		G1271	C1207	A1143	C1079	U1019	C955		G809	G741	U667	G602	G533	G463
C1476	C1411	G1344	A1272	C1208	G1144	C1080	A1020	G956	G883	U810	G742	G668	A603	U534	U464
A1477	A1412	C1345	U1273	G1209	C1145	U1081	A1021	A957	C884	U811	G743	G669	G604	C535	G465
G1478	G1413	G1346	A1274	A1210	C1146	U1082	G1022	U958	G892	C812	G744	A670	C605	A536	
	G1414	G1347	A1275	U1211	C1147	U1083	U1023	A959	C893	U813	G745	C671	U606	C537	G468
U1481	U1415	G1348	A1276		A1148	A1084	G1024	A960	C894	C814	A746	C672	U607	G538	G469
G1482	G1416	A1349	G1277	G1215	G1149	A1085	G1025	C961	U895	C815	U747	C673	A608	G539	A470
G1484	C1417	C1350	A1278	G1216	C1150	A1086	U1026	G962	A896	C816		G674	A609	C540	A471

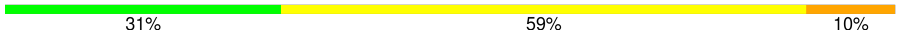


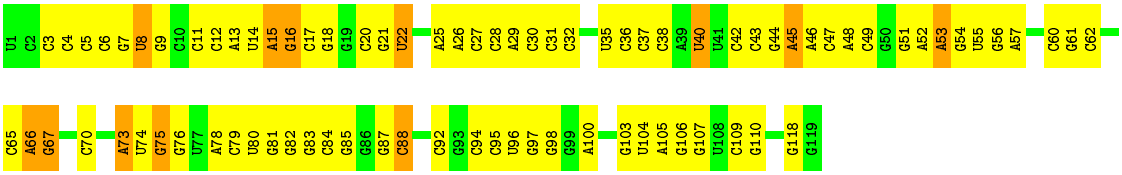
WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



- Molecule 39: 5S rRNA

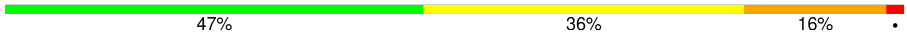
Chain BB:

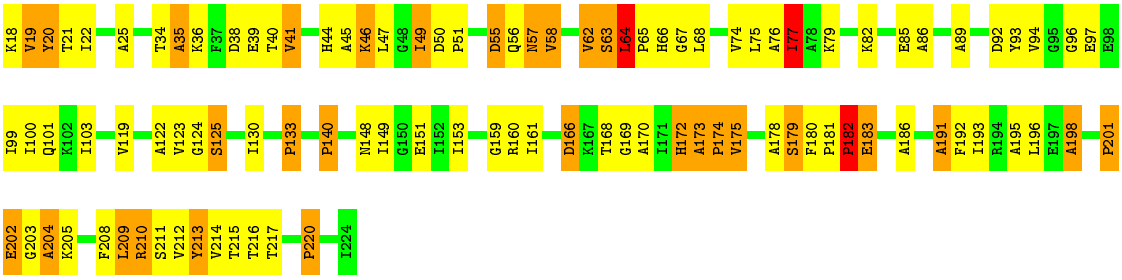




- Molecule 40: 50S ribosomal protein L1

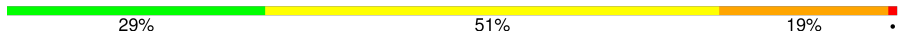
Chain BC:

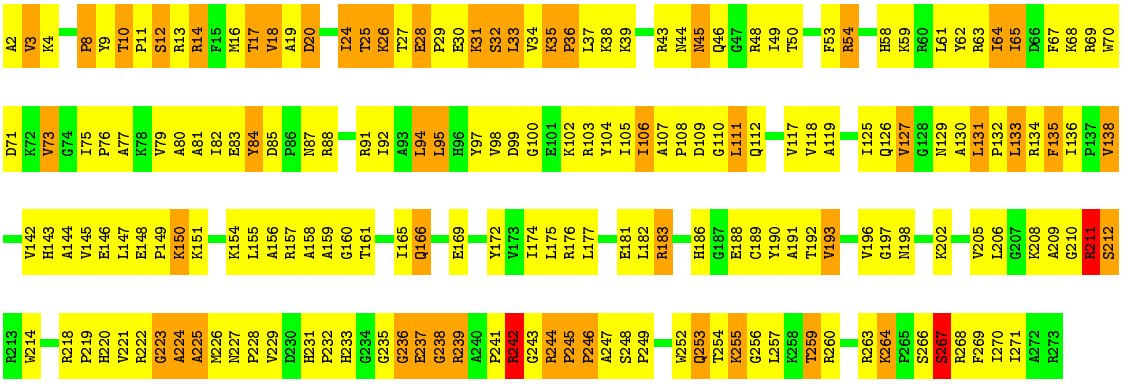




- Molecule 41: 50S ribosomal protein L2

Chain BD:





- Molecule 42: 50S ribosomal protein L3

Chain BE: 23% 52% 23%

M1 K2 G3 I4 L5 G6 V7 K8 V9 G10 M11 T12 R13 I14 F15 R16 D17 D18 V21 P22 V23 T24 V25 I26 L27 A28 G29 P30 C31 P32 V33 V34 Q35 R36 R37 T38 P39 E40 K41 D42 G43 Y44 T45 A46 V47 Q48 L49 G50 F51 L52 P53 Q54 N55 P56 K57 R58 V59 N60 R61

P62 L63 K64 G65 H66 E67 A68 K69 A70 G71 V72 E73 P74 V75 R76 I77 L78 R79 E80 I81 R82 D83 F84 E87 G88 D89 T90 V91 T92 V93 E94 I95 P96 K97 E100 R101 V102 D103 V104 T107 S108 K109 G110 R111 G112 F113 A114 G115 V116 M117 K118 R119 W120 N121 F122 A123 G124

G125 P126 D127 S128 H129 G130 A131 H132 K133 I134 H135 I141 G142 N143 R144 K145 R149 V150 G153 K154 K155 M156 A157 G158 H159 Y160 G161 A162 E163 V167 M168 N169 L170 E171 V172 V173 D174 V175 I176 P177 E178 E179 N180 L181 L182 L183 V184 K185 G186 A187 V188 P189 G190 P191 N192 G193

