



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2018 – 04:39 AM EST

PDB ID : 4V8Q  
Title : Complex of SmpB, a tmRNA fragment and EF-Tu-GDP-Kirromycin with the 70S ribosome  
Authors : Neubauer, C.; Gillet, R.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2011-12-10  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

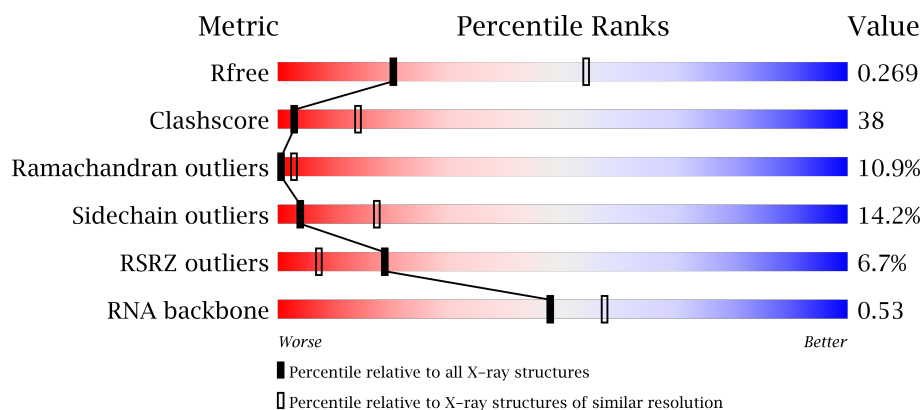
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	85	
2	A1	98	
3	A2	72	
4	A3	60	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A4	71	
6	A5	60	
7	A6	54	
8	A7	49	
9	A8	65	
10	A9	37	
11	AA	2915	
12	AB	122	
13	AC	229	
14	AD	276	
15	AE	206	
16	AF	210	
17	AG	182	
18	AH	180	
19	AJ	130	
20	AK	140	
21	AN	140	
22	AO	122	
23	AP	150	
24	AQ	141	
25	AR	118	
26	AS	112	
27	AT	146	
28	AU	118	
29	AV	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	AW	113	
31	AX	96	
32	AY	110	
33	AZ	206	
34	B2	144	
35	BA	1522	
36	BB	256	
37	BC	239	
38	BD	209	
39	BE	162	
40	BF	101	
41	BG	156	
42	BH	138	
43	BI	128	
44	BJ	105	
45	BK	129	
46	BL	135	
47	BM	126	
48	BN	61	
49	BO	89	
50	BP	88	
51	BQ	105	
52	BR	88	
53	BS	93	
54	BT	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	BU	27	<div><div></div><div>4%</div><div>52%</div><div>26%</div><div>11%</div><div>7%</div></div>
56	BV	77	<div><div></div><div>%</div><div>38%</div><div>48%</div><div>13%</div></div>
56	BW	77	<div><div></div><div>27%</div><div>87%</div><div>58%</div><div>10%</div></div>
57	BX	19	<div><div></div><div>5%</div><div>16%</div><div>5%</div><div>74%</div></div>
58	BY	90	<div><div></div><div>7%</div><div>32%</div><div>23%</div><div>7%</div><div>31%</div></div>
59	BZ	405	<div><div></div><div>2%</div><div>32%</div><div>50%</div><div>10%</div><div>7%</div></div>

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 154205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	A7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	A8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 11 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AA	2901	Total	C	N	O	P	0	0	0
			62479	27808	11685	20086	2900			

- Molecule 12 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AC	228	Total	C	N	O	S	0	0	0
			1742	1101	318	319	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	19	ILE	VAL	conflict	UNP Q5SLP7
AC	27	HIS	ARG	conflict	UNP Q5SLP7
AC	127	MET	LEU	conflict	UNP Q5SLP7

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AJ	130	Total	C	N	O		0	0	0
			654	393	130	131				

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L11.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AK	140	Total	C	N	O	0	0	0
			701	420	140	141			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	AR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	AX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AZ	184	Total	C	N	O	S	0	0	1
			1460	932	261	265	2			

- Molecule 34 is a protein called SMALL PROTEIN B SMPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B2	144	Total	C	N	O	S	0	0	0
			1184	754	219	210	1			

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	1504	Total	C	N	O	P	0	0	0
			32330	14391	5994	10442	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1489	A	G	conflict	GB NC_006461
BA	1490	A	C	conflict	GB NC_006461

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	1	MET	-	expression tag	UNP Q5SHN3
BL	2	VAL	-	expression tag	UNP Q5SHN3
BL	3	ALA	-	expression tag	UNP Q5SHN3
BL	4	LEU	-	expression tag	UNP Q5SHN3

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 52 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 53 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 54 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 55 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 56 is a RNA chain called E-SITE or P-SITE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
56	BW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 57 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BX	5	Total	C	N	O	P	0	0	0
			104	48	19	33	4			

- Molecule 58 is a RNA chain called TMRNA DELA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BY	62	Total	C	N	O	P	0	0	0
			1305	582	233	429	61			

- Molecule 59 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BZ	378	Total	C	N	O	S	0	0	1
			2929	1854	510	553	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	181	GLU	GLN	conflict	UNP Q5SHN6
BZ	184	LYS	ARG	conflict	UNP Q5SHN6
BZ	189	LYS	ARG	conflict	UNP Q5SHN6
BZ	264	LYS	ARG	conflict	UNP Q5SHN6
BZ	288	LEU	VAL	conflict	UNP Q5SHN6
BZ	322	ILE	VAL	conflict	UNP Q5SHN6
BZ	336	THR	SER	conflict	UNP Q5SHN6
BZ	354	ARG	GLN	conflict	UNP Q5SHN6
BZ	357	GLN	PRO	conflict	UNP Q5SHN6

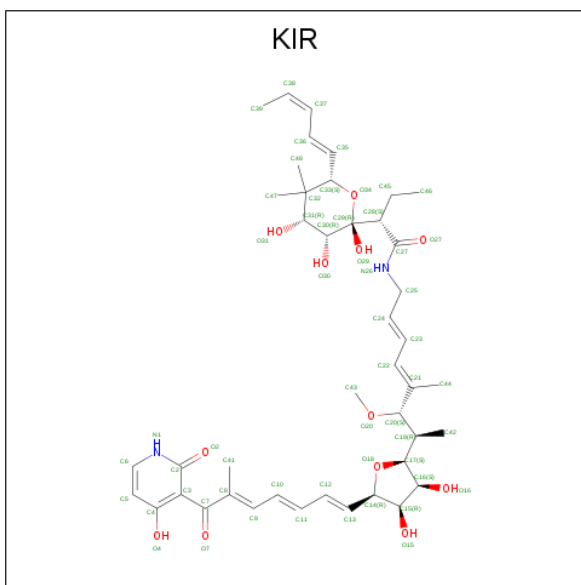
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	A9	1	Total Zn 1 1	0	0
60	BN	1	Total Zn 1 1	0	0
60	BD	1	Total Zn 1 1	0	0

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

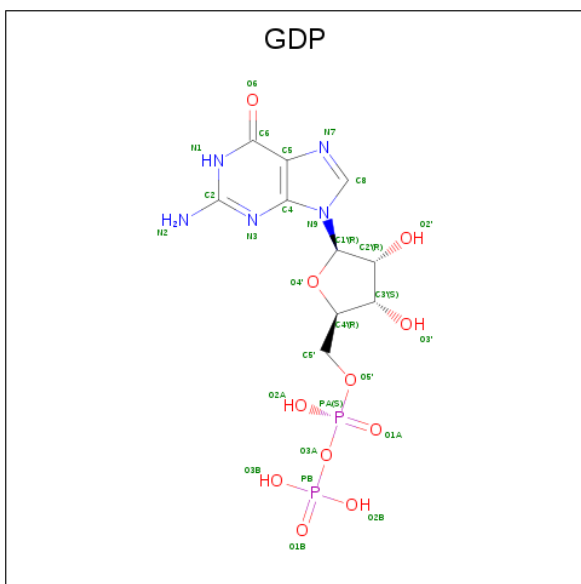
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BZ	1	Total Mg 1 1	0	0
61	AA	1	Total Mg 1 1	0	0

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: C<sub>43</sub>H<sub>60</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
62	BZ	1	Total	C	N	O	0	0
			57	43	2	12		

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



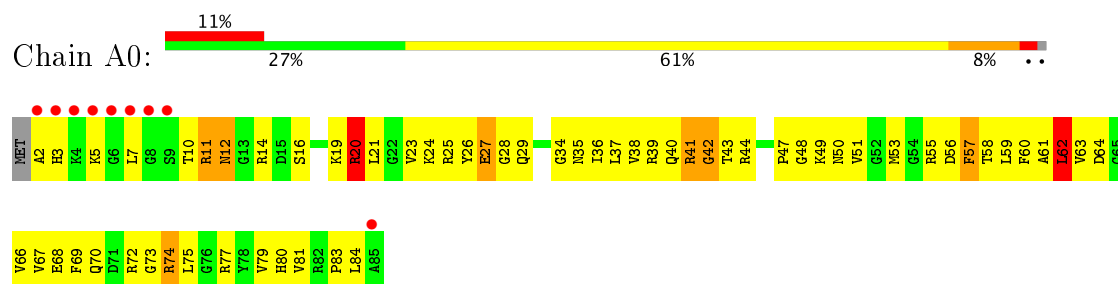
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
63	BZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		



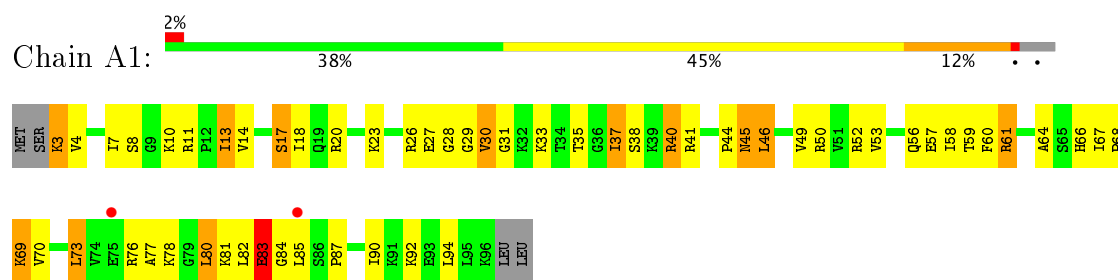
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

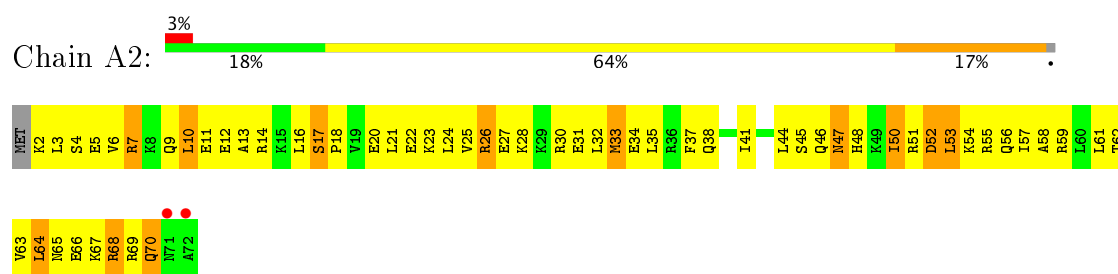
#### • Molecule 1: 50S RIBOSOMAL PROTEIN L27



