



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:35 PM BST

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 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/ValidationPDFNotes.html>

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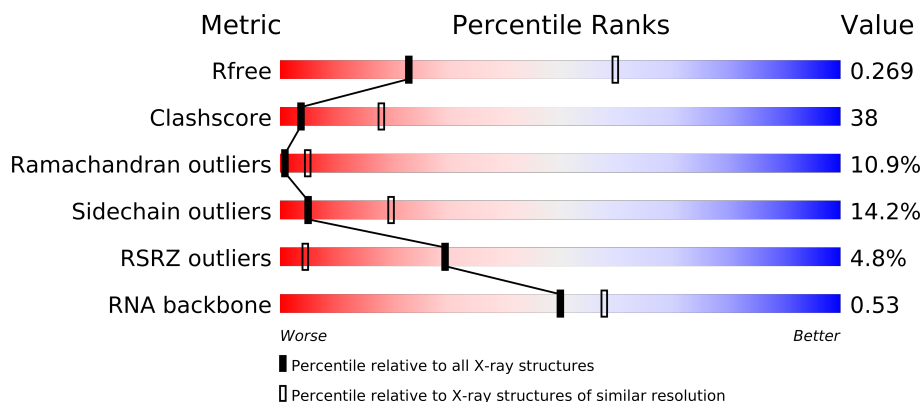
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A0	85	
2	A1	98	
3	A2	72	
4	A3	60	
5	A4	71	
6	A5	60	
7	A6	54	
8	A7	49	
9	A8	65	
10	A9	37	
11	AA	2915	
12	AB	122	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
55	BU	27	<div><div></div></div>
56	BV	77	<div><div></div></div>
56	BW	77	<div><div></div></div>
57	BX	19	<div><div></div></div>
58	BY	90	<div><div></div></div>
59	BZ	405	<div><div></div></div>

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 154206 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RRNA.

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 TRNA FMET 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
			1306	582	233	430	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

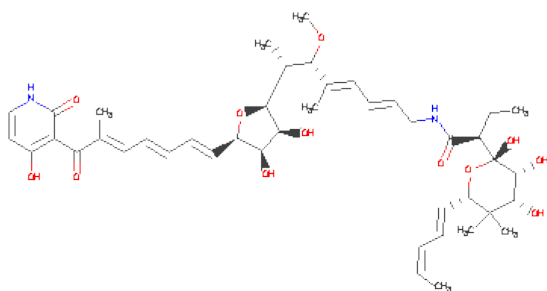
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

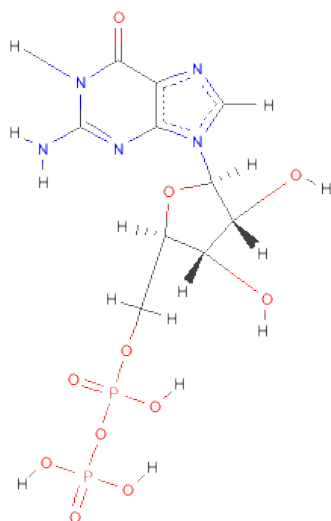
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BZ	1	Total Mg 1 1	0	0
61	AA	1	Total Mg 1 1	0	0

- 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:  $C_{10}H_{15}N_5O_{11}P_2$ ).

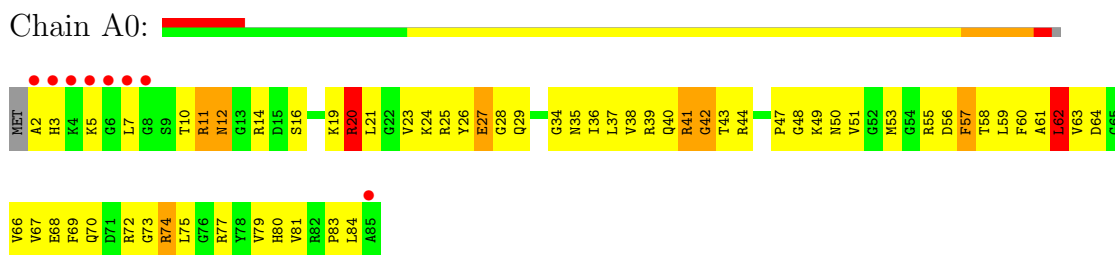


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
63	BZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

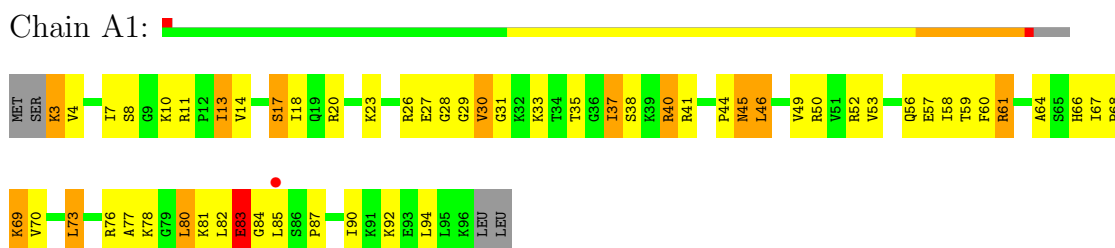
### 3 Residue-property plots

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 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.

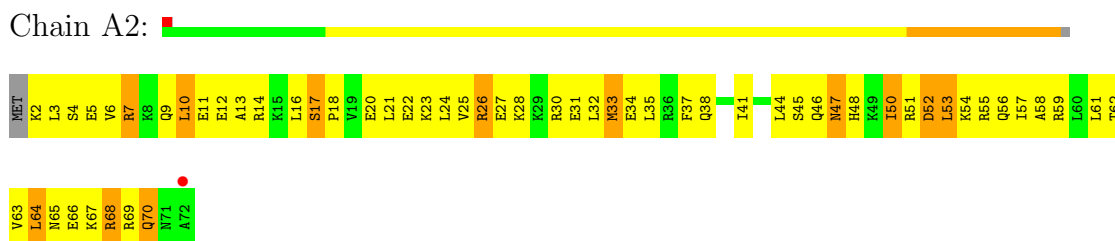
- Molecule 1: 50S RIBOSOMAL PROTEIN L27



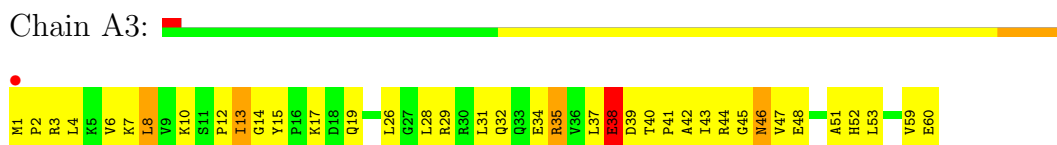
- Molecule 2: 50S RIBOSOMAL PROTEIN L28



- Molecule 3: 50S RIBOSOMAL PROTEIN L29



- Molecule 4: 50S RIBOSOMAL PROTEIN L30



- Molecule 5: 50S RIBOSOMAL PROTEIN L31

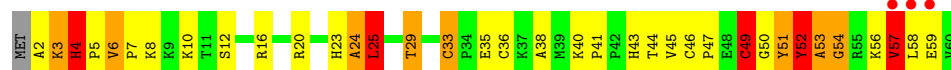






• Molecule 6: 50S RIBOSOMAL PROTEIN L32

Chain A5:



• Molecule 7: 50S RIBOSOMAL PROTEIN L33

Chain A6:



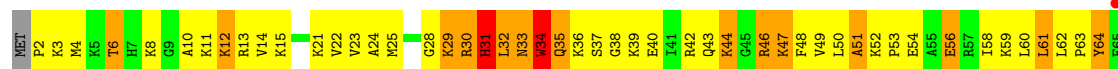
• Molecule 8: 50S RIBOSOMAL PROTEIN L34

Chain A7:



• Molecule 9: 50S RIBOSOMAL PROTEIN L35

Chain A8:



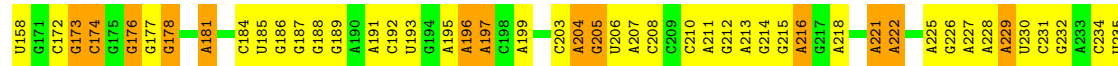
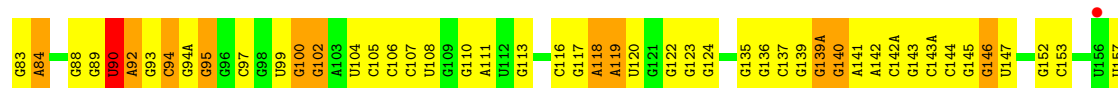
• Molecule 10: 50S RIBOSOMAL PROTEIN L36

Chain A9:



• Molecule 11: 23S RIBOSOMAL RNA

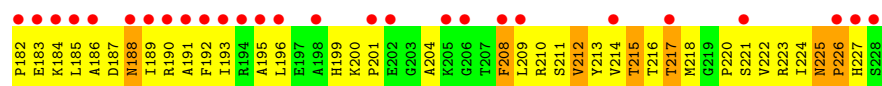
Chain AA:



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A1174	U1097	G1034	U963	C889	G616	U554	A479	C409	G333	U272A	C237
U1175	A1098	U1035	C964	A890	C618	U555	A480	G410	C334	G272B	C238
A1176	G1099	C964	C965	U826	G619	U556	A481	G411	C335	G272C	U239
C1177	U1100	C1038	U969	U827	G620	G556	A482	A412	C336	G272D	G240
U1101	U1101	G1039	C970	U828	A621	U557	A483	C413	C337		A241
C1102	A1102	G1040	C971	A895	G622	G558	C484	C414			G242
A1103	G1041	G1041	C972	A896	G623	U562	C485	A415	A340	C272H	U243
U1104	G1042	G1042	G973	C897	C624	G563		G418	G341	U272I	A244
U1105	C1043	G1043	G974	U832	U625	C564	G491	G419	G342	C272J	G245
G1106	G1044	G1044	C975	U833	A627	C565	A492	C420	G343	G274	G246
U1107	A1045	C975	C975A	U834	G628	U566	A493	U421	G352	G275	G247
U1108	A1046	G975A		A675	G629	A567	G494	A422	G353	A276	G248
C1109	G1047	G978		A676	G630	U568	G495	A423	G354	G277	C249
G1110	A1048	A983		G631	A631	U569	G496	G424		C278	G250
A1111	C1049	A983		G632	A632	U570	A497	G425	A251	G279	G252
U1112	A1050	A983		G633	A633	A571	G498	G426		G280	C253
G1113	G1051	A983		G634	A634	A572	U499	U427		G281	G254
U1114	C1052	C986		C635	A646	G573	A502	A428		U284	A255
A1115	C1053	G987		G636	G647	A575	A505	C435		C285	A256
C1116	A1054	A988		G637	G648	A576	A506	C436		C286	A257
U1119	G1055	G989		G638	G649		A507	C437		C287	G258
G1120	G1056	A990		U688	G650		A508	G438		C291	G259
C1121	A1057	C991		G689	A639		A509	G440		C292	G260
G1125	G1058	C995		G690	U639		A512	U441		U293	G261
A1128	U1060	A996		C691	G642		A517	G442		G296	C262
U1204	A1061	G997		G692	A643		A518	G443		C297	C264
A1129	G1062	C998		C693	A644		A519	G444		C298	A265
U1130	G1063	U999		U694	C645		A520	G445		G299	G266
G1131	C1064	A1000		G695	A646		A521	G446		C300	C267
A1132	U1065	A1000		U703	G647		A522	U447		G301	G268
U1133	G1066	G1003		G704	G648		A523	U448		C302	U269
U1136	A1067	C1004		G705	G649		A524	C451		A271	A270
G1137	G1068	C1005		A706	G650		A525	G452		C303	A271A
A1069	A1069	C1006		U707	C651		A526	G453		U306	C271B
C1070	G1071	C1007		G708	A653		A527	C454		G307	G271C
G1139	U1072	G1008		G709	A654		A528	C455		G308	U271D
C1140	C1073	A1009		U710	C654B		A529	C456		G309	U271E
U1141	A1073	U1010		G717	G654C		A530	A457		A310	C271F
U1142	G1074	G1011		A718	G654D		A531	C458		G387	G271G
A1142A	C1076	U1012		C719	G654E		A532	U459		G388	G271H
C1145	U1077	C1013		C720	G654F		A533			G389	C271I
C1146	U1078	U1014		C721	G654G		A534			G390	U271J
G1147	C1079	U1014		A722	C654H		A535			G391	U271K
A1151	U1080	U1019		G725	G654I		A536			C392	G271L
C1152	C1152	G1019		G726	A654J		A537			G393	U271M
G1153	C1153	A1020		A727	C654K		A538			A320	G271N
U1154	A1084	A1021		G728	G654L		A539			A322	C271O
A1155	A1085	U1022		U877	C654M		A540			A324	G271P
A1156	C1087	G1023		G730	G654N		A541			G395	U271Q
G1164	U1088	U1024		G733	G654O		A542			G396	G271R
U1165	A1089	G1025		U879	G654P		A543			G397	G271S
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U1167	G1091	G1027		A735	G654R		A545			U328	G271U
G1168	U1092	A1028		C736	C654S		A546			G329	C271V
C1169	C1093	A1029		C737	G654T		A547			A330	G271W
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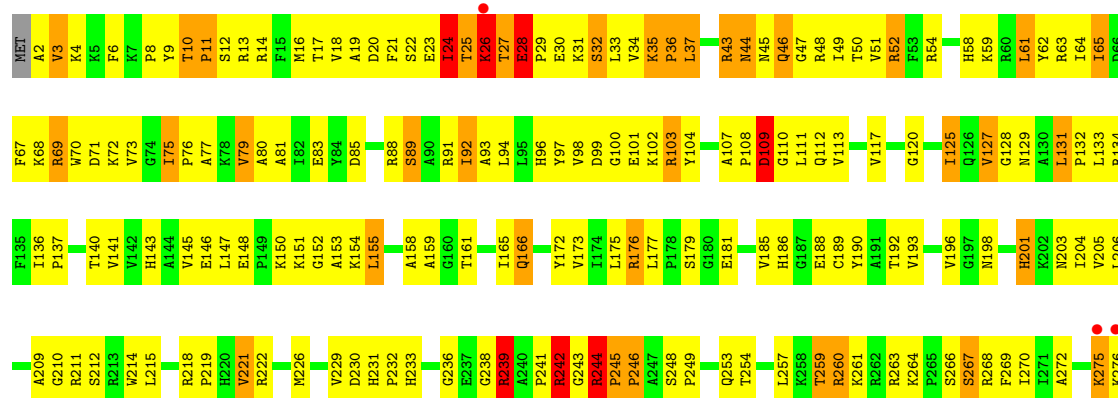
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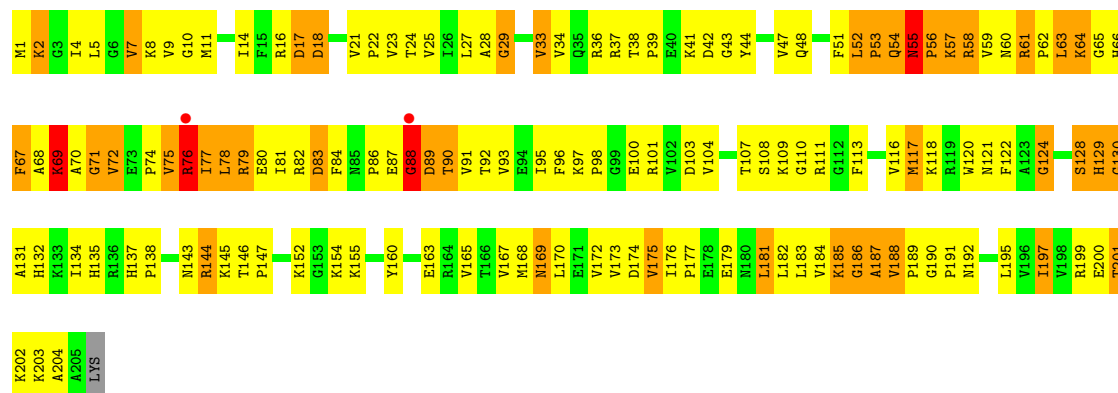
• Molecule 14: 50S RIBOSOMAL PROTEIN L2

Chain AD:



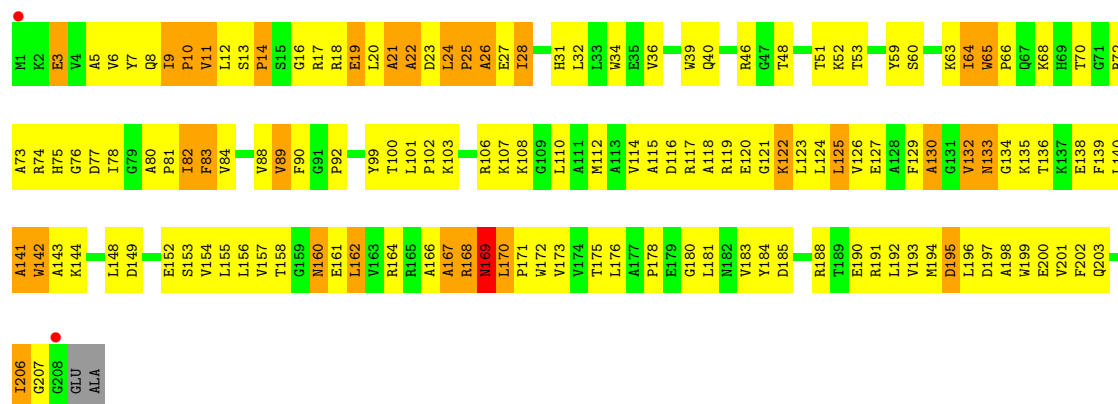
• Molecule 15: 50S RIBOSOMAL PROTEIN L3

Chain AE:



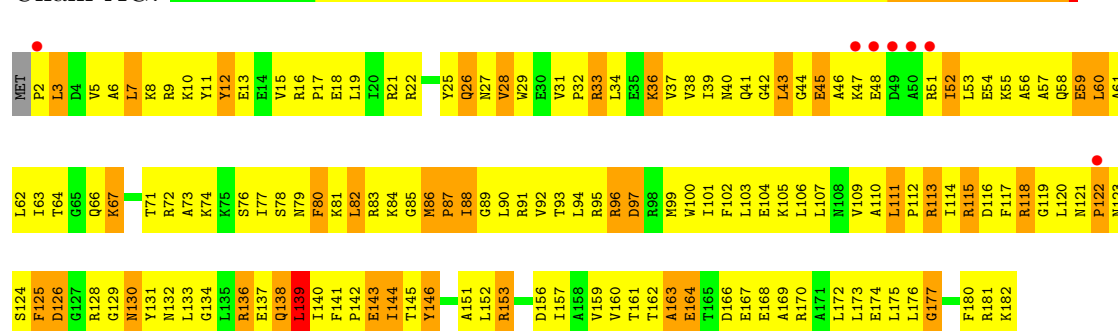
• Molecule 16: 50S RIBOSOMAL PROTEIN L4

Chain AF:



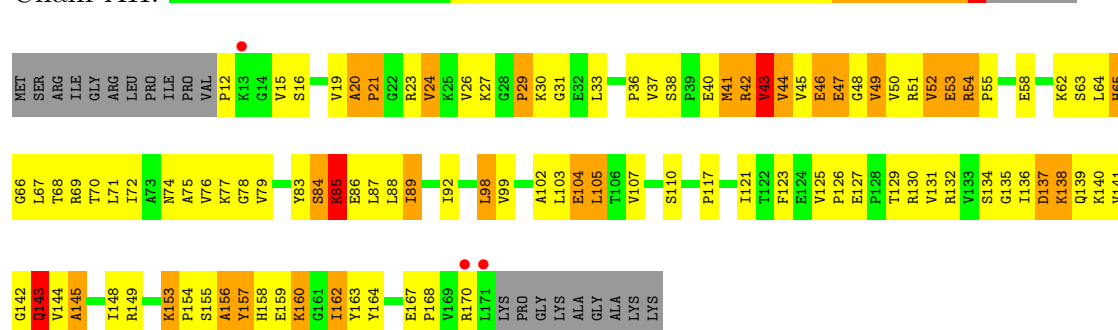
- Molecule 17: 50S RIBOSOMAL PROTEIN L5

Chain AG:



- Molecule 18: 50S RIBOSOMAL PROTEIN L6

Chain AH:



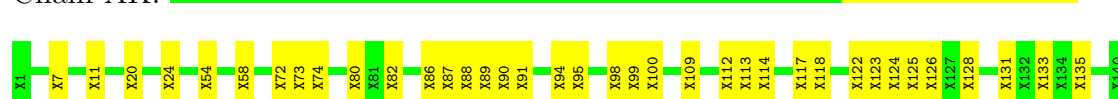
- Molecule 19: 50S RIBOSOMAL PROTEIN L10

Chain AJ:



- Molecule 20: 50S RIBOSOMAL PROTEIN L11

Chain AK:



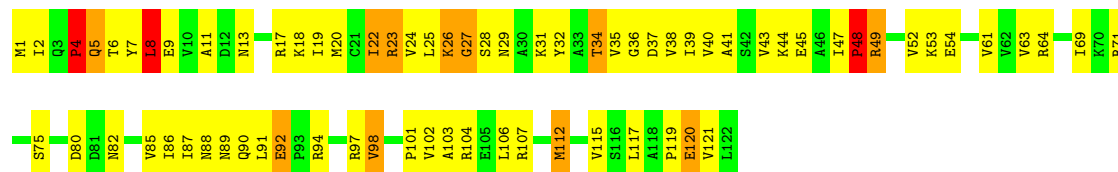
- Molecule 21: 50S RIBOSOMAL PROTEIN L13

Chain AN:



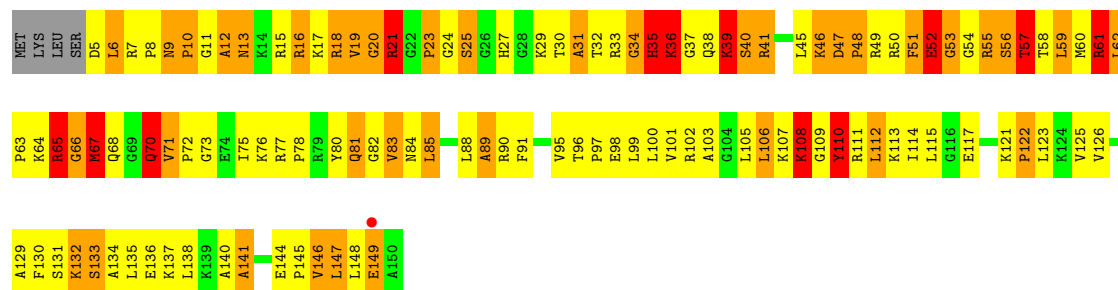
- Molecule 22: 50S RIBOSOMAL PROTEIN L14

Chain AO:



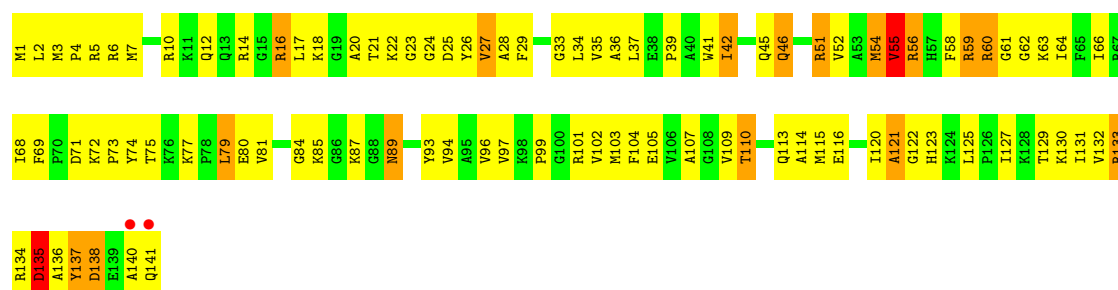
- Molecule 23: 50S RIBOSOMAL PROTEIN L15

Chain AP:



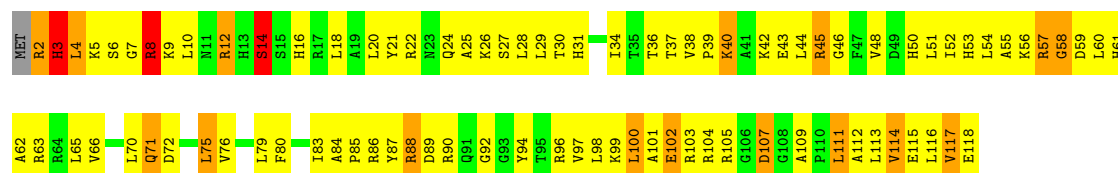
- Molecule 24: 50S RIBOSOMAL PROTEIN L16

Chain AQ:



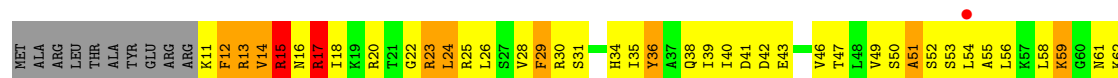
- Molecule 25: 50S RIBOSOMAL PROTEIN L17

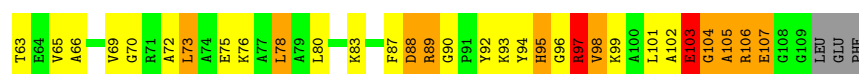
Chain AR:



- Molecule 26: 50S RIBOSOMAL PROTEIN L18

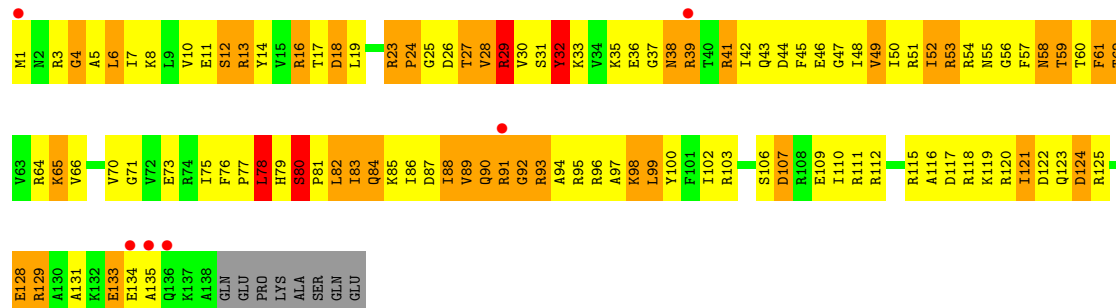
Chain AS:





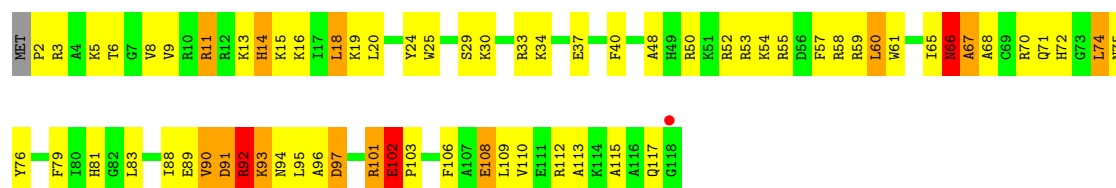
• Molecule 27: 50S RIBOSOMAL PROTEIN L19

Chain AT:



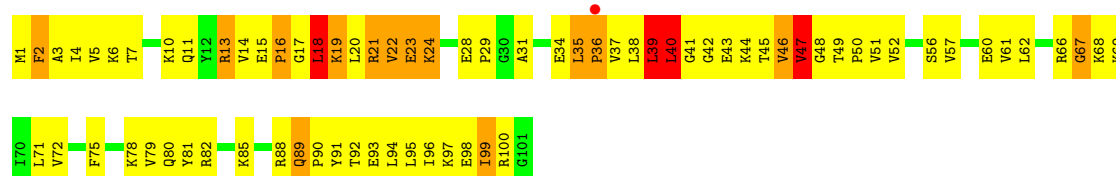
• Molecule 28: 50S RIBOSOMAL PROTEIN L20

Chain AU:



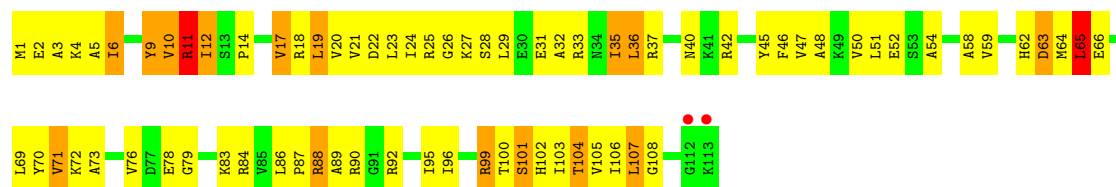
• Molecule 29: 50S RIBOSOMAL PROTEIN L21

Chain AV:



• Molecule 30: 50S RIBOSOMAL PROTEIN L22

Chain AW:



• Molecule 31: 50S RIBOSOMAL PROTEIN L23

Chain AX:

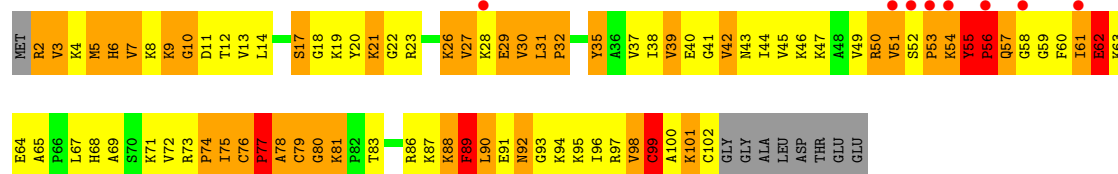






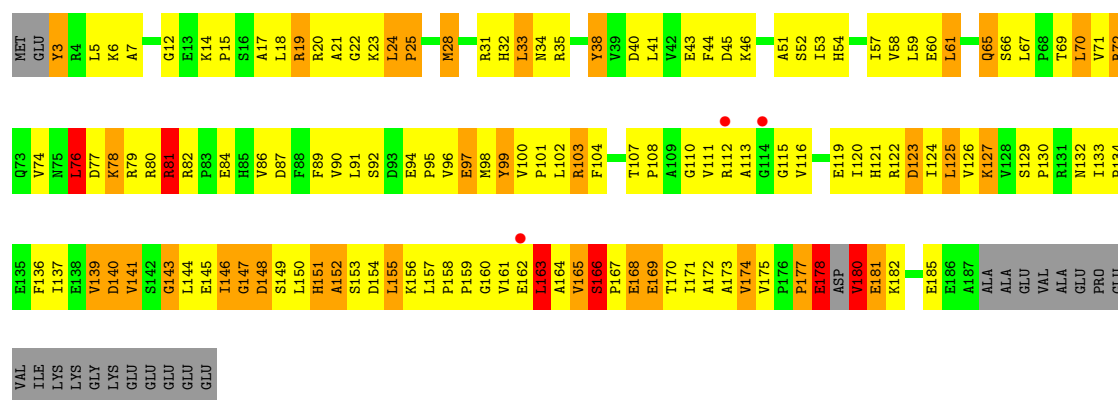
• Molecule 32: 50S RIBOSOMAL PROTEIN L24

Chain AY:



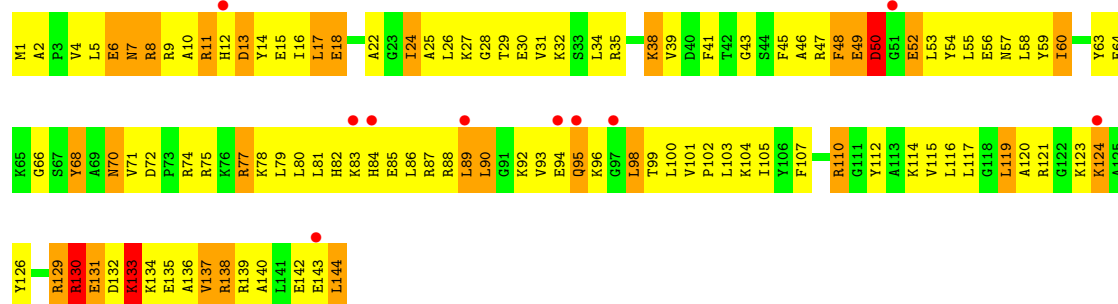
• Molecule 33: 50S RIBOSOMAL PROTEIN L25

Chain AZ:



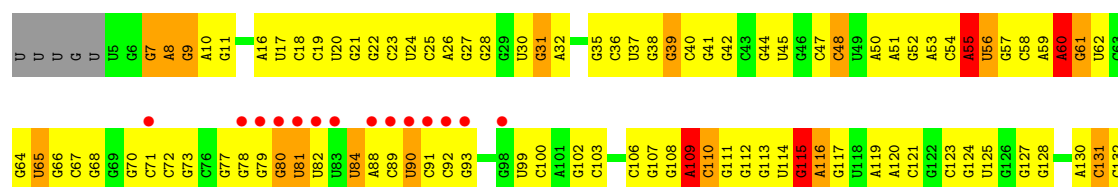
• Molecule 34: SMALL PROTEIN B SMPB

Chain B2:



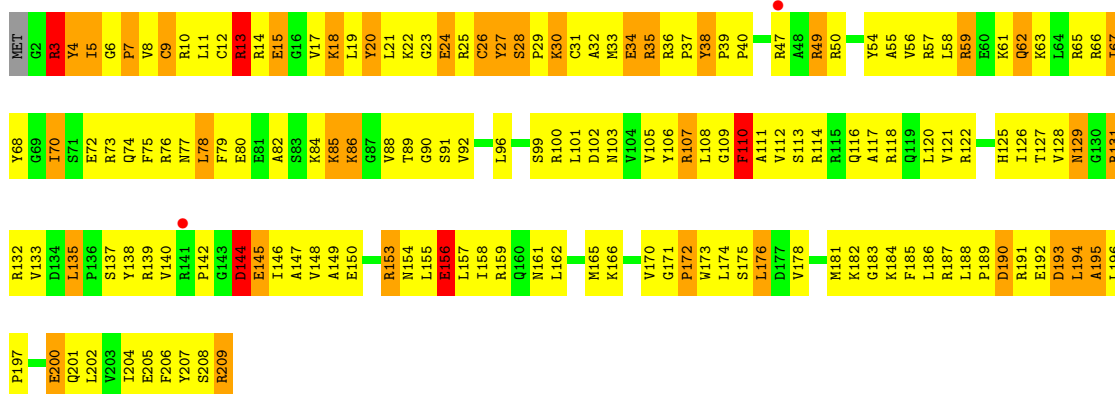
• Molecule 35: 16S RRNA

Chain BA:

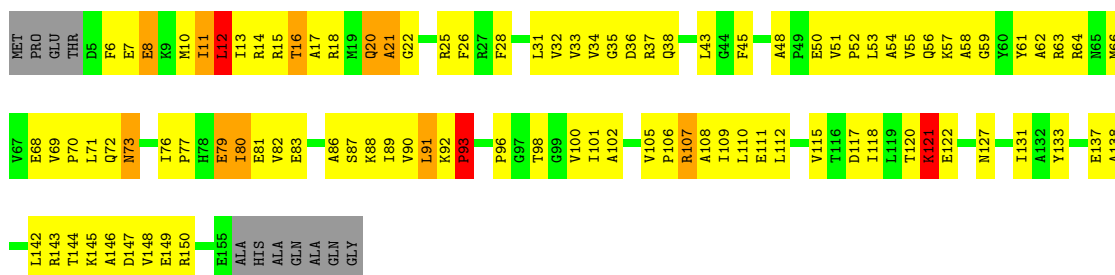


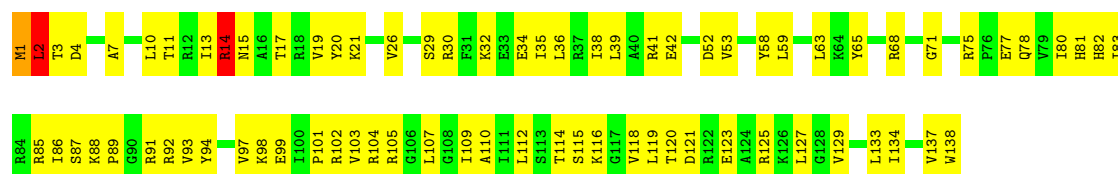
G1181	G1042	C980	A918	C840	C764	C689	G624	A547	U480	U405	U343	C272	A195	U133
C1118	G1046	U981	A919	U841	G765	G690	G625	G548	G490	G406	A344	A273	A196	A134
C1120	A1046	U982	U920	C948	A766	G626	U626	G549	G484	G407	C345	A274	A197	C135
U1121	G1047	A983	U921	C949	G767	U627	G627	G550	G485	A408	C346	G275	G198	C136
U1122	G1048	U984	G922	U850	G769	G628	G628	U551	U486	G409	G347	G276	G199	C137
U1123	G1049	A985	A923	G851	C770	G629	G629	U552	A487	G410	G348	G277	G200	G138
G1124	G1050	G987	C924	G852	G771	G698	G630	U553	G488	A411	A349	G278	C201	G139
U1125	U1052	U991	G925	G853	U772	G699	G631	C556	G490	A412	G350	C283	U202	
A1191	U1053	G926	G926	G854	G776	C701	A632	G557	G491	A413	G351		U203	A143
C1127	G1054	U992	G927	A702	A777	A702	G633	G558	G492	G414	C352	U287	U204	G144
C1128	C1054	G928	G928	C857	G778	G703	G634	A559	A353	A415	A353	U288	G216	G147
G1129	A1055	G929	G929	G858	G779	A704	G635	U560	A495	A416	A288	A288	C217	G148
C1130	C995	C930	C930	A859	C779	U705	G636	U561	A496	C417	G289	G289	C218	A149
U1131	G1057	C931	C931	A860	A780	A706	G637	C562	U498	C418	C290	G290	C219	C150
	G1058		C934	G861	A781	C707	G638	C566	A499	C419	G357	C291	G220	
G1134	C1059	G942	G942	A872	A782	C708	G639	C567	G500	U420	U358	G292	G221	
U1135	C1060	A935	A935	A864	C783	G709	A640	C568	C501	U421	U359	G293	U222	A151
U1136	G1061	G936	G936	A865	C784	G710	U641	A572	G502	G422	G361	U294	U223	A152
C1137	U1062	A937	A937	C866	G785	G711	A642	A573	C503	G423	G362	U295	C224	G158
G1138	C1063	A938	A938	G867	G786	A712	G643	A574	C504	G424	A363	U296	C225	G159
C1139	G1064	G939	G939	C868	A787	G713	G644	A575	G505	G425	A364	G297	G226	
C1140	U1065	C940	C940	G869	U788	G714	C645	C576	G506	G426	A298	A298	G227	A161
U1141	C1066	G941	G941	G870	U789	A716	U646	C577	C507	U427	U367	G299		A162
G1142				A872	A790		C647	C578	C508	U428	U368	A300		C163
G1143	U1070	G1009	G945	C875	G791	C719	A648	U580	A509	U429	C369	G301	G233	
G1144		G1010	G946		A792	C720	G649	C581	A510	A430	C370	G302	G234	G167
C1145	C1075	U1011	A947	G878	U793	G721	G650	C582	C511	A431	G371	A303	C235	G168
A1146	G1076	G1012	G948	G879	A722	A722		C583	U512	A432	C372	U304	G236	C169
C1147	G1077	U1013	C948	C880	G723	U723	A653	C584	C513	C433	C373	A304	C237	U170
U1148	A1014	A1014	A949	G881	C797	G724	G654	C585	U516	U434	A374	C307	G238	A171
A1015	A1015	A1015	U950	G882	G798	G725	A655	C586	C517	C435	U375	C308	U239	A172
U1150	G1081	C951	G951	C883	G799	C726	C656	C587	C518	C436	G376	C309	C240	U173
A1151	G1082	U952	U952	U884	G800	G727	C657	C588	C519	U437	G377	G310	C241	G174
C1152	C1018	G953	G953	U885	U801	A802	U658	C589	G521	A438	C378	C311	C242	C175
U1153	U1019	G954	G954	A889	G803	C731	U659	C590	G522	A441	C380	C312	C243	C176
G1154	U1091	U955	U955	G890	G808	C732	G661	C591	C523	U442	C381	A313	U244	C177
G1155			U956	G891	G809	A733	G662	C592	C524	C443	C382	C314	C245	C178
G1156	U1094	G1023	U957	U893	G808	C736	A663	C593	G527	U444	A383	G316	A246	A179
A1157	U1095	U1024	A958	A892	G809	C737	A664	C594	G528	C445	A384		G247	U180
C1158	C1096	U1025	A959	C893	A737	C738	G665	C595	U531	A452	C385	A321	A250	G184
U1159	C1097	G1026	U960	G894	A814	C739	A666	C600	A532	A453	C386	C322	G251	A185
C1160	C1098	C1027	U961	G895	A815	C739	A667	C601	A533	C456	C387	U323	G252	C186
C1161	G1099	G1028	G962	C896	C817	U740	G668	A602	U534	C457	C388	G324	G253	C187
C1162	C1100	C1029	G963		C818	G741		U603	A535	C458	C389	A325	G254	C188
C1163	A1101	C1030	A964	C899	G818	G742		U604	U536	A461	A389	A326	G255	
G1164	A1102	U1030A	A965	A900	A819		G671	U605	A537	C459	C390	G326	U256	
C1165	C1103	C1030B	G966	A901	U820	C748	U672	U606	A538	C460	C391	A327	G257	C189B
C1166	G1104	G1030C	G967	G902	G821	C749	G673	A607	U539	C461	C392	C328	G258	C189C
U1234	A1105	A1030D	A968	G903	C822	G750	G674	A608	A535	C462	C393	C329	G259	C189D
U1235	G1106	G1031	A969	C904	G823		A675	A609	C536	C463	C394	C330		
A1236	C1107	G1032	C970			C754	A676	G610	G537	A464	C395	G331	A262	G189H
C1237	G1108	U1033	G971	A909	C826	G755	U677	G611	G538	C470	C396	G332	A263	G189I
A1238		G1034	G972	C910	U827	C756		G612	A539	C471	C397	G333	U264	G189J
U1239	U1172	A1035	G973	U911	A828	U757	C681	C613	G540	A472	C398	C334	G265	U189K
U1240	G1111	G1036	A974	C912	G758	G758	G682	U619	G541	C473	G399	C335	G266	G189L
G1241	C1112	C1037	A975	A913	U833	A759		C620	G542	C474	C400	C336	C267	U190
C1242	C1113	C1038	G976	A914	C834		G685	A621	C543	C475	C401	C337	C268	G191
C1243	C1114	G1039	G977	A915	G838		U686	A622	C544	C476	C402	A388	C269	U192
C1244	C1115	U1040	A978	A916	C762		U687	A623	C545	A477	C403	C339	A270	C193
A1245	G1117	A1041	C979	G917	U839	G763	G688	C623	G546	C479	U404		C271	C194