G194 L195 V196 I197 V198 R199 E200 T201 K202 K203 A204 A205

- Molecule 43: 50S ribosomal protein L4

Chain BF: 26% 60% 13%

M1 K2 E3 V4 A5 V6 Y7 Q8 I9 P10 V11 L12 S13 P14 S15 G16 R17 R18 E19 L20 A21 A22 D23 L24 P25 A26 E27 I28 H31 L32 L33 W34 E35 V36 V37 R38 W39 Q40 L41 A42 K43 R44 R45 R46 G47 T48 T51 K52 T53 R54 G55 E56 V57 A58 Y59 S60 G61 R62

K63 I64 W65 P66 Q67 K68 H69 R74 H75 G76 D77 I78 G79 A80 F83 V84 G85 G86 V89 F90 G91 P92 K93 P94 R95 Y99 T100 L101 P102 K103 K104 V105 R106 K107 K108 G109 L110 A111 M112 A113 V114 A115 D116 R117 A118 R119 K122 L123 L124 L125 V126 E127 A128 V132

N133 G134 K135 T136 F139 L140 A143 A146 G147 L148 S153 V154 L155 L156 V157 T158 G159 N160 E161 L162 V163 R164 R165 A166 A167 R168 N169 L170 P171 W172 V173 V174 T175 L176 A177 P178 E179 G180 L181 N182 V183 Y184 D185 I186 V187 R188 T189 E190 R191 L192 V193 M194 D195 L196 D197 A198

W199 E200 V201 F202 Q203 N204 R205 I206 G207 G208

- Molecule 44: 50S ribosomal protein L5

Chain BG: 19% 60% 18%

P2 L3 D4 V5 A6 L7 K8 R9 K10 Y11 Y12 E13 E14 V15 R16 P17 E18 L19 I20 R21 R22 F23 G24 Y25 Q26 N27 V28 W29 E30 V31 P32 R33 L34 E35 I39 N40 Q41 G42 L43 G44 E45 A46 K47 E48 D49 A50 R51 E54 K55 A56 A57 Q58 E59 L60 A61 L62 I63 T64

G65 Q66 K67 P68 A69 V70 T71 R72 S76 I77 S78 N79 F80 K81 L82 R83 K84 G85 M86 P87 I88 G89 L90 R91 L94 R95 R96 D97 R98 M99 W100 I101 F102 L103 E104 K105 L106 L107 N108 V109 A110 L111 P112 R113 I114 R115 D116 F117 L120 N121 P122 N123 S124 F125 D126 G127 R128

G129 N130 Y131 N132 L133 G134 L135 R136 E137 Q138 L139 I140 E143 I144 T145 Y146 D147 M148 V149 L152 R153 G154 M155 D156 I157 A158 V159 V160 T161 T162 A163 E164 T165 D166 E167 E168 A169 R170 A171 L172 L173 E174 L175 L176 G177 F178 P179 F180 R181 K182

- Molecule 45: 50S ribosomal protein L6

Chain BH: 24% 55% 18%

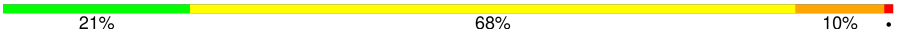
P12 K13 G14 V15 S16 V17 E18 V19 A20 P21 K25 V26 K27 G28 P29 K30 G31 E32 L33 E34 V35 P36 V37 S38 P39 E40 N41 R42 V43 V44 V45 E46 E47 G48 V49 V50 R51 V52 E53 R54 P55 S56 D57 E58 R59 R60 H61 K62 S63 L64 H65 G66 L67 T68 R69 T70 L71 I72 A73

N74 A75 V76 K77 G78 V79 S80 E81 G82 Y83 S84 K85 E86 L87 L88 I89 K90 G91 I92 G93 Y94 R95 A96 R97 L98 A102 L103 E104 L105 T106 V107 P112 Y113 V114 V115 E116 P117 P118 I121 T122 F123 E124 V125 P126 E127 P128 T129 R130 V131 R132 V133 S134 G135 I136 D137 K138 Q139

K140 V141 G142 Q143 V144 A145 A146 N147 I148 R149 A150 I151 R152 K153 P154 S155 A156 Y157 H158 E159 K160 G161 I162 Y163 V169 R170 L171

- Molecule 46: 50S ribosomal protein L9

Chain BI:



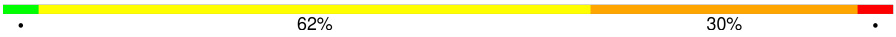
M1 K2 V3 I4 L5 L6 E7 P8 L9 E10 N11 L12 G13 D14 V15 G16 Q17 V18 V19 D20 V21 K22 P23 G24 Y25 N28 Y29 L30 L31 P32 R33 V37 L38 A39 T40 E41 L44 K45 A46 L47 E48 A49 R50 I51 R52 A53 Q54 A55 K56 R57 L58 A59 E60 R61 K62 E66

R67 L68 K69 E70 I71 L72 L75 T76 L77 T78 I79 P80 V81 R82 A83 G84 E85 T86 K87 I88 Y89 G90 S91 V92 T93 A94 K95 D96 I97 A98 E99 A100 L101 S102 R103 Q104 H105 G106 V107 T108 I109 D110 P111 K112 R113 L114 A115 P119 I120 K121 E122 L123 G124 E125 Y126 V127 L128 T129

Y130 K131 P132 H133 P134 E135 V136 P137 I138 Q139 L140 K141 V142 S143 V144 V145 V146

- Molecule 47: 50S ribosomal protein L11

Chain BL:



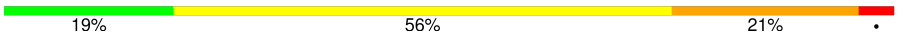
K2 K3 V4 V5 A6 V7 V8 K9 L10 Q11 L12 P13 A14 G15 K16 A17 T18 P19 A20 P21 P22 V23 G24 P25 A26 L27 G28 Q29 H30 G31 A32 N33 I34 M35 E36 F37 V38 K39 A40 F41 N42 A43 A44 T45 A46 N47 M48 G49 D50 A51 I52 V53 P54 V55 E56 I57 T58 I59 Y60 A61

