wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 04:12 pm GMT

PDB ID	:	4V8O
Title	:	Crystal structure of the hybrid state of ribosome in complex with the guanosine triphosphatase release factor 3
Authors	:	Jin, H.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2011-07-26
Resolution	:	3.80 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:

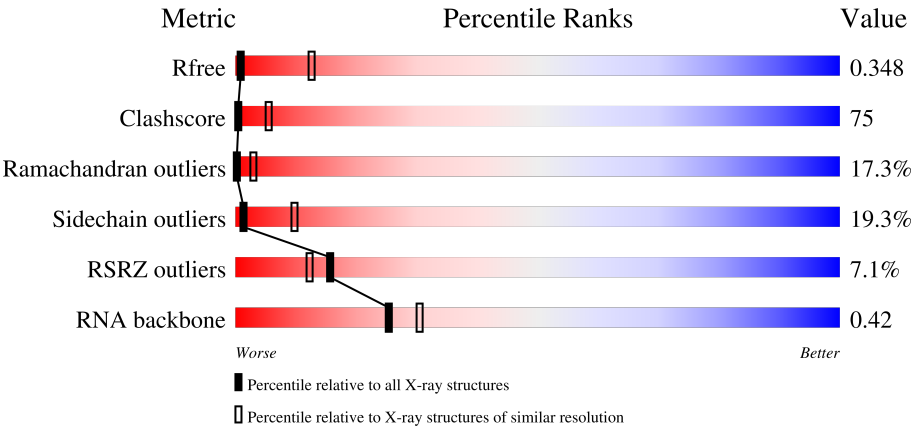
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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% 11% 64% 20%
2	AB	256	9% 46% 31% 5% 8%
3	AC	239	18% 46% 21% 13%
4	AD	209	6% 20% 60% 19%

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Mol	Chain	Length	Quality of chain
5	AE	162	2% 17% 57% 18% 7%
6	AF	101	20% 60% 19%
7	AG	156	2% 18% 65% 15%
8	AH	138	4% 17% 63% 17%
9	AI	128	2% 12% 68% 16%
10	AJ	105	10% 15% 56% 19% 6%
11	AK	129	4% 17% 59% 14% 8%
12	AL	135	4% 21% 46% 19% 6% 7%
13	AM	126	9% 19% 48% 30%
14	AN	61	8% 57% 25% 8%
15	AO	89	4% 10% 56% 30%
16	AP	88	20% 11% 65% 19% 5%
17	AQ	105	12% 18% 64% 13% 5%
18	AR	88	2% 10% 55% 13% 20%
19	AS	93	4% 57% 23% 15%
20	AT	106	9% 14% 58% 20% 7%
21	AU	27	15% 19% 52% 15% 7% 7%
22	AV	77	% 53% 45%
23	AX	9	11% 44% 44%
24	AY	529	10% 12% 47% 29% 5% 6%
25	B0	85	21% 16% 60% 19%
26	B1	98	8% 14% 63% 15%
27	B2	72	10% 6% 81% 11%
28	B3	60	10% 15% 67% 15%
29	B4	71	4% 14% 34% 11% 37%

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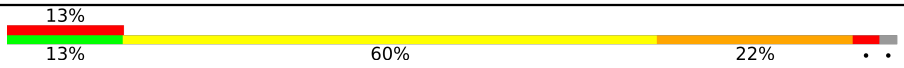
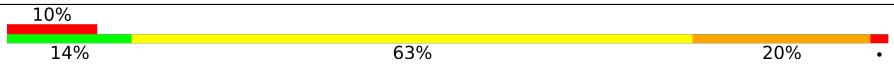
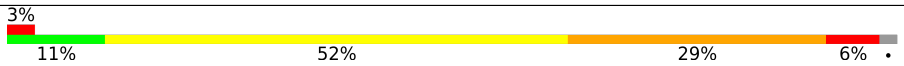
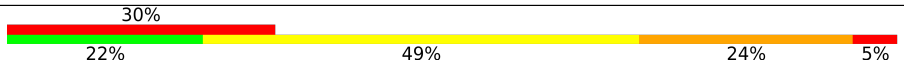
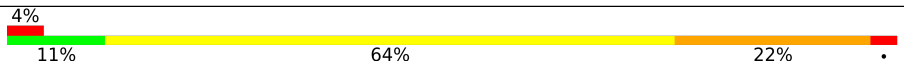
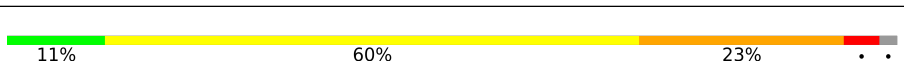
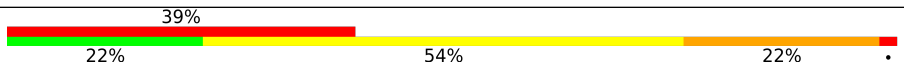
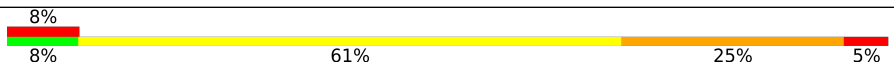
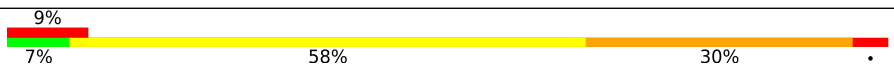
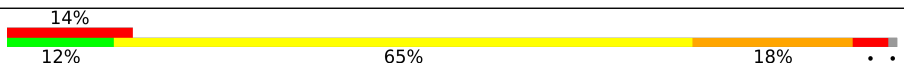
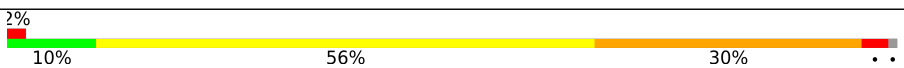
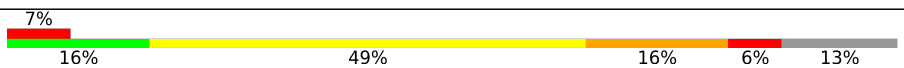
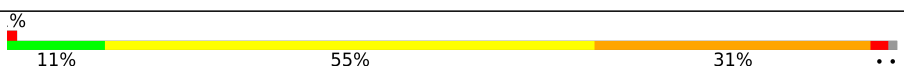
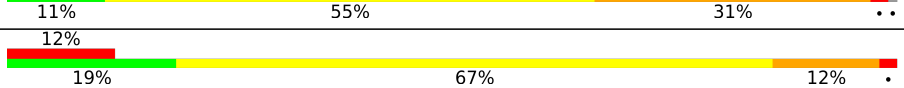
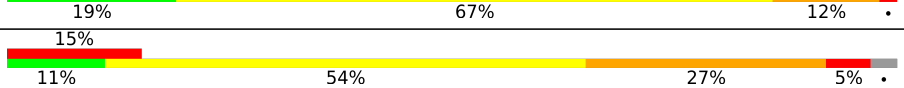
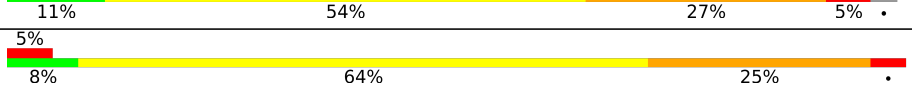
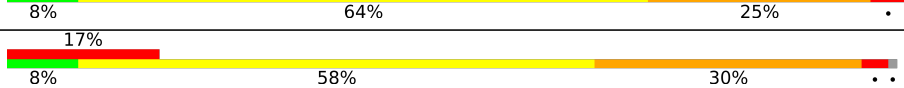
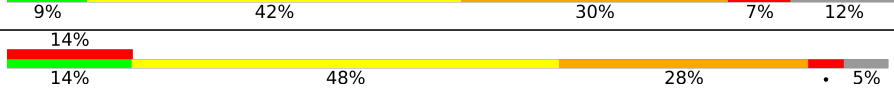
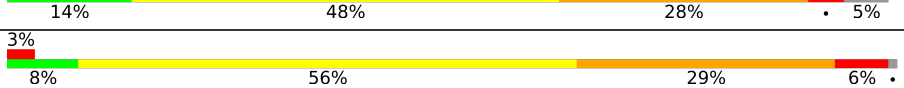
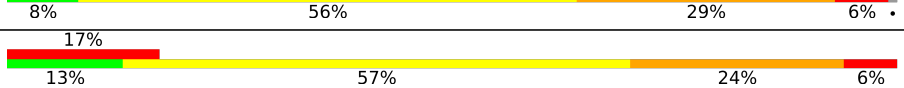
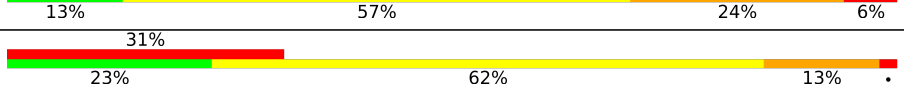
Mol	Chain	Length	Quality of chain
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BJ	173	
44	BK	147	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	

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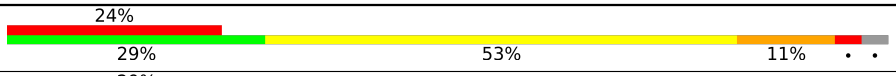
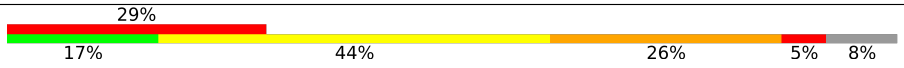
Mol	Chain	Length	Quality of chain
55	BX	96	
56	BY	110	
57	BZ	206	

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
58	GCP	AY	1000	-	-	X	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 151017 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	235	1901	1213	342	341	5	0	0	1

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

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

- 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	151	1147	724	218	201	4	0	0	1

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	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	79	Total	C	N	O	S	0	0	1
			630	403	115	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	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called PE HYBRID STATE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			192	88	39	57	8			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	496	Total	C	N	O	S	0	0	0
			3934	2492	677	744	21			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

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

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	156	Total	C	N	O	S	0	0	1
			1189	752	222	214	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	131	Total	C	N	O	0	0	1
			654	393	131	130			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BK	141	Total	C	N	O	0	0	1
			701	420	141	140			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

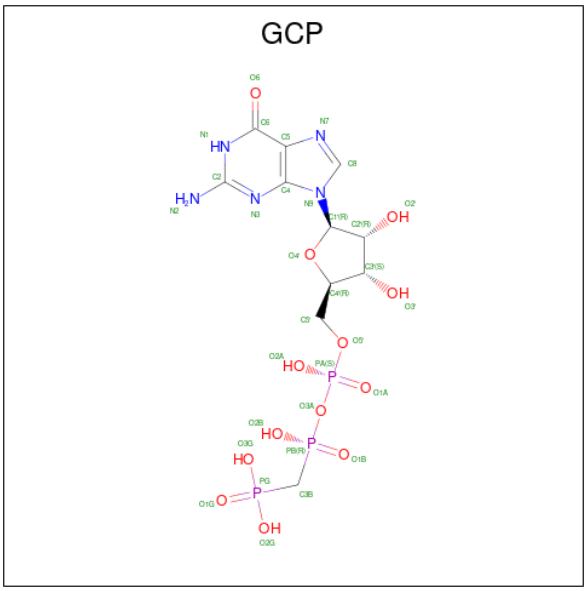
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



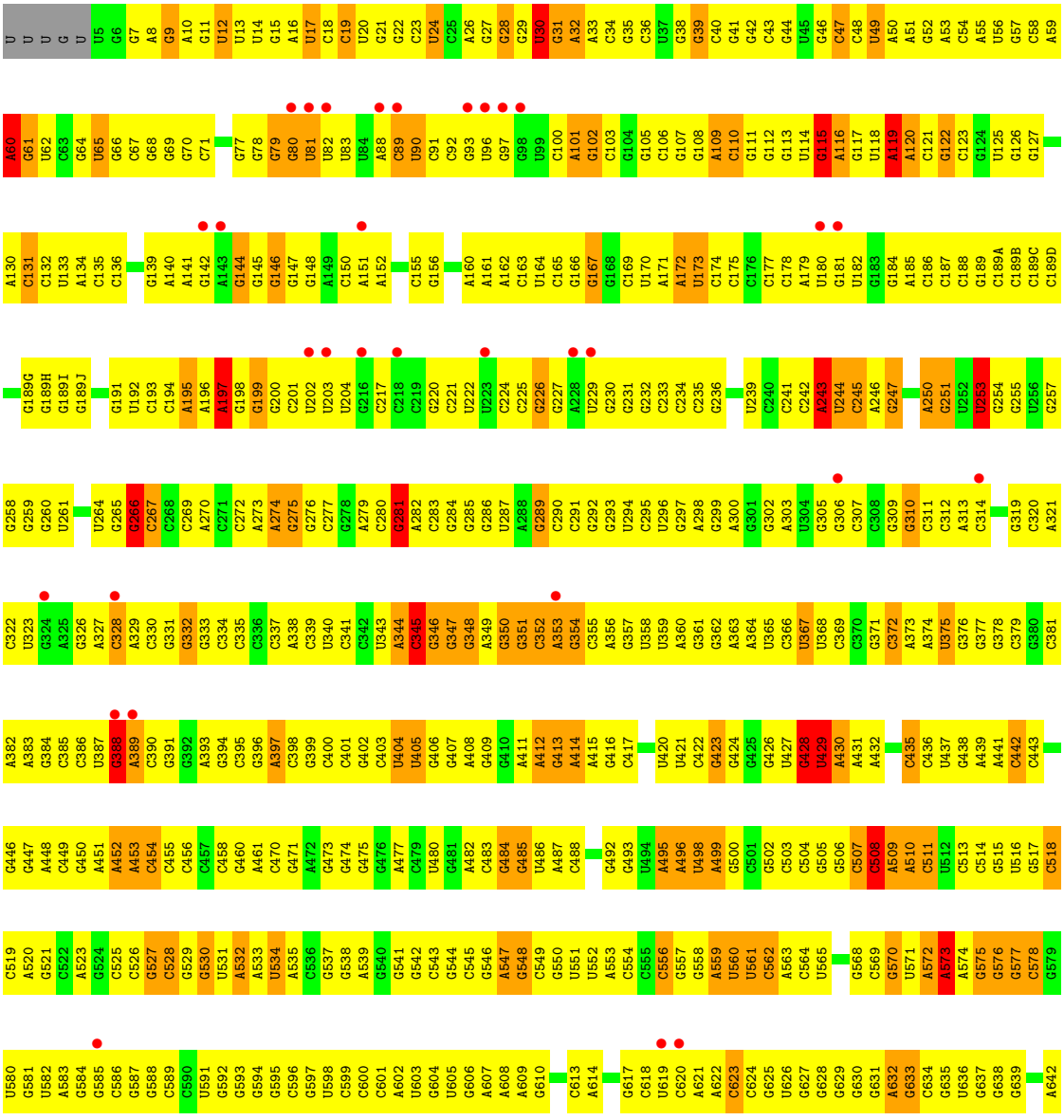
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