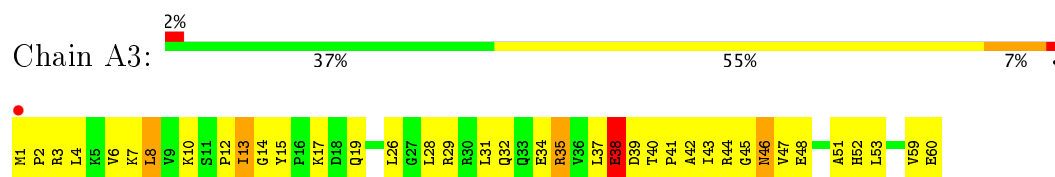
#### • Molecule 2: 50S RIBOSOMAL PROTEIN L28



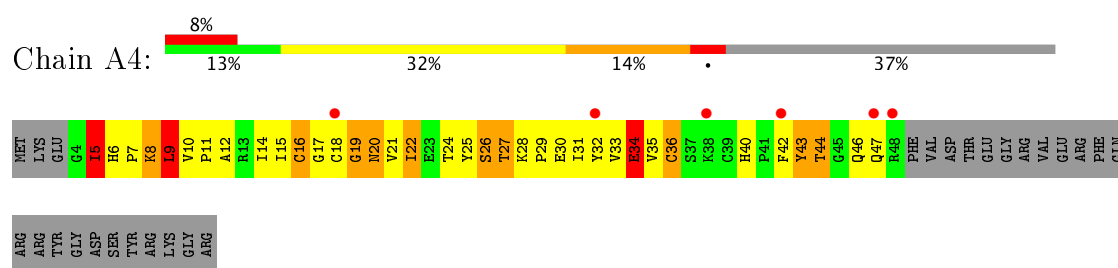
#### • Molecule 3: 50S RIBOSOMAL PROTEIN L29



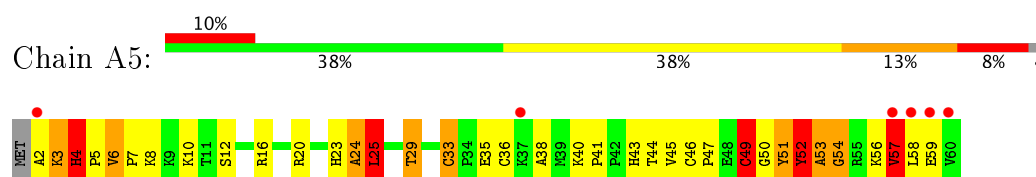
#### • Molecule 4: 50S RIBOSOMAL PROTEIN L30



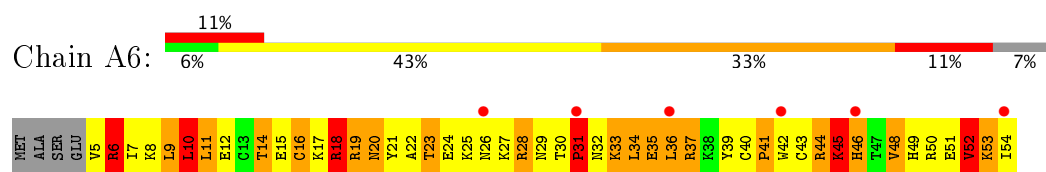
#### • Molecule 5: 50S RIBOSOMAL PROTEIN L31



