



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:33 am BST

PDB ID : 4V5L  
Title : The structure of EF-Tu and aminoacyl-tRNA bound to the 70S ribosome with a GTP analog  
Authors : Voorhees, R.M.; Schmeing, T.M.; Ramakrishnan, V.  
Deposited on : 2010-09-02  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

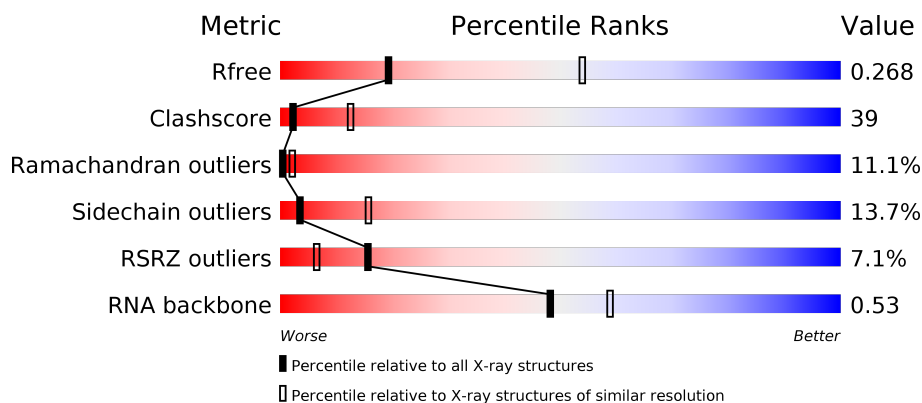
# 1 Overall quality at a glance

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.





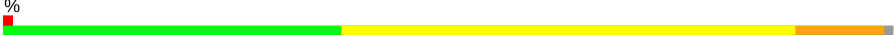

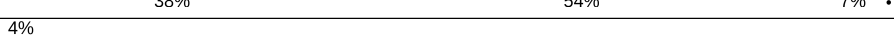
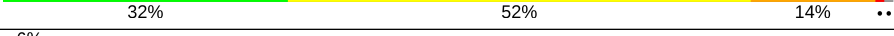
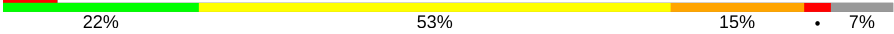


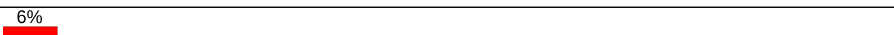
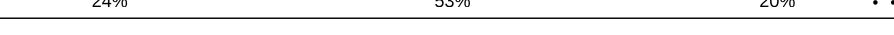
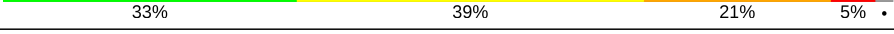
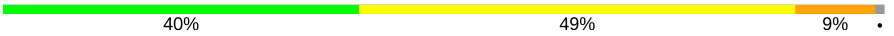
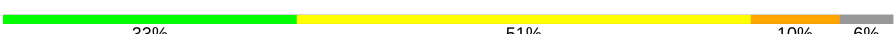


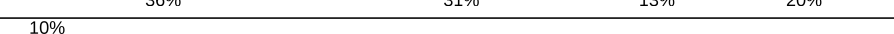

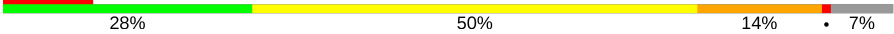
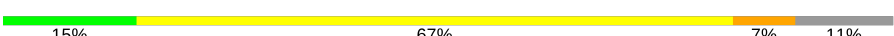


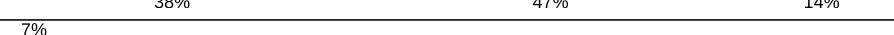
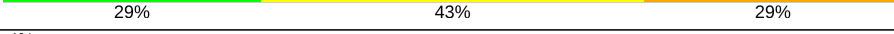
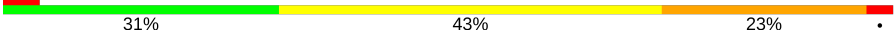
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	AA	1522	<div> <div>2%</div> <div>33% 52% 11%</div> </div>
2	AB	256	<div> <div>5%</div> <div>20% 54% 15% 9%</div> </div>
3	AC	239	<div> <div>29% 48% 9% 14%</div> </div>
4	AD	209	<div> <div>38% 47% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
22	AW	76	
23	AX	14	
24	AY	77	
25	AZ	405	
26	B0	85	
27	B1	98	
28	B2	72	

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Mol	Chain	Length	Quality of chain
29	B3	60	
30	B4	71	
31	B5	60	
32	B6	54	
33	B7	49	
34	B8	65	
35	B9	37	
36	BA	2915	
37	BB	122	
38	BC	229	
39	BD	276	
40	BE	206	
41	BF	210	
42	BG	182	
43	BH	180	
44	BJ	130	
45	BK	140	
46	BN	140	
47	BO	122	
48	BP	150	
49	BQ	141	
50	BR	118	
51	BS	112	
52	BT	146	
53	BU	118	

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Mol	Chain	Length	Quality of chain
54	BV	101	
55	BW	113	
56	BX	96	
57	BY	110	
58	BZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	H2U	AY	16	-	-	-	X
24	H2U	AY	17	-	-	-	X

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 153628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	expression tag	UNP P17293
AL	2	VAL	-	expression tag	UNP P17293
AL	3	ALA	-	expression tag	UNP P17293
AL	4	LEU	-	expression tag	UNP P17293

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.



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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	14	Total	C	N	O	P	0	0	0
			298	135	56	94	13			

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0
			1644	742	289	535	76	2		

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	405	Total	C	N	O	S	0	0	0
			3142	1983	550	597	12			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	27	ARG	LEU	conflict	UNP Q5SLP7

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O		0	0	0
			651	391	130	130				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O		0	0	0
			700	420	140	140				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	98	Total	C	N	O		0	0	0
			770	486	154	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

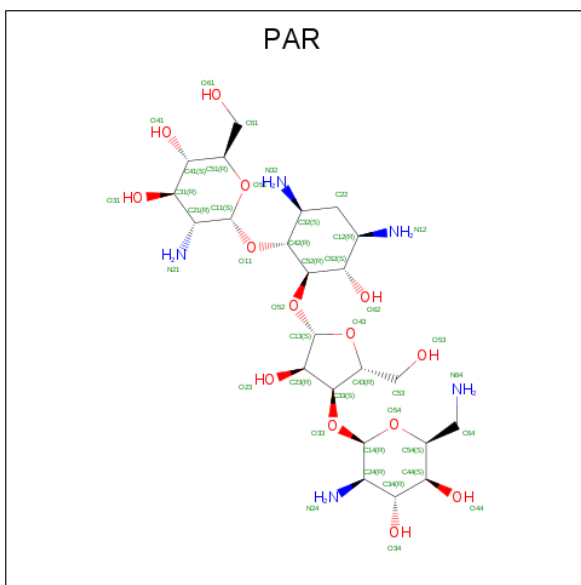
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).

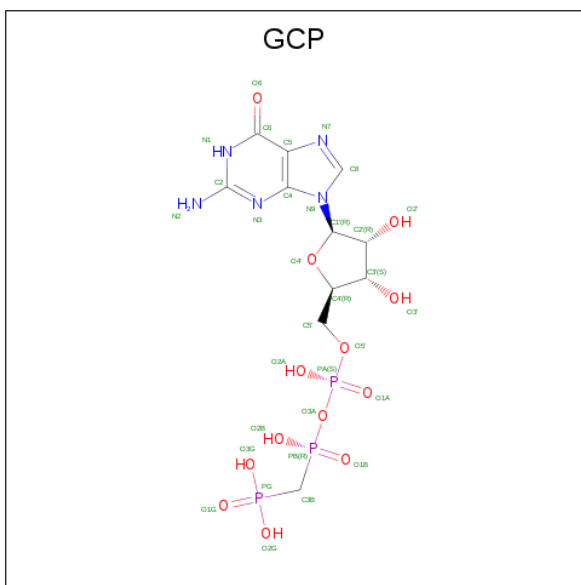


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	N	O	0	0
			42	23	5	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B9	1	Total	Zn	0	0
			1	1		
60	B4	1	Total	Zn	0	0
			1	1		
60	AD	1	Total	Zn	0	0
			1	1		
60	AN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AZ	1	Total Mg 1 1	0	0

- Molecule 63 is water.

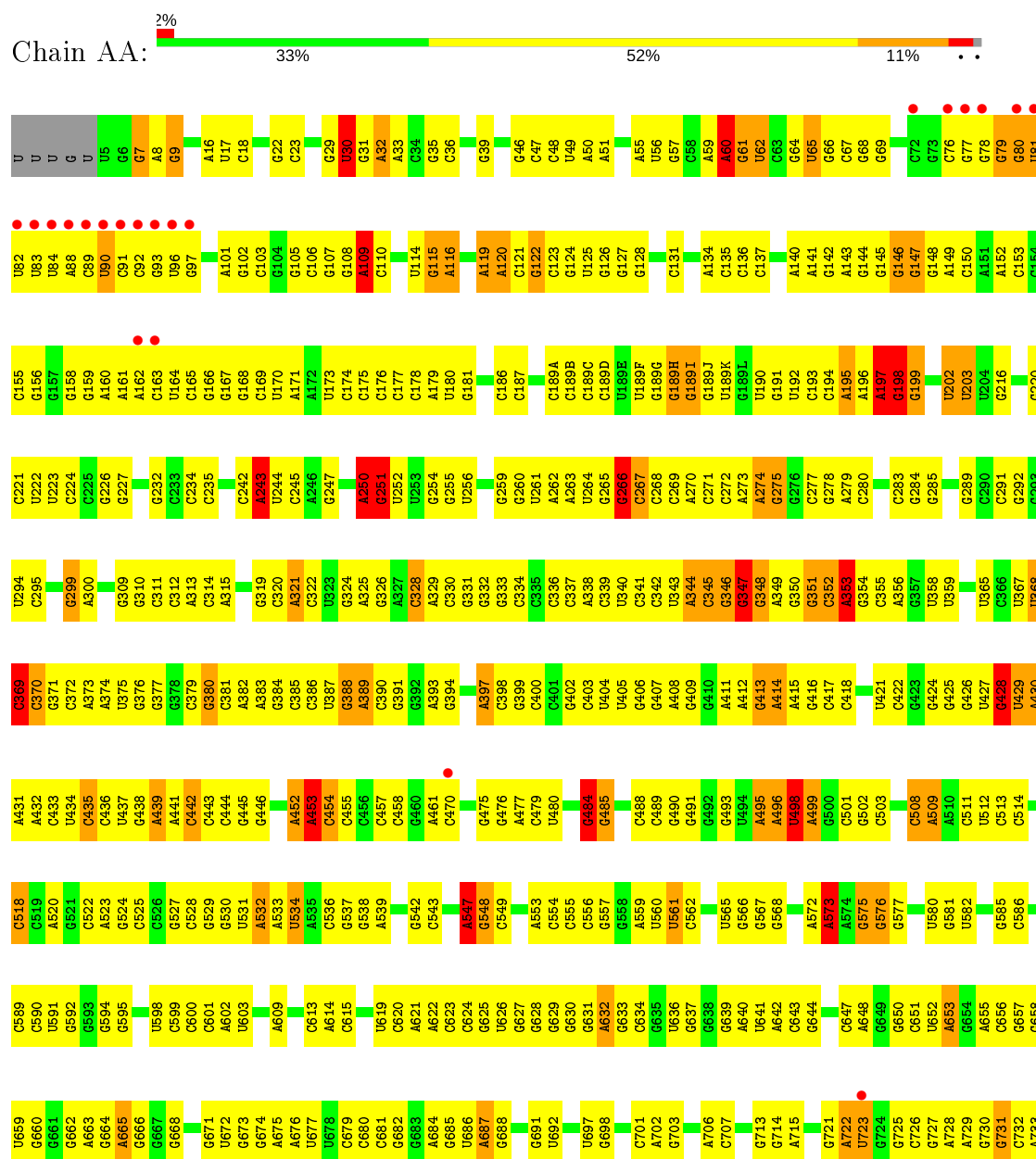
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	AZ	1	Total O 1 1	0	0

