wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:47 PM GMT

PDB ID	:	4V8Q
Title	:	COMPLEX OF SMPB, A TMRNA FRAGMENT AND EF-TU-GDP-KIRROMYCIN WITH THE 70S RIBOSOME
Authors	:	Neubauer, C.; Gillet, R.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2011-12-10
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

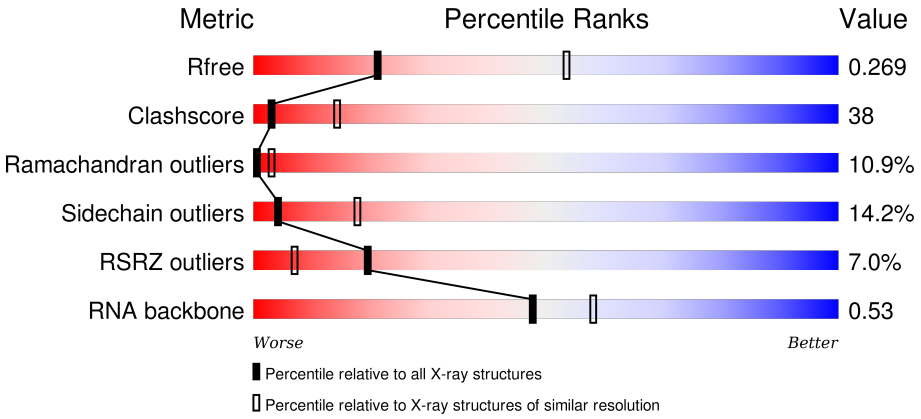
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	85	11% 27% 61% 8%
2	A1	98	2% 38% 45% 12%
3	A2	72	3% 18% 64% 17%
4	A3	60	2% 37% 55% 7%

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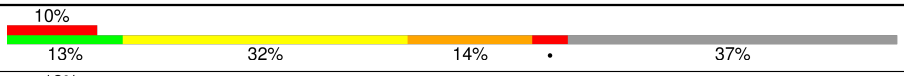
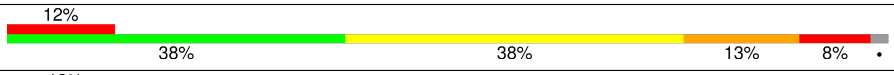
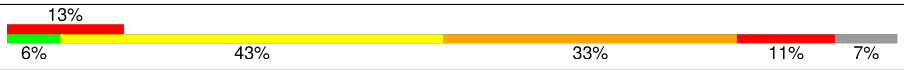
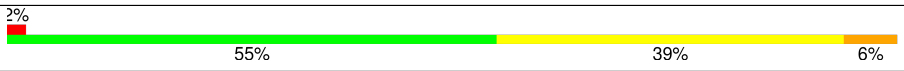
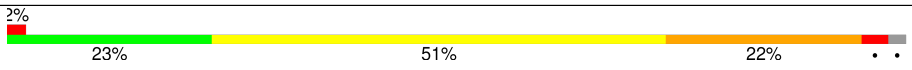
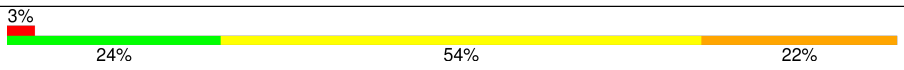
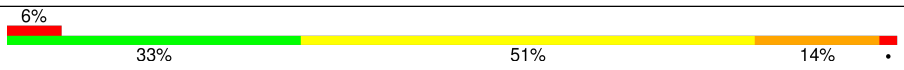
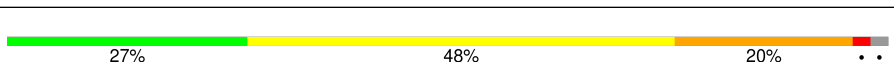
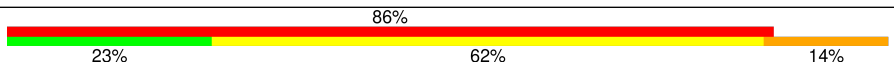
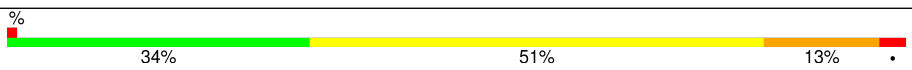
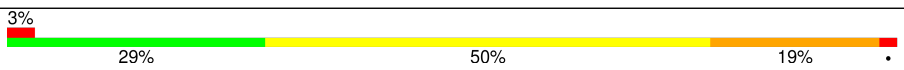
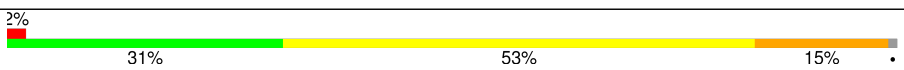
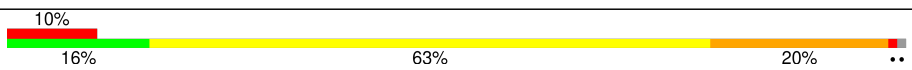
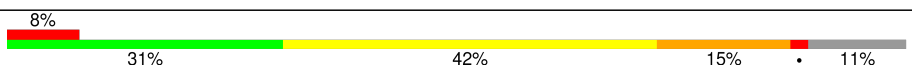
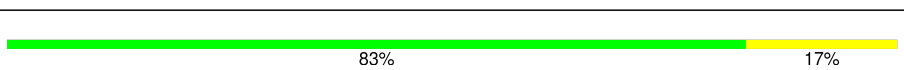
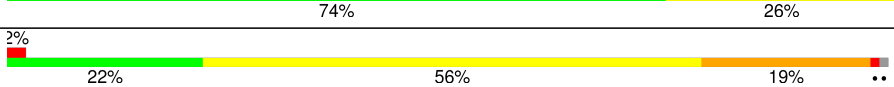
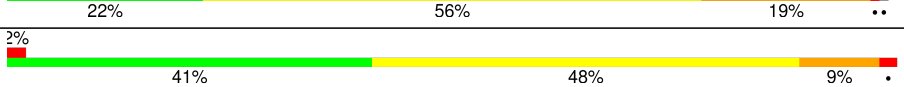
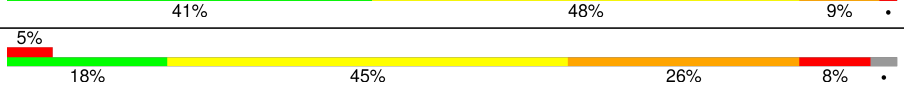
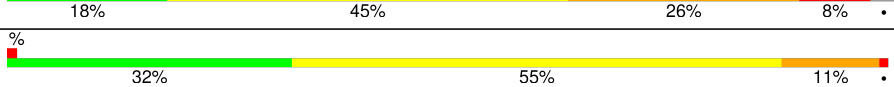
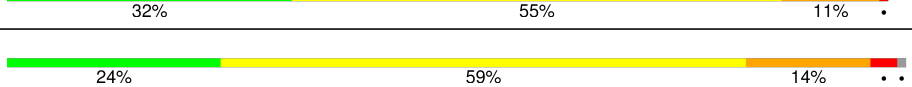
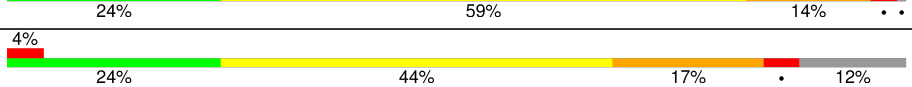
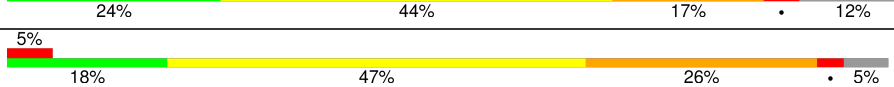
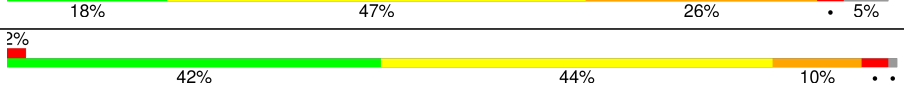
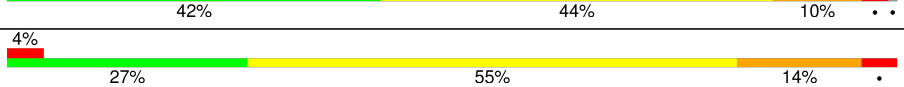
Mol	Chain	Length	Quality of chain
5	A4	71	
6	A5	60	
7	A6	54	
8	A7	49	
9	A8	65	
10	A9	37	
11	AA	2915	
12	AB	122	
13	AC	229	
14	AD	276	
15	AE	206	
16	AF	210	
17	AG	182	
18	AH	180	
19	AJ	130	
20	AK	140	
21	AN	140	
22	AO	122	
23	AP	150	
24	AQ	141	
25	AR	118	
26	AS	112	
27	AT	146	
28	AU	118	
29	AV	101	

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Mol	Chain	Length	Quality of chain
30	AW	113	2% 34% 51% 13%
31	AX	96	41% 49% 7%
32	AY	110	12% 12% 42% 33% 5% 8%
33	AZ	206	4% 23% 47% 17% 11%
34	B2	144	16% 22% 56% 19%
35	BA	1522	3% 26% 58% 13%
36	BB	256	4% 22% 52% 18% 8%
37	BC	239	34% 46% 5% 13%
38	BD	209	7% 23% 56% 18%
39	BE	162	% 33% 52% 6% 7%
40	BF	101	2% 38% 49% 13%
41	BG	156	8% 42% 48% 8%
42	BH	138	45% 53%
43	BI	128	6% 22% 61% 16%
44	BJ	105	16% 19% 56% 18% 6%
45	BK	129	6% 32% 53% 8% 8%
46	BL	135	3% 38% 40% 11% 7%
47	BM	126	8% 20% 59% 17%
48	BN	61	3% 25% 49% 20% 5%
49	BO	89	44% 47% 7%
50	BP	88	% 28% 56% 11% 5%
51	BQ	105	42% 49% 5% 5%
52	BR	88	% 24% 48% 8% 20%
53	BS	93	11% 14% 51% 19% 15%
54	BT	106	4% 25% 58% 11% 7%

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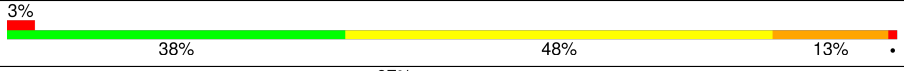
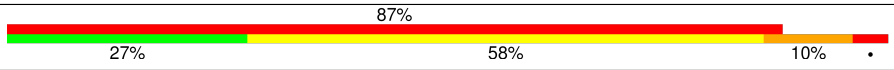
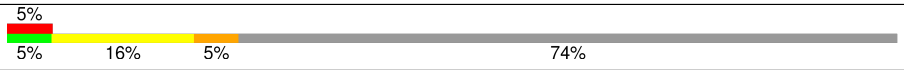
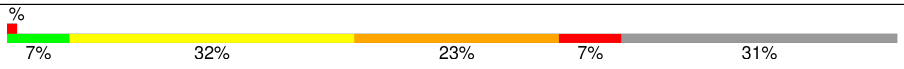
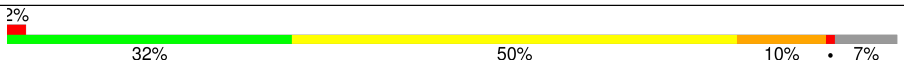
Mol	Chain	Length	Quality of chain
55	BU	27	
56	BV	77	
56	BW	77	
57	BX	19	
58	BY	90	
59	BZ	405	

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is a RNA chain called MRNA.

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

- Molecule 58 is a RNA chain called TMRNA DELA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BY	62	Total	C	N	O	P	0	0	0
			1306	582	233	430	61			

- Molecule 59 is a protein called ELONGATION FACTOR TU.

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

There are 9 discrepancies between the modelled and reference sequences:

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

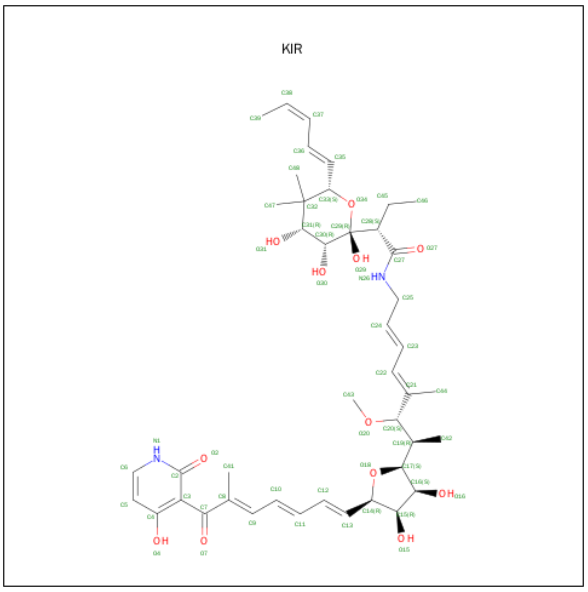
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

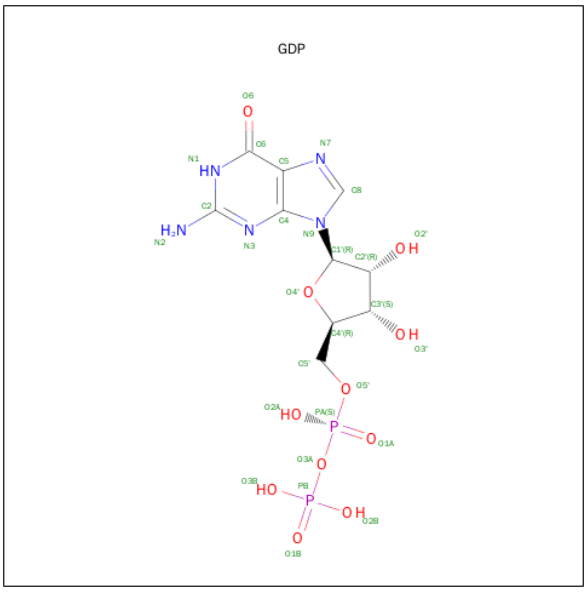
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BZ	1	Total Mg 1 1	0	0
61	AA	1	Total Mg 1 1	0	0

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).