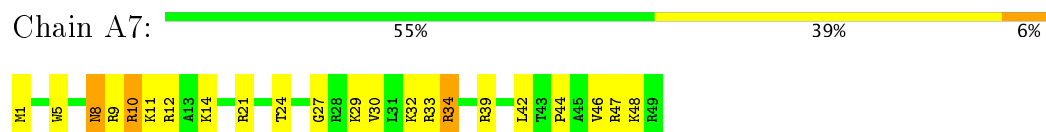
- Molecule 6: 50S RIBOSOMAL PROTEIN L32



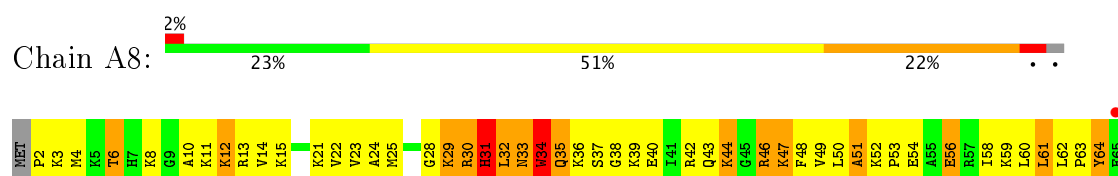
- Molecule 7: 50S RIBOSOMAL PROTEIN L33



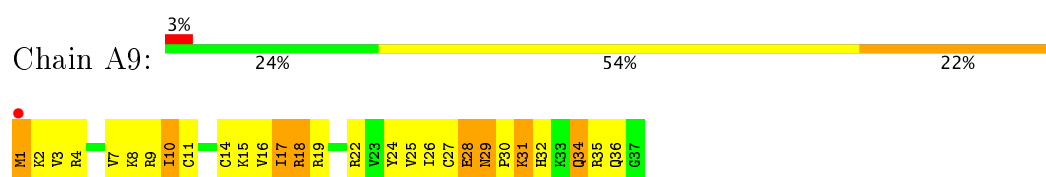
- Molecule 8: 50S RIBOSOMAL PROTEIN L34



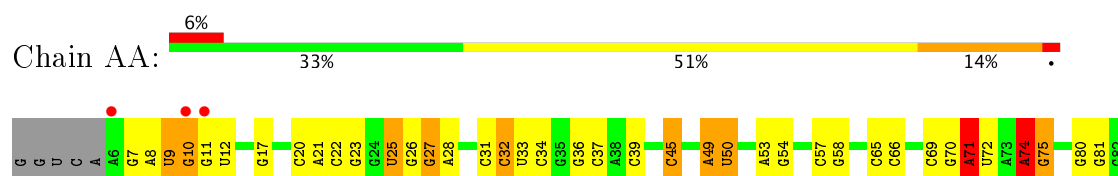
- Molecule 9: 50S RIBOSOMAL PROTEIN L35



- Molecule 10: 50S RIBOSOMAL PROTEIN L36

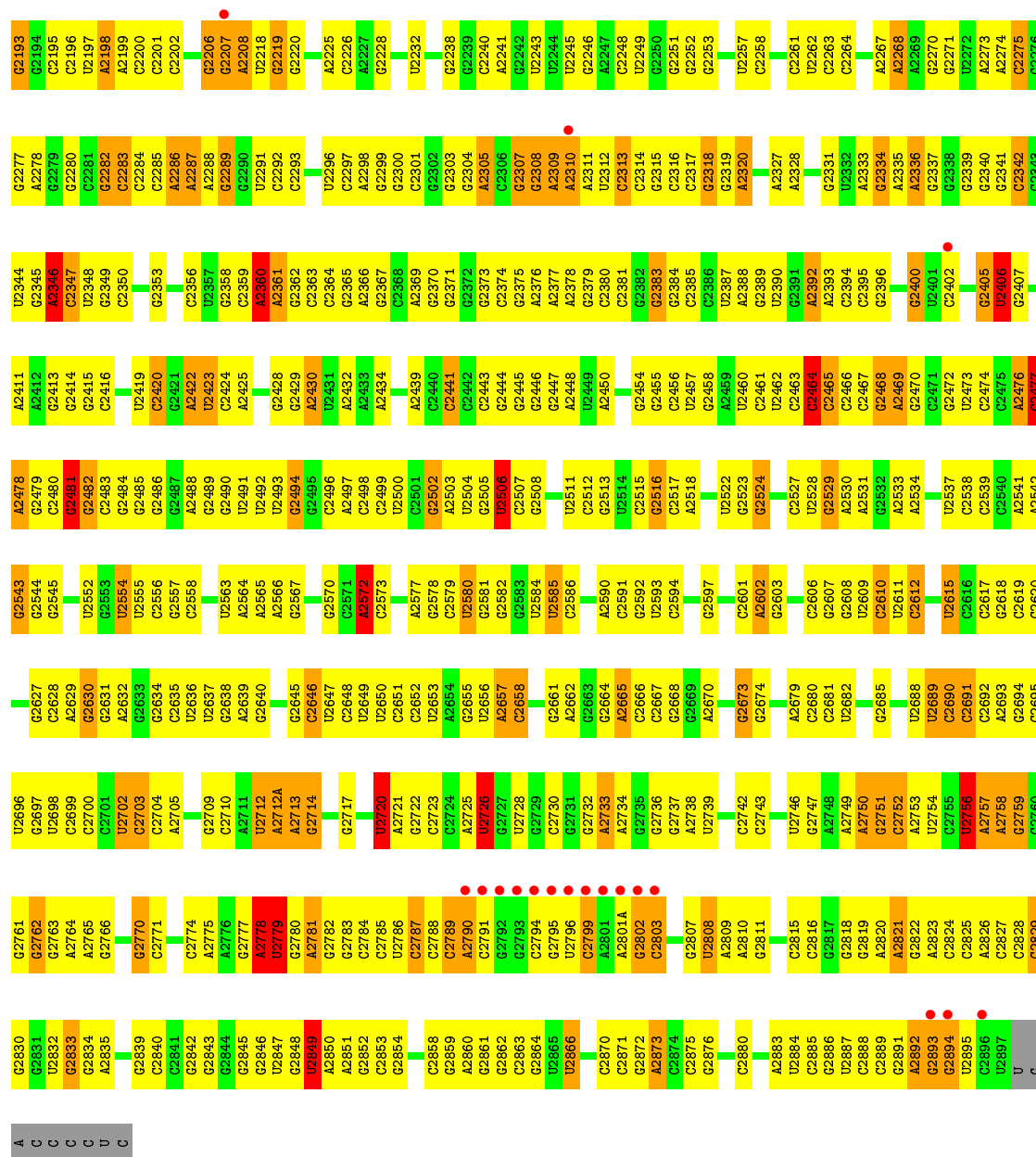


- Molecule 11: 23S ribosomal RNA



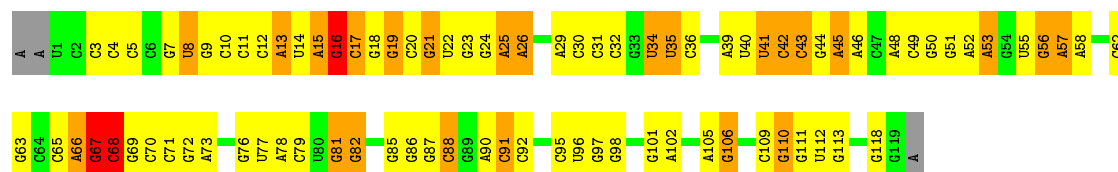
U1033	G962	C888	G615	G551	G406	A332	U271Y	C236	U158	G83
G1034	U963	C889	G616	U554	A479	G333	U272A	C237	G171	A84
U1035	C964	A890	G618	U555	A480	C334	G272B	U239	G172	
	G965	U826	G619	G481	G410	C335	G272C	G240	G173	G88
C1038	U969	C993	G620	A482	G411	C336	G272D	A241	G174	G89
G1039	U970	U827	A621	U557	A412	C337	G272E	G242	G175	G90
C1040	A829	G622	G623	G558	C413			G243	G176	G91
G971	G830	G624	U562	U563	G414	A340	C272H	G244	G177	A92
G1042	G831	G625	G563	G564	A415	G341	U272I	G245	G178	G93
G832	U833	U626	C564	U565	G418	G342	G272J	G246	G94	G94A
G1043	G832	G627	U566	G493	G419	C343	G272K	G247	G95	G95
G974	U833	A627	A567	G494	C420	G352	G272L	G248	A181	
G975	G833	G628	U568	G495	A421	G353	A276	G249	G96	G97
G975A	U833	A675	G629	G496	A422	G354	C277	G250	G98	G98
		G674	G630	U569	G423	U358	A278	A251	U185	
		A676	A631	G497	A424	G359	G280	G252	U186	G99
		G675	G632	A498	G425	U358	G281	G253	G100	G100
		A676	G633	A571	G426	G360		G254	G102	G102
		G680	G634	A572	A427	G361	U284	G255	U104	U104
		G681	G635	G573	U428	U362	C285	A256	C105	C105
		G682	G636	A574	A429	G363	C286	A257	C106	C106
		G683	U639	A575	U430	G364	C287	G258	U107	U107
		G684	G640	G576	C435	G365	C288	G259	G108	G108
		G685	G641	G577	A436	G366		G260	G109	G109
		G686	G642	A578	G437	G367		G261	G110	G110
		G687	G643	G579	A438	G368	C291	A262	A111	A111
		G688	G644	G580	G439	G369	C292	G263	U112	U112
		G689	G645	G581	G440	C36A	U293	G264	U113	U113
		G690	G646	G582	U441			C265	C116	C116
		G691	A646	G583	A442	A371	C296	A266	G117	G117
		G692	G647	A586	G443	G372	C297	G267	A204	A204
		G693	G648	C587	C444	U373	C298	C268	G205	G205
		G694	G649	U588	G445	A374	A299	G269	U206	U206
		G695	G650	C589	U446		A300	A270	A207	A207
		G696	G651	G590	A447	C378	G301	A271	G208	G208
		G697	G652	C591	U448	G379	C302	A272	G209	G209
		G698	G653	G592	U449	U380	U303	A273	C210	C210
		G699	A654	G593	U450	G381		A274	A211	A211
		G700	G655	U594	G451	U382	U306	A275	G212	G212
		G701	G656	G602	G452	U383	G307	A276	G213	G213
		G702	G657	A603	C453	U384	G308	U271E	G214	G214
		G703	G658	G604	C454	C385	G309	C271F	G215	G215
		G704	G659	U597	C455	G386	A310	G271G	G216	G216
		G705	G660	G598	A456	U387	A311	C271H	G139A	G139A
		G706	G661	G599	U457	G388		G271I	G140	G140
		G707	G662	G605	U458	G389	A314	A221	A141	A141
		G708	G663	A606	G463	A390	G315	A222	C142A	C142A
		G709	G664	G607	U464	C391	A320	G271M	G143	G143
		G710	G665	U606	G465	G392	G321	U271N	C143A	C143A
		G711	G666	U607	A466	C393	A322	C271O	G144	G144
		G712	G667	A608	G467	A394	G323	C271P	U147	U147
		G713	G668	G609	G468	U395	A324	G271Q	G226	G226
		G714	G669	A609	G469	G396	G325	G271R	A228	A228
		G715	G670	G610	A470	G397	G326	G271S	G230	G230
		G716	G671	C611	C541	G398	G327	C271T	C231	C231
		G717	G672	G612	C542		U328	G271U	G232	G232
		G718	G673	G613	C543	A402	G329	G271V	A233	A233
		G719	G674	U614	G472	U403	A330	G271W	C234	C234
		G720	G675	U615	G473	G404	A331	G271X	U235	U235
		G721	G676	U616	G474					
		G722	G677	U617	G475					
		G723	G678	U618	G476					
		G724	G679	U619	G477					
		G725	G680	U620	G478					
		G726	G681	U621	G479					
		G727	G682	U622	G480					
		G728	G683	U623	G481					
		G729	G684	U624	G482					
		G730	G685	U625	G483					
		G731	G686	U626	G484					
		G732	G687	U627	G485					
		G733	G688	U628	G486					
		G734	G689	U629	G487					
		G735	G690	U630	G488					
		G736	G691	U631	G489					
		G737	G692	U632	G490					
		G738	G693	U633	G491					
		G739	G694	U634	G492					
		G740	G695	U635	G493					
		G741	G696	U636	G494					
		G742	G697	U637	G495					
		G743	G698	U638	G496					
		G744	G699	U639	G497					
		G745	G700	U640	G498					
		G746	G701	U641	G499					
		G747	G702	U642	G500					
		G748	G703	U643	G501					
		G749	G704	U644	G502					
		G750	G705	U645	G503					
		G751	G706	U646	G504					
		G752	G707	U647	G505					
		G753	G708	U648	G506					
		G754	G709	U649	G507					
		G755	G710	U650	G508					
		G756	G711	U651	G509					
		G757	G712	U652	G510					
		G758	G713	U653	G511					
		G759	G714	U654	G512					
		G760	G715	U655	G513					
		G761	G716	U656	G514					
		G762	G717	U657	G515					
		G763	G718	U658	G516					
		G764	G719	U659	G517					
		G765	G720	U660	G518					
		G766	G721	U661	G519					
		G767	G722	U662	G520					
		G768	G723	U663	G521					
		G769	G724	U664	G522					
		G770	G725	U665	G523					
		G771	G726	U666	G524					
		G772	G727	U667	G525					
		G773	G728	U668	G526					
		G774	G729	U669	G527					
		G775	G730	U670	G528					
		G776	G731	U671	G529					
		G777	G732	U672	G530					
		G778	G733	U673	G531					
		G779	G734	U674	G532					
		G780	G735	U675	G533					
		G781	G736	U676	G534					
		G782	G737	U677	G535					
		G783	G738	U678	G536					
		G784	G739	U679	G537					
		G785	G740	U680	G538					
		G786	G741	U681	G539					
		G787	G742	U682	G540					
		G788	G743	U683	G541					
		G789	G744	U684	G542					
		G790	G745	U685	G543					
		G791	G746	U686	G544					
		G792	G747	U687	G545					
		G793	G748	U688	G546					
		G794	G749	U689	G547					
		G795	G750	U690	G548					
		G796	G751	U691	G549					
		G797	G752	U692	G550					
		G798	G753	U693	G551					
		G799	G754	U694	G552					
		G800	G755	U695	G553					
		G801	G756	U696	G554					
		G802	G757	U697	G555					
		G803	G758	U698	G556					
		G804	G759	U699	G557					
		G805	G760	U700	G558					
		G806	G761	U701	G559					
		G807	G762	U702	G560					
		G808	G763	U703	G561					
		G809	G764	U704	G562					
		G810	G765	U705	G563					
		G811	G766	U706	G564					
		G812	G767	U707	G565					
		G813	G768	U708	G566					
		G814	G769	U709	G567					
		G815	G770	U710	G568					
		G816	G771	U711	G569					
		G817	G772	U712	G570					
		G818	G773	U713	G571					
		G819	G774	U714	G572					
		G820	G775	U715	G573					
		G821	G776	U716	G574					
		G822	G777	U717	G575					
		G823	G778	U718	G576					
		G824	G779	U719	G577					
		G825	G780	U720	G578					
		G826	G781	U721	G579					
		G827	G782	U722	G580					
		G828	G783	U723	G581					
		G829	G784	U724	G582					
		G830	G785	U725	G583					





