wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 03:35 pm GMT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

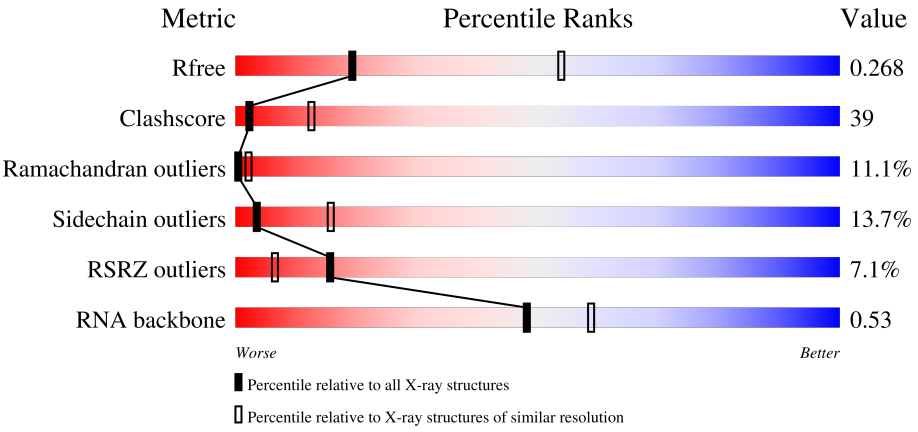
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	2% 33% 52% 11%
2	AB	256	5% 20% 54% 15% 9%
3	AC	239	29% 48% 9% 14%
4	AD	209	38% 47% 14%

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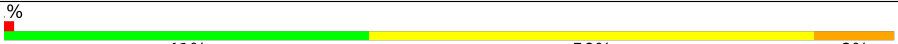
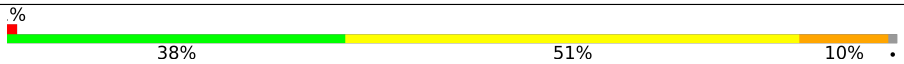
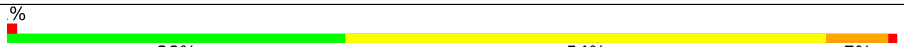
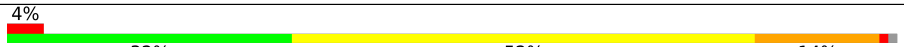
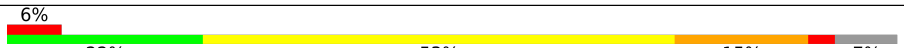
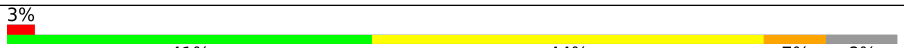
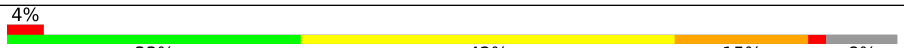
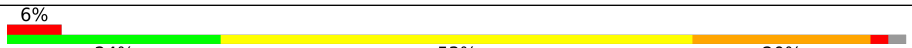
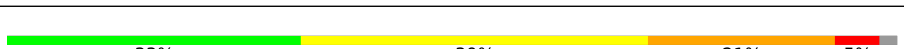
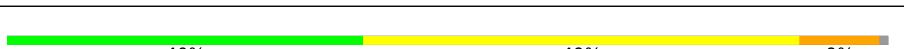
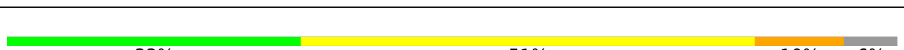
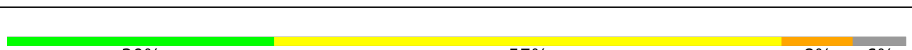
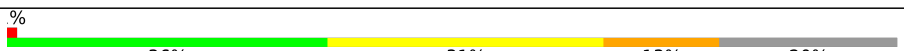
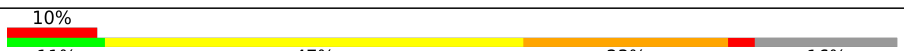
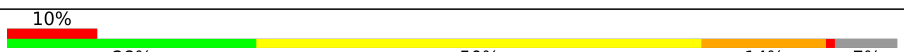
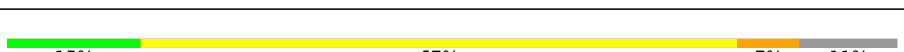
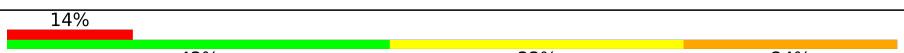
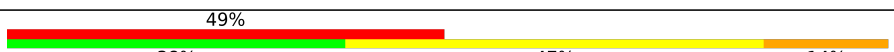
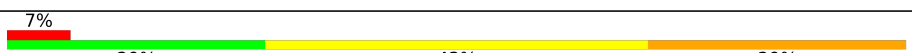
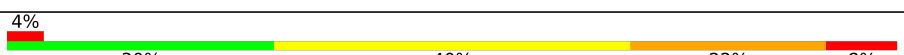
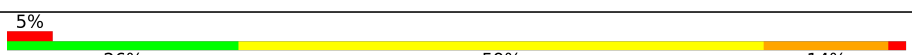
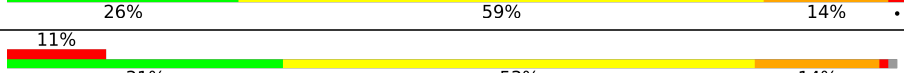
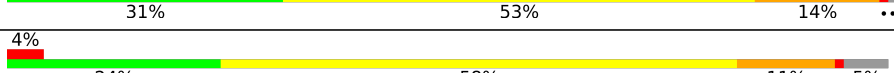
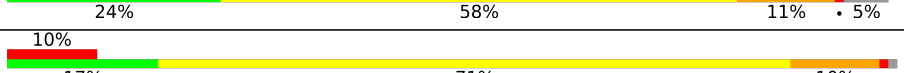
Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
22	AW	76	
23	AX	14	
24	AY	77	
25	AZ	405	
26	B0	85	
27	B1	98	
28	B2	72	

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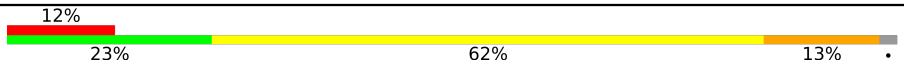
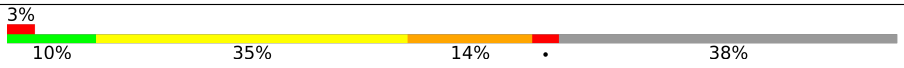
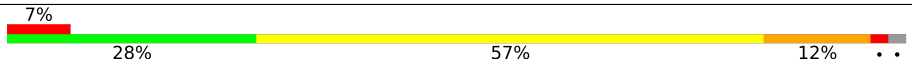
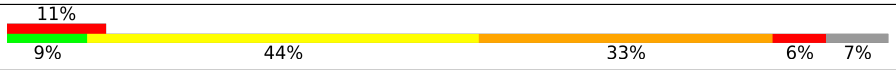
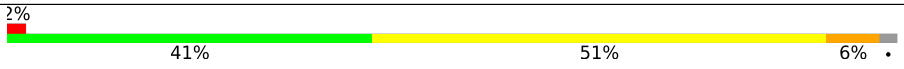
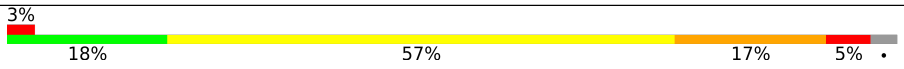
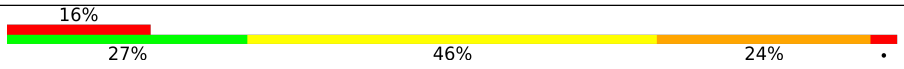
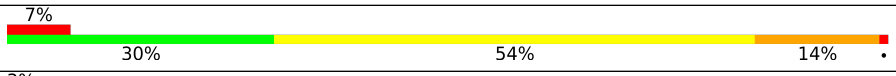
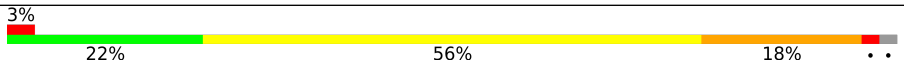
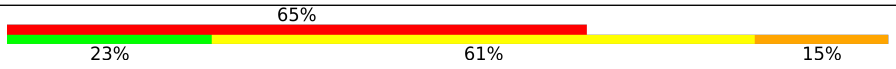
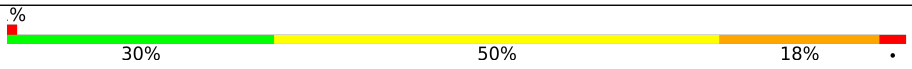
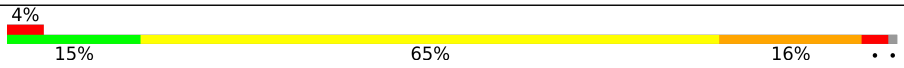
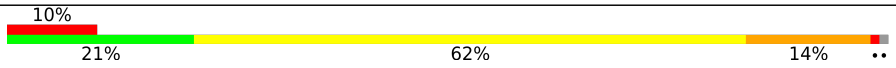
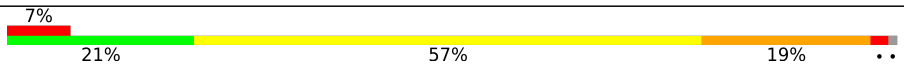
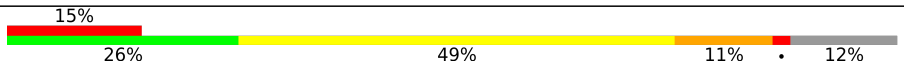
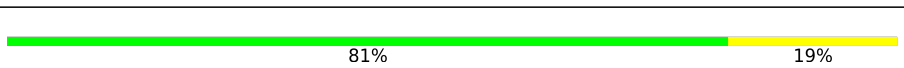
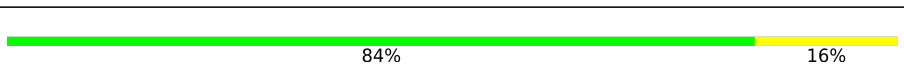
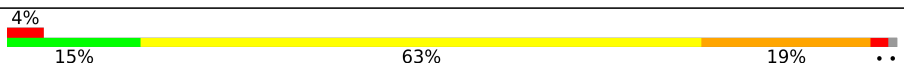
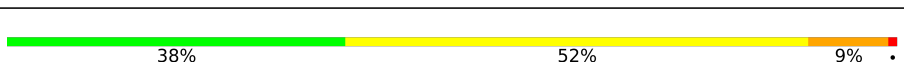
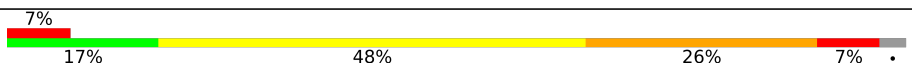
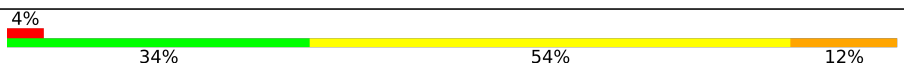
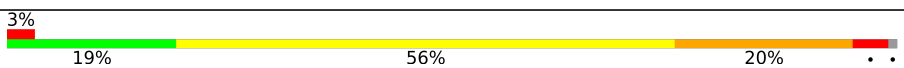
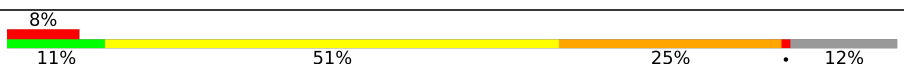
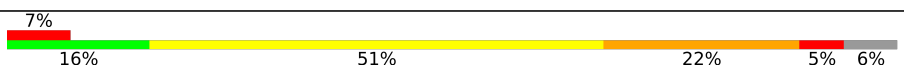
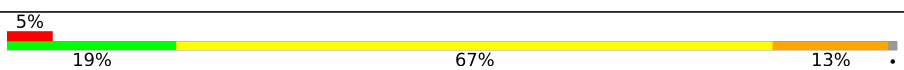
Mol	Chain	Length	Quality of chain
29	B3	60	
30	B4	71	
31	B5	60	
32	B6	54	
33	B7	49	
34	B8	65	
35	B9	37	
36	BA	2915	
37	BB	122	
38	BC	229	
39	BD	276	
40	BE	206	
41	BF	210	
42	BG	182	
43	BH	180	
44	BJ	130	
45	BK	140	
46	BN	140	
47	BO	122	
48	BP	150	
49	BQ	141	
50	BR	118	
51	BS	112	
52	BT	146	
53	BU	118	

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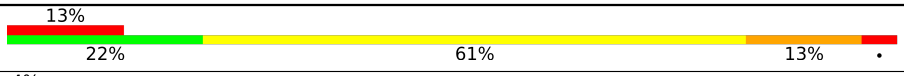
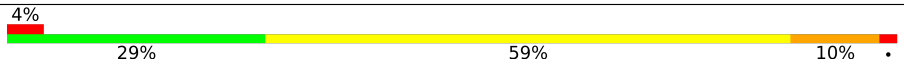
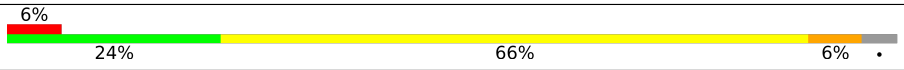
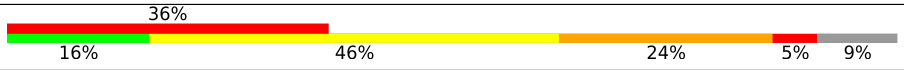
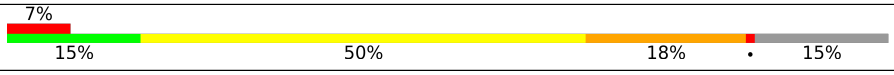
Mol	Chain	Length	Quality of chain
54	BV	101	
55	BW	113	
56	BX	96	
57	BY	110	
58	BZ	206	

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 (i)

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
			Total	C	N	O	P			
1	AA	1504	32329	14390	5992	10444	1503	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	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	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	0	0	0
			725	471	131	123			

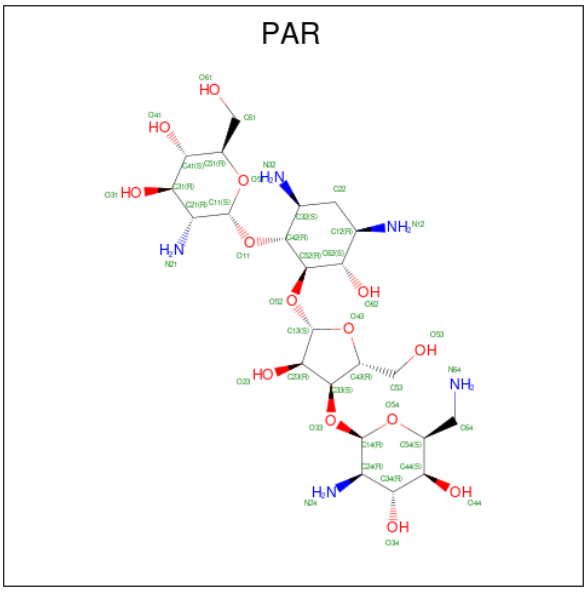
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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: $C_{23}H_{45}N_5O_{14}$).

