



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:04 PM BST

PDB ID : 4V5S
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a cognate codon on the 70S ribosome.
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2010-12-07
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

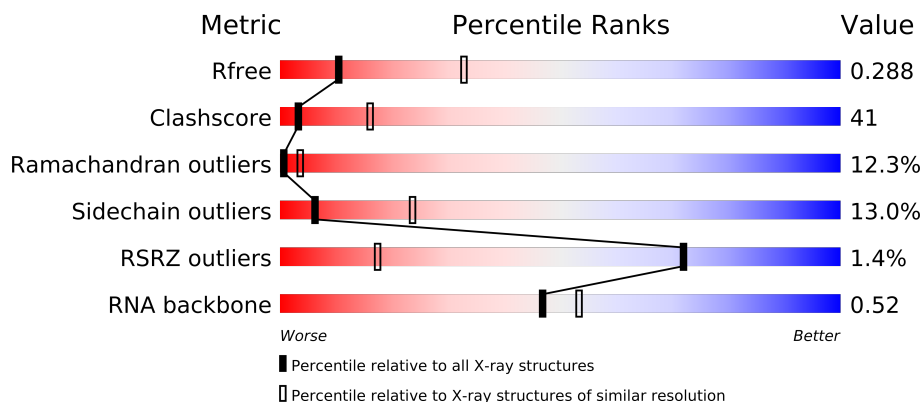
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	405	
25	CZ	405	
26	B0	85	
26	D0	85	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307196 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	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			
8	CH	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
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	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			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	16			
23	CX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	16			

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

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

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			
25	CZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
27	D1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
29	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			
30	D4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
33	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
34	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

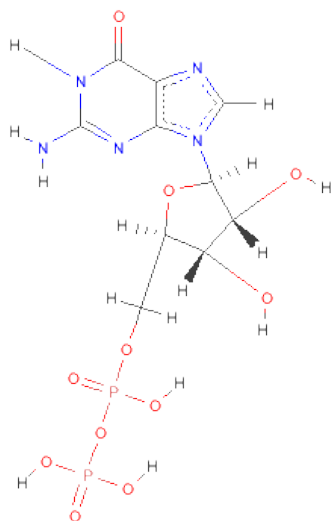
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			
58	DZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

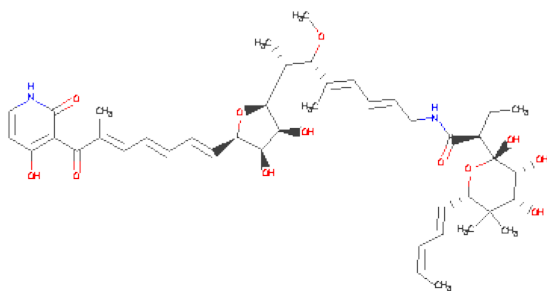
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
60	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).

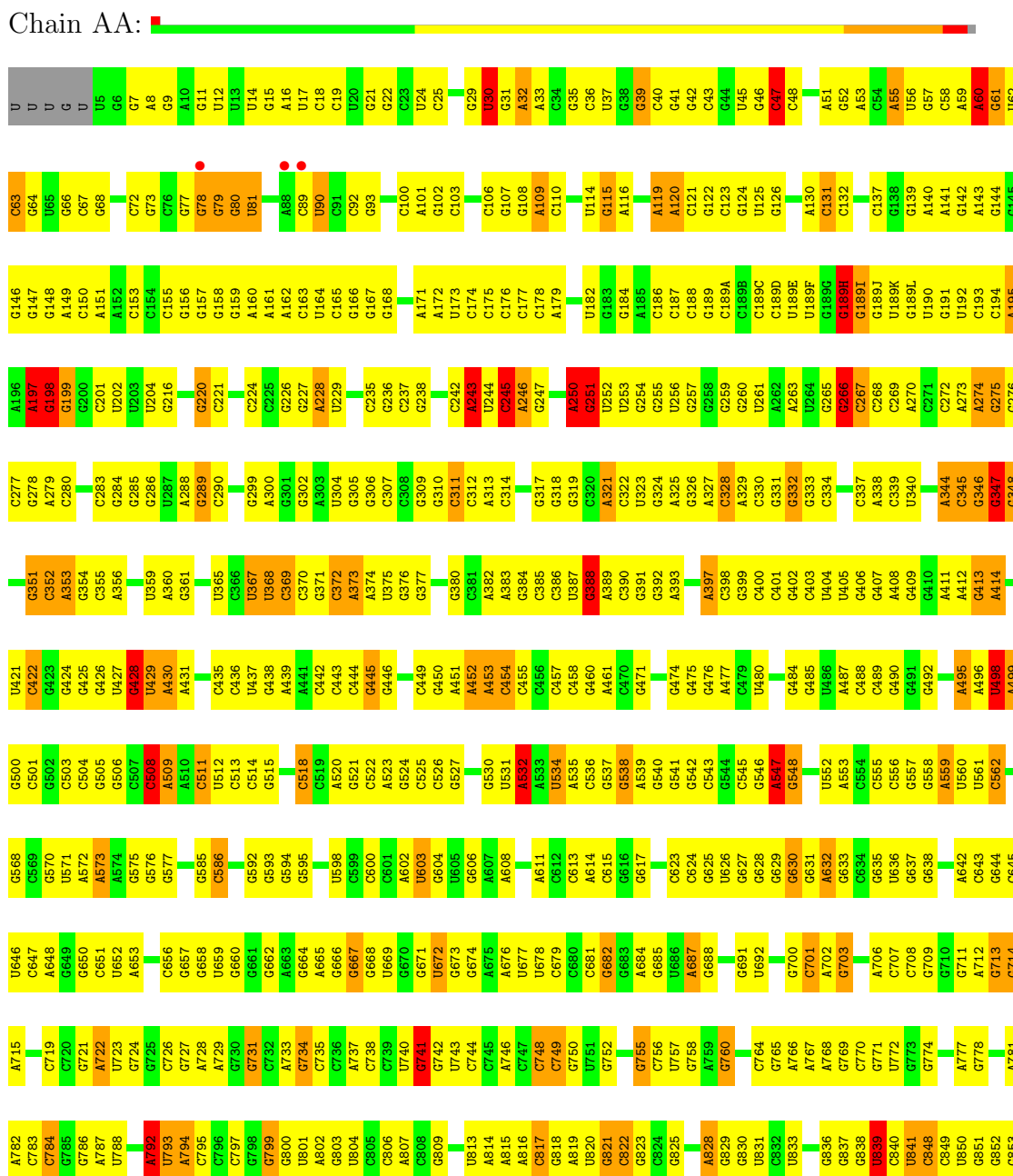


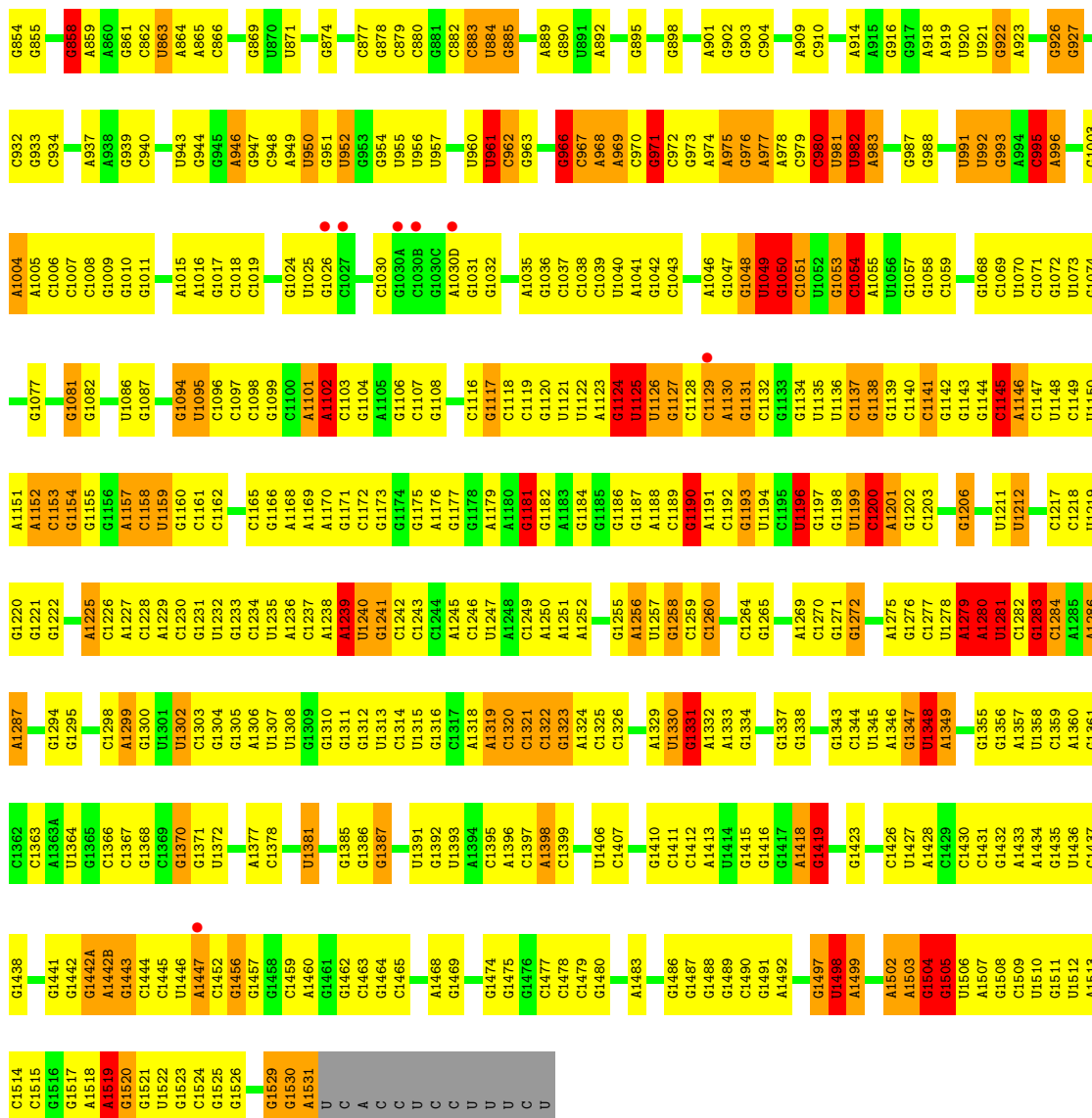
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
61	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

3 Residue-property plots

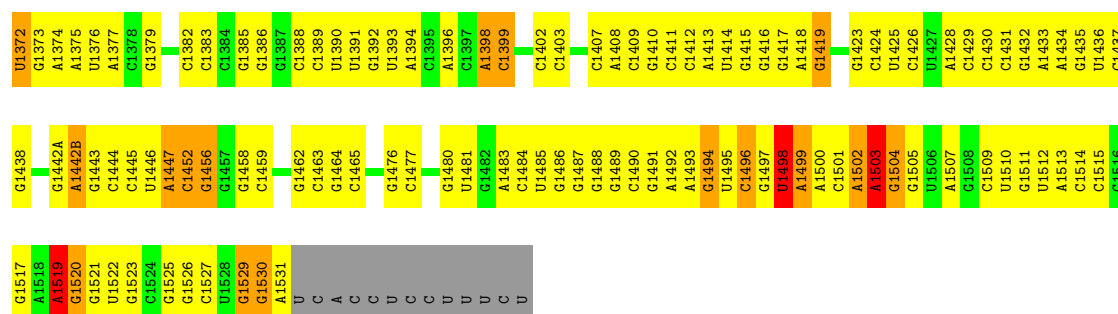
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S RRNA