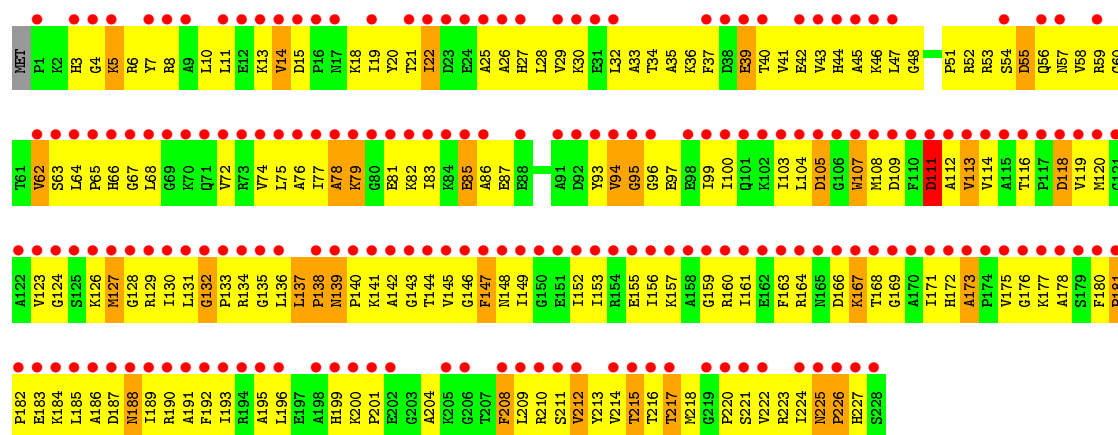
### • Molecule 12: 5S ribosomal RNA

Chain AB: 27% 48% 20%

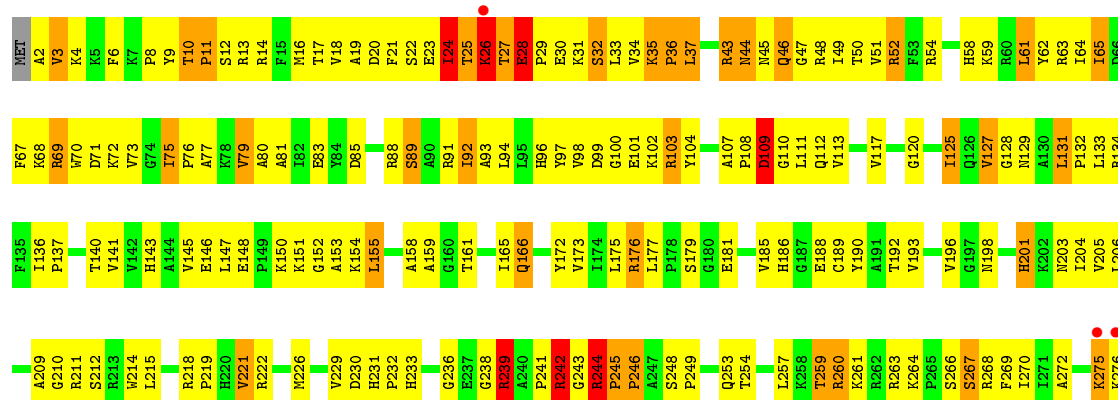


### • Molecule 13: 50S RIBOSOMAL PROTEIN L1

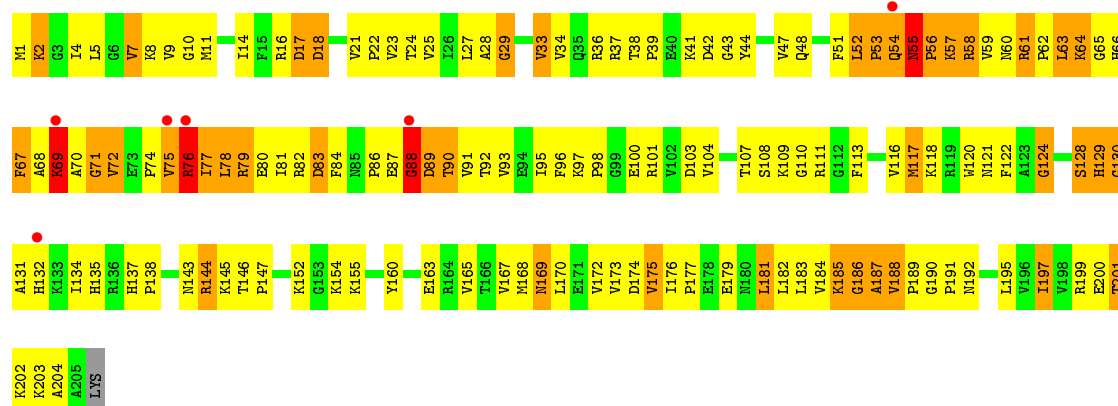
Chain AC: 23% 85% 62% 14%



• Molecule 14: 50S RIBOSOMAL PROTEIN L2

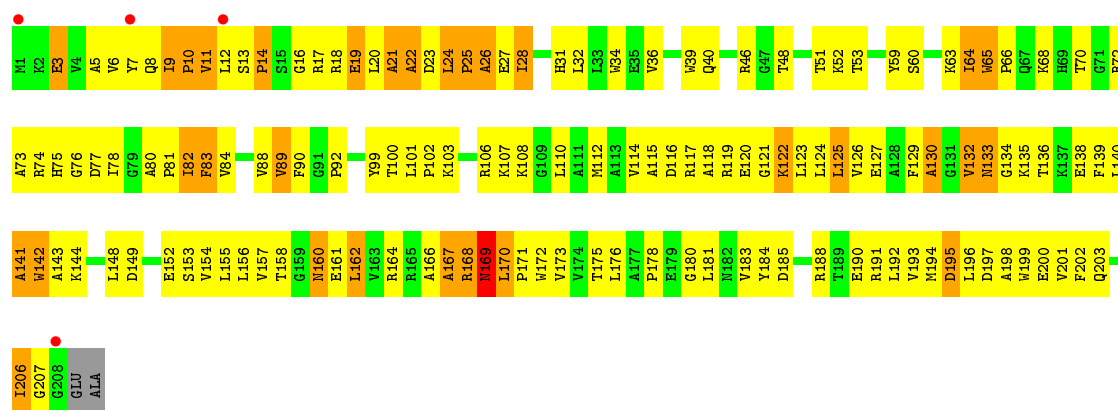


• Molecule 15: 50S RIBOSOMAL PROTEIN L3

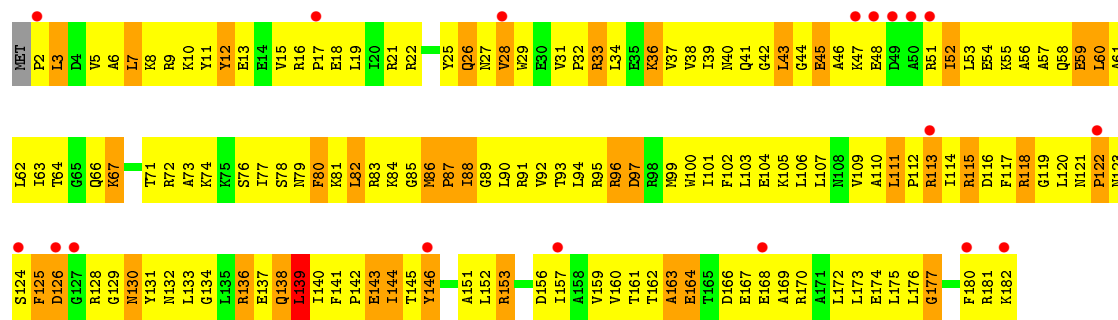


• Molecule 16: 50S RIBOSOMAL PROTEIN L4

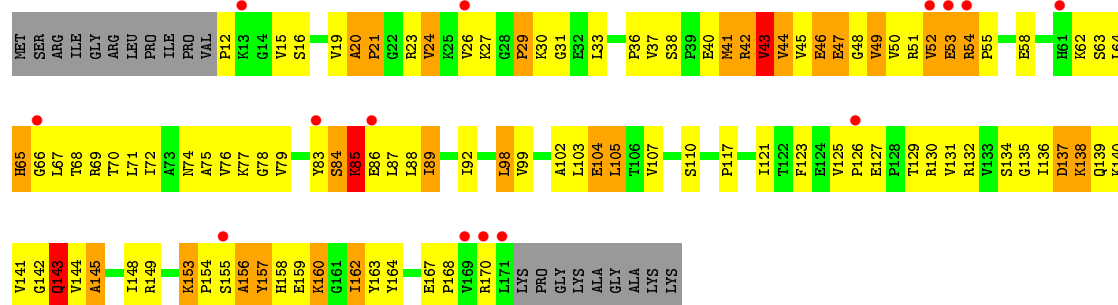




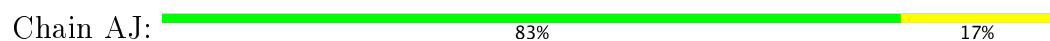
• Molecule 17: 50S RIBOSOMAL PROTEIN L5



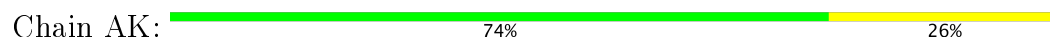
• Molecule 18: 50S RIBOSOMAL PROTEIN L6



• Molecule 19: 50S RIBOSOMAL PROTEIN L10



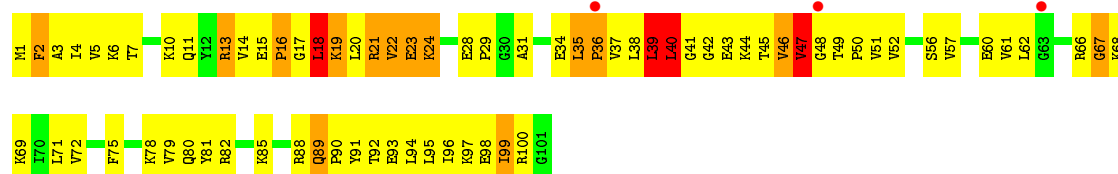
• Molecule 20: 50S RIBOSOMAL PROTEIN L11



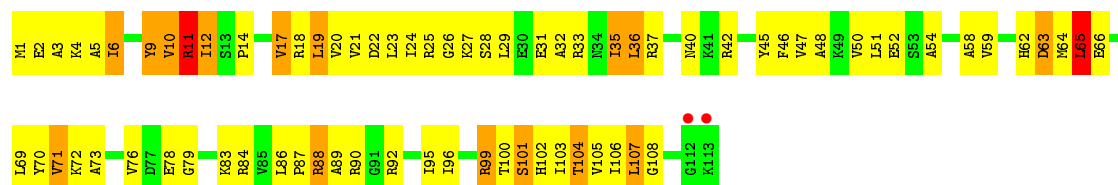




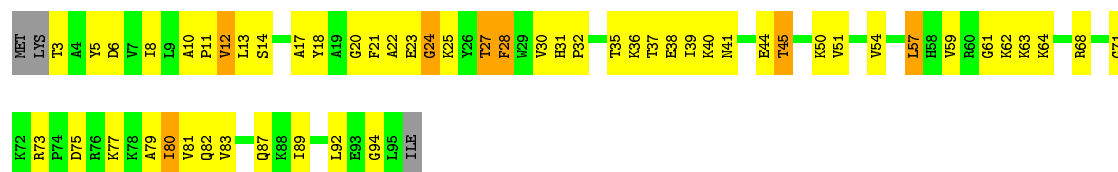




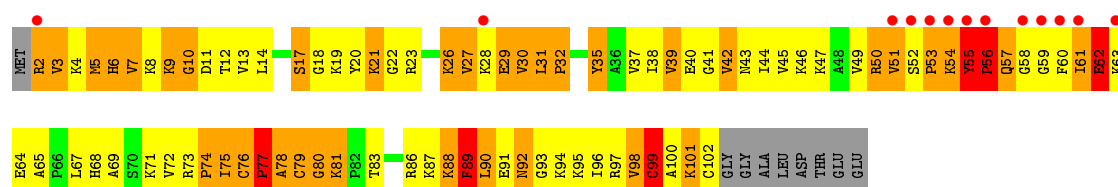
• Molecule 30: 50S RIBOSOMAL PROTEIN L22



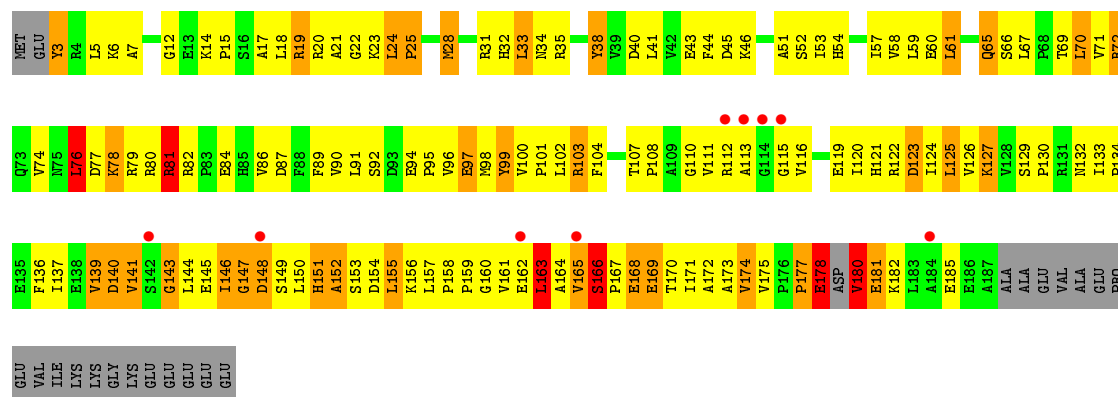
• Molecule 31: 50S RIBOSOMAL PROTEIN L23



• Molecule 32: 50S RIBOSOMAL PROTEIN L24



• Molecule 33: 50S RIBOSOMAL PROTEIN L25

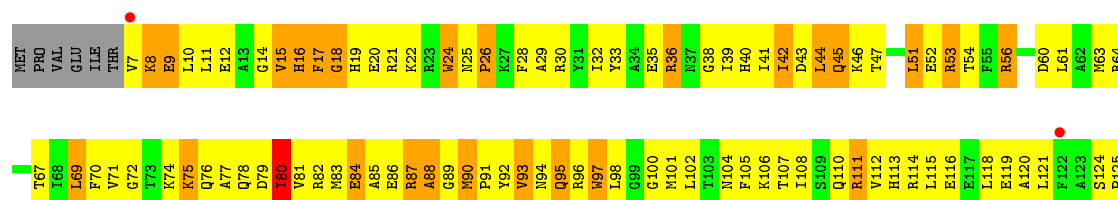


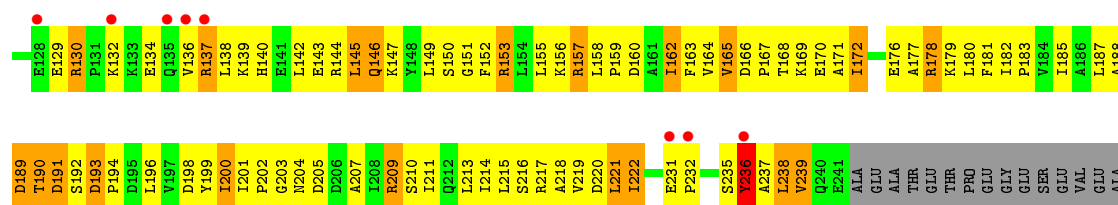
Chain B2:

15% 22% 56% 19%

M1 A2 P3 V4 E6 N7 R8 A10 H12 D13 Y14 E15 I16 L17 E18 A22 G23 I24 A25 L26 K27 G28 T29 V30 E31 K32 S33 L34 R35 K38 V39 D40 F41 T42 G43 S44 F45 A46 R47 F48 E49 D50 G51 E52 L53 Y54 L55 E56 N57 L58 Y59 I60 Y63 E64 K65 G66 S67 Y68 A69 W70 V71 D72 R73 P74 R75 K76 R77 K78 L79 L80 L81 H82 K83 H84 E85 L86 R87 R88 L89 L90 K91 K92 V93 E94 Q95 K96 G97 L98 T99 L100 V101 P102 L103 K104 I105 Y106 F107 R110 G111 Y112 A113 K114 V115 L116 L117 G118 L119 A120 R121 G122 K123 K124 A125 Y126 R129 R130 E131 D132 K133 K134 E135 A136 V137 R138 R139 L141 E142 E143 L144

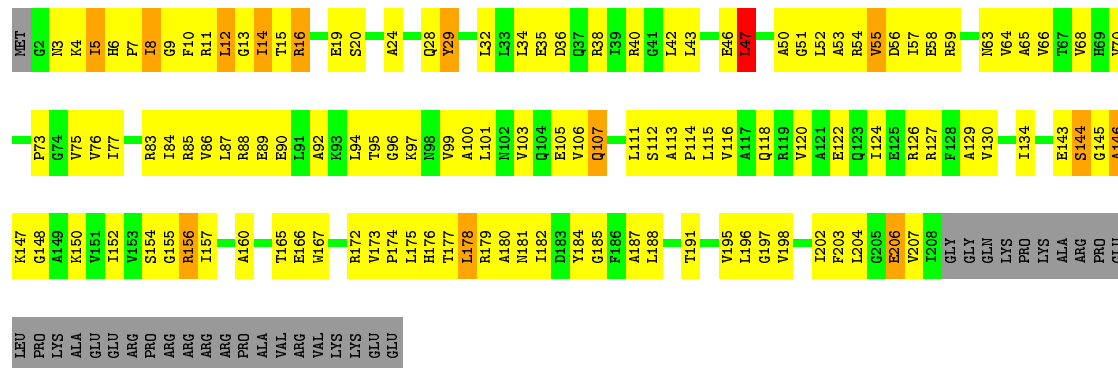
[illegible]





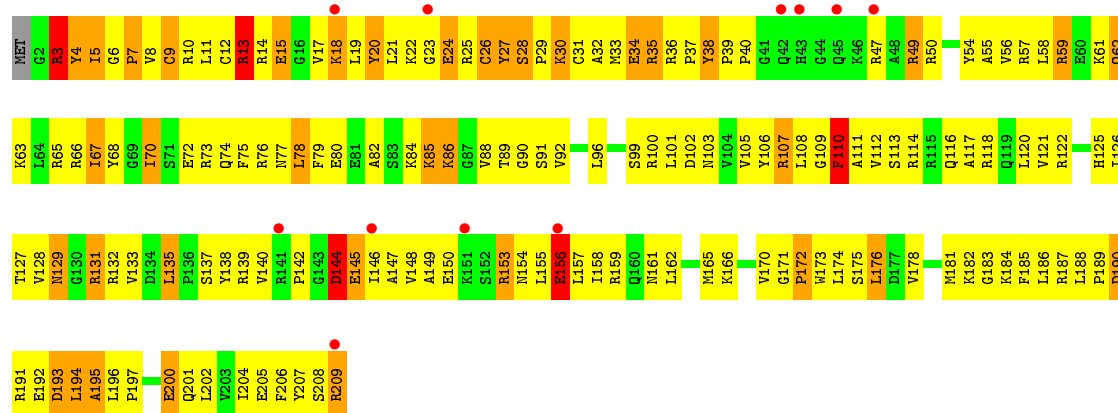
• Molecule 37: 30S RIBOSOMAL PROTEIN S3

Chain BC: 34% 46% 5% 13%



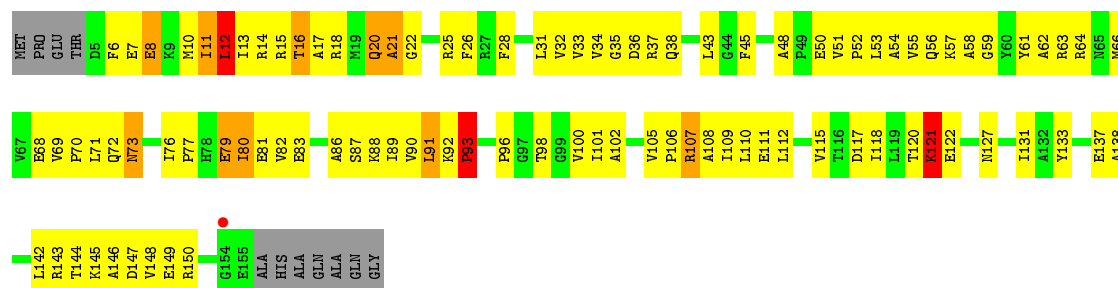
• Molecule 38: 30S RIBOSOMAL PROTEIN S4

Chain BD: 5% 23% 56% 18%

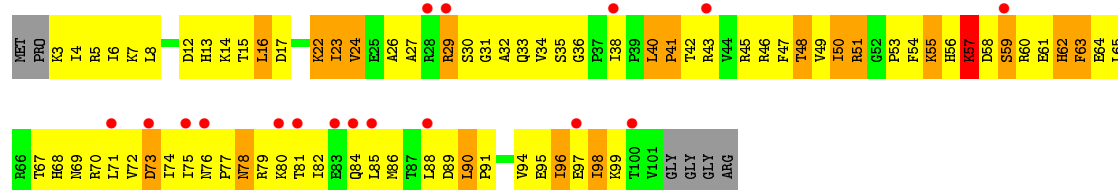


• Molecule 39: 30S RIBOSOMAL PROTEIN S5

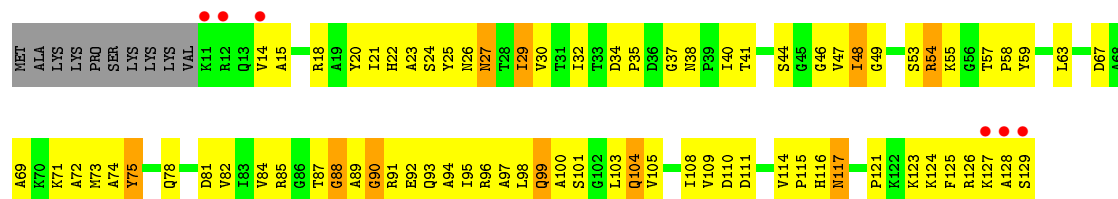
Chain BE: 33% 52% 6% 7%



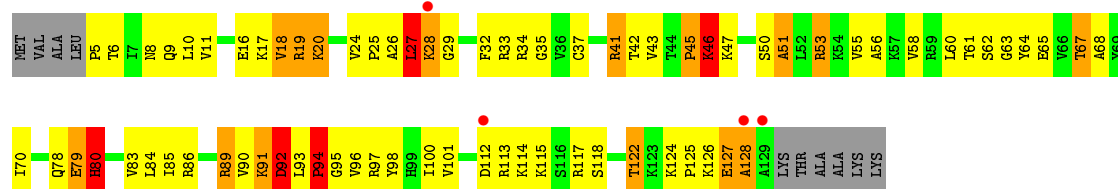




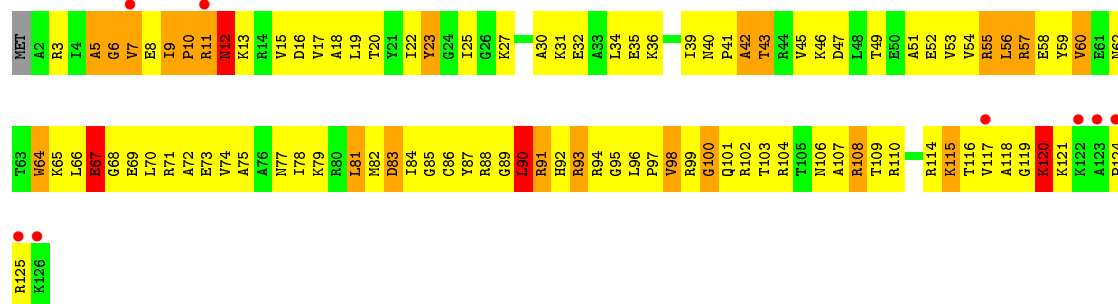
• Molecule 45: 30S RIBOSOMAL PROTEIN S11



• Molecule 46: 30S RIBOSOMAL PROTEIN S12



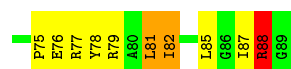
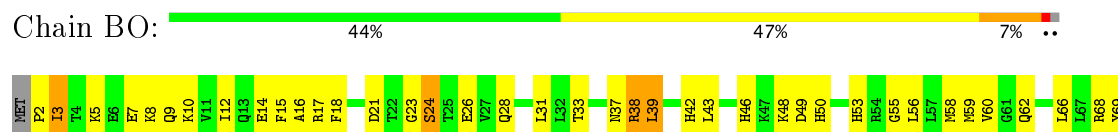
• Molecule 47: 30S RIBOSOMAL PROTEIN S13



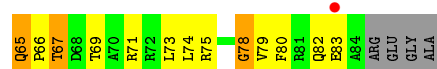
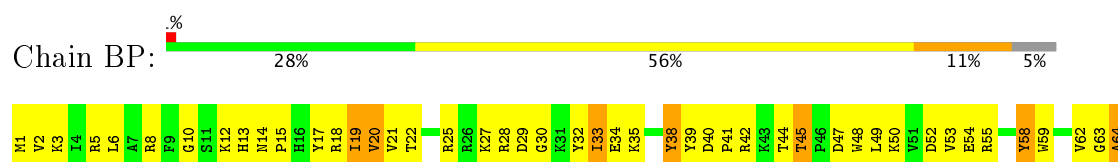
• Molecule 48: 30S RIBOSOMAL PROTEIN S14



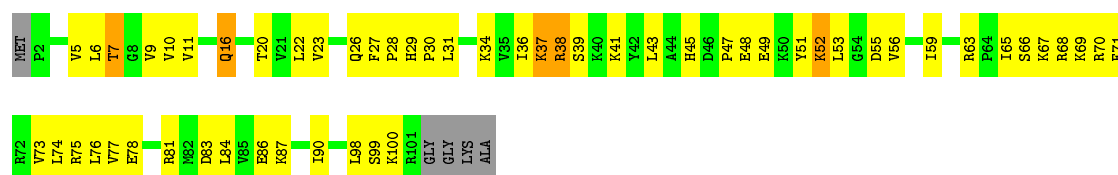
• Molecule 49: 30S RIBOSOMAL PROTEIN S15