D62 R63 S64 F65 T66 F67 V68 T69 K70 T71 P72 P73 A74 S75 Y76 L77 I78 R79 K80 A81 A82 G83 L84 E85 K86 G87 A88 H89 K90 P91 G92 R93 E94 K95 V96 G97 R98 I99 T100 W101 E102 Q103 V104 L105 E106 I107 A108 K109 Q110 K111 M112 P113 D114 L115 N116 T117 T118 D119 L120 E121

A122 A123 A124 R125 M126 I127 A128 G129 S130 A131 R132 S133 M134 G135 V136 E137 V138 V139

- Molecule 48: 50S ribosomal protein L13

Chain BN:



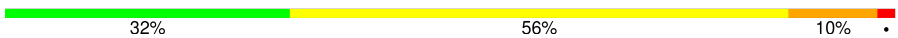
M1 K2 T3 Y4 V5 P6 Y9 E10 P11 R12 W13 V14 L15 I16 D17 A18 E19 G20 K21 T22 L23 G24 R25 L26 A27 T28 K29 I30 A31 T32 L33 L34 R35 G36 K37 H38 R39 P40 D41 W42 T43 V46 A47 M48 G49 D50 F51 V52 V53 V54 V55 N56 A57 D58 K59 I60 R61 V62

T63 G64 K65 K66 L67 E68 Q69 K70 I71 Y72 T73 R74 Y75 S76 G77 Y78 P79 G80 G81 L82 K83 K84 I85 P86 L87 E88 K89 M90 T93 H94 P95 E96 R97 V98 L99 E100 H101 A102 V103 K104 G105 M106 L107 P108 P111 L112 G113 R114 R115 L116 F117 K118 R119 L120 K121 V122 Y123 A124

G125 P126 D127 H128 P129 H130 Q131 A132 Q133 R134 P135 E136 E139

- Molecule 49: 50S ribosomal protein L14

Chain BO:



M1 I2 Q3 P4 Q5 T6 Y7 L8 E9 V10 A11 D12 N13 T14 G15 A16 R17 K18 I19 M20 C21 I22 R23 V24 L25 K26 G27 S28 N29 A30 K31 Y32 A33 T34 V35 G36 V40 A41 S42 V43 K44 E45 A46 I47 P48 V52 K53 E54 G55 D56 V63 R64 T65 K66 K67 E68 I69

K70 R71 P72 D73 G74 S75 A76 I77 R78 F79 N82 V85 I86 I87 N88 N89 Q90 L91 E92 P93 R97 V98 F99 G100 P101 V102 A103 R104 E105 L106 R107 E108 K109 M112 K113 I114 V115 S116 L117 A118 P119 E120 V121 L122

- Molecule 50: 50S ribosomal protein L15

Chain BP: 14% 55% 26% 5%

D5 L6 R7 P8 N9 P10 G11 A12 N13 K14 R15 R16 K17 R18 V19 G20 R21 G22 P23 G24 S25 G26 H27 G28 K29 T30 A31 T32 R33 G34 H35 K36 G37 Q38 K39 S40 R41 S42 G43 G44 L45 K46 D47 P48 R49 R50 F51 E52 G53 G54 R55 S56 T57 T58 L59 M60 R61 L62 P63 K64

R65 G66 M67 Q68 G69 Q70 V71 P72 G73 E74 I75 R79 Y80 Q81 G82 V83 N84 L85 L88 A89 R90 F91 E92 G93 E94 V95 T96 P97 E98 L99 L100 V101 R102 A103 G104 L105 L106 K107 K108 G109 Y110 R111 L112 K113 I114 L115 G116 E117 A120 K121 P122 L123 K124 V125 V126 A127 H128

A129 F130 S131 K132 S133 A134 L135 E136 K137 L138 K139 A140 A141 G142 G143 E144 P145 V146 L147 L148 E149 A150

- Molecule 51: 50S ribosomal protein L16

Chain BQ: 19% 59% 21%

R6 M7 K8 Y9 R10 K11 Q12 Q13 R14 G15 R16 L17 A20 T21 K22 G23 G24 D25 Y26 V27 A28 F29 G30 D31 Y32 G33 L34 V35 A36 L37 E38 P39 A40 W41 I42 T43 A44 Q45 Q46 I47 E48 A49 A50 R51 V52 A53 M54 V55 R56 H57 F58 R59 G62 K63 I64 F65 I66 R67

I68 F69 P70 D71 K72 F73 Y74 T75 K76 K77 P78 L79 E80 V81 R82 M83 G84 K85 G86 K87 G88 N89 V90 E91 G92 Y93 V94 V97 K98 P99 G100 R101 V102 M103 F104 E105 V106 A107 G108 V109 T110 E111 E112 Q113 A114 A117 L118 R119 I120 A121 G122 H123 K124 L125 P126 I127 K128 T129

K130 I131 V132 R133 R134 D135 A136 Y137 D138 E139 A140 Q141

- Molecule 52: 50S ribosomal protein L17

Chain BR: 21% 58% 19%

R2 H3 L4 K5 S6 G7 R8 K9 L10 N11 R12 H13 S14 S15 H16 R17 L18 A19 I20 Y21 R22 N23 Q24 S27 L28 L29 T30 R33 T36 T37 V38 P39 K40 A41 K42 E43 L44 R45 G46 F47 V48 D49 H50 L51 I52 H53 L54 A55 K56 L60 H61 A62 R63 R64 L65 V66

L67 R68 D69 L70 V73 K74 L75 V76 R77 K78 L79 F80 D81 E82 I83 A84 P85 R86 Y87 R88 D89 G92 G93 Y94 T95 R96 V97 L98 K99 L100 A101 E102 R103 R104 R105 G106 D107 G108 L111 A112 L113 V114 E115 L116 V117 E118

- Molecule 53: 50S ribosomal protein L18

Chain BS: 12% 51% 35%

K11 F12 R13 V14 R15 N16 R17 I18 K19 R20 R23 L24 R25 L26 S27 V28 F29 R30 S31 L32 K33 H34 I35 Y36 A37 Q38 I39 D42 E43 K44 G45 V46 T47 L48 V49 S50 A51 S52 S53 L54 A55 L56 K57 L58 K59 G60 N61 K62 T63 E64 V65 A66 R67 Q68 V69 G70 R71 A72