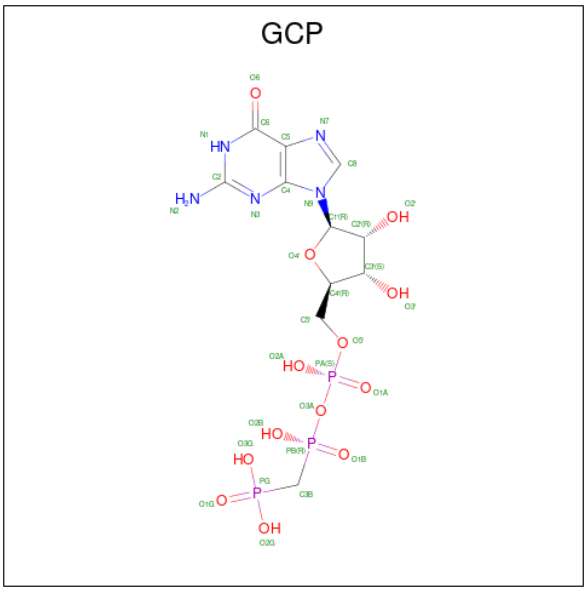


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	1	Total C N O 42 23 5 14	0	0

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

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

- Molecule 61 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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	0	0
			1	1		

- Molecule 63 is water.

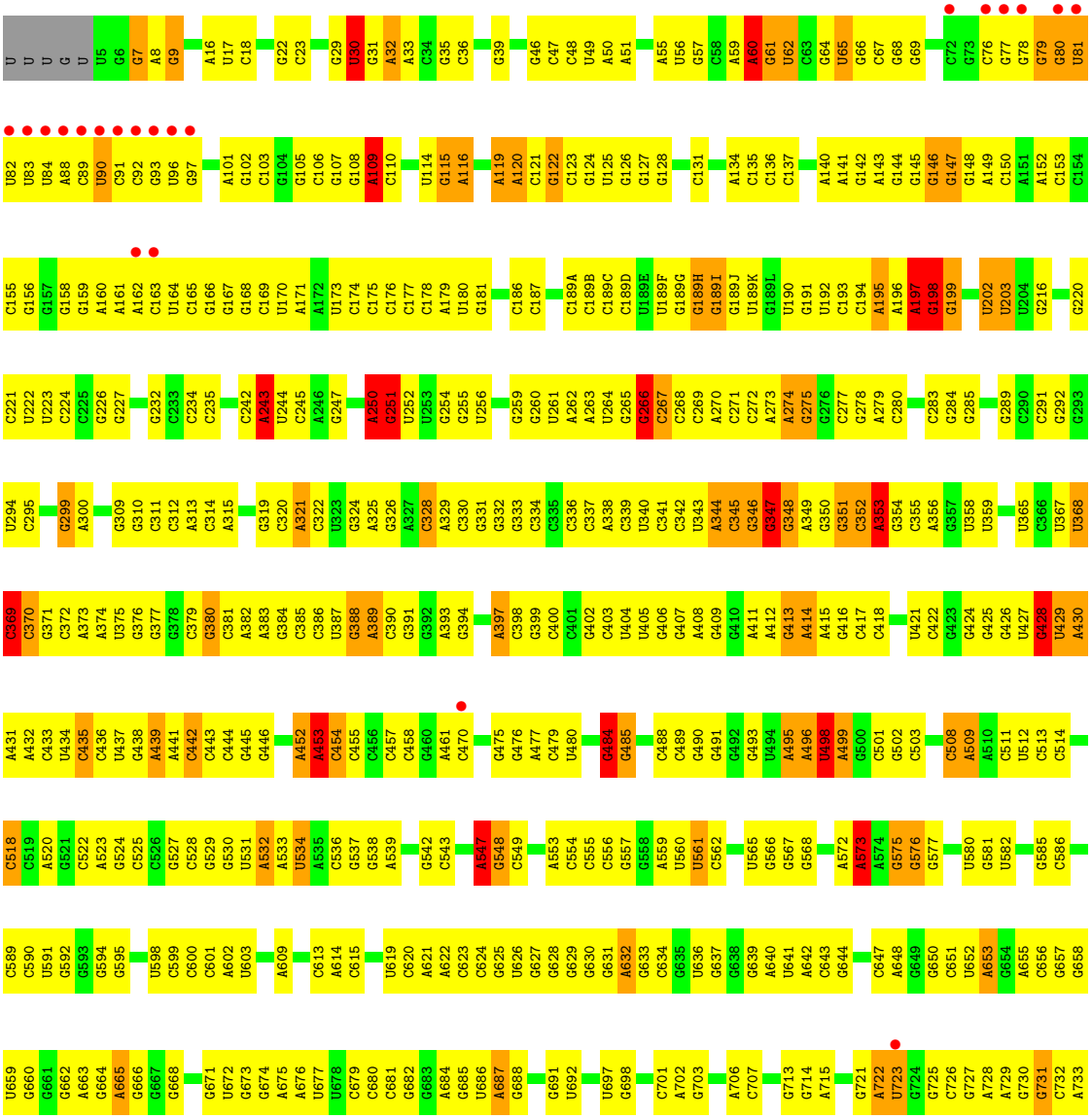
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AZ	1	Total	O	0	0
			1	1		

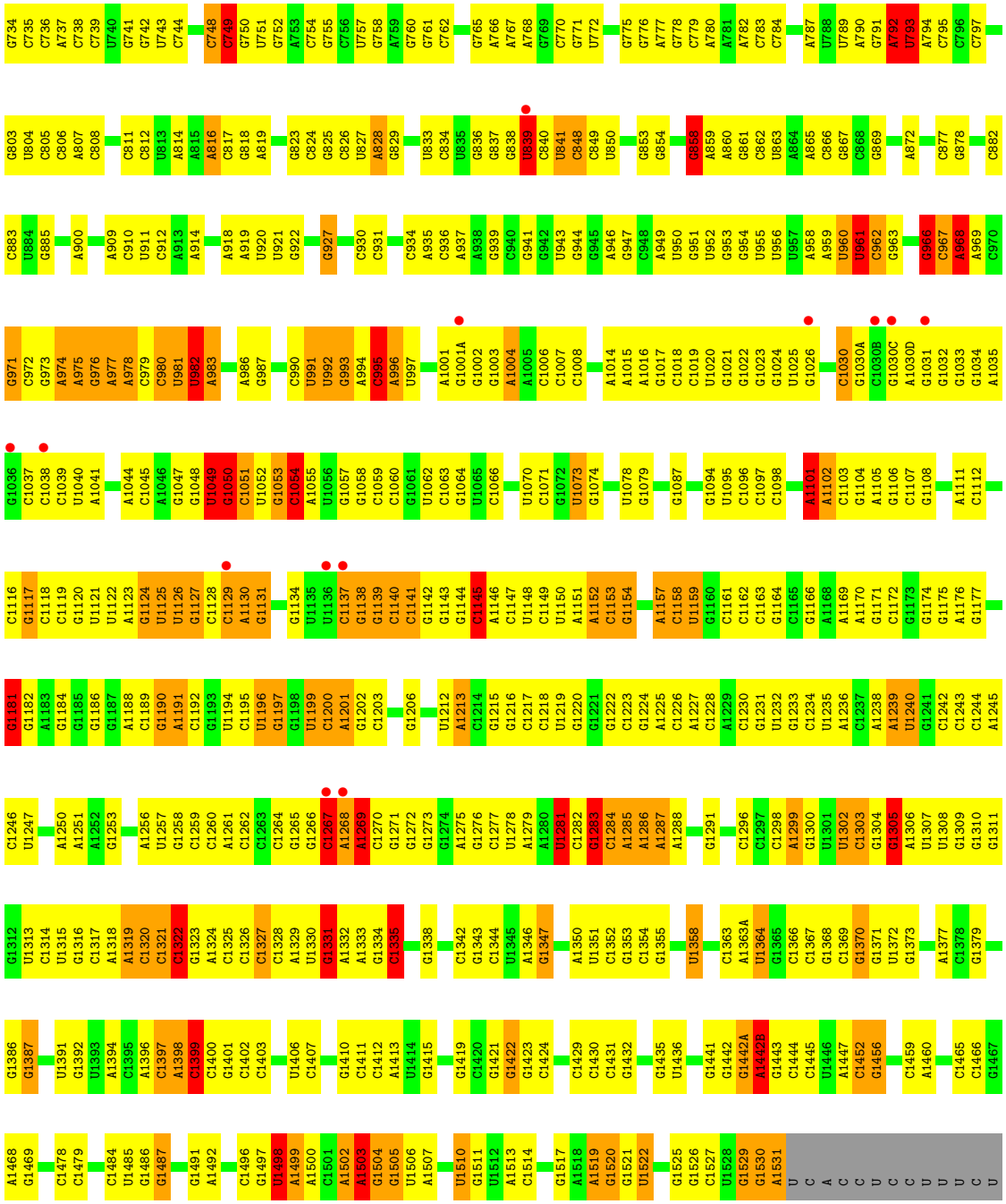
3 Residue-property plots (i)

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

- Molecule 1: 16S RRNA

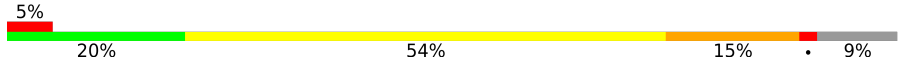
Chain AA: 

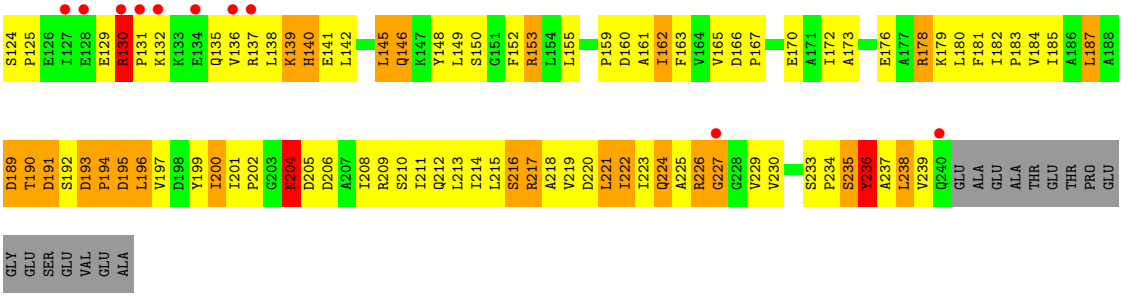




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

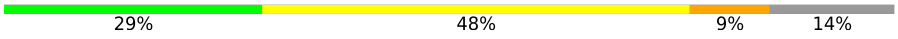
Chain AB:

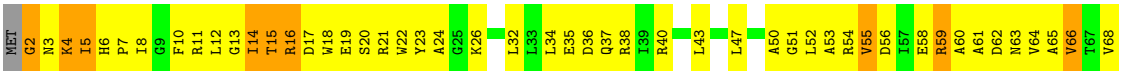


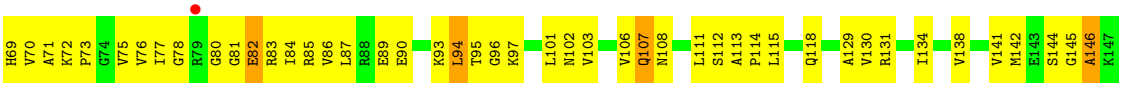


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:

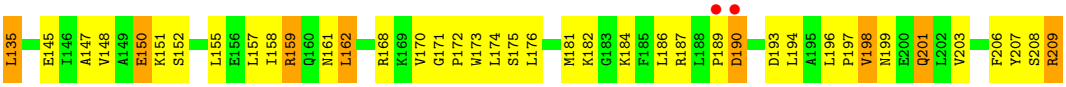






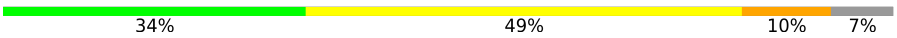
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

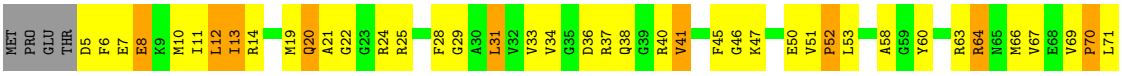
Chain AD:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

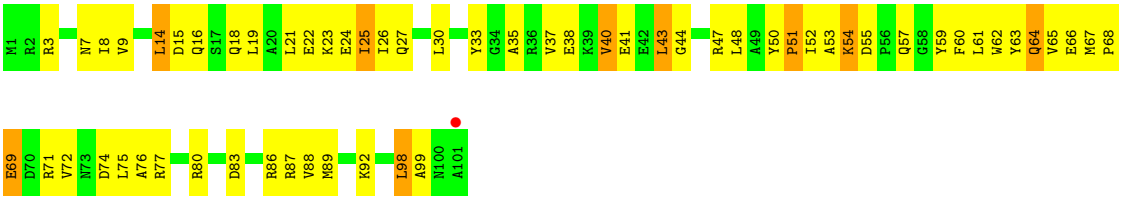
Chain AE:





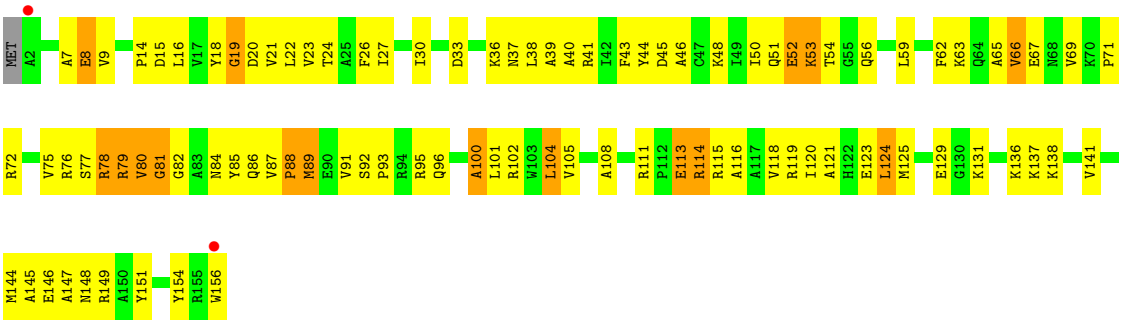
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



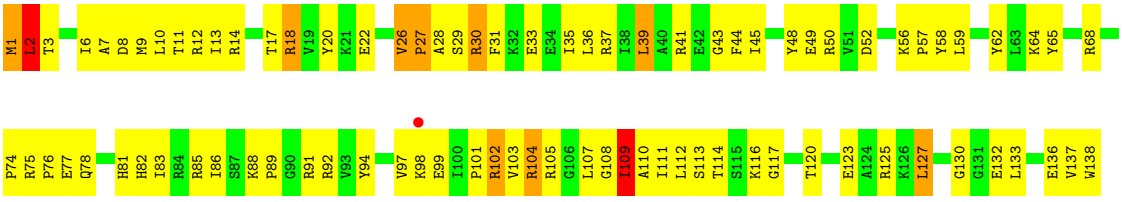
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



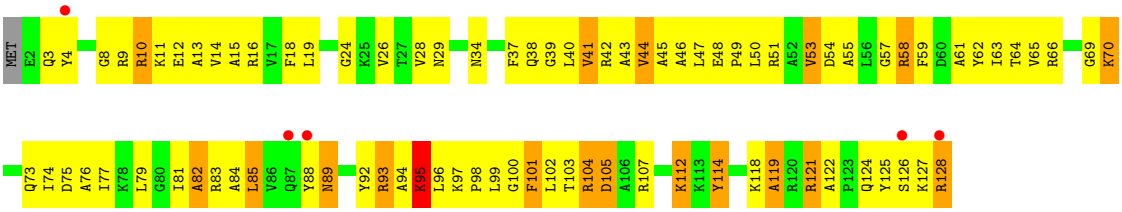
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



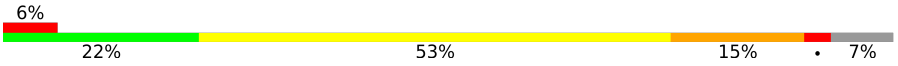
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

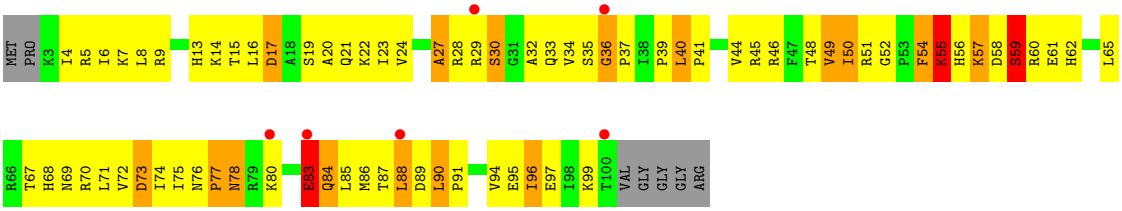
Chain AI:



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

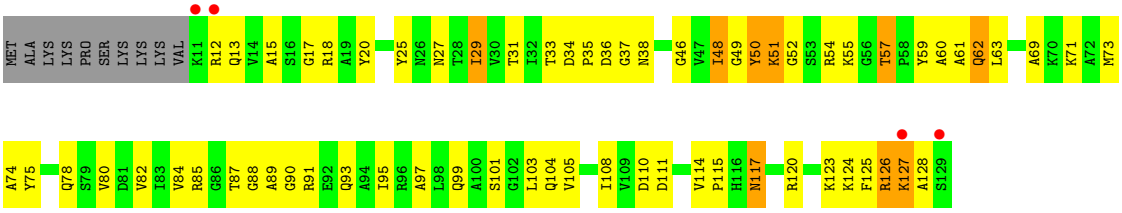
Chain AJ:





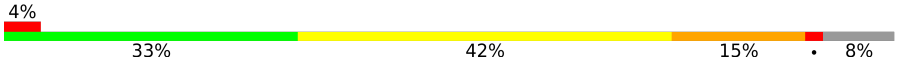
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

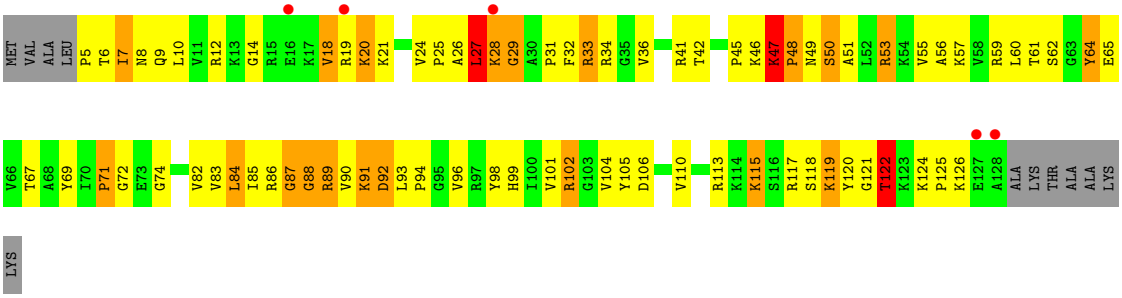
Chain AK:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

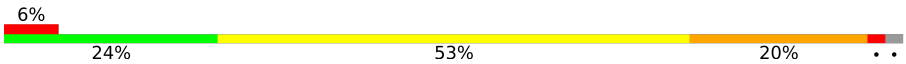
Chain AL:

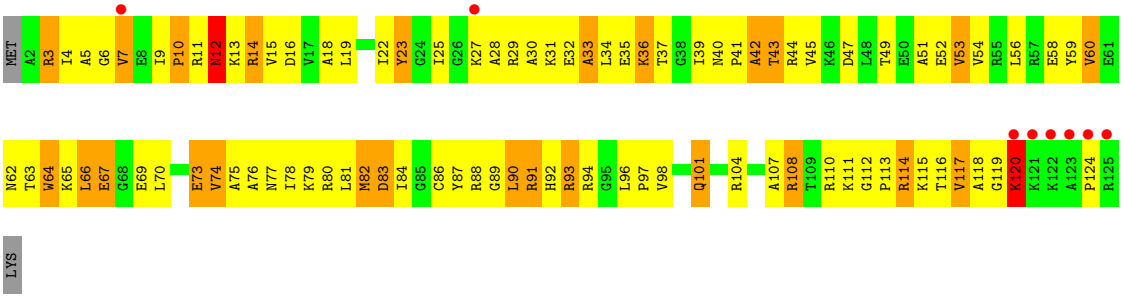




• Molecule 13: 30S RIBOSOMAL PROTEIN S13

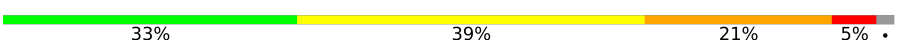
Chain AM:

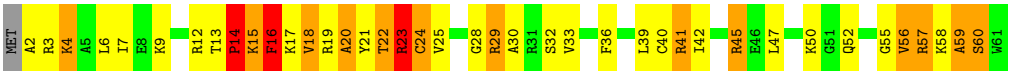




• Molecule 14: 30S RIBOSOMAL PROTEIN S14

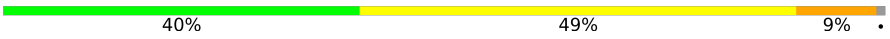
Chain AN:

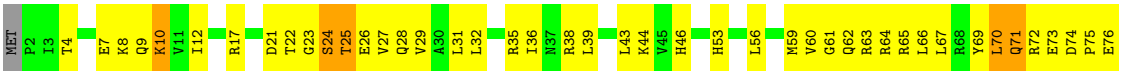


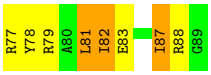


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:

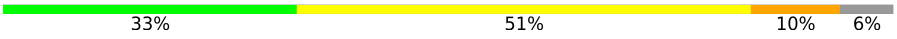


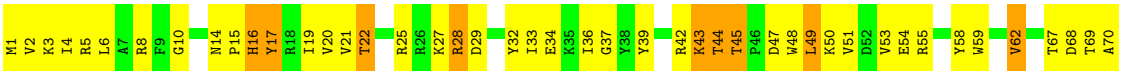




• Molecule 16: 30S RIBOSOMAL PROTEIN S16

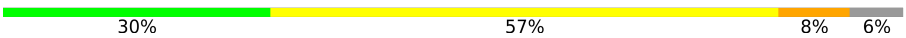
Chain AP:

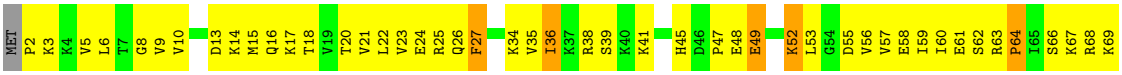


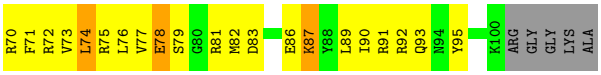


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:

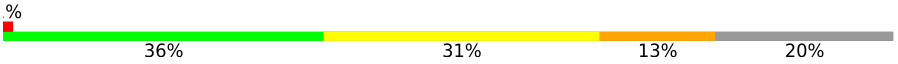


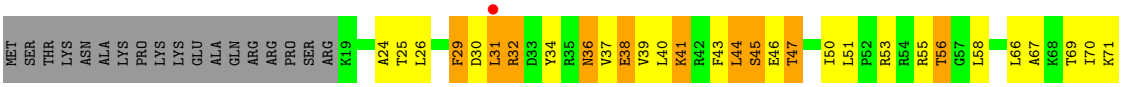


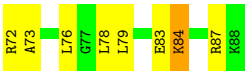


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:

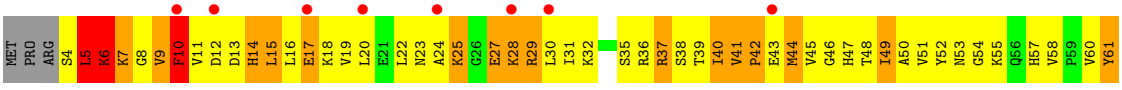


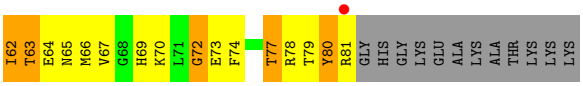




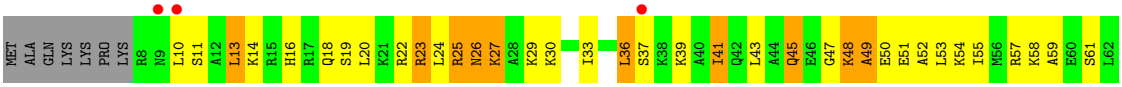
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

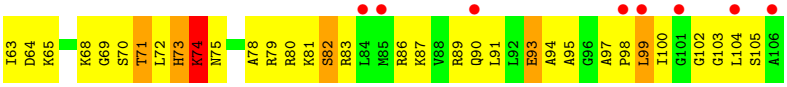
Chain AS:



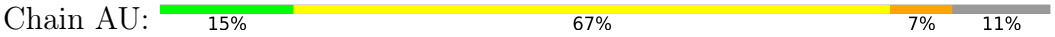


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

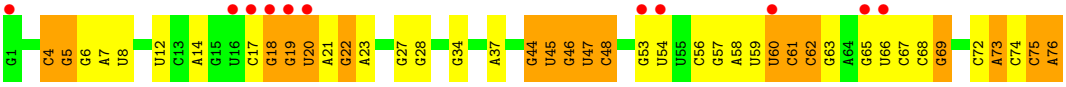




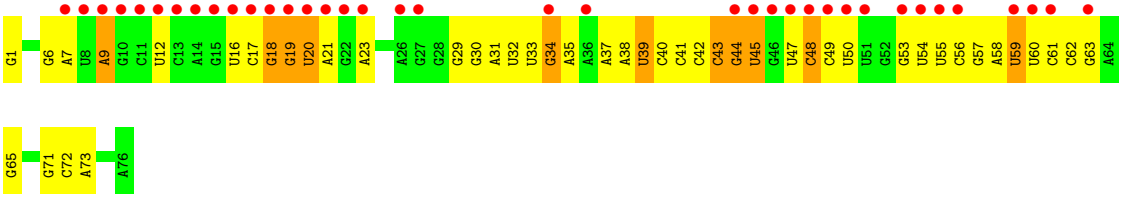
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



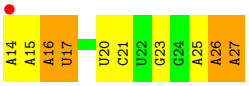
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



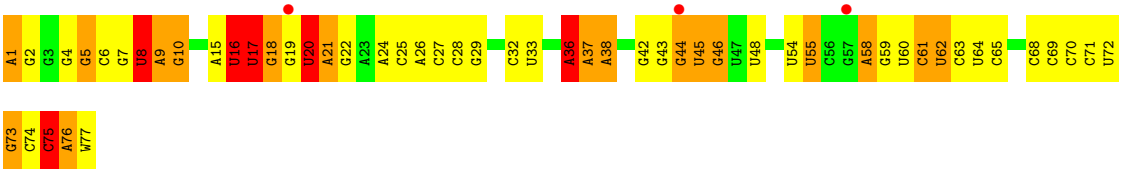
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