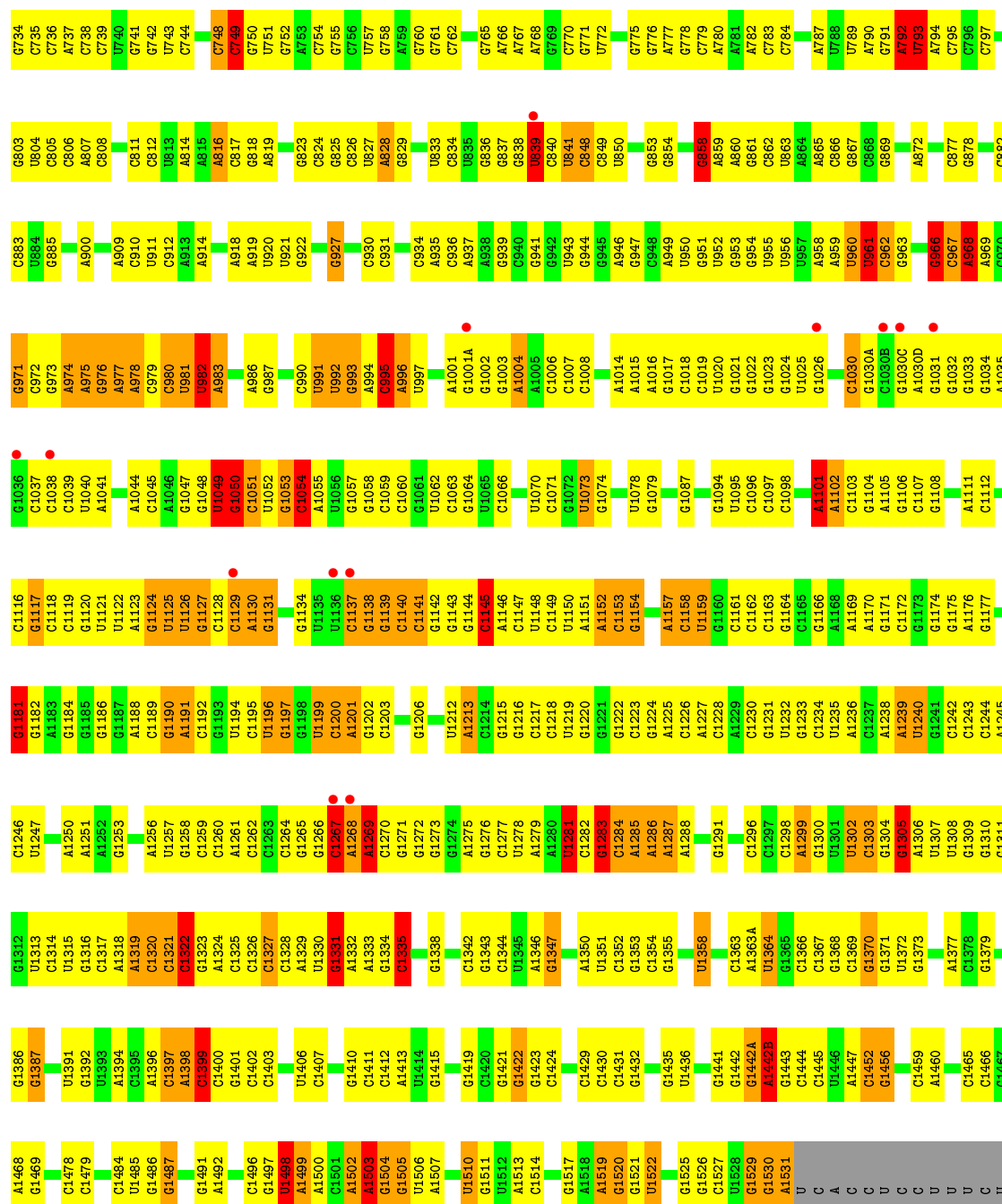


### 3 Residue-property plots

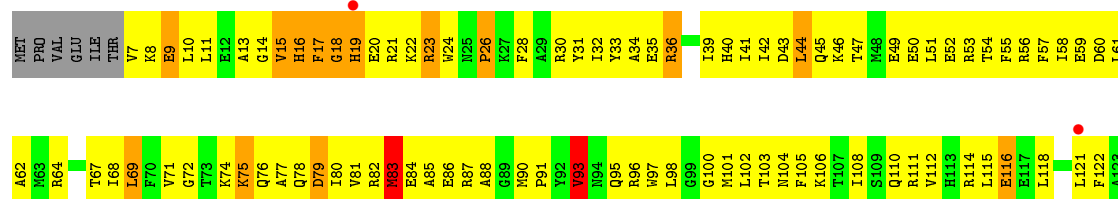
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

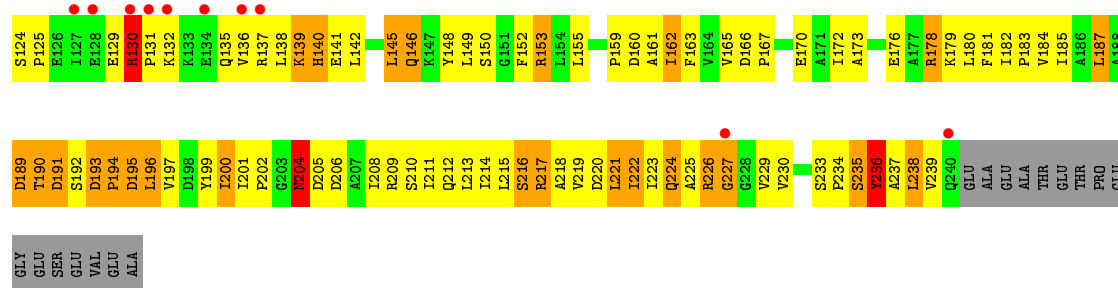
#### • Molecule 1: 16S rRNA





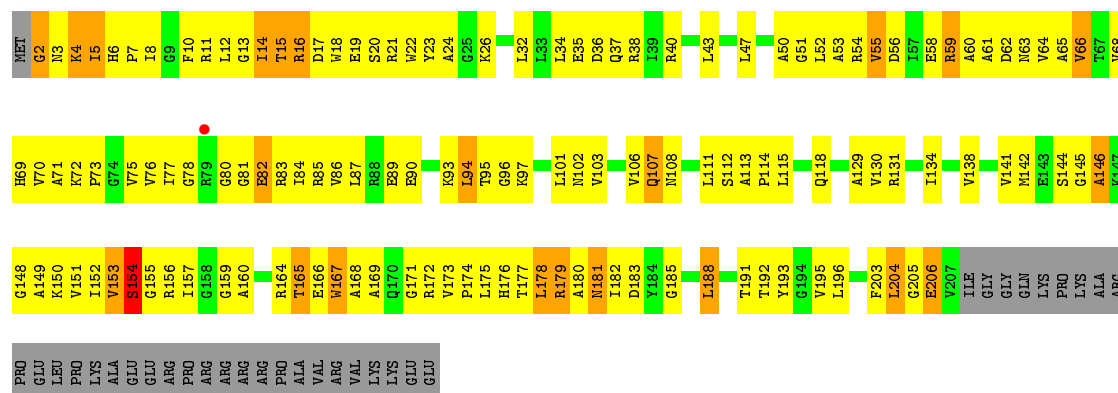
• Molecule 2: 30S RIBOSOMAL PROTEIN S2





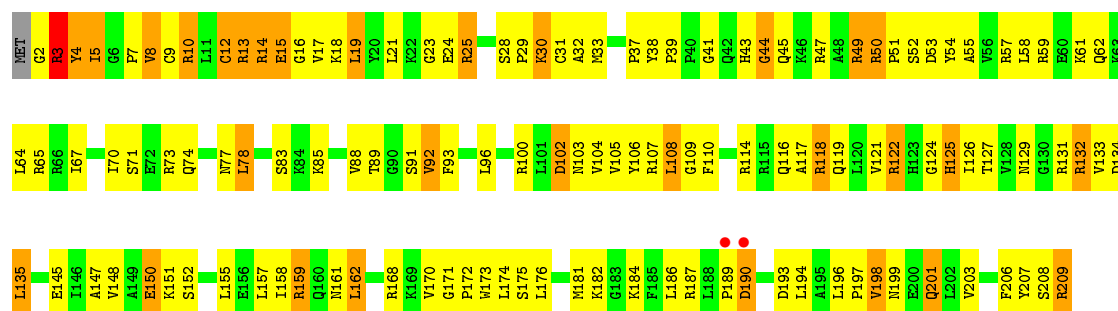
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 29% 48% 9% 14%



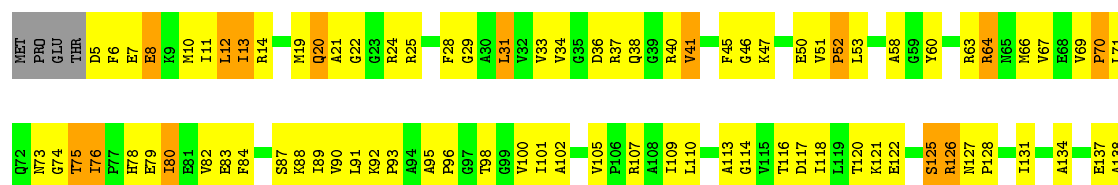
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

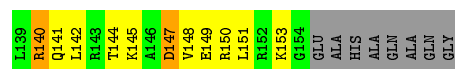
Chain AD: 38% 47% 14%



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE: 34% 49% 10% 7%

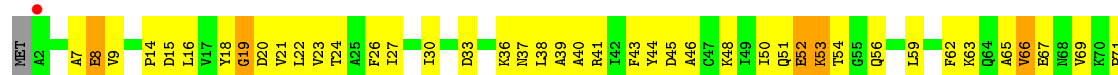




• Molecule 6: 30S RIBOSOMAL PROTEIN S6



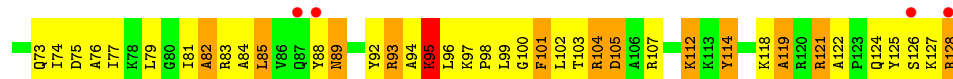
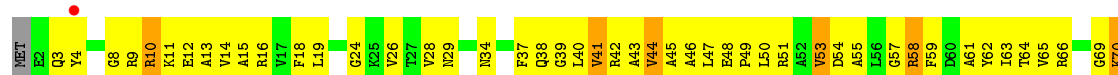
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



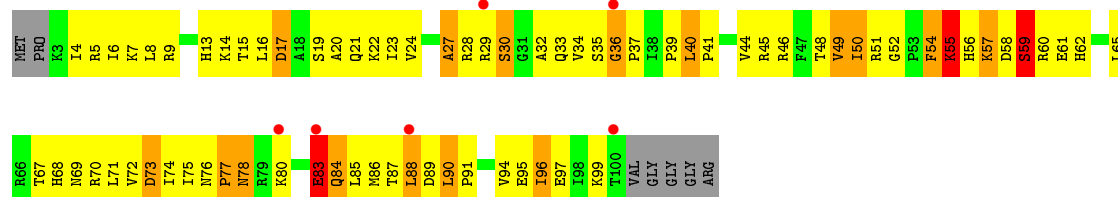
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



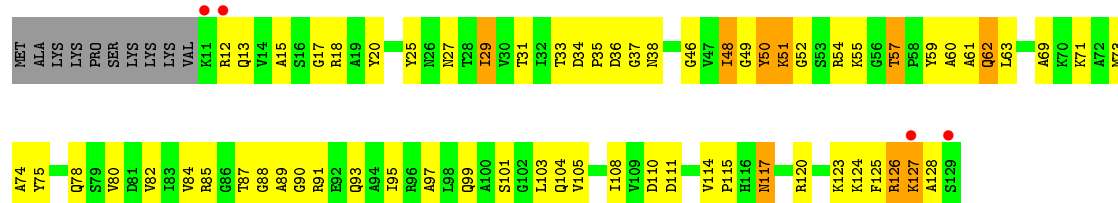
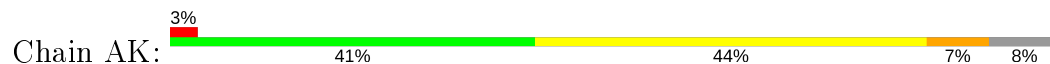
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



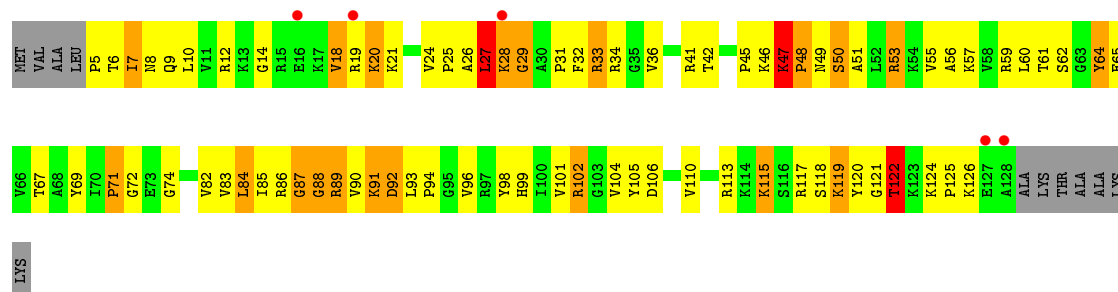
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