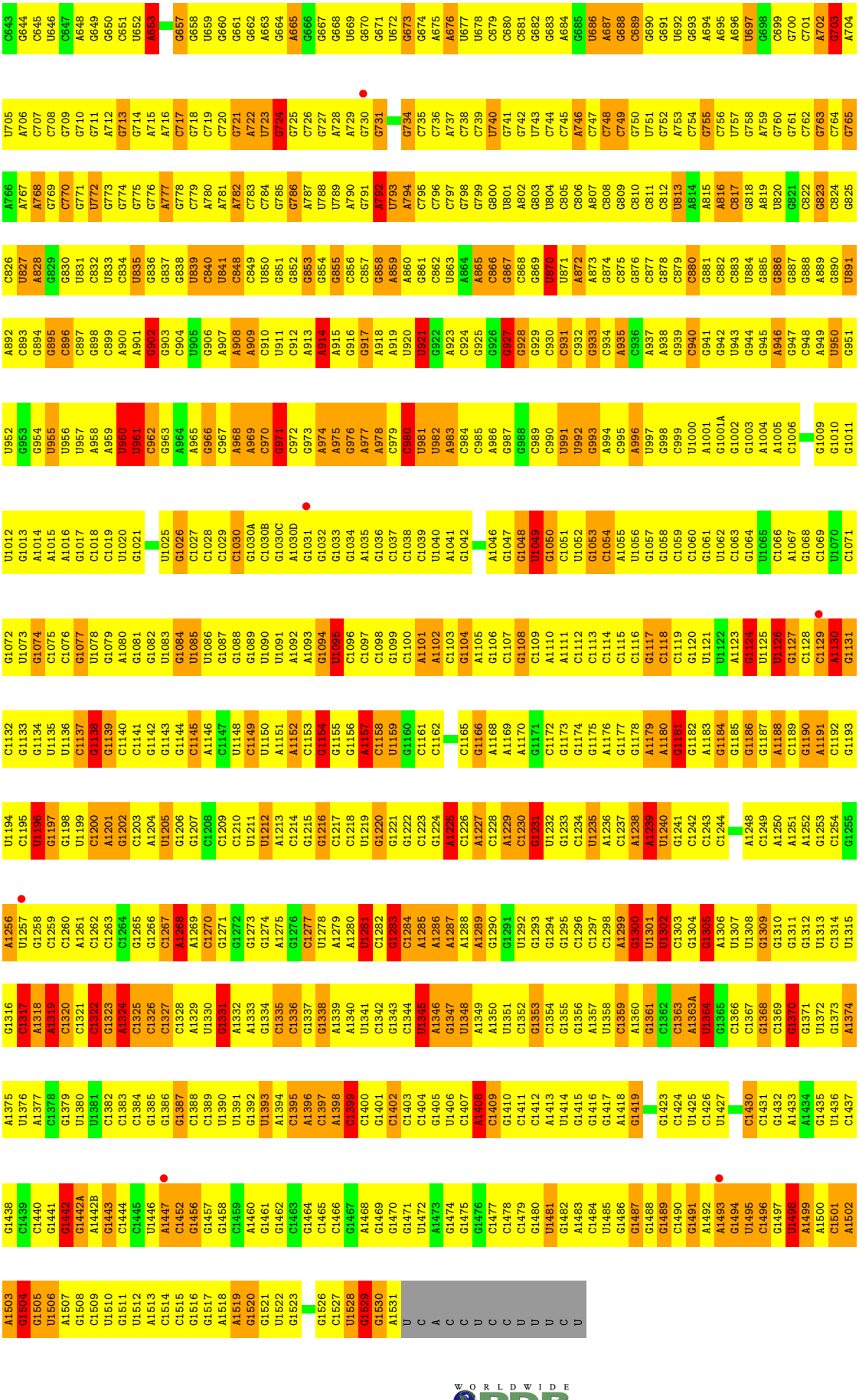
3 Residue-property plots (i)

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

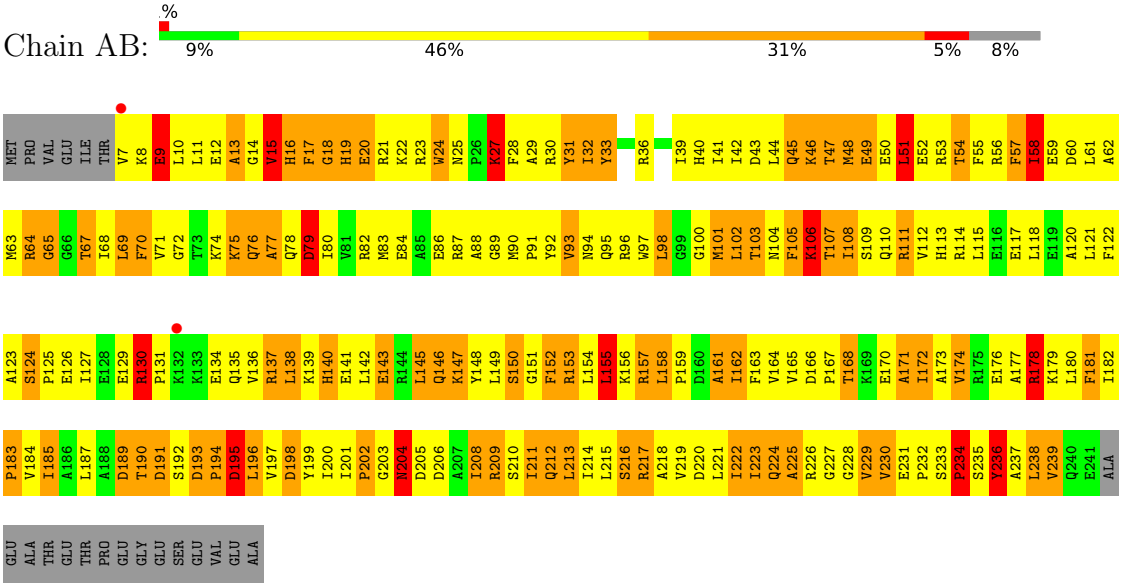
Chain AA: 





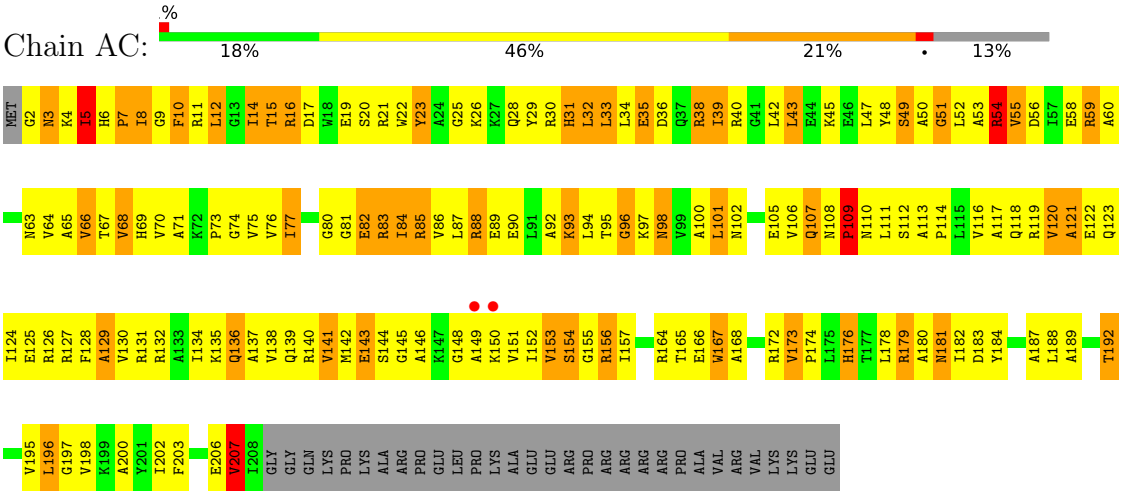
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



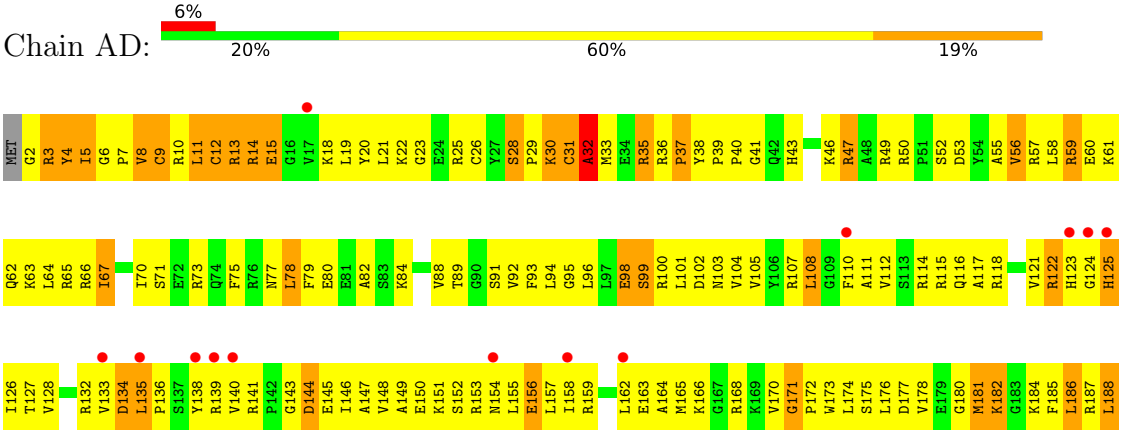
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



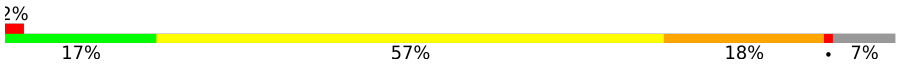
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

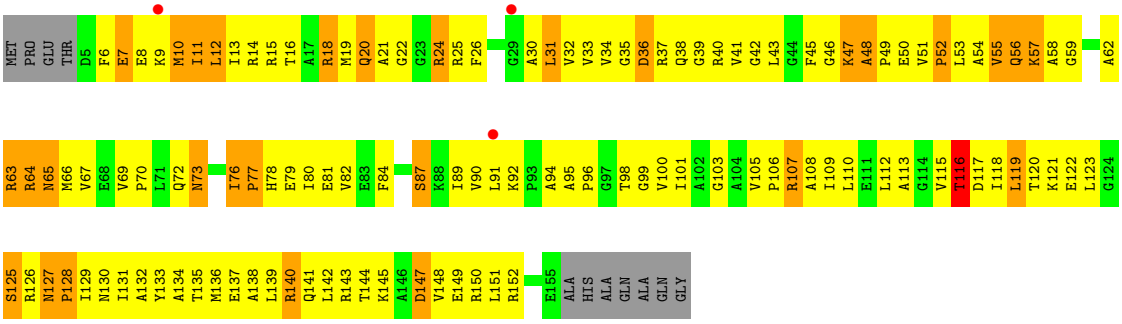
Chain AD:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

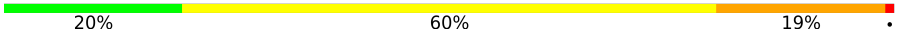
Chain AE:





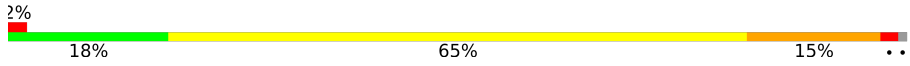
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

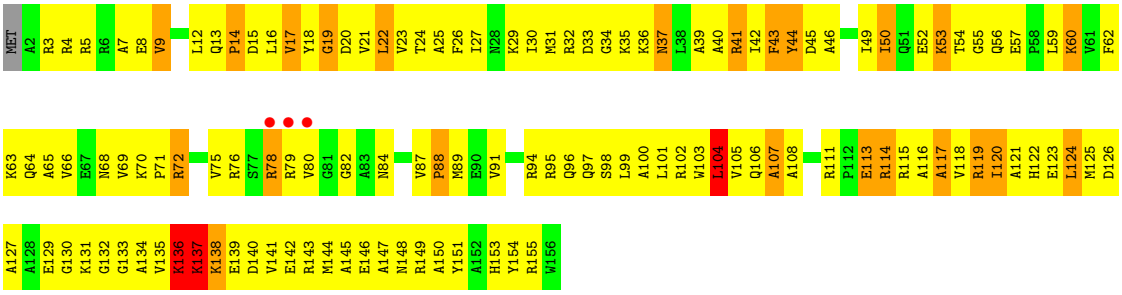
Chain AF:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

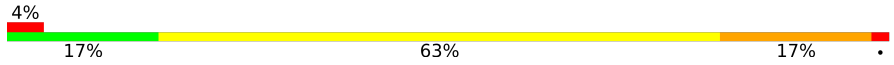
Chain AG:

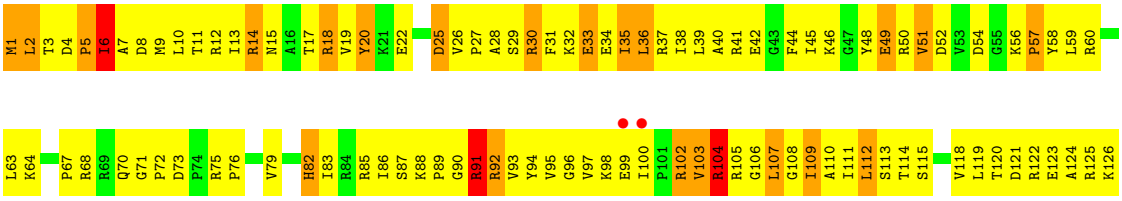


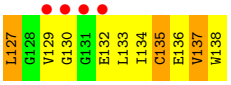


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

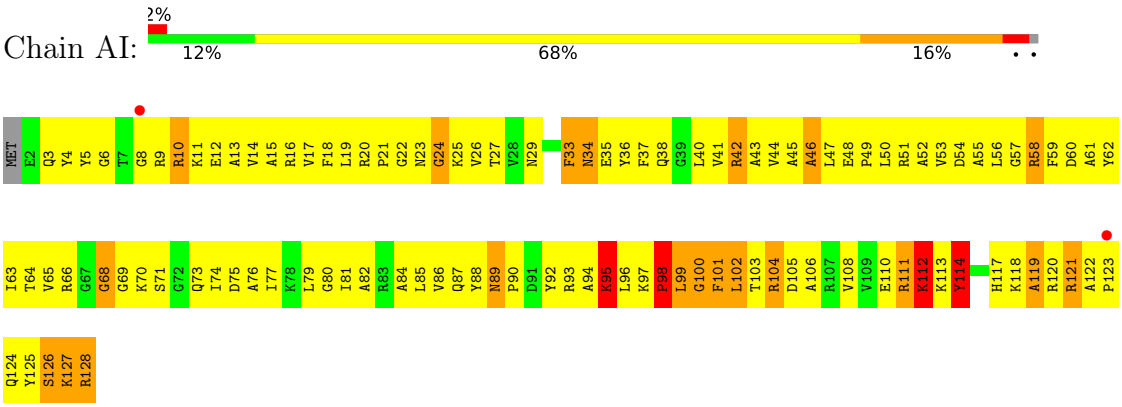
Chain AH:



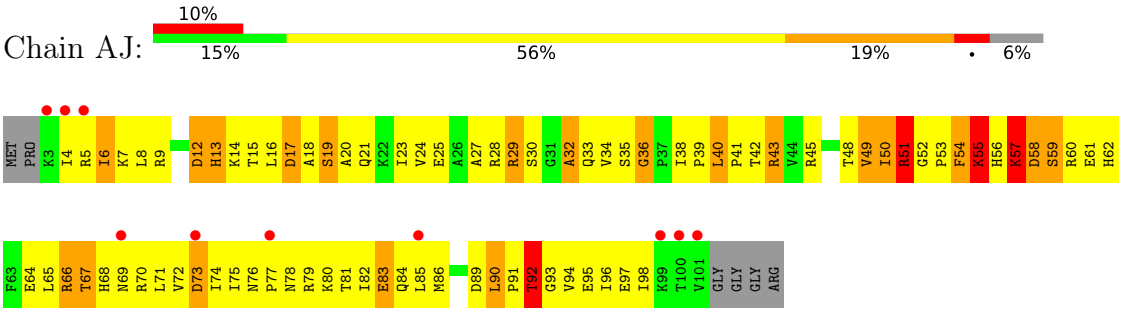




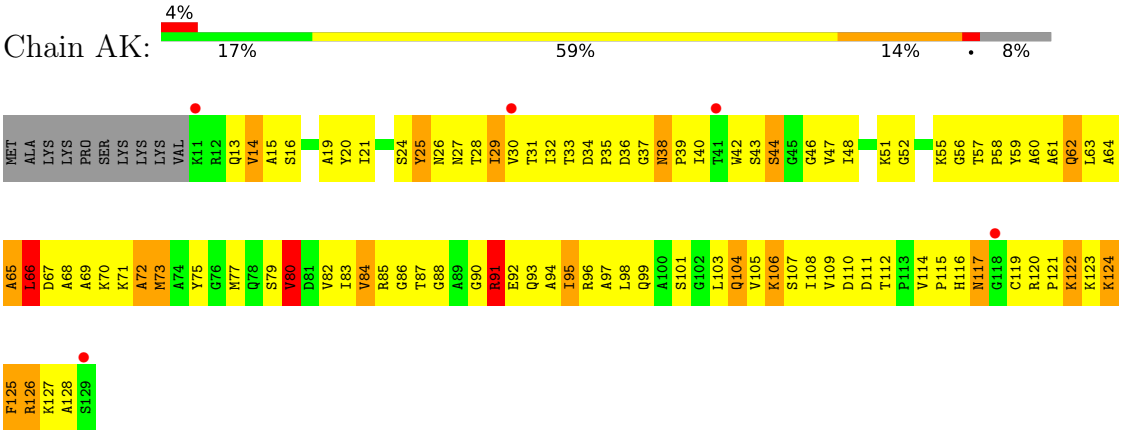
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



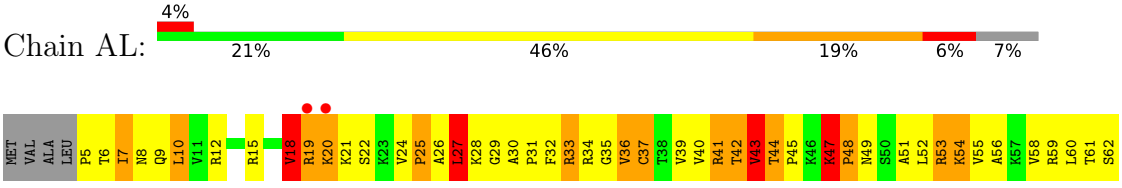
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

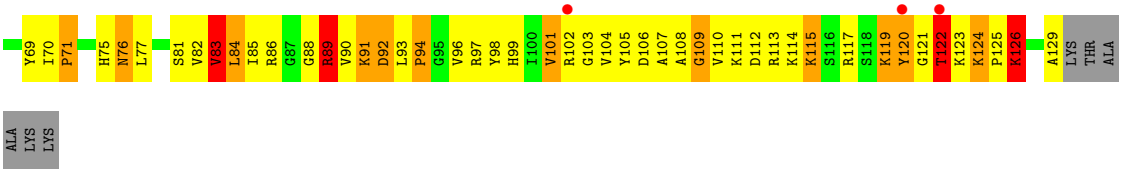


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

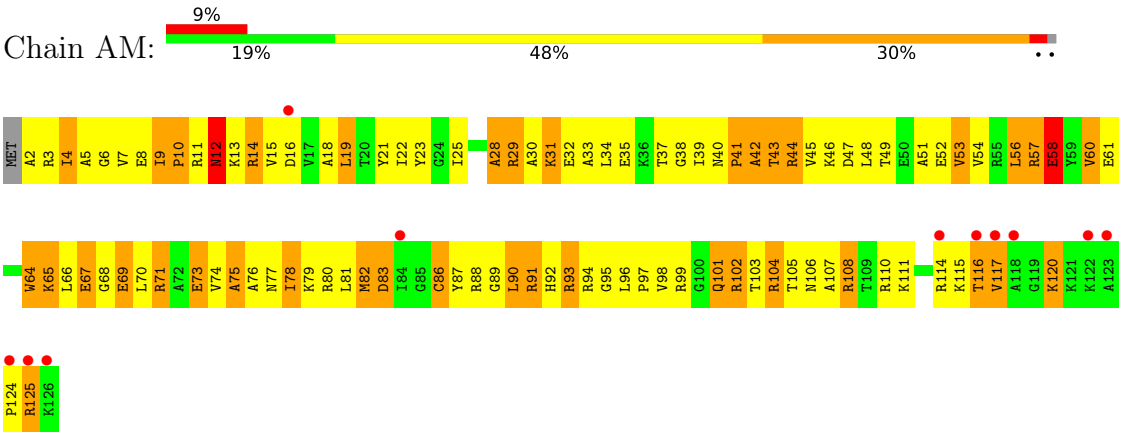


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

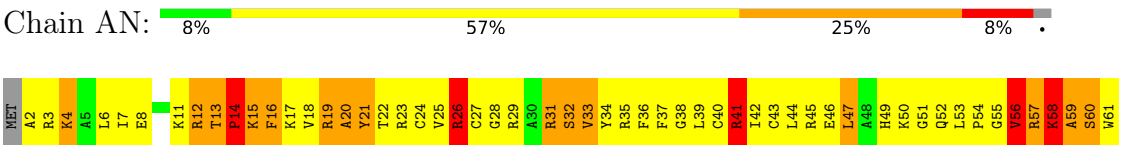




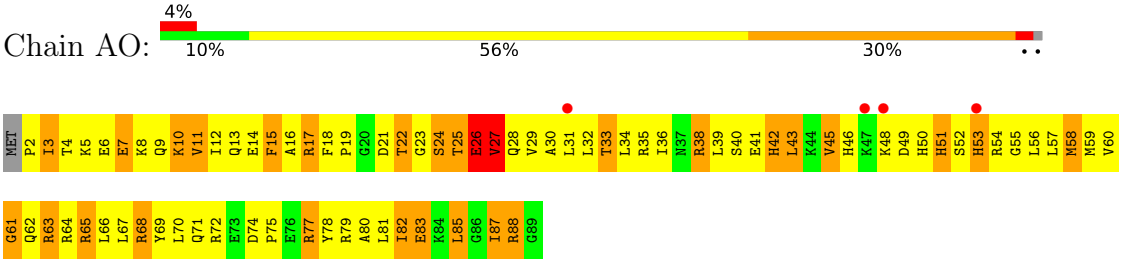
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



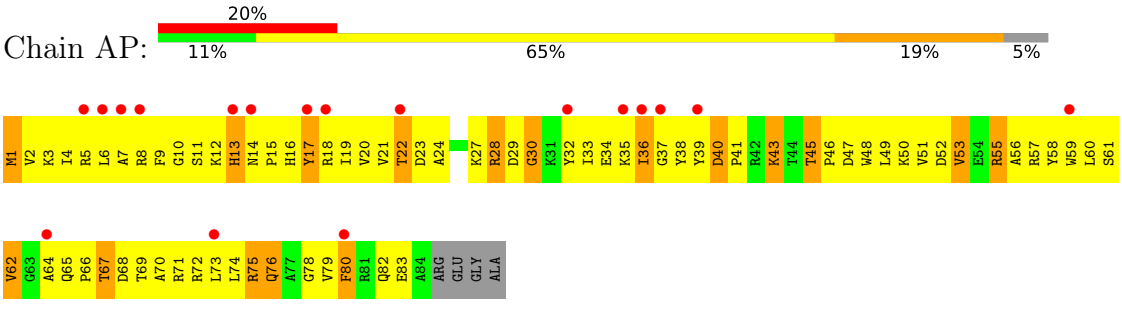
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



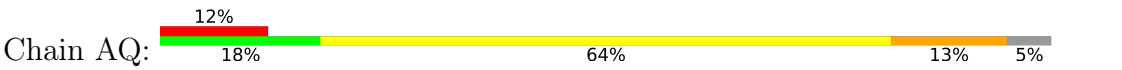
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

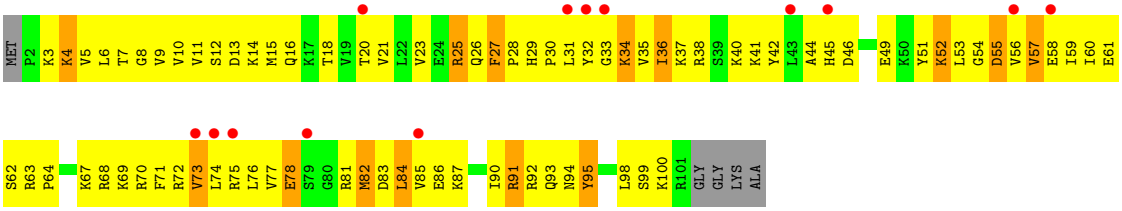


• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



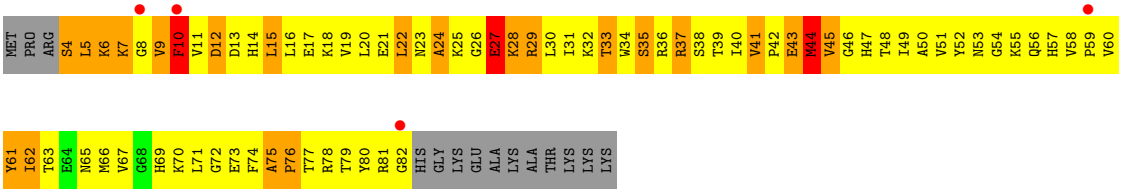


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:

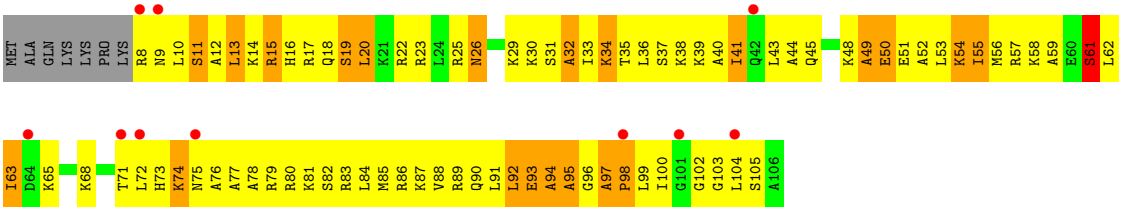
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



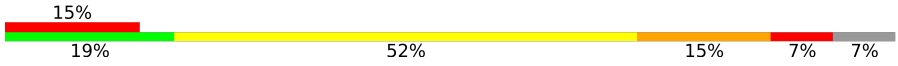
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

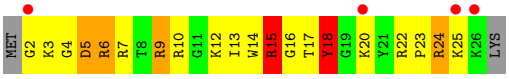
Chain AT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

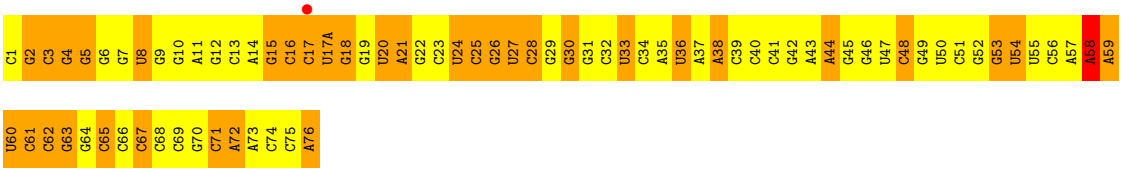
Chain AU:



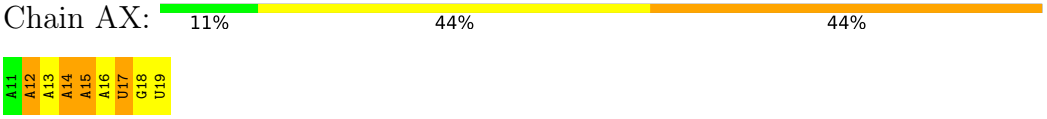


• Molecule 22: PE HYBRID STATE TRNA FMET

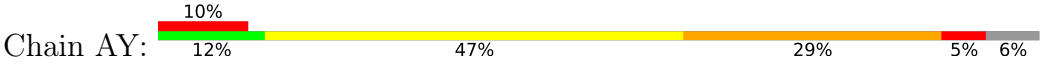
Chain AV:

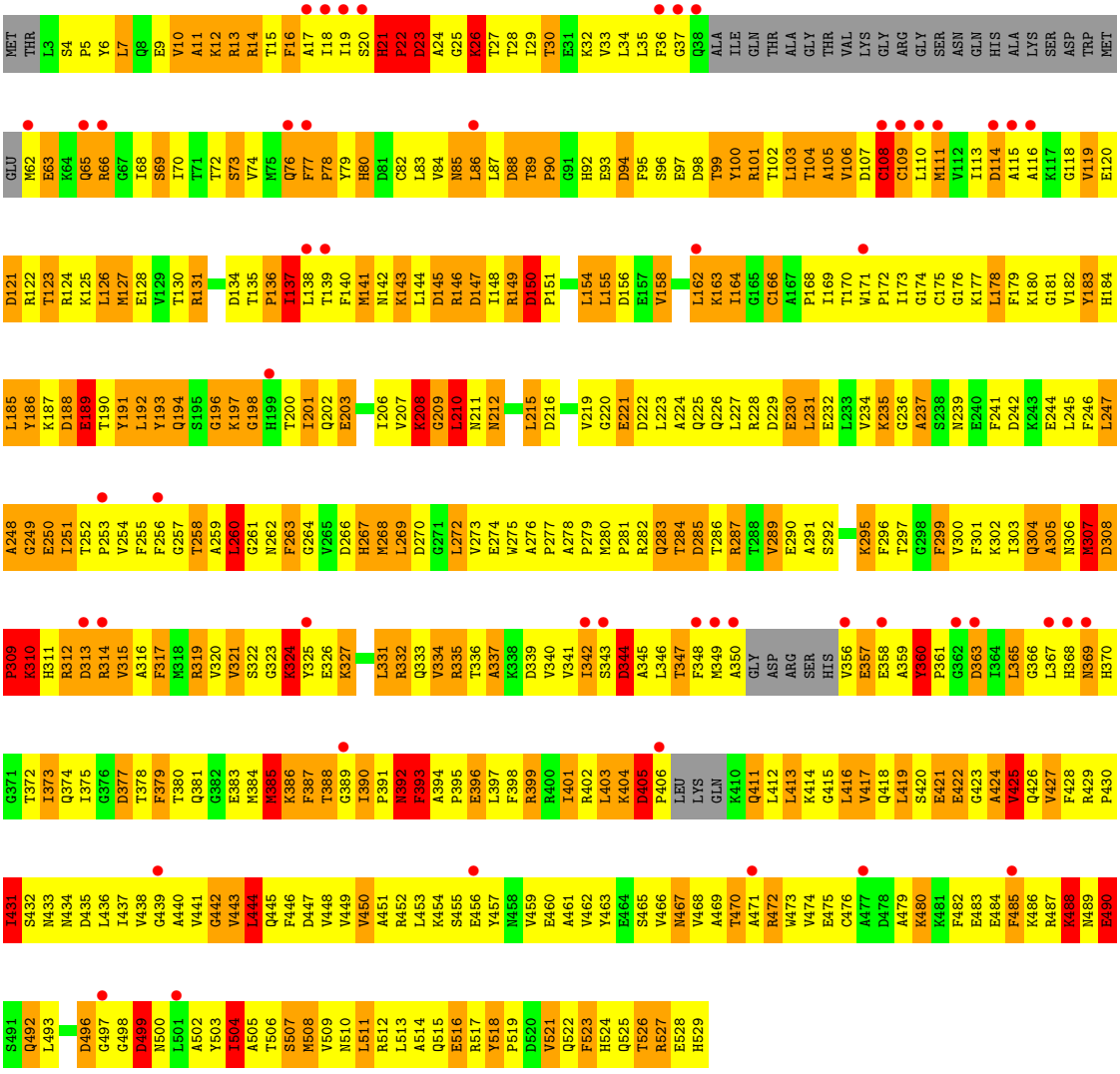


• Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

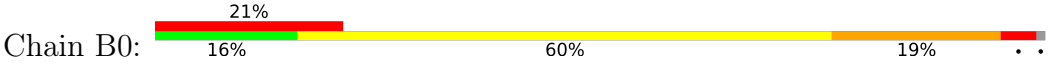


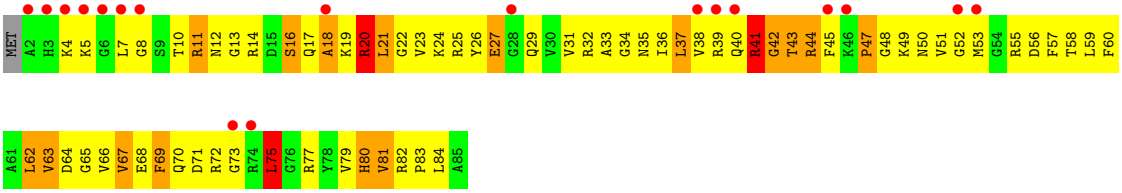
• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3





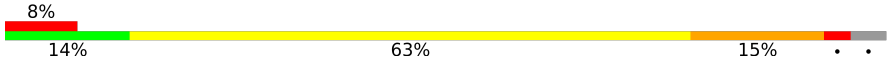
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

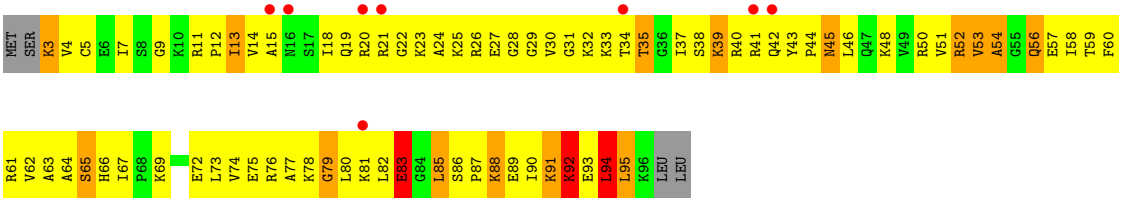




• Molecule 26: 50S RIBOSOMAL PROTEIN L28

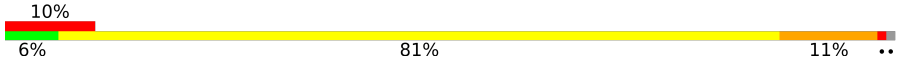
Chain B1:

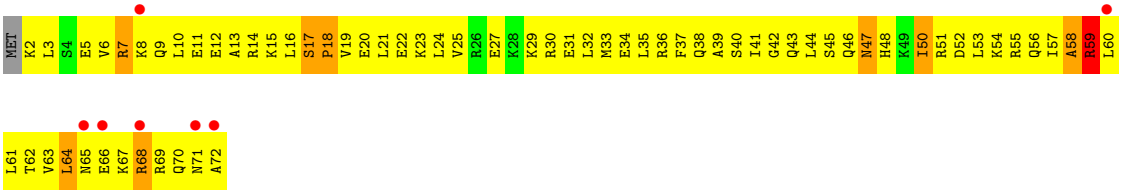




• Molecule 27: 50S RIBOSOMAL PROTEIN L29

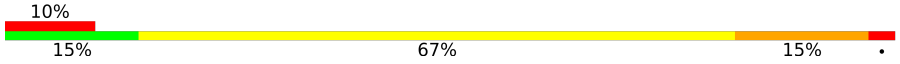
Chain B2:





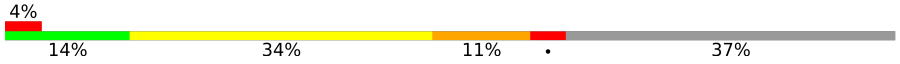
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

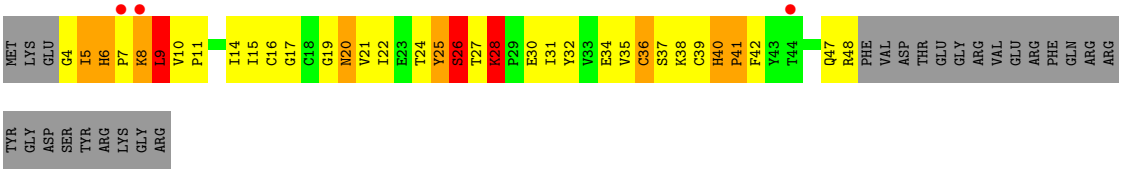
Chain B3:



• Molecule 29: 50S RIBOSOMAL PROTEIN L31

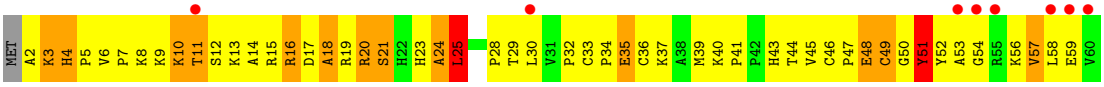
Chain B4:





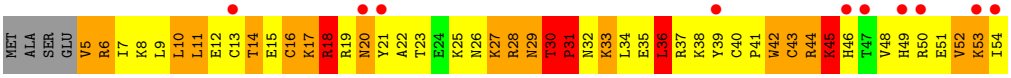
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



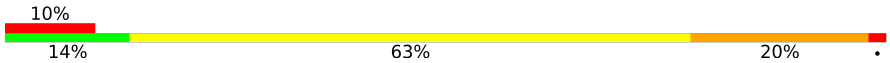
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

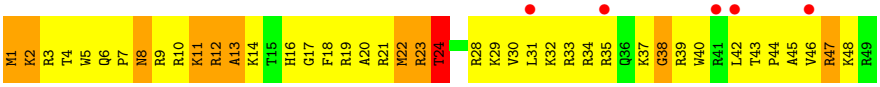
Chain B6:



• Molecule 32: 50S RIBOSOMAL PROTEIN L34

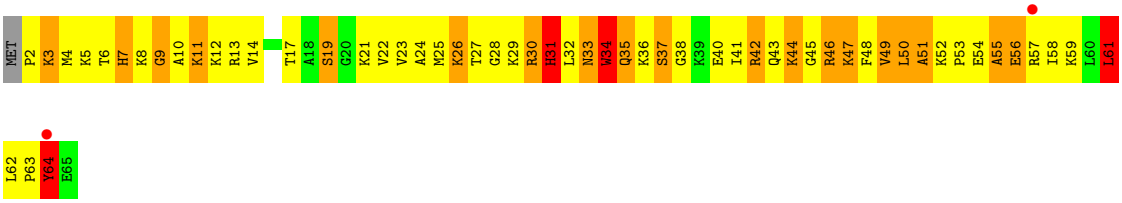
Chain B7:





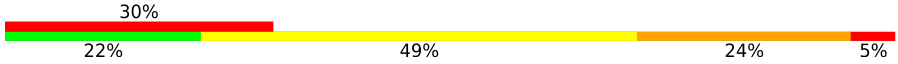
• Molecule 33: 50S RIBOSOMAL PROTEIN L35

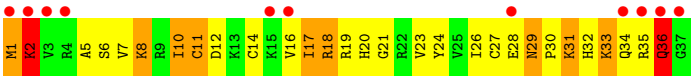
Chain B8:



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

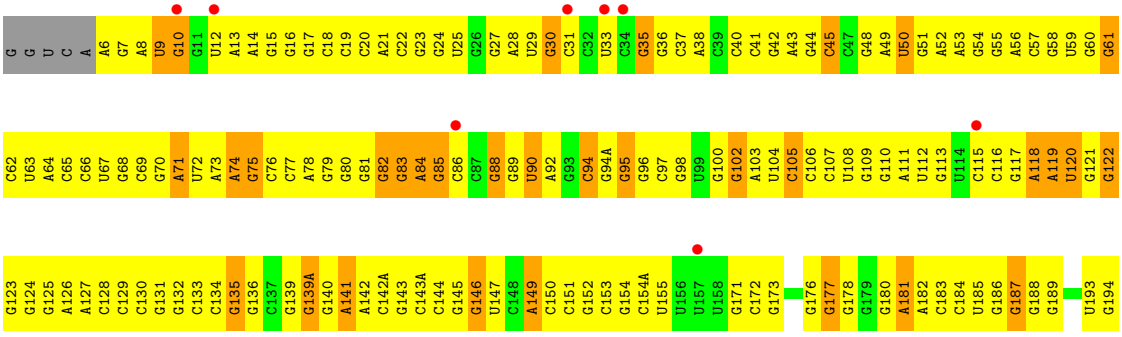
Chain B9:

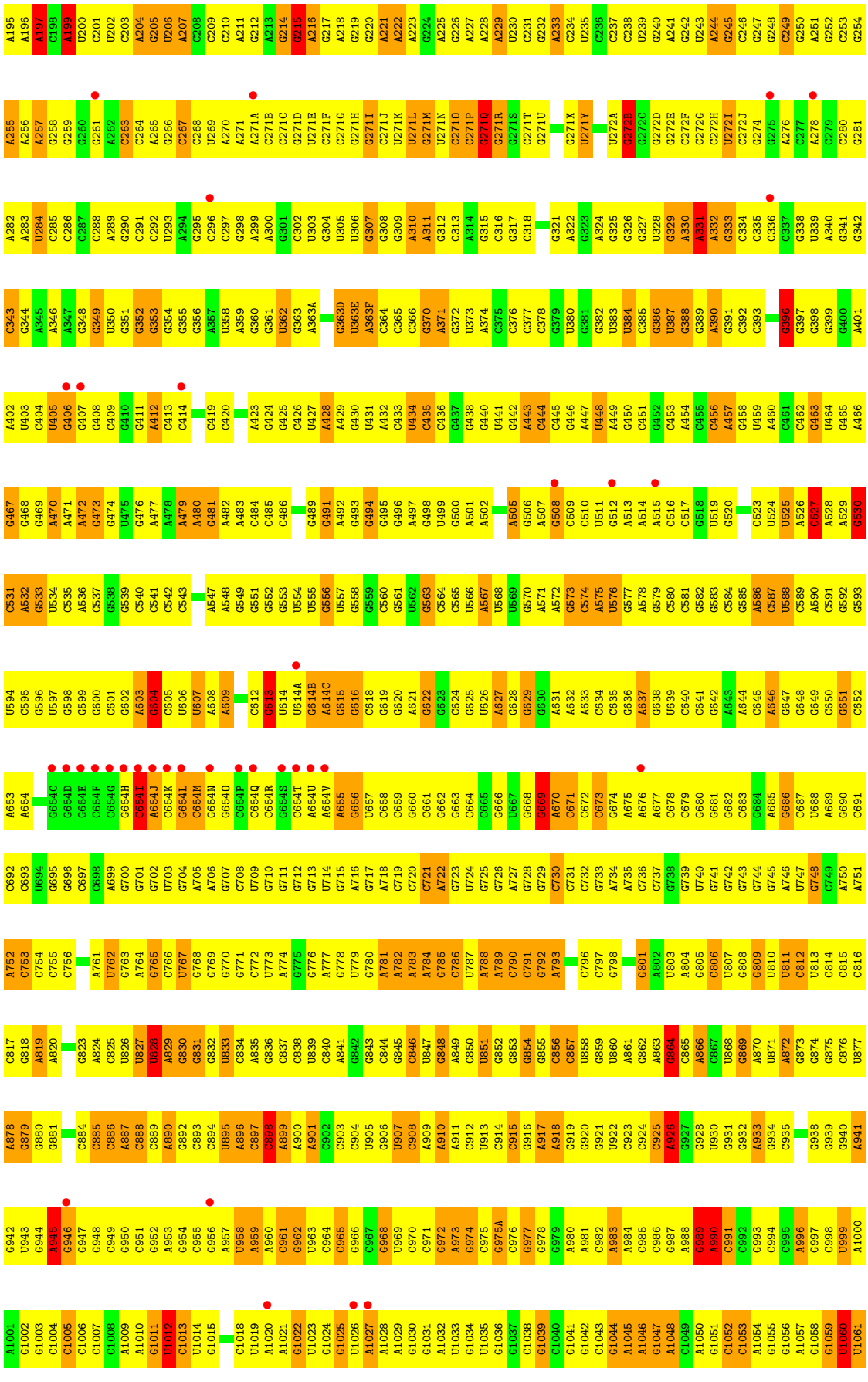


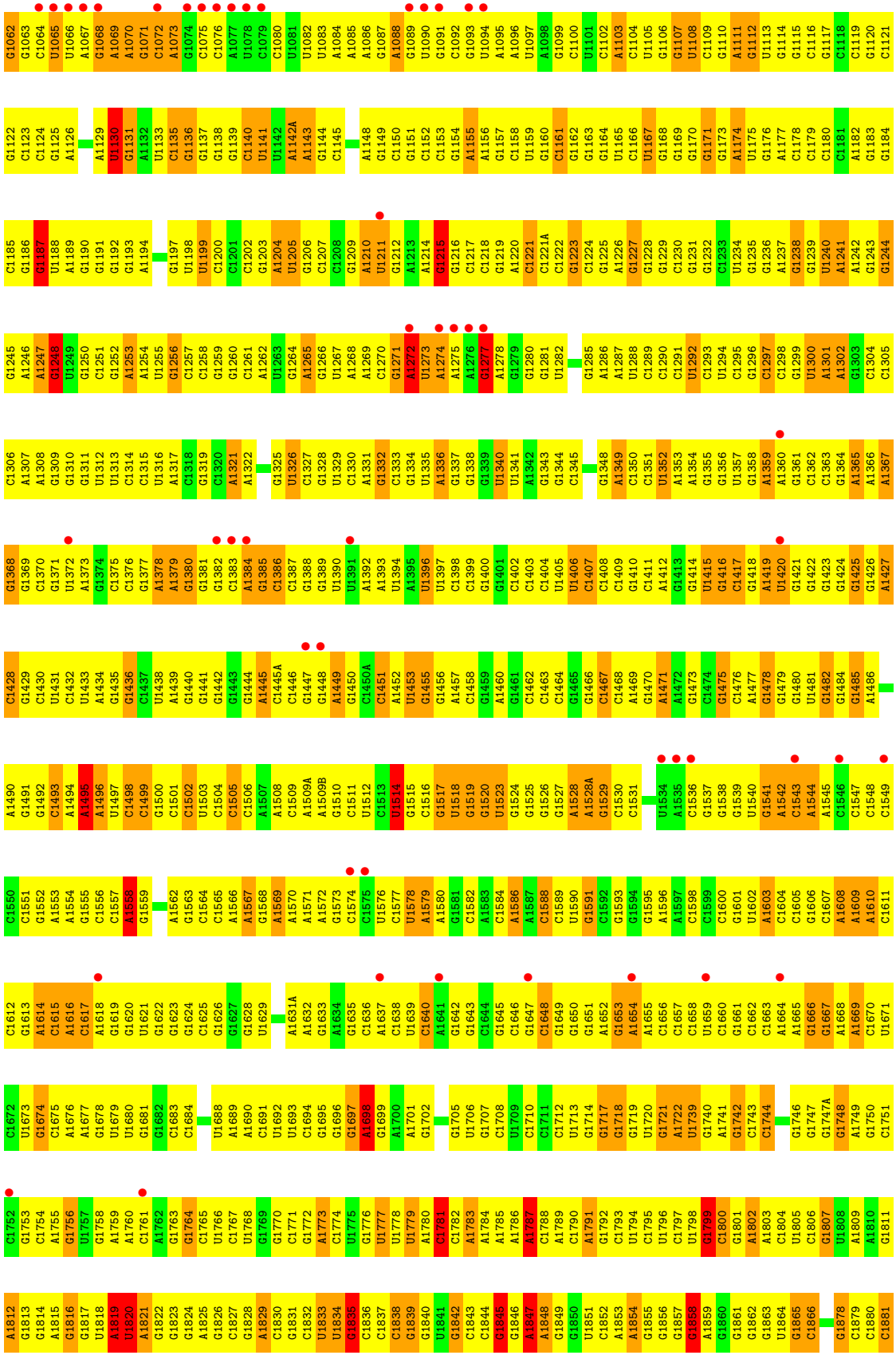


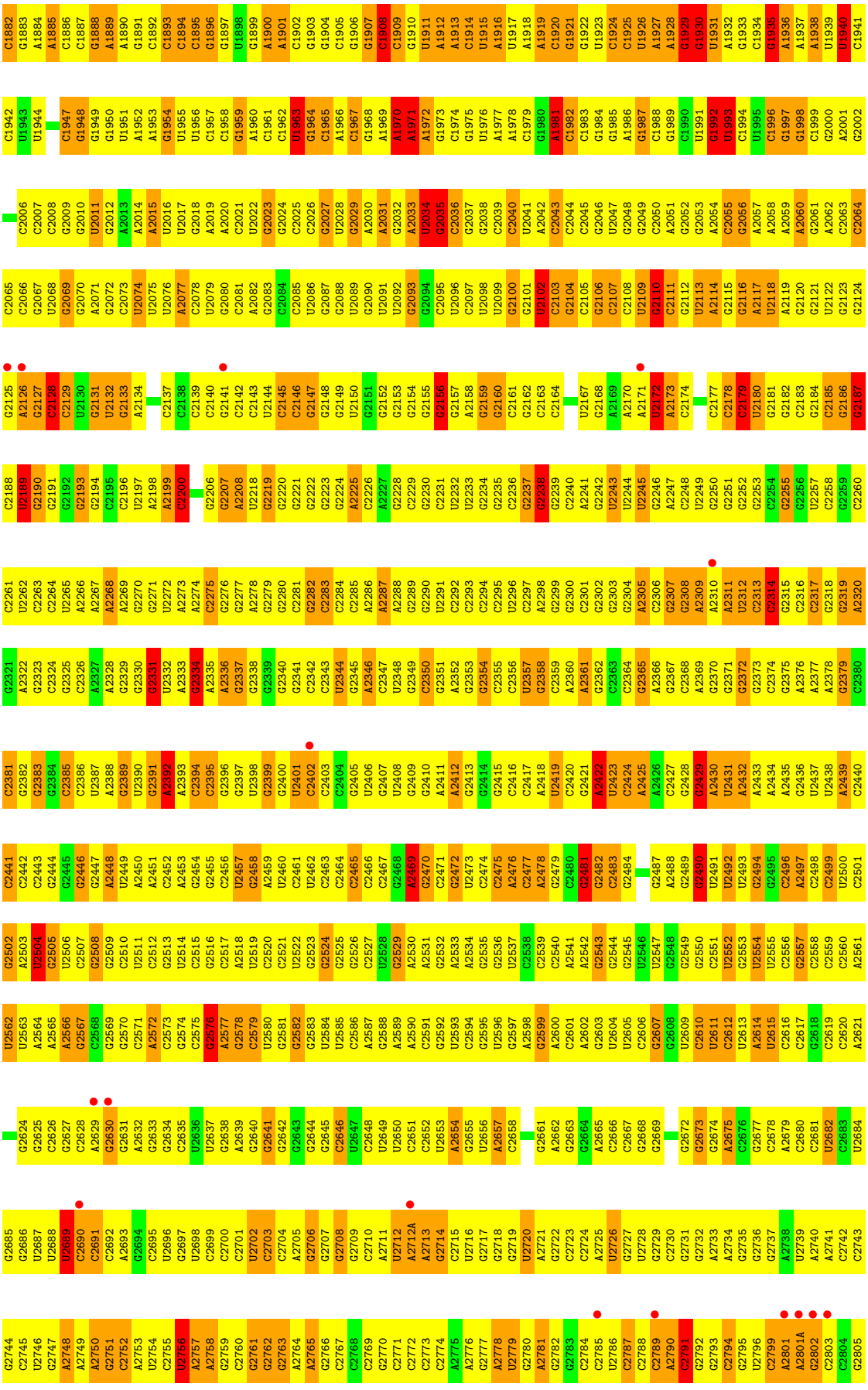
• Molecule 35: 23S RIBOSOMAL RNA

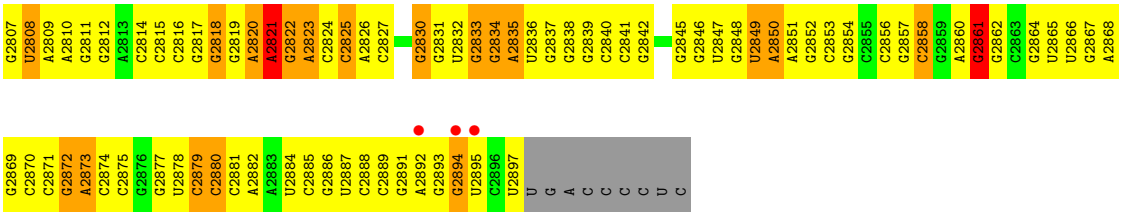
Chain BA:





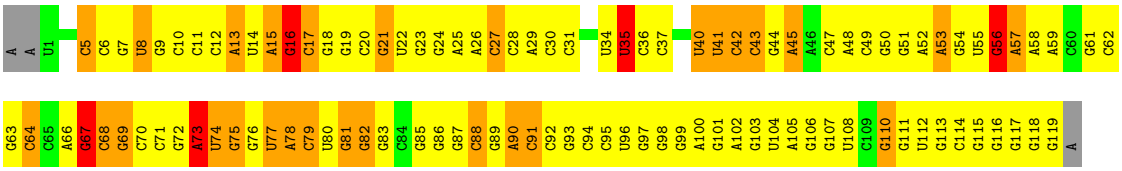






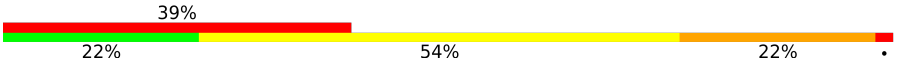
• Molecule 36: 5S RIBOSOMAL RNA

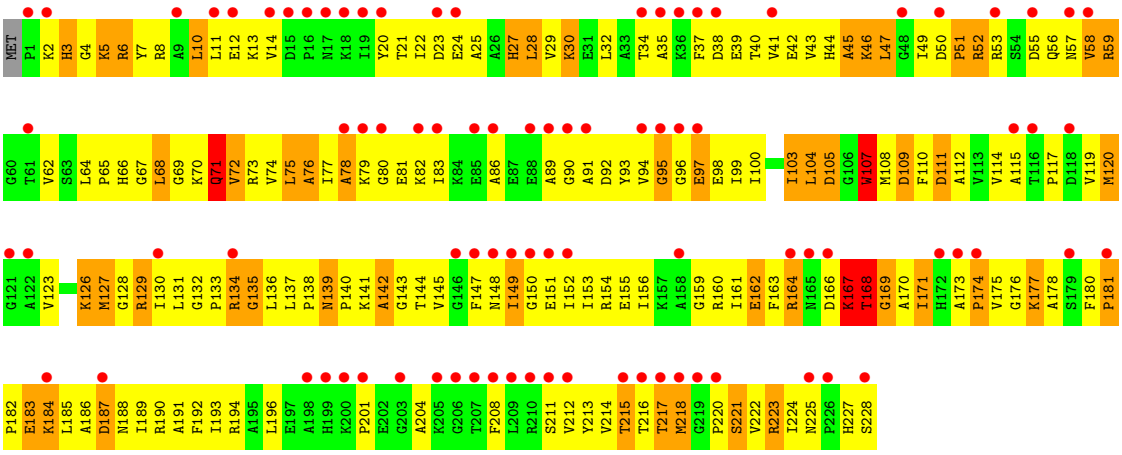
Chain BB:



• Molecule 37: 50S RIBOSOMAL PROTEIN L1

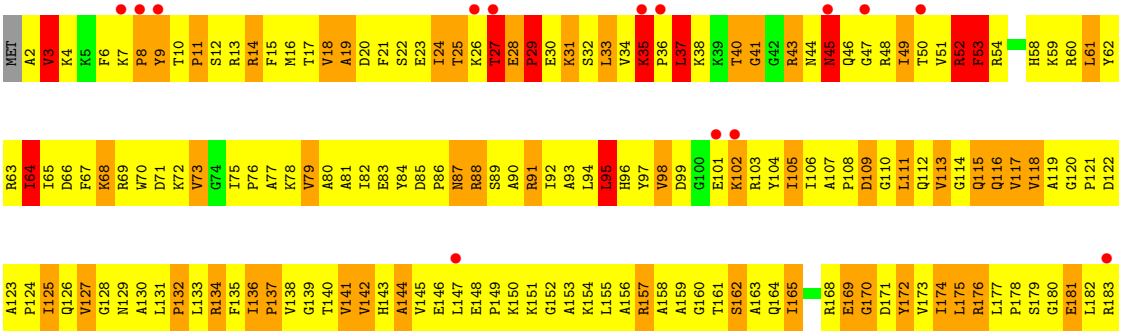
Chain BC:

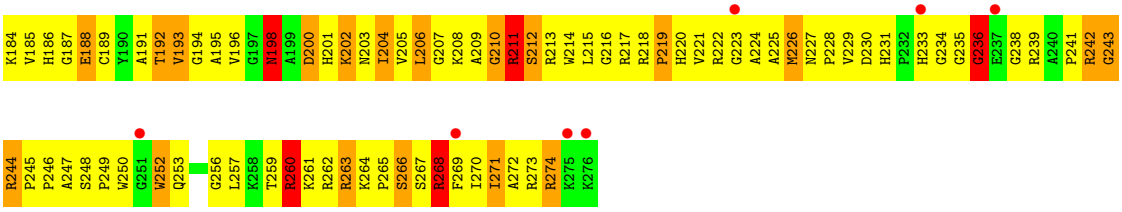




• Molecule 38: 50S RIBOSOMAL PROTEIN L2

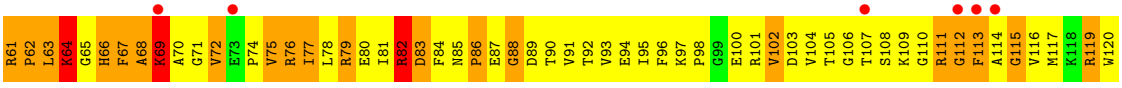
Chain BD:

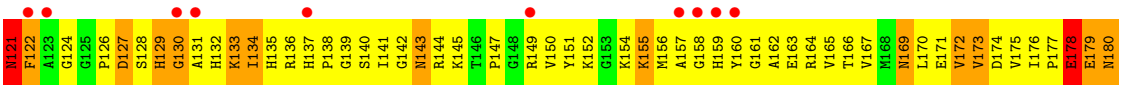




• Molecule 39: 50S RIBOSOMAL PROTEIN L3

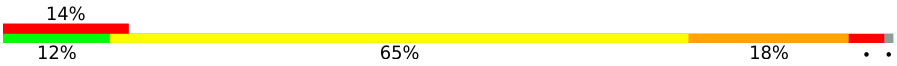
Chain BE:

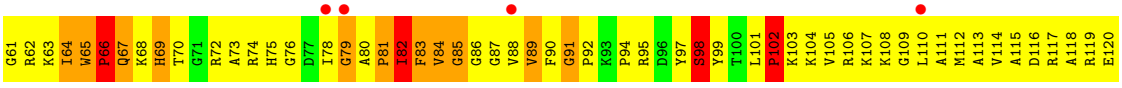


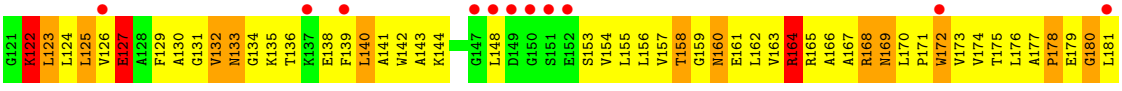


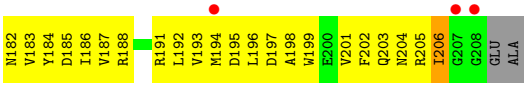
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



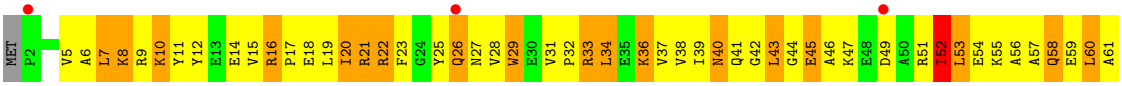






• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



P122 N123 S124 F125 D126 G127 R128 G129 N130 Y131 N132 L133 G134 L135 R136 E137 Q138 L139 I140 F141 P142 E143 I144 T145 Y146 D147 M148 V149 D150 A151 L152 R153 G154 M155 D156 I157 A158 V159 V160 T161 T162 A163 D166 E167 E168 A169 R170 A171 L172 L173 E174 L175 L176 G177 F178 P179 F180 R181 K182