Chain BD: 

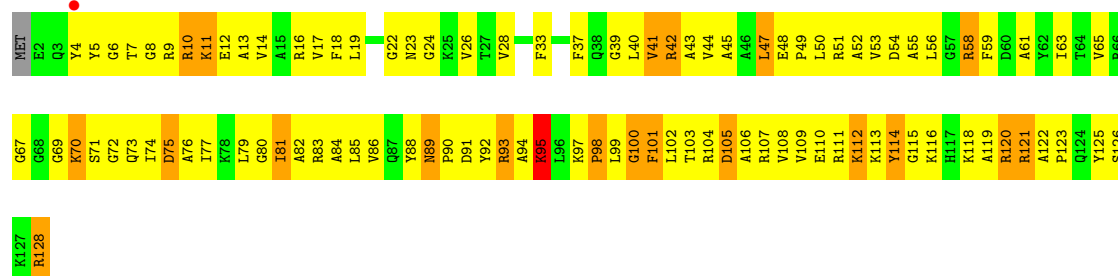
- Molecule 39: 30S RIBOSOMAL PROTEIN S5

Chain BE: 



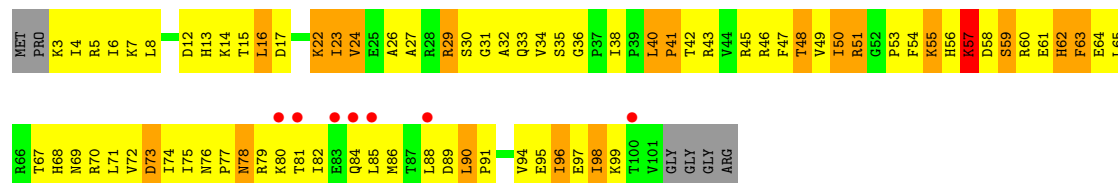
• Molecule 43: 30S RIBOSOMAL PROTEIN S9

Chain BI:



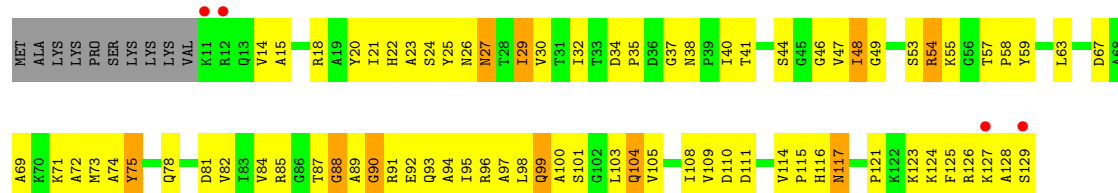
• Molecule 44: 30S RIBOSOMAL PROTEIN S10

Chain BJ:



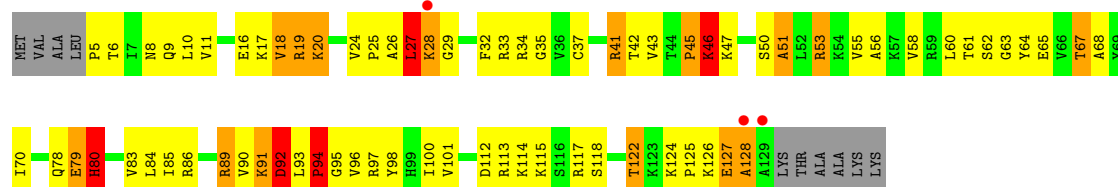
• Molecule 45: 30S RIBOSOMAL PROTEIN S11

Chain BK:



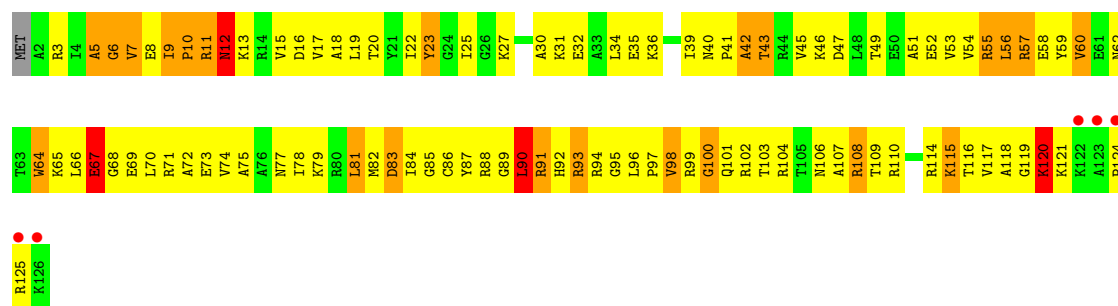
• Molecule 46: 30S RIBOSOMAL PROTEIN S12

Chain BL:



• Molecule 47: 30S RIBOSOMAL PROTEIN S13

Chain BM:



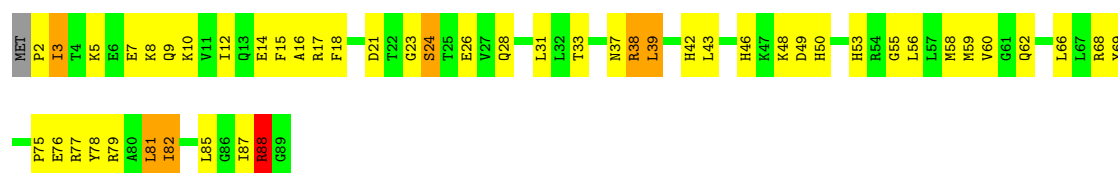
- Molecule 48: 30S RIBOSOMAL PROTEIN S14

Chain BN:



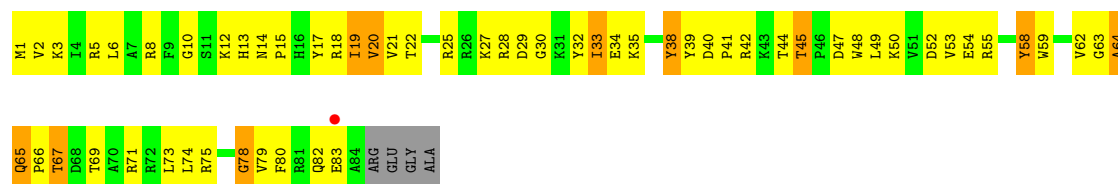
- Molecule 49: 30S RIBOSOMAL PROTEIN S15

Chain BO:



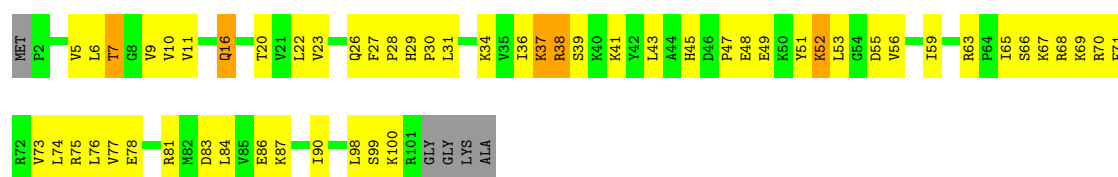
- Molecule 50: 30S RIBOSOMAL PROTEIN S16

Chain BP:



- Molecule 51: 30S RIBOSOMAL PROTEIN S17

Chain BQ:



- Molecule 52: 30S RIBOSOMAL PROTEIN S18

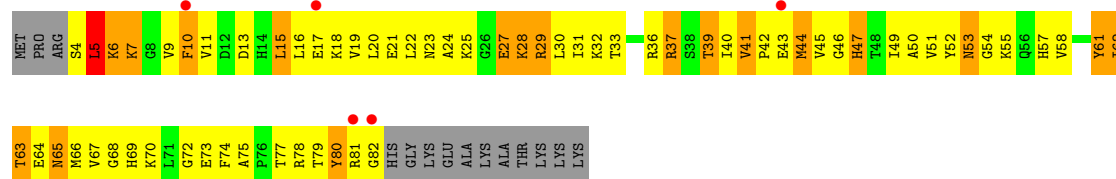
Chain BR:





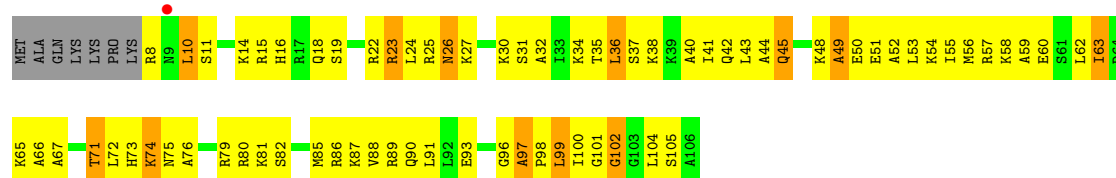
• Molecule 53: 30S RIBOSOMAL PROTEIN S19

Chain BS:



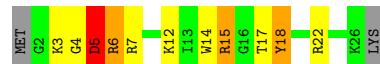
• Molecule 54: 30S RIBOSOMAL PROTEIN S20

Chain BT:



• Molecule 55: 30S RIBOSOMAL PROTEIN THX

Chain BU:



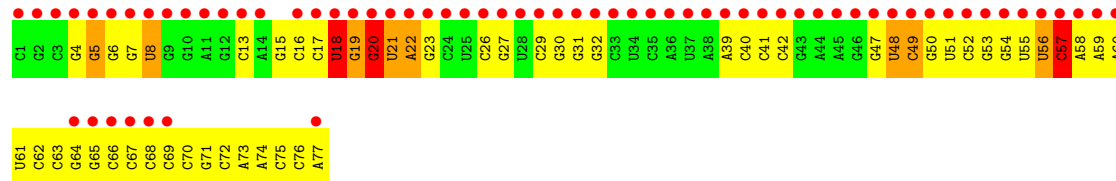
• Molecule 56: E-SITE TRNA FMET OR P-SITE TRNA FMET

Chain BV:



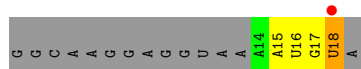
• Molecule 56: E-SITE TRNA FMET OR P-SITE TRNA FMET

Chain BW:



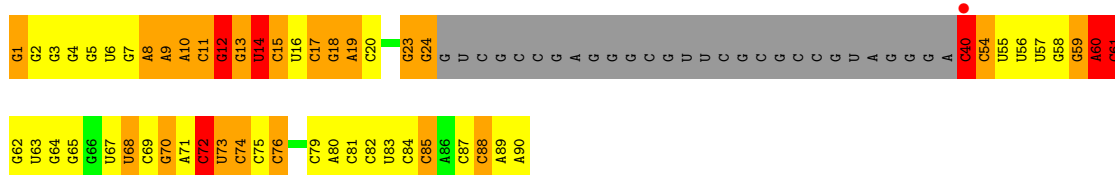
• Molecule 57: MRNA

Chain BX:



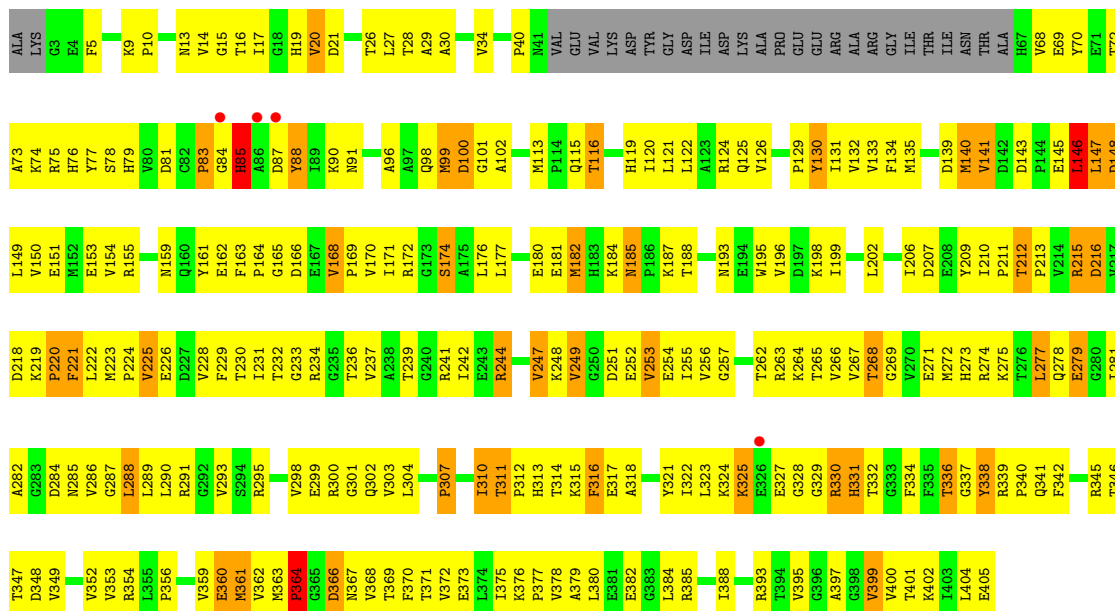
● Molecule 58: TMRNA DELA

Chain BY:



● Molecule 59: ELONGATION FACTOR TU

Chain BZ:





## 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> )	0.28 , 18.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 503945 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	154206	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.

## 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	0.82	5/1455 (0.3%)	0.97	5/2258 (0.2%)
59	BZ	0.42	0/2986	0.69	0/4050
All	All	0.52	12/165829 (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 12 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	40	C	OP3-P	-6.93	1.52	1.61
58	BY	1	G	OP3-P	-6.81	1.52	1.61
11	AA	761	A	C6-N6	-6.64	1.28	1.33

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	2217	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	1298	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BB	1901	0	1951	255	0
37	BC	1613	0	1677	152	0
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	161	0
57	BX	104	0	55	4	0
58	BY	1306	0	663	88	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	154206	0	105206	9942	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 9942 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

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

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

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

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

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

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%)	5	21
2	A1	78/83 (94%)	63 (81%)	15 (19%)	2	9
3	A2	66/67 (98%)	57 (86%)	9 (14%)	5	21
4	A3	51/52 (98%)	46 (90%)	5 (10%)	12	40
5	A4	39/63 (62%)	30 (77%)	9 (23%)	1	5
6	A5	51/52 (98%)	41 (80%)	10 (20%)	2	8
7	A6	49/52 (94%)	34 (69%)	15 (31%)	0	1
8	A7	41/42 (98%)	35 (85%)	6 (15%)	5	18
9	A8	53/55 (96%)	42 (79%)	11 (21%)	2	7
10	A9	34/34 (100%)	26 (76%)	8 (24%)	1	5
13	AC	180/181 (99%)	164 (91%)	16 (9%)	14	47
14	AD	217/218 (100%)	183 (84%)	34 (16%)	4	14
15	AE	165/166 (99%)	138 (84%)	27 (16%)	3	12
16	AF	165/166 (99%)	150 (91%)	15 (9%)	14	45
17	AG	155/156 (99%)	135 (87%)	20 (13%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AH	132/148 (89%)	116 (88%)	16 (12%)	7	27
21	AN	117/119 (98%)	101 (86%)	16 (14%)	5	21
22	AO	100/100 (100%)	88 (88%)	12 (12%)	7	27
23	AP	112/116 (97%)	89 (80%)	23 (20%)	2	8
24	AQ	111/111 (100%)	90 (81%)	21 (19%)	2	9
25	AR	100/101 (99%)	85 (85%)	15 (15%)	4	17
26	AS	77/88 (88%)	67 (87%)	10 (13%)	6	23
27	AT	120/127 (94%)	91 (76%)	29 (24%)	1	4
28	AU	92/94 (98%)	82 (89%)	10 (11%)	9	34
29	AV	82/82 (100%)	72 (88%)	10 (12%)	7	26
30	AW	91/92 (99%)	77 (85%)	14 (15%)	4	15
31	AX	74/78 (95%)	67 (90%)	7 (10%)	12	42
32	AY	84/91 (92%)	69 (82%)	15 (18%)	2	10
33	AZ	161/179 (90%)	132 (82%)	29 (18%)	2	10
34	B2	120/120 (100%)	81 (68%)	39 (32%)	0	0
36	BB	202/220 (92%)	172 (85%)	30 (15%)	4	17
37	BC	160/188 (85%)	149 (93%)	11 (7%)	22	62
38	BD	180/181 (99%)	152 (84%)	28 (16%)	4	14
39	BE	115/123 (94%)	99 (86%)	16 (14%)	5	21
40	BF	90/90 (100%)	76 (84%)	14 (16%)	4	14
41	BG	126/127 (99%)	115 (91%)	11 (9%)	15	49
42	BH	119/119 (100%)	108 (91%)	11 (9%)	13	45
43	BI	98/99 (99%)	87 (89%)	11 (11%)	9	33
44	BJ	88/92 (96%)	74 (84%)	14 (16%)	4	13
45	BK	90/99 (91%)	84 (93%)	6 (7%)	23	63
46	BL	104/111 (94%)	91 (88%)	13 (12%)	7	25
47	BM	99/101 (98%)	84 (85%)	15 (15%)	4	16
48	BN	49/50 (98%)	41 (84%)	8 (16%)	3	12
49	BO	79/80 (99%)	72 (91%)	7 (9%)	14	47
50	BP	72/74 (97%)	64 (89%)	8 (11%)	9	33
51	BQ	94/97 (97%)	89 (95%)	5 (5%)	32	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	BR	61/77 (79%)	56 (92%)	5 (8%)	17 53
53	BS	69/80 (86%)	57 (83%)	12 (17%)	3 11
54	BT	76/82 (93%)	68 (90%)	8 (10%)	10 35
55	BU	19/22 (86%)	16 (84%)	3 (16%)	4 14
59	BZ	316/338 (94%)	275 (87%)	41 (13%)	6 23
All	All	5289/5550 (95%)	4537 (86%)	752 (14%)	5 20