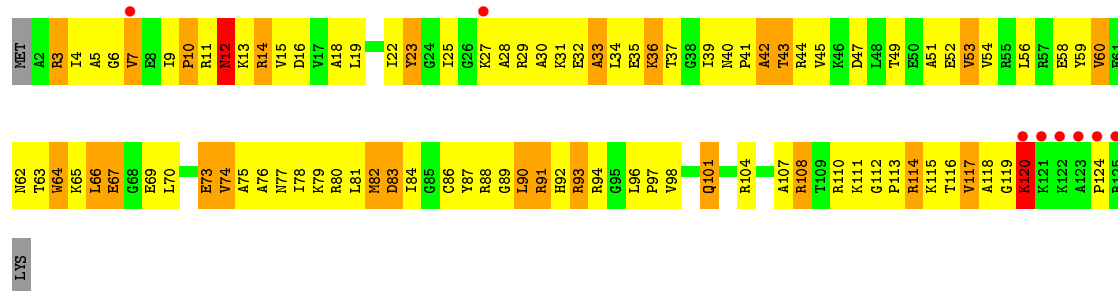
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

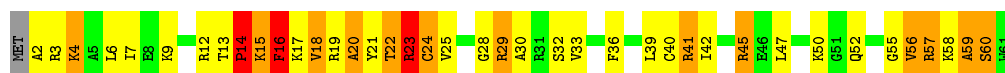


• Molecule 13: 30S RIBOSOMAL PROTEIN S13



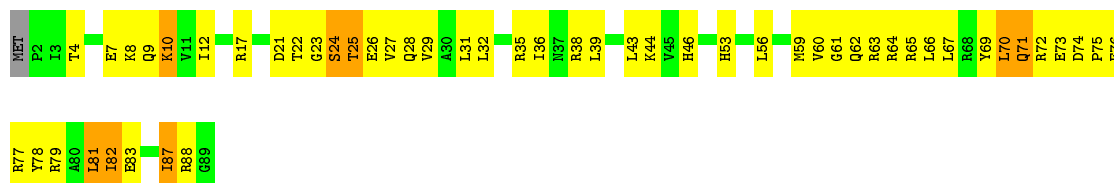
• Molecule 14: 30S RIBOSOMAL PROTEIN S14





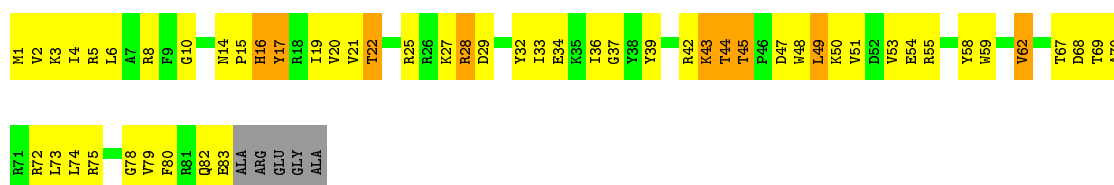
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 40% 49% 9%



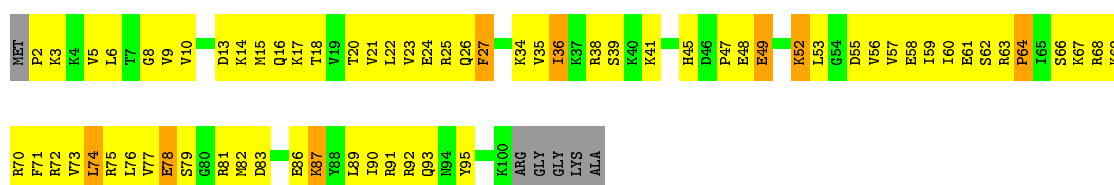
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 33% 51% 10% 6%



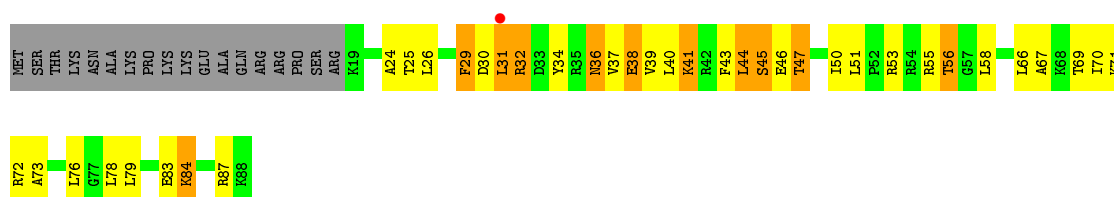
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 30% 57% 8% 6%



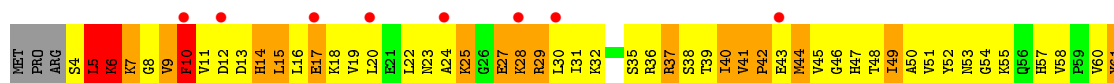
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 36% 31% 13% 20%

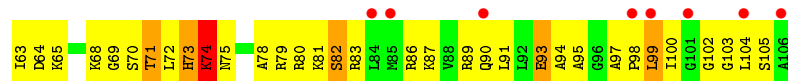


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

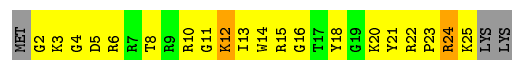
Chain AS: 10% 11% 47% 23% 16%



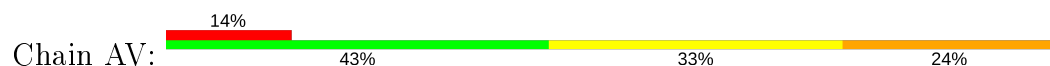
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



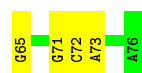
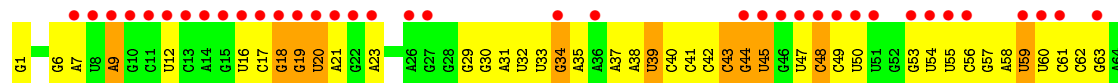
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



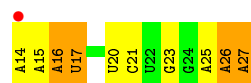
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

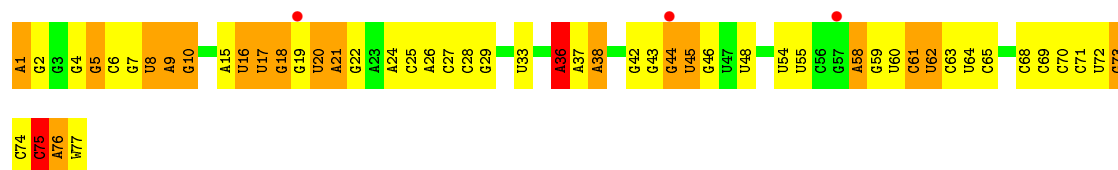


- Molecule 23: mRNA

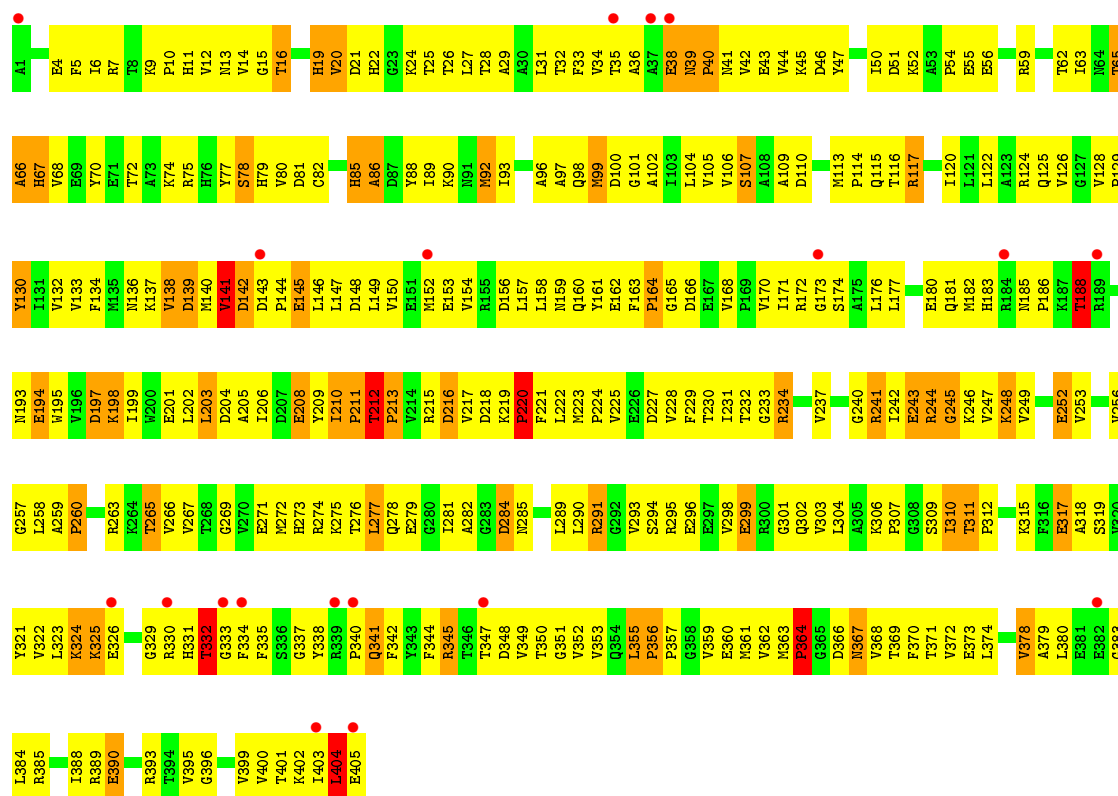


- Molecule 24: A-SITE tRNA G24A TRP-tRNA TRP

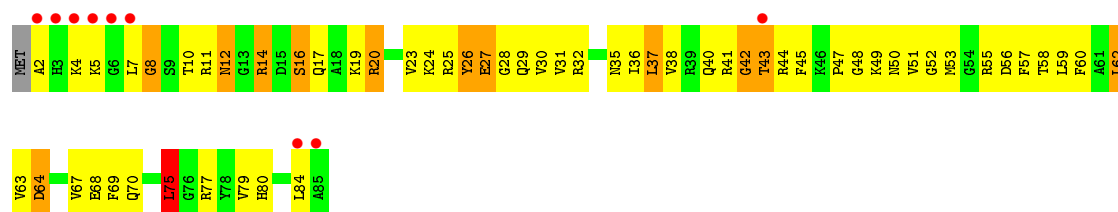




• Molecule 25: ELONGATION FACTOR TU



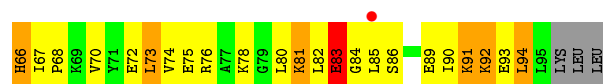
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



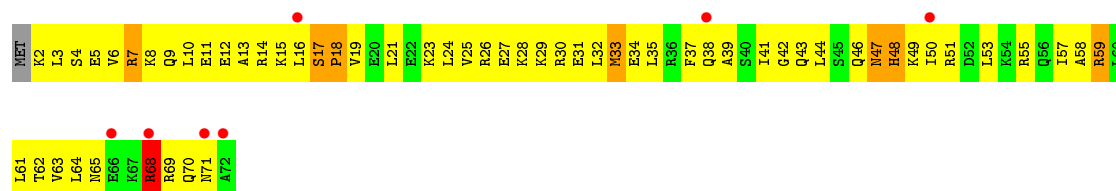
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



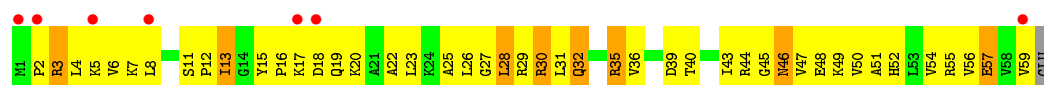




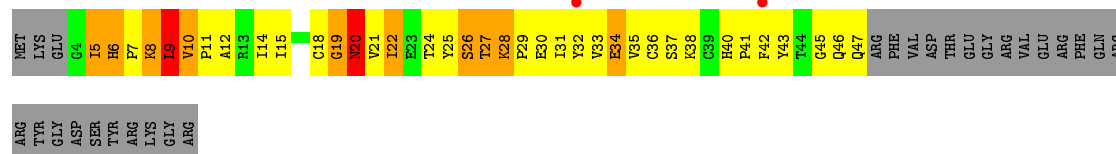
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



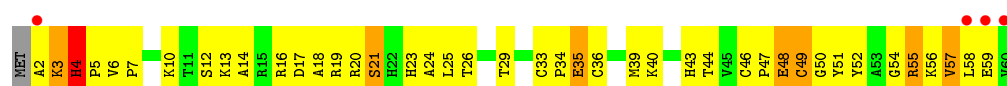
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 31: 50S RIBOSOMAL PROTEIN L32