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

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



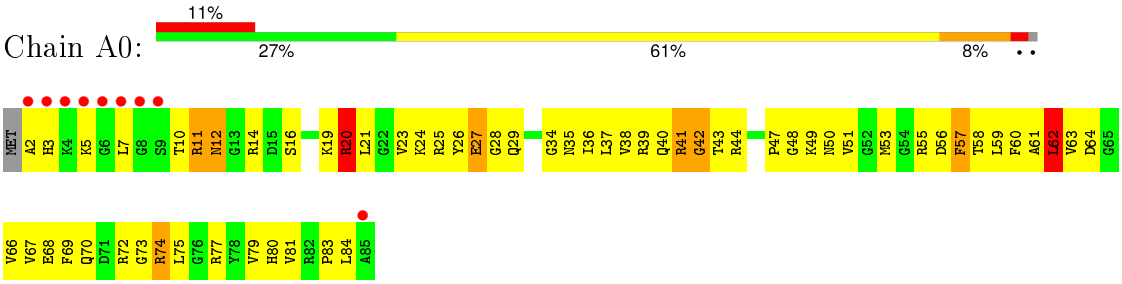
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
63	BZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

3 Residue-property plots (i)

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

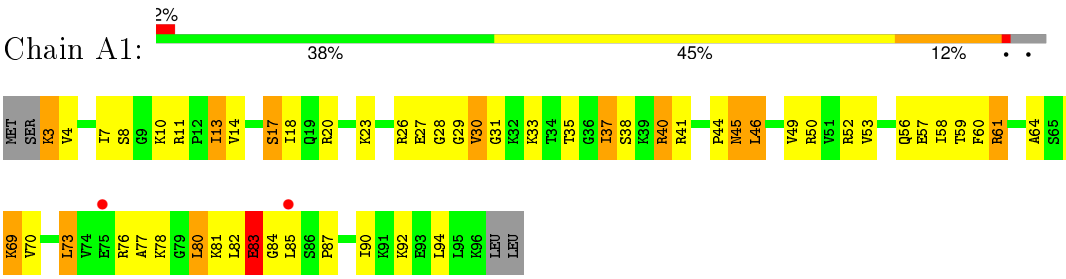
- Molecule 1: 50S RIBOSOMAL PROTEIN L27

Chain A0:



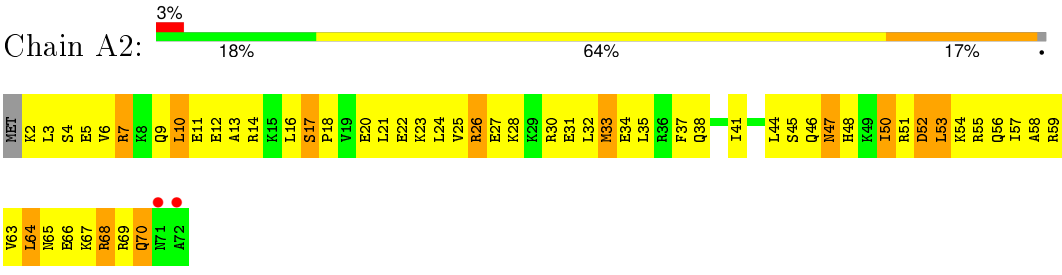
- Molecule 2: 50S RIBOSOMAL PROTEIN L28

Chain A1:



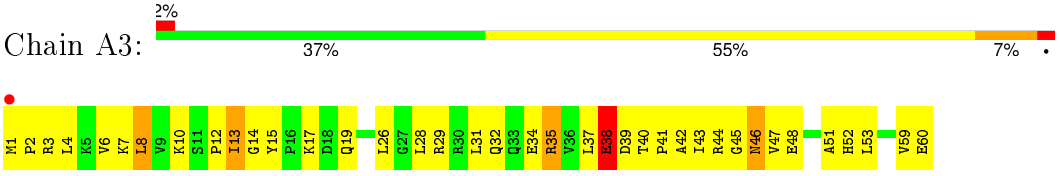
- Molecule 3: 50S RIBOSOMAL PROTEIN L29

Chain A2:



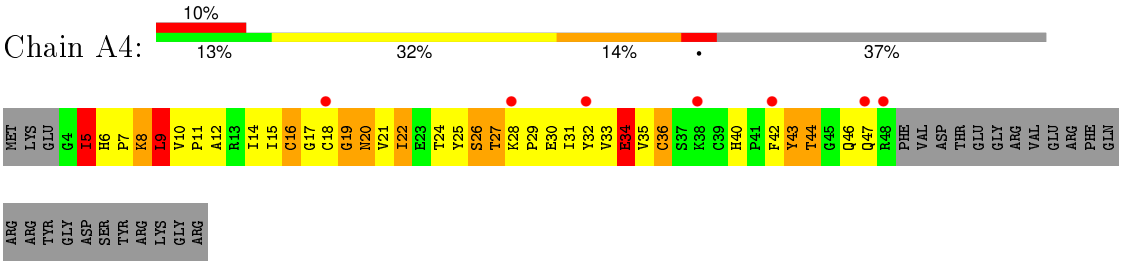
- Molecule 4: 50S RIBOSOMAL PROTEIN L30

Chain A3:



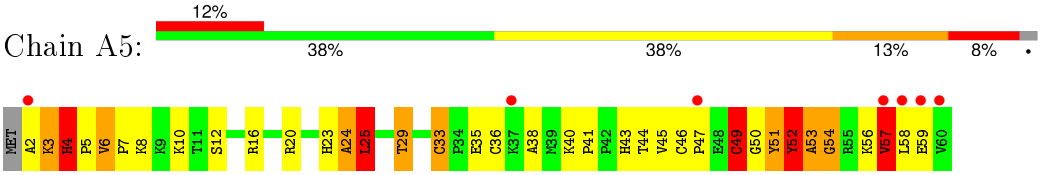
- Molecule 5: 50S RIBOSOMAL PROTEIN L31

Chain A4:



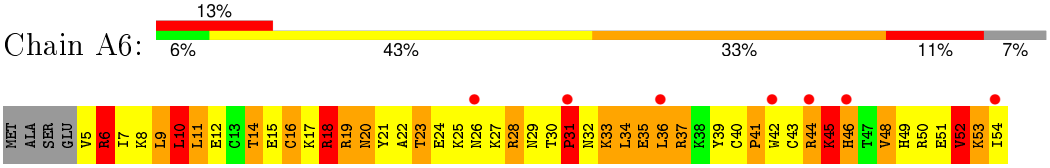
- Molecule 6: 50S RIBOSOMAL PROTEIN L32

Chain A5:



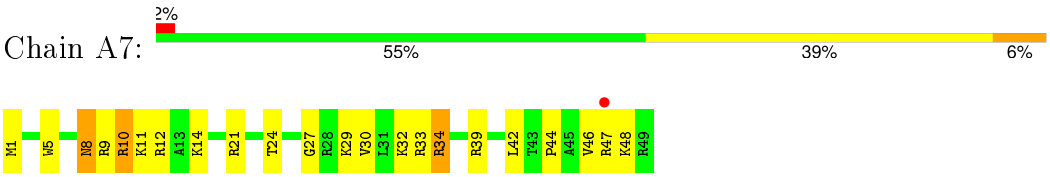
- Molecule 7: 50S RIBOSOMAL PROTEIN L33

Chain A6:



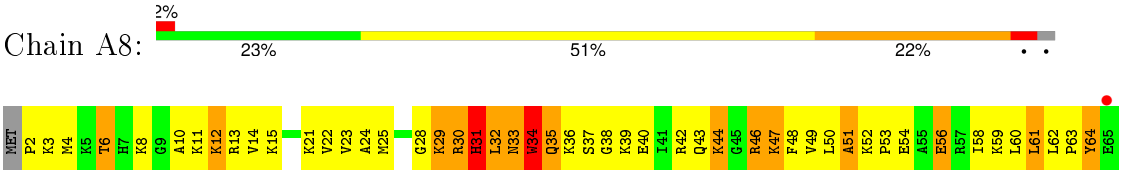
- Molecule 8: 50S RIBOSOMAL PROTEIN L34

Chain A7:



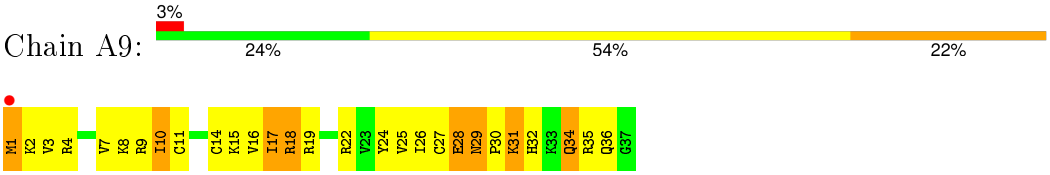
- Molecule 9: 50S RIBOSOMAL PROTEIN L35

Chain A8:



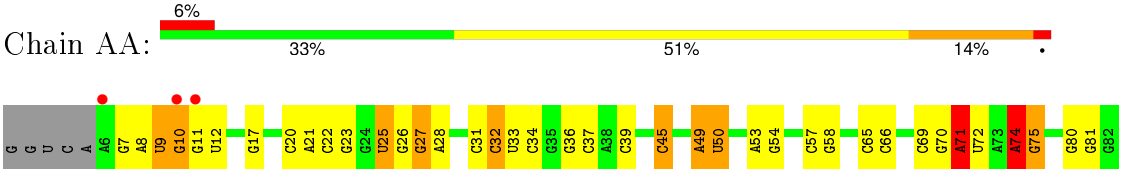
- Molecule 10: 50S RIBOSOMAL PROTEIN L36

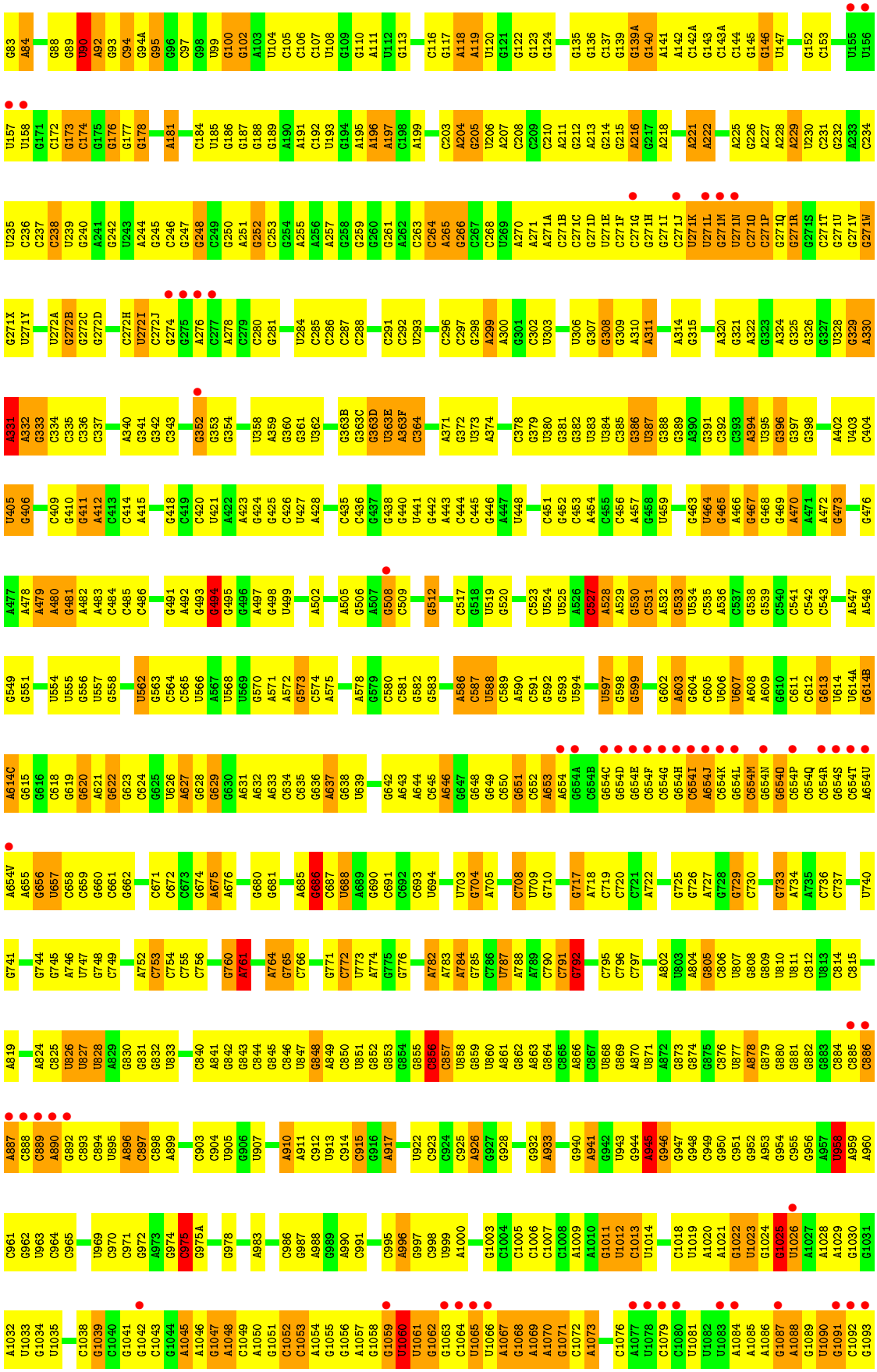
Chain A9:

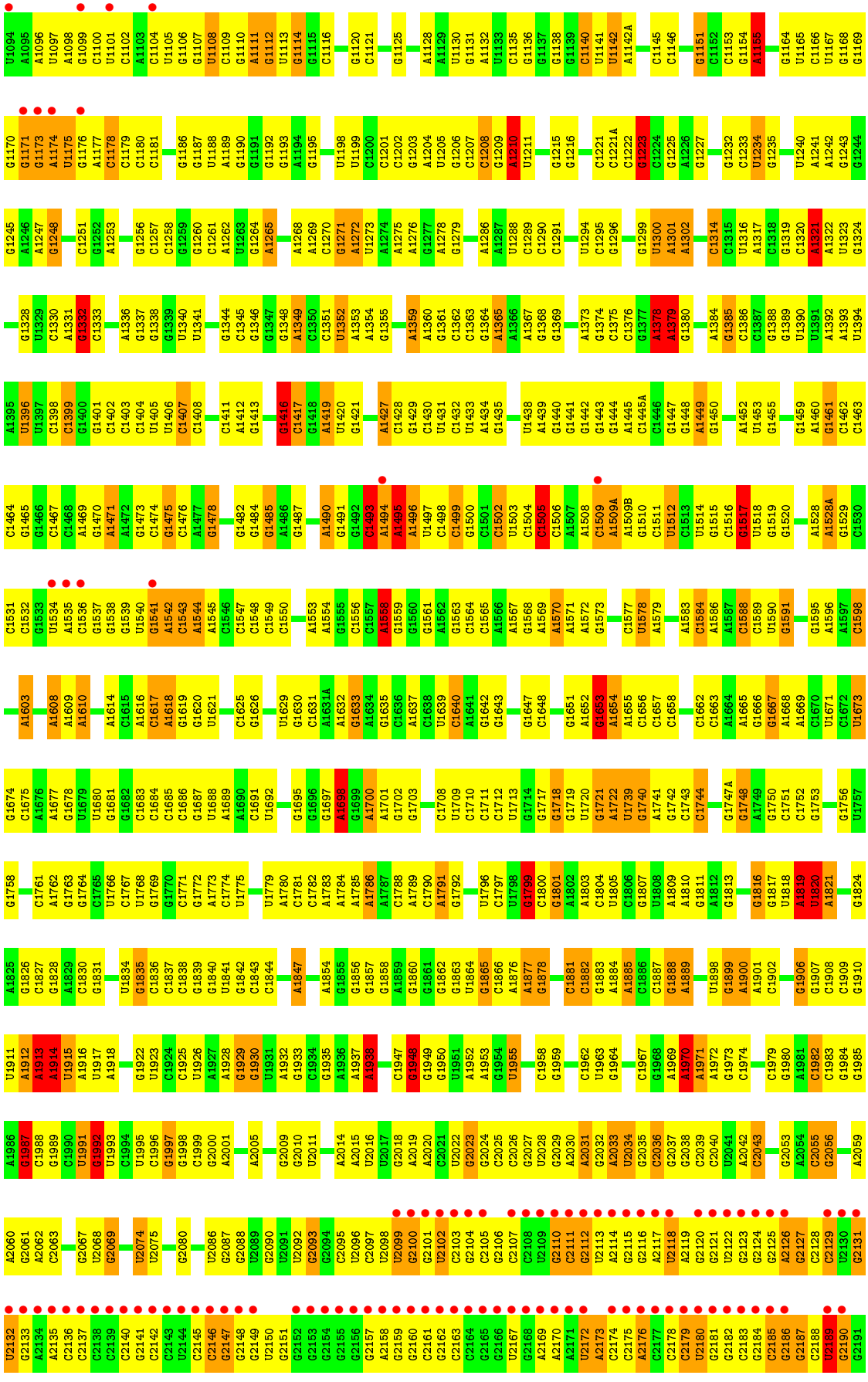


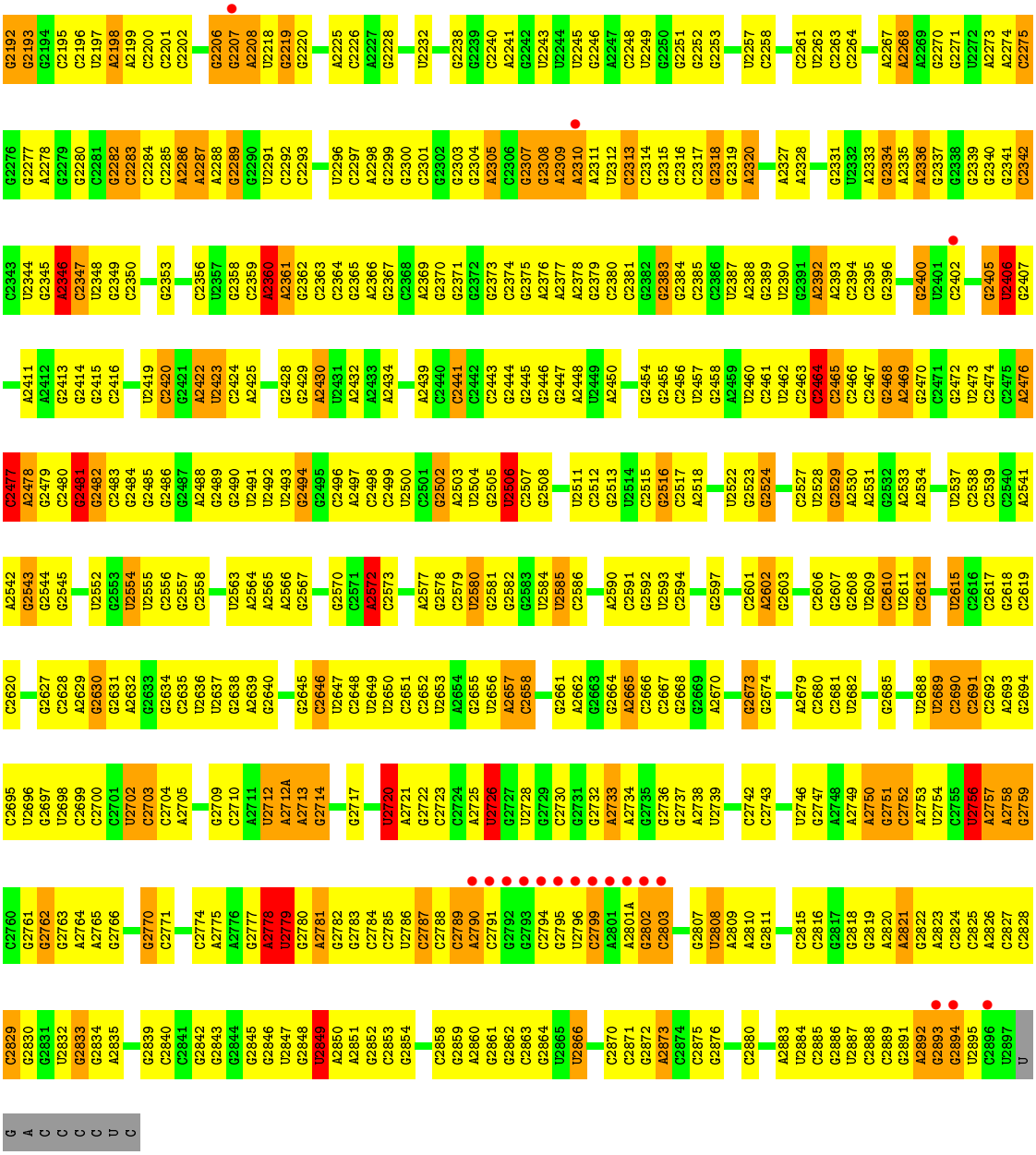
- Molecule 11: 23S RIBOSOMAL RNA

Chain AA:



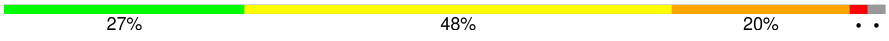

G83 A84 G88 G89 U90 A92 G93 C94 G94A G95 G96 C97 G98 U99 G100 G102 A103 U104 C105 C106 C107 U108 G109 G110 A111 U112 G113 C116 G117 A118 A119 U120 G121 G122 G123 G124 G135 G136 C137 G139 G139A G140 A141 A142 C142A G143 C143A C144 G145 G146 U147 G152 C153 U155 U156
U157 U158 G171 C172 G173 C174 G175 G176 G177 G178 A181 C184 U185 G186 G187 G188 G189 A190 A191 C192 U193 G194 A195 A196 A197 C198 A199 C203 A204 G205 U206 A207 C208 C209 C210 A211 G212 A213 G214 G215 A216 G217 A218 A221 A222 A225 G226 A227 A228 A229 U230 C231 C232 A233 C234
U235 C236 C237 C238 U239 G240 A241 G242 U243 A244 G245 C246 G247 G248 G249 G250 A251 G252 C253 G254 A255 A256 A257 G258 G259 G260 C261 A262 C263 C264 A265 G266 C267 C268 U269 A270 A271 A271A C271B C271C C271D U271E C271F C271G G271H G271I C271J U271K U271L G271M U271N C271O C271P G271Q G271R G271S C271T G271U G271V G271W
G271X U271Y U272A G272B G272C G272D C272H U272I C272J G274 G275 A276 C277 A278 C279 C280 G281 U284 C285 C286 C287 C288 C291 C292 U293 C296 C297 G298 A299 A300 G301 C302 U303 U306 G307 G308 G309 A310 A311 A314 G315 A320 G321 A322 G323 A324 G325 G326 G327 U328 G329 A330
A331 A332 G333 C334 C335 C336 C337 A340 G341 G342 C343 G352 G353 G354 U358 A359 G360 G361 U362 G363B G363C G363D U363E A363F C364 A371 G372 U373 A374 C378 G379 U380 G381 G382 U383 U384 C385 G386 U387 G388 G389 A390 G391 C392 G393 A394 U395 G396 G397 G398 A402 U403 C404
U405 G406 C409 G410 G411 A412 C413 C414 A415 G418 C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 C435 C436 G437 G438 G440 U441 G442 A443 C444 C445 G446 A447 U448 C451 G452 C453 A454 G455 C456 A457 G458 U459 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 G473 G476
A477 A478 A479 A480 G481 A482 A483 C484 C485 C486 G491 A492 G493 G494 G495 G496 A497 G498 U499 A502 A505 G506 A507 G508 C509 G512 C517 G518 U519 G520 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 C541 C542 C543 A547 A548
G549 G551 U554 U555 G556 U557 G558 U562 G563 C564 C565 U566 A567 U568 U569 G570 A571 A572 G573 C574 A575 A578 G579 C580 C581 G582 G583 A586 C587 U588 C589 A590 C591 G592 G593 U594 U597 G598 G599 G602 A603 G604 C605 U606 U607 A608 A609 G610 C611 C612 G613 U614 U614A G614B
A614C G615 G616 C618 G619 G620 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 G642 A643 A644 C645 A646 G647 G648 G649 C650 G651 C652 A653 A654 G654A C654B G654C G654D G654E C654F C654G G654H C654I A654J C654K G654L C654M G654N G654O C654P C654Q C654R G654S C654T A654U
A654V A655 G656 U657 C658 C659 G660 C661 G662 C671 C672 C673 G674 A675 A676 G680 G681 A685 G686 C687 U688 A689 G690 C691 C692 C693 U694 U703 G704 A705 C708 U709 G710 G717 A718 C719 C720 C721 A722 G725 G726 A727 G728 G729 C730 G733 A734 A735 C736 C737 U740
G741 G744 G745 A746 U747 G748 C749 A752 C753 C754 C755 C756 G760 A761 A764 G765 C766 G771 C772 U773 A774 G775 G776 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 C795 C796 C797 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815
A819 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C840 A841 G842 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852 G853 G854 G855 G856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 U871 A872 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886
A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 G898 A899 C903 C904 U905 G906 U907 A910 A911 C912 U913 C914 C915 G916 A917 U922 C923 C924 C925 A926 G927 G928 G932 A933 G940 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951 G952 A953 G954 C955 C956 A957 U958 A959 A960
C961 G962 U963 C964 C965 G972 A973 G974 G975 G975A G978 A983 C986 G987 A988 G989 A990 C991 C995 A996 G997 C998 U999 A1000 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031
A1032 U1033 G1034 U1035 C1038 G1039 C1040 G1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 A1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093

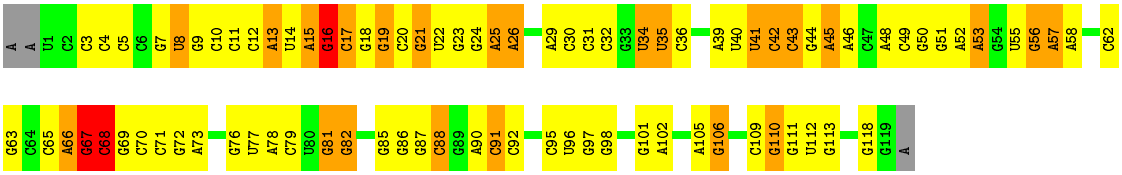




• Molecule 12: 5S RIBOSOMAL RNA

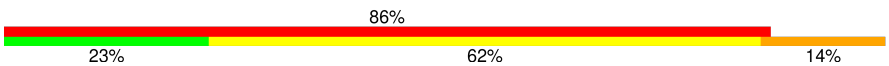
Chain AB:

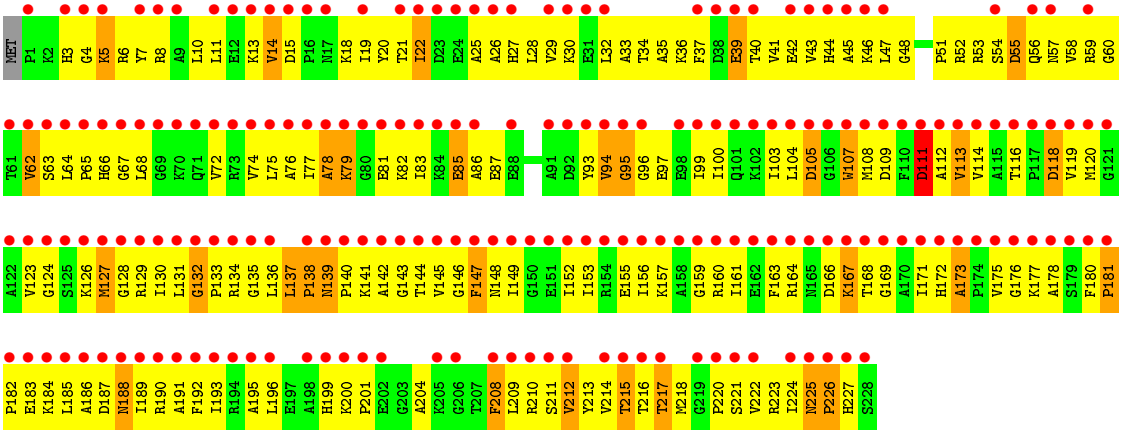




• Molecule 13: 50S RIBOSOMAL PROTEIN L1

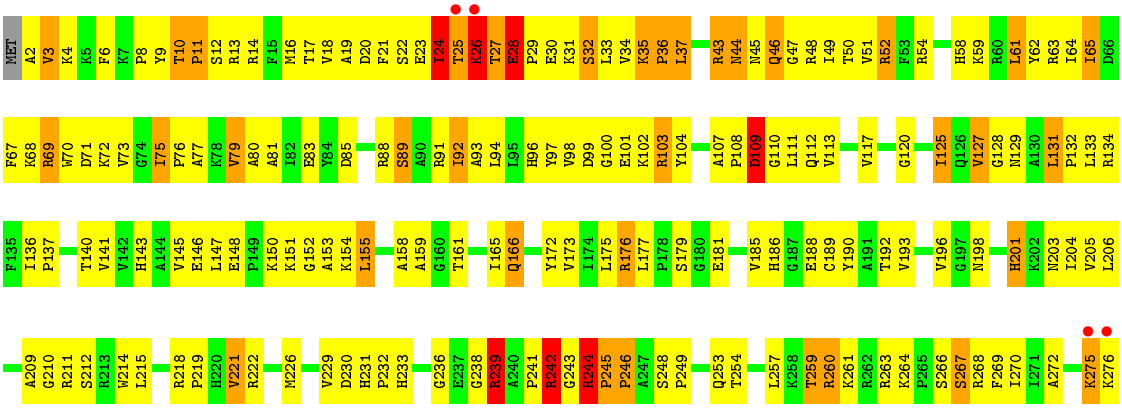
Chain AC:





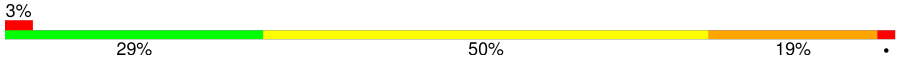
- Molecule 14: 50S RIBOSOMAL PROTEIN L2

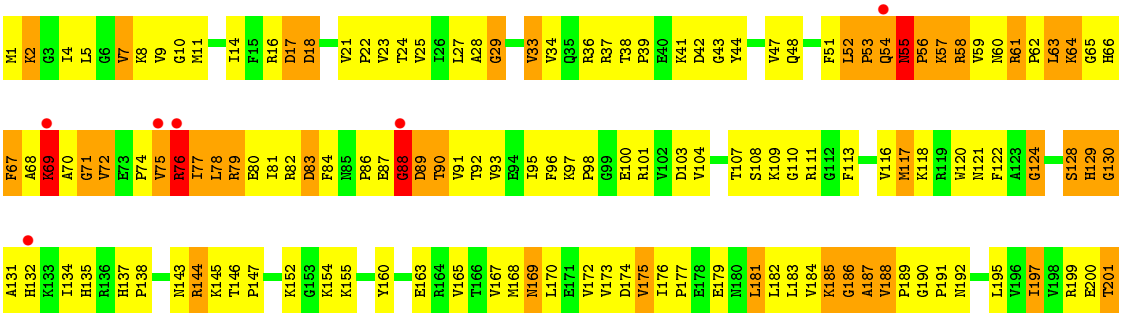
Chain AD:



- Molecule 15: 50S RIBOSOMAL PROTEIN L3

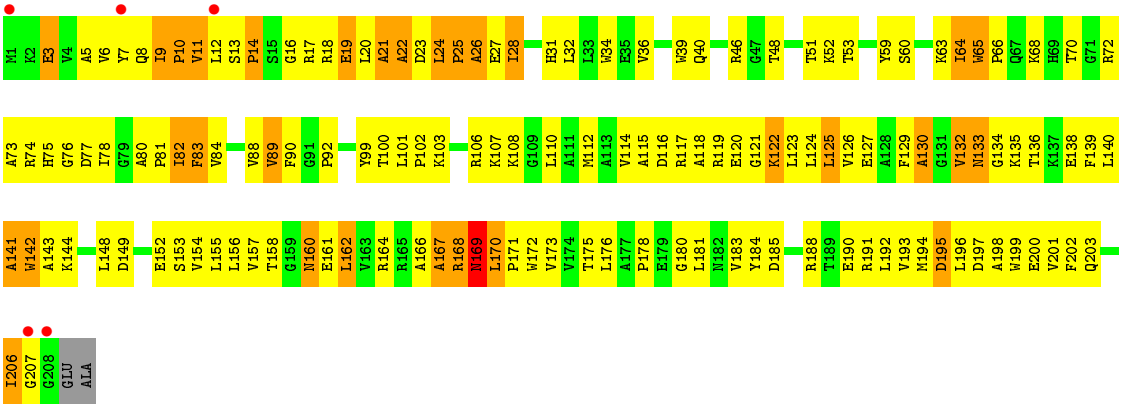
Chain AE:



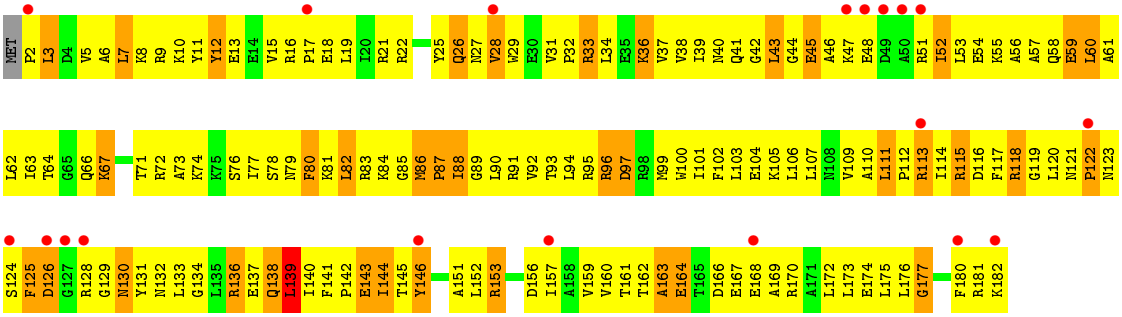


- Molecule 16: 50S RIBOSOMAL PROTEIN L4

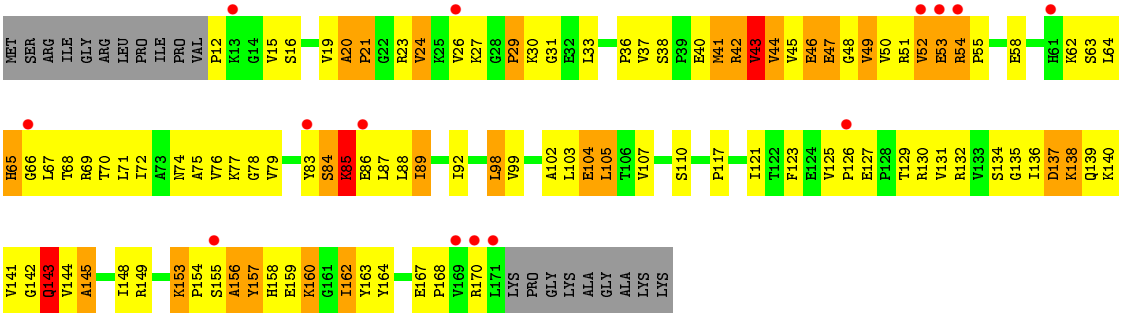
Chain AF:



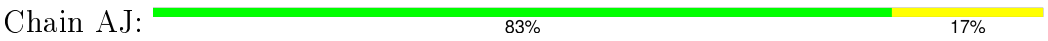
• Molecule 17: 50S RIBOSOMAL PROTEIN L5

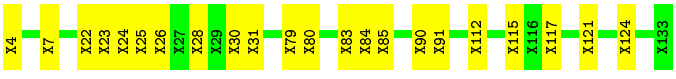


• Molecule 18: 50S RIBOSOMAL PROTEIN L6

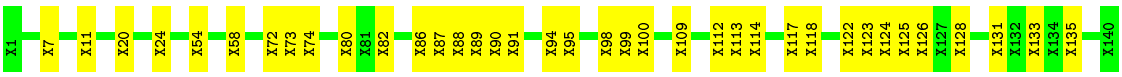


• Molecule 19: 50S RIBOSOMAL PROTEIN L10



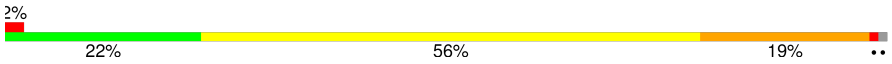


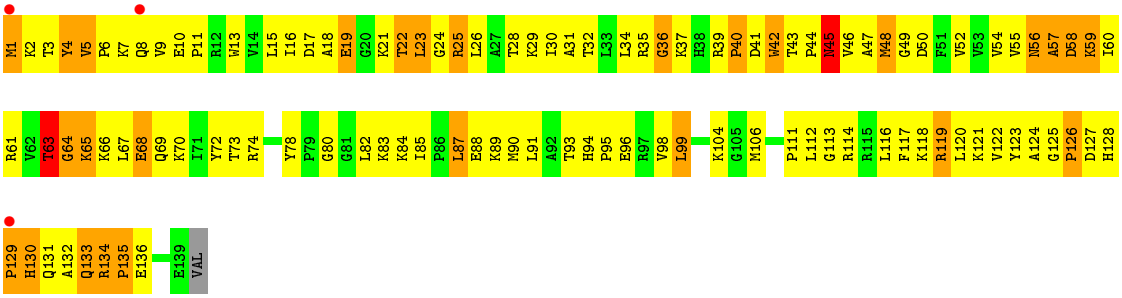
• Molecule 20: 50S RIBOSOMAL PROTEIN L11



- Molecule 21: 50S RIBOSOMAL PROTEIN L13

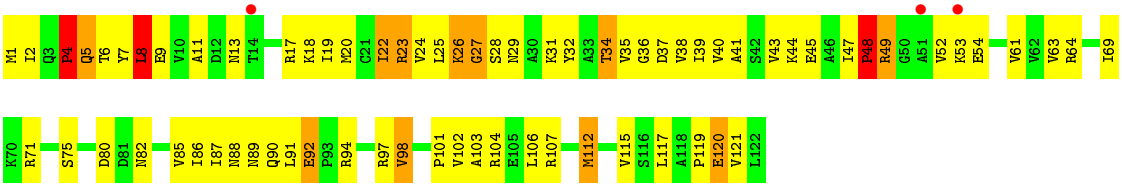
Chain AN:





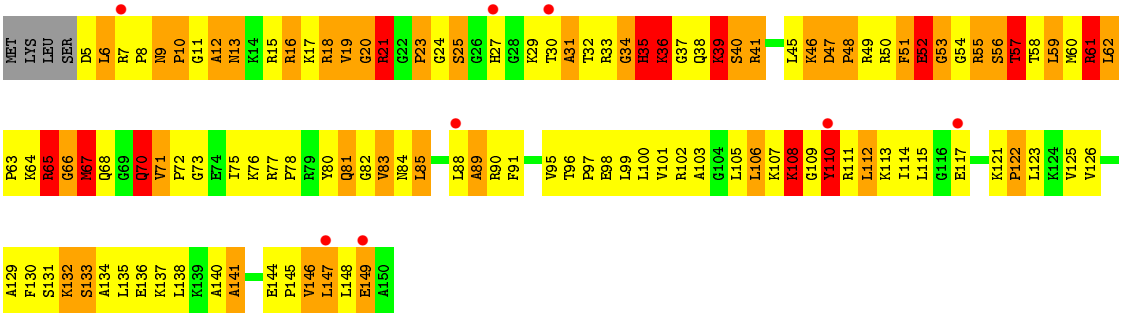
- Molecule 22: 50S RIBOSOMAL PROTEIN L14

Chain AO:



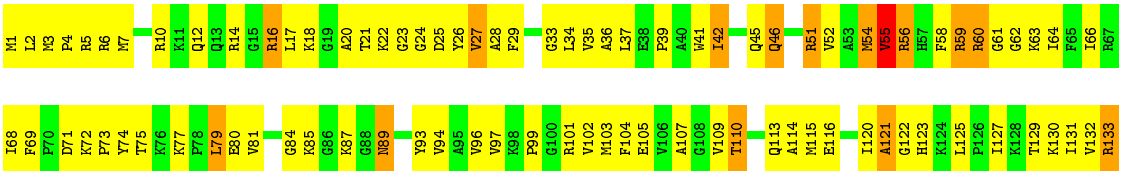
- Molecule 23: 50S RIBOSOMAL PROTEIN L15

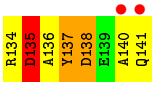
Chain AP:



- Molecule 24: 50S RIBOSOMAL PROTEIN L16

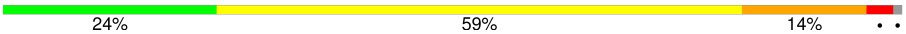
Chain AQ:

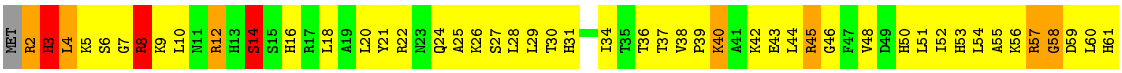




- Molecule 25: 50S RIBOSOMAL PROTEIN L17

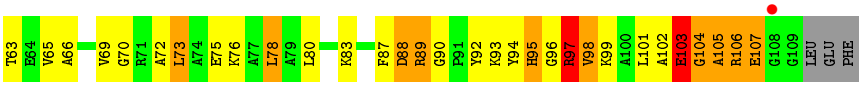
Chain AR:





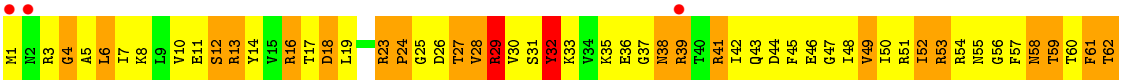
- Molecule 26: 50S RIBOSOMAL PROTEIN L18

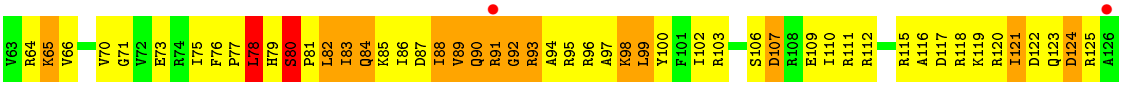
Chain AS:

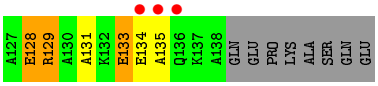


- Molecule 27: 50S RIBOSOMAL PROTEIN L19

Chain AT:

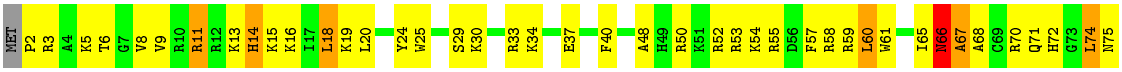


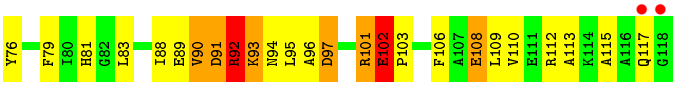




- Molecule 28: 50S RIBOSOMAL PROTEIN L20

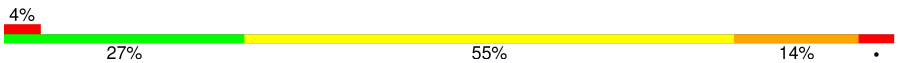
Chain AU:

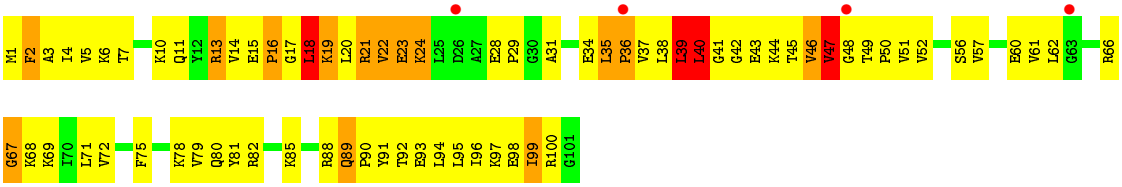




- Molecule 29: 50S RIBOSOMAL PROTEIN L21

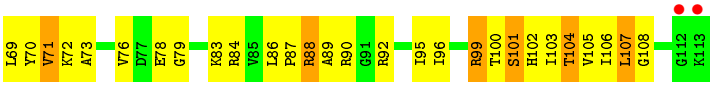
Chain AV:





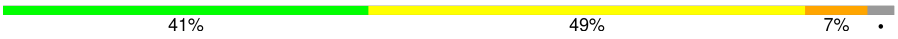
• Molecule 30: 50S RIBOSOMAL PROTEIN L22