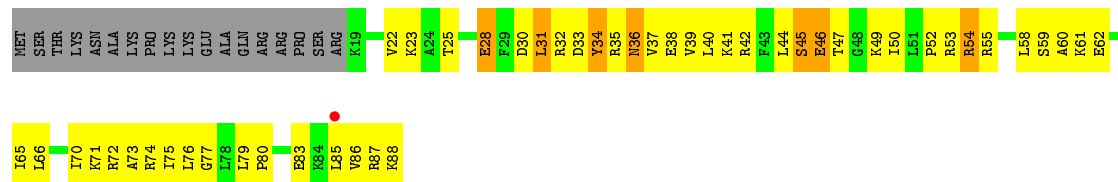
• Molecule 50: 30S RIBOSOMAL PROTEIN S16



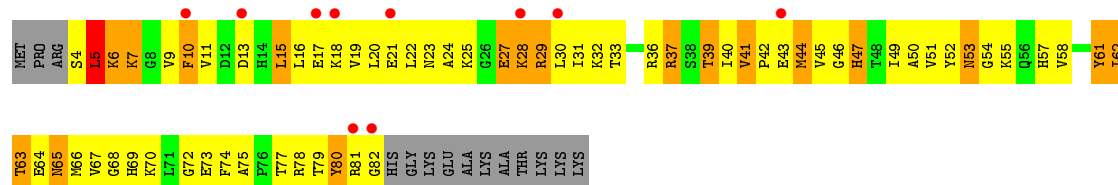
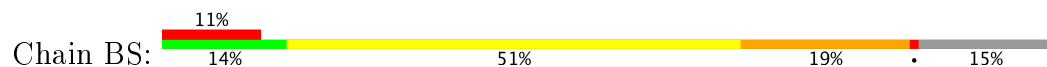
• Molecule 51: 30S RIBOSOMAL PROTEIN S17



• Molecule 52: 30S RIBOSOMAL PROTEIN S18



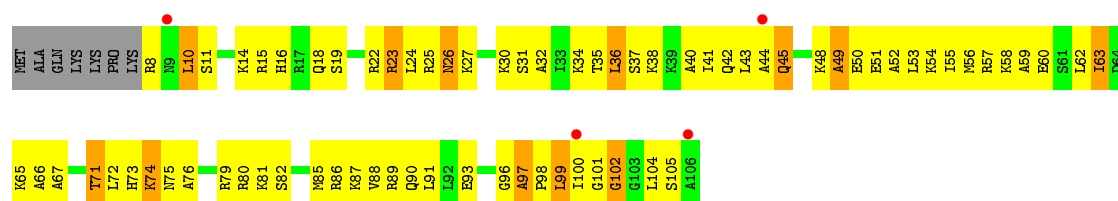
• Molecule 53: 30S RIBOSOMAL PROTEIN S19



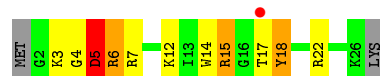
• Molecule 54: 30S RIBOSOMAL PROTEIN S20



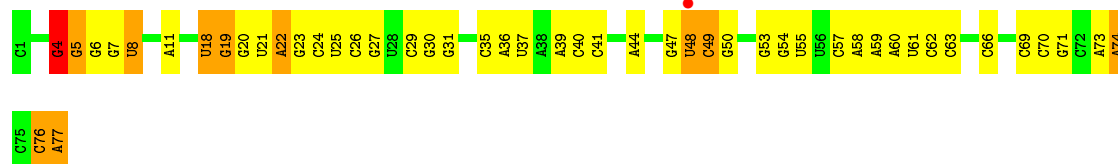




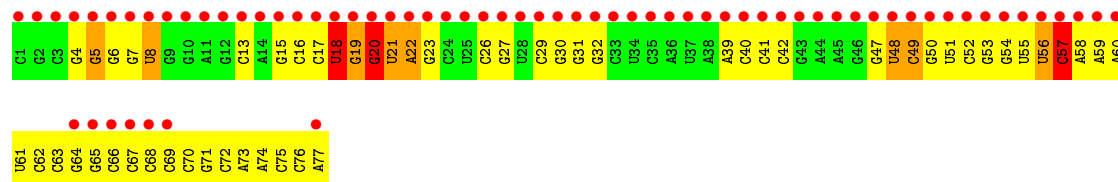
• Molecule 55: 30S RIBOSOMAL PROTEIN THX



• Molecule 56: E-SITE or P-SITE TRNA FMET



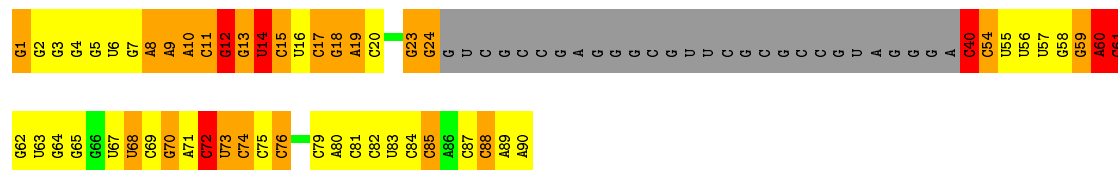
• Molecule 56: E-SITE or P-SITE TRNA FMET



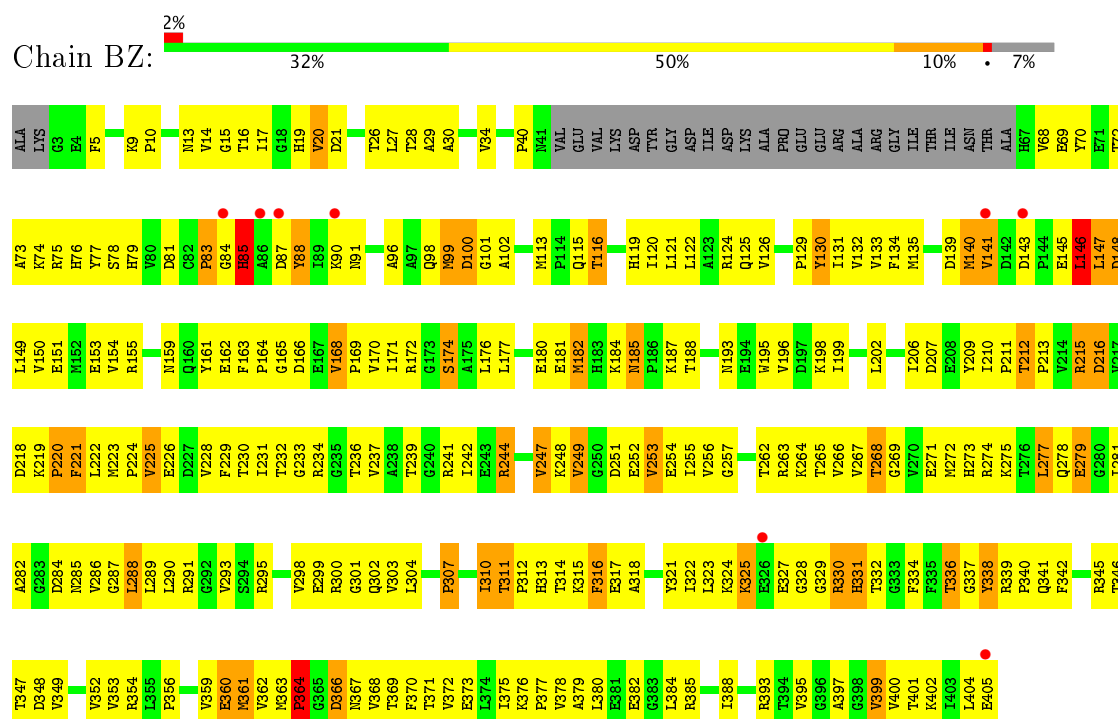
• Molecule 57: MRNA



• Molecule 58: TMRNA DELA



• Molecule 59: ELONGATION FACTOR TU



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.17Å 290.76Å 250.65Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.10) 97.4 (49.68-3.10)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.230 , 0.270 0.229 , 0.269	Depositor DCC
$R_{free}$ test set	24443 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	154205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, KIR, ZN, MG

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	A0	0.46	0/671	0.72	1/892 (0.1%)
2	A1	0.46	0/739	0.74	0/983
3	A2	0.43	0/600	0.73	0/793
4	A3	0.45	0/473	0.70	0/636
5	A4	0.47	0/350	0.62	0/476
6	A5	0.53	0/473	0.86	1/639 (0.2%)
7	A6	0.69	0/440	0.99	1/586 (0.2%)
8	A7	0.49	0/427	0.69	0/563
9	A8	0.59	0/516	0.94	1/681 (0.1%)
10	A9	0.48	0/310	0.75	0/407
11	AA	0.57	5/69979 (0.0%)	0.81	83/109249 (0.1%)
12	AB	0.44	0/2853	0.79	2/4451 (0.0%)
13	AC	0.46	1/1775 (0.1%)	0.65	0/2392
14	AD	0.53	0/2195	0.83	2/2955 (0.1%)
15	AE	0.54	0/1597	0.84	1/2155 (0.0%)
16	AF	0.45	0/1659	0.78	1/2246 (0.0%)
17	AG	0.38	0/1499	0.69	1/2016 (0.0%)
18	AH	0.44	0/1246	0.77	0/1684
21	AN	0.49	0/1132	0.82	0/1527
22	AO	0.50	0/943	0.77	1/1269 (0.1%)
23	AP	0.54	0/1131	1.06	6/1504 (0.4%)
24	AQ	0.51	0/1143	0.74	0/1527
25	AR	0.45	0/974	0.82	1/1302 (0.1%)
26	AS	0.43	0/779	0.75	0/1038
27	AT	0.54	0/1156	0.88	2/1544 (0.1%)
28	AU	0.56	0/975	0.80	0/1297
29	AV	0.49	0/790	0.86	1/1057 (0.1%)
30	AW	0.54	0/907	0.83	2/1216 (0.2%)
31	AX	0.52	0/740	0.74	0/995
32	AY	0.59	0/789	0.95	3/1053 (0.3%)
33	AZ	0.47	0/1492	0.76	0/2026
34	B2	0.49	0/1203	0.71	1/1606 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	BA	0.48	1/36192 (0.0%)	0.78	39/56489 (0.1%)
36	BB	0.46	0/1936	0.72	0/2611
37	BC	0.43	0/1637	0.69	0/2207
38	BD	0.40	0/1733	0.68	0/2318
39	BE	0.49	0/1163	0.72	0/1566
40	BF	0.43	0/856	0.68	1/1154 (0.1%)
41	BG	0.36	0/1276	0.61	0/1709
42	BH	0.45	0/1136	0.75	0/1527
43	BI	0.41	0/1029	0.67	0/1378
44	BJ	0.42	0/808	0.69	0/1087
45	BK	0.39	0/900	0.65	0/1213
46	BL	0.45	0/987	0.74	0/1322
47	BM	0.38	0/999	0.71	0/1338
48	BN	0.45	0/501	0.75	0/664
49	BO	0.45	0/745	0.70	0/992
50	BP	0.42	0/717	0.65	0/965
51	BQ	0.42	0/837	0.67	0/1119
52	BR	0.42	0/579	0.70	0/768
53	BS	0.45	0/643	0.67	1/867 (0.1%)
54	BT	0.37	0/765	0.65	0/1007
55	BU	0.48	0/213	0.63	0/279
56	BV	0.45	0/1832	0.79	1/2855 (0.0%)
56	BW	0.45	0/1832	0.81	3/2855 (0.1%)
57	BX	0.71	0/116	0.89	0/179
58	BY	0.80	4/1454 (0.3%)	0.97	5/2258 (0.2%)
59	BZ	0.42	0/2986	0.69	0/4050
All	All	0.52	11/165828 (0.0%)	0.79	161/247542 (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
11	AA	9	95
12	AB	0	3
14	AD	0	1
30	AW	0	1
33	AZ	0	1
35	BA	4	40
56	BV	0	1
56	BW	0	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
58	BY	0	3
All	All	13	148