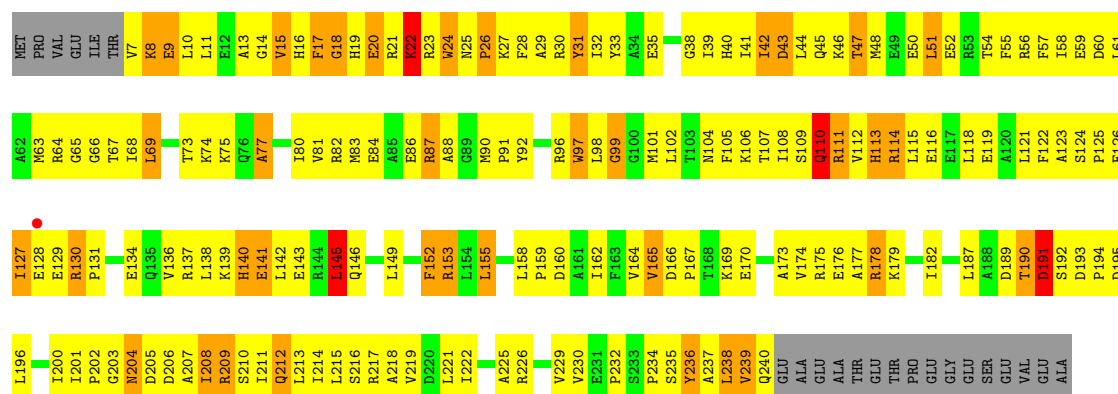


G1312	C1249	G1184	G1120	C1054	A886	A923	U841	A777	C708	G638	G566	G492	C418	G351	G285
U1313	A1250	G1185	A1123	A1055	G987	C924	C848	G778	G711	C644	G666	G493	C419	C352	A288
C1314	A1251	G1186	G1187	U1056	G988	G925	C849	G779	A712	G643	G568	U494	U420	A353	G289
U1315	A1252	G1187	G1124	G1057	G989	G926		A780	G713	G645	G576	A495	U421	C355	C290
G1316	G1255	A1188	U1125	G1058	C990	G927	G853	A781	G714	U646	A572	U488	G423	C356	C291
C1317	A1256	C1189	U1126	G1059	U991	G928	G854	A782	G715	C647	A573	A499	G424	G357	G292
A1318	U1257	G1190	G1127	C1060	U992	G929		C783	A716		A574	G500	G425	U358	G293
A1319	U1258		G1128	U1061	U993	C930	G858	G784	C717	G650	G575	C501	G426	U359	U294
C1320	C1259	G1193	C1129	U1062	G993		A859	G785	G718	G651	G576	G502	A427	A360	C295
C1321	U1196		A1130	G995	A994	C934	G860	A786	C719	U652	G577	C503	G428	G361	U296
C1322	G1197	U1198	G1132	U1065	A996	A935	C862	U788	G720	A653	G585	G504	U429		G297
G1323	G1198	G1183	G1133	A1067	U997	C936	U863	U789	G721	G654	G586	G505	A430	U365	A298
A1324	U1199	G1134	G1134	G1068	U997	A937	A864	A790	A722	A655	C586	G506	U431	C366	G299
C1325	G1264	U1199	U1135	C1069	G1002	A938	A865	G791	U723	G656		C507	U434	U367	A300
C1326	G1265	A1200	U1136	U1070	G1003	A939	C966	A792	G724	G657	C592	C508	U435	U368	G301
C1327	G1266	A1201	C1137	C1071	A1004	C940		U793	G725	G658	C593	A509	C436	C369	G302
C1328	A1267	G1202	G1138	G1072	A1005	C941	G869	A794	G726	U659	C594	A510	C437	C370	A303
A1329	C1268	C1203	U1073	U1073	C1006	G942	U870	C795	G727	G660	C595	C511	U437	G371	U304
U1330	A1269	A1204			C1007	U943		C796		G661	C596		G438	C372	G305
G1331	C1270	U1205	C1140	G1077	C1008	G944	G874	C797	G731	G662	C597	C518	G439	A373	G309
A1332	G1271	G1206	C1141	U1078	G1009	G945			C732	A663	C598	C519	A441	A374	G310
A1333	G1272	G1207	G1142	U1079	G1010	A946	C877	U801	A733	G664	C599	A520	C442	U375	G311
G1334	G1273	C1208	G1143	A1080	G1011	A947	G878		G734	A665	C600	G521	C443	G376	C312
C1335	G1274		G1144	A1081		C948	C879	U804	G735	G666		G522	C444	G377	C313
C1336	A1275	U1211	C1145	G1077	A1014	A949			C736	G667	U603	A523	G445	G378	A313
G1337	G1276	U1212	A1146	U1086	A1015	U950	C882	A807	A737	G673	G604	G524	G446	C379	G314
G1338	U1277	G1215	U1148	U1087	A1016	G951	C883	C808	C738	G674	U605	C525	G447	G380	A315
A1339	U1278	G1216	G1149	G1088	G1017	U952	U884	G809			G606	C526	A448	C381	
C1342	A1280	C1217	U1150	G1089	C1018	G953	G885	C810	U740		A607	G527	A449	C392	G319
G1343	U1281	C1218	A1151	U1090	C1019	G954	G886	C811	G741	U677	A608		G450	A392	C320
C1344	C1282	U1219	A1152	U1091		U955	G887	C812		U678	A609	G530	A451	C383	A321
U1345	G1283	G1220	A1153	A1092	G1024	U956	G888	U813	C744	C679	G610	U531	A452	C385	C322
A1346	C1284	G1221	G1094	A1093	U1025	U957	G889	A814	A745	C680	C611	A532	A453	C386	U323
G1347	A1285	G1222	U1095	A1094	G1026	A958	G890	A815	A746	C681	C612	U534	A454	U387	G324
U1348	A1286		U1157	U1096	G1030	A959	A892	A816	C747	G682	C613	A535	C455	G388	A325
A1349	A1287	A1225	U1158	C1096	G1030A	U960	A893	C817	G748	G683	A614	A536	C456	A399	A326
A1350	C1226	C1226	U1159	C1097		U961	C993	G818	C749	A684	C615	A537	C457	C390	A327
U1351	A1227	C1228	G1160	C1098	G1030B	C962		A819	U751	G685	G616	G537	C458	G391	C328
G1353	U1292	C1229	C1161	G1099	A1030D	G963	A900	U820		U686	C617	G538	G460	A393	C330
C1354	G1293	C1230	C1162	C1100	G1031	A964	A901	G821	C754	A687	C618	A539	G471	G394	G331
G1355	G1294	G1231	C1165	A1102	G1032	A965	G902	G822	G755	C689	C620	G541	A472		G332
G1356	C1295	U1292	G1166	C1103	G1033	C966	G906	G823	G756	C690	G621	G542	G473	A397	G333
A1357	C1296	G1233	A1168	G1104	A1035	A968	A907	C824	C757	G691	A622	C543	G474	C398	C334
U1358	C1297	U1234	A1169	A1105	G1036	A969	A908	G825	U757	U692	C623	G544	G475		
C1359	C1298	U1235	A1170	G1106	C1037	C970	A909	C826	A759	G693	C624	G545	G476		
A1360	A1299	A1236	G1171	C1107	C1038	G971	C910	U827	G760	A694	G625	A547	U480	U403	C337
G1361	G1300	C1237	C1172	G1108	C1039	C972	U911	A828		A695	G626	A548	U481	U404	C338
C1362	U1301	U1238	G1173	C1109	U1040	G973	C912	G829	G763	A696	G627	G549	G482	U405	C339
C1363	U1302	A1239	G1174	A1110	A1041	A974	A913	G830		A697	G628		G483	G406	U340
A1363A	A1303	U1240	G1175	A1111		A975	A914	U831	C764	G698	G629		A482	A408	C341
U1364	G1304	G1241	A1176	C1112	A1046	G976	A915	C832	G765	C699	G630	C555	G484	G409	U342
G1365	G1305	C1242	G1177	C1113	G1047	A977	G916	U833	A766	G700	G631	C556	G485	A410	U343
C1366	G1306	C1243	G1178	C1114	U1048	A978	G917	C834	A767	C701	A632	G557	U486	A411	A344
C1367	U1307	C1244	A1179	C1115	U1049	C979	A918	U835	G770	A702	G633	G558	U487	A412	G345
G1368	U1308	A1245	A1180	C1116	G1050	C880	A919	G837	G771	G703	C634	A559	C488	C413	G346
C1369	G1309	C1246	G1181	C1117	U1051	U981	U920	G838	G774	A706	U636	U560	C489	A414	G347
G1370	G1310	U1247	U1182	U1052	U1052	U982	U921	U839			U636	U561	G490	A349	G348
G1371	G1311	A1248	A1193	C1119	G1053	A983	G922	C840			G637	C562	G491	A415	G350



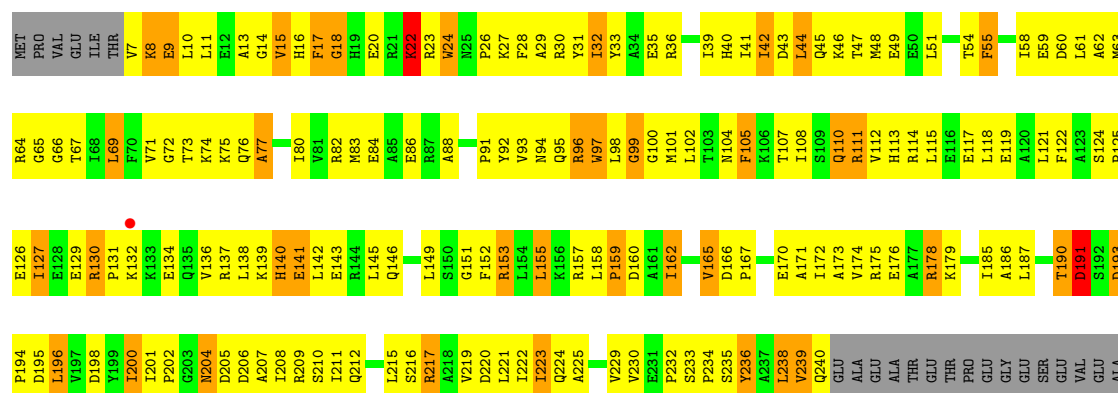
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



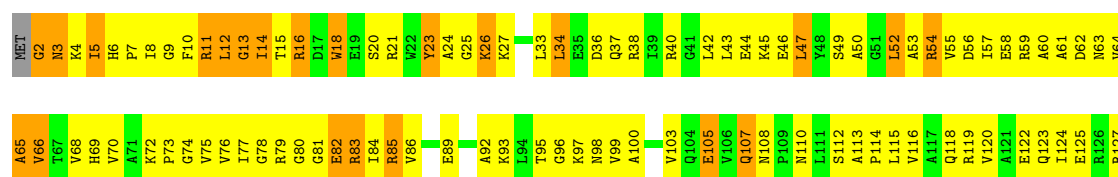
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

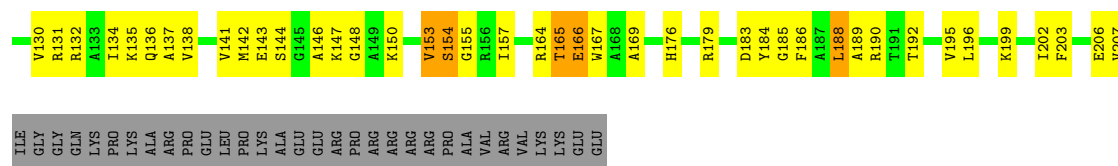
Chain CB:



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

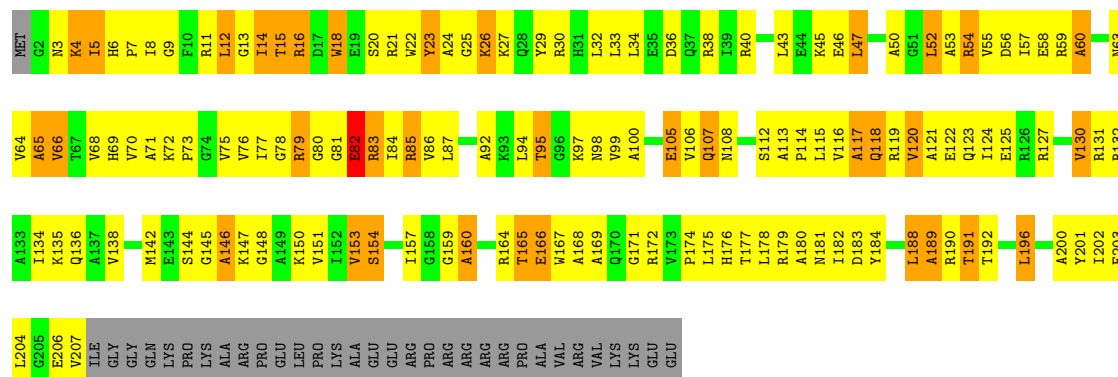
Chain AC:





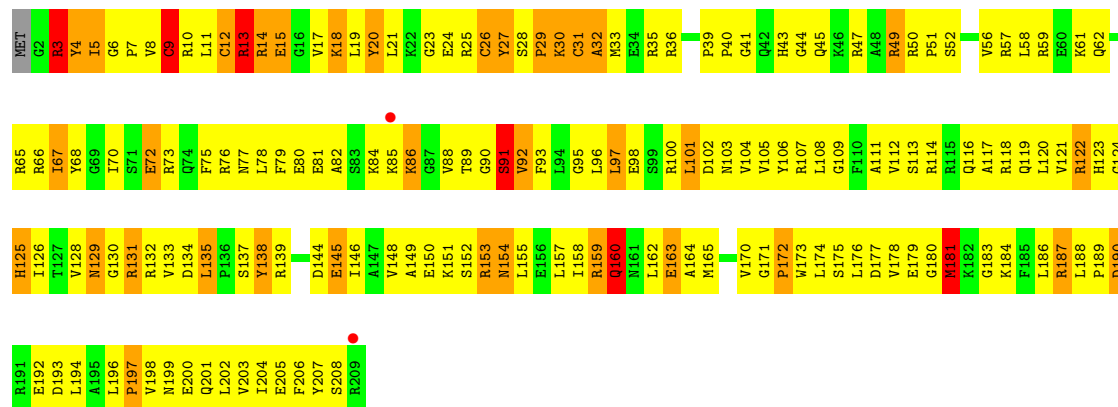
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



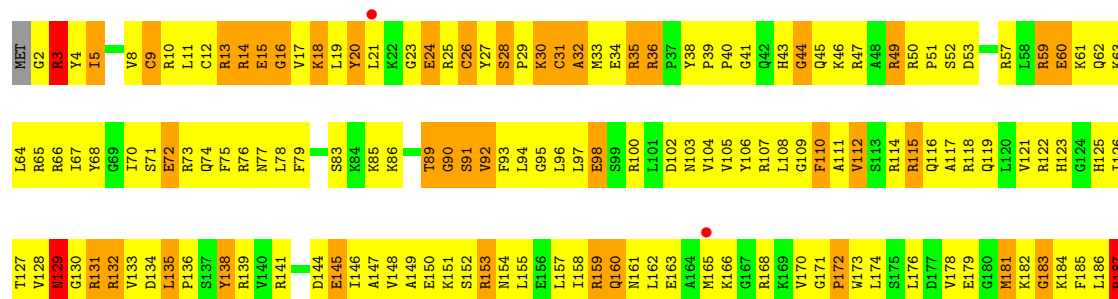
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

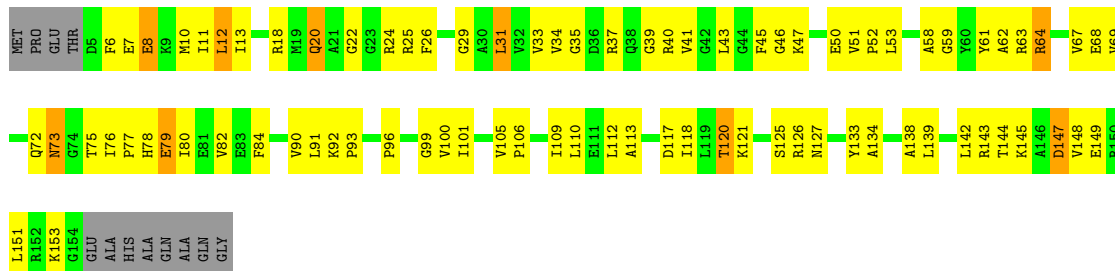
Chain CD:





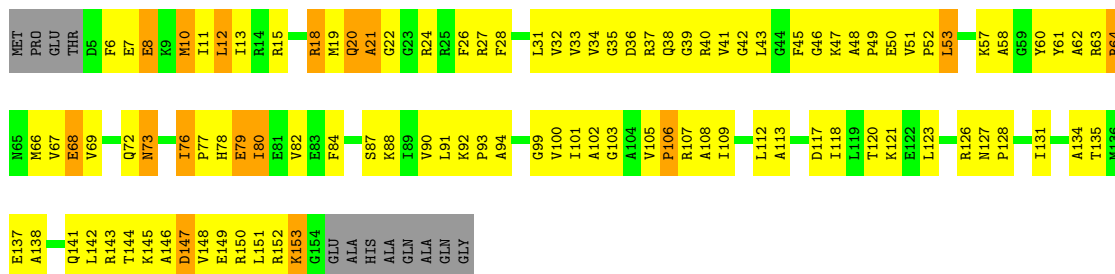
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



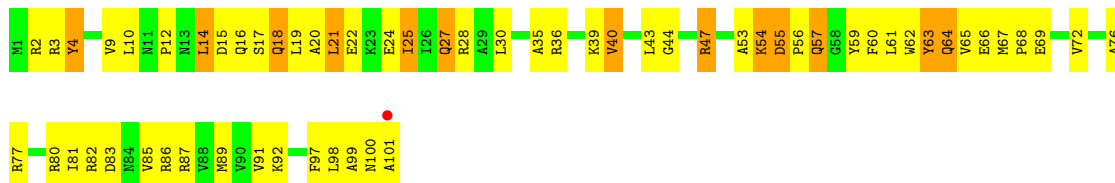
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



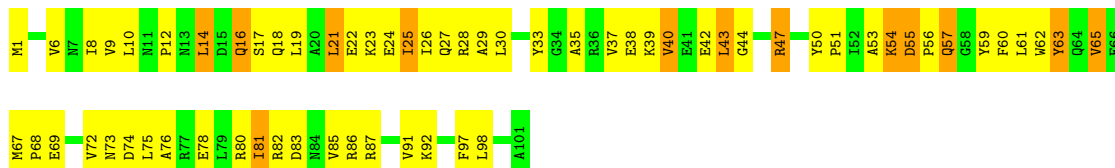
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

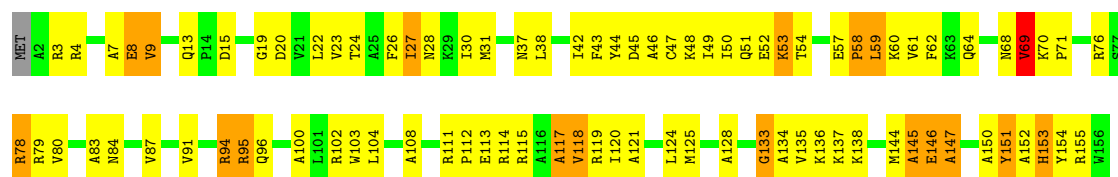
Chain CF:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:





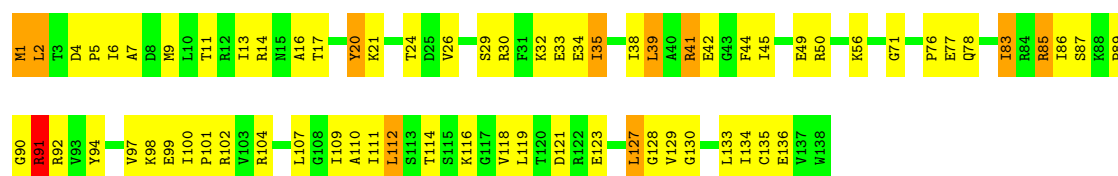
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



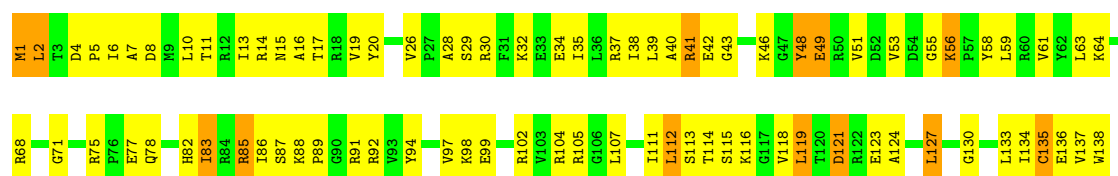
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



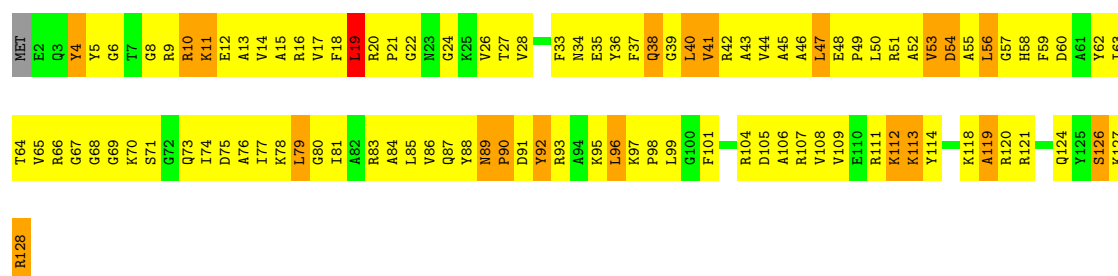
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



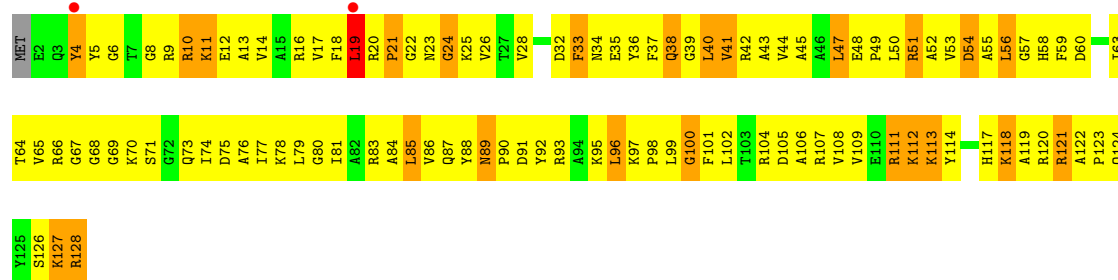
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



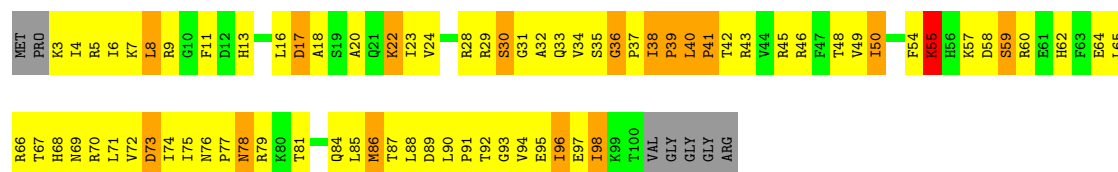
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



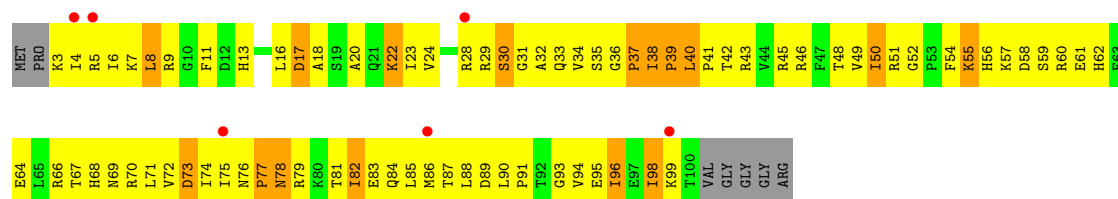
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



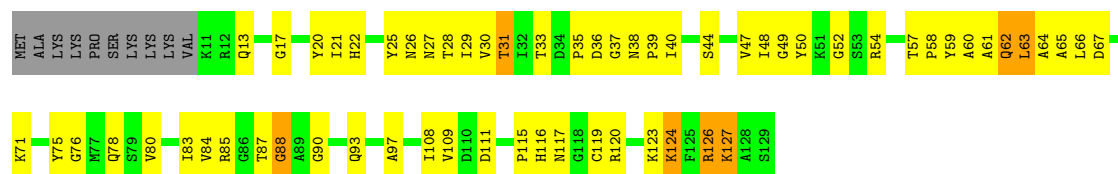
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



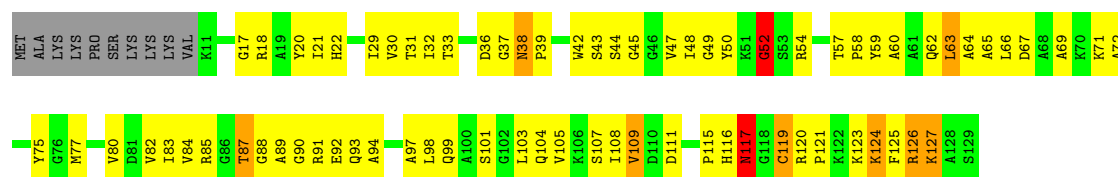
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



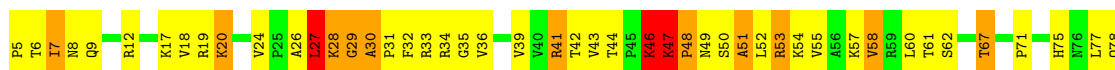
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



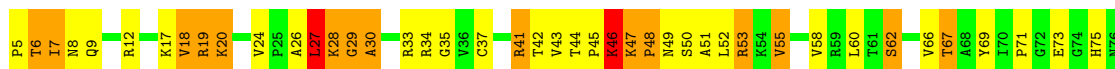
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



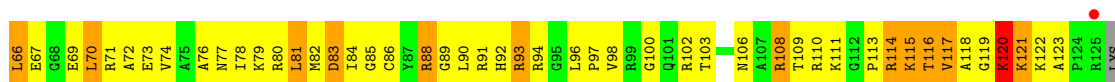
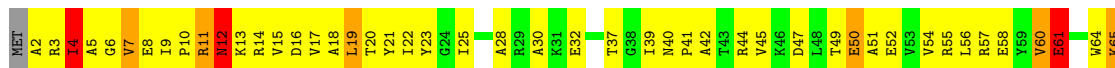
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



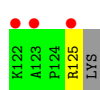
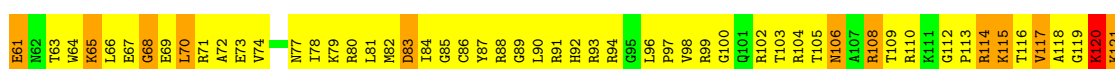
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



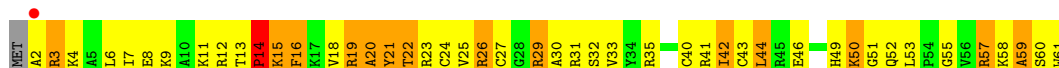
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

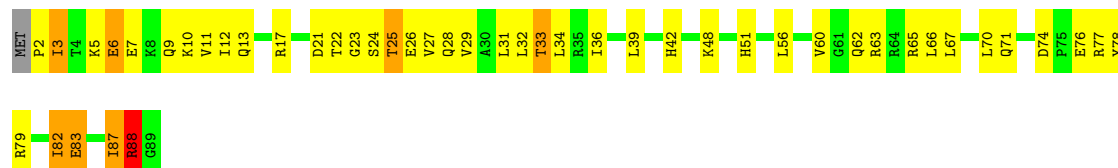
Chain CN:



W61

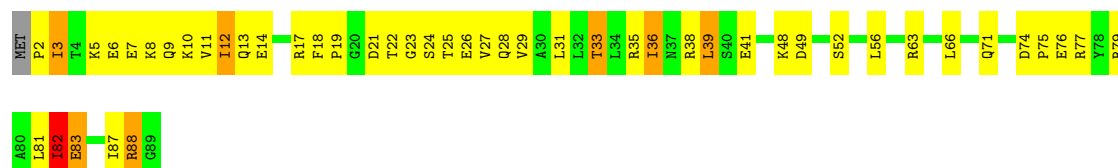
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



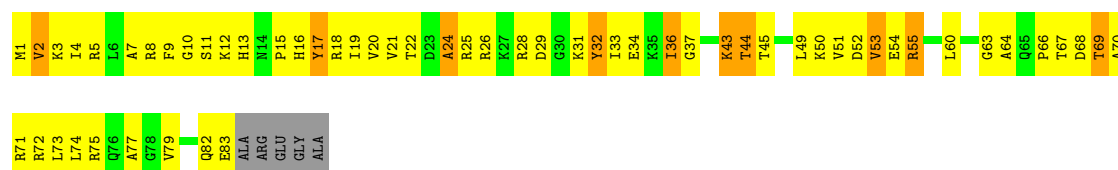
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



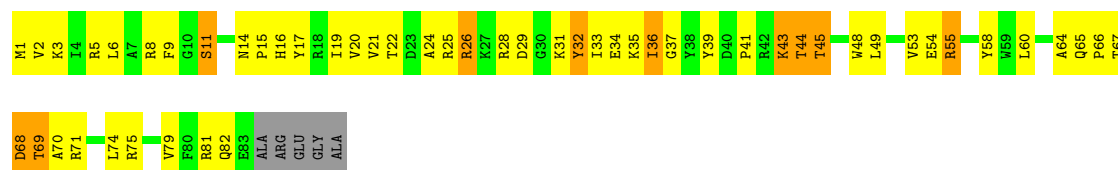
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



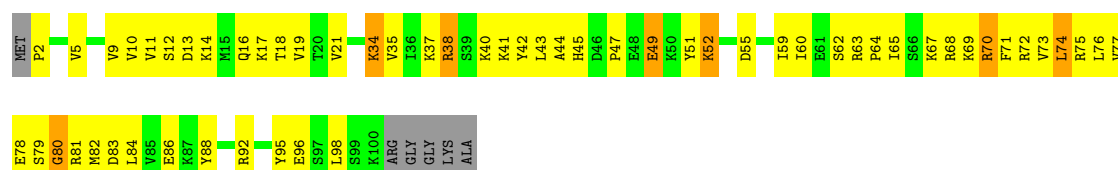
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

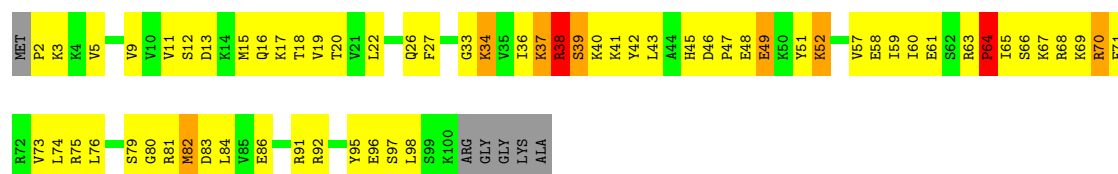
Chain AQ:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

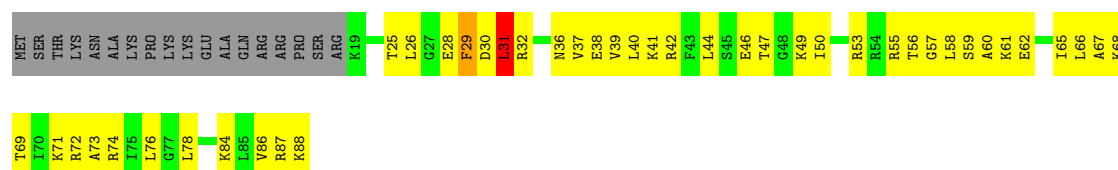
Chain CQ:





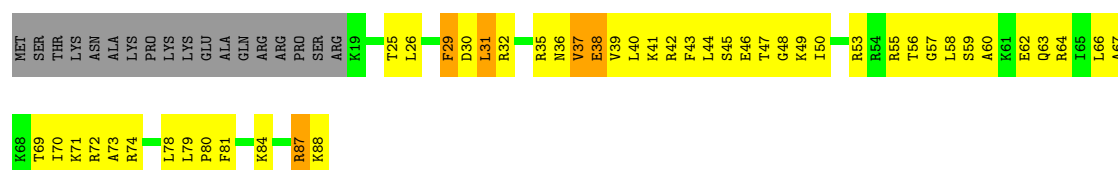
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



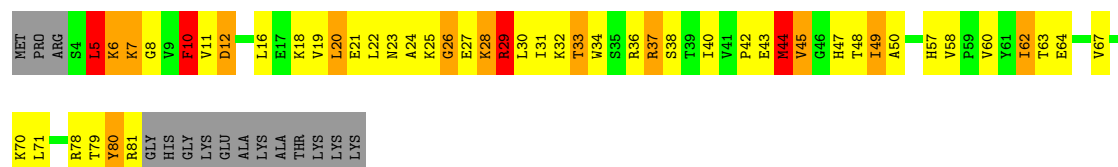
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



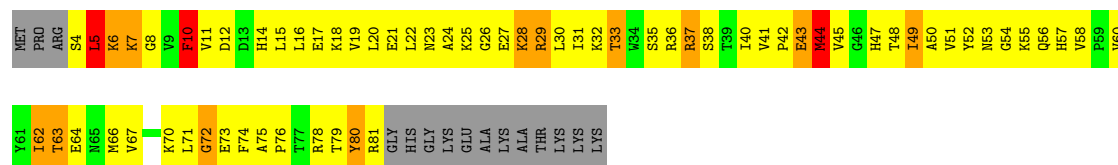
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



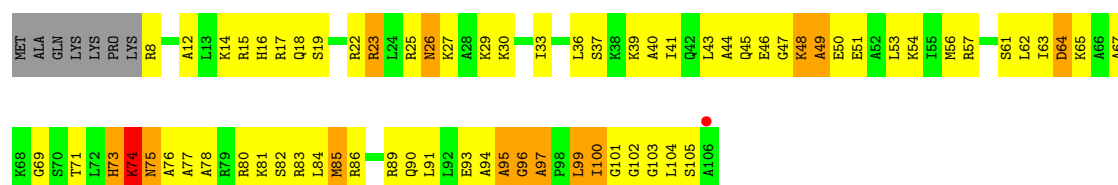
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