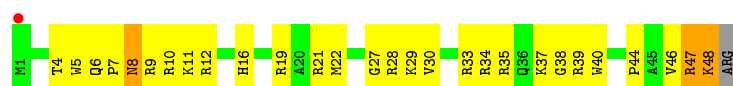


• Molecule 32: 50S RIBOSOMAL PROTEIN L33



• Molecule 33: 50S RIBOSOMAL PROTEIN L34

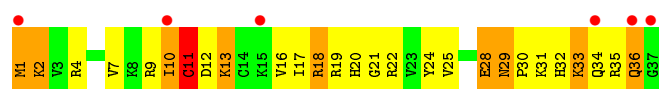




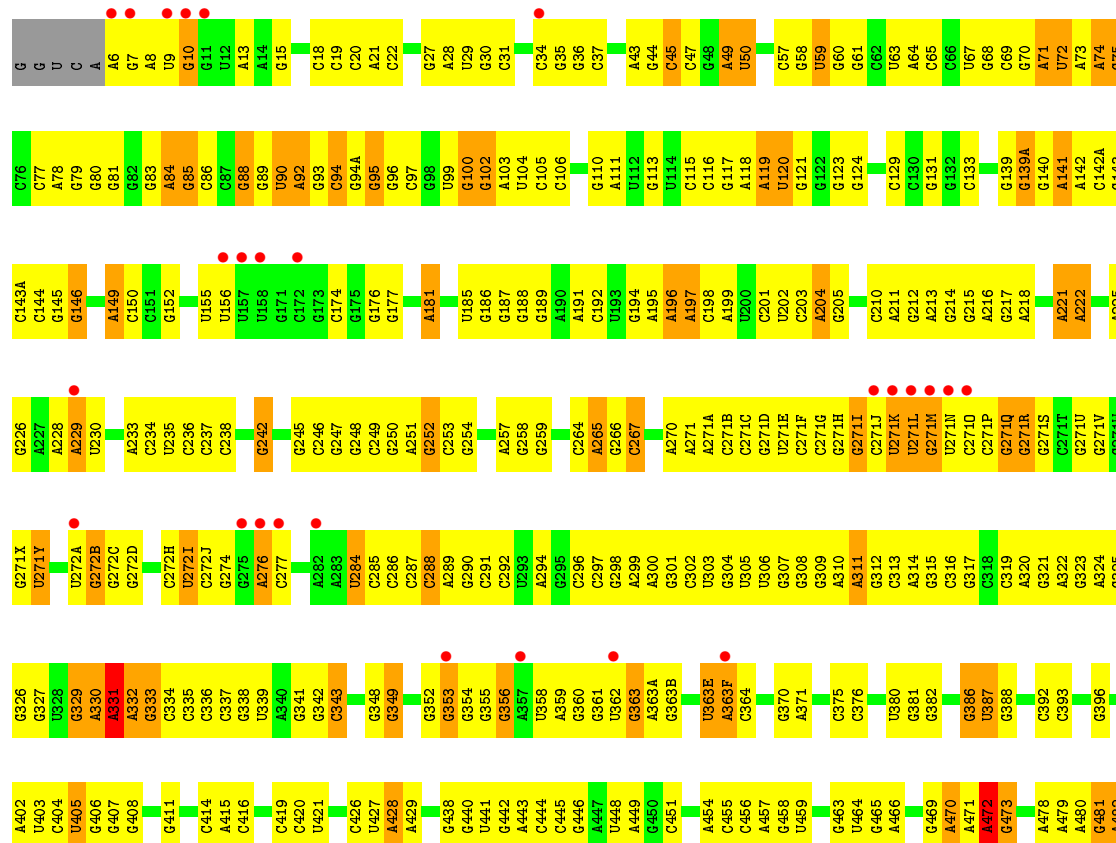
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



• Molecule 35: 50S RIBOSOMAL PROTEIN L36

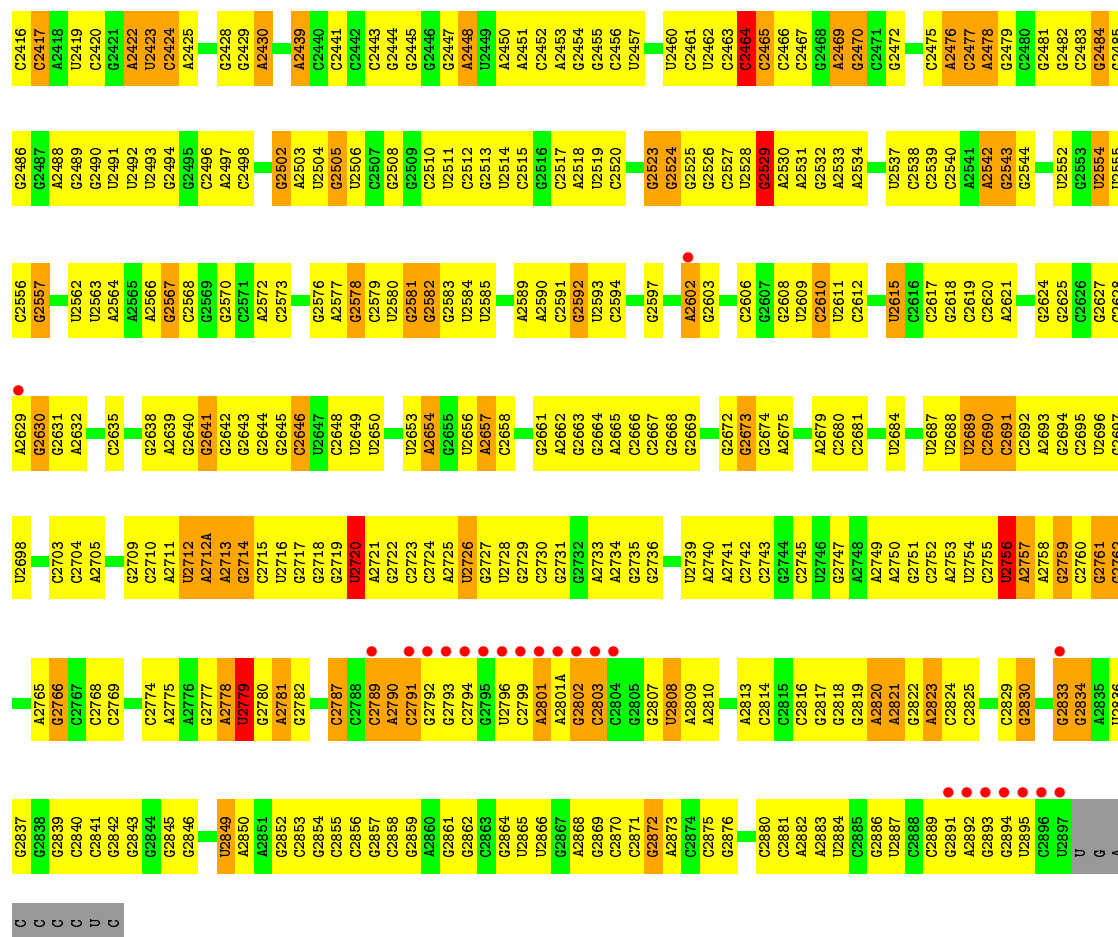


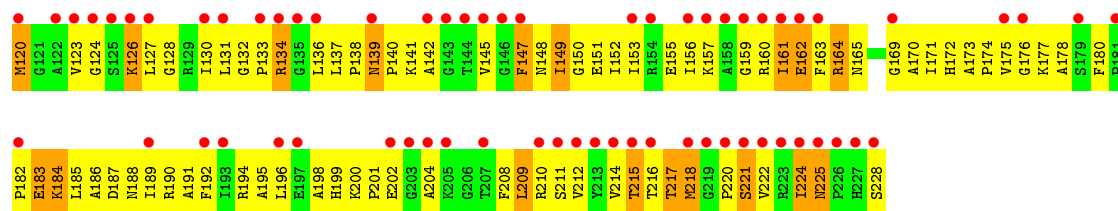
• Molecule 36: 23S RIBOSOMAL RNA



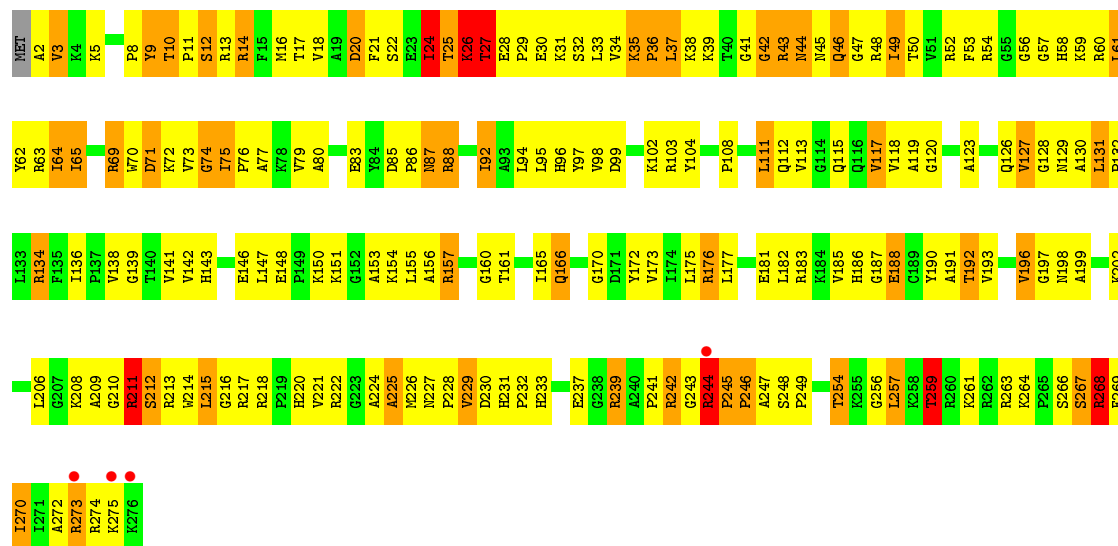
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G2349	G2350	G2351	G2354	G2355	G2356	G2357	A2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	A2376	A2377	A2378	G2379	G2383	G2384	G2385	G2386	G2387	G2391	A2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	U2401	G2402	G2405	G2406	U2408	G2409	G2410	G2411	A2412	G2413	G2414	G2415																																																																																																																																																																																																																																																																																																																								
G2279	G2280	G2281	G2282	G2283	G2284	G2285	A2286	A2287	A2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2303	G2304	A2305	G2306	G2307	G2308	A2309	A2310	A2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	A2319	A2320	A2327	G2328	G2329	G2330	G2331	A2332	A2333	A2336	G2339	G2340	G2341	G2342	G2343	G2344	G2345	A2346	G2347	U2348																																																																																																																																																																																																																																																																																																																					
U2203	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2252	G2257	G2258	G2261	G2262	G2263	G2264	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278																																																																																																																																																																																																																																																																																																															
G2141	G2142	G2143	U2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	A2198	G2199	G2200																																																																																																																																																																																																																																																																																																																		
G2078	U2079	G2080	G2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140																																																																																																																																																																																																																																																																																																																			
G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019	A2020	U2021	U2022	G2023	G2024	G2025	G2026	G2027	U2028	G2029	A2030	A2031	A2032	A2033	U2034	G2035	G2036	G2037	A2038	A2039	A2040	G2041	G2042	G2043	G2046	U2047	G2048	G2049	G2050	A2051	G2052	G2053	A2054	G2055	G2056	A2059	A2060	G2061	G2062	G2063	G2064	G2065	G2066	G2067	U2068	G2069	G2072	G2073	U2074	U2011																																																																																																																																																																																																																																																																																																																				
A1936	A1937	A1938	U1939	U1940	U1943	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1980	U1981	U1982	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	G2000	A2001	G2002	U2006	G2007	G2008	G2009	G2010	U2011																																																																																																																																																																																																																																																																																																																						
U1851	G1852	A1853	A1854	G1858	A1859	G1861	G1862	U1863	U1864	U1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1881	G1882	G1883	G1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893	G1894	G1895	G1896	G1897	G1898	G1899	G1900	G1901	G1902	G1903	G1906	G1907	G1908	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1927	A1928	A1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	G2000	A2001	G2002	U2006	G2007	G2008	G2009	G2010	U2011																																																																																																																																																																																																																															
C1781	C1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	A1790	A1791	U1794	C1795	U1796	U1797	U1798	U1799	C1800	G1801	G1802	G1803	C1804	U1805	U1806	C1807	U1808	U1809	A1810	U1811	U1812	G1813	G1816	U1817	U1818	U1819	U1820	G1824	G1825	G1826	G1827	G1828	A1829	C1830	G1831	C1832	G1835	G1836	C1837	G1842	G1843	G1844	G1845	G1846	A1847	A1848	U1851	G1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1906	A1907	A1908	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1927	A1928	A1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	G2000	A2001	G2002	U2006	G2007	G2008	G2009	G2010	U2011																																																																																																																																																																		
U1692	G1696	G1697	A1698	A1701	G1702	C1708	U1709	C1710	G1714	G1717	G1718	G1719	U1720	G1721	G1722	U1739	G1740	A1741	G1742	C1743	G1744	G1745	G1746	G1747	G1748	A1749	G1750	C1751	G1754	A1755	G1756	U1757	G1758	A1762	G1763	G1764	G1765	U1766	U1767	U1768	U1769	G1770	G1771	G1772	A1773	G1774	U1775	U1776	U1777	U1778	U1779	A1780	U1851	G1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1906	A1907	A1908	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1927	A1928	A1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	G2000	A2001	G2002	U2006	G2007	G2008	G2009	G2010	U2011																																																																																																																																																																				
A1542	C1543	A1544	C1547	C1548	C1549	C1550	C1551	C1552	C1553	A1554	G1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	U1602	A1603	A1604	C1605	G1606	C1607	A1608	A1609	U1610	C1611	G1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911