• Molecule 23: MRNA

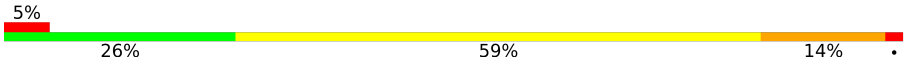


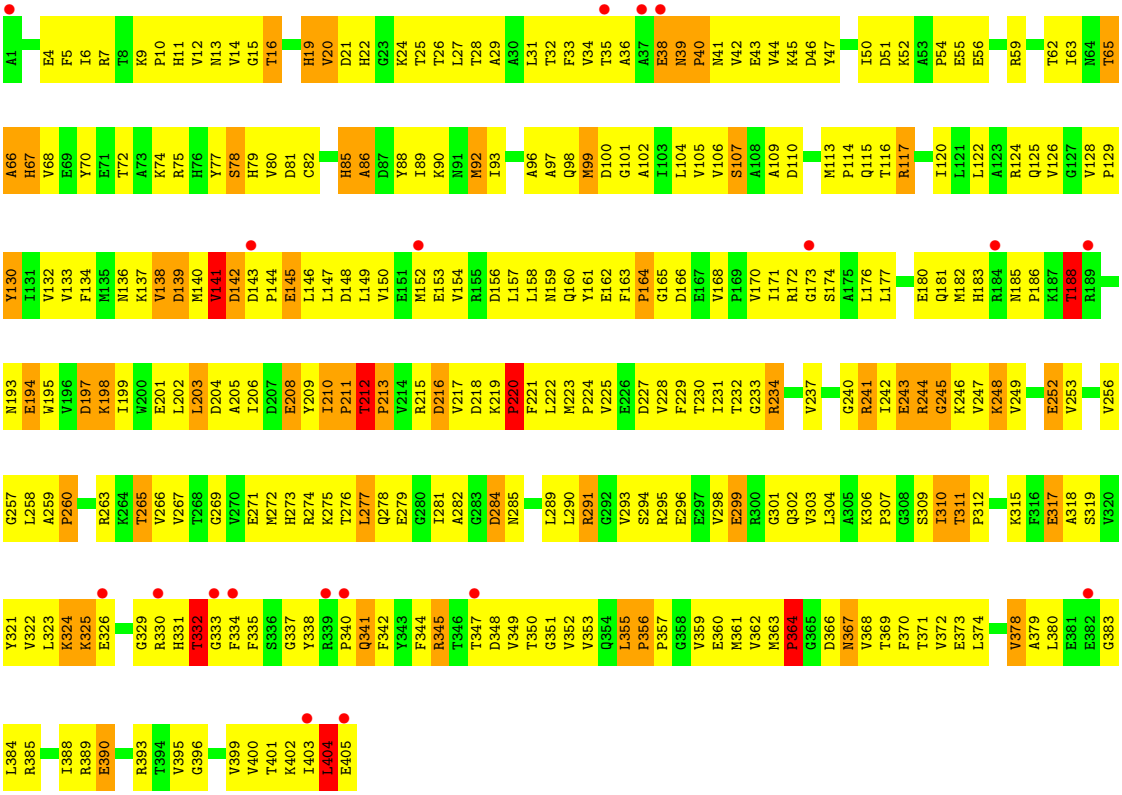
• Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP



• Molecule 25: ELONGATION FACTOR TU

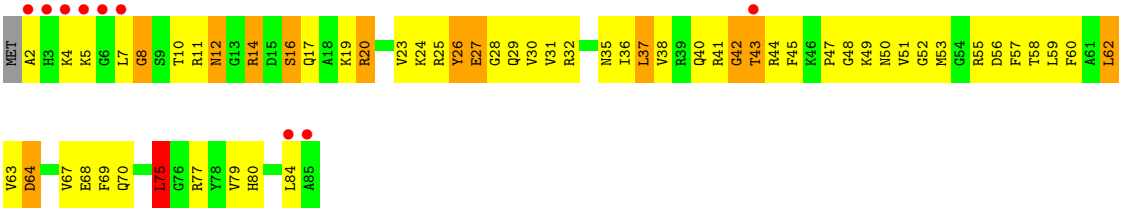
Chain AZ:





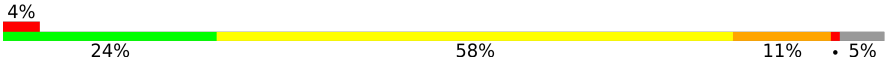
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

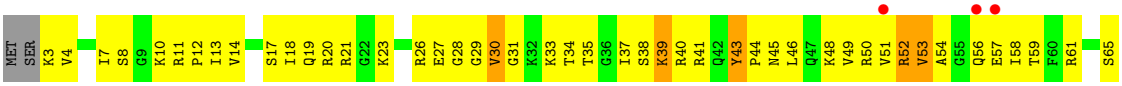
Chain B0:

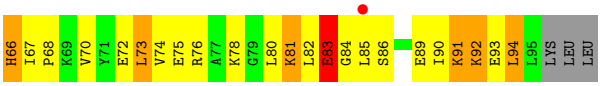


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:

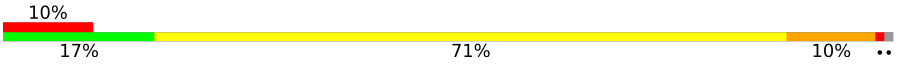


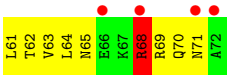




• Molecule 28: 50S RIBOSOMAL PROTEIN L29

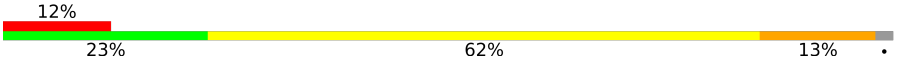
Chain B2:





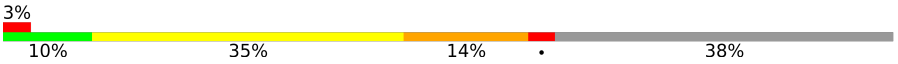
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

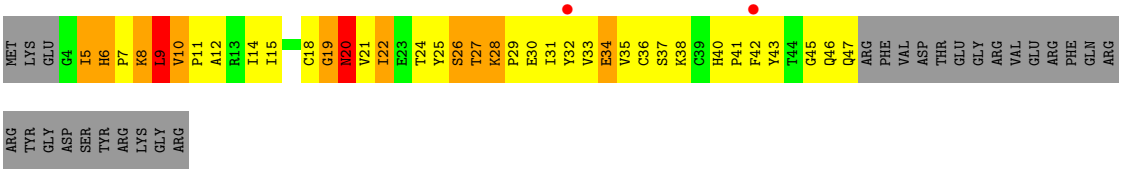
Chain B3:



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

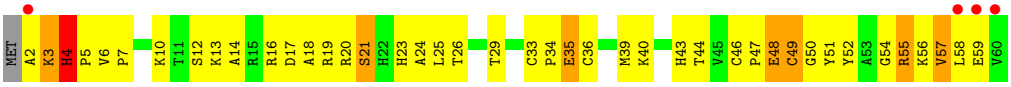
Chain B4:





• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:

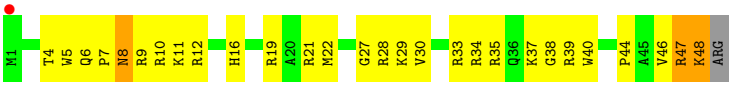


• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:

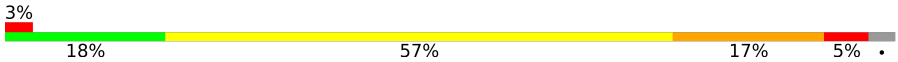
• Molecule 33: 50S RIBOSOMAL PROTEIN L34

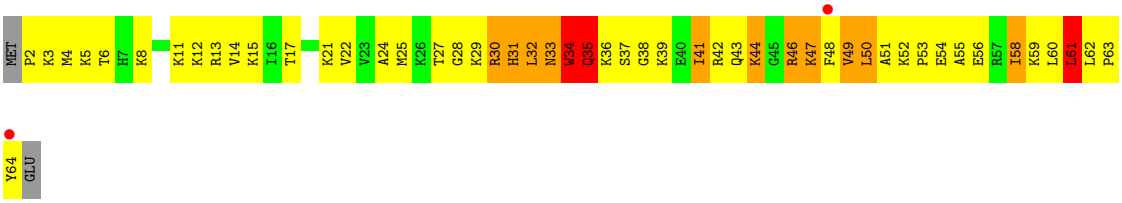
Chain B7:



• Molecule 34: 50S RIBOSOMAL PROTEIN L35

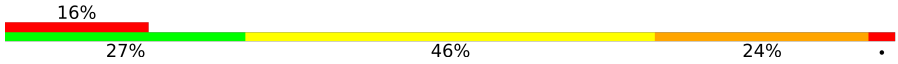
Chain B8:

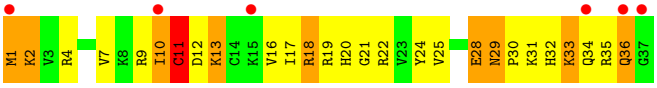




• Molecule 35: 50S RIBOSOMAL PROTEIN L36

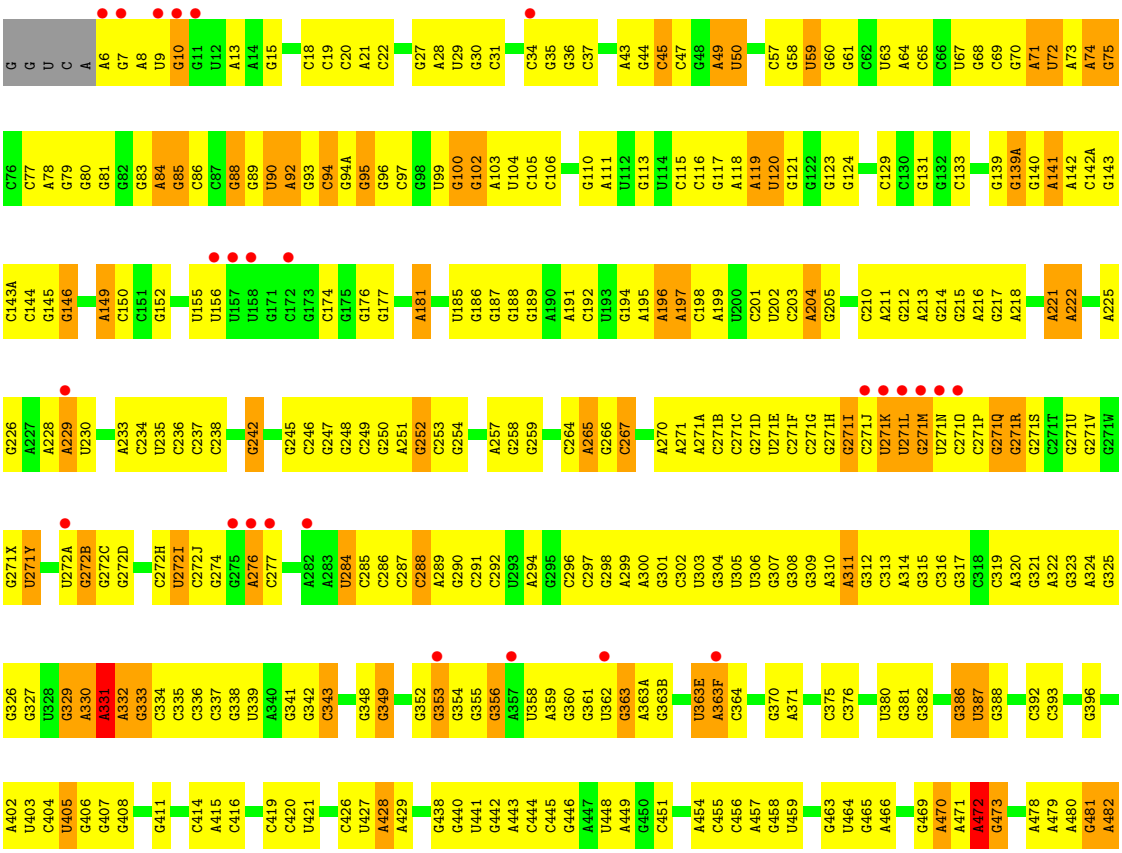
Chain B9:

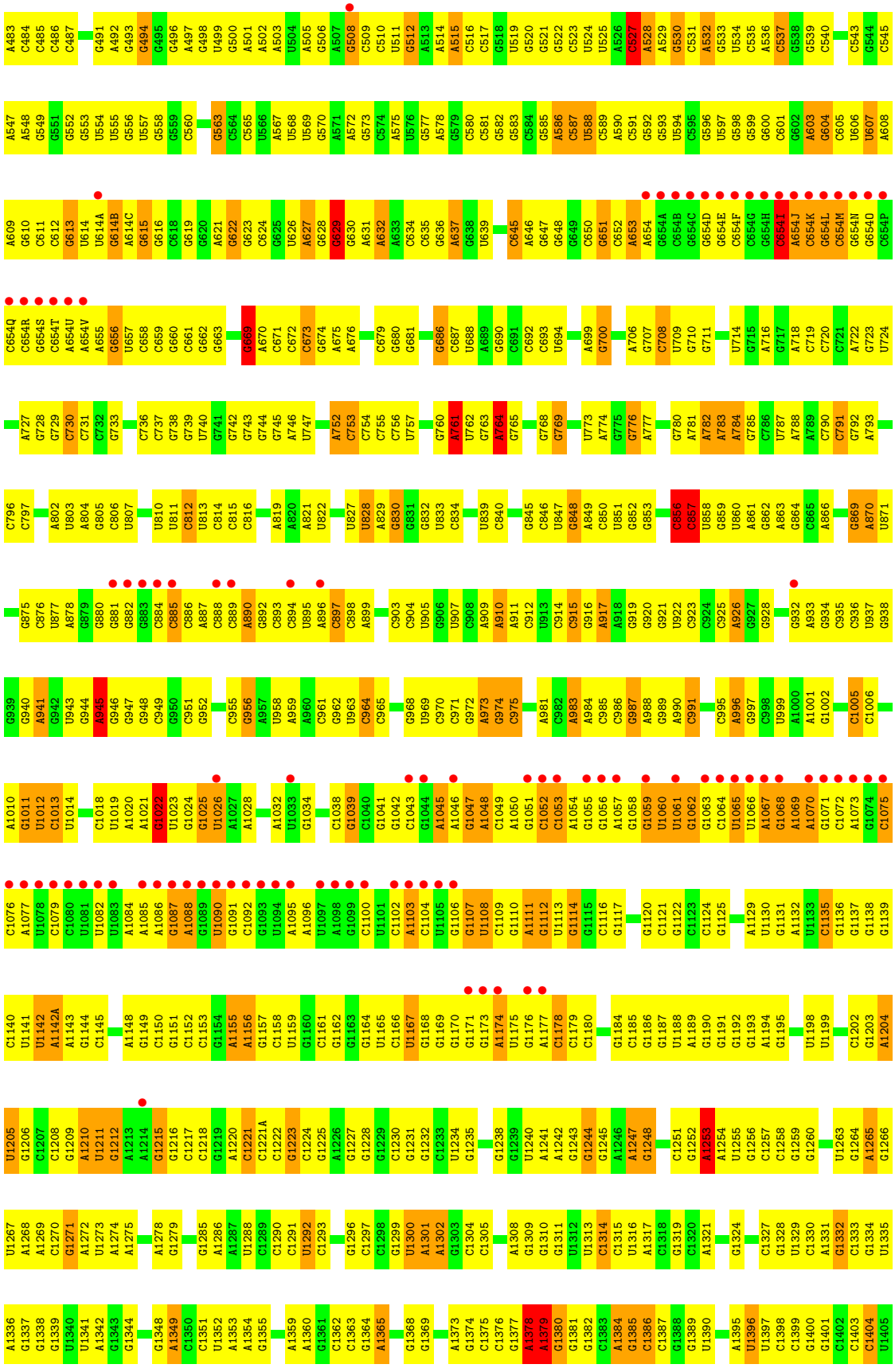


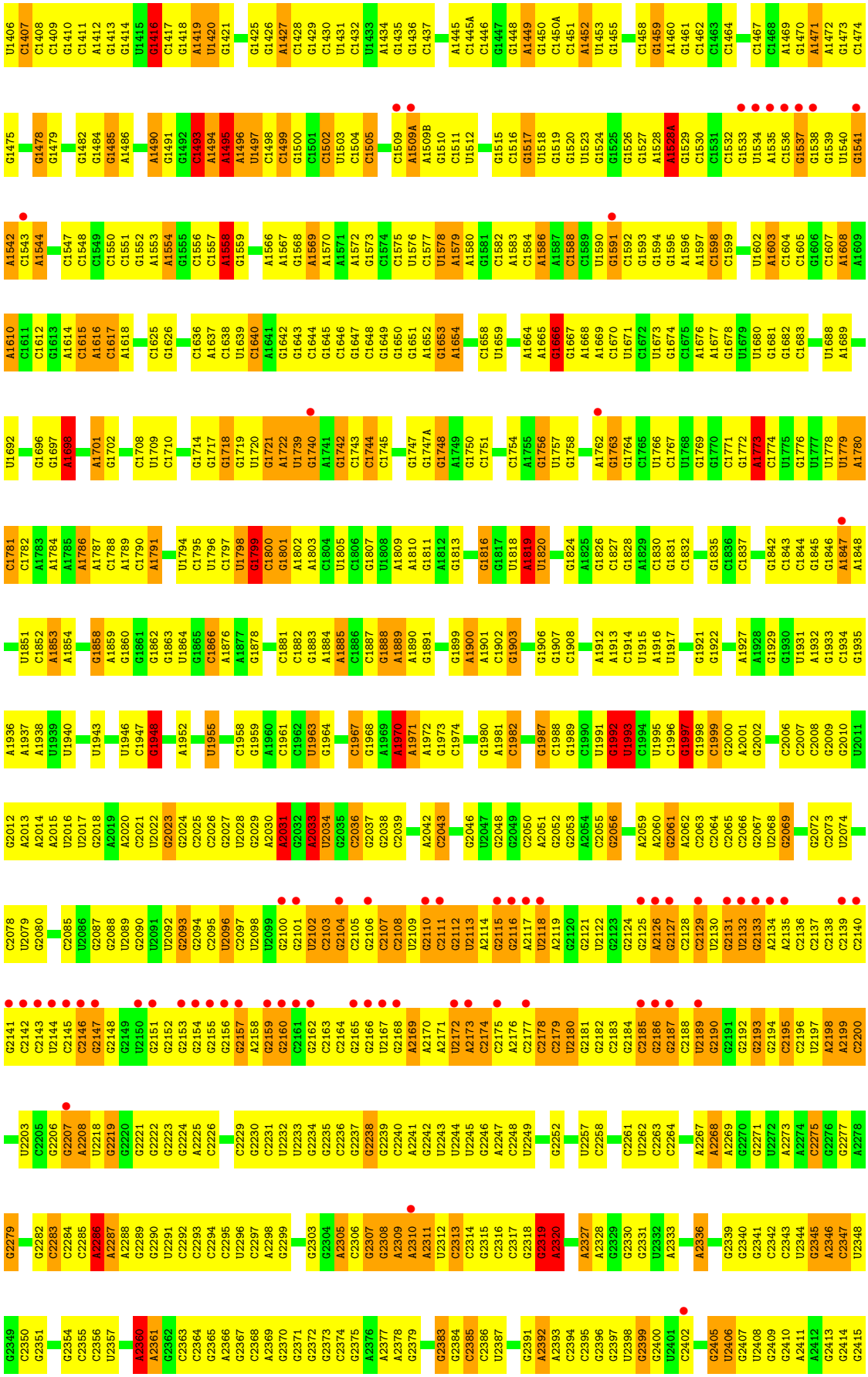


• Molecule 36: 23S RIBOSOMAL RNA

Chain BA:






U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 C1437 A1445 C1445A C1446 G1447 G1448 A1449 G1450 C1450A C1451 A1452 U1453 G1455 C1458 G1459 A1460 G1461 C1462 C1463 C1464 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474
G1475 G1478 G1479 G1482 G1484 G1485 A1486 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 C1501 C1502 U1503 C1504 C1505 C1509 A1509A A1509B G1510 C1511 U1512 G1515 C1516 G1517 U1518 G1519 G1520 U1523 G1524 G1525 G1526 G1527 A1528 A1528A G1529 C1530 C1531 C1532 G1533 U1534 A1535 C1536 G1537 G1538 G1539 U1540 G1541
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A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 C1625 G1626 C1636 A1637 C1638 U1639 C1640 A1641 G1642 G1643 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 C1658 U1659 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 C1675 A1676 A1677 G1678 U1679 U1680 G1681 G1682 C1683 U1688 A1689
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C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 U1808 A1809 A1810 G1811 A1812 G1813 G1816 G1817 U1818 A1819 U1820 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 G1835 C1836 C1837 G1842 C1843 C1844 G1845 G1846 A1847 A1848
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A1936 A1937 A1938 U1939 U1940 U1943 U1946 C1947 G1948 A1952 U1955 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1980 A1981 C1982 G1987 C1988 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 A2001 G2002 C2006 C2007 C2008 G2009 G2010 U2011
G2012 A2013 A2014 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 C2029 A2030 A2031 C2032 A2033 U2034 C2035 C2036 G2037 G2038 C2039 A2042 C2043 G2046 U2047 G2048 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2072 C2073 U2074
C2078 U2079 G2080 C2085 U2086 G2087 G2088 U2089 G2090 U2091 U2092 G2093 G2094 C2095 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140
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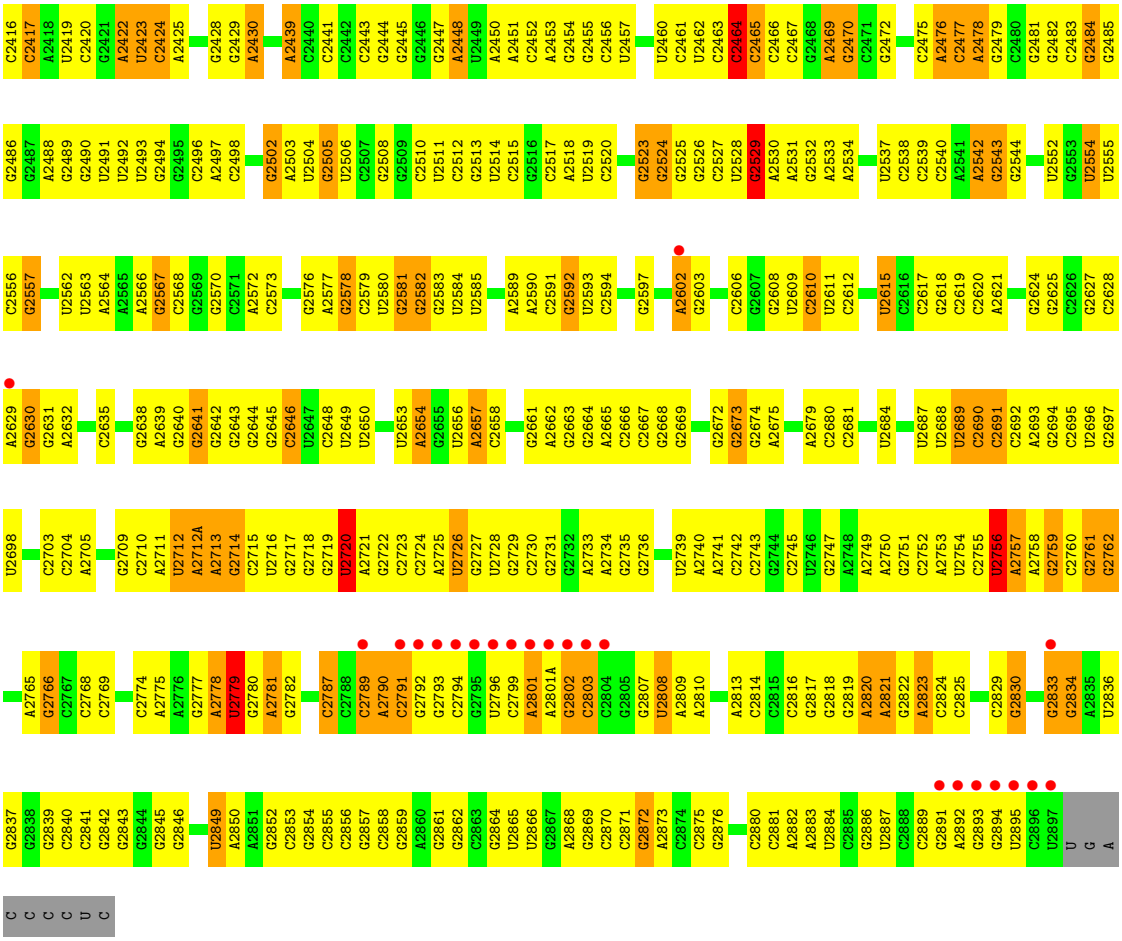
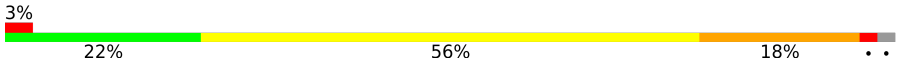
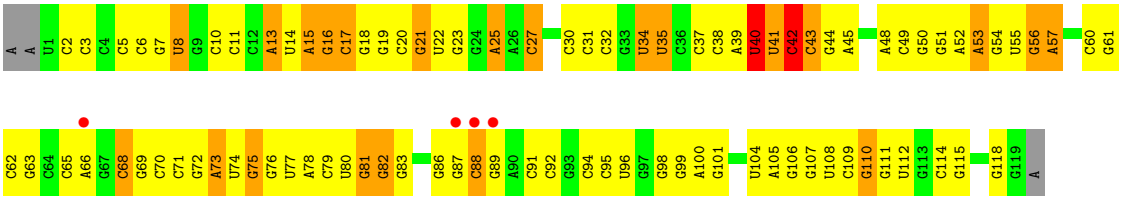
U2203 C2205 G2206 G2207 A2208 U2218 G2219 G2220 G2221 G2222 G2223 G2224 A2225 C2226 C2229 G2230 C2231 U2232 U2233 G2234 C2235 C2236 G2237 G2238 G2239 C2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2252 U2257 C2258 C2261 U2262 C2263 C2264 A2267 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278
G2279 G2282 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 C2297 A2298 G2299 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 A2327 A2328 G2329 G2330 G2331 U2332 A2333 A2336 G2339 G2340 G2341 C2342 C2343 U2344 G2345 A2346 C2347 U2348
G2349 C2350 G2351 G2354 C2355 C2356 U2357 A2360 A2361 G2362 C2363 C2364 G2365 A2366 G2367 C2368 A2369 G2370 G2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 G2379 G2383 G2384 C2385 C2386 U2387 G2391 A2392 A2393 C2394 C2395 G2396 G2397 U2398 G2399 G2400 U2401 C2402 G2405 U2406 G2407 U2408 G2409 G2410 A2411 A2412 G2413 G2414 G2415



• Molecule 37: 5S RIBOSOMAL RNA

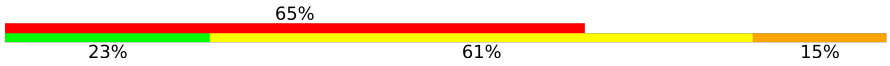
Chain BB:

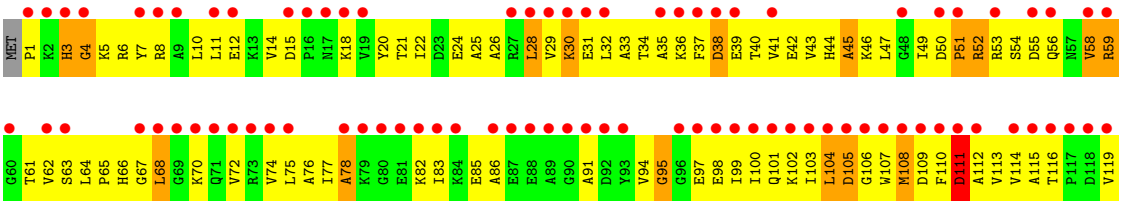


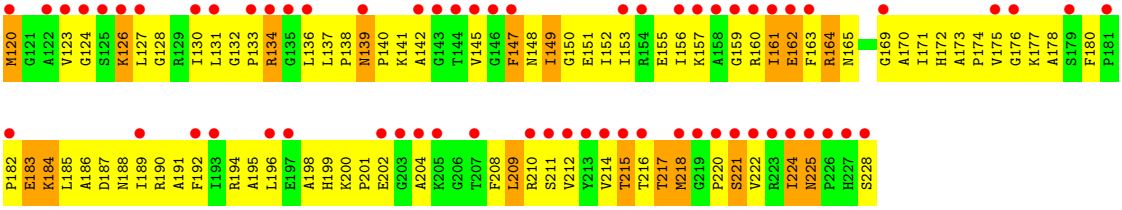


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC:

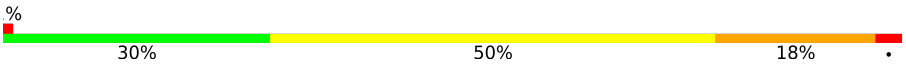


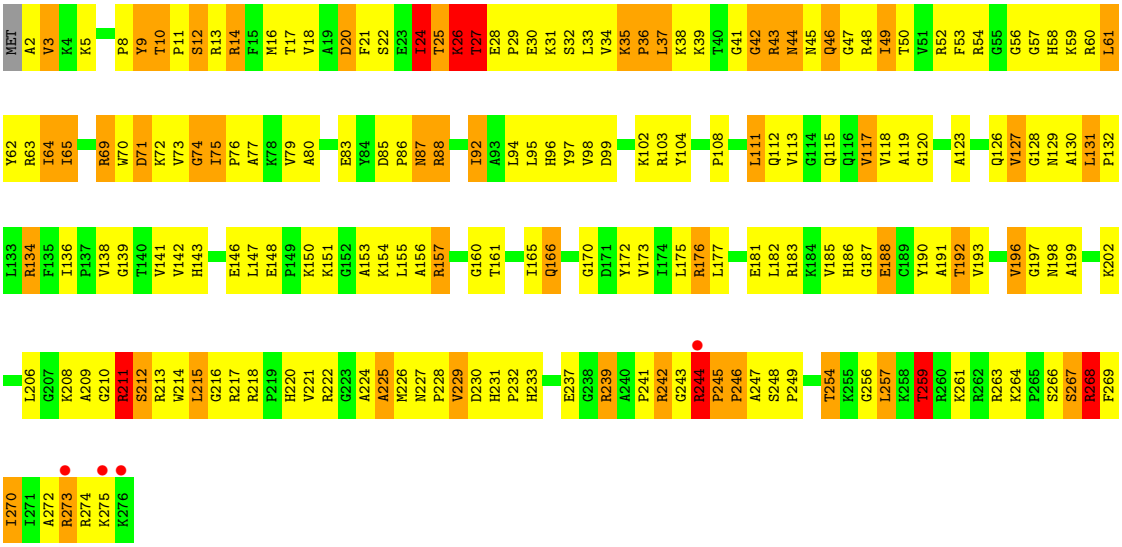




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

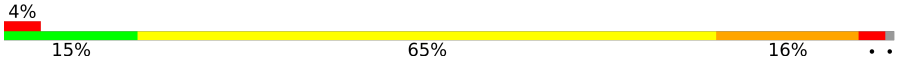
Chain BD:

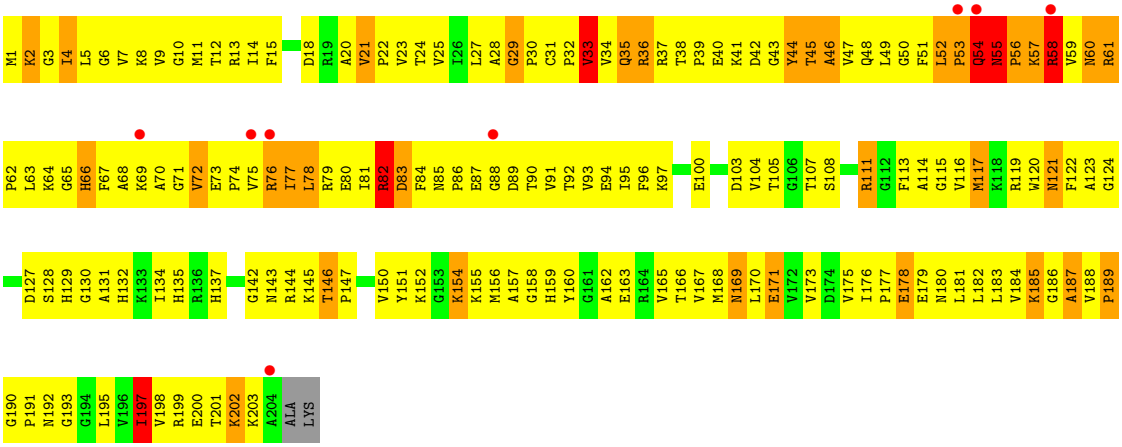




• Molecule 40: 50S RIBOSOMAL PROTEIN L3

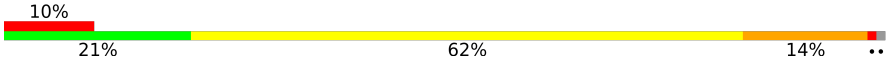
Chain BE:

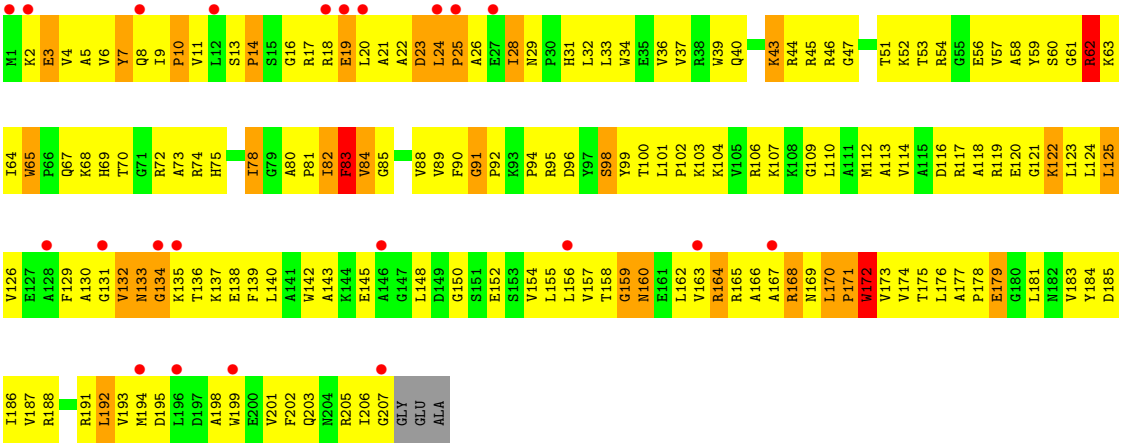




• Molecule 41: 50S RIBOSOMAL PROTEIN L4

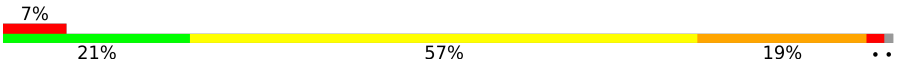
Chain BF:

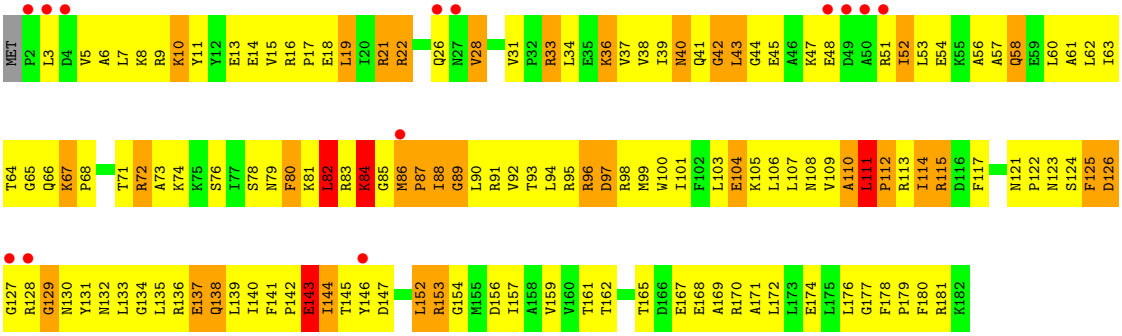




• Molecule 42: 50S RIBOSOMAL PROTEIN L5

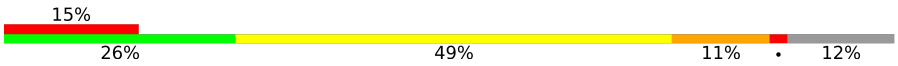
Chain BG:

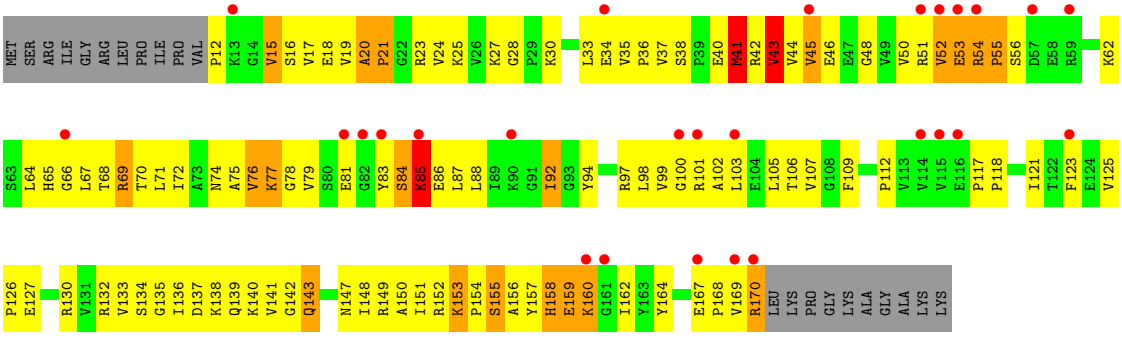




• Molecule 43: 50S RIBOSOMAL PROTEIN L6

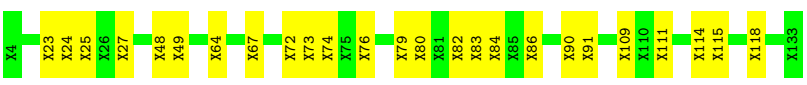
Chain BH:





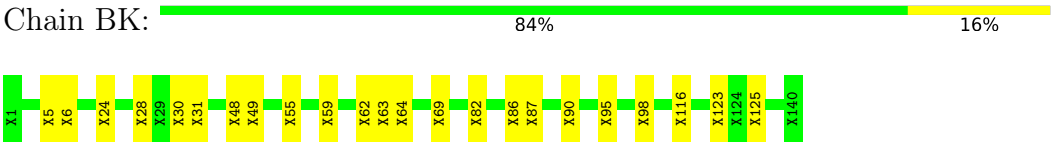
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



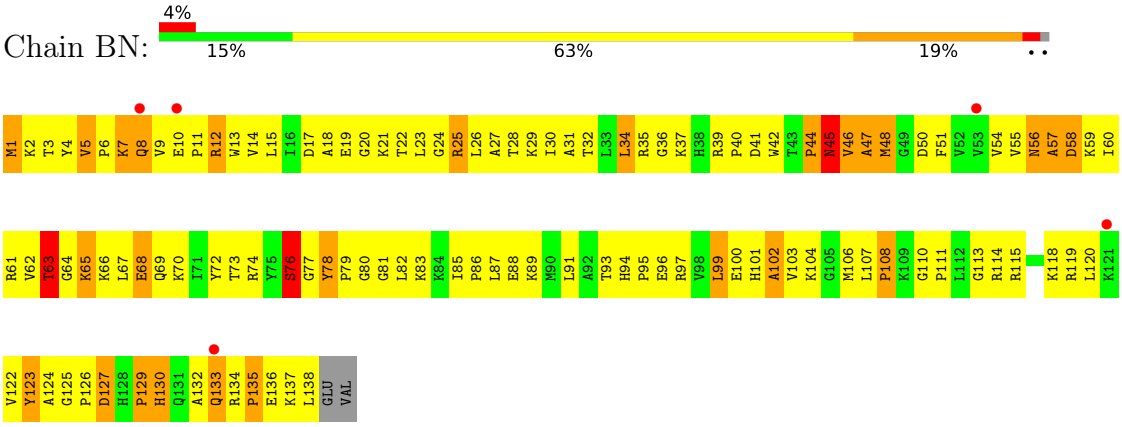
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:



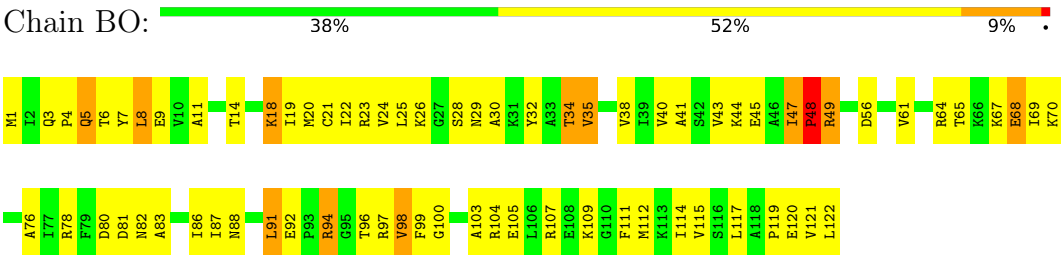
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