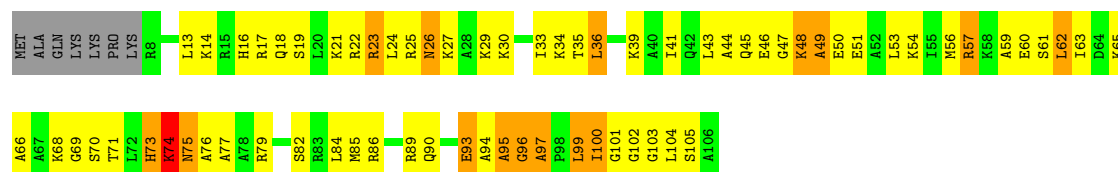
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



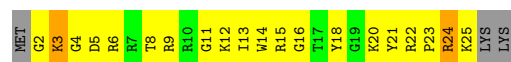
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT: 



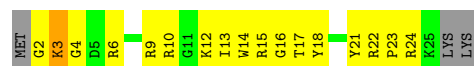
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU: 



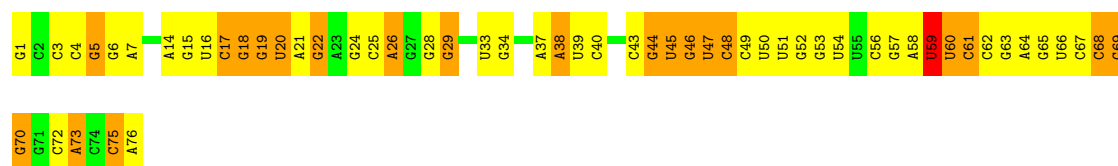
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU: 



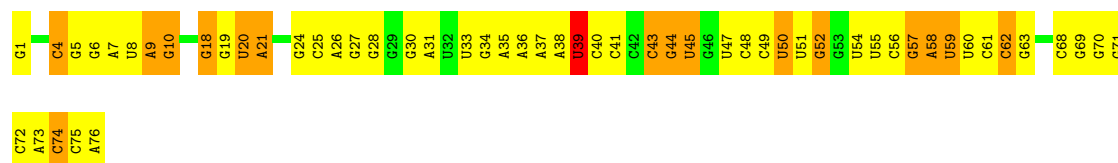
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV: 



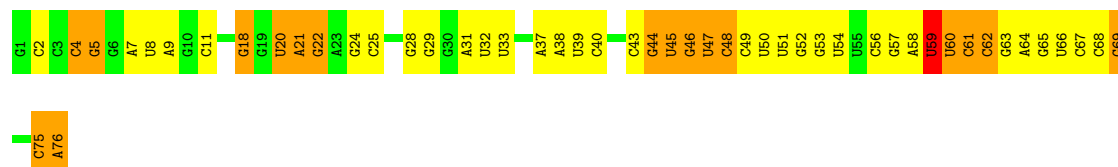
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AW: 



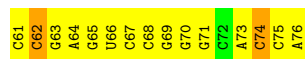
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CV: 

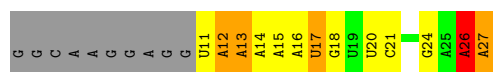


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CW: 



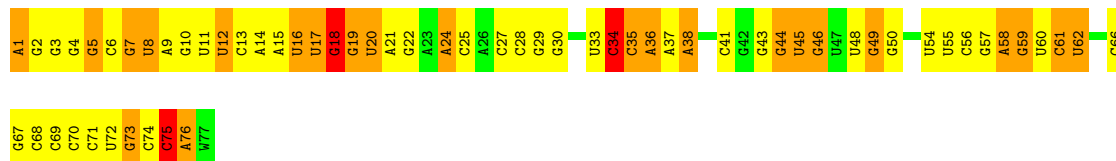
Chain AX:



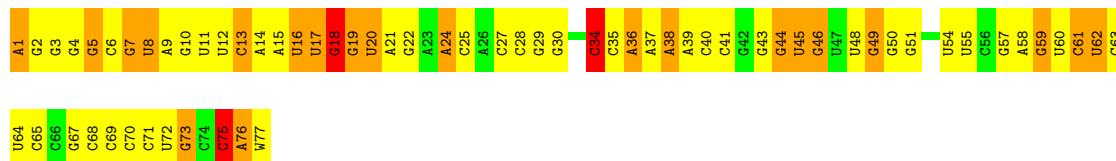
Chain CX:



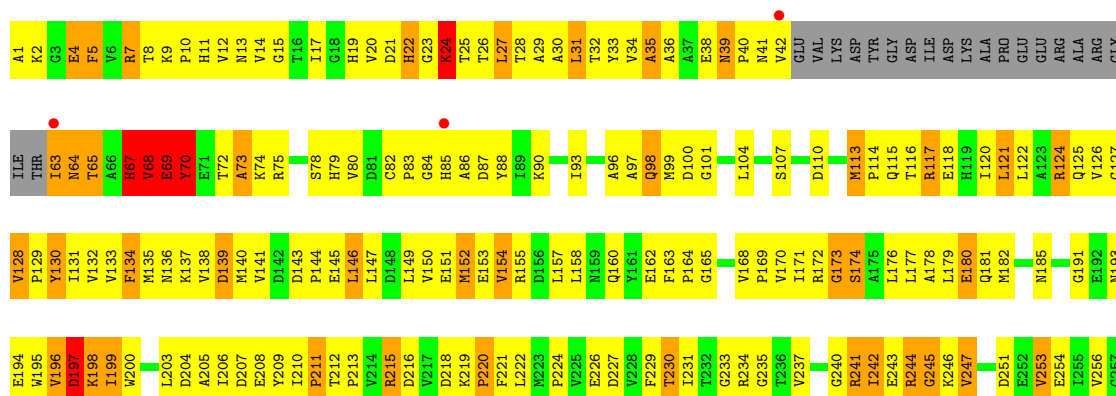
Chain AY:

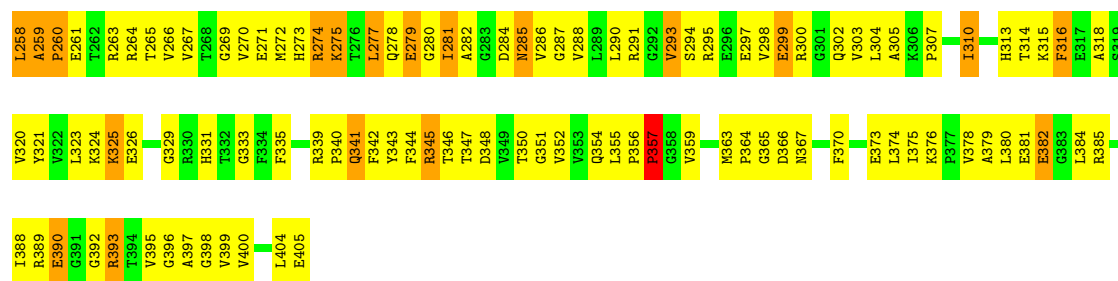


Chain CY:



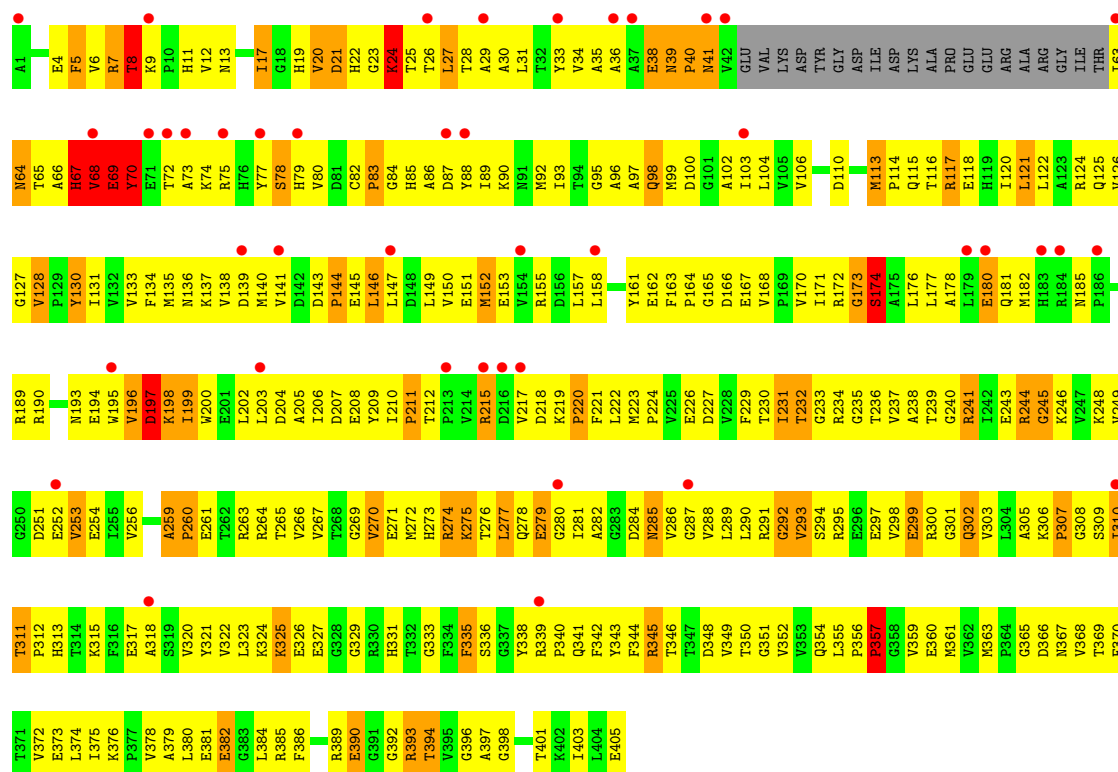
Chain AZ:





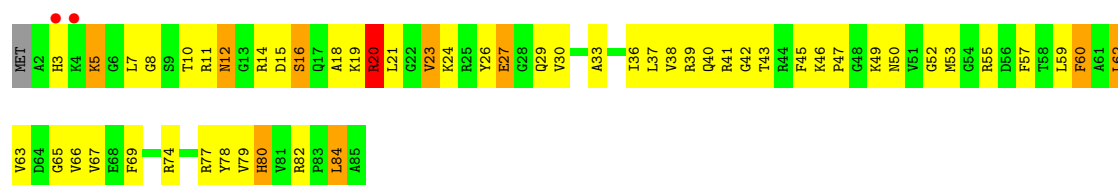
• Molecule 25: ELONGATION FACTOR TU

Chain CZ:



• Molecule 26: 50S RIBOSOMAL PROTEIN L27

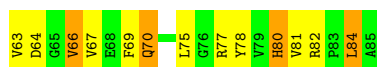
Chain B0:



• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:





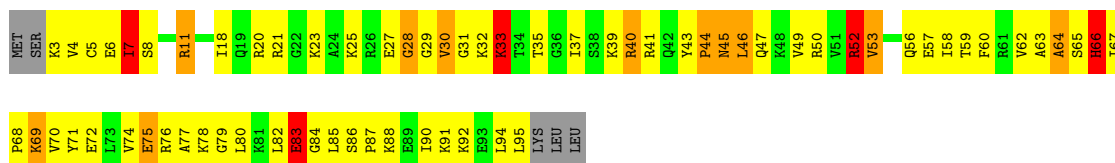
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



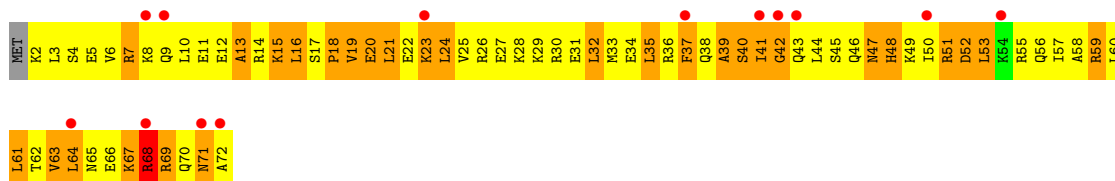
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



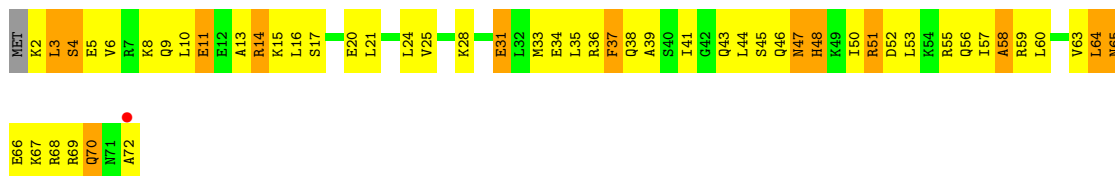
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



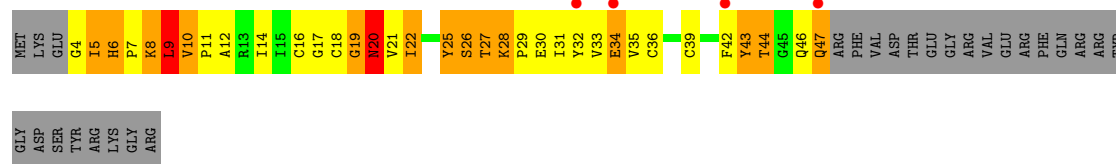
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



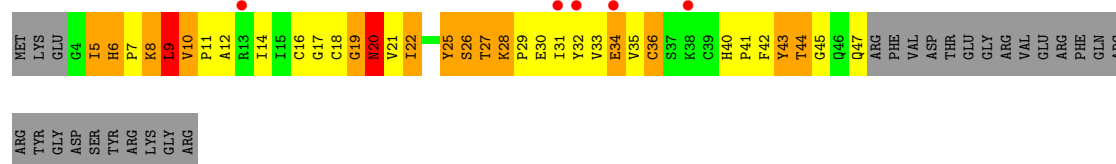
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



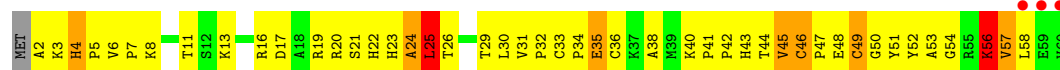
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:



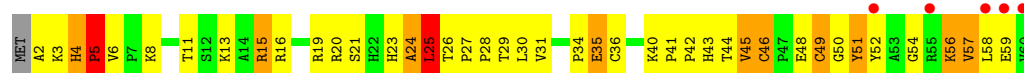
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:



• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5:



• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:



• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:



• Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



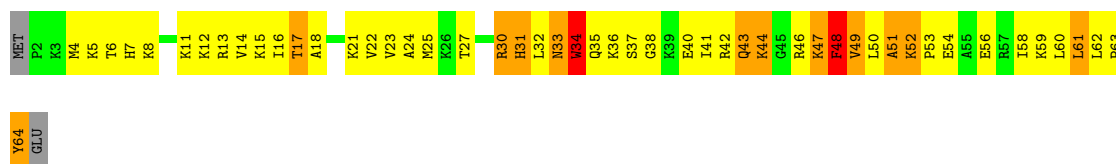
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:



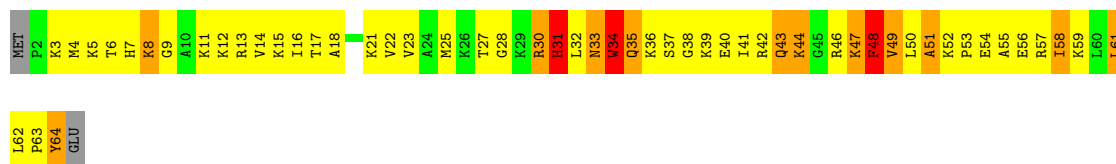
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



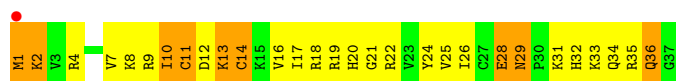
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8:



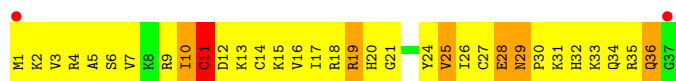
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



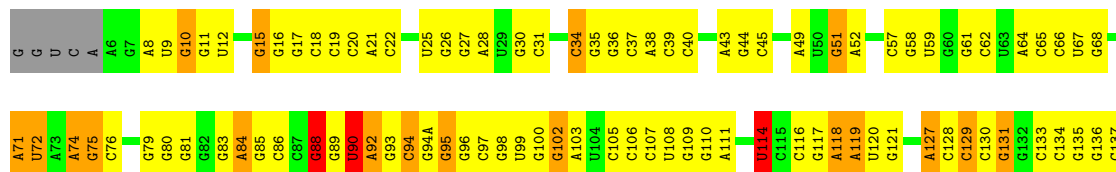
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



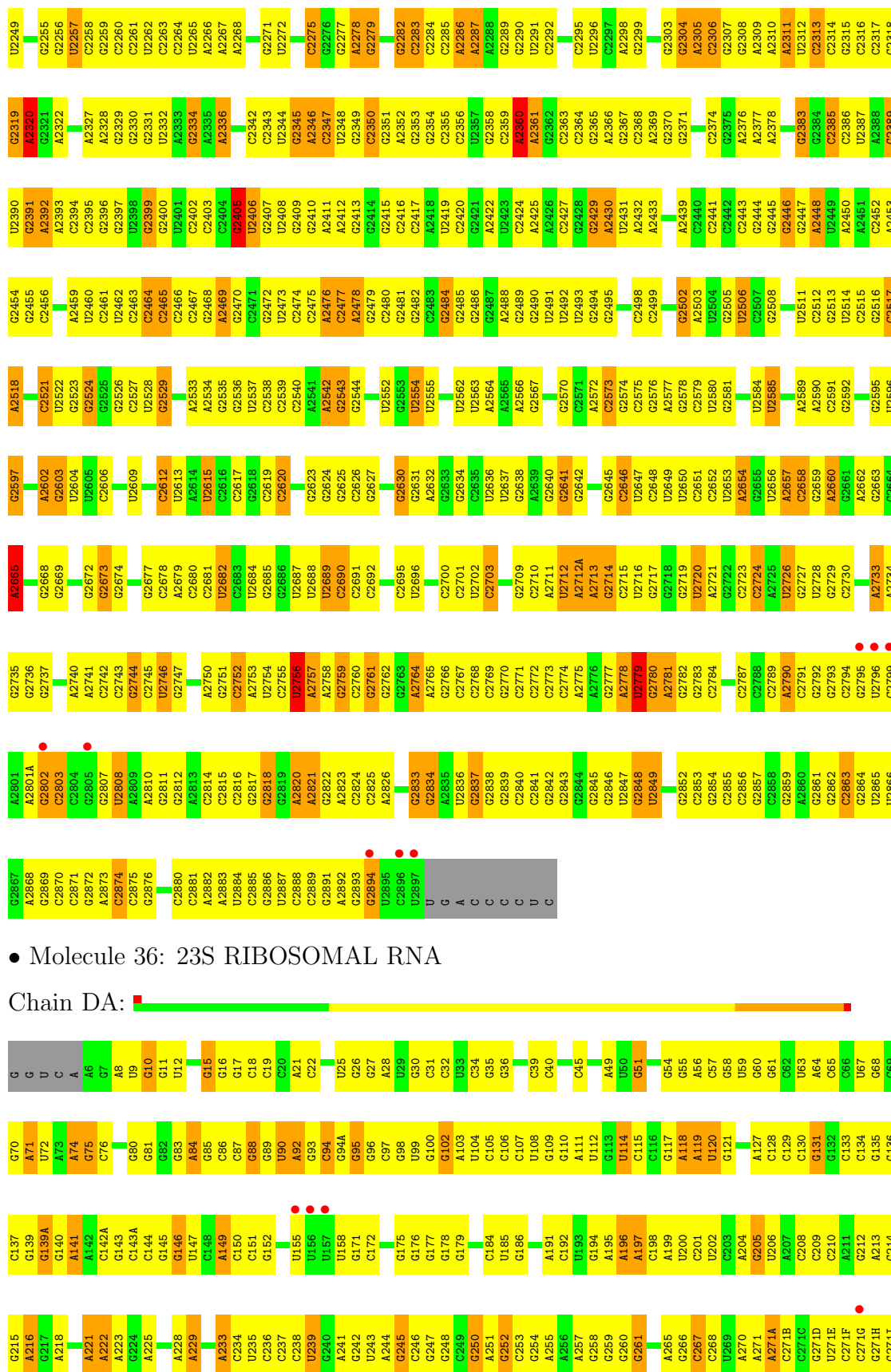
- Molecule 36: 23S RIBOSOMAL RNA

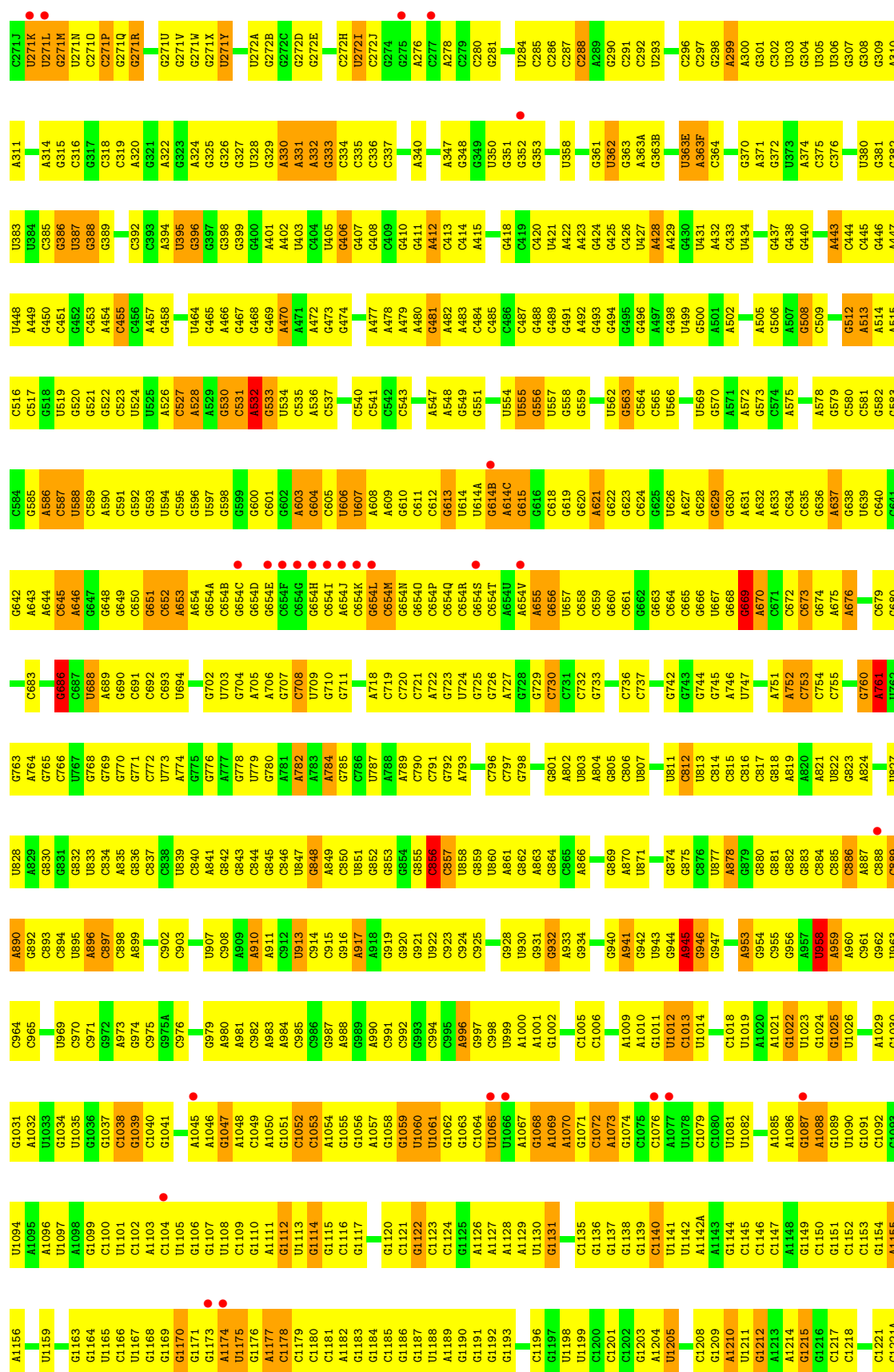
Chain BA:



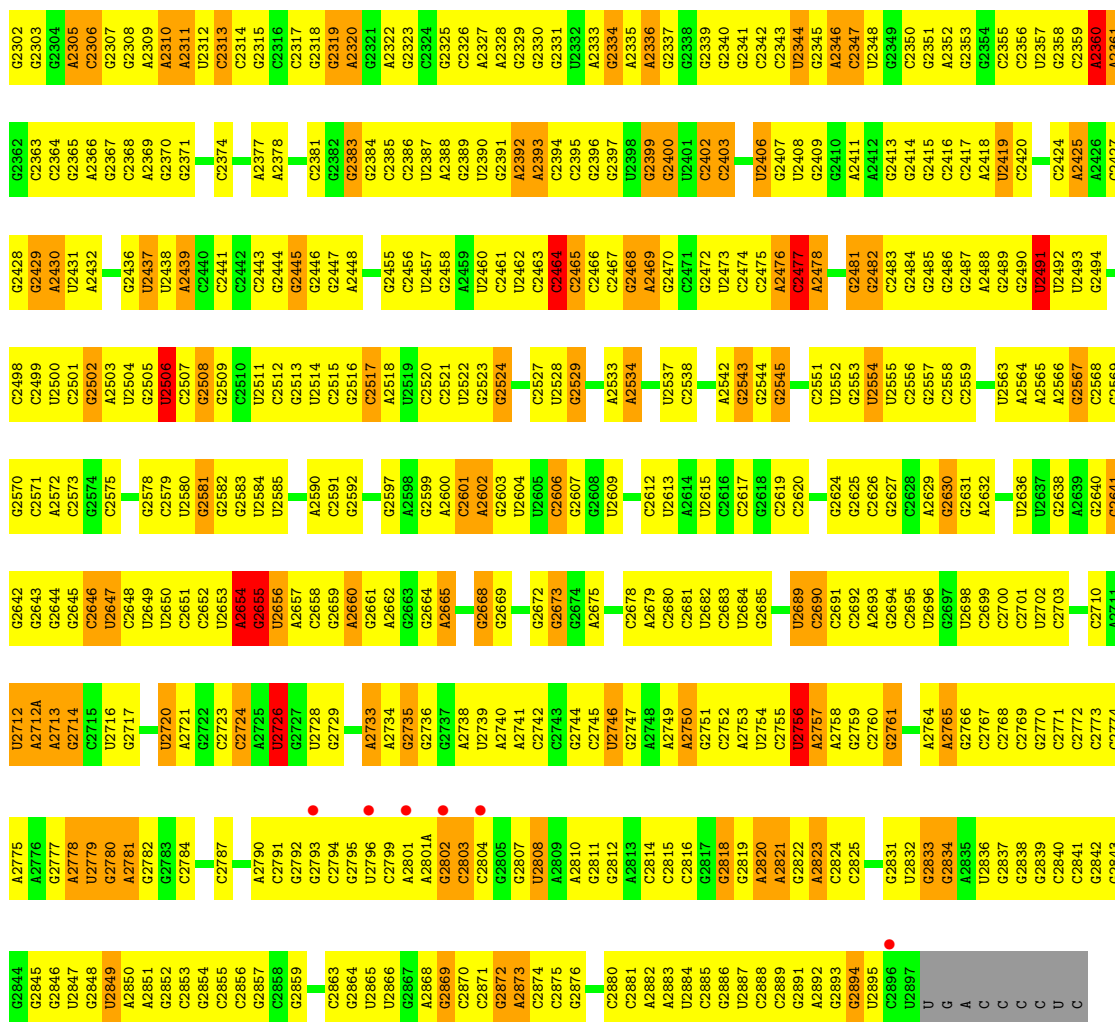
A1098	A1028	A960	G892	C825	G759	U688	A643	C584	G518	C450	U387	G308	U271E	G211	G139
G1099	A1029	C961	C893	U826	G760	A689	A644	G585	U519	C451	G388	G309	C271F	G212	G139A
C1100	G1030	G962	C894	U827	A761	G690	C645	A586	G520	C455	G389	A310	C271G	A213	A141
U1101	U895	U963	U896	U828	A764	C691	A646	A587	G521	C456	A390	A311	G271H	G214	A142
C1102	A896	C964	A897	A829	G765	C692	C650	U588	G522	A457	G391		G271I	G215	C142A
A1103	U1033	C965	C897	G830		C693	G651	A590	C523	C458	C592	C318	G271J	G216	G143
C1104	G1034		C898	G831		U694	G652	C591	U524	C459	C593	C319	U271K	G217	
U1105			A899	G832	G768	G695	C653	C592	U525	U459	A594	A320	G271L	A218	
G1106	G1037		U969	U833	G769	G696	A653	G592	A526	A460	U395	G321	G271M	G219	C143A
U1107	C1038	C970	C903	C834	G770	C697	A654	G593	C527	C461	G396	A322	U271N	G220	C144
G1108	G1039	C971	C904	C835	G771	C698	G654A	U594	A528	C462	G397	G323	G271O	A221	G145
C1109	U1040		U905	C837	G772	A699	G654B	G595	A529	C463	G398	A324	G271P	U147	G146
G1110	G1041		G906	C838	U773	G700	G654C	G596	G530	U464	G399	G326	G271Q	U148	
A1111		C975		U839	A774	G701	G654D	U597	C531	C465		A225	G271R	A149	
	A1045		A909	C840	G775	G702	G654E	G598	A532	A466	A402	G327		A150	
U1113	A1046		A910	C841	G776	G703	G654F	G599	G533	U403	U403	U328	G271U	A226	C151
G1114	G1047		A911	G842	G777	G704	C654G	G600	U534	C468	U405	A329	G271V	A228	
G1115	A1048		G912	G843	A780	A705	G654H	C601	C535	C469	C404	A330	G271W	A229	
C1116	C1049	A980	U913	C844	A781	A706	G654I	G602	A536	A470	G406	A331	G271X	U230	
G1117	A1050		C914	G845	A782	G707	A654J	A603		A471	G407	A332	U271Y	C231	U155
	U1051		C915	C846	A783	C708	C654K	G604	G539	A472	G408	G333		G232	U156
C1120	C1052		G916	U847	A784	U709	G654L	C605	C540	C473	C409	C334	U272A	A233	U157
G1121	C1053		A917	G848	G785	G710	C654M	U606	C541	C474	G410	C335	G272B	U158	
C1122	A1054		A918	C786	G787	G711	G654N	U607	C542	U475	G411	C336	G272C	G171	
			G919	C850	U787		G654O		C543	C476	A412		G272D	C236	C172
C1124	A1057		G920	U851	A788	G715	G654P	G610		A477	C413	A340		C237	G175
G1125	G1058		G921	G852	A789	A716	C654Q	C611	A547	A478	C414		G272H	C238	G176
	U1059		U922	G853	C790	G717	C654R	C612	A548	A479	A415	A347	U272I	U239	G177
U1130	U1060	C991	C923	G854	C791	A718	G654S	G613	G549	A480	C416		G272J		G178
C1131	U1061	C992	G924	G855	G792	C719	C654T	G614	G551	C417	C418	U350	G274	G242	G179
A1132	G1062		G928	C856	A793	C720	A654U	U614A		A482	G419	G351	G275	U243	
U1133	G1063		U930	C857	G794	C721	A654V	G614B	U554	A483	C420	G352	A276	A244	A182
C1135	U1064		G931	C858	A795	A722	A655	A614C	U555	C484	C425	G353	G277	G245	C183
G1136	U1065		G932	G859	C796	G723	G656	G615	U557	C485	U421		A278	C246	C184
U1137	C1066		A933	C797		U724	U657	G616			A422	U358	G279	G247	U185
G1138	U1067		G934				C658	C618	G558	C489	A423		C280	G248	G186
C1139	A1068		U937	G862	G801	A727	C659	G619	G559	C491	G424	G361	G281	C249	G187
A1140	A1069		G938	A863	A802	G728		G620		A492	G425	U362		G250	G188
U1141	G1070	G1002	G939	G864	U803	G729	C664	A621	U562	C493	U426	A363A	U284	A251	G189
C1142	C1071		G940	C865	A804	C730	C665	G622	G563	C494			C285	G252	A190
A1143	C1072	C1006	G941	A866	G805	C731	U666	G623	C564		A428	U363E	C286	A255	C192
G1144	G1073		G942	G873	C806	G732	G667	G624	C565	C498	A429	A363F	C287	A256	U193
C1145	U1074		U943	G874	U807	G733	G668	G625	U566	U499	G430	C364	A289	A257	G194
U1146	C1075		G944	C875	G808	A734	G669	U626	A567	G500	U431	C365	G290	G258	A196
C1147	U1076		A945	C876	U810	U740	A670	A627	U568	A501	A432		G291	G259	C197
A1148	U1077		G946	U877	U811	G741	C671	G628	G570	A502		A371	C292	G260	A198
G1149	U1078		G947	A878	C812	G742	C672	G629	A571		C436	G372	U293	G261	C199
C1150	C1079		U948	G879	U813	G743	G673	G630	A572	A505	G437				A199
G1151	G1079		C949	G880	C814	G744	A675	A632	G573	G506	C438	C376	C296	A265	U200
	U1080		G950	G881	C815	G745	A676	A633	C574	A507	G440	C377	C297	G266	C201
C1152	G1088		C951	G882	A746			A634	C575	G508	U441	C378	C298	G267	U202
G1153	U1089		G952	G883	A747	G747	G680	C635	U576	C509	A442	G379	A299	C268	C203
C1154	U1090		A953	C884	G748	G748	G681	G636	G577	U511	A443	U380	A300	U269	A204
A1155	G1091		G954	C885	G749	C749	G682	A637	A578	G512	G381	G381	G301	A270	G205
U1156	C1092		U1023	C886	A819	G750	G683	G638	G579	A513	C445	G382	C302	A271	U206
G1157	G1093		C955	A887	A820	A751	G684	U639	C580	A514	G446	U383	U303	A271A	A207
C1158	U1094		G956	A887	A821	A752	A685	C640	G581	A515	U447	U384	G304	G271B	C208
	A1095		A957	G888	U822	C753	A686	G641	G582	C516	A448	C385	U305	G271C	C209
C1161	U1096		G823	C889	G823		C687	G642	G583	C517	A449	G386		G271D	C210