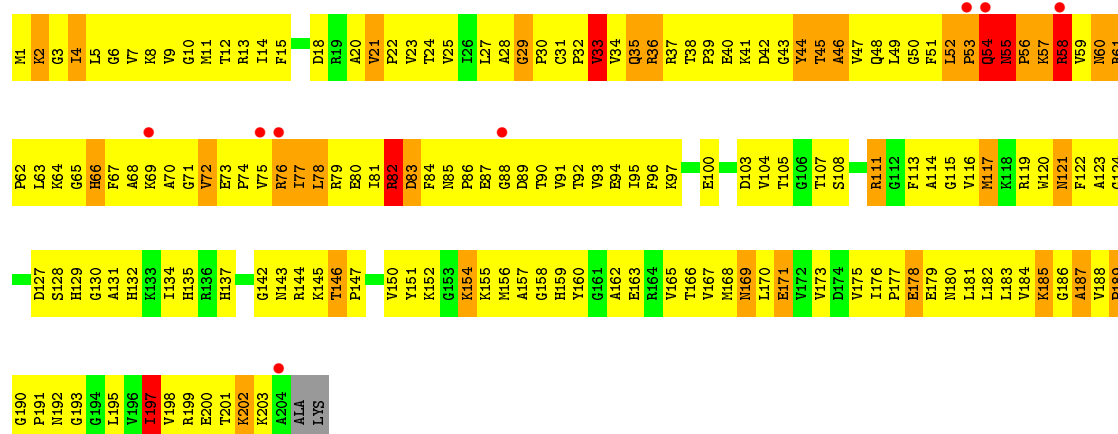




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

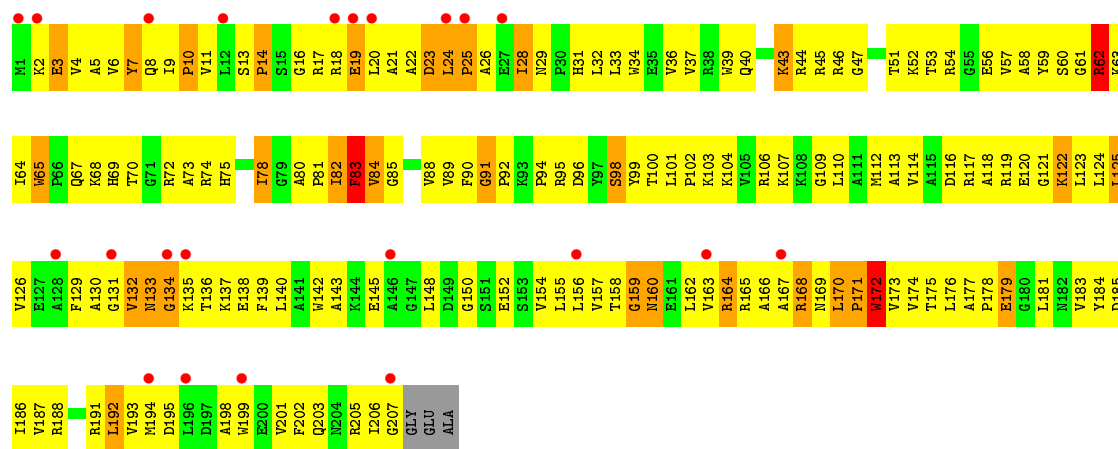


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

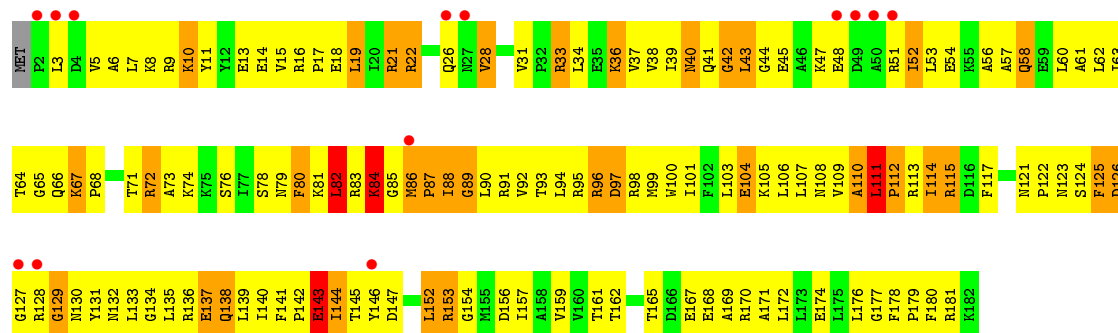


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

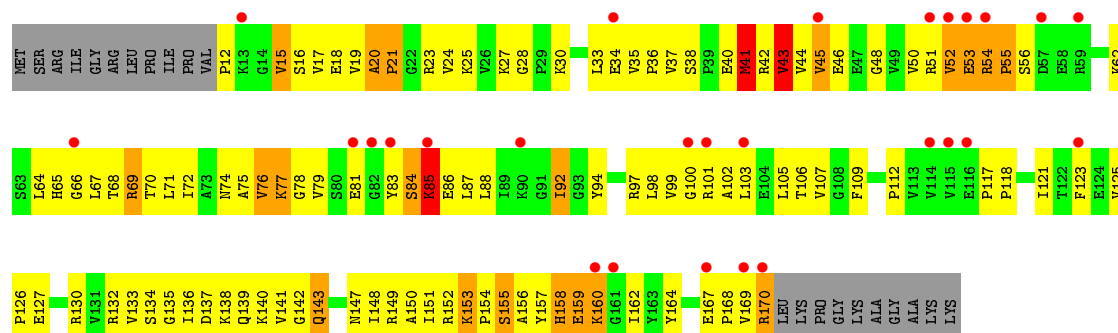




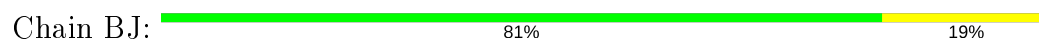
• Molecule 42: 50S RIBOSOMAL PROTEIN L5




• Molecule 43: 50S RIBOSOMAL PROTEIN L6

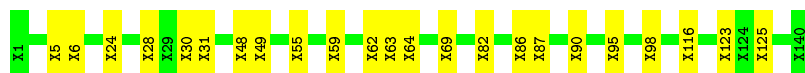


• Molecule 44: 50S RIBOSOMAL PROTEIN L10



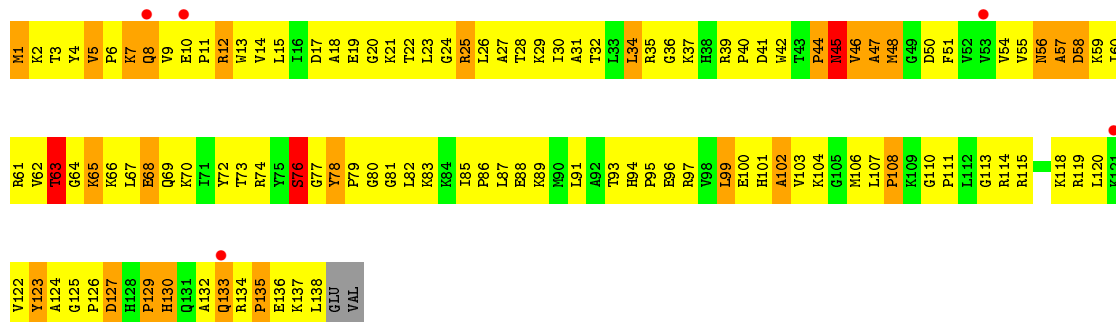
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:  84% 16%



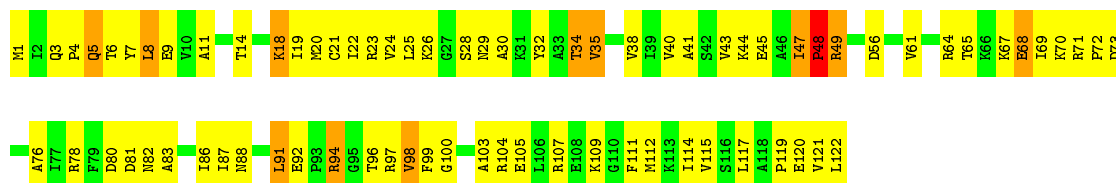
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:  4% 15% 63% 19%




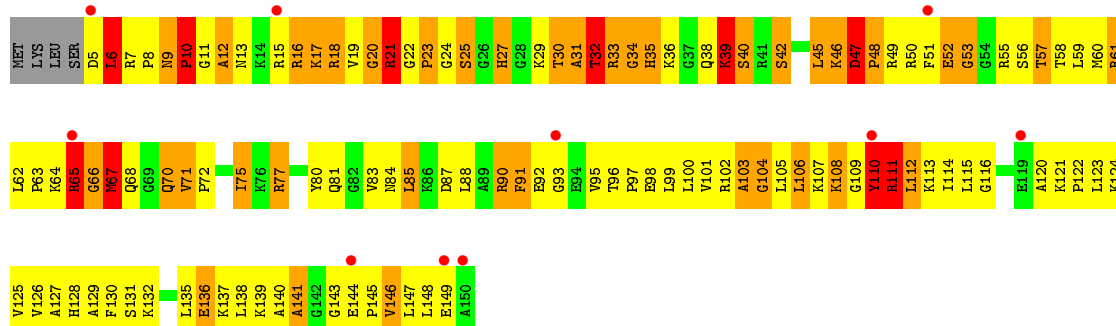
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:  38% 52% 9%



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:  7% 17% 48% 26% 7%

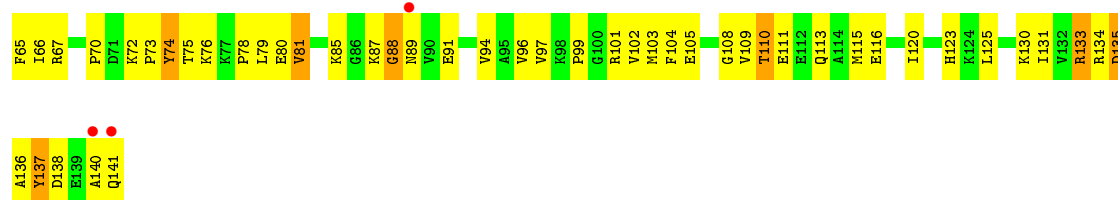


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

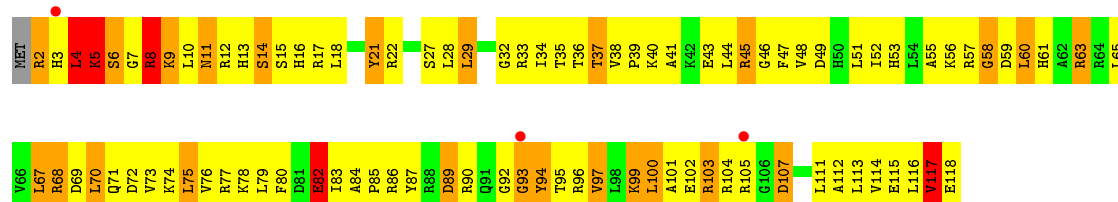
Chain BQ:  4% 34% 54% 12%



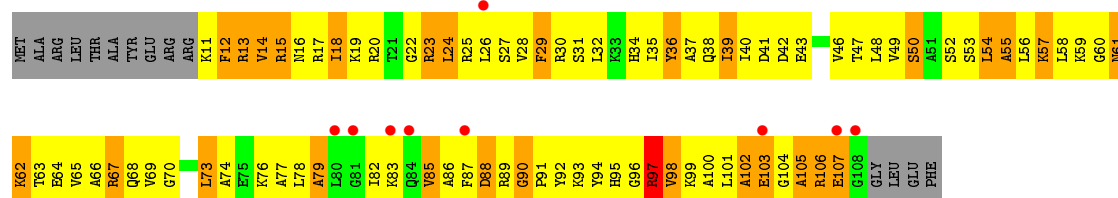
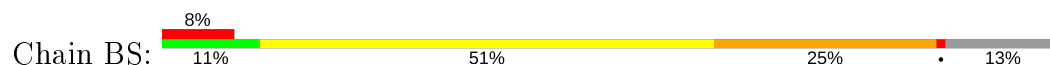




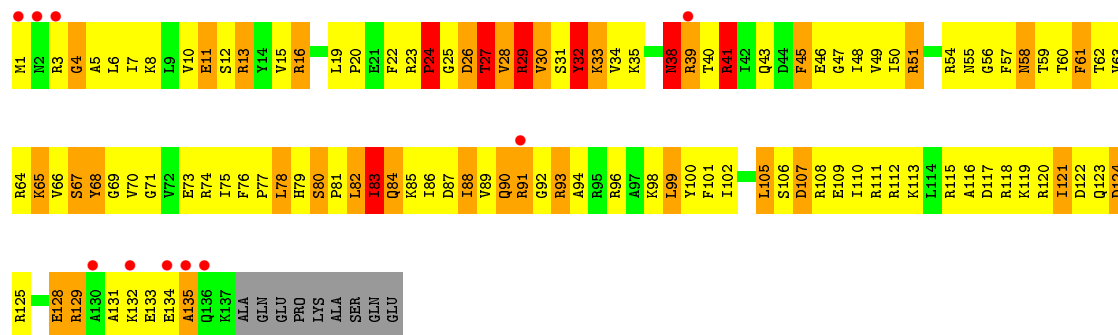
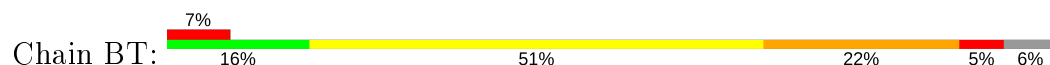
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