- Molecule 42: 50S RIBOSOMAL PROTEIN L6

7%

Chain BH: 16% 49% 16% 6% 13%

MET SER ARG ILE GLY ARG LEU PRO ILE PRO VAL P12 V15 S16 V17 E18 V19 A20 P21 G22 R23 V24 K25 V26 K27 G28 P29 K30 G31 E32 L33 E34 V35 P36 V37 S38 P39 E40 M41 R42 V43 V44 V45 E46 E47 G48 V49 V50 R51 V52 E53 R54 P55 S56 D57 E58 R59 R60 H61

K62 S63 L64 H65 G66 L67 T68 R69 T70 L71 I72 A73 N74 A75 V76 V79 S80 Y83 S84 K85 E86 L87 L88 G91 I92 G93 Y94 R95 A96 R97 L98 V99 G100 R101 A102 L103 E104 L105 T106 V107 G108 F109 S110 H111 P112 V113 V114 V115 E116 P117 P118 E119 G120 I121 T122 F123 E124

V125 P126 E127 P128 T129 R130 V131 R132 V133 S134 G135 I136 D137 K138 Q139 K140 V141 G142 Q143 V144 A145 A146 N147 I148 R149 A150 I151 R152 K153 P154 S155 A156 Y157 H158 E159 K160 G161 I162 Y163 Y164 E167 PRO VAL ARG LEU LYS PRO GLY LYS ALA GLY ALA LYS LYS

- Molecule 43: 50S RIBOSOMAL PROTEIN L10

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Chain BJ: 47% 29% 24%

UNK UNK UNK X4 X15 X16 X17 X18 X19 X20 X24 X25 X26 X27 X28 X45 X48 X49 X54 X55 X56 X57 X58 X59 X60 X61 X64 X65 X66 X67 X68 X69 X70 X71 X72 X73 X74 X75 X76 X80 X81 X82 X83 X84 L85 X91 X92 X93 X94 X95 X99

X100 X103 X108 X113 X118 X119 X120 X121 X122 X127 X130 X131 X132 X133 X134 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain BK: 71% 24% •

X1 X2 X5 X6 X7 X8 X9 X22 X23 X24 X25 X30 X31 X55 X69 X73 X81 X82 X83 X86 X87 X91 X92 X97 X98 X99 X100 X101 X115 X116 X117 X118 X125 X129 X130 X131 X134 X135 X136 X137 X138 X141 UNK UNK UNK

UNK UNK UNK

- Molecule 45: 50S RIBOSOMAL PROTEIN L13

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Chain BN: 11% 55% 31% ••

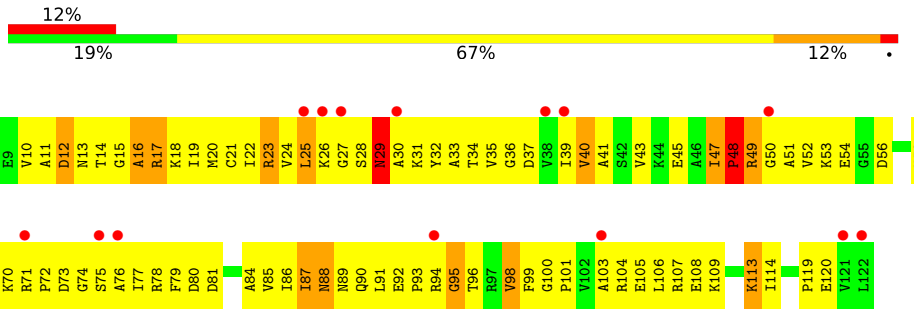
M1 K2 T3 Y4 V5 P6 K7 Q8 V9 E10 P11 R12 W13 V14 L15 I16 D17 A18 E19 G20 K21 T22 L23 G24 R25 L26 A27 T28 K29 I30 A31 L34 R35 G36 K37 H38 R39 P40 D41 W42 T43 P44 N45 V46 A47 M48 G49 D50 F51 V52 V53 V54 V55 N56 A57 D58 K59 I60 R61

V62 T63 G64 K65 K66 L67 E68 Q69 K70 I71 Y72 T73 R74 Y75 S76 G77 G81 L82 K83 K84 I85 P86 L87 E88 K89 M90 L91 A92 T93 H94 P95 E96 R97 V98 L99 E100 H101 A102 V103 K104 G105 M106 L107 P108 K109 G110 P111 L112 G113 R114 R115 L116 F117 K118 R119 L120 K121 V122 Y123

A124 G125 P126 D127 H128 P129 H130 Q131 A132 Q133 R134 P135 E136 K137 L138 E139 VAL

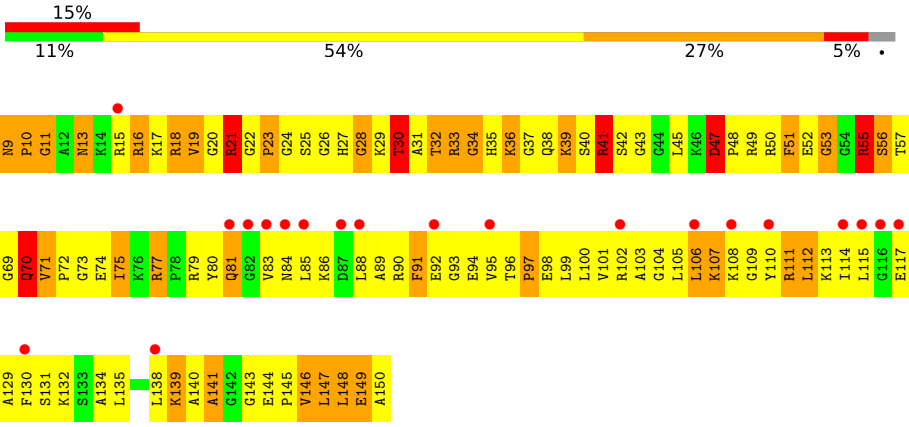
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:



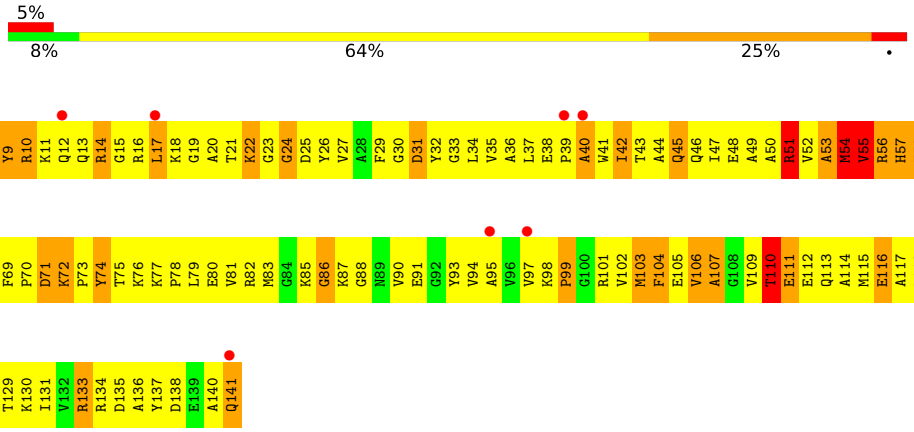
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain BP:



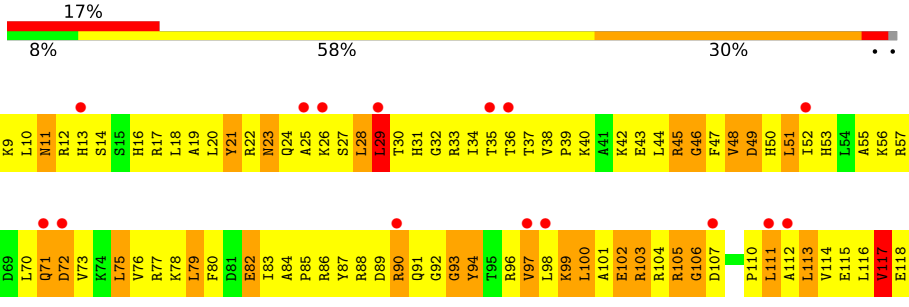
• Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



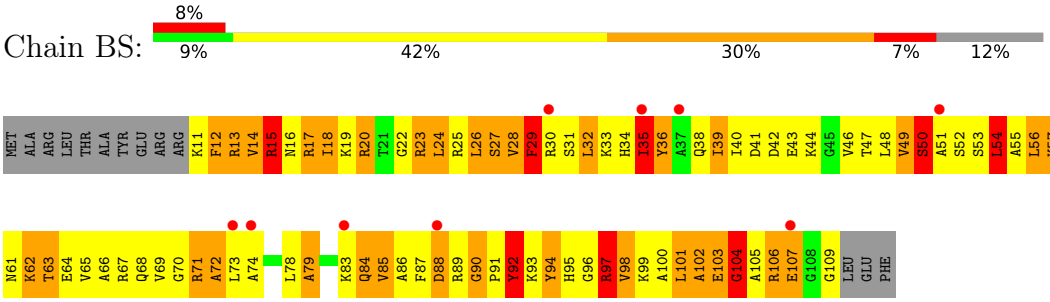
• Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR:



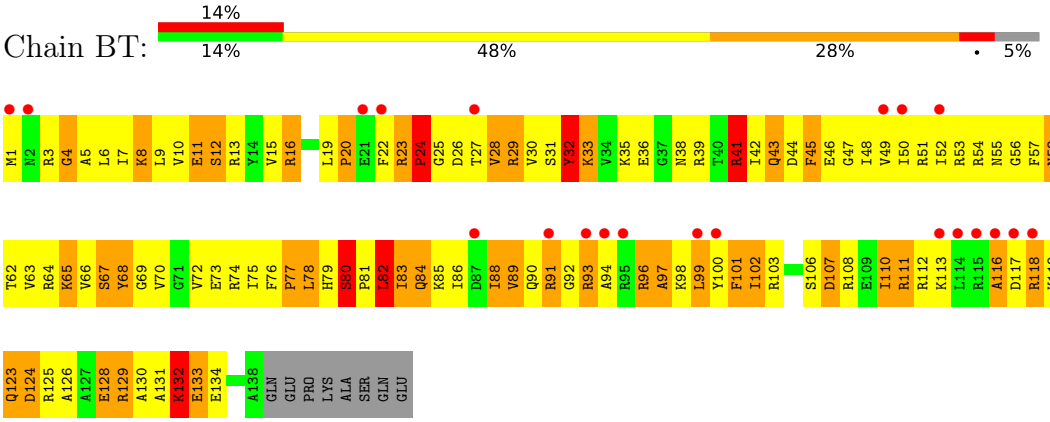
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain BS:



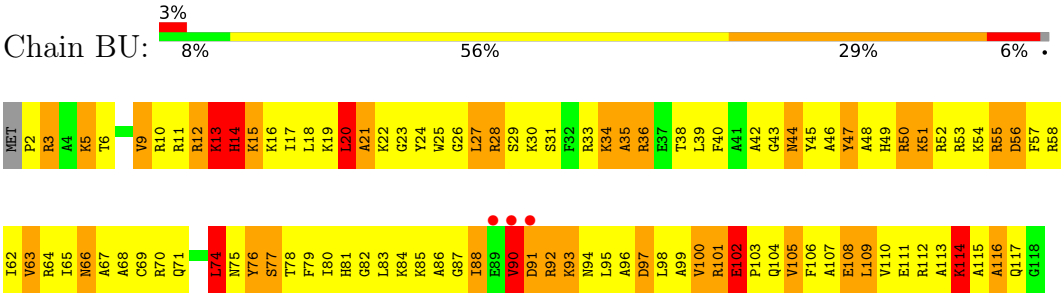
• Molecule 51: 50S RIBOSOMAL PROTEIN L19

Chain BT:



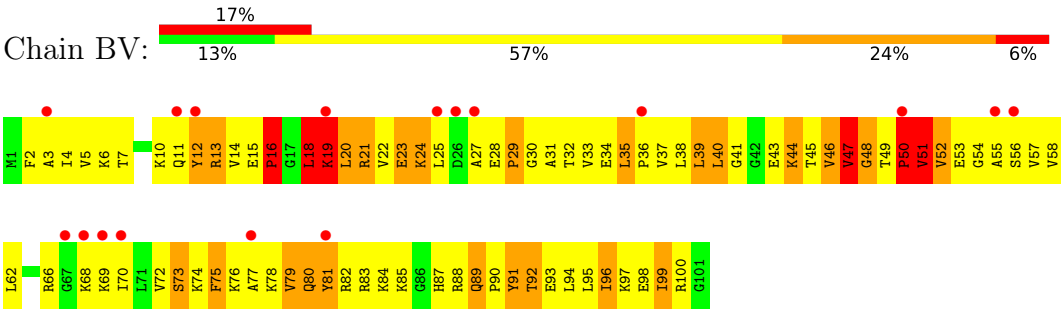
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:



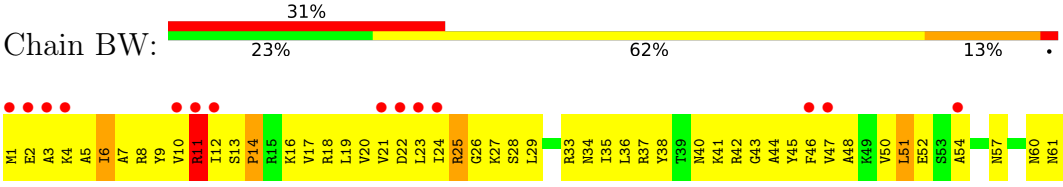
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

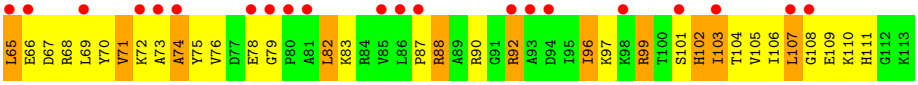
Chain BV:



• Molecule 54: 50S RIBOSOMAL PROTEIN L22

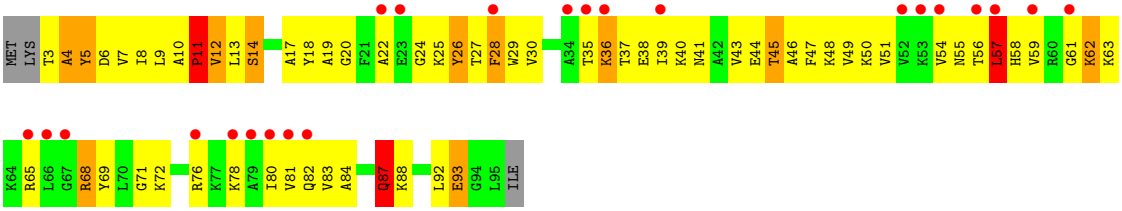
Chain BW:





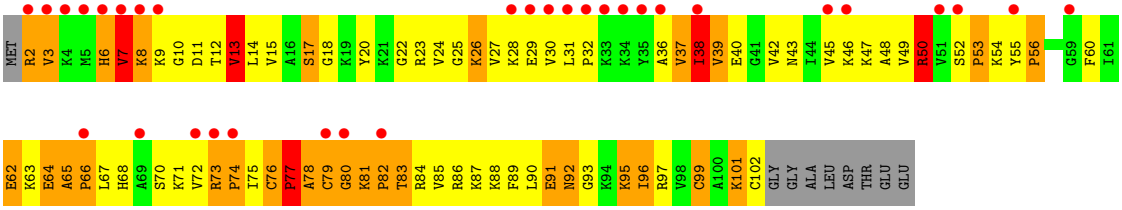
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain BX:



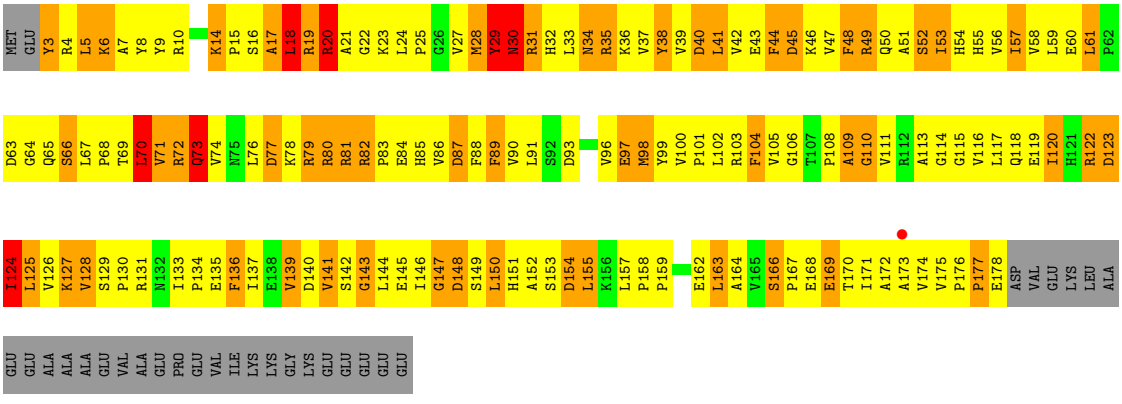
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	204.70Å 229.30Å 307.00Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	44.90 – 3.80 44.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.90-3.80) 96.6 (44.91-3.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.351 0.298 , 0.348	Depositor DCC
R_{free} test set	53888 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å^2)	110.2	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	151017	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: GCP

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	0.79	12/36190 (0.0%)	0.89	56/56486 (0.1%)
2	AB	0.62	0/1936	0.96	1/2611 (0.0%)
3	AC	0.60	0/1637	0.93	3/2207 (0.1%)
4	AD	0.50	0/1733	0.86	2/2318 (0.1%)
5	AE	0.63	0/1163	0.94	1/1566 (0.1%)
6	AF	0.56	0/856	0.88	0/1154
7	AG	0.59	0/1276	0.85	0/1709
8	AH	0.56	0/1136	0.91	1/1527 (0.1%)
9	AI	0.56	0/1029	0.83	0/1378
10	AJ	0.59	0/808	0.88	0/1087
11	AK	0.57	0/900	0.89	0/1213
12	AL	0.59	0/987	1.01	2/1322 (0.2%)
13	AM	0.59	0/999	0.95	0/1338
14	AN	0.71	0/501	1.03	1/664 (0.2%)
15	AO	0.65	0/745	0.86	0/992
16	AP	0.53	0/717	0.88	0/965
17	AQ	0.61	0/837	0.92	1/1119 (0.1%)
18	AR	0.60	0/579	0.89	1/768 (0.1%)
19	AS	0.68	0/643	0.91	1/867 (0.1%)
20	AT	0.54	0/765	0.80	0/1007
21	AU	0.70	0/213	0.95	1/279 (0.4%)
22	AV	0.65	0/1832	0.82	0/2855
23	AX	0.66	0/216	0.77	0/335
24	AY	1.05	19/4005 (0.5%)	1.16	32/5407 (0.6%)
25	B0	0.61	0/671	0.98	2/892 (0.2%)
26	B1	0.49	0/739	0.85	0/983
27	B2	0.51	0/600	0.82	0/793
28	B3	0.57	0/473	0.93	0/636
29	B4	0.69	0/350	0.80	0/476
30	B5	0.64	0/473	0.89	0/639
31	B6	0.79	0/440	1.09	2/586 (0.3%)
32	B7	0.53	0/427	0.79	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	B8	0.68	0/516	0.92	0/681
34	B9	0.53	0/310	0.85	0/407
35	BA	0.76	16/69976 (0.0%)	0.86	82/109244 (0.1%)
36	BB	0.76	1/2853 (0.0%)	0.89	5/4451 (0.1%)
37	BC	0.81	4/1775 (0.2%)	0.94	4/2392 (0.2%)
38	BD	0.69	0/2195	1.07	9/2955 (0.3%)
39	BE	0.59	0/1597	0.95	1/2155 (0.0%)
40	BF	0.61	0/1659	0.88	0/2246
41	BG	0.58	0/1499	0.92	3/2016 (0.1%)
42	BH	0.66	0/1211	0.88	0/1636
43	BJ	0.53	0/7	0.70	0/8
45	BN	0.57	0/1132	0.91	1/1527 (0.1%)
46	BO	0.60	0/943	0.90	0/1269
47	BP	0.57	0/1131	1.08	6/1504 (0.4%)
48	BQ	0.63	0/1143	1.00	3/1527 (0.2%)
49	BR	0.49	0/974	0.92	1/1302 (0.1%)
50	BS	0.66	0/779	1.12	6/1038 (0.6%)
51	BT	0.60	0/1156	0.92	3/1544 (0.2%)
52	BU	0.63	0/975	0.91	1/1297 (0.1%)
53	BV	0.54	0/790	0.97	2/1057 (0.2%)
54	BW	0.59	0/907	0.82	0/1216
55	BX	0.63	0/740	0.83	1/995 (0.1%)
56	BY	0.61	0/789	0.90	0/1053
57	BZ	0.62	0/1435	0.95	0/1949
All	All	0.73	52/162368 (0.0%)	0.89	235/242211 (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	125
9	AI	0	1
11	AK	0	1
17	AQ	0	1
21	AU	0	1
22	AV	0	5
24	AY	0	5
30	B5	0	1
35	BA	3	160
36	BB	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BH	0	1
45	BN	0	1
48	BQ	0	1
53	BV	0	1
All	All	6	316

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	191	TYR	CE2-CZ	11.85	1.53	1.38
24	AY	189	GLU	CG-CD	-10.57	1.36	1.51
24	AY	191	TYR	CD1-CE1	10.46	1.55	1.39
24	AY	504	ILE	C-N	-9.62	1.11	1.34
24	AY	444	LEU	C-N	-9.54	1.12	1.34

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AY	191	TYR	CB-CG-CD1	-18.01	110.19	121.00
24	AY	307	MET	CG-SD-CE	13.35	121.55	100.20
24	AY	319	ARG	NE-CZ-NH1	12.45	126.52	120.30
24	AY	504	ILE	C-N-CA	-12.18	91.26	121.70
1	AA	1498	U	C2'-C3'-O3'	11.78	135.42	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1049	U	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'

5 of 316 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	19	C	Sidechain
1	AA	28	G	Sidechain
1	AA	96	U	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	2580	0
2	AB	1901	0	1951	513	1
3	AC	1613	0	1677	306	0
4	AD	1703	0	1767	335	0
5	AE	1147	0	1207	231	0
6	AF	843	0	857	144	0
7	AG	1257	0	1296	177	0
8	AH	1116	0	1177	205	0
9	AI	1011	0	1043	205	0
10	AJ	795	0	840	196	0
11	AK	885	0	904	152	0
12	AL	971	0	1057	217	0
13	AM	988	0	1059	192	0
14	AN	492	0	533	153	0
15	AO	734	0	771	229	0
16	AP	701	0	720	131	0
17	AQ	824	0	891	158	0
18	AR	574	0	644	122	0
19	AS	630	0	652	209	0
20	AT	763	0	861	150	0
21	AU	209	0	221	48	0
22	AV	1640	0	837	195	0
23	AX	192	0	99	22	0
24	AY	3934	0	3922	1256	0
25	B0	662	0	688	138	0
26	B1	732	0	808	131	0
27	B2	598	0	653	126	0
28	B3	468	0	523	108	0
29	B4	341	0	339	89	0
30	B5	459	0	480	131	0
31	B6	433	0	461	109	0
32	B7	419	0	467	110	0
33	B8	508	0	576	154	0
34	B9	307	0	338	70	0
35	BA	62477	0	31497	5283	0
36	BB	2551	0	1295	229	0
37	BC	1742	0	1794	377	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	780	0
39	BE	1564	0	1629	448	0
40	BF	1624	0	1677	415	0
41	BG	1474	0	1535	340	0
42	BH	1189	0	1247	282	0
43	BJ	654	0	157	36	0
44	BK	701	0	168	41	0
45	BN	1105	0	1180	270	0
46	BO	933	0	996	182	0
47	BP	1114	0	1187	361	0
48	BQ	1122	0	1179	291	0
49	BR	960	0	1021	236	0
50	BS	771	0	832	206	0
51	BT	1142	0	1202	332	0
52	BU	958	0	1015	317	0
53	BV	779	0	852	219	0
54	BW	896	0	953	173	0
55	BX	726	0	778	114	0
56	BY	776	0	870	193	0
57	BZ	1403	0	1432	371	0
58	AY	32	0	14	11	0
All	All	151017	0	103381	18971	1

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 75.

The worst 5 of 18971 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)
24:AY:111:MET:CE	24:AY:139:THR:HG23	1.18	1.62
24:AY:331:LEU:CD2	24:AY:379:PHE:HD2	1.19	1.51
24:AY:331:LEU:HD22	24:AY:379:PHE:CD2	1.46	1.47
37:BC:127:MET:SD	37:BC:127:MET:CG	2.03	1.45
24:AY:135:THR:CG2	24:AY:136:PRO:HD2	1.44	1.45

All (1) 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)
2:AB:62:ALA:O	37:BC:30:LYS:O[2_656]	2.18	0.02

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	233/256 (91%)	110 (47%)	62 (27%)	61 (26%)	0 1
3	AC	205/239 (86%)	134 (65%)	39 (19%)	32 (16%)	0 4
4	AD	206/209 (99%)	131 (64%)	51 (25%)	24 (12%)	0 6
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	1 19
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1 14
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0 3
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0 6
9	AI	125/128 (98%)	78 (62%)	28 (22%)	19 (15%)	0 4
10	AJ	97/105 (92%)	60 (62%)	23 (24%)	14 (14%)	0 4
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	0 7
12	AL	123/135 (91%)	66 (54%)	33 (27%)	24 (20%)	0 2
13	AM	123/126 (98%)	63 (51%)	31 (25%)	29 (24%)	0 1
14	AN	58/61 (95%)	33 (57%)	12 (21%)	13 (22%)	0 1
15	AO	86/89 (97%)	59 (69%)	21 (24%)	6 (7%)	1 17
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	0 6
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	1 20
18	AR	68/88 (77%)	37 (54%)	18 (26%)	13 (19%)	0 2
19	AS	77/93 (83%)	42 (54%)	18 (23%)	17 (22%)	0 1
20	AT	97/106 (92%)	46 (47%)	32 (33%)	19 (20%)	0 2
21	AU	23/27 (85%)	11 (48%)	8 (35%)	4 (17%)	0 3
24	AY	488/529 (92%)	314 (64%)	88 (18%)	86 (18%)	0 2
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	0 8
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0 4
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0 5
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	B4	43/71 (61%)	26 (60%)	9 (21%)	8 (19%)	0 2
30	B5	57/60 (95%)	34 (60%)	11 (19%)	12 (21%)	0 1
31	B6	48/54 (89%)	18 (38%)	16 (33%)	14 (29%)	0 0
32	B7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0 3
33	B8	62/65 (95%)	30 (48%)	16 (26%)	16 (26%)	0 1
34	B9	35/37 (95%)	19 (54%)	10 (29%)	6 (17%)	0 3
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0 5
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	0 6
39	BE	203/206 (98%)	99 (49%)	48 (24%)	56 (28%)	0 0
40	BF	206/210 (98%)	134 (65%)	35 (17%)	37 (18%)	0 2
41	BG	179/182 (98%)	95 (53%)	47 (26%)	37 (21%)	0 2
42	BH	154/180 (86%)	111 (72%)	23 (15%)	20 (13%)	0 5
43	BJ	1/173 (1%)	1 (100%)	0	0	100 100
45	BN	137/140 (98%)	78 (57%)	28 (20%)	31 (23%)	0 1
46	BO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0 8
47	BP	144/150 (96%)	70 (49%)	37 (26%)	37 (26%)	0 1
48	BQ	139/141 (99%)	79 (57%)	40 (29%)	20 (14%)	0 4
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0 3
50	BS	97/112 (87%)	41 (42%)	23 (24%)	33 (34%)	0 0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0 1
52	BU	115/118 (98%)	59 (51%)	27 (24%)	29 (25%)	0 1
53	BV	99/101 (98%)	56 (57%)	21 (21%)	22 (22%)	0 1
54	BW	111/113 (98%)	72 (65%)	25 (22%)	14 (13%)	0 5
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	0 10
56	BY	99/110 (90%)	33 (33%)	36 (36%)	30 (30%)	0 0
57	BZ	174/206 (84%)	88 (51%)	48 (28%)	38 (22%)	0 1
All	All	6255/6850 (91%)	3758 (60%)	1413 (23%)	1084 (17%)	0 3

5 of 1084 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	19	HIS
2	AB	24	TRP

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%)	152 (75%)	50 (25%)	0 5
3	AC	160/188 (85%)	133 (83%)	27 (17%)	2 14
4	AD	180/181 (99%)	154 (86%)	26 (14%)	3 20
5	AE	115/123 (94%)	94 (82%)	21 (18%)	1 11
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2 17
7	AG	126/127 (99%)	114 (90%)	12 (10%)	8 34
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3 18
9	AI	98/99 (99%)	82 (84%)	16 (16%)	2 15
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1 10
11	AK	90/99 (91%)	73 (81%)	17 (19%)	1 10
12	AL	104/111 (94%)	86 (83%)	18 (17%)	2 13
13	AM	99/101 (98%)	79 (80%)	20 (20%)	1 9
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0 3
15	AO	79/80 (99%)	52 (66%)	27 (34%)	0 1
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6 29
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8 34
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5 27
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2 16
20	AT	76/82 (93%)	69 (91%)	7 (9%)	9 35
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7 30
24	AY	427/453 (94%)	308 (72%)	119 (28%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	B0	66/67 (98%)	49 (74%)	17 (26%)	0 4
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2 15
27	B2	66/67 (98%)	61 (92%)	5 (8%)	13 43
28	B3	51/52 (98%)	42 (82%)	9 (18%)	2 13
29	B4	39/63 (62%)	29 (74%)	10 (26%)	0 4
30	B5	51/52 (98%)	47 (92%)	4 (8%)	12 42
31	B6	49/52 (94%)	37 (76%)	12 (24%)	0 5
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5 25
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1 8
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1 5
37	BC	180/181 (99%)	150 (83%)	30 (17%)	2 15
38	BD	217/218 (100%)	150 (69%)	67 (31%)	0 2
39	BE	165/166 (99%)	134 (81%)	31 (19%)	1 10
40	BF	165/166 (99%)	142 (86%)	23 (14%)	3 21
41	BG	155/156 (99%)	127 (82%)	28 (18%)	1 12
42	BH	128/148 (86%)	90 (70%)	38 (30%)	0 2
43	BJ	1/1 (100%)	1 (100%)	0	100 100
45	BN	117/119 (98%)	99 (85%)	18 (15%)	2 17
46	BO	100/100 (100%)	89 (89%)	11 (11%)	6 29
47	BP	112/116 (97%)	91 (81%)	21 (19%)	1 10
48	BQ	111/111 (100%)	87 (78%)	24 (22%)	1 7
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1 7
50	BS	77/88 (88%)	60 (78%)	17 (22%)	1 6
51	BT	120/127 (94%)	96 (80%)	24 (20%)	1 9
52	BU	92/94 (98%)	74 (80%)	18 (20%)	1 9
53	BV	82/82 (100%)	65 (79%)	17 (21%)	1 8
54	BW	91/92 (99%)	81 (89%)	10 (11%)	6 29
55	BX	74/78 (95%)	63 (85%)	11 (15%)	3 18
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2 12
57	BZ	155/179 (87%)	117 (76%)	38 (24%)	0 5
All	All	5271/5546 (95%)	4255 (81%)	1016 (19%)	1 10