L73 A74 E75 K76 A77 L78 A79 L80 G81 I82 K83 Q84 V85 A86 F87 D88 R89 G90 P91 Y92 K93 Y94 R95 G96 R97 V98 K99 A100 L101 A102 E103 G104 A105 R106 E107 G108 G109

- Molecule 54: 50S ribosomal protein L19

Chain BT: 19% 54% 22% 5%

M1 N2 R3 G4 A5 L6 I7 K8 L9 V10 E11 S12 R13 Y14 V15 R16 T17 D18 F22 R23 P24 G25 D26 T27 V28 R29 V30 S31 Y32 R33 V34 K35 E36 G37 N38 R39 T40 R41 I42 Q43 D44 F45 E46 G47 I48 V49 I50 R51 I52 R53 R54 N55 G56 F57 N58 T59 T60 F61 T62

V63 R64 K65 V66 S67 Y68 G69 V70 G71 V72 E73 R74 I75 F76 P77 L78 H79 S80 P81 L82 I83 Q84 K85 I86 D87 I88 V89 Q90 R91 G92 R93 A94 R95 R96 A97 K98 L99 Y100 F101 I102 R103 S106 D107 R108 E109 R112 K113 L114 R115 A116 D117 R118 K119 R120 I121 D122 Q123 D124

E128 R129 A130 A131 K132 E133 E134 A135 A138

- Molecule 55: 50S ribosomal protein L20

Chain BU: 29% 58% 12%

P2 T6 G7 V8 V9 R10 R11 R12 K13 H14 K15 K16 I17 L18 K19 L20 A21 K22 G23 Y24 W25 G26 L27 R28 S29 K30 S31 F32 R33 K34 A35 R36 E37 T38 L39 F40 N44 Y45 H49 R50 K51 R52 R53 K54 R55 D56 F57 R58 R59 L60 W61 I62 V63 R64 I65 N66 A67

A68 C69 L74 N75 Y76 F79 I80 H81 G82 L83 G87 I88 E89 V90 D91 R92 K93 N94 L95 A96 D97 L98 R101 E102 V105 F106 A107 E108 L109 V110 E111 R112 A113 K114 A115 G118

- Molecule 56: 50S ribosomal protein L21

Chain BV: 14% 48% 36%

M1 P2 A3 I4 V5 K6 T7 G8 G9 K10 Q11 Y12 R13 V14 E15 P16 G17 L18 K19 L20 R21 V22 E23 K24 L25 D26 A27 E28 P29 T32 V33 E34 L35 P36 V37 L38 L39 L40 G41 G42 E43 K44 T45 V46 V47 G48 T49 P50 V51 V52 E53 G54 A55 S56 V57 E60 V61 L62

G63 H64 G65 R66 G67 K68 K69 I70 L71 V72 S73 K74 F75 K76 A77 K78 V79 Q80 Y81 R82 R83 K84 K85 G86 H87 R88 Q89 P90 Y91 T92 E93 L94 L95 I96 K97 E98 I99 R100 G101

- Molecule 57: 50S ribosomal protein L22

Chain BW: 25% 61% 13%

M1 E2 A3 K4 A5 I6 A7 R8 Y9 V10 R11 I12 S13 P14 R15 K16 V17 R18 L19 V20 V21 D22 L23 I24 R25 G26 K27 S28 L29 E30 E31 A32 R33 N34 I35 L36 R37 N40 K41 A44 Y45 F46 V47 A48 K49 V50 L51 E52 S53 A54 A55 A56 N57 A58 V59 N60 N61 H62

D63 E66 L69 Y70 V71 K72 A73 A74 Y75 V76 G79 L82 K83 R84 V85 L86 P87 R88 A89 R90 G91 R92 A93 D94 I95 I96 R99 T100 S101 H102 I103 T104 V105 I106 L107 K110 H111 G112 K113

- Molecule 58: 50S ribosomal protein L23

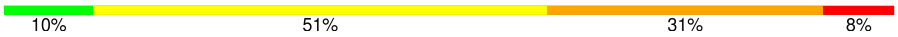
Chain BX: 14% 56% 23% 8%

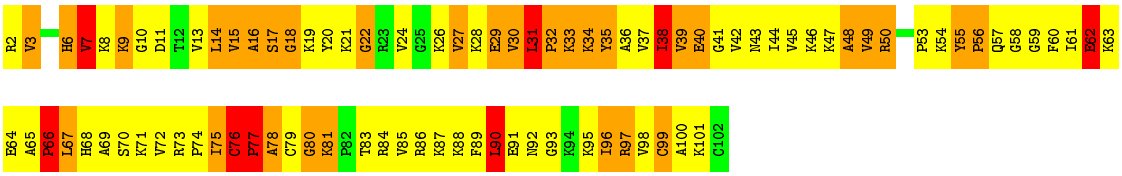
T3 A4 Y5 D6 V7 I8 L9 A10 P11 V12 L13 S14 E15 K16 A17 Y18 A19 G20 F21 A22 E23 G24 K25 Y26 T27 F28 W29 V30 H31 P32 K33 A34 T35 K36 T37 E38 I39 K40 N41 A42 V43 E44 K48 W49 K50 V51 V52 K53 V54 N55 T56 L57 H58 V59 R60 G61 K62 K63 K64

R65 L66 G67 R68 Y69 L70 G71 K72 R73 P74 D75 R76 K77 K78 A79 I80 V81 Q82 V83 A84 P85 G86 Q87 K88 I89 E90 A91 L92 E93 G94 L95

- Molecule 59: 50S ribosomal protein L24

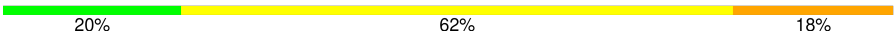
Chain BY:

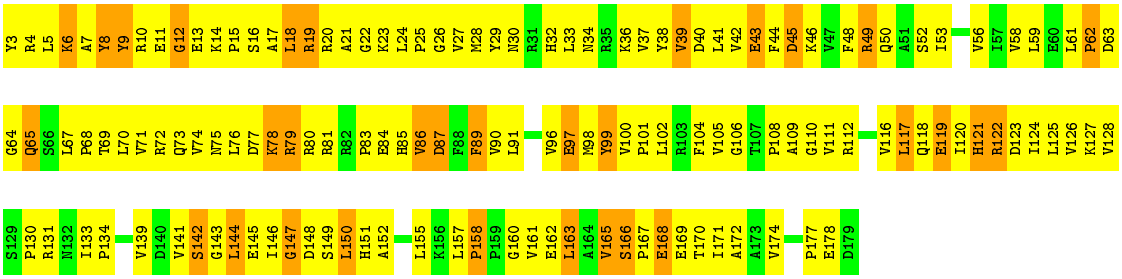




- Molecule 60: 50S ribosomal protein L25

Chain BZ:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of each defocus group volume prior to back projection.	Depositor
Microscope	Tecnai Polara F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2300	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	39000	Depositor
Image detector	Kodak SO-163	Depositor

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: 5MU, OMC, OMG, BME, PHA, GDP, YG, 2MG, 5MC, 1MA, MAU, M2G, 7MG, PSU

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	$\#\|Z\| >2$	RMSZ	$\#\|Z\| >2$
1	AA	0.51	0/36190	0.73	27/56486 (0.0%)
10	AP	0.43	0/717	0.70	0/965
11	AQ	0.42	0/837	0.67	0/1119
12	AR	0.40	0/579	0.71	0/768
13	AT	0.34	0/765	0.59	0/1007
14	AC	0.35	0/1637	0.58	0/2207
15	AG	0.34	0/1276	0.55	0/1709
16	AI	0.32	0/1027	0.56	0/1372
17	AJ	0.36	0/808	0.62	0/1087
18	AM	0.35	0/994	0.63	0/1322
19	AN	0.39	0/501	0.66	0/664
2	AB	0.33	0/1936	0.59	0/2611
20	AS	0.37	0/643	0.61	0/867
21	AU	0.46	0/213	0.56	0/279
22	AV	0.52	1/1814 (0.1%)	0.72	0/2825
23	AX	0.85	1/147 (0.7%)	0.83	0/223
24	AW	0.45	1/1813 (0.1%)	0.78	6/2823 (0.2%)
25	AY	1.12	4/1407 (0.3%)	2.35	13/2177 (0.6%)
26	A0	2.23	2/65 (3.1%)	1.08	0/98
27	AZ	0.30	0/3052	0.65	1/4141 (0.0%)
28	B0	0.39	0/658	0.65	0/878
29	B1	0.61	0/700	1.04	1/931 (0.1%)
3	AD	0.42	0/1733	0.67	0/2318
30	B2	0.45	0/423	0.99	3/560 (0.5%)
31	B3	0.37	0/473	0.61	0/636
32	B4	0.47	0/241	0.88	4/334 (1.2%)
33	B5	0.43	0/473	0.74	0/639
34	B6	0.39	0/387	0.62	0/517
35	B7	0.51	0/427	0.73	0/563
36	B8	0.50	0/516	0.81	0/681
37	B9	0.55	0/297	0.61	0/392
38	BA	0.66	8/68796 (0.0%)	0.80	76/107396 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
39	BB	0.39	0/2853	0.70	0/4451
4	AE	0.42	0/1163	0.66	0/1566
40	BC	0.38	0/1145	0.68	7/1556 (0.4%)
41	BD	0.52	0/2155	0.87	3/2907 (0.1%)
42	BE	0.43	0/1597	0.76	0/2155
43	BF	0.44	0/1659	0.70	0/2246
44	BG	0.39	0/1498	0.72	1/2013 (0.0%)
45	BH	0.33	0/1246	0.69	0/1684
46	BI	0.35	0/1147	0.66	0/1553
47	BL	0.50	0/1044	0.92	1/1415 (0.1%)
48	BN	0.41	0/1132	0.78	0/1527
49	BO	0.48	0/943	0.74	0/1269
5	AF	0.37	0/856	0.64	0/1154
50	BP	0.42	0/1131	1.00	6/1504 (0.4%)
51	BQ	0.37	0/1100	0.72	1/1470 (0.1%)
52	BR	0.40	0/974	0.74	1/1302 (0.1%)
53	BS	0.40	0/779	0.73	0/1038
54	BT	0.43	0/1156	0.77	2/1544 (0.1%)
55	BU	0.38	0/975	0.68	0/1297
56	BV	0.38	0/789	0.73	0/1054
57	BW	0.43	0/907	0.72	0/1216
58	BX	0.53	0/740	0.89	3/995 (0.3%)
59	BY	0.41	0/789	0.78	0/1053
6	AH	0.36	0/1136	0.62	0/1527
60	BZ	0.35	0/1436	0.64	0/1951
7	AK	0.38	0/900	0.64	0/1213
8	AL	0.42	0/987	0.72	0/1322
9	AO	0.38	0/745	0.63	0/992
All	All	0.56	17/164527 (0.0%)	0.79	156/245569 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	2	37
22	AV	0	2
24	AW	3	1
25	AY	0	5
29	B1	0	1
38	BA	29	93
All	All	34	139

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	BA	1051	G	O3'-P	37.08	2.05	1.61
38	BA	2190	G	O3'-P	-29.41	1.25	1.61
38	BA	2653	U	O3'-P	-27.37	1.28	1.61
25	AY	46	7MG	O3'-P	-19.71	1.37	1.61
25	AY	34	OMG	O3'-P	19.70	1.84	1.61

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	47	U	P-O3'-C3'	-79.00	24.90	119.70
38	BA	1051	G	P-O3'-C3'	-45.69	64.87	119.70
25	AY	35	A	P-O3'-C3'	41.14	169.07	119.70
38	BA	2190	G	P-O3'-C3'	27.80	153.06	119.70
25	AY	46	7MG	P-O3'-C3'	23.58	147.99	119.70

5 of 34 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	410	G	C3'
1	AA	412	A	C1'
24	AW	17	C	C1'
24	AW	47	U	C1'
24	AW	70	G	C3'