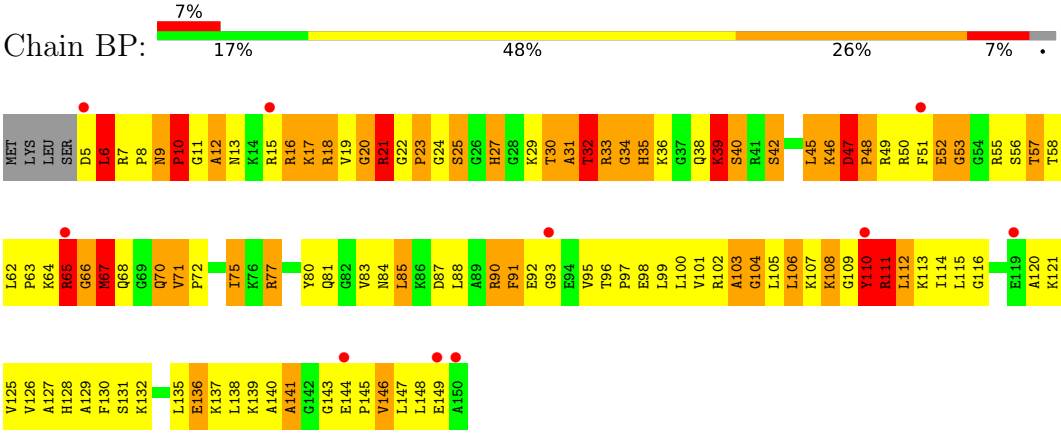
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



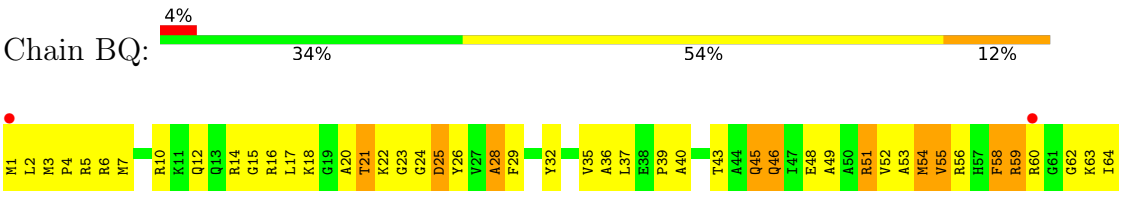
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

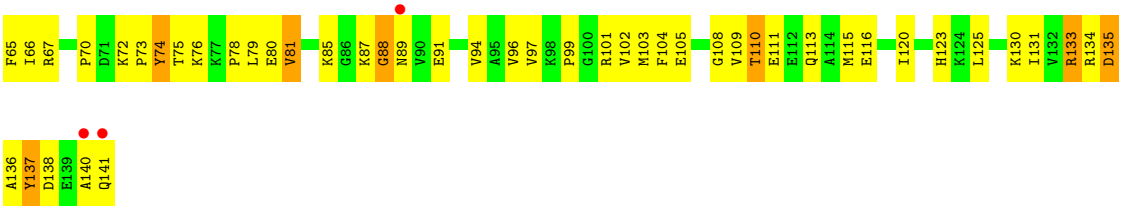
Chain BP:



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

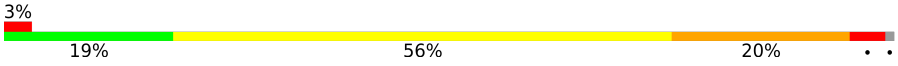
Chain BQ:

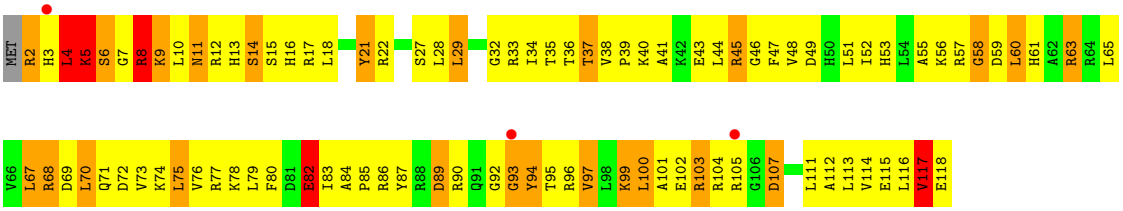




• Molecule 50: 50S RIBOSOMAL PROTEIN L17

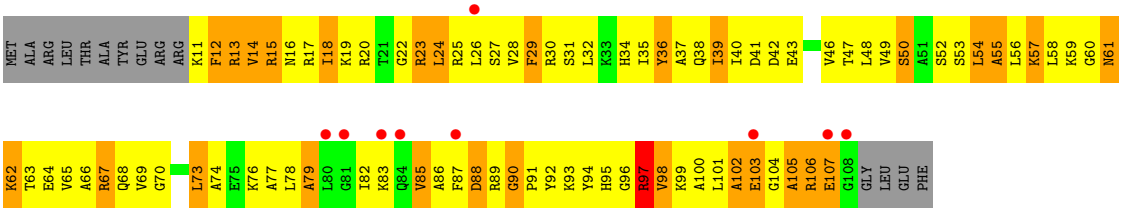
Chain BR:





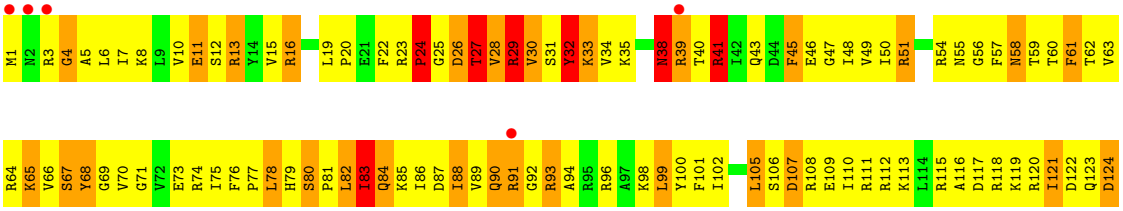
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

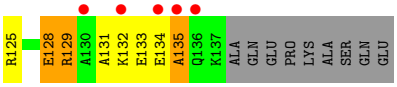
Chain BS:



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

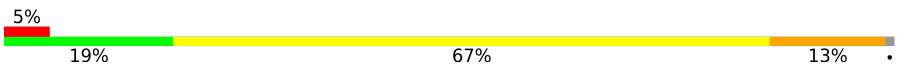
Chain BT:

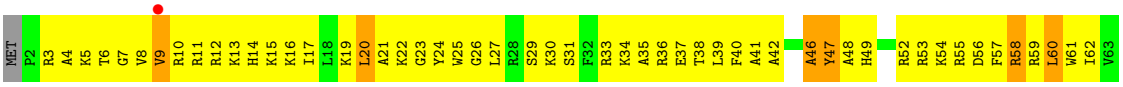


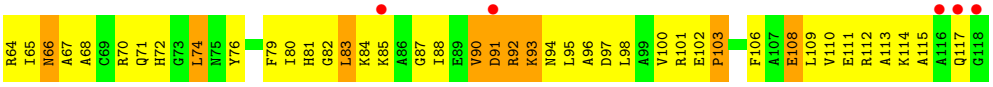


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

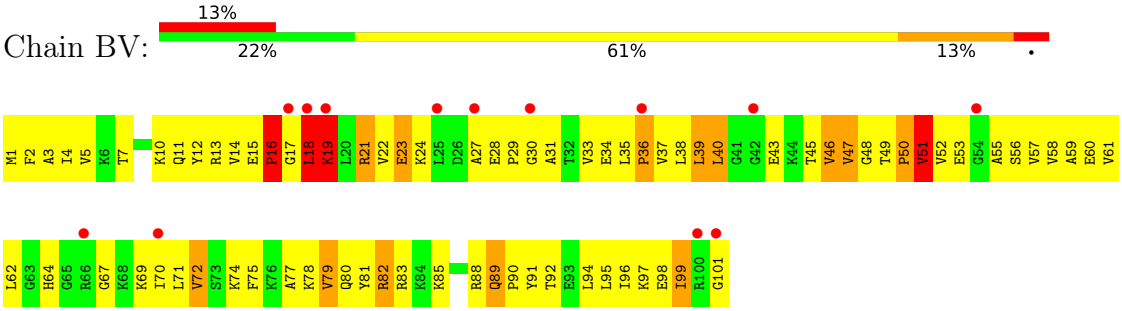
Chain BU:



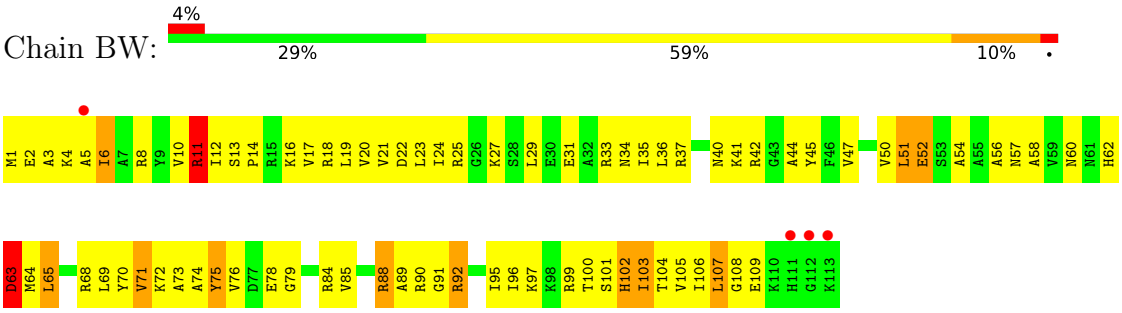




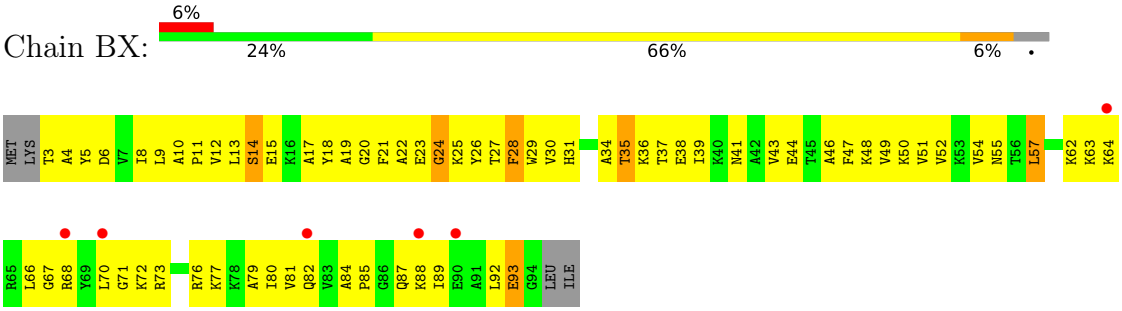
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



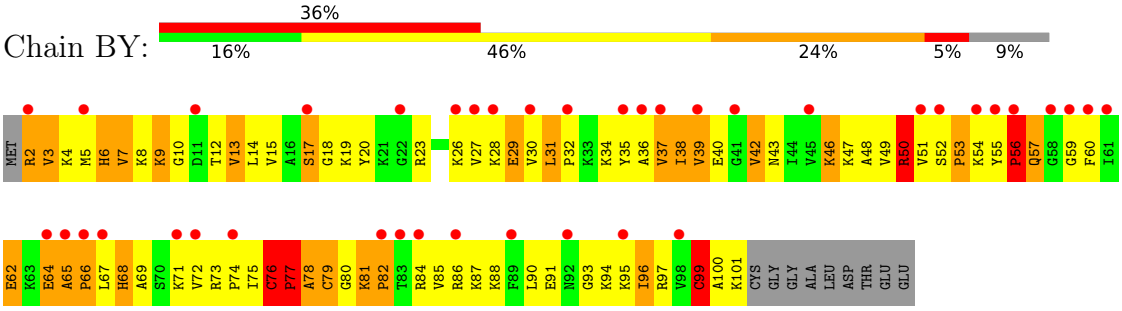
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



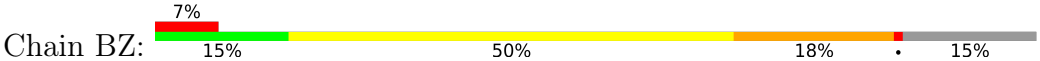
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

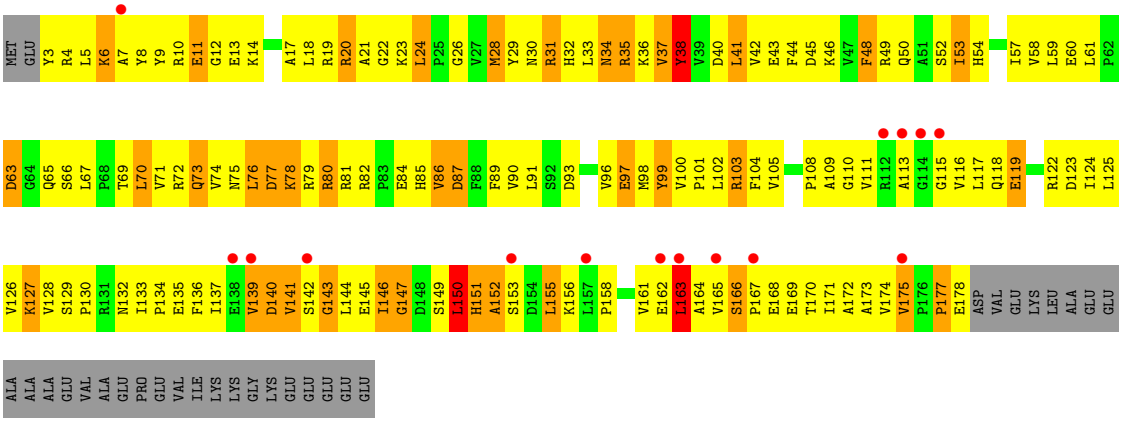


• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

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D63 G64 Q65 S66 L67 P68 T69 L70 V71 R72 Q73 V74 N75 L76 D77 K78 R79 R80 R81 R82 P83 E84 H85 V86 D87 P88 F89 V90 L91 S92 D93 V96 E97 M98 Y99 V100 P101 L102 R103 F104 V105 P108 A109 G110 V111 R112 A113 G114 G115 V116 L117 Q118 E119 R122 D123 I124 L125
V126 K127 V128 S129 P130 R131 N132 I133 P134 E135 F136 I137 E138 V139 D140 V141 S142 G143 L144 E145 I146 G147 D148 S149 L150 H151 A152 S153 D154 L155 K156 L157 P158 V161 E162 L163 A164 V165 S166 P167 E168 E169 T170 I171 A172 A173 V174 V175 P176 P177 E178 ASP VAL GLU LYS LEU ALA GLU GLU
ALA ALA ALA GLU VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	64.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 85.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, GCP, 4SU, OMC, 5MU, ZN, PSU, MG, PAR, H2U, MIA