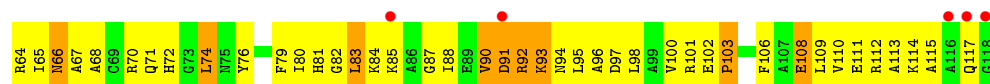


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

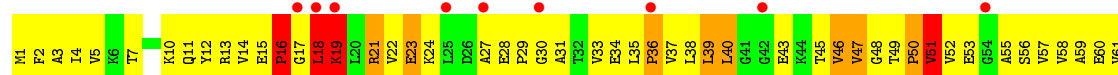


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

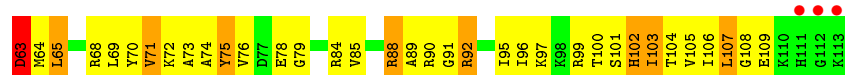
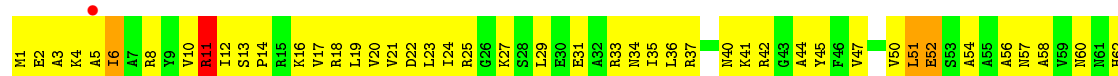




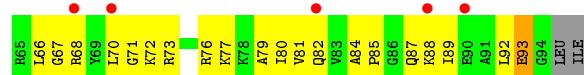
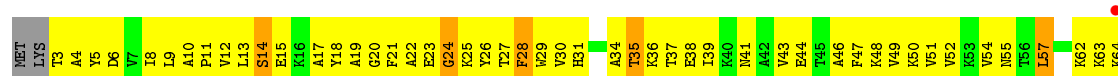
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



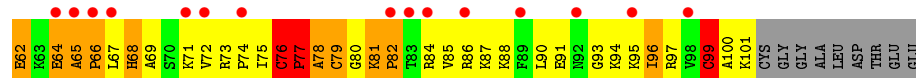
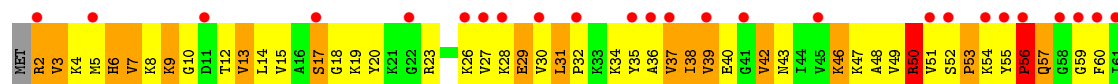
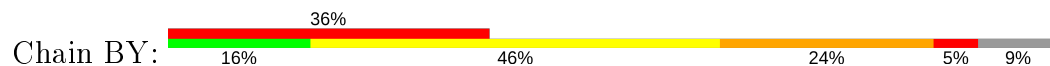
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



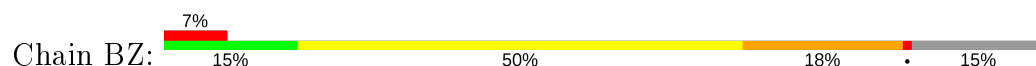
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.60Å 274.93Å 282.46Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 48.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.10) 95.9 (48.00-3.01)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.231 , 0.268 0.232 , 0.268	Depositor DCC
$R_{free}$ test set	28503 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 85.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k 0.019 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	153628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: OMC, 5MU, PAR, 4SU, GCP, MIA, MG, H2U, ZN, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.58	3/36190 (0.0%)	0.77	49/56486 (0.1%)
2	AB	0.44	0/1935	0.72	1/2609 (0.0%)
3	AC	0.50	1/1636 (0.1%)	0.75	0/2205
4	AD	0.44	0/1733	0.71	1/2318 (0.0%)
5	AE	0.54	0/1162	0.75	0/1564
6	AF	0.45	0/856	0.69	1/1154 (0.1%)
7	AG	0.43	0/1276	0.66	0/1709
8	AH	0.45	0/1136	0.73	0/1527
9	AI	0.45	0/1029	0.71	0/1378
10	AJ	0.49	0/807	0.78	0/1085
11	AK	0.45	0/900	0.72	0/1213
12	AL	0.58	0/986	0.88	2/1320 (0.2%)
13	AM	0.42	0/998	0.79	2/1336 (0.1%)
14	AN	0.54	0/501	0.79	0/664
15	AO	0.42	0/745	0.66	0/992
16	AP	0.44	0/716	0.74	0/963
17	AQ	0.44	0/836	0.70	0/1117
18	AR	0.47	0/579	0.76	0/768
19	AS	0.44	0/642	0.72	0/865
20	AT	0.39	0/765	0.72	1/1007 (0.1%)
21	AU	0.45	0/212	0.69	0/277
22	AV	0.49	0/1809	0.75	0/2819
22	AW	0.45	0/1809	0.73	0/2819
23	AX	0.65	0/334	0.81	0/519
24	AY	0.49	1/1618 (0.1%)	0.78	3/2514 (0.1%)
25	AZ	0.41	0/3203	0.68	1/4346 (0.0%)
26	B0	0.39	0/671	0.73	0/892
27	B1	0.44	0/738	0.74	0/981
28	B2	0.35	0/600	0.63	0/793
29	B3	0.37	0/472	0.66	0/634
30	B4	0.41	0/349	0.60	0/474
31	B5	0.38	0/473	0.72	0/639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	B6	0.66	0/440	0.98	2/586 (0.3%)
33	B7	0.43	0/426	0.71	0/561
34	B8	0.55	0/515	0.83	1/679 (0.1%)
35	B9	0.45	0/310	0.65	0/407
36	BA	0.51	2/69976 (0.0%)	0.74	57/109244 (0.1%)
37	BB	0.40	0/2853	0.72	0/4451
38	BC	0.42	2/1774 (0.1%)	0.67	0/2391
39	BD	0.57	0/2195	0.91	3/2955 (0.1%)
40	BE	0.41	0/1596	0.71	0/2153
41	BF	0.37	0/1658	0.68	0/2244
42	BG	0.37	0/1499	0.68	1/2016 (0.0%)
43	BH	0.36	0/1245	0.70	0/1682
46	BN	0.36	0/1131	0.69	0/1525
47	BO	0.50	0/943	0.76	0/1269
48	BP	0.48	0/1131	0.98	4/1504 (0.3%)
49	BQ	0.45	0/1143	0.69	0/1527
50	BR	0.35	0/974	0.74	1/1302 (0.1%)
51	BS	0.42	0/778	0.77	0/1036
52	BT	0.44	0/1155	0.80	2/1542 (0.1%)
53	BU	0.39	0/975	0.65	0/1297
54	BV	0.36	0/790	0.70	0/1057
55	BW	0.37	0/907	0.68	0/1216
56	BX	0.43	0/739	0.66	1/993 (0.1%)
57	BY	0.38	0/788	0.73	0/1051
58	BZ	0.39	0/1435	0.67	0/1949
All	All	0.50	9/165092 (0.0%)	0.74	133/246624 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	3	51
23	AX	0	1
24	AY	2	1
36	BA	4	70
37	BB	0	2
All	All	9	125

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	761	A	C5-C6	-8.40	1.33	1.41
24	AY	1	A	OP3-P	-6.72	1.53	1.61
38	BC	120	MET	CG-SD	6.37	1.97	1.81
1	AA	1267	C	C5'-C4'	6.34	1.58	1.51
36	BA	2506	U	N1-C2	5.99	1.44	1.38

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	10.24	132.03	109.50
1	AA	508	C	C2'-C3'-O3'	10.16	131.85	109.50
36	BA	654(I)	C	N1-C1'-C2'	10.03	127.04	114.00
24	AY	75	C	C2'-C3'-O3'	9.40	130.19	109.50
36	BA	1799	G	C2'-C3'-O3'	9.36	130.09	109.50

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1498	U	C3'
1	AA	1504	G	C3'
24	AY	36	A	C3'
24	AY	75	C	C3'

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	198	G	Sidechain
1	AA	250	A	Sidechain
1	AA	50	A	Sidechain
1	AA	62	U	Sidechain
1	AA	7	G	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1085	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1900	0	1951	250	0
3	AC	1612	0	1677	139	0
4	AD	1703	0	1764	151	0
5	AE	1146	0	1207	100	0
6	AF	843	0	857	52	0
7	AG	1257	0	1296	120	0
8	AH	1116	0	1177	91	0
9	AI	1011	0	1043	128	0
10	AJ	794	0	840	135	0
11	AK	885	0	904	76	0
12	AL	970	0	1057	110	0
13	AM	987	0	1059	131	0
14	AN	492	0	529	66	0
15	AO	734	0	771	61	0
16	AP	700	0	720	65	0
17	AQ	823	0	891	82	0
18	AR	574	0	644	37	0
19	AS	629	0	652	125	0
20	AT	763	0	861	107	0
21	AU	208	0	221	29	0
22	AV	1619	0	822	61	0
22	AW	1619	0	822	85	0
23	AX	298	0	152	26	0
24	AY	1644	0	853	68	0
25	AZ	3142	0	3152	385	0
26	B0	662	0	688	107	0
27	B1	731	0	808	83	0
28	B2	598	0	653	77	0
29	B3	467	0	523	59	0
30	B4	340	0	337	57	0
31	B5	459	0	480	79	0
32	B6	433	0	461	135	0
33	B7	418	0	467	31	0
34	B8	507	0	576	104	0
35	B9	307	0	335	48	0
36	BA	62477	0	31497	2447	2
37	BB	2551	0	1295	115	0
38	BC	1742	0	1800	349	0
39	BD	2145	0	2234	324	0
40	BE	1563	0	1629	273	0
41	BF	1623	0	1677	250	0
42	BG	1474	0	1535	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BH	1222	0	1282	170	0
44	BJ	651	0	152	15	0
45	BK	700	0	166	13	0
46	BN	1104	0	1180	181	0
47	BO	933	0	996	92	0
48	BP	1114	0	1187	297	0
49	BQ	1122	0	1179	149	0
50	BR	960	0	1021	148	0
51	BS	770	0	832	169	0
52	BT	1141	0	1202	250	0
53	BU	958	0	1015	159	0
54	BV	779	0	852	127	0
55	BW	896	0	953	104	0
56	BX	725	0	778	97	0
57	BY	775	0	870	197	0
58	BZ	1403	0	1432	241	0
59	AA	42	0	45	2	0
60	AD	1	0	0	1	0
60	AN	1	0	0	0	0
60	B4	1	0	0	0	0
60	B9	1	0	0	0	0
61	AZ	32	0	14	5	0
62	AZ	1	0	0	0	0
63	AZ	1	0	0	0	0
All	All	153628	0	104391	9953	2

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 39.

The worst 5 of 9953 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)
36:BA:1899:G:N2	36:BA:1902:C:H41	1.36	1.21
36:BA:2833:G:H3'	36:BA:2834:G:H5''	1.24	1.20
24:AY:1:A:H5'	25:AZ:90:LYS:HZ2	1.06	1.17
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.22	1.17
55:BW:14:PRO:HG2	55:BW:78:GLU:HG3	1.22	1.17

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1267:C:O5'	36:BA:654(I):C:O4'[2_746]	1.83	0.37
1:AA:1266:G:O3'	36:BA:654(I):C:O4'[2_746]	2.16	0.04