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BY	12	G	C2-N2	-13.61	1.21	1.34
11	AA	761	A	C5-C6	-11.47	1.30	1.41
58	BY	1	G	OP3-P	-6.81	1.52	1.61
11	AA	761	A	C6-N6	-6.64	1.28	1.33
11	AA	1332	G	N9-C4	-6.30	1.32	1.38

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	1992	G	C2'-C3'-O3'	10.04	131.59	109.50
35	BA	115	G	C2'-C3'-O3'	9.61	130.64	109.50
11	AA	1786	A	N9-C1'-C2'	9.57	126.44	114.00
11	AA	527	C	O4'-C1'-N1	9.54	115.83	108.20
35	BA	966	G	N9-C1'-C2'	-9.47	101.58	112.00

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	AA	614(C)	A	C3'
11	AA	1300	U	C3'
11	AA	1378	A	C3'
11	AA	1427	A	C3'
11	AA	1799	G	C3'

5 of 148 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AA	122	G	Sidechain
11	AA	25	U	Sidechain
11	AA	27	G	Sidechain
11	AA	50	U	Sidechain
11	AA	90	U	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	662	0	688	113	0
2	A1	732	0	808	72	0
3	A2	598	0	653	74	0
4	A3	468	0	523	35	0
5	A4	341	0	339	67	0
6	A5	459	0	480	71	0
7	A6	433	0	461	148	0
8	A7	419	0	467	30	0
9	A8	508	0	576	97	0
10	A9	307	0	335	40	0
11	AA	62479	0	31495	2218	0
12	AB	2551	0	1295	109	0
13	AC	1742	0	1794	315	0
14	AD	2145	0	2234	279	0
15	AE	1564	0	1629	224	0
16	AF	1624	0	1677	194	0
17	AG	1474	0	1535	276	0
18	AH	1223	0	1282	159	0
19	AJ	654	0	142	11	0
20	AK	701	0	163	25	0
21	AN	1105	0	1180	160	0
22	AO	933	0	996	95	0
23	AP	1114	0	1187	270	0
24	AQ	1122	0	1179	154	0
25	AR	960	0	1021	136	0
26	AS	771	0	832	122	0
27	AT	1142	0	1202	267	0
28	AU	958	0	1015	128	0
29	AV	779	0	852	147	0
30	AW	896	0	953	83	0
31	AX	726	0	778	77	0
32	AY	776	0	870	193	0
33	AZ	1460	0	1488	183	0
34	B2	1184	0	1235	205	0
35	BA	32330	0	16318	1299	0
36	BB	1901	0	1951	255	0
37	BC	1613	0	1677	152	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	1703	0	1764	264	0
39	BE	1147	0	1207	135	0
40	BF	843	0	857	69	0
41	BG	1257	0	1296	103	0
42	BH	1116	0	1177	77	0
43	BI	1011	0	1043	155	0
44	BJ	795	0	840	176	0
45	BK	885	0	904	83	0
46	BL	971	0	1057	105	0
47	BM	988	0	1059	186	0
48	BN	492	0	529	90	0
49	BO	734	0	771	61	0
50	BP	701	0	720	70	0
51	BQ	824	0	891	54	0
52	BR	574	0	644	62	0
53	BS	630	0	652	103	0
54	BT	763	0	861	83	0
55	BU	209	0	221	14	0
56	BV	1640	0	837	44	0
56	BW	1640	0	837	160	0
57	BX	104	0	55	4	0
58	BY	1305	0	663	87	0
59	BZ	2929	0	2941	341	0
60	A9	1	0	0	0	0
60	BD	1	0	0	0	0
60	BN	1	0	0	0	0
61	AA	1	0	0	0	0
61	BZ	1	0	0	0	0
62	BZ	57	0	58	7	0
63	BZ	28	0	12	2	0
All	All	154205	0	105206	9942	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 38.

The worst 5 of 9942 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)
38:BD:20:TYR:HA	38:BD:26:CYS:SG	1.82	1.19
14:AD:44:ASN:HB3	14:AD:49:ILE:HA	1.21	1.18
1:A0:40:GLN:HE22	1:A0:43:THR:HA	1.02	1.17

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A6:11:LEU:HD22	7:A6:12:GLU:H	1.08	1.15
13:AC:167:LYS:HB2	56:BW:18:U:H5"	1.18	1.15

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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	82/85 (96%)	62 (76%)	14 (17%)	6 (7%)	1	7
2	A1	92/98 (94%)	80 (87%)	7 (8%)	5 (5%)	2	14
3	A2	69/72 (96%)	47 (68%)	13 (19%)	9 (13%)	0	1
4	A3	58/60 (97%)	46 (79%)	8 (14%)	4 (7%)	1	8
5	A4	43/71 (61%)	23 (54%)	10 (23%)	10 (23%)	0	0
6	A5	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
7	A6	48/54 (89%)	18 (38%)	15 (31%)	15 (31%)	0	0
8	A7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
9	A8	62/65 (95%)	37 (60%)	14 (23%)	11 (18%)	0	0
10	A9	35/37 (95%)	27 (77%)	6 (17%)	2 (6%)	2	12
13	AC	226/229 (99%)	159 (70%)	46 (20%)	21 (9%)	1	4
14	AD	273/276 (99%)	210 (77%)	39 (14%)	24 (9%)	1	5
15	AE	203/206 (98%)	136 (67%)	40 (20%)	27 (13%)	0	1
16	AF	206/210 (98%)	147 (71%)	34 (16%)	25 (12%)	0	2
17	AG	179/182 (98%)	110 (62%)	46 (26%)	23 (13%)	0	1
18	AH	158/180 (88%)	98 (62%)	35 (22%)	25 (16%)	0	0
21	AN	137/140 (98%)	89 (65%)	27 (20%)	21 (15%)	0	0
22	AO	120/122 (98%)	103 (86%)	9 (8%)	8 (7%)	1	8

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AP	144/150 (96%)	74 (51%)	28 (19%)	42 (29%)	0	0
24	AQ	139/141 (99%)	104 (75%)	27 (19%)	8 (6%)	2	12
25	AR	115/118 (98%)	80 (70%)	21 (18%)	14 (12%)	0	2
26	AS	97/112 (87%)	57 (59%)	20 (21%)	20 (21%)	0	0
27	AT	136/146 (93%)	89 (65%)	28 (21%)	19 (14%)	0	1
28	AU	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	6
29	AV	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0	0
30	AW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	7
31	AX	91/96 (95%)	78 (86%)	8 (9%)	5 (6%)	2	13
32	AY	99/110 (90%)	47 (48%)	18 (18%)	34 (34%)	0	0
33	AZ	182/206 (88%)	107 (59%)	40 (22%)	35 (19%)	0	0
34	B2	142/144 (99%)	124 (87%)	14 (10%)	4 (3%)	6	29
36	BB	233/256 (91%)	153 (66%)	55 (24%)	25 (11%)	0	3
37	BC	205/239 (86%)	141 (69%)	49 (24%)	15 (7%)	1	7
38	BD	206/209 (99%)	126 (61%)	52 (25%)	28 (14%)	0	1
39	BE	149/162 (92%)	121 (81%)	21 (14%)	7 (5%)	3	17
40	BF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	15
41	BG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	9
42	BH	136/138 (99%)	120 (88%)	14 (10%)	2 (2%)	12	45
43	BI	125/128 (98%)	73 (58%)	33 (26%)	19 (15%)	0	0
44	BJ	97/105 (92%)	69 (71%)	18 (19%)	10 (10%)	0	3
45	BK	117/129 (91%)	87 (74%)	21 (18%)	9 (8%)	1	6
46	BL	123/135 (91%)	84 (68%)	23 (19%)	16 (13%)	0	1
47	BM	123/126 (98%)	76 (62%)	28 (23%)	19 (15%)	0	0
48	BN	58/61 (95%)	43 (74%)	5 (9%)	10 (17%)	0	0
49	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	4	23
50	BP	82/88 (93%)	53 (65%)	23 (28%)	6 (7%)	1	7
51	BQ	98/105 (93%)	76 (78%)	20 (20%)	2 (2%)	9	37
52	BR	68/88 (77%)	53 (78%)	10 (15%)	5 (7%)	1	7
53	BS	77/93 (83%)	53 (69%)	14 (18%)	10 (13%)	0	1
54	BT	97/106 (92%)	72 (74%)	17 (18%)	8 (8%)	1	6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	5
59	BZ	374/405 (92%)	295 (79%)	58 (16%)	21 (6%)	2	12
All	All	6294/6697 (94%)	4435 (70%)	1170 (19%)	689 (11%)	0	3

5 of 689 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A1	30	VAL
2	A1	83	GLU
3	A2	47	ASN
3	A2	70	GLN
4	A3	13	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	66/67 (98%)	57 (86%)	9 (14%)	4	19
2	A1	78/83 (94%)	63 (81%)	15 (19%)	1	7
3	A2	66/67 (98%)	57 (86%)	9 (14%)	4	19
4	A3	51/52 (98%)	46 (90%)	5 (10%)	9	35
5	A4	39/63 (62%)	30 (77%)	9 (23%)	1	4
6	A5	51/52 (98%)	41 (80%)	10 (20%)	1	7
7	A6	49/52 (94%)	34 (69%)	15 (31%)	0	1
8	A7	41/42 (98%)	35 (85%)	6 (15%)	3	16
9	A8	53/55 (96%)	42 (79%)	11 (21%)	1	6
10	A9	34/34 (100%)	26 (76%)	8 (24%)	1	3
13	AC	180/181 (99%)	164 (91%)	16 (9%)	11	41
14	AD	217/218 (100%)	183 (84%)	34 (16%)	3	13
15	AE	165/166 (99%)	138 (84%)	27 (16%)	2	12
16	AF	165/166 (99%)	150 (91%)	15 (9%)	11	39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AG	155/156 (99%)	135 (87%)	20 (13%)	5	21
18	AH	132/148 (89%)	116 (88%)	16 (12%)	6	24
21	AN	117/119 (98%)	101 (86%)	16 (14%)	4	19
22	AO	100/100 (100%)	88 (88%)	12 (12%)	6	24
23	AP	112/116 (97%)	89 (80%)	23 (20%)	1	6
24	AQ	111/111 (100%)	90 (81%)	21 (19%)	2	7
25	AR	100/101 (99%)	85 (85%)	15 (15%)	3	15
26	AS	77/88 (88%)	67 (87%)	10 (13%)	5	21
27	AT	120/127 (94%)	91 (76%)	29 (24%)	1	3
28	AU	92/94 (98%)	82 (89%)	10 (11%)	7	30
29	AV	82/82 (100%)	72 (88%)	10 (12%)	6	23
30	AW	91/92 (99%)	77 (85%)	14 (15%)	3	14
31	AX	74/78 (95%)	67 (90%)	7 (10%)	10	37
32	AY	84/91 (92%)	69 (82%)	15 (18%)	2	9
33	AZ	161/179 (90%)	132 (82%)	29 (18%)	2	9
34	B2	120/120 (100%)	81 (68%)	39 (32%)	0	0
36	BB	202/220 (92%)	172 (85%)	30 (15%)	3	15
37	BC	160/188 (85%)	149 (93%)	11 (7%)	18	53
38	BD	180/181 (99%)	152 (84%)	28 (16%)	3	13
39	BE	115/123 (94%)	99 (86%)	16 (14%)	4	18
40	BF	90/90 (100%)	76 (84%)	14 (16%)	3	13
41	BG	126/127 (99%)	115 (91%)	11 (9%)	12	43
42	BH	119/119 (100%)	108 (91%)	11 (9%)	11	39
43	BI	98/99 (99%)	87 (89%)	11 (11%)	7	29
44	BJ	88/92 (96%)	74 (84%)	14 (16%)	3	13
45	BK	90/99 (91%)	84 (93%)	6 (7%)	19	54
46	BL	104/111 (94%)	91 (88%)	13 (12%)	5	22
47	BM	99/101 (98%)	84 (85%)	15 (15%)	3	14
48	BN	49/50 (98%)	41 (84%)	8 (16%)	3	12
49	BO	79/80 (99%)	72 (91%)	7 (9%)	11	41
50	BP	72/74 (97%)	64 (89%)	8 (11%)	7	29