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(^{o})	Ideal(^{o})
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
40	BE	146	THR
49	BQ	59	ARG
41	BF	70	THR
40	BE	121	ASN
46	BN	25	ARG

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

Mol	Chain	Res	Type
41	BF	133	ASN
52	BT	79	HIS
42	BG	121	ASN
48	BP	81	GLN
54	BV	80	GLN

5.3.3 RNA (i)

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
24	AY	18	G
36	BA	2762	G
36	BA	614(C)	A
36	BA	2756	U
36	BA	2126	A

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	H2U	AY	17	24	18,21,22	0.91	1 (5%)	21,30,33	1.77	4 (19%)
24	5MU	AY	54	24	19,22,23	0.39	0	28,32,35	0.43	0
24	H2U	AY	20	24	18,21,22	0.87	0	21,30,33	1.93	6 (28%)
24	H2U	AY	16	24	18,21,22	0.81	0	21,30,33	1.87	5 (23%)
24	PSU	AY	55	24	18,21,22	0.91	2 (11%)	22,30,33	1.79	5 (22%)
24	4SU	AY	8	24	18,21,22	0.47	0	26,30,33	0.85	2 (7%)
24	OMC	AY	32	24	19,22,23	0.34	0	26,31,34	0.64	1 (3%)
24	7MG	AY	46	24	22,26,27	3.02	2 (9%)	29,39,42	1.62	2 (6%)
24	MIA	AY	37	24	24,31,32	1.02	1 (4%)	26,44,47	1.74	4 (15%)

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	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	5MU	AY	54	24	-	0/7/25/26	0/2/2/2
24	H2U	AY	20	24	-	4/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	2/7/25/26	0/2/2/2
24	4SU	AY	8	24	-	1/7/25/26	0/2/2/2
24	OMC	AY	32	24	-	0/9/27/28	0/2/2/2
24	7MG	AY	46	24	-	5/7/37/38	0/3/3/3
24	MIA	AY	37	24	-	3/11/33/34	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-13.69	1.38	1.46
24	AY	46	7MG	C5-N7	3.42	1.39	1.35
24	AY	55	PSU	C6-C5	2.50	1.38	1.35
24	AY	55	PSU	C6-N1	2.31	1.40	1.36
24	AY	17	H2U	C2-N1	2.23	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AY	46	7MG	N9-C8-N7	6.89	113.23	103.38
24	AY	37	MIA	C11-S10-C2	4.91	105.94	102.27
24	AY	17	H2U	C4-N3-C2	-4.75	121.85	125.79
24	AY	16	H2U	C4-N3-C2	-4.56	122.01	125.79
24	AY	20	H2U	C4-N3-C2	-4.47	122.08	125.79

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C6
24	AY	20	H2U	O4'-C1'-N1-C6
24	AY	37	MIA	C5-C6-N6-C12
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	17	H2U	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	54	5MU	2	0
24	AY	20	H2U	3	0
24	AY	16	H2U	1	0
24	AY	55	PSU	1	0
24	AY	8	4SU	3	0
24	AY	37	MIA	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
61	GCP	AZ	501	62	27,34,34	2.03	6 (22%)	34,54,54	1.94	9 (26%)
59	PAR	AA	1601	-	45,45,45	1.57	7 (15%)	64,67,67	1.26	6 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GCP	AZ	501	62	-	11/15/38/38	0/3/3/3
59	PAR	AA	1601	-	-	4/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	501	GCP	C6-N1	6.86	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AA	1601	PAR	C64-C54	5.14	1.59	1.52
61	AZ	501	GCP	PG-O2G	-3.93	1.45	1.54
59	AA	1601	PAR	C52-C42	3.44	1.59	1.52
61	AZ	501	GCP	C8-N7	-3.12	1.29	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	AZ	501	GCP	C4-C5-C6	-5.41	115.64	120.80
61	AZ	501	GCP	C5-C6-N1	-4.85	116.79	123.43
59	AA	1601	PAR	O33-C14-C24	4.78	116.45	108.22
61	AZ	501	GCP	C2-N3-C4	-4.25	110.50	115.36
59	AA	1601	PAR	O54-C54-C64	3.88	113.23	106.01

There are no chirality outliers.

5 of 15 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.

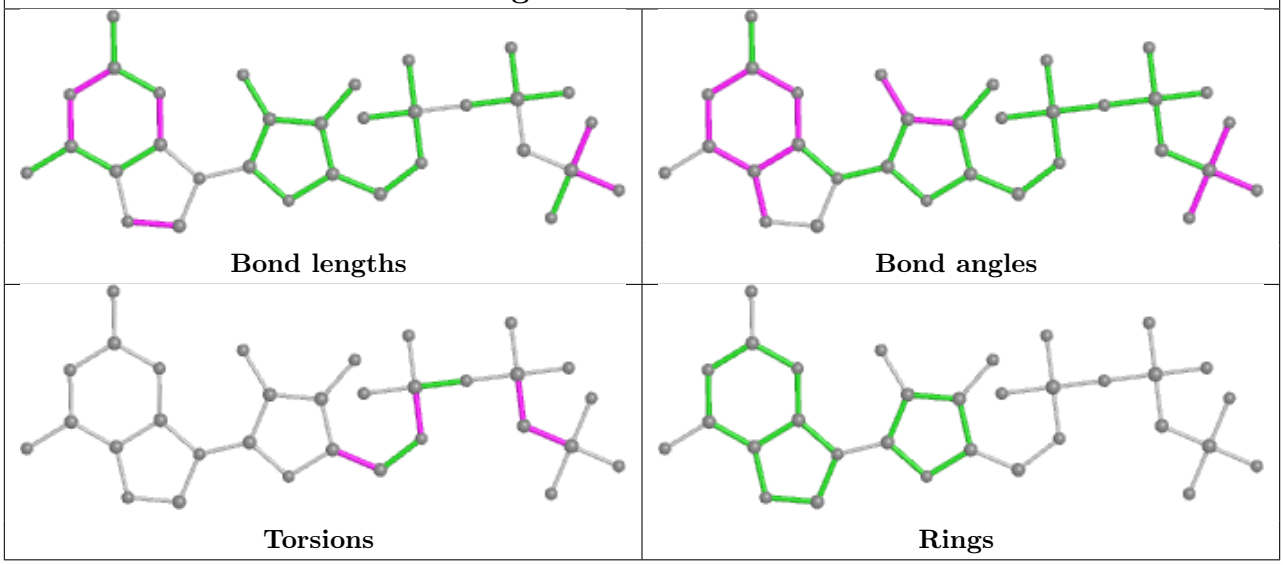
2 monomers are involved in 7 short contacts:

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

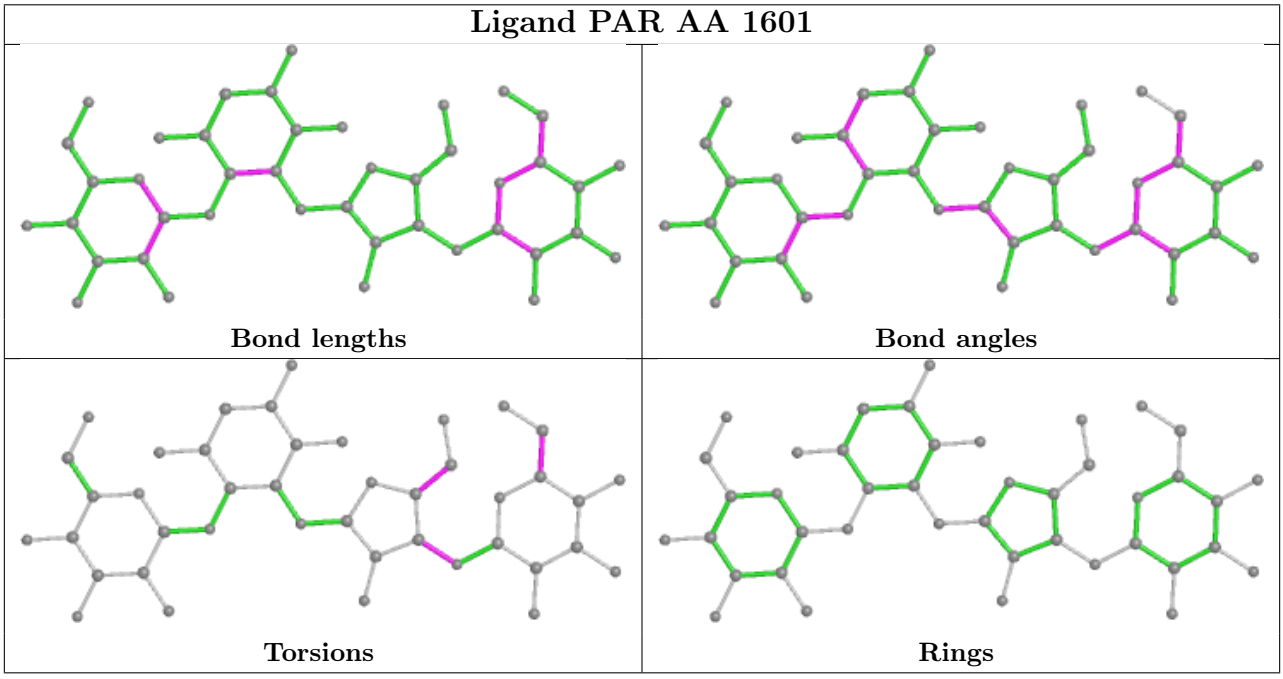
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand GCP AZ 501



Ligand PAR AA 1601



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	0.03	34 (2%) 60 39	24, 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	34, 57, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	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^2)	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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^2)	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

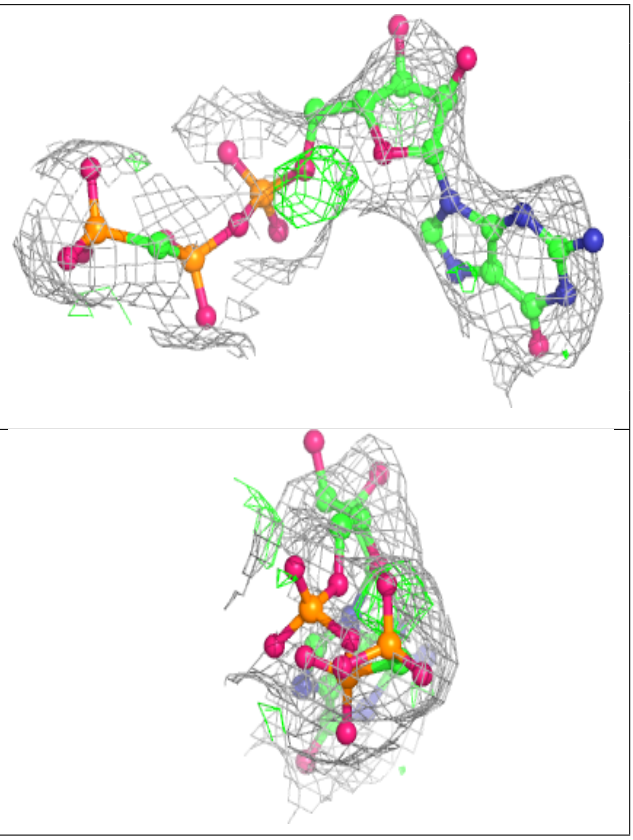
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	B4	101	1/1	0.92	0.08	132,132,132,132	0
61	GCP	AZ	501	32/32	0.93	0.23	89,110,116,117	0
62	MG	AZ	502	1/1	0.93	0.24	55,55,55,55	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.

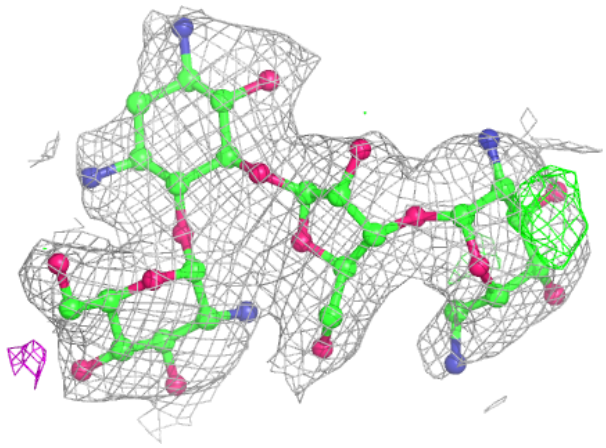
Electron density around GCP AZ 501:

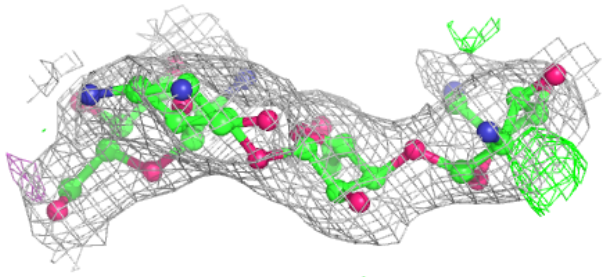
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

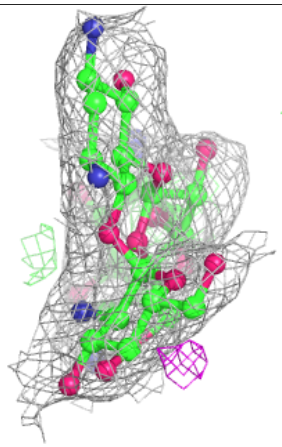


Electron density around PAR AA 1601:

$2mF_o$-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 (i)

There are no such residues in this entry.