5 of 139 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	107	G	Sidechain
1	AA	253	U	Sidechain
1	AA	371	G	Sidechain
1	AA	38	G	Sidechain
1	AA	9	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1554	0
2	AB	1901	0	1951	280	0
3	AD	1703	0	1767	184	0
4	AE	1147	0	1207	167	0
5	AF	843	0	857	94	0
6	AH	1116	0	1177	129	0
7	AK	885	0	904	116	0
8	AL	971	0	1057	122	0
9	AO	734	0	771	76	0
10	AP	701	0	720	82	0
11	AQ	824	0	891	86	0
12	AR	574	0	644	97	0
13	AT	763	0	861	104	0
14	AC	1613	0	1677	212	0
15	AG	1257	0	1296	129	0
16	AI	1011	0	1041	140	0
17	AJ	795	0	840	145	0
18	AM	988	0	1055	179	0
19	AN	492	0	533	62	0
20	AS	630	0	652	104	0
21	AU	209	0	221	22	0
22	AV	1645	0	836	146	0
23	AX	132	0	67	15	0
24	AW	1623	0	821	97	0
25	AY	1546	0	801	196	0
26	A0	60	0	30	22	0
27	AZ	2962	0	2975	133	0
28	B0	650	0	654	82	0
29	B1	693	0	764	179	0
30	B2	421	0	461	124	0
31	B3	468	0	523	52	0
32	B4	242	0	103	20	0
33	B5	459	0	480	75	0
34	B6	381	0	390	55	0
35	B7	419	0	467	35	0
36	B8	508	0	576	111	0
37	B9	294	0	316	182	0
38	BA	61426	0	30956	3131	0
39	BB	2551	0	1295	107	0
40	BC	1142	0	865	99	0
41	BD	2105	0	2182	360	0
42	BE	1564	0	1629	326	0
43	BF	1624	0	1677	233	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BG	1474	0	1534	270	0
45	BH	1223	0	1282	205	0
46	BI	1132	0	1218	203	0
47	BL	1025	0	1074	426	0
48	BN	1105	0	1180	213	0
49	BO	933	0	996	136	0
50	BP	1114	0	1187	325	0
51	BQ	1080	0	1127	225	0
52	BR	960	0	1021	176	0
53	BS	771	0	832	185	0
54	BT	1142	0	1202	238	0
55	BU	958	0	1015	188	0
56	BV	779	0	851	216	0
57	BW	896	0	953	112	0
58	BX	726	0	778	205	0
59	BY	776	0	870	220	0
60	BZ	1404	0	1429	241	0
61	AY	11	0	10	5	0
62	AZ	28	0	12	1	0
63	AZ	58	0	60	0	0
64	AZ	4	0	5	3	0
All	All	152000	0	103944	12176	0

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 48.

The worst 5 of 12176 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)
37:B9:33:LYS:CD	38:BA:2527:C:H4'	1.25	1.66
25:AY:65:G:C5'	27:AZ:391:GLY:HA2	1.20	1.60
37:B9:4:ARG:CZ	38:BA:2465:C:C4'	1.78	1.56
37:B9:33:LYS:HD3	38:BA:2527:C:C4'	1.34	1.54
25:AY:65:G:H5'	27:AZ:391:GLY:CA	1.08	1.53

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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
2	AB	233/235 (99%)	148 (64%)	53 (23%)	32 (14%)	0 6
3	AD	206/208 (99%)	130 (63%)	51 (25%)	25 (12%)	0 8
4	AE	149/151 (99%)	108 (72%)	28 (19%)	13 (9%)	1 17
5	AF	99/101 (98%)	72 (73%)	21 (21%)	6 (6%)	2 26
6	AH	136/138 (99%)	103 (76%)	27 (20%)	6 (4%)	3 33
7	AK	117/119 (98%)	87 (74%)	25 (21%)	5 (4%)	3 34
8	AL	123/125 (98%)	83 (68%)	22 (18%)	18 (15%)	0 6
9	AO	86/88 (98%)	48 (56%)	34 (40%)	4 (5%)	3 32
10	AP	82/84 (98%)	53 (65%)	24 (29%)	5 (6%)	2 26
11	AQ	98/100 (98%)	74 (76%)	15 (15%)	9 (9%)	1 16
12	AR	68/70 (97%)	38 (56%)	21 (31%)	9 (13%)	0 7
13	AT	97/99 (98%)	54 (56%)	29 (30%)	14 (14%)	0 6
14	AC	205/207 (99%)	130 (63%)	55 (27%)	20 (10%)	1 14
15	AG	153/155 (99%)	99 (65%)	42 (28%)	12 (8%)	1 20
16	AI	121/127 (95%)	80 (66%)	30 (25%)	11 (9%)	1 17
17	AJ	97/99 (98%)	70 (72%)	18 (19%)	9 (9%)	1 16
18	AM	113/125 (90%)	68 (60%)	26 (23%)	19 (17%)	0 5
19	AN	58/60 (97%)	35 (60%)	17 (29%)	6 (10%)	1 12
20	AS	77/79 (98%)	52 (68%)	15 (20%)	10 (13%)	0 7
21	AU	23/25 (92%)	18 (78%)	4 (17%)	1 (4%)	3 34
27	AZ	382/405 (94%)	373 (98%)	8 (2%)	1 (0%)	46 83
28	B0	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	2 26
29	B1	87/89 (98%)	43 (49%)	25 (29%)	19 (22%)	0 2
30	B2	49/51 (96%)	16 (33%)	16 (33%)	17 (35%)	0 0
31	B3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	1 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B4	48/50 (96%)	14 (29%)	11 (23%)	23 (48%)	0	0
33	B5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	0	8
34	B6	41/45 (91%)	18 (44%)	16 (39%)	7 (17%)	0	4
35	B7	47/49 (96%)	36 (77%)	10 (21%)	1 (2%)	9	50
36	B8	62/64 (97%)	38 (61%)	13 (21%)	11 (18%)	0	4
37	B9	33/35 (94%)	22 (67%)	5 (15%)	6 (18%)	0	4
40	BC	183/191 (96%)	87 (48%)	53 (29%)	43 (24%)	0	2
41	BD	270/272 (99%)	193 (72%)	51 (19%)	26 (10%)	1	15
42	BE	203/205 (99%)	116 (57%)	49 (24%)	38 (19%)	0	3
43	BF	206/208 (99%)	142 (69%)	40 (19%)	24 (12%)	0	9
44	BG	177/181 (98%)	93 (52%)	56 (32%)	28 (16%)	0	5
45	BH	158/160 (99%)	100 (63%)	31 (20%)	27 (17%)	0	4
46	BI	144/146 (99%)	98 (68%)	36 (25%)	10 (7%)	1	22
47	BL	136/138 (99%)	66 (48%)	32 (24%)	38 (28%)	0	0
48	BN	137/139 (99%)	75 (55%)	35 (26%)	27 (20%)	0	3
49	BO	120/122 (98%)	92 (77%)	17 (14%)	11 (9%)	1	16
50	BP	144/146 (99%)	72 (50%)	37 (26%)	35 (24%)	0	2
51	BQ	134/136 (98%)	82 (61%)	33 (25%)	19 (14%)	0	6
52	BR	115/117 (98%)	74 (64%)	20 (17%)	21 (18%)	0	3
53	BS	97/99 (98%)	49 (50%)	19 (20%)	29 (30%)	0	0
54	BT	136/138 (99%)	77 (57%)	34 (25%)	25 (18%)	0	3
55	BU	115/117 (98%)	61 (53%)	42 (36%)	12 (10%)	1	12
56	BV	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
57	BW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	8
58	BX	91/93 (98%)	45 (50%)	23 (25%)	23 (25%)	0	1
59	BY	99/101 (98%)	41 (41%)	24 (24%)	34 (34%)	0	0
60	BZ	175/177 (99%)	99 (57%)	48 (27%)	28 (16%)	0	5
All	All	6336/6487 (98%)	4034 (64%)	1428 (22%)	874 (14%)	1	6