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	B0	27	GLU
51	BT	24	PRO
37	BC	162	GLU
50	BS	56	LEU
54	BW	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
38	BD	166	GLN
46	BO	5	GLN
39	BE	48	GLN
40	BF	169	ASN
48	BQ	46	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	273 (18%)	58 (3%)
22	AV	76/77 (98%)	36 (47%)	3 (3%)
23	AX	8/9 (88%)	5 (62%)	0
35	BA	2900/2915 (99%)	654 (22%)	73 (2%)
36	BB	118/122 (96%)	24 (20%)	1 (0%)
All	All	4605/4645 (99%)	992 (21%)	135 (2%)

5 of 992 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 135 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	1996	C
35	BA	2126	A

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Mol	Chain	Res	Type
35	BA	2689	U
1	AA	1285	A
1	AA	1283	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
58	GCP	AY	1000	-	27,34,34	2.58	7 (25%)	34,54,54	2.04	10 (29%)

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
58	GCP	AY	1000	-	-	10/15/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	C6-N1	8.37	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PB-O3A	5.84	1.64	1.58
58	AY	1000	GCP	C2-N1	4.88	1.44	1.35
58	AY	1000	GCP	C4-N3	4.57	1.42	1.35
58	AY	1000	GCP	PG-O2G	-2.81	1.48	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	AY	1000	GCP	C5-C6-N1	-6.21	114.93	123.43
58	AY	1000	GCP	C2-N1-C6	4.62	123.27	115.93
58	AY	1000	GCP	N3-C2-N1	-4.35	121.42	127.22
58	AY	1000	GCP	O3G-PG-O1G	-2.67	105.32	112.39
58	AY	1000	GCP	O3G-PG-O2G	2.66	115.84	108.08

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AY	1000	GCP	PB-C3B-PG-O1G
58	AY	1000	GCP	PB-C3B-PG-O2G
58	AY	1000	GCP	PG-C3B-PB-O1B
58	AY	1000	GCP	PG-C3B-PB-O3A
58	AY	1000	GCP	C5'-O5'-PA-O3A

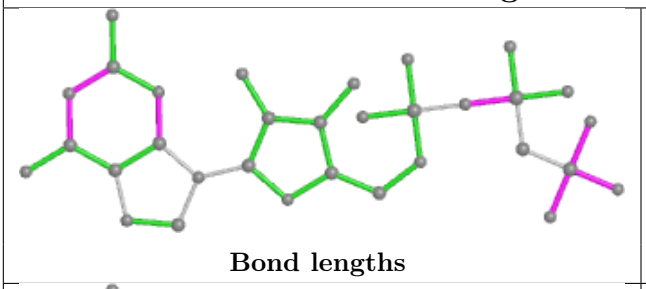
There are no ring outliers.

1 monomer is involved in 11 short contacts:

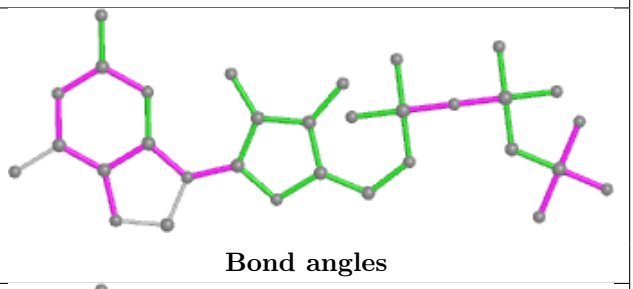
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AY	1000	GCP	11	0

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.

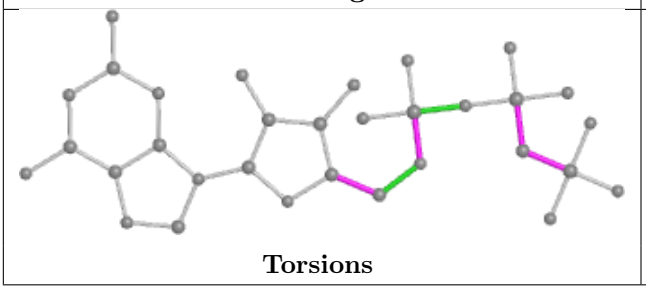
Ligand GCP AY 1000



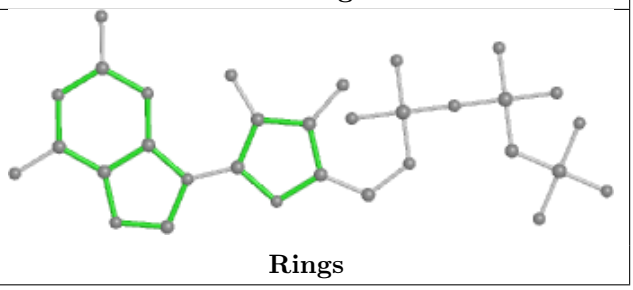
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	AY	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AY	444:LEU	C	445:GLN	N	1.12
1	AY	504:ILE	C	505:ALA	N	1.11

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%)	-0.14	37 (2%) 57 49	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.44	2 (0%) 84 79	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.49	2 (0%) 82 76	37, 117, 174, 200	0
4	AD	208/209 (99%)	0.22	13 (6%) 20 15	48, 158, 200, 200	0
5	AE	151/162 (93%)	-0.18	3 (1%) 65 58	38, 112, 171, 200	0
6	AF	101/101 (100%)	-0.60	0 100 100	59, 135, 188, 200	0
7	AG	155/156 (99%)	-0.37	3 (1%) 66 59	46, 128, 189, 200	0
8	AH	138/138 (100%)	-0.10	6 (4%) 35 30	36, 114, 180, 200	0
9	AI	127/128 (99%)	-0.12	2 (1%) 72 64	32, 121, 172, 200	0
10	AJ	99/105 (94%)	0.40	10 (10%) 7 6	32, 125, 191, 200	0
11	AK	119/129 (92%)	-0.10	5 (4%) 36 30	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.24	5 (4%) 38 32	45, 119, 192, 200	0
13	AM	125/126 (99%)	0.29	11 (8%) 10 8	64, 127, 200, 200	0
14	AN	60/61 (98%)	-0.28	0 100 100	28, 104, 172, 200	0
15	AO	88/89 (98%)	0.04	4 (4%) 33 28	59, 130, 188, 200	0
16	AP	84/88 (95%)	1.03	18 (21%) 0 1	79, 156, 200, 200	0
17	AQ	100/105 (95%)	0.70	13 (13%) 3 4	66, 141, 200, 200	0
18	AR	70/88 (79%)	-0.01	2 (2%) 51 42	59, 124, 176, 200	0
19	AS	79/93 (84%)	0.13	4 (5%) 28 24	57, 118, 197, 200	0
20	AT	99/106 (93%)	0.55	10 (10%) 7 6	87, 153, 200, 200	0
21	AU	25/27 (92%)	0.70	4 (16%) 1 2	46, 117, 175, 185	0
22	AV	77/77 (100%)	-0.68	1 (1%) 77 70	77, 151, 189, 199	0
23	AX	9/9 (100%)	0.18	0 100 100	79, 156, 192, 199	0
24	AY	496/529 (93%)	0.42	51 (10%) 6 6	71, 170, 202, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	B0	84/85 (98%)	1.13	18 (21%) 0 1	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.59	8 (8%) 10 9	65, 143, 197, 200	0
27	B2	71/72 (98%)	0.13	7 (9%) 7 6	101, 153, 200, 200	0
28	B3	60/60 (100%)	0.68	6 (10%) 7 6	54, 126, 198, 200	0
29	B4	45/71 (63%)	-0.05	3 (6%) 17 14	108, 174, 200, 200	0
30	B5	59/60 (98%)	0.40	8 (13%) 3 3	62, 150, 200, 200	0
31	B6	50/54 (92%)	0.79	10 (20%) 1 1	62, 139, 186, 200	0
32	B7	49/49 (100%)	0.56	5 (10%) 6 6	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.13	2 (3%) 49 40	66, 129, 179, 200	0
34	B9	37/37 (100%)	1.39	11 (29%) 0 0	71, 142, 178, 194	0
35	BA	2901/2915 (99%)	0.09	112 (3%) 39 32	51, 159, 201, 202	0
36	BB	119/122 (97%)	-0.48	0 100 100	66, 123, 172, 190	0
37	BC	228/229 (99%)	2.01	89 (39%) 0 0	87, 182, 200, 200	0
38	BD	275/276 (99%)	0.15	21 (7%) 13 11	40, 117, 175, 200	0
39	BE	205/206 (99%)	0.19	18 (8%) 10 8	51, 143, 199, 200	0
40	BF	208/210 (99%)	0.51	29 (13%) 2 3	51, 156, 200, 200	0
41	BG	181/182 (99%)	-0.08	4 (2%) 62 54	47, 134, 194, 200	0
42	BH	156/180 (86%)	0.30	12 (7%) 13 11	78, 165, 200, 200	0
43	BJ	1/173 (0%)	3.32	1 (100%) 0 0	174, 174, 174, 174	0
44	BK	0/147	-	-	-	-
45	BN	139/140 (99%)	0.01	2 (1%) 75 68	69, 131, 190, 200	0
46	BO	122/122 (100%)	0.47	15 (12%) 4 4	59, 133, 198, 200	0
47	BP	146/150 (97%)	0.86	22 (15%) 2 2	65, 147, 200, 200	0
48	BQ	141/141 (100%)	0.05	7 (4%) 28 25	20, 107, 171, 200	0
49	BR	117/118 (99%)	0.80	20 (17%) 1 1	81, 169, 200, 200	0
50	BS	99/112 (88%)	0.05	9 (9%) 9 7	49, 123, 194, 200	0
51	BT	138/146 (94%)	0.51	21 (15%) 2 2	89, 162, 200, 200	0
52	BU	117/118 (99%)	-0.05	3 (2%) 56 47	47, 121, 179, 200	0
53	BV	101/101 (100%)	0.82	17 (16%) 1 2	42, 146, 200, 200	0
54	BW	113/113 (100%)	1.30	35 (30%) 0 0	78, 165, 200, 200	0
55	BX	93/96 (96%)	1.10	23 (24%) 0 0	38, 167, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	BY	101/110 (91%)	1.53	32 (31%) 0 0	86, 169, 200, 200	0
57	BZ	176/206 (85%)	-0.29	1 (0%) 89 85	43, 122, 195, 200	0
All	All	10971/11642 (94%)	0.18	777 (7%) 16 12	20, 146, 200, 202	0

The worst 5 of 777 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	165	ASN	14.2
37	BC	173	ALA	12.2
37	BC	216	THR	11.9
28	B3	1	MET	11.0
24	AY	349	MET	10.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

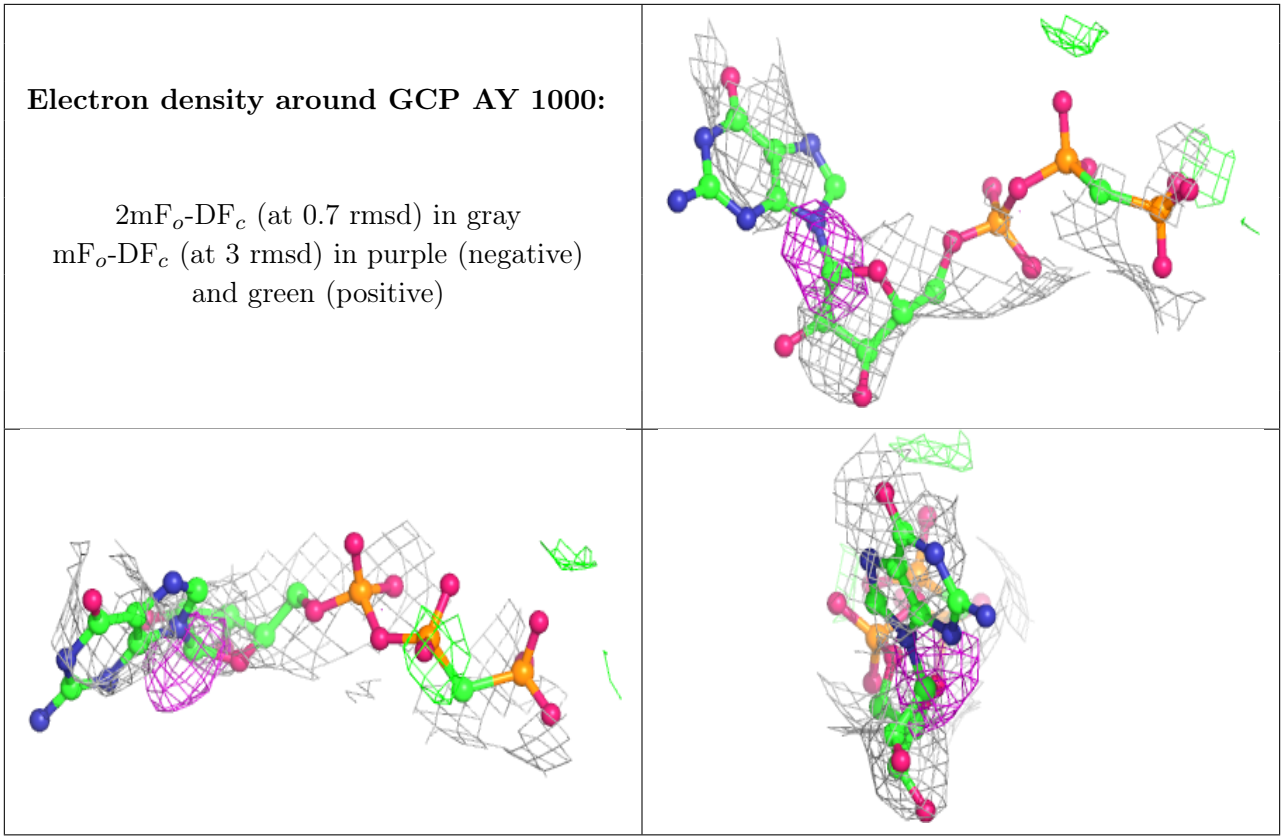
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	GCP	AY	1000	32/32	0.82	0.24	95,109,121,122	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 AY 1000:

$2mF_o$-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.