U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	G2203	G2204	G2205	G2206	G2207	G2208	A2208	U2218	C2219	G2222	G2223	G2224	A2225	C2226	U2233	U2234	C2235	C2236	G2237	G2238	C2238	G2238	C2240	A2241	G2242	A2158	G2159	G2160	G2166	U2167				
U1955	U1956	U1957	U1958	U1959	U1960	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1977	U1978	U1981	U1982	C1983	C2050	A2051	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	A2136	A2062	C2063	U2068	C2069	C2070	A2071	C2006	C2007	U2074	U2075	C2008	C2078	U2109	U2110	G2080	C2081	A2013	A2014	A2015	G2087	U2017	G2088	U2089	C2090	U2091	U2092	G2093	C2097	U2098			
G1799	G1800	G1801	G1802	G1803	C1804	U1805	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	C1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1840	U1841	U1842	U1843	C1847	U1848	U2011	U2012	G2012	G2013	A2014	A2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	G2023	C2024	U2025			
G1642	G1643	G1647	C1648	C1649	C1650	G1651	U1652	C1653	C1654	A1655	C1655	C1656	C1657	C1658	C1659	U1660	C1661	C1662	C1663	A1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	G1678	U1679	U1680	C1681	C1682	C1683	C1684	C1685	U1688	A1689	U1693	C1694	C1695	C1696	C1697	C1698	U1700	U1701	U1702	C1703	U1709	C1710	C1711	C1712	U1713								
A1572	A1573	U1576	U1577	U1578	U1579	A1580	C1581	C1582	A1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	A1603	U1608	A1609	C1610	C1611	C1612	C1613	C1614	C1615	A1616	C1617	A1618	C1619	C1620	C1621	C1622	C1623	C1624	U1628	C1632	C1633	C1634	C1635	C1638	C1639	C1640	C1641	C1642								
U1497	C1498	C1499	C1500	C1501	C1502	U1503	C1504	C1505	C1506	C1507	A1508	C1509	A1509B	C1510	C1511	U1512	U1513	C1514	C1515	C1516	C1517	C1518	U1523	C1524	C1525	C1526	C1527	C1528	A1528A	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	U1539	U1540	C1541	C1542	C1543	C1544	C1547	C1548	A1554	C1553	C1559	A1567	C1568	A1569	C1570	C1571	C1572								
A1427	C1428	U1431	C1432	U1433	U1434	U1435	U1440	C1441	C1442	U1443	U1444	A1445	C1445A	C1446	C1447	C1448	A1449	A1452	C1453	C1454	C1455	C1456	A1457	C1458	C1459	C1460	C1461	C1462	A1465	C1466	C1467	C1468	C1469	C1470	A1471	C1472	C1473	C1474	C1475	C1477	C1478	C1479	C1480	U1481	C1482	C1484	C1485	A1486	C1487	U1488	U1489	A1490	C1491	C1492	C1493	C1494	C1495	C1496						
C1293	C1294	C1295	C1296	C1297	U1300	U1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359
A1360	C1361	C1362	C1363	C1364	A1365	U1368	U1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	A1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	U1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1423	C1424	C1425	C1426		
G1163	G1164	U1165	C1166	U1167	G1168	C1169	C1170	C1171	C1173	U1174	U1175	G1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1196	C1197	U1198	U1199	C1203	U1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1221A	C1222	C1223	C1224	C1225	C1226	C1227					



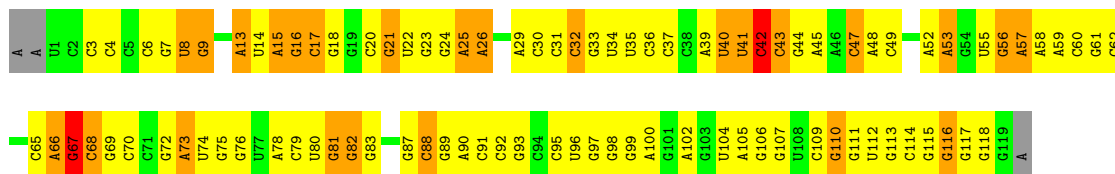






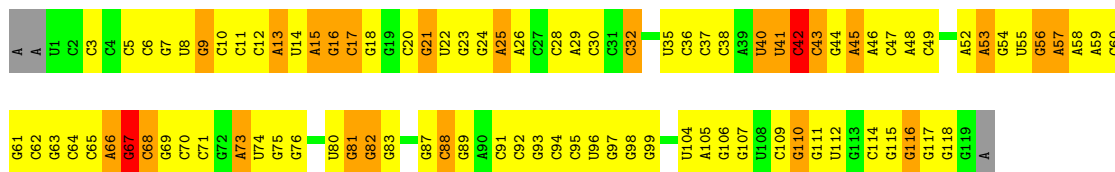
• Molecule 37: 5S RIBOSOMAL RNA

Chain BB:



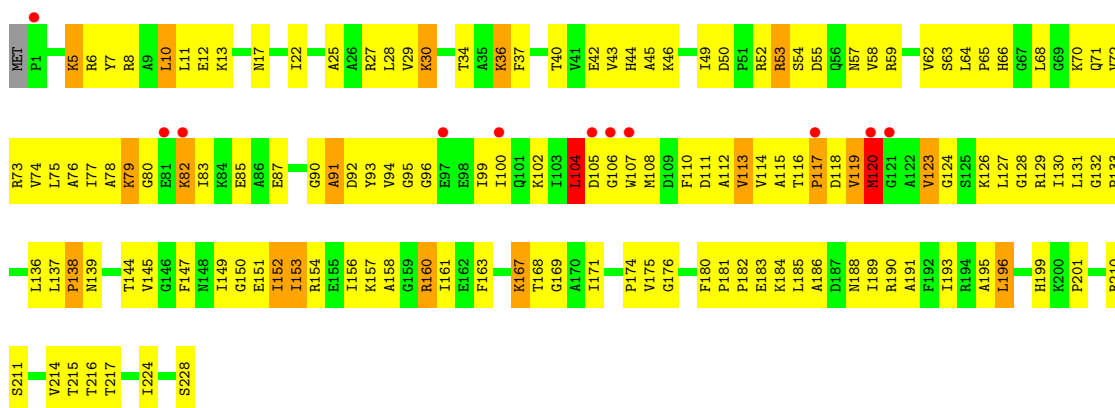
• Molecule 37: 5S RIBOSOMAL RNA

Chain DB:



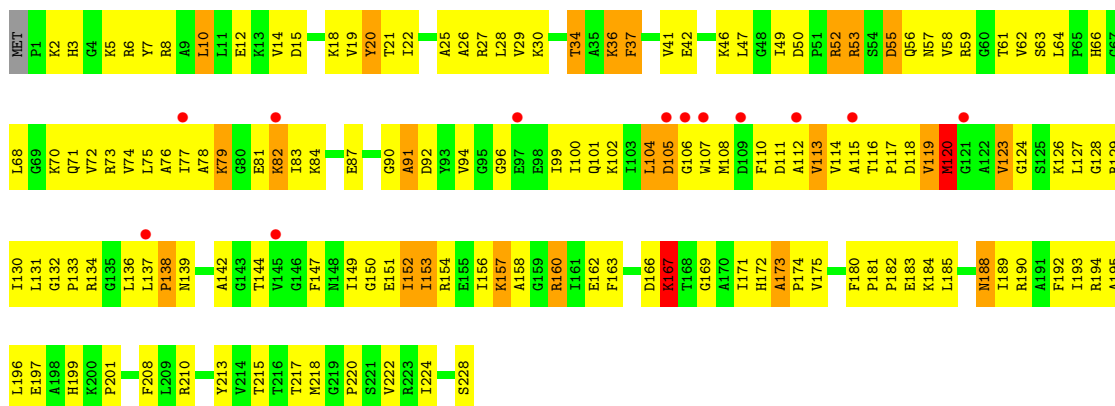
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC:



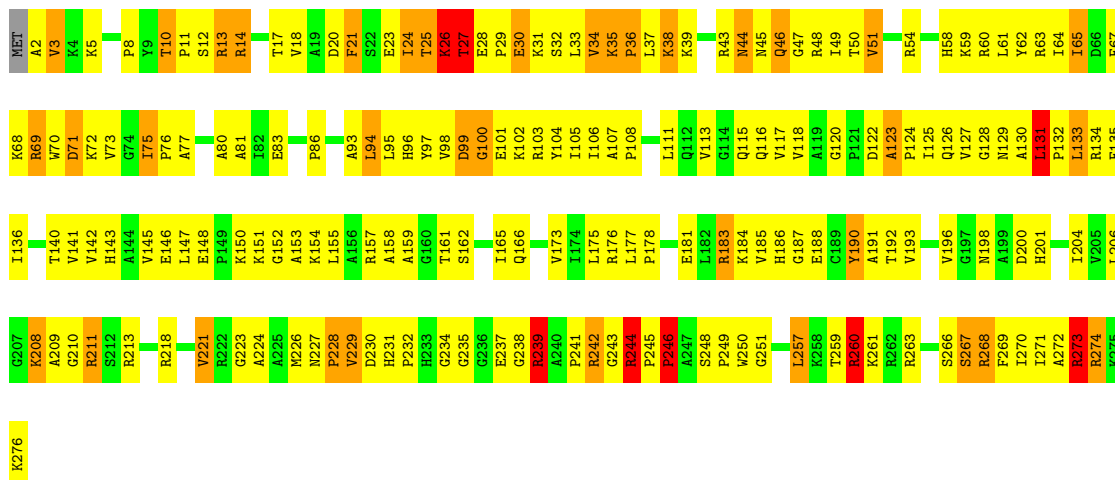
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain DC:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

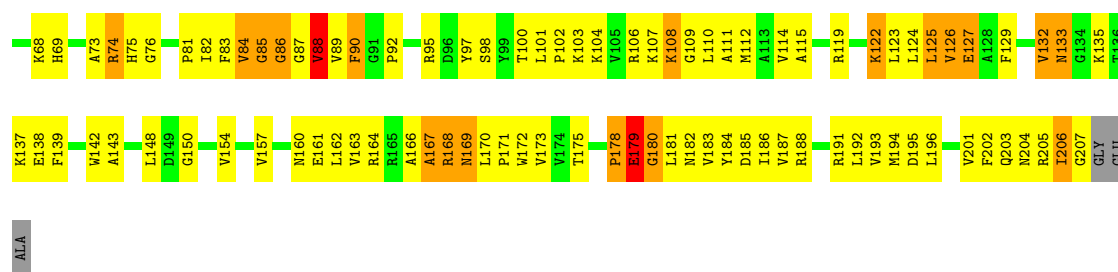
Chain BD:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

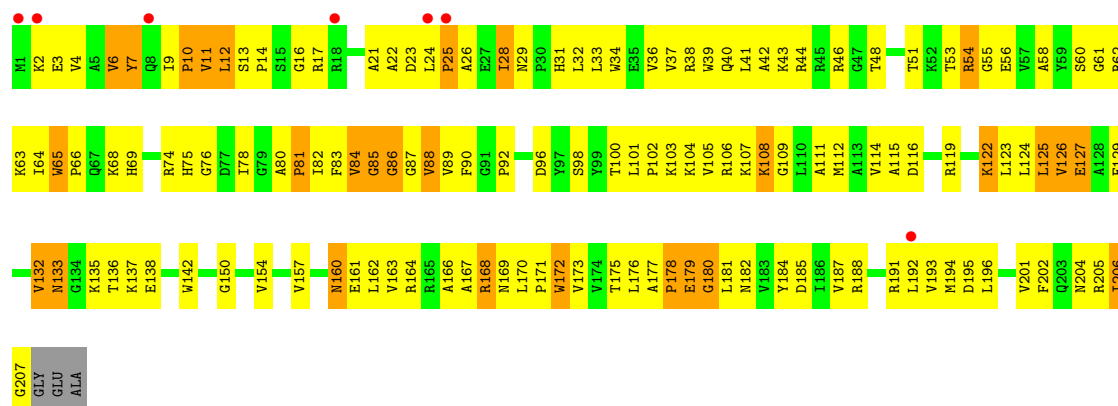
Chain DD:





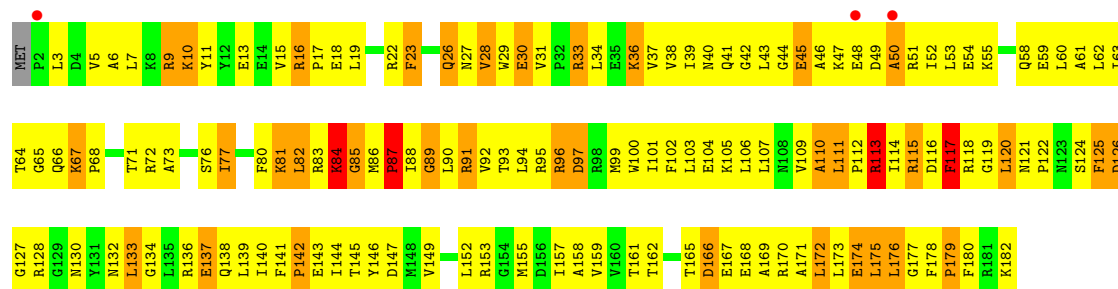
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:

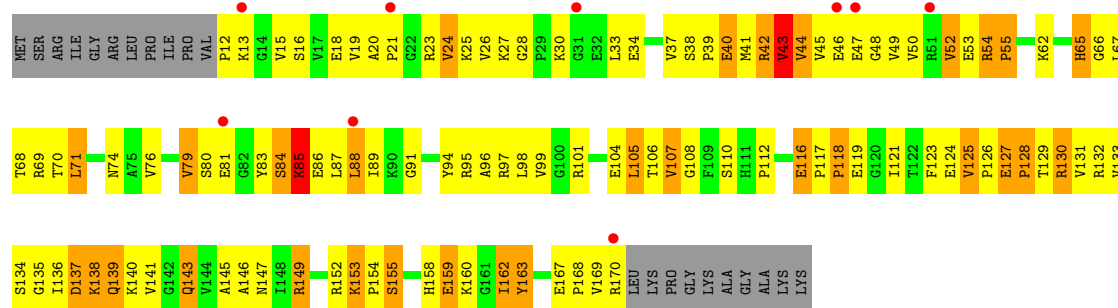


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain BG:

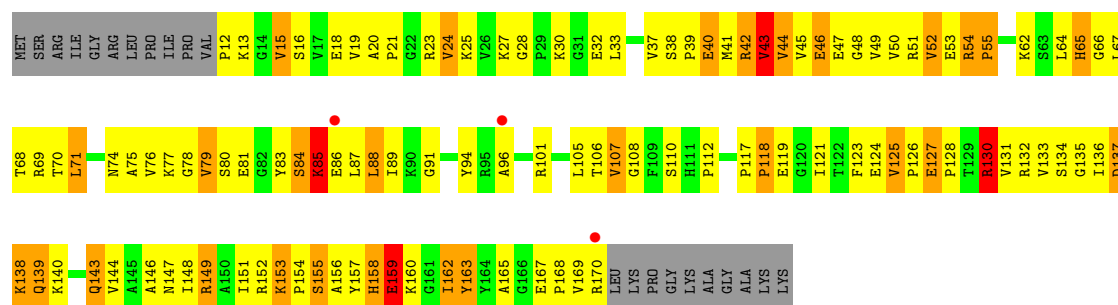


Chain BH:



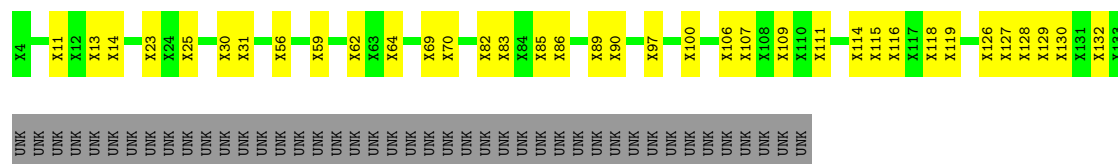
- Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain DH:



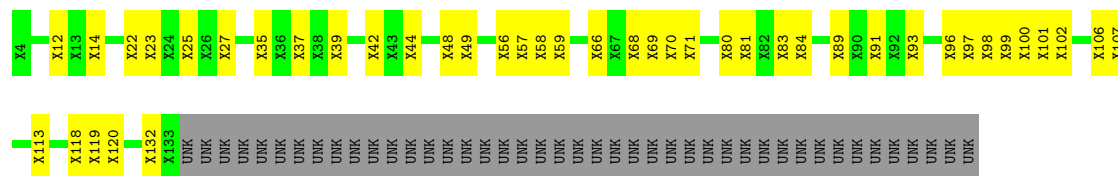
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:

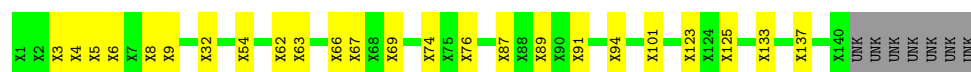


- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:

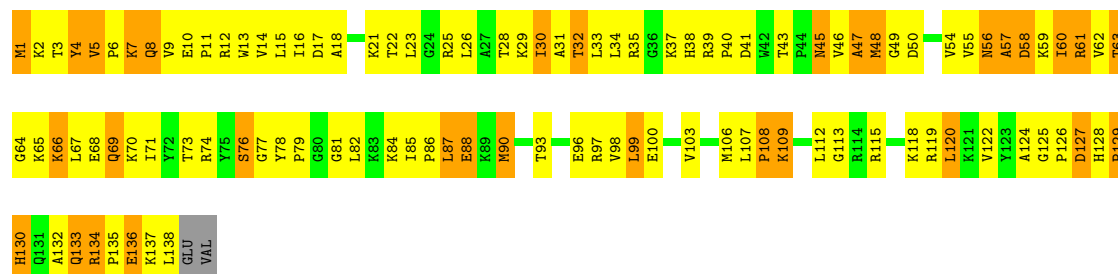


Chain DK: 



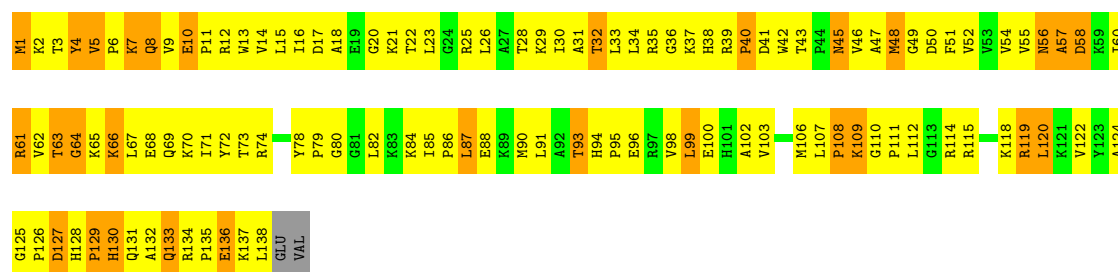
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 



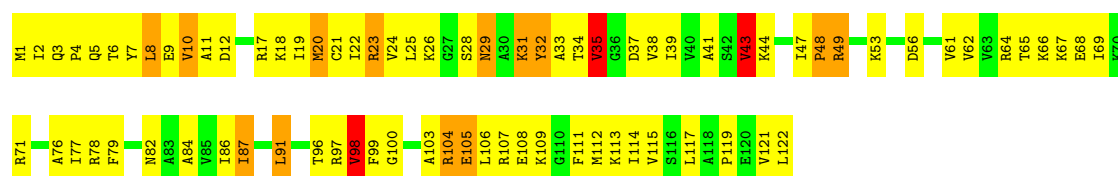
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 



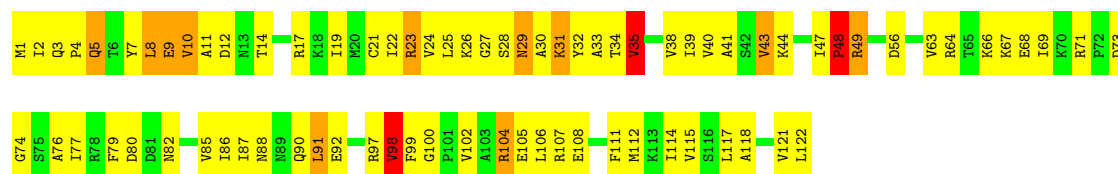
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 



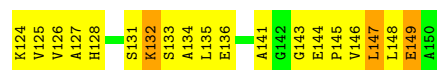
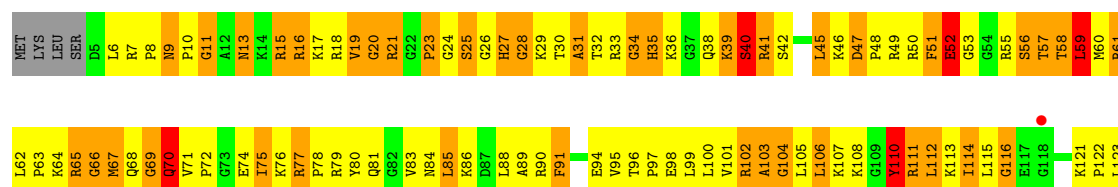
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 



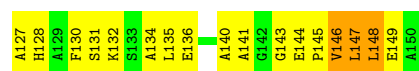
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



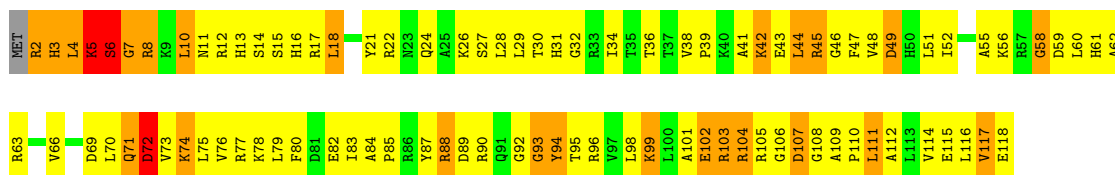
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



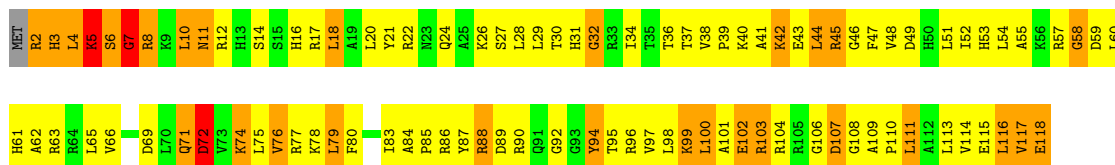
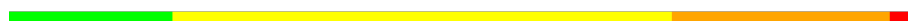
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



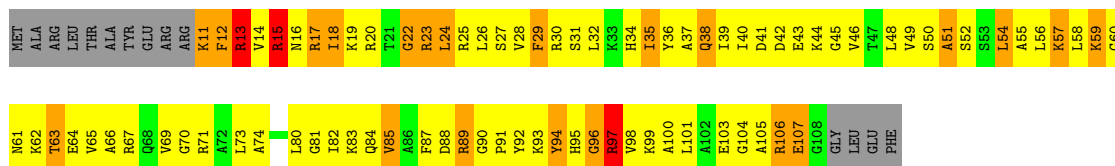
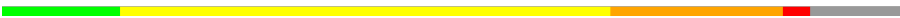
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



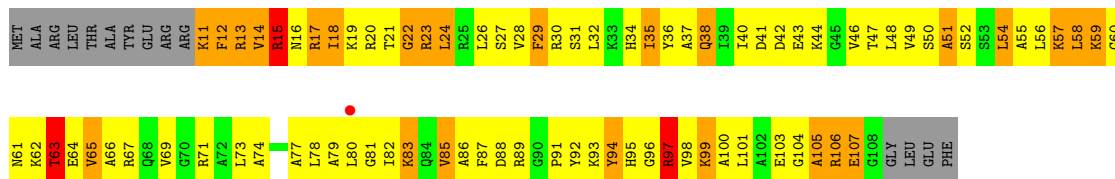
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



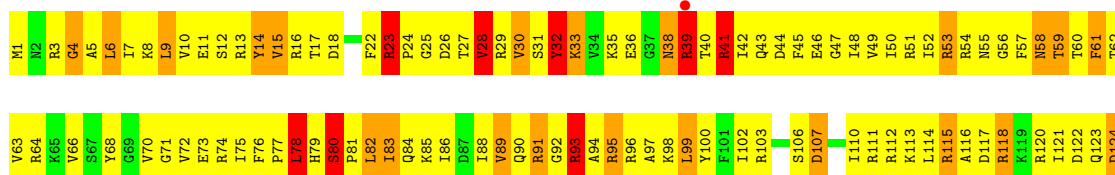
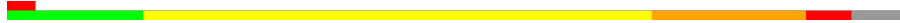
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



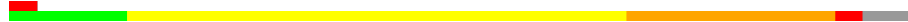
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:

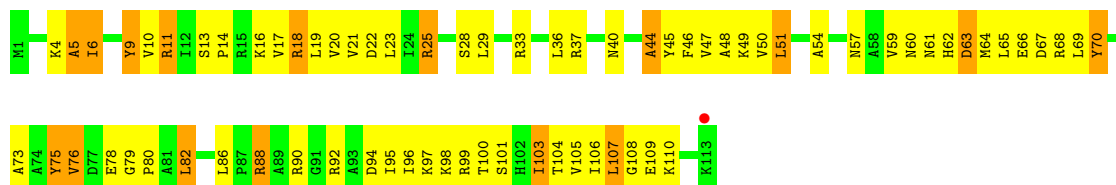






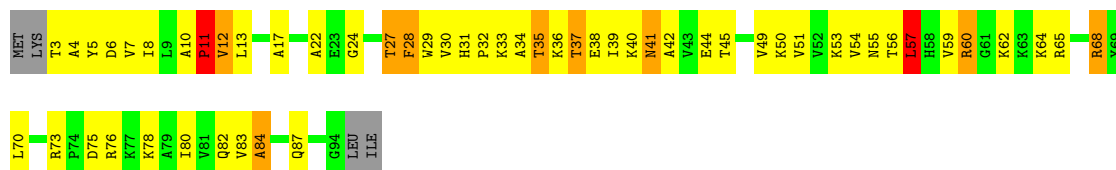
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



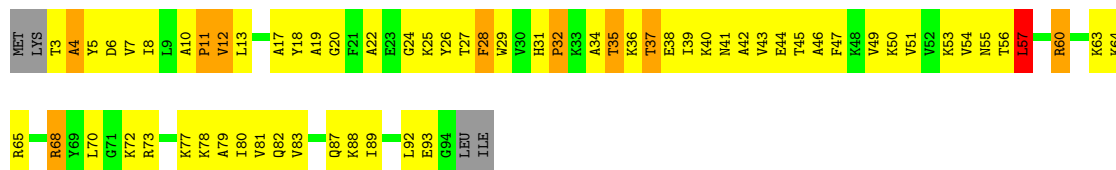
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



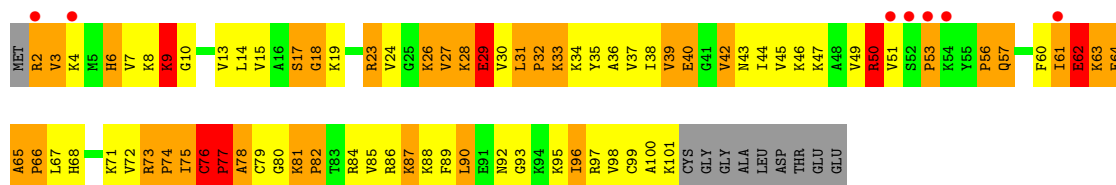
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



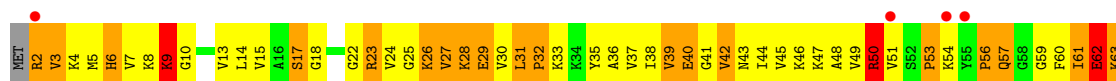
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