5 of 874 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	52	GLU
2	AB	77	ALA
2	AB	84	GLU
2	AB	154	LEU

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 PDB entries followed by that with respect to all EM entries.

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	
2	AB	202/203 (100%)	182 (90%)	20 (10%)	10	39
3	AD	180/180 (100%)	159 (88%)	21 (12%)	7	32
4	AE	115/116 (99%)	102 (89%)	13 (11%)	7	33
5	AF	90/90 (100%)	84 (93%)	6 (7%)	20	57
6	AH	119/119 (100%)	114 (96%)	5 (4%)	36	70
7	AK	90/90 (100%)	85 (94%)	5 (6%)	26	62
8	AL	104/104 (100%)	95 (91%)	9 (9%)	13	45
9	AO	79/79 (100%)	74 (94%)	5 (6%)	22	59
10	AP	72/72 (100%)	65 (90%)	7 (10%)	10	40
11	AQ	94/95 (99%)	92 (98%)	2 (2%)	61	84
12	AR	61/61 (100%)	55 (90%)	6 (10%)	10	39
13	AT	76/76 (100%)	65 (86%)	11 (14%)	4	25
14	AC	160/161 (99%)	151 (94%)	9 (6%)	26	62
15	AG	126/126 (100%)	122 (97%)	4 (3%)	46	76
16	AI	98/98 (100%)	88 (90%)	10 (10%)	9	37
17	AJ	88/89 (99%)	82 (93%)	6 (7%)	20	57
18	AM	99/100 (99%)	93 (94%)	6 (6%)	23	60
19	AN	49/49 (100%)	47 (96%)	2 (4%)	37	71
20	AS	69/69 (100%)	62 (90%)	7 (10%)	9	38
21	AU	19/20 (95%)	17 (90%)	2 (10%)	8	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	AZ	325/339 (96%)	323 (99%)	2 (1%)	90	95
28	B0	61/67 (91%)	54 (88%)	7 (12%)	7	32
29	B1	73/74 (99%)	62 (85%)	11 (15%)	3	23
30	B2	46/47 (98%)	35 (76%)	11 (24%)	1	7
31	B3	51/52 (98%)	49 (96%)	2 (4%)	39	72
33	B5	51/51 (100%)	41 (80%)	10 (20%)	1	12
34	B6	43/44 (98%)	35 (81%)	8 (19%)	2	14
35	B7	41/42 (98%)	37 (90%)	4 (10%)	10	39
36	B8	53/54 (98%)	45 (85%)	8 (15%)	3	23
37	B9	33/33 (100%)	30 (91%)	3 (9%)	12	43
40	BC	61/148 (41%)	54 (88%)	7 (12%)	7	32
41	BD	213/214 (100%)	180 (84%)	33 (16%)	3	22
42	BE	165/165 (100%)	145 (88%)	20 (12%)	6	31
43	BF	165/165 (100%)	153 (93%)	12 (7%)	17	54
44	BG	155/155 (100%)	135 (87%)	20 (13%)	5	28
45	BH	132/133 (99%)	117 (89%)	15 (11%)	7	32
46	BI	122/123 (99%)	113 (93%)	9 (7%)	17	53
47	BL	105/105 (100%)	85 (81%)	20 (19%)	2	13
48	BN	117/118 (99%)	98 (84%)	19 (16%)	3	20
49	BO	100/100 (100%)	92 (92%)	8 (8%)	15	50
50	BP	112/112 (100%)	92 (82%)	20 (18%)	2	15
51	BQ	106/106 (100%)	93 (88%)	13 (12%)	6	30
52	BR	100/100 (100%)	91 (91%)	9 (9%)	12	44
53	BS	77/77 (100%)	65 (84%)	12 (16%)	3	22
54	BT	120/120 (100%)	99 (82%)	21 (18%)	2	16
55	BU	92/93 (99%)	85 (92%)	7 (8%)	16	53
56	BV	82/82 (100%)	64 (78%)	18 (22%)	1	9
57	BW	91/92 (99%)	85 (93%)	6 (7%)	21	57
58	BX	74/75 (99%)	59 (80%)	15 (20%)	1	11
59	BY	84/85 (99%)	67 (80%)	17 (20%)	1	11
60	BZ	155/156 (99%)	144 (93%)	11 (7%)	18	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5195/5324 (98%)	4661 (90%)	534 (10%)	13 37