## 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	
2	AB	232/256 (91%)	163 (70%)	41 (18%)	28 (12%)	0	1
3	AC	204/239 (85%)	155 (76%)	33 (16%)	16 (8%)	1	5
4	AD	206/209 (99%)	157 (76%)	34 (16%)	15 (7%)	1	6
5	AE	148/162 (91%)	125 (84%)	16 (11%)	7 (5%)	2	14
6	AF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	1	6
7	AG	153/156 (98%)	118 (77%)	25 (16%)	10 (6%)	1	8
8	AH	136/138 (99%)	118 (87%)	16 (12%)	2 (2%)	10	39
9	AI	125/128 (98%)	83 (66%)	29 (23%)	13 (10%)	0	3
10	AJ	96/105 (91%)	67 (70%)	17 (18%)	12 (12%)	0	1
11	AK	117/129 (91%)	94 (80%)	19 (16%)	4 (3%)	3	21
12	AL	122/135 (90%)	89 (73%)	20 (16%)	13 (11%)	0	2
13	AM	122/126 (97%)	74 (61%)	27 (22%)	21 (17%)	0	0
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	0
15	AO	86/89 (97%)	65 (76%)	17 (20%)	4 (5%)	2	14
16	AP	81/88 (92%)	62 (76%)	14 (17%)	5 (6%)	1	9
17	AQ	97/105 (92%)	74 (76%)	18 (19%)	5 (5%)	2	12
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	1	6
19	AS	76/93 (82%)	41 (54%)	21 (28%)	14 (18%)	0	0
20	AT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	1	5
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	AZ	403/405 (100%)	285 (71%)	83 (21%)	35 (9%)	1	4
26	B0	82/85 (96%)	65 (79%)	12 (15%)	5 (6%)	1	9
27	B1	91/98 (93%)	73 (80%)	9 (10%)	9 (10%)	0	3
28	B2	69/72 (96%)	46 (67%)	15 (22%)	8 (12%)	0	2
29	B3	57/60 (95%)	40 (70%)	9 (16%)	8 (14%)	0	1
30	B4	42/71 (59%)	23 (55%)	11 (26%)	8 (19%)	0	0
31	B5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	1
32	B6	48/54 (89%)	23 (48%)	12 (25%)	13 (27%)	0	0
33	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
34	B8	61/65 (94%)	34 (56%)	17 (28%)	10 (16%)	0	0
35	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	1
38	BC	226/229 (99%)	161 (71%)	46 (20%)	19 (8%)	1	5
39	BD	273/276 (99%)	219 (80%)	28 (10%)	26 (10%)	0	3
40	BE	202/206 (98%)	116 (57%)	53 (26%)	33 (16%)	0	0
41	BF	205/210 (98%)	144 (70%)	35 (17%)	26 (13%)	0	1
42	BG	179/182 (98%)	107 (60%)	47 (26%)	25 (14%)	0	1
43	BH	157/180 (87%)	96 (61%)	42 (27%)	19 (12%)	0	1
46	BN	136/140 (97%)	93 (68%)	21 (15%)	22 (16%)	0	0
47	BO	120/122 (98%)	97 (81%)	16 (13%)	7 (6%)	1	10
48	BP	144/150 (96%)	74 (51%)	36 (25%)	34 (24%)	0	0
49	BQ	139/141 (99%)	108 (78%)	24 (17%)	7 (5%)	2	13
50	BR	115/118 (98%)	72 (63%)	28 (24%)	15 (13%)	0	1
51	BS	96/112 (86%)	37 (38%)	37 (38%)	22 (23%)	0	0
52	BT	135/146 (92%)	85 (63%)	27 (20%)	23 (17%)	0	0
53	BU	115/118 (98%)	72 (63%)	34 (30%)	9 (8%)	1	5
54	BV	99/101 (98%)	69 (70%)	13 (13%)	17 (17%)	0	0
55	BW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	5
56	BX	90/96 (94%)	67 (74%)	15 (17%)	8 (9%)	1	4
57	BY	98/110 (89%)	45 (46%)	26 (26%)	27 (28%)	0	0
58	BZ	174/206 (84%)	108 (62%)	39 (22%)	27 (16%)	0	0
All	All	6150/6553 (94%)	4274 (70%)	1193 (19%)	683 (11%)	0	2

5 of 683 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	191	ASP
2	AB	194	PRO
2	AB	195	ASP
3	AC	146	ALA
4	AD	4	TYR

### 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	
2	AB	202/220 (92%)	171 (85%)	31 (15%)	2	12
3	AC	160/188 (85%)	139 (87%)	21 (13%)	4	17
4	AD	180/181 (99%)	159 (88%)	21 (12%)	5	22
5	AE	115/123 (94%)	96 (84%)	19 (16%)	2	10
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	19
7	AG	126/127 (99%)	118 (94%)	8 (6%)	18	48
8	AH	119/119 (100%)	104 (87%)	15 (13%)	4	18
9	AI	98/99 (99%)	85 (87%)	13 (13%)	4	16
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	3	13
11	AK	90/99 (91%)	80 (89%)	10 (11%)	6	24
12	AL	104/111 (94%)	88 (85%)	16 (15%)	2	11
13	AM	99/101 (98%)	85 (86%)	14 (14%)	3	15
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	5
15	AO	79/80 (99%)	73 (92%)	6 (8%)	13	41
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	24
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
18	AR	61/77 (79%)	55 (90%)	6 (10%)	8	29
19	AS	69/80 (86%)	54 (78%)	15 (22%)	1	4
20	AT	76/82 (93%)	66 (87%)	10 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	54
25	AZ	339/339 (100%)	289 (85%)	50 (15%)	3	13
26	B0	66/67 (98%)	55 (83%)	11 (17%)	2	9
27	B1	78/83 (94%)	65 (83%)	13 (17%)	2	9
28	B2	66/67 (98%)	61 (92%)	5 (8%)	13	41
29	B3	51/52 (98%)	48 (94%)	3 (6%)	19	50
30	B4	39/63 (62%)	30 (77%)	9 (23%)	1	3
31	B5	51/52 (98%)	46 (90%)	5 (10%)	8	29
32	B6	49/52 (94%)	39 (80%)	10 (20%)	1	5
33	B7	41/42 (98%)	35 (85%)	6 (15%)	3	13
34	B8	53/55 (96%)	43 (81%)	10 (19%)	1	6
35	B9	34/34 (100%)	27 (79%)	7 (21%)	1	5
38	BC	180/181 (99%)	159 (88%)	21 (12%)	5	22
39	BD	217/218 (100%)	175 (81%)	42 (19%)	1	6
40	BE	165/166 (99%)	142 (86%)	23 (14%)	3	15
41	BF	165/166 (99%)	149 (90%)	16 (10%)	8	30
42	BG	155/156 (99%)	132 (85%)	23 (15%)	3	13
43	BH	132/148 (89%)	124 (94%)	8 (6%)	18	49
46	BN	117/119 (98%)	102 (87%)	15 (13%)	4	18
47	BO	100/100 (100%)	92 (92%)	8 (8%)	12	40
48	BP	112/116 (97%)	87 (78%)	25 (22%)	1	3
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	18
50	BR	100/101 (99%)	81 (81%)	19 (19%)	1	6
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	14
52	BT	120/127 (94%)	96 (80%)	24 (20%)	1	5
53	BU	92/94 (98%)	81 (88%)	11 (12%)	5	20
54	BV	82/82 (100%)	72 (88%)	10 (12%)	5	19
55	BW	91/92 (99%)	80 (88%)	11 (12%)	5	20
56	BX	74/78 (95%)	68 (92%)	6 (8%)	11	39
57	BY	84/91 (92%)	71 (84%)	13 (16%)	2	11
58	BZ	155/179 (87%)	129 (83%)	26 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5186/5431 (96%)	4476 (86%)	710 (14%)	3 16

5 of 710 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	B1	43	TYR
38	BC	147	PHE
55	BW	52	GLU
28	B2	7	ARG
32	B6	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
26	B0	50	ASN
34	B8	35	GLN
55	BW	57	ASN
27	B1	45	ASN
29	B3	52	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	247 (16%)	56 (3%)
22	AV	75/76 (98%)	22 (29%)	0
22	AW	75/76 (98%)	17 (22%)	0
23	AX	13/14 (92%)	2 (15%)	1 (7%)
24	AY	74/77 (96%)	23 (31%)	2 (2%)
36	BA	2900/2915 (99%)	547 (18%)	52 (1%)
37	BB	118/122 (96%)	24 (20%)	2 (1%)
All	All	4758/4802 (99%)	882 (18%)	113 (2%)

5 of 882 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1319	A
36	BA	221	A
36	BA	2439	A
1	AA	1399	C
24	AY	18	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PSU	AY	55	24	17,21,22	1.20	2 (11%)	20,30,33	3.37	7 (35%)
24	H2U	AY	17	24	18,21,22	0.91	1 (5%)	21,30,33	1.77	4 (19%)
24	MIA	AY	37	24	24,31,32	1.02	1 (4%)	26,44,47	1.74	4 (15%)
24	OMC	AY	32	24	15,22,23	0.78	0	17,31,34	1.15	2 (11%)
24	5MU	AY	54	24	15,22,23	1.20	1 (6%)	16,32,35	3.76	2 (12%)
24	H2U	AY	20	24	18,21,22	0.87	0	21,30,33	1.93	6 (28%)
24	7MG	AY	46	24	22,26,27	1.21	2 (9%)	28,39,42	2.31	5 (17%)
24	H2U	AY	16	24	18,21,22	0.81	0	21,30,33	1.87	5 (23%)
24	4SU	AY	8	24	14,21,22	1.39	3 (21%)	15,30,33	2.58	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	MIA	AY	37	24	-	3/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OMC	AY	32	24	-	0/7/27/28	0/2/2/2
24	5MU	AY	54	24	-	0/5/25/26	0/2/2/2
24	H2U	AY	20	24	-	4/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	6/7/37/38	0/3/3/3
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	4SU	AY	8	24	-	1/5/25/26	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C6-N1	3.81	1.39	1.33
24	AY	8	4SU	C5-C4	3.53	1.42	1.38
24	AY	54	5MU	C4-N3	3.46	1.39	1.33
24	AY	55	PSU	C4-N3	3.20	1.38	1.33
24	AY	46	7MG	C8-N9	-3.13	1.38	1.45

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	54	5MU	C4-N3-C2	14.70	127.55	115.14
24	AY	55	PSU	N1-C2-N3	-10.53	120.06	128.43
24	AY	8	4SU	C2-N3-C4	7.83	126.50	115.15
24	AY	46	7MG	N7-C8-N9	6.89	113.23	103.38
24	AY	55	PSU	C4-N3-C2	6.80	120.89	115.14

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C6
24	AY	37	MIA	C5-C6-N6-C12
24	AY	20	H2U	O4'-C1'-N1-C6
24	AY	20	H2U	O4'-C4'-C5'-O5'
24	AY	46	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	55	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	17	H2U	1	0
24	AY	37	MIA	2	0
24	AY	54	5MU	2	0
24	AY	20	H2U	3	0
24	AY	16	H2U	1	0
24	AY	8	4SU	3	0

## 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
59	PAR	AA	1601	-	45,45,45	1.57	7 (15%)	64,67,67	1.26	6 (9%)
61	GCP	AZ	501	62	26,34,34	2.53	7 (26%)	31,54,54	2.00	7 (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
59	PAR	AA	1601	-	-	4/18/94/94	0/4/4/4
61	GCP	AZ	501	62	-	14/18/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	501	GCP	C6-N1	7.35	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	501	GCP	C5-C6	-5.81	1.42	1.52
61	AZ	501	GCP	C4-N9	-5.68	1.40	1.47
59	AA	1601	PAR	C64-C54	5.14	1.59	1.52
61	AZ	501	GCP	PG-O2G	-3.93	1.45	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AZ	501	GCP	C4-C5-N7	7.75	112.74	102.46
59	AA	1601	PAR	O33-C14-C24	4.78	116.45	108.22
59	AA	1601	PAR	O54-C54-C64	3.88	113.23	106.01
61	AZ	501	GCP	O6-C6-N1	-3.59	117.86	122.69
59	AA	1601	PAR	C14-O54-C54	3.57	120.69	113.69

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AA	1601	PAR	C44-C54-C64-N64
59	AA	1601	PAR	O54-C54-C64-N64
61	AZ	501	GCP	PB-C3B-PG-O1G
61	AZ	501	GCP	PB-C3B-PG-O2G
61	AZ	501	GCP	PG-C3B-PB-O1B