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	BQ	94/97 (97%)	89 (95%)	5 (5%)	26	63
52	BR	61/77 (79%)	56 (92%)	5 (8%)	13	45
53	BS	69/80 (86%)	57 (83%)	12 (17%)	2	10
54	BT	76/82 (93%)	68 (90%)	8 (10%)	8	31
55	BU	19/22 (86%)	16 (84%)	3 (16%)	3	13
59	BZ	316/338 (94%)	275 (87%)	41 (13%)	5	21
All	All	5289/5550 (95%)	4537 (86%)	752 (14%)	4	17

5 of 752 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	AT	65	LYS
33	AZ	87	ASP
53	BS	39	THR
27	AT	133	GLU
30	AW	99	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
27	AT	79	HIS
31	AX	87	GLN
51	BQ	16	GLN
28	AU	14	HIS
30	AW	34	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	2900/2915 (99%)	536 (18%)	63 (2%)
12	AB	118/122 (96%)	27 (22%)	4 (3%)
35	BA	1503/1522 (98%)	248 (16%)	56 (3%)
56	BV	76/77 (98%)	12 (15%)	2 (2%)
56	BW	76/77 (98%)	11 (14%)	2 (2%)
57	BX	4/19 (21%)	1 (25%)	0
58	BY	60/90 (66%)	22 (36%)	13 (21%)
All	All	4737/4822 (98%)	857 (18%)	140 (2%)

5 of 857 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	9	U
11	AA	10	G
11	AA	32	C
11	AA	34	C
11	AA	45	C

5 of 140 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	AB	16	G
35	BA	266	G
58	BY	11	C
12	AB	42	C
35	BA	109	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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
62	KIR	BZ	1002	-	53,59,59	3.36	20 (37%)	57,84,84	1.87	18 (31%)
63	GDP	BZ	1003	61	25,30,30	1.30	2 (8%)	26,47,47	1.95	6 (23%)

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
62	KIR	BZ	1002	-	-	0/54/98/98	0/3/3/3
63	GDP	BZ	1003	61	-	0/12/32/32	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	1002	KIR	O18-C17	-13.54	1.24	1.44
62	BZ	1002	KIR	O30-C30	-12.78	1.16	1.42
62	BZ	1002	KIR	O4-C4	-3.31	1.29	1.36
62	BZ	1002	KIR	C3-C7	2.13	1.54	1.50
62	BZ	1002	KIR	C44-C21	2.20	1.54	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	1002	KIR	O29-C29-O34	-5.66	100.64	110.22
63	BZ	1003	GDP	N3-C2-N1	-5.00	120.16	127.46
63	BZ	1003	GDP	C5-C6-N1	-3.46	118.56	123.48
62	BZ	1002	KIR	O7-C7-C3	-3.06	112.68	120.22
62	BZ	1002	KIR	O27-C27-C28	-2.92	118.12	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	BZ	1002	KIR	7	0
63	BZ	1003	GDP	2	0

## 5.7 Other polymers ⓘ

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
58	BY	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BY	89:A	O3'	90:ALA	N	3.53



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A0	84/85 (98%)	0.49	9 (10%) 7 2	25, 44, 110, 136	0
2	A1	94/98 (95%)	0.19	2 (2%) 64 43	23, 43, 88, 95	0
3	A2	71/72 (98%)	0.13	2 (2%) 53 29	34, 61, 88, 98	0
4	A3	60/60 (100%)	0.01	1 (1%) 70 49	21, 36, 55, 87	0
5	A4	45/71 (63%)	0.67	6 (13%) 4 1	98, 118, 132, 138	0
6	A5	59/60 (98%)	0.40	6 (10%) 7 2	14, 39, 121, 137	0
7	A6	50/54 (92%)	0.69	6 (12%) 5 2	31, 61, 79, 82	0
8	A7	49/49 (100%)	-0.22	0 100 100	14, 24, 77, 93	0
9	A8	64/65 (98%)	-0.05	1 (1%) 72 51	21, 40, 55, 83	0
10	A9	37/37 (100%)	0.33	1 (2%) 55 30	33, 49, 68, 72	0
11	AA	2901/2915 (99%)	0.11	168 (5%) 24 10	8, 36, 159, 189	0
12	AB	119/122 (97%)	0.00	0 100 100	26, 77, 104, 137	0
13	AC	228/229 (99%)	4.97	195 (85%) 0 0	131, 151, 164, 168	0
14	AD	275/276 (99%)	-0.38	3 (1%) 80 65	8, 27, 53, 87	0
15	AE	205/206 (99%)	-0.09	6 (2%) 52 28	10, 29, 75, 88	0
16	AF	208/210 (99%)	-0.11	4 (1%) 67 46	11, 49, 116, 129	0
17	AG	181/182 (99%)	0.54	18 (9%) 8 3	55, 86, 112, 132	0
18	AH	160/180 (88%)	0.61	14 (8%) 11 4	39, 83, 124, 134	0
19	AJ	0/130	-	-	-	-
20	AK	0/140	-	-	-	-
21	AN	139/140 (99%)	-0.20	3 (2%) 62 41	17, 37, 86, 94	0
22	AO	122/122 (100%)	-0.32	2 (1%) 72 51	15, 31, 49, 66	0
23	AP	146/150 (97%)	0.49	7 (4%) 31 14	18, 60, 93, 119	0
24	AQ	141/141 (100%)	-0.23	2 (1%) 75 57	22, 32, 57, 106	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	AR	117/118 (99%)	-0.34	0 100 100	19, 31, 54, 67	0
26	AS	99/112 (88%)	0.51	4 (4%) 39 19	53, 76, 107, 109	0
27	AT	138/146 (94%)	0.10	8 (5%) 24 10	15, 48, 124, 143	0
28	AU	117/118 (99%)	-0.25	2 (1%) 70 49	15, 30, 57, 97	0
29	AV	101/101 (100%)	0.25	3 (2%) 51 27	9, 56, 76, 82	0
30	AW	113/113 (100%)	-0.29	2 (1%) 69 47	12, 29, 61, 106	0
31	AX	93/96 (96%)	-0.30	0 100 100	22, 41, 61, 75	0
32	AY	101/110 (91%)	0.77	13 (12%) 4 2	25, 56, 108, 128	0
33	AZ	184/206 (89%)	0.23	9 (4%) 30 14	28, 63, 98, 115	0
34	B2	144/144 (100%)	0.92	21 (14%) 3 1	49, 78, 118, 124	0
35	BA	1504/1522 (98%)	0.03	49 (3%) 47 24	14, 52, 128, 187	0
36	BB	235/256 (91%)	0.09	10 (4%) 36 17	27, 51, 114, 128	0
37	BC	207/239 (86%)	-0.07	0 100 100	36, 59, 86, 96	0
38	BD	208/209 (99%)	0.53	11 (5%) 27 12	47, 74, 111, 116	0
39	BE	151/162 (93%)	-0.34	1 (0%) 87 75	23, 40, 70, 92	0
40	BF	101/101 (100%)	-0.21	2 (1%) 65 44	33, 56, 71, 95	0
41	BG	155/156 (99%)	0.25	13 (8%) 12 4	52, 75, 107, 129	0
42	BH	138/138 (100%)	-0.36	0 100 100	17, 36, 54, 67	0
43	BI	127/128 (99%)	0.49	8 (6%) 21 8	46, 82, 107, 111	0
44	BJ	99/105 (94%)	0.88	17 (17%) 2 1	42, 82, 119, 122	0
45	BK	119/129 (92%)	0.22	6 (5%) 30 13	26, 56, 90, 107	0
46	BL	125/135 (92%)	0.03	4 (3%) 48 25	24, 50, 69, 112	0
47	BM	125/126 (99%)	0.53	8 (6%) 20 7	42, 80, 107, 139	0
48	BN	60/61 (98%)	0.06	2 (3%) 47 24	38, 48, 70, 77	0
49	BO	88/89 (98%)	-0.16	0 100 100	22, 41, 64, 69	0
50	BP	84/88 (95%)	0.20	1 (1%) 79 61	39, 58, 77, 102	0
51	BQ	100/105 (95%)	-0.27	0 100 100	27, 47, 68, 73	0
52	BR	70/88 (79%)	0.16	1 (1%) 75 57	28, 46, 71, 79	0
53	BS	79/93 (84%)	0.52	10 (12%) 4 2	55, 73, 101, 111	0
54	BT	99/106 (93%)	0.33	4 (4%) 39 19	46, 65, 101, 104	0
55	BU	25/27 (92%)	0.59	1 (4%) 39 19	52, 65, 83, 84	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BV	77/77 (100%)	0.02	1 (1%) 77 59	36, 57, 97, 104	0
56	BW	77/77 (100%)	5.36	67 (87%) 0 0	95, 192, 197, 199	0
57	BX	5/19 (26%)	0.76	1 (20%) 1 0	34, 36, 69, 80	0
58	BY	62/90 (68%)	0.13	0 100 100	55, 85, 125, 135	0
59	BZ	378/405 (93%)	-0.04	8 (2%) 64 43	23, 56, 92, 124	0
All	All	11143/11789 (94%)	0.24	743 (6%) 19 7	8, 50, 137, 199	0

The worst 5 of 743 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AC	111	ASP	20.0
13	AC	73	ARG	18.6
13	AC	173	ALA	18.5
11	AA	2182	G	18.2
13	AC	172	HIS	17.6

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
62	KIR	BZ	1002	57/57	0.89	0.36	1.25	101,117,134,134	0
63	GDP	BZ	1003	28/28	0.97	0.14	-0.62	36,43,44,45	0
60	ZN	BN	1001	1/1	0.99	0.13	-1.09	51,51,51,51	0
60	ZN	A9	1001	1/1	0.99	0.07	-1.75	58,58,58,58	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	ZN	BD	1001	1/1	0.98	0.19	-2.00	59,59,59,59	0
61	MG	BZ	1001	1/1	0.97	0.14	-	25,25,25,25	0
61	MG	AA	3001	1/1	0.99	0.22	-	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.