5 of 534 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BD	73	VAL
44	BG	39	ILE
58	BX	28	PHE
41	BD	131	LEU
42	BE	89	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
34	B6	26	ASN
42	BE	143	ASN
57	BW	57	ASN
36	B8	35	GLN
41	BD	164	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	200 (13%)	36 (2%)
22	AV	76/77 (98%)	18 (23%)	0
23	AX	4/6 (66%)	2 (50%)	0
24	AW	75/76 (98%)	15 (20%)	3 (4%)
25	AY	65/72 (90%)	11 (16%)	3 (4%)
26	A0	2/3 (66%)	0	0
38	BA	2849/2852 (99%)	589 (20%)	78 (2%)
39	BB	118/119 (99%)	14 (11%)	1 (0%)
All	All	4692/4709 (99%)	849 (18%)	121 (2%)

5 of 849 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

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Mol	Chain	Res	Type
1	AA	47	C

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	BA	387	U
38	BA	1051	G
38	BA	2481	G
38	BA	474	G
38	BA	669	G

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

13 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	$\#\|Z\| > 2$
22	5MU	AV	54	22	13,22,23	1.11	2 (15%)	16,32,35	4.76	3 (18%)
25	2MG	AY	10	25	18,26,27	1.09	2 (11%)	21,38,41	2.77	5 (23%)
25	M2G	AY	26	25	18,27,28	1.24	3 (16%)	22,40,43	2.19	3 (13%)
25	OMC	AY	32	25	15,22,23	0.76	0	20,31,34	0.65	0
25	OMG	AY	34	26	18,26,27	1.24	2 (11%)	21,38,41	2.85	3 (14%)
25	YG	AY	37	25	28,42,43	1.01	1 (3%)	28,62,65	2.26	8 (28%)
25	PSU	AY	39	25	15,21,22	1.23	2 (13%)	16,30,33	3.35	2 (12%)
25	5MC	AY	40	25	14,22,23	0.91	1 (7%)	17,32,35	0.98	2 (11%)
25	7MG	AY	46	25	20,26,27	1.61	3 (15%)	23,39,42	2.48	2 (8%)
25	5MC	AY	49	25	14,22,23	0.81	0	17,32,35	1.06	2 (11%)
25	5MU	AY	54	25	13,22,23	1.11	1 (7%)	16,32,35	4.95	2 (12%)
25	PSU	AY	55	25	15,21,22	1.47	3 (20%)	16,30,33	3.25	4 (25%)
25	1MA	AY	58	25	15,25,26	3.16	3 (20%)	15,37,40	2.34	2 (13%)

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
22	5MU	AV	54	22	-	0/3/25/26	0/2/2/2
25	2MG	AY	10	25	-	0/5/27/28	0/3/3/3
25	M2G	AY	26	25	-	0/7/29/30	0/3/3/3
25	OMC	AY	32	25	-	0/5/27/28	0/2/2/2
25	OMG	AY	34	26	-	0/5/27/28	0/3/3/3
25	YG	AY	37	25	-	0/20/42/43	0/4/4/4
25	PSU	AY	39	25	-	0/7/25/26	0/2/2/2
25	5MC	AY	40	25	-	0/3/25/26	0/2/2/2
25	7MG	AY	46	25	-	0/7/37/38	0/3/3/3
25	5MC	AY	49	25	-	0/3/25/26	0/2/2/2
25	5MU	AY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
25	1MA	AY	58	25	-	0/3/25/26	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AY	46	7MG	C8-N9	-5.08	1.38	1.45
25	AY	39	PSU	C6-C5	-3.27	1.33	1.38
25	AY	55	PSU	C6-C5	-3.00	1.34	1.38
25	AY	46	7MG	C8-N7	-2.85	1.30	1.43
22	AV	54	5MU	C6-C5	-2.18	1.34	1.40

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	54	5MU	C5-C4-N3	-13.31	114.18	125.35
22	AV	54	5MU	C5-C4-N3	-11.99	115.29	125.35
25	AY	34	OMG	C5-C6-N1	-9.32	111.34	123.52
25	AY	10	2MG	C5-C6-N1	-9.03	111.72	123.52
25	AY	26	M2G	C5-C6-N1	-8.90	111.89	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0
25	AY	10	2MG	3	0
25	AY	26	M2G	18	0
25	AY	32	OMC	1	0
25	AY	34	OMG	12	0
25	AY	37	YG	20	0
25	AY	39	PSU	1	0
25	AY	40	5MC	3	0
25	AY	46	7MG	8	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
61	PHA	AY	101	-	9,11,11	0.43	0	11,13,13	0.60	0
62	GDP	AZ	501	-	24,30,30	1.23	2 (8%)	26,47,47	2.53	4 (15%)
63	MAU	AZ	502	-	55,60,60	3.78	13 (23%)	54,86,86	1.55	9 (16%)
64	BME	AZ	503	-	3,3,3	0.35	0	1,2,2	0.03	0

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
61	PHA	AY	101	-	-	0/4/6/6	0/1/1/1
62	GDP	AZ	501	-	-	0/12/32/32	0/3/3/3
63	MAU	AZ	502	-	-	0/54/98/98	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	BME	AZ	503	-	-	0/1/1/1	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	AZ	502	MAU	O18-C17	-16.16	1.20	1.44
63	AZ	502	MAU	O34-C33	-14.56	1.21	1.44
63	AZ	502	MAU	O30-C30	-13.64	1.15	1.42
62	AZ	501	GDP	C8-N7	-2.02	1.30	1.34
63	AZ	502	MAU	C6-C5	2.08	1.42	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	AZ	501	GDP	C5-C6-N1	-8.85	111.96	123.52
63	AZ	502	MAU	C29-C30-C31	-4.07	104.76	110.80
63	AZ	502	MAU	C23-C22-C21	-3.75	123.09	127.69
63	AZ	502	MAU	O29-C29-O34	-2.99	105.54	110.33
62	AZ	501	GDP	N3-C2-N1	-2.84	123.69	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	101	PHA	5	0
62	AZ	501	GDP	1	0
64	AZ	503	BME	3	0

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
25	AY	6
18	AM	5
38	BA	4
40	BC	3
16	AI	2
44	BG	1
56	BV	1
23	AX	1
34	B6	1

The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BC	110:PHE	C	119:VAL	N	11.81
1	AY	14:A	O3'	18:G	P	11.44
1	AX	14:A	O3'	16:A	P	8.56
1	AY	19:G	O3'	21:A	P	5.14
1	BC	27:ARG	C	34:THR	N	5.01