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	59,59,59	3.49	23 (38%)	82,84,84	2.05	23 (28%)
63	GDP	BZ	1003	61	30,30,30	1.43	6 (20%)	45,47,47	2.56	10 (22%)

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	-	0/16/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	1002	KIR	O18-C17	-12.72	1.24	1.44
62	BZ	1002	KIR	O30-C30	-12.31	1.16	1.42
62	BZ	1002	KIR	O34-C33	-11.40	1.28	1.44
62	BZ	1002	KIR	C45-C28	5.65	1.61	1.54
62	BZ	1002	KIR	C5-C4	4.88	1.48	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	BZ	1003	GDP	C6-C5-N7	-12.71	132.43	134.14
62	BZ	1002	KIR	C3-C2-N1	6.95	122.86	115.86
62	BZ	1002	KIR	O29-C29-O34	-5.87	100.64	110.32
62	BZ	1002	KIR	C4-C3-C7	5.39	133.90	120.31
63	BZ	1003	GDP	C5-C4-N3	-4.92	120.41	126.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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%)	0.23	8 (9%) 8 2	25, 44, 110, 136	0
2	A1	94/98 (95%)	0.07	1 (1%) 77 22	23, 43, 88, 95	0
3	A2	71/72 (98%)	0.03	1 (1%) 72 17	34, 61, 88, 98	0
4	A3	60/60 (100%)	-0.08	1 (1%) 67 15	21, 36, 55, 87	0
5	A4	45/71 (63%)	0.43	2 (4%) 33 5	98, 118, 132, 138	0
6	A5	59/60 (98%)	0.14	3 (5%) 27 4	14, 39, 121, 137	0
7	A6	50/54 (92%)	0.35	2 (4%) 36 5	31, 61, 79, 82	0
8	A7	49/49 (100%)	-0.17	0 100 100	14, 24, 77, 93	0
9	A8	64/65 (98%)	-0.02	1 (1%) 68 15	21, 40, 55, 83	0
10	A9	37/37 (100%)	0.23	1 (2%) 52 8	33, 49, 68, 72	0
11	AA	2901/2915 (99%)	0.01	157 (5%) 25 4	8, 36, 159, 189	0
12	AB	119/122 (97%)	-0.03	0 100 100	26, 77, 104, 137	0
13	AC	228/229 (99%)	2.75	146 (64%) 0 0	131, 151, 164, 168	0
14	AD	275/276 (99%)	-0.26	3 (1%) 77 22	8, 27, 53, 87	0
15	AE	205/206 (99%)	-0.11	2 (0%) 79 23	10, 29, 75, 88	0
16	AF	208/210 (99%)	-0.13	2 (0%) 79 23	11, 49, 116, 129	0
17	AG	181/182 (99%)	0.24	7 (3%) 37 5	55, 86, 112, 132	0
18	AH	160/180 (88%)	0.30	3 (1%) 64 13	39, 83, 124, 134	0
19	AJ	0/130	-	-	-	-
20	AK	0/140	-	-	-	-
21	AN	139/140 (99%)	-0.17	1 (0%) 84 32	17, 37, 86, 94	0
22	AO	122/122 (100%)	-0.27	0 100 100	15, 31, 49, 66	0
23	AP	146/150 (97%)	0.24	1 (0%) 84 32	18, 60, 93, 119	0
24	AQ	141/141 (100%)	-0.18	2 (1%) 72 17	22, 32, 57, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	AR	117/118 (99%)	-0.24	0 100 100	19, 31, 54, 67	0
26	AS	99/112 (88%)	0.21	1 (1%) 79 23	53, 76, 107, 109	0
27	AT	138/146 (94%)	0.06	6 (4%) 34 5	15, 48, 124, 143	0
28	AU	117/118 (99%)	-0.18	1 (0%) 81 25	15, 30, 57, 97	0
29	AV	101/101 (100%)	0.13	1 (0%) 79 23	9, 56, 76, 82	0
30	AW	113/113 (100%)	-0.22	2 (1%) 65 14	12, 29, 61, 106	0
31	AX	93/96 (96%)	-0.19	0 100 100	22, 41, 61, 75	0
32	AY	101/110 (91%)	0.36	8 (7%) 13 2	25, 56, 108, 128	0
33	AZ	184/206 (89%)	0.12	3 (1%) 68 15	28, 63, 98, 115	0
34	B2	144/144 (100%)	0.61	10 (6%) 17 3	49, 78, 118, 124	0
35	BA	1504/1522 (98%)	-0.06	44 (2%) 49 7	14, 52, 128, 187	0
36	BB	235/256 (91%)	0.02	5 (2%) 60 11	27, 51, 114, 128	0
37	BC	207/239 (86%)	-0.11	0 100 100	36, 59, 86, 96	0
38	BD	208/209 (99%)	0.30	2 (0%) 79 23	47, 74, 111, 116	0
39	BE	151/162 (93%)	-0.27	0 100 100	23, 40, 70, 92	0
40	BF	101/101 (100%)	-0.20	0 100 100	33, 56, 71, 95	0
41	BG	155/156 (99%)	0.12	9 (5%) 22 3	52, 75, 107, 129	0
42	BH	138/138 (100%)	-0.29	0 100 100	17, 36, 54, 67	0
43	BI	127/128 (99%)	0.29	1 (0%) 83 28	46, 82, 107, 111	0
44	BJ	99/105 (94%)	0.57	7 (7%) 16 3	42, 82, 119, 122	0
45	BK	119/129 (92%)	0.15	4 (3%) 43 6	26, 56, 90, 107	0
46	BL	125/135 (92%)	-0.00	3 (2%) 56 9	24, 50, 69, 112	0
47	BM	125/126 (99%)	0.29	5 (4%) 36 5	42, 80, 107, 139	0
48	BN	60/61 (98%)	-0.04	1 (1%) 67 15	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%)	0.05	1 (1%) 75 20	39, 58, 77, 102	0
51	BQ	100/105 (95%)	-0.20	0 100 100	27, 47, 68, 73	0
52	BR	70/88 (79%)	0.04	0 100 100	28, 46, 71, 79	0
53	BS	79/93 (84%)	0.30	5 (6%) 19 3	55, 73, 101, 111	0
54	BT	99/106 (93%)	0.11	1 (1%) 79 23	46, 65, 101, 104	0
55	BU	25/27 (92%)	0.45	0 100 100	52, 65, 83, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BV	77/77 (100%)	-0.13	1 (1%) 74 19	36, 57, 97, 104	0
56	BW	77/77 (100%)	5.08	66 (85%) 0 0	95, 192, 197, 199	0
57	BX	5/19 (26%)	0.58	1 (20%) 2 0	34, 36, 69, 80	0
58	BY	62/90 (68%)	0.04	1 (1%) 68 15	55, 85, 125, 136	0
59	BZ	378/405 (93%)	-0.07	4 (1%) 77 22	23, 56, 92, 124	0
All	All	11143/11789 (94%)	0.10	537 (4%) 29 4	8, 50, 137, 199	0

The worst 5 of 537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	AA	2182	G	16.9
11	AA	2181	G	15.2
56	BW	35	C	14.6
56	BW	37	U	14.5
11	AA	2123	G	14.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
61	MG	AA	3001	1/1	0.22	-	10,10,10,10	0
61	MG	BZ	1001	1/1	0.15	-	25,25,25,25	0
63	GDP	BZ	1003	28/28	0.14	-	36,43,44,45	0
60	ZN	A9	1001	1/1	0.06	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
62	KIR	BZ	1002	57/57	0.36	-	101,117,134,134	0
60	ZN	BD	1001	1/1	0.19	-	59,59,59,59	0
60	ZN	BN	1001	1/1	0.12	-	51,51,51,51	0

## 6.5 Other polymers

There are no such residues in this entry.