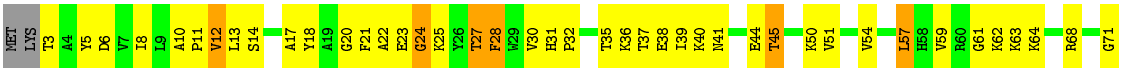
Chain AW:

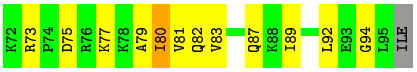


• Molecule 31: 50S RIBOSOMAL PROTEIN L23

Chain AX:

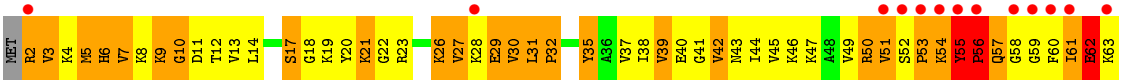






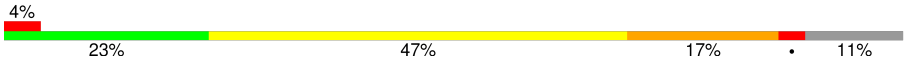
• Molecule 32: 50S RIBOSOMAL PROTEIN L24

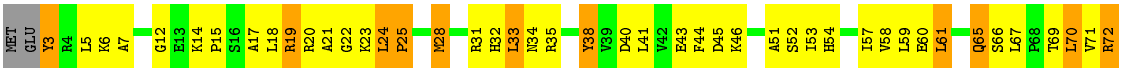
Chain AY:



• Molecule 33: 50S RIBOSOMAL PROTEIN L25

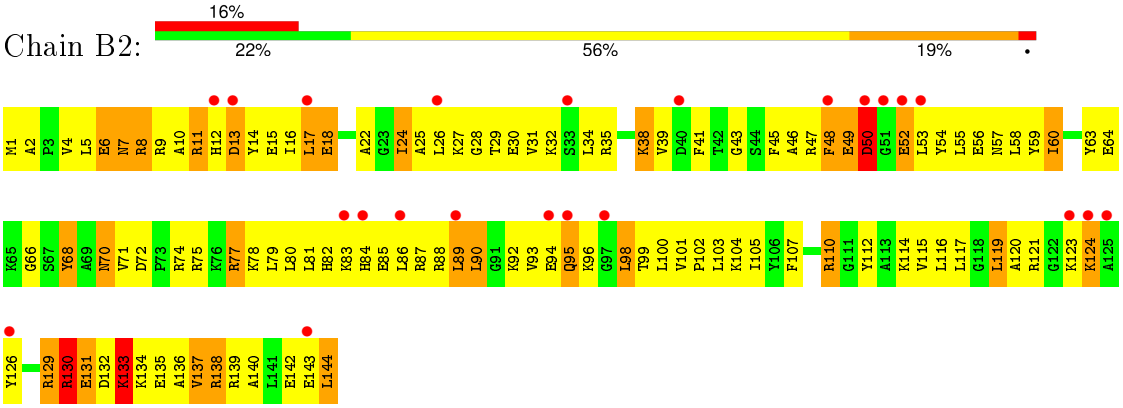
Chain AZ:





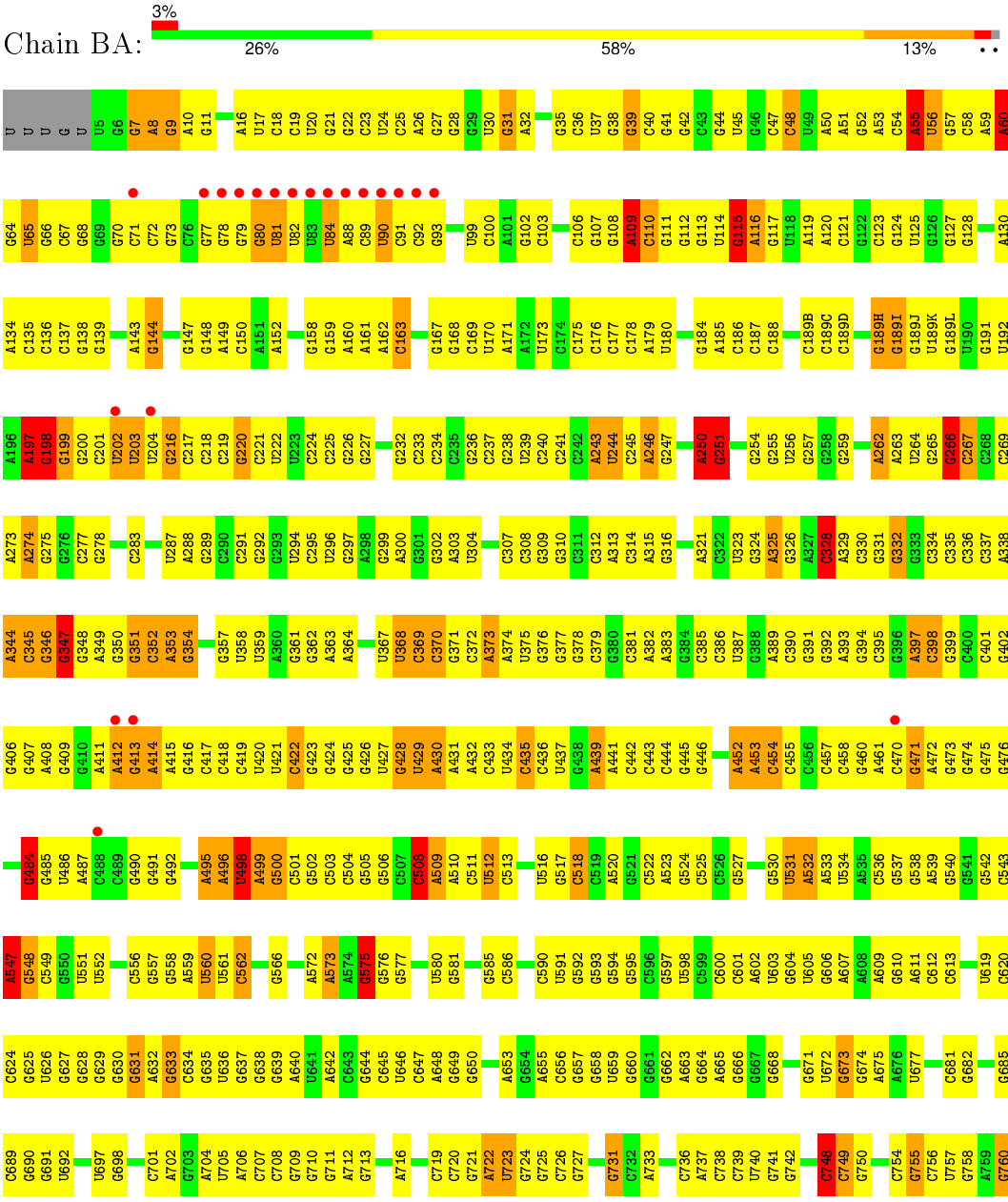
- Molecule 34: SMALL PROTEIN B SMPB

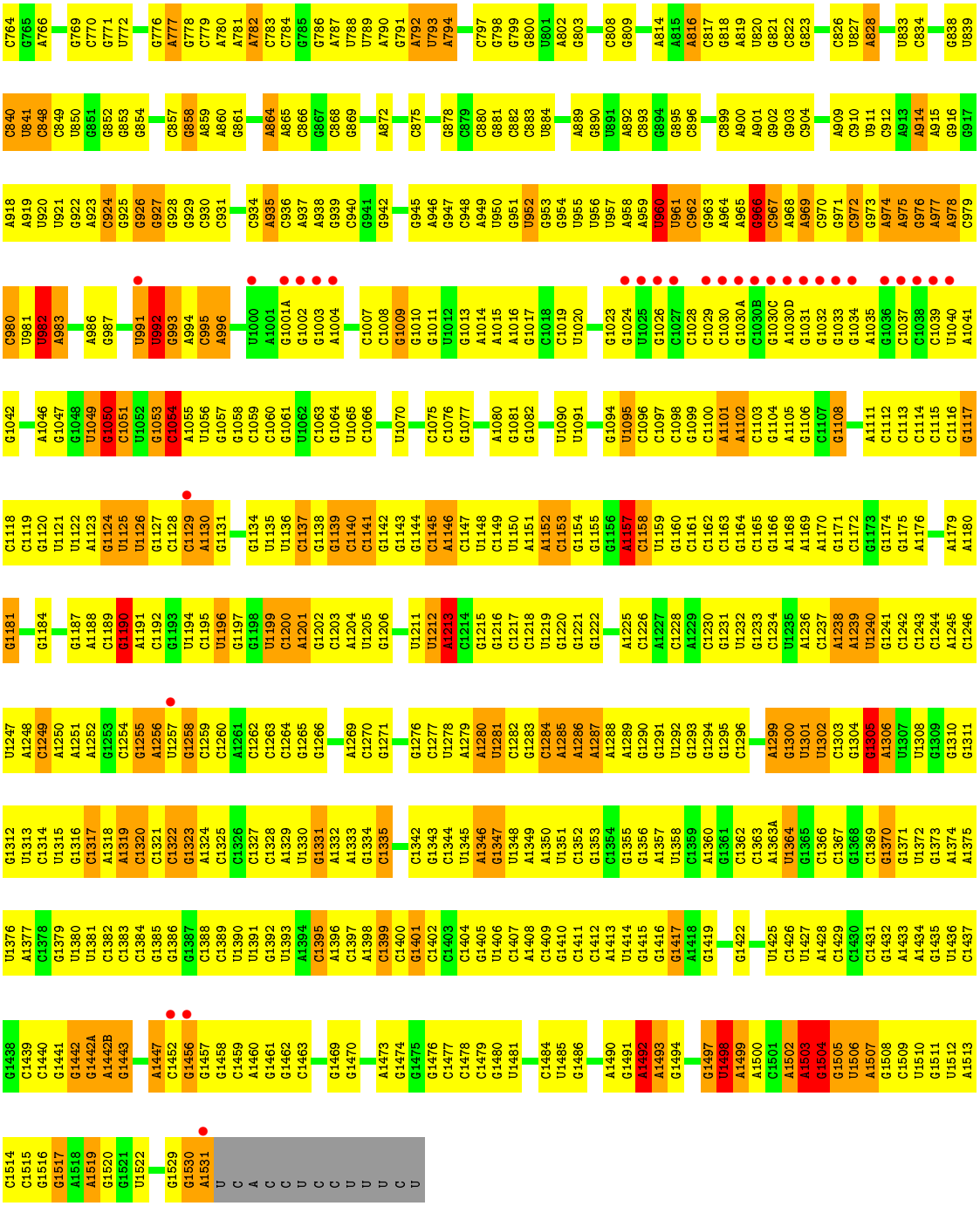
Chain B2:



- Molecule 35: 16S RRNA

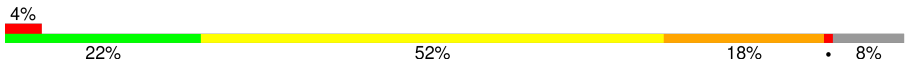
Chain BA:

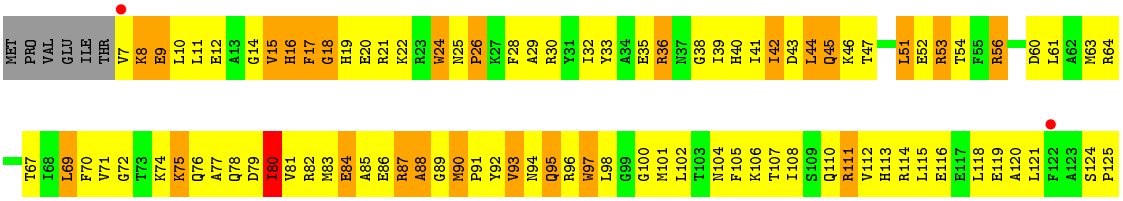


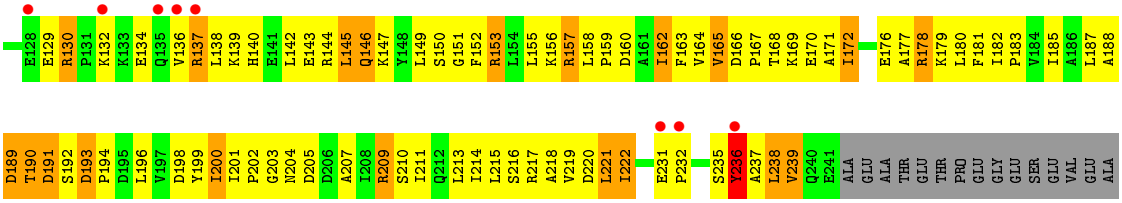


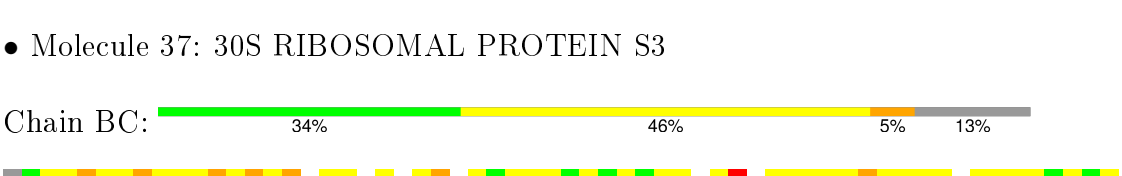
• Molecule 36: 30S RIBOSOMAL PROTEIN S2

Chain BB:



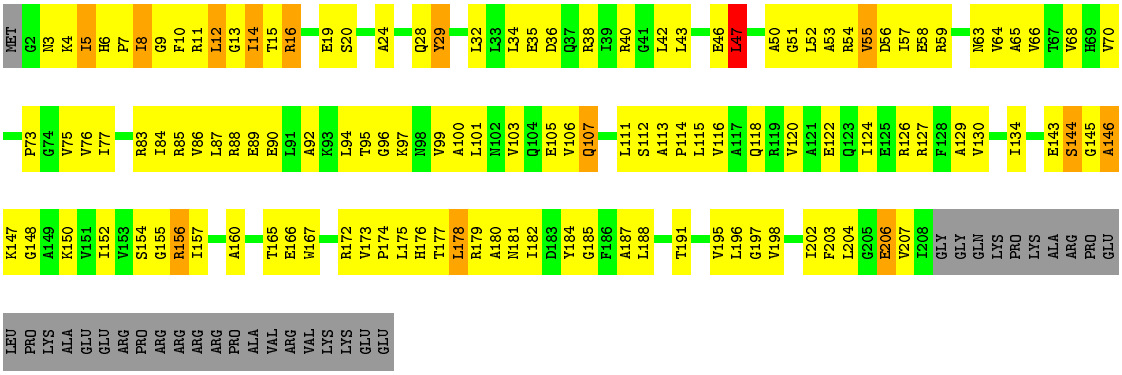






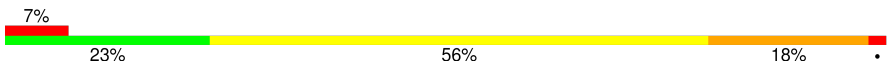
• Molecule 37: 30S RIBOSOMAL PROTEIN S3

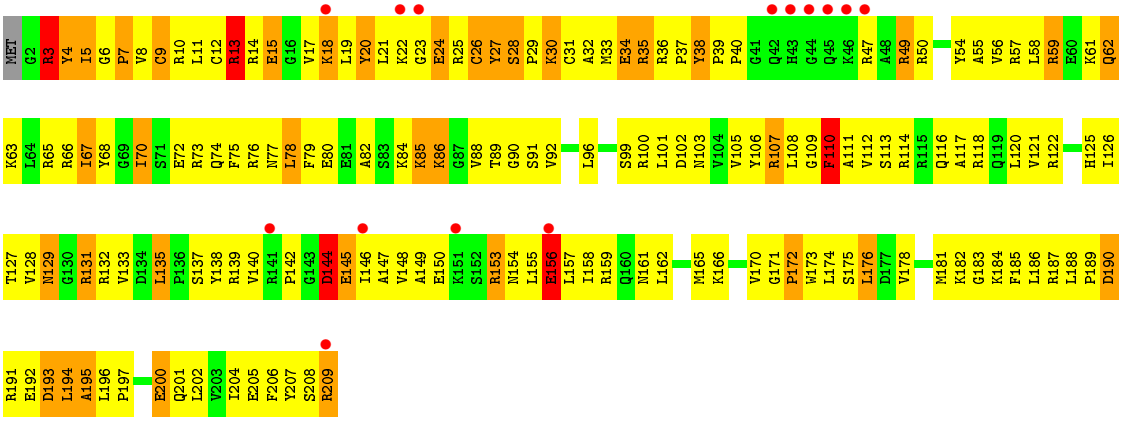
Chain BC:



• Molecule 38: 30S RIBOSOMAL PROTEIN S4

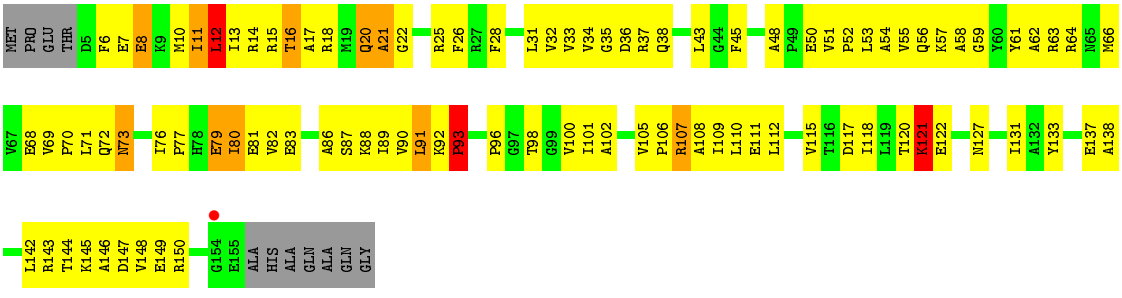
Chain BD:





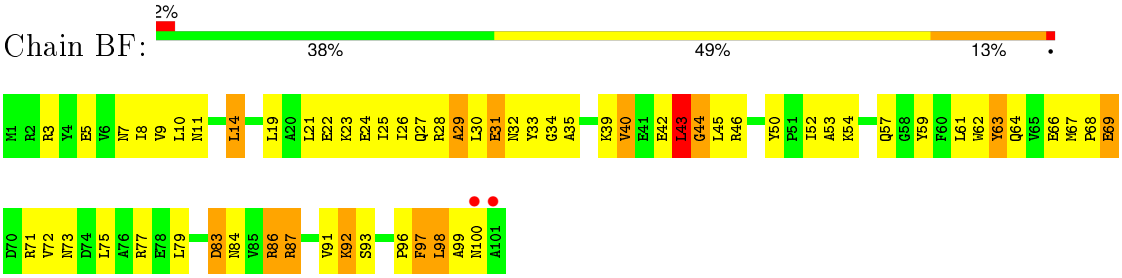
• Molecule 39: 30S RIBOSOMAL PROTEIN S5

Chain BE:



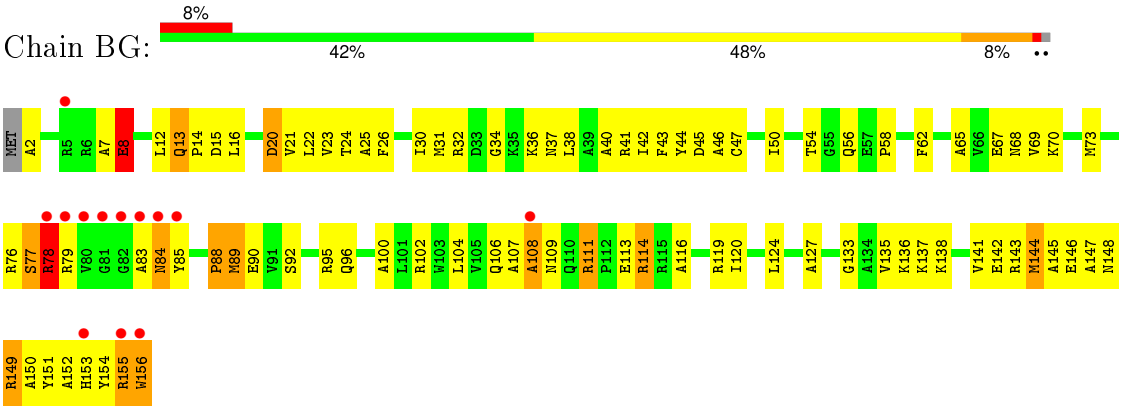
- Molecule 40: 30S RIBOSOMAL PROTEIN S6

Chain BF:



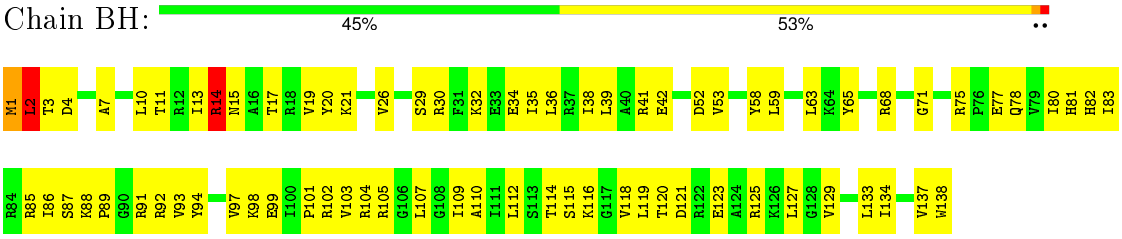
- Molecule 41: 30S RIBOSOMAL PROTEIN S7

Chain BG:



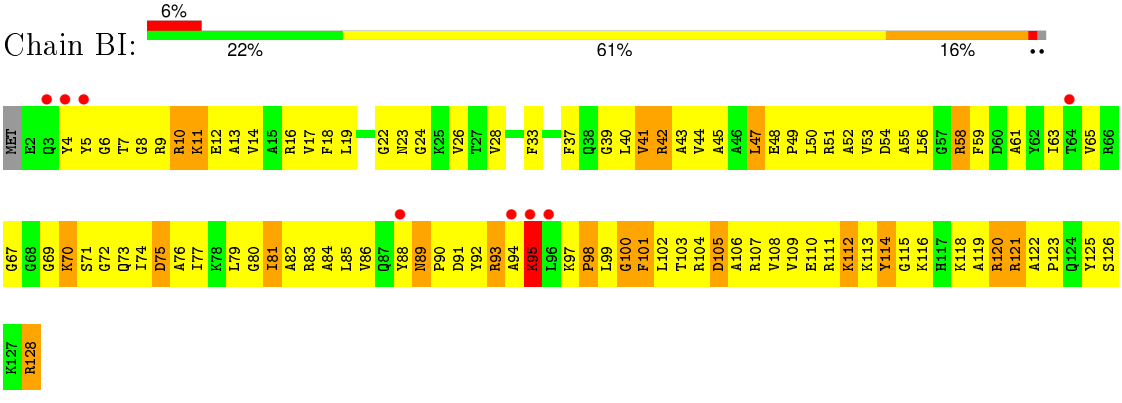
- Molecule 42: 30S RIBOSOMAL PROTEIN S8

Chain BH:



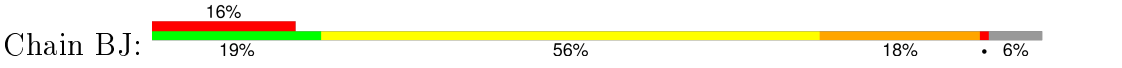
- Molecule 43: 30S RIBOSOMAL PROTEIN S9

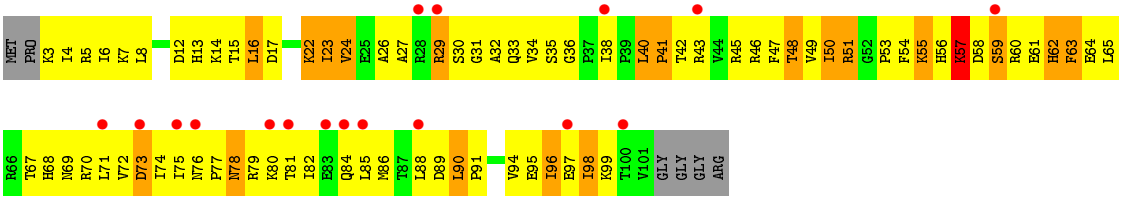
Chain BI:



- Molecule 44: 30S RIBOSOMAL PROTEIN S10

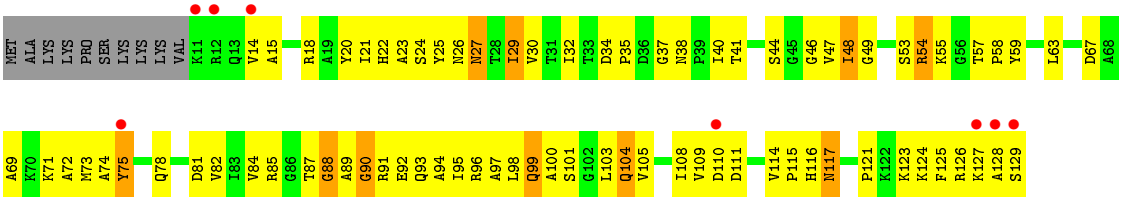
Chain BJ:





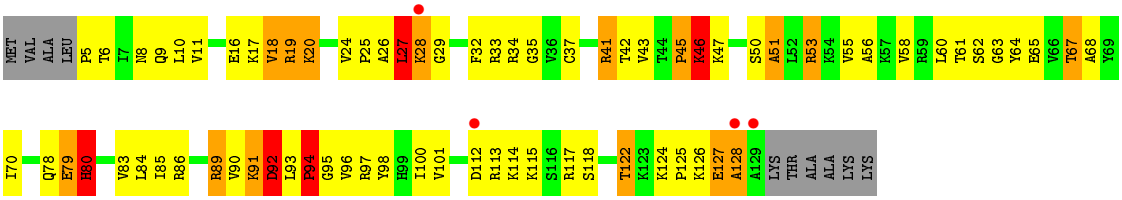
• Molecule 45: 30S RIBOSOMAL PROTEIN S11

Chain BK:



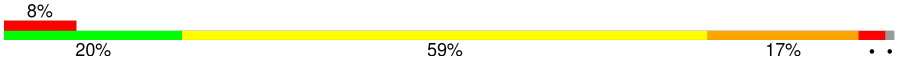
• Molecule 46: 30S RIBOSOMAL PROTEIN S12

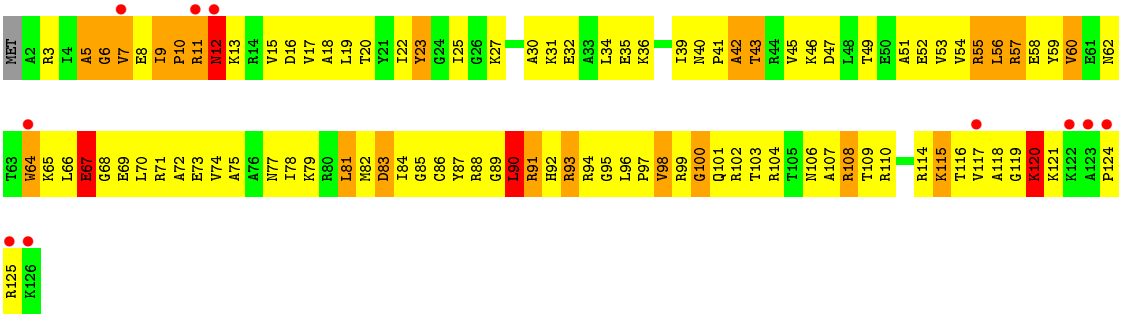
Chain BL:



• Molecule 47: 30S RIBOSOMAL PROTEIN S13

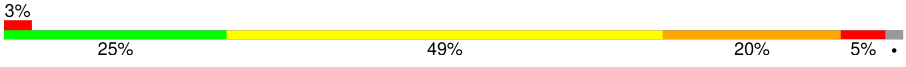
Chain BM:





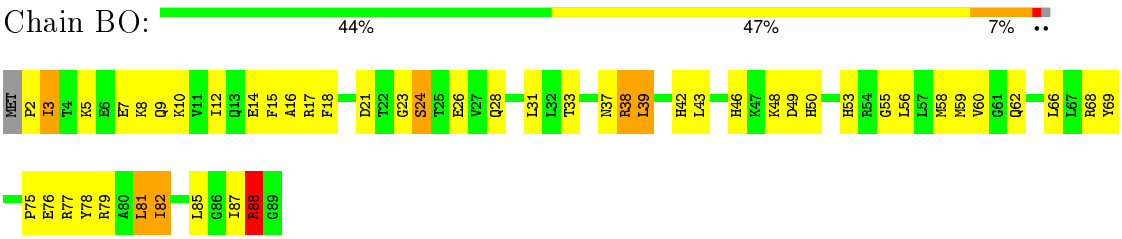
• Molecule 48: 30S RIBOSOMAL PROTEIN S14

Chain BN:



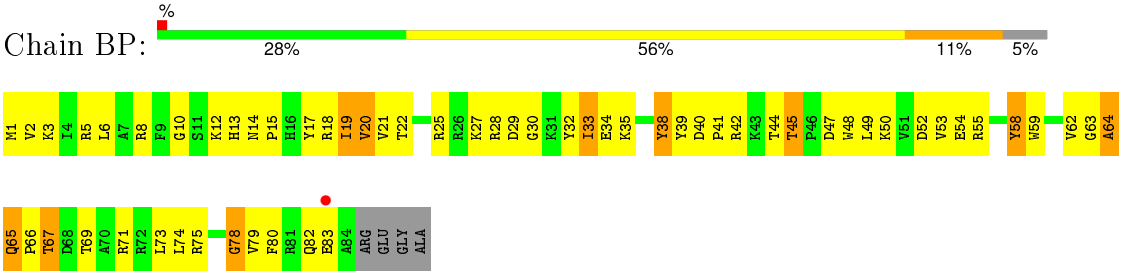
• Molecule 49: 30S RIBOSOMAL PROTEIN S15

Chain BO:



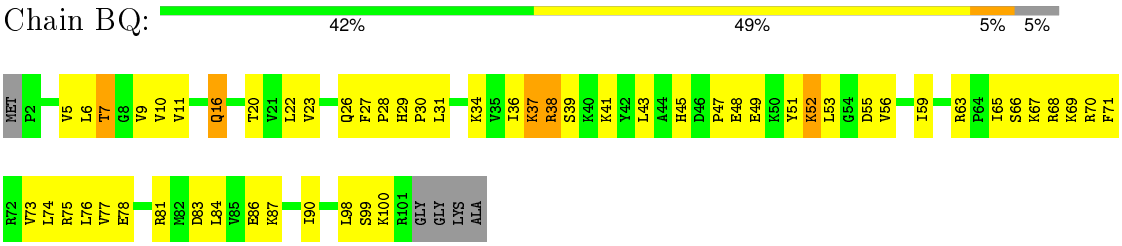
- Molecule 50: 30S RIBOSOMAL PROTEIN S16

Chain BP:



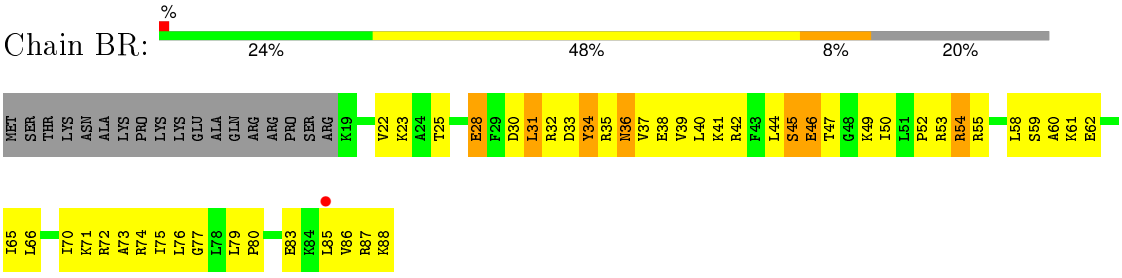
- Molecule 51: 30S RIBOSOMAL PROTEIN S17

Chain BQ:



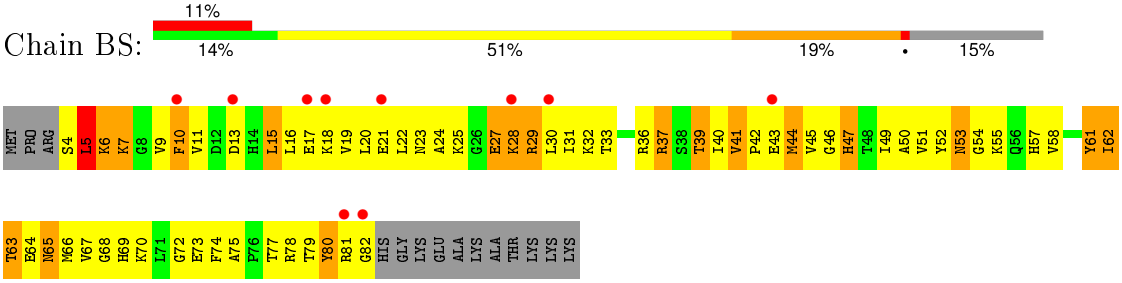
- Molecule 52: 30S RIBOSOMAL PROTEIN S18

Chain BR:



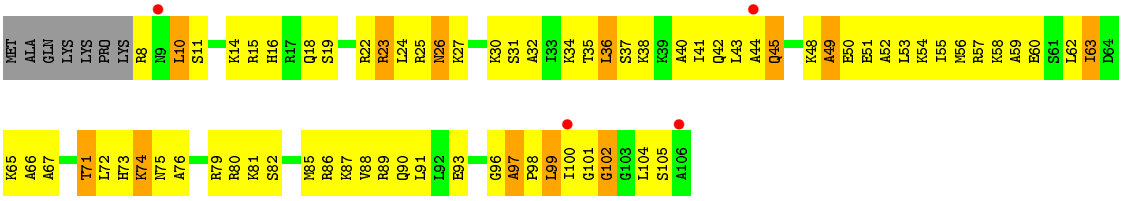
- Molecule 53: 30S RIBOSOMAL PROTEIN S19

Chain BS:

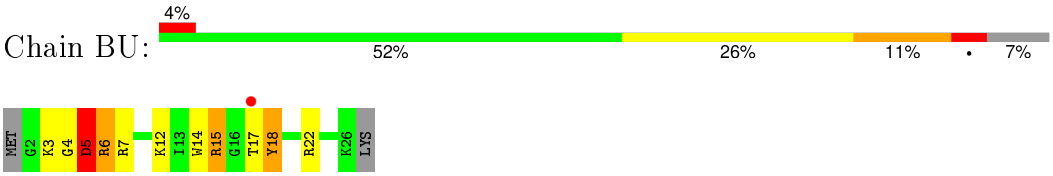


- Molecule 54: 30S RIBOSOMAL PROTEIN S20

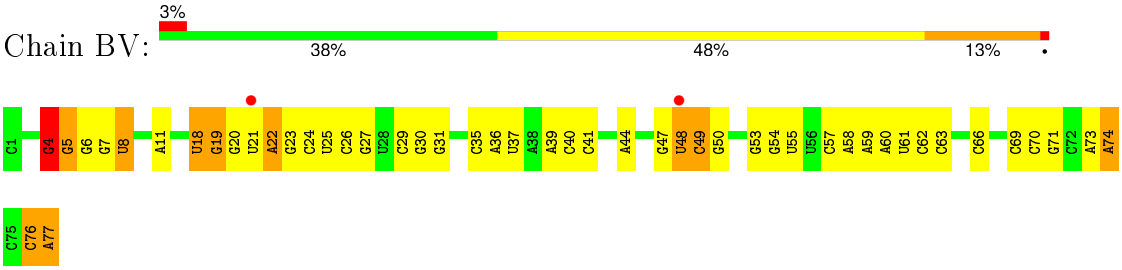
Chain BT:



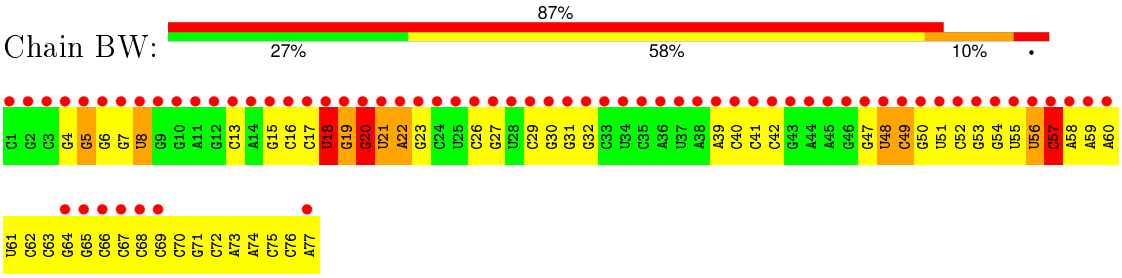
- Molecule 55: 30S RIBOSOMAL PROTEIN THX



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

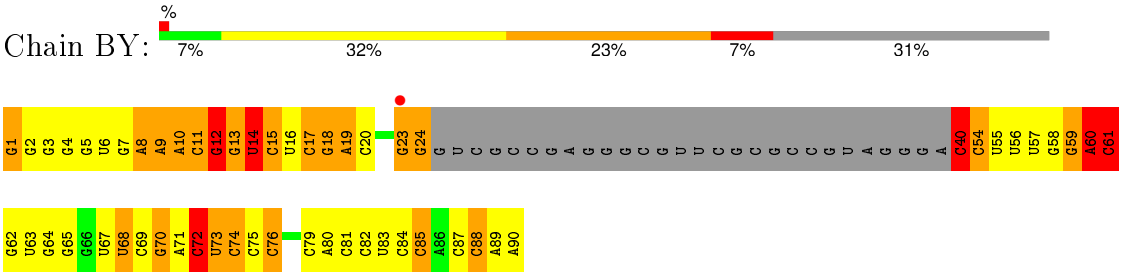


- Molecule 56: E-SITE TRNA FMET OR P-SITE TRNA FMET



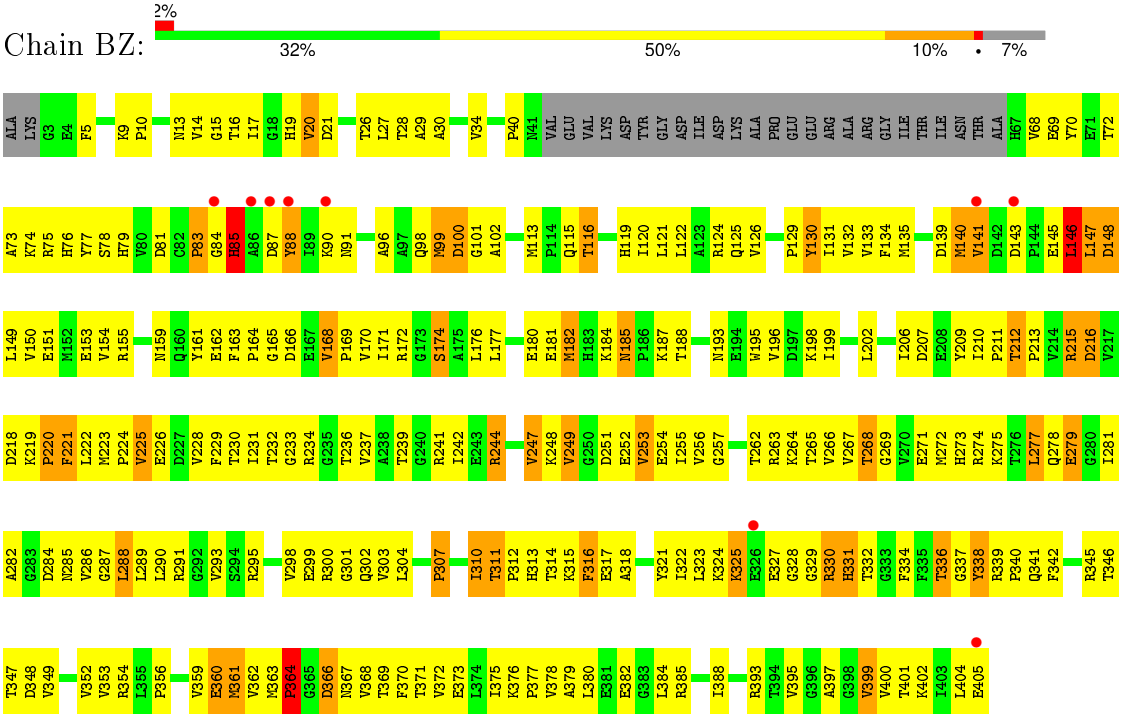
- Molecule 57: MRNA

- Molecule 58: TMRNA DELA



- Molecule 59: ELONGATION FACTOR TU

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	202.17Å 290.76Å 250.65Å 90.00° 97.63° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.10) 97.4 (49.68-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.270 0.229 , 0.269	Depositor DCC
R_{free} test set	24443 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 503945 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	154206	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	BA	0.48	1/36192 (0.0%)	0.78	39/56489 (0.1%)
36	BB	0.46	0/1936	0.72	0/2611
37	BC	0.43	0/1637	0.69	0/2207
38	BD	0.40	0/1733	0.68	0/2318
39	BE	0.49	0/1163	0.72	0/1566
40	BF	0.43	0/856	0.68	1/1154 (0.1%)
41	BG	0.36	0/1276	0.61	0/1709
42	BH	0.45	0/1136	0.75	0/1527
43	BI	0.41	0/1029	0.67	0/1378
44	BJ	0.42	0/808	0.69	0/1087
45	BK	0.39	0/900	0.65	0/1213
46	BL	0.45	0/987	0.74	0/1322
47	BM	0.38	0/999	0.71	0/1338
48	BN	0.45	0/501	0.75	0/664
49	BO	0.45	0/745	0.70	0/992
50	BP	0.42	0/717	0.65	0/965
51	BQ	0.42	0/837	0.67	0/1119
52	BR	0.42	0/579	0.70	0/768
53	BS	0.45	0/643	0.67	1/867 (0.1%)
54	BT	0.37	0/765	0.65	0/1007
55	BU	0.48	0/213	0.63	0/279
56	BV	0.45	0/1832	0.79	1/2855 (0.0%)
56	BW	0.45	0/1832	0.81	3/2855 (0.1%)
57	BX	0.71	0/116	0.89	0/179
58	BY	0.82	5/1455 (0.3%)	0.97	5/2258 (0.2%)
59	BZ	0.42	0/2986	0.69	0/4050
All	All	0.52	12/165829 (0.0%)	0.79	161/247542 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	AA	9	95
12	AB	0	3
14	AD	0	1
30	AW	0	1
33	AZ	0	1
35	BA	4	40
56	BV	0	1
56	BW	0	3

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BY	12	G	C2-N2	-13.61	1.21	1.34
11	AA	761	A	C5-C6	-11.47	1.30	1.41
58	BY	40	C	OP3-P	-6.93	1.52	1.61
58	BY	1	G	OP3-P	-6.81	1.52	1.61
11	AA	761	A	C6-N6	-6.64	1.28	1.33

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

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

5 of 13 chirality outliers are listed below:

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

5 of 148 planarity outliers are listed below:

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

5.2 Too-close contacts (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	A0	662	0	688	113	0
2	A1	732	0	808	72	0
3	A2	598	0	653	74	0
4	A3	468	0	523	35	0
5	A4	341	0	339	67	0
6	A5	459	0	480	71	0
7	A6	433	0	461	148	0
8	A7	419	0	467	30	0
9	A8	508	0	576	97	0
10	A9	307	0	335	40	0
11	AA	62479	0	31495	2217	0
12	AB	2551	0	1295	109	0
13	AC	1742	0	1794	315	0
14	AD	2145	0	2234	279	0
15	AE	1564	0	1629	224	0
16	AF	1624	0	1677	194	0
17	AG	1474	0	1535	276	0
18	AH	1223	0	1282	159	0
19	AJ	654	0	142	11	0
20	AK	701	0	163	25	0
21	AN	1105	0	1180	160	0
22	AO	933	0	996	95	0
23	AP	1114	0	1187	270	0
24	AQ	1122	0	1179	154	0
25	AR	960	0	1021	136	0
26	AS	771	0	832	122	0
27	AT	1142	0	1202	267	0
28	AU	958	0	1015	128	0
29	AV	779	0	852	147	0
30	AW	896	0	953	83	0
31	AX	726	0	778	77	0
32	AY	776	0	870	193	0
33	AZ	1460	0	1488	183	0
34	B2	1184	0	1235	205	0
35	BA	32330	0	16318	1298	0
36	BB	1901	0	1951	255	0
37	BC	1613	0	1677	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	1703	0	1764	264	0
39	BE	1147	0	1207	135	0
40	BF	843	0	857	69	0
41	BG	1257	0	1296	103	0
42	BH	1116	0	1177	77	0
43	BI	1011	0	1043	155	0
44	BJ	795	0	840	176	0
45	BK	885	0	904	83	0
46	BL	971	0	1057	105	0
47	BM	988	0	1059	186	0
48	BN	492	0	529	90	0
49	BO	734	0	771	61	0
50	BP	701	0	720	70	0
51	BQ	824	0	891	54	0
52	BR	574	0	644	62	0
53	BS	630	0	652	103	0
54	BT	763	0	861	83	0
55	BU	209	0	221	14	0
56	BV	1640	0	837	44	0
56	BW	1640	0	837	161	0
57	BX	104	0	55	4	0
58	BY	1306	0	663	88	0
59	BZ	2929	0	2941	341	0
60	A9	1	0	0	0	0
60	BD	1	0	0	0	0
60	BN	1	0	0	0	0
61	AA	1	0	0	0	0
61	BZ	1	0	0	0	0
62	BZ	57	0	58	7	0
63	BZ	28	0	12	2	0
All	All	154206	0	105206	9942	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 9942 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BD:20:TYR:HA	38:BD:26:CYS:SG	1.82	1.19
14:AD:44:ASN:HB3	14:AD:49:ILE:HA	1.21	1.18
1:A0:40:GLN:HE22	1:A0:43:THR:HA	1.02	1.17

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
55	BU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1 5
59	BZ	374/405 (92%)	295 (79%)	58 (16%)	21 (6%)	2 13
All	All	6294/6697 (94%)	4435 (70%)	1170 (19%)	689 (11%)	0 3

5 of 689 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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
1	A0	66/67 (98%)	57 (86%)	9 (14%)	5 19
2	A1	78/83 (94%)	63 (81%)	15 (19%)	2 8
3	A2	66/67 (98%)	57 (86%)	9 (14%)	5 19
4	A3	51/52 (98%)	46 (90%)	5 (10%)	10 36
5	A4	39/63 (62%)	30 (77%)	9 (23%)	1 4
6	A5	51/52 (98%)	41 (80%)	10 (20%)	1 7
7	A6	49/52 (94%)	34 (69%)	15 (31%)	0 1
8	A7	41/42 (98%)	35 (85%)	6 (15%)	4 16
9	A8	53/55 (96%)	42 (79%)	11 (21%)	1 6
10	A9	34/34 (100%)	26 (76%)	8 (24%)	1 4
13	AC	180/181 (99%)	164 (91%)	16 (9%)	12 42
14	AD	217/218 (100%)	183 (84%)	34 (16%)	3 13
15	AE	165/166 (99%)	138 (84%)	27 (16%)	3 12
16	AF	165/166 (99%)	150 (91%)	15 (9%)	12 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	AG	155/156 (99%)	135 (87%)	20 (13%)	5 21
18	AH	132/148 (89%)	116 (88%)	16 (12%)	6 24
21	AN	117/119 (98%)	101 (86%)	16 (14%)	4 19
22	AO	100/100 (100%)	88 (88%)	12 (12%)	6 24
23	AP	112/116 (97%)	89 (80%)	23 (20%)	1 6
24	AQ	111/111 (100%)	90 (81%)	21 (19%)	2 8
25	AR	100/101 (99%)	85 (85%)	15 (15%)	3 15
26	AS	77/88 (88%)	67 (87%)	10 (13%)	5 21
27	AT	120/127 (94%)	91 (76%)	29 (24%)	1 3
28	AU	92/94 (98%)	82 (89%)	10 (11%)	8 30
29	AV	82/82 (100%)	72 (88%)	10 (12%)	6 24
30	AW	91/92 (99%)	77 (85%)	14 (15%)	3 14
31	AX	74/78 (95%)	67 (90%)	7 (10%)	11 38
32	AY	84/91 (92%)	69 (82%)	15 (18%)	2 10
33	AZ	161/179 (90%)	132 (82%)	29 (18%)	2 10
34	B2	120/120 (100%)	81 (68%)	39 (32%)	0 0
36	BB	202/220 (92%)	172 (85%)	30 (15%)	4 15
37	BC	160/188 (85%)	149 (93%)	11 (7%)	19 55
38	BD	180/181 (99%)	152 (84%)	28 (16%)	3 14
39	BE	115/123 (94%)	99 (86%)	16 (14%)	4 19
40	BF	90/90 (100%)	76 (84%)	14 (16%)	3 14
41	BG	126/127 (99%)	115 (91%)	11 (9%)	13 44
42	BH	119/119 (100%)	108 (91%)	11 (9%)	11 40
43	BI	98/99 (99%)	87 (89%)	11 (11%)	7 29
44	BJ	88/92 (96%)	74 (84%)	14 (16%)	3 13
45	BK	90/99 (91%)	84 (93%)	6 (7%)	20 56
46	BL	104/111 (94%)	91 (88%)	13 (12%)	6 22
47	BM	99/101 (98%)	84 (85%)	15 (15%)	3 14
48	BN	49/50 (98%)	41 (84%)	8 (16%)	3 12
49	BO	79/80 (99%)	72 (91%)	7 (9%)	12 42
50	BP	72/74 (97%)	64 (89%)	8 (11%)	8 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	BQ	94/97 (97%)	89 (95%)	5 (5%)	28 64
52	BR	61/77 (79%)	56 (92%)	5 (8%)	14 47
53	BS	69/80 (86%)	57 (83%)	12 (17%)	2 11
54	BT	76/82 (93%)	68 (90%)	8 (10%)	8 31
55	BU	19/22 (86%)	16 (84%)	3 (16%)	3 13
59	BZ	316/338 (94%)	275 (87%)	41 (13%)	5 21
All	All	5289/5550 (95%)	4537 (86%)	752 (14%)	4 18

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

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

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

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

5.3.3 RNA (i)

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

5 of 857 RNA backbone outliers are listed below:

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

5 of 140 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	AB	16	G
35	BA	266	G
58	BY	11	C
12	AB	42	C
35	BA	109	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	KIR	BZ	1002	-	55,59,59	3.65	22 (40%)	53,84,84	1.83	15 (28%)
63	GDP	BZ	1003	61	23,30,30	1.37	3 (13%)	30,47,47	1.76	7 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	KIR	BZ	1002	-	-	0/54/98/98	0/3/3/3
63	GDP	BZ	1003	61	-	0/12/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	1002	KIR	O18-C17	-13.45	1.24	1.44
62	BZ	1002	KIR	O30-C30	-12.40	1.16	1.42
62	BZ	1002	KIR	O34-C33	-11.38	1.28	1.44
62	BZ	1002	KIR	O4-C4	-3.27	1.29	1.36
62	BZ	1002	KIR	C3-C7	2.13	1.54	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	BZ	1002	KIR	O29-C29-O34	-5.77	100.64	110.18
63	BZ	1003	GDP	N3-C2-N1	-4.78	120.16	127.44
63	BZ	1003	GDP	C5-C6-N1	-3.68	118.56	123.59
63	BZ	1003	GDP	PA-O3A-PB	-3.67	120.37	132.67
62	BZ	1002	KIR	O7-C7-C3	-2.93	112.68	120.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	A0	84/85 (98%)	0.52	9 (10%) 8 3	25, 44, 110, 136	0
2	A1	94/98 (95%)	0.22	2 (2%) 67 44	23, 43, 88, 95	0
3	A2	71/72 (98%)	0.16	2 (2%) 56 32	34, 61, 88, 98	0
4	A3	60/60 (100%)	0.04	1 (1%) 73 52	21, 36, 55, 87	0
5	A4	45/71 (63%)	0.71	7 (15%) 3 1	98, 118, 132, 138	0
6	A5	59/60 (98%)	0.43	7 (11%) 6 2	14, 39, 121, 137	0
7	A6	50/54 (92%)	0.73	7 (14%) 4 2	31, 61, 79, 82	0
8	A7	49/49 (100%)	-0.20	1 (2%) 68 46	14, 24, 77, 93	0
9	A8	64/65 (98%)	-0.03	1 (1%) 74 55	21, 40, 55, 83	0
10	A9	37/37 (100%)	0.37	1 (2%) 58 34	33, 49, 68, 72	0
11	AA	2901/2915 (99%)	0.14	176 (6%) 25 10	8, 36, 159, 189	0
12	AB	119/122 (97%)	0.03	0 100 100	26, 77, 104, 137	0
13	AC	228/229 (99%)	5.11	196 (85%) 0 0	131, 151, 164, 168	0
14	AD	275/276 (99%)	-0.36	4 (1%) 76 58	8, 27, 53, 87	0
15	AE	205/206 (99%)	-0.07	7 (3%) 49 24	10, 29, 75, 88	0
16	AF	208/210 (99%)	-0.09	5 (2%) 62 39	11, 49, 116, 129	0
17	AG	181/182 (99%)	0.58	19 (10%) 8 3	55, 86, 112, 132	0
18	AH	160/180 (88%)	0.65	14 (8%) 12 4	39, 83, 124, 134	0
19	AJ	0/130	-	-	-	-
20	AK	0/140	-	-	-	-
21	AN	139/140 (99%)	-0.17	3 (2%) 65 42	17, 37, 86, 94	0
22	AO	122/122 (100%)	-0.30	3 (2%) 61 37	15, 31, 49, 66	0
23	AP	146/150 (97%)	0.52	8 (5%) 29 12	18, 60, 93, 119	0
24	AQ	141/141 (100%)	-0.21	2 (1%) 78 60	22, 32, 57, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	AR	117/118 (99%)	-0.32	0 100 100	19, 31, 54, 67	0
26	AS	99/112 (88%)	0.55	4 (4%) 42 20	53, 76, 107, 109	0
27	AT	138/146 (94%)	0.13	8 (5%) 26 11	15, 48, 124, 143	0
28	AU	117/118 (99%)	-0.24	2 (1%) 73 52	15, 30, 57, 97	0
29	AV	101/101 (100%)	0.28	4 (3%) 42 20	9, 56, 76, 82	0
30	AW	113/113 (100%)	-0.27	2 (1%) 71 50	12, 29, 61, 106	0
31	AX	93/96 (96%)	-0.28	0 100 100	22, 41, 61, 75	0
32	AY	101/110 (91%)	0.81	13 (12%) 5 2	25, 56, 108, 128	0
33	AZ	184/206 (89%)	0.26	9 (4%) 33 14	28, 63, 98, 115	0
34	B2	144/144 (100%)	0.96	23 (15%) 3 1	49, 78, 118, 124	0
35	BA	1504/1522 (98%)	0.05	51 (3%) 49 24	14, 52, 128, 187	0
36	BB	235/256 (91%)	0.11	10 (4%) 39 18	27, 51, 114, 128	0
37	BC	207/239 (86%)	-0.05	0 100 100	36, 59, 86, 96	0
38	BD	208/209 (99%)	0.57	14 (6%) 21 7	47, 74, 111, 116	0
39	BE	151/162 (93%)	-0.32	1 (0%) 89 78	23, 40, 70, 92	0
40	BF	101/101 (100%)	-0.19	2 (1%) 68 46	33, 56, 71, 95	0
41	BG	155/156 (99%)	0.28	13 (8%) 14 4	52, 75, 107, 129	0
42	BH	138/138 (100%)	-0.34	0 100 100	17, 36, 54, 67	0
43	BI	127/128 (99%)	0.52	8 (6%) 23 9	46, 82, 107, 111	0
44	BJ	99/105 (94%)	0.92	17 (17%) 2 1	42, 82, 119, 122	0
45	BK	119/129 (92%)	0.25	8 (6%) 21 7	26, 56, 90, 107	0
46	BL	125/135 (92%)	0.05	4 (3%) 51 27	24, 50, 69, 112	0
47	BM	125/126 (99%)	0.57	10 (8%) 15 5	42, 80, 107, 139	0
48	BN	60/61 (98%)	0.09	2 (3%) 50 26	38, 48, 70, 77	0
49	BO	88/89 (98%)	-0.14	0 100 100	22, 41, 64, 69	0
50	BP	84/88 (95%)	0.23	1 (1%) 81 64	39, 58, 77, 102	0
51	BQ	100/105 (95%)	-0.25	0 100 100	27, 47, 68, 73	0
52	BR	70/88 (79%)	0.19	1 (1%) 78 60	28, 46, 71, 79	0
53	BS	79/93 (84%)	0.56	10 (12%) 5 2	55, 73, 101, 111	0
54	BT	99/106 (93%)	0.36	4 (4%) 42 20	46, 65, 101, 104	0
55	BU	25/27 (92%)	0.64	1 (4%) 42 20	52, 65, 83, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	BV	77/77 (100%)	0.05	2 (2%) 59 35	36, 57, 97, 104	0
56	BW	77/77 (100%)	5.54	67 (87%) 0 0	95, 192, 197, 199	0
57	BX	5/19 (26%)	0.81	1 (20%) 1 0	34, 36, 69, 80	0
58	BY	62/90 (68%)	0.16	1 (1%) 74 55	55, 85, 125, 136	0
59	BZ	378/405 (93%)	-0.01	9 (2%) 62 39	23, 56, 92, 124	0
All	All	11143/11789 (94%)	0.27	777 (6%) 19 7	8, 50, 137, 199	0

The worst 5 of 777 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AC	111	ASP	20.4
13	AC	73	ARG	19.2
13	AC	173	ALA	19.0
11	AA	2182	G	18.8
13	AC	172	HIS	17.9

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
62	KIR	BZ	1002	57/57	0.89	0.36	1.25	101,117,134,134	0
63	GDP	BZ	1003	28/28	0.97	0.14	-0.62	36,43,44,45	0
60	ZN	BN	1001	1/1	0.98	0.13	-1.09	51,51,51,51	0
60	ZN	A9	1001	1/1	0.99	0.07	-1.75	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
60	ZN	BD	1001	1/1	0.98	0.19	-2.01	59,59,59,59	0
61	MG	BZ	1001	1/1	0.97	0.14	-	25,25,25,25	0
61	MG	AA	3001	1/1	0.99	0.22	-	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.