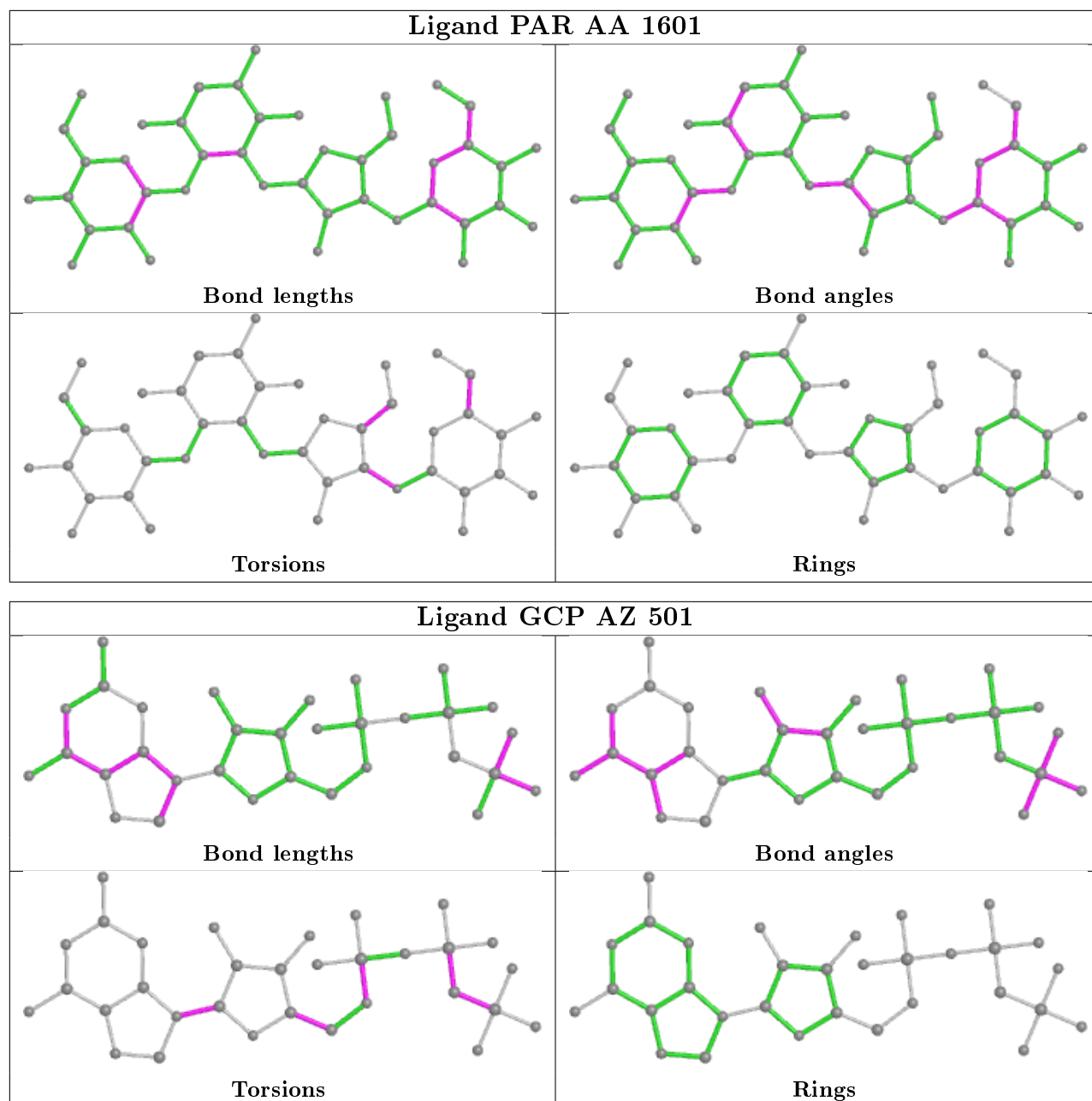
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AA	1601	PAR	2	0
61	AZ	501	GCP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	AA	1504/1522 (98%)	0.03	34 (2%) 60 39	25, 58, 149, 200	0
2	AB	234/256 (91%)	0.03	12 (5%) 28 13	35, 74, 133, 147	0
3	AC	206/239 (86%)	-0.35	1 (0%) 91 81	34, 57, 91, 103	0
4	AD	208/209 (99%)	-0.08	2 (0%) 82 67	44, 68, 96, 102	0
5	AE	150/162 (92%)	-0.34	0 100 100	33, 52, 82, 102	0
6	AF	101/101 (100%)	-0.12	1 (0%) 82 67	52, 74, 89, 100	0
7	AG	155/156 (99%)	-0.24	2 (1%) 77 59	46, 71, 96, 119	0
8	AH	138/138 (100%)	-0.19	1 (0%) 87 75	38, 58, 78, 87	0
9	AI	127/128 (99%)	0.12	5 (3%) 39 20	41, 74, 103, 112	0
10	AJ	98/105 (93%)	0.21	6 (6%) 21 9	35, 75, 111, 117	0
11	AK	119/129 (92%)	-0.09	4 (3%) 45 24	39, 59, 95, 117	0
12	AL	124/135 (91%)	-0.12	5 (4%) 38 19	36, 48, 77, 112	0
13	AM	124/126 (98%)	0.39	8 (6%) 18 8	50, 80, 107, 132	0
14	AN	60/61 (98%)	-0.18	0 100 100	32, 48, 76, 83	0
15	AO	88/89 (98%)	-0.02	0 100 100	42, 64, 89, 93	0
16	AP	83/88 (94%)	0.02	0 100 100	50, 65, 85, 114	0
17	AQ	99/105 (94%)	0.10	0 100 100	45, 70, 95, 97	0
18	AR	70/88 (79%)	-0.02	1 (1%) 75 56	46, 65, 97, 111	0
19	AS	78/93 (83%)	0.41	9 (11%) 4 2	58, 84, 115, 123	0
20	AT	99/106 (93%)	0.73	11 (11%) 5 2	56, 86, 128, 131	0
21	AU	24/27 (88%)	0.05	0 100 100	52, 64, 79, 91	0
22	AV	76/76 (100%)	1.00	11 (14%) 2 1	35, 127, 168, 176	0
22	AW	76/76 (100%)	2.16	37 (48%) 0 0	60, 175, 200, 200	0
23	AX	14/14 (100%)	0.74	1 (7%) 16 6	35, 57, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
24	AY	68/77 (88%)	0.40	3 (4%) 34 17	47, 110, 160, 196	0
25	AZ	405/405 (100%)	0.22	19 (4%) 31 15	57, 100, 135, 143	0
26	B0	84/85 (98%)	0.75	9 (10%) 6 2	59, 75, 116, 136	0
27	B1	93/98 (94%)	0.25	4 (4%) 35 17	44, 65, 106, 114	0
28	B2	71/72 (98%)	0.71	7 (9%) 7 2	75, 108, 124, 146	0
29	B3	59/60 (98%)	0.79	7 (11%) 4 2	72, 93, 110, 135	0
30	B4	44/71 (61%)	0.52	2 (4%) 33 16	103, 134, 142, 149	0
31	B5	59/60 (98%)	0.54	4 (6%) 17 7	57, 89, 151, 155	0
32	B6	50/54 (92%)	0.93	6 (12%) 4 2	52, 81, 99, 108	0
33	B7	48/49 (97%)	0.27	1 (2%) 63 43	49, 59, 99, 117	0
34	B8	63/65 (96%)	0.35	2 (3%) 47 25	53, 73, 91, 106	0
35	B9	37/37 (100%)	0.97	6 (16%) 1 1	61, 82, 96, 97	0
36	BA	2901/2915 (99%)	0.37	211 (7%) 15 6	28, 76, 190, 200	0
37	BB	119/122 (97%)	0.14	4 (3%) 45 24	74, 103, 134, 150	0
38	BC	228/229 (99%)	3.41	148 (64%) 0 0	125, 160, 177, 186	0
39	BD	275/276 (99%)	-0.20	4 (1%) 73 54	24, 45, 71, 93	0
40	BE	204/206 (99%)	0.34	8 (3%) 39 20	50, 77, 128, 135	0
41	BF	207/210 (98%)	0.66	22 (10%) 6 2	47, 97, 149, 155	0
42	BG	181/182 (99%)	0.42	13 (7%) 15 6	79, 101, 126, 137	0
43	BH	159/180 (88%)	0.86	27 (16%) 1 0	80, 119, 144, 150	0
44	BJ	0/130	-	-	-	-
45	BK	0/140	-	-	-	-
46	BN	138/140 (98%)	0.42	5 (3%) 42 22	68, 93, 127, 132	0
47	BO	122/122 (100%)	-0.23	0 100 100	42, 59, 72, 83	0
48	BP	146/150 (97%)	0.70	10 (6%) 17 7	55, 90, 121, 146	0
49	BQ	141/141 (100%)	0.05	5 (3%) 44 23	50, 68, 100, 134	0
50	BR	117/118 (99%)	0.29	3 (2%) 56 33	58, 81, 100, 105	0
51	BS	98/112 (87%)	0.55	9 (9%) 9 3	70, 93, 121, 126	0
52	BT	137/146 (93%)	0.35	10 (7%) 15 6	54, 80, 139, 161	0
53	BU	117/118 (99%)	0.31	6 (5%) 28 13	68, 88, 113, 120	0
54	BV	101/101 (100%)	0.96	13 (12%) 3 1	67, 117, 132, 137	0
55	BW	113/113 (100%)	0.35	4 (3%) 44 23	65, 88, 115, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BX	92/96 (95%)	0.48	6 (6%) 18 8	65, 85, 101, 107	0
57	BY	100/110 (90%)	1.72	40 (40%) 0 0	94, 125, 149, 158	0
58	BZ	176/206 (85%)	0.60	15 (8%) 10 4	69, 102, 125, 134	0
All	All	11008/11625 (94%)	0.34	784 (7%) 16 6	24, 77, 158, 200	0

The worst 5 of 784 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	BC	220	PRO	12.6
58	BZ	114	GLY	12.1
38	BC	111	ASP	11.3
38	BC	123	VAL	11.1
36	BA	654(P)	C	11.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
24	H2U	AY	16	20/21	0.55	0.42	171,185,187,190	0
24	H2U	AY	17	20/21	0.61	0.80	191,199,200,200	0
24	5MU	AY	54	21/22	0.65	0.36	145,152,154,155	0
24	PSU	AY	55	20/21	0.71	0.31	154,158,159,160	0
24	H2U	AY	20	20/21	0.75	0.31	185,187,191,191	0
24	4SU	AY	8	20/21	0.79	0.24	104,105,107,108	0
24	7MG	AY	46	24/25	0.88	0.24	112,114,120,121	0
24	OMC	AY	32	21/22	0.91	0.24	76,80,87,88	0
24	MIA	AY	37	29/30	0.94	0.27	48,63,74,86	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

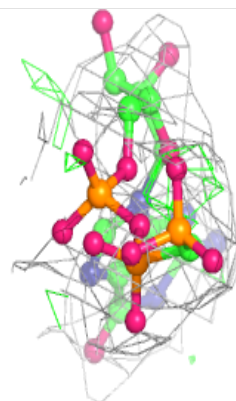
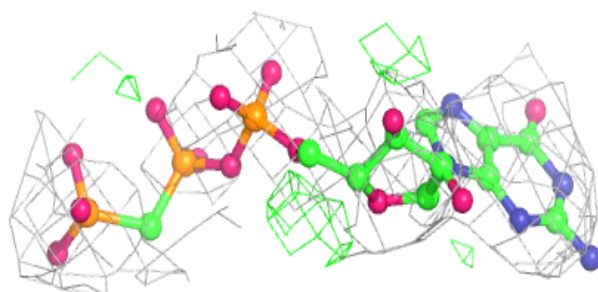
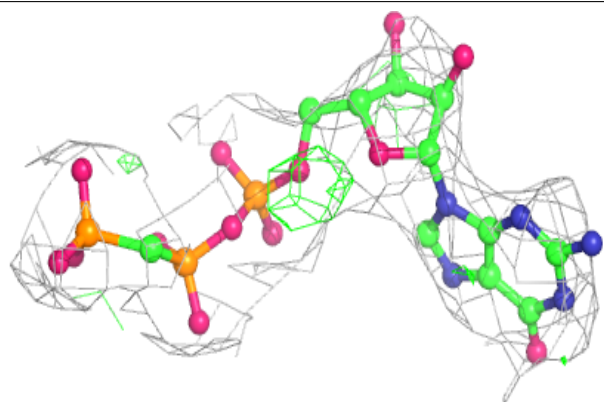
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	ZN	B4	101	1/1	0.92	0.08	132,132,132,132	0
62	MG	AZ	502	1/1	0.93	0.24	55,55,55,55	0
61	GCP	AZ	501	32/32	0.93	0.23	89,110,116,117	0
59	PAR	AA	1601	42/42	0.95	0.21	33,42,58,62	0
60	ZN	AD	301	1/1	0.98	0.33	58,58,58,58	0
60	ZN	B9	101	1/1	0.99	0.12	92,92,92,92	0
60	ZN	AN	101	1/1	1.00	0.19	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

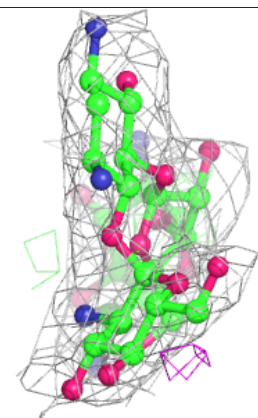
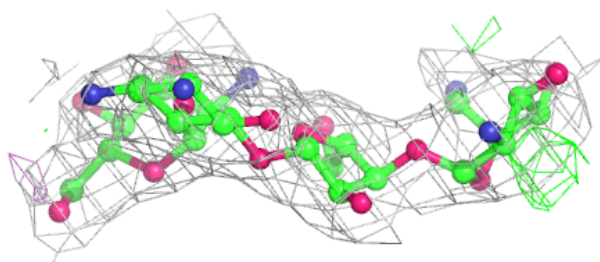
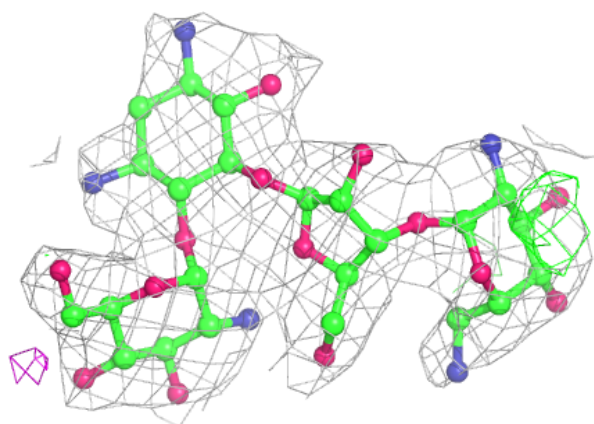
### Electron density around GCP AZ 501:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR AA 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.