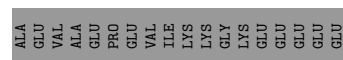
Chain BY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	289.80Å 269.10Å 403.90Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.83 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.10) 89.6 (49.83-2.93)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.247 , 0.285 0.252 , 0.288	Depositor DCC
R_{free} test set	58969 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.1	EDS
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 1182846 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	307196	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.63	5/36190 (0.0%)	0.80	59/56486 (0.1%)
1	CA	0.60	4/36190 (0.0%)	0.78	33/56486 (0.1%)
2	AB	0.51	0/1935	0.76	2/2609 (0.1%)
2	CB	0.49	0/1935	0.76	0/2609
3	AC	0.57	1/1636 (0.1%)	0.81	0/2205
3	CC	0.54	0/1636	0.76	0/2205
4	AD	0.51	0/1733	0.81	2/2318 (0.1%)
4	CD	0.56	0/1733	0.84	1/2318 (0.0%)
5	AE	0.58	0/1162	0.85	0/1564
5	CE	0.56	0/1162	0.84	0/1564
6	AF	0.45	0/856	0.70	0/1154
6	CF	0.45	0/856	0.74	0/1154
7	AG	0.46	0/1276	0.68	2/1709 (0.1%)
7	CG	0.50	0/1276	0.63	0/1709
8	AH	0.51	0/1136	0.80	0/1527
8	CH	0.51	0/1136	0.80	0/1527
9	AI	0.50	0/1029	0.77	0/1379
9	CI	0.49	0/1029	0.74	0/1379
10	AJ	0.51	0/807	0.80	0/1085
10	CJ	0.48	0/807	0.74	0/1085
11	AK	0.56	0/900	0.84	1/1213 (0.1%)
11	CK	0.51	0/900	0.77	1/1213 (0.1%)
12	AL	0.53	0/986	0.90	2/1320 (0.2%)
12	CL	0.54	0/986	0.87	1/1320 (0.1%)
13	AM	0.43	0/998	0.75	0/1336
13	CM	0.42	0/998	0.75	0/1336
14	AN	0.56	0/501	0.87	1/664 (0.2%)
14	CN	0.70	0/501	0.92	0/664
15	AO	0.49	0/745	0.71	0/992
15	CO	0.50	0/745	0.71	0/992
16	AP	0.44	0/716	0.73	0/963
16	CP	0.40	0/716	0.71	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.47	0/836	0.73	0/1117
17	CQ	0.48	0/836	0.76	0/1117
18	AR	0.54	0/579	0.76	0/768
18	CR	0.52	0/579	0.76	0/768
19	AS	0.49	0/642	0.74	1/865 (0.1%)
19	CS	0.45	0/642	0.71	0/865
20	AT	0.40	0/765	0.72	0/1007
20	CT	0.37	0/765	0.70	0/1007
21	AU	0.43	0/212	0.75	0/277
21	CU	0.60	0/212	0.81	0/277
22	AV	0.64	0/1809	0.80	1/2819 (0.0%)
22	AW	0.47	1/1809 (0.1%)	0.74	0/2819
22	CV	0.58	0/1809	0.79	1/2819 (0.0%)
22	CW	0.40	0/1809	0.73	0/2819
23	AX	0.80	0/406	0.89	2/631 (0.3%)
23	CX	0.78	0/406	0.94	2/631 (0.3%)
24	AY	0.80	7/1618 (0.4%)	0.91	7/2514 (0.3%)
24	CY	0.76	4/1618 (0.2%)	0.91	7/2514 (0.3%)
25	AZ	0.72	7/3042 (0.2%)	0.84	8/4129 (0.2%)
25	CZ	0.79	6/3042 (0.2%)	0.88	7/4129 (0.2%)
26	B0	0.44	0/671	0.68	0/892
26	D0	0.45	0/671	0.72	0/892
27	B1	0.47	0/738	0.77	0/981
27	D1	0.42	0/738	0.70	0/981
28	B2	0.39	0/600	0.77	0/793
28	D2	0.34	0/600	0.66	0/793
29	B3	0.43	0/472	0.69	0/634
29	D3	0.39	0/472	0.71	0/634
30	B4	0.53	0/349	0.67	0/474
30	D4	0.52	0/349	0.65	0/474
31	B5	0.44	0/473	0.76	0/639
31	D5	0.43	0/473	0.77	0/639
32	B6	0.62	0/440	0.93	0/586
32	D6	0.60	0/440	0.91	0/586
33	B7	0.51	0/426	0.74	0/561
33	D7	0.47	0/426	0.71	0/561
34	B8	0.59	0/515	0.87	0/679
34	D8	0.56	0/515	0.87	0/679
35	B9	0.53	0/310	0.74	0/407
35	D9	0.61	0/310	0.92	0/407
36	BA	0.55	2/69976 (0.0%)	0.75	50/109244 (0.0%)
36	DA	0.54	3/69976 (0.0%)	0.75	43/109244 (0.0%)
37	BB	0.47	0/2853	0.75	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.49	0/2853	0.75	0/4451
38	BC	0.42	1/1774 (0.1%)	0.68	0/2391
38	DC	0.46	2/1774 (0.1%)	0.65	0/2391
39	BD	0.55	0/2195	0.89	4/2955 (0.1%)
39	DD	0.55	0/2195	0.90	5/2955 (0.2%)
40	BE	0.47	0/1596	0.76	0/2153
40	DE	0.49	0/1596	0.78	1/2153 (0.0%)
41	BF	0.41	0/1658	0.69	0/2244
41	DF	0.39	0/1658	0.67	0/2244
42	BG	0.43	0/1499	0.72	0/2016
42	DG	0.39	0/1499	0.71	0/2016
43	BH	0.40	0/1245	0.68	0/1682
43	DH	0.38	0/1245	0.71	0/1682
46	BN	0.44	0/1131	0.74	0/1525
46	DN	0.41	0/1131	0.72	0/1525
47	BO	0.52	0/943	0.76	1/1269 (0.1%)
47	DO	0.51	0/943	0.77	0/1269
48	BP	0.48	0/1131	1.00	6/1504 (0.4%)
48	DP	0.46	0/1131	1.00	6/1504 (0.4%)
49	BQ	0.51	0/1143	0.77	0/1527
49	DQ	0.50	0/1143	0.79	0/1527
50	BR	0.40	0/974	0.77	0/1302
50	DR	0.39	0/974	0.74	2/1302 (0.2%)
51	BS	0.41	0/778	0.74	0/1036
51	DS	0.41	0/778	0.70	0/1036
52	BT	0.44	0/1155	0.78	2/1542 (0.1%)
52	DT	0.43	0/1155	0.76	1/1542 (0.1%)
53	BU	0.46	0/975	0.75	0/1297
53	DU	0.49	0/975	0.74	0/1297
54	BV	0.40	0/790	0.75	0/1057
54	DV	0.41	0/790	0.73	0/1057
55	BW	0.39	0/907	0.70	0/1216
55	DW	0.40	0/907	0.67	0/1216
56	BX	0.45	0/739	0.70	1/993 (0.1%)
56	DX	0.45	0/739	0.72	1/993 (0.1%)
57	BY	0.38	0/788	0.70	0/1051
57	DY	0.38	0/788	0.73	1/1051 (0.1%)
58	BZ	0.46	0/1491	0.80	1/2024 (0.0%)
58	DZ	0.46	0/1491	0.74	1/2024 (0.0%)
All	All	0.55	43/330118 (0.0%)	0.77	267/493190 (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	6	89
1	CA	4	91
8	AH	0	1
8	CH	0	1
19	AS	0	1
22	AV	0	7
22	CV	0	1
22	CW	0	1
23	AX	0	1
23	CX	0	4
24	AY	2	1
24	CY	2	2
25	AZ	0	2
25	CZ	0	2
36	BA	0	123
36	DA	1	104
37	BB	0	3
37	DB	0	3
39	BD	0	1
49	BQ	0	1
49	DQ	0	1
All	All	15	440

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DA	761	A	C5-C6	-10.85	1.31	1.41
24	AY	34	C	C5-C6	10.54	1.42	1.34
25	AZ	69	GLU	N-CA	9.82	1.66	1.46
25	CZ	67	HIS	C-O	9.21	1.40	1.23
25	CZ	69	GLU	N-CA	8.60	1.63	1.46

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1054	C	N1-C1'-C2'	12.37	130.09	114.00
1	AA	1054	C	N3-C2-O2	12.20	130.44	121.90
1	AA	1498	U	C2'-C3'-O3'	11.43	134.65	109.50
1	CA	1054	C	N1-C1'-C2'	11.34	128.74	114.00
1	CA	1503	A	N9-C1'-C2'	-11.14	99.52	114.00

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	243	A	C3'
1	AA	508	C	C3'
1	AA	687	A	C3'
1	AA	968	A	C3'
1	AA	1498	U	C3'

5 of 440 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	114	U	Sidechain
1	AA	122	G	Sidechain
1	AA	14	U	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	47	C	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1145	0
1	CA	32329	0	16317	1397	0
2	AB	1900	0	1951	238	3
2	CB	1900	0	1951	239	3
3	AC	1612	0	1677	194	0
3	CC	1612	0	1677	201	0
4	AD	1703	0	1765	249	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	111	0
5	CE	1146	0	1207	159	0
6	AF	843	0	857	75	0
6	CF	843	0	857	82	0
7	AG	1257	0	1296	81	0
7	CG	1257	0	1296	109	0
8	AH	1116	0	1177	72	0
8	CH	1116	0	1177	99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	1010	0	1037	145	0
9	CI	1010	0	1037	159	0
10	AJ	794	0	840	146	0
10	CJ	794	0	840	155	0
11	AK	885	0	904	58	0
11	CK	885	0	904	86	0
12	AL	970	0	1057	118	0
12	CL	970	0	1057	124	0
13	AM	987	0	1059	158	0
13	CM	987	0	1059	179	0
14	AN	492	0	529	70	0
14	CN	492	0	530	115	0
15	AO	734	0	771	64	0
15	CO	734	0	771	61	0
16	AP	700	0	720	71	0
16	CP	700	0	720	77	0
17	AQ	823	0	891	63	0
17	CQ	823	0	891	73	0
18	AR	574	0	644	51	0
18	CR	574	0	644	77	0
19	AS	629	0	652	73	0
19	CS	629	0	652	98	0
20	AT	763	0	861	84	0
20	CT	763	0	861	88	0
21	AU	208	0	221	28	0
21	CU	208	0	221	23	0
22	AV	1619	0	822	88	0
22	AW	1619	0	822	89	0
22	CV	1619	0	822	64	0
22	CW	1619	0	822	97	0
23	AX	362	0	184	13	0
23	CX	362	0	184	11	0
24	AY	1644	0	853	74	0
24	CY	1644	0	853	92	0
25	AZ	2984	0	2997	411	0
25	CZ	2984	0	2997	510	0
26	B0	662	0	688	90	0
26	D0	662	0	688	104	0
27	B1	731	0	808	104	0
27	D1	731	0	808	101	0
28	B2	598	0	653	192	0
28	D2	598	0	653	98	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B3	467	0	523	58	0
29	D3	467	0	523	34	0
30	B4	340	0	336	62	0
30	D4	340	0	337	55	0
31	B5	459	0	480	90	0
31	D5	459	0	480	73	0
32	B6	433	0	461	134	0
32	D6	433	0	461	134	0
33	B7	418	0	467	37	0
33	D7	418	0	467	31	0
34	B8	507	0	576	115	0
34	D8	507	0	576	130	0
35	B9	307	0	336	53	0
35	D9	307	0	338	83	0
36	BA	62477	0	31497	2437	0
36	DA	62477	0	31497	2528	0
37	BB	2551	0	1295	127	0
37	DB	2551	0	1295	122	0
38	BC	1742	0	1800	167	3
38	DC	1742	0	1800	184	3
39	BD	2145	0	2234	266	0
39	DD	2145	0	2234	290	0
40	BE	1563	0	1629	263	0
40	DE	1563	0	1629	276	0
41	BF	1623	0	1677	212	0
41	DF	1623	0	1677	226	0
42	BG	1474	0	1535	247	0
42	DG	1474	0	1535	278	0
43	BH	1222	0	1282	178	0
43	DH	1222	0	1282	193	0
44	BJ	651	0	170	25	0
44	DJ	651	0	157	32	0
45	BK	700	0	180	17	0
45	DK	700	0	176	16	0
46	BN	1104	0	1180	178	0
46	DN	1104	0	1180	205	0
47	BO	933	0	996	116	0
47	DO	933	0	996	108	0
48	BP	1114	0	1187	292	0
48	DP	1114	0	1187	290	0
49	BQ	1122	0	1179	166	0
49	DQ	1122	0	1179	165	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BR	960	0	1021	150	0
50	DR	960	0	1021	154	0
51	BS	770	0	832	148	0
51	DS	770	0	832	140	0
52	BT	1141	0	1202	257	0
52	DT	1141	0	1202	227	0
53	BU	958	0	1015	165	0
53	DU	958	0	1015	154	0
54	BV	779	0	852	122	0
54	DV	779	0	852	122	0
55	BW	896	0	953	98	0
55	DW	896	0	953	93	0
56	BX	725	0	778	91	0
56	DX	725	0	778	108	0
57	BY	775	0	870	165	0
57	DY	775	0	870	168	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	254	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	1	0
60	AZ	28	0	12	7	0
60	CZ	28	0	12	17	0
61	AZ	57	0	58	5	0
61	CZ	57	0	58	7	0
All	All	307196	0	208708	20881	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 20881 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:AZ:357:PRO:CB	25:AZ:357:PRO:CG	1.77	1.43
38:DC:100:ILE:HG23	38:DC:127:LEU:CD1	1.68	1.23
4:CD:187:ARG:NH1	4:CD:187:ARG:HB3	1.52	1.22
15:AO:87:ILE:HG22	15:AO:88:ARG:H	1.08	1.18
24:CY:76:A:H1'	25:CZ:287:GLY:HA3	1.26	1.18

The worst 5 of 6 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	Distance(Å)	Clash(Å)
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_646]	1.45	0.75
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_445]	1.59	0.61
2:CB:66:GLY:CA	38:DC:27:ARG:NH2[2_646]	1.87	0.33
2:AB:66:GLY:CA	38:BC:27:ARG:NH2[2_445]	1.94	0.26
2:CB:65:GLY:C	38:DC:27:ARG:NH2[2_646]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/256 (91%)	163 (70%)	43 (18%)	26 (11%)	1	5
2	CB	232/256 (91%)	157 (68%)	52 (22%)	23 (10%)	1	6
3	AC	204/239 (85%)	148 (72%)	37 (18%)	19 (9%)	1	7
3	CC	204/239 (85%)	136 (67%)	43 (21%)	25 (12%)	1	3
4	AD	206/209 (99%)	130 (63%)	48 (23%)	28 (14%)	0	2
4	CD	206/209 (99%)	124 (60%)	53 (26%)	29 (14%)	0	2
5	AE	148/162 (91%)	131 (88%)	13 (9%)	4 (3%)	8	39
5	CE	148/162 (91%)	125 (84%)	18 (12%)	5 (3%)	6	32
6	AF	99/101 (98%)	79 (80%)	14 (14%)	6 (6%)	2	16
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	2	12
7	AG	153/156 (98%)	113 (74%)	27 (18%)	13 (8%)	1	9
7	CG	153/156 (98%)	113 (74%)	23 (15%)	17 (11%)	1	5
8	AH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	7	38
8	CH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	5	31
9	AI	125/128 (98%)	79 (63%)	29 (23%)	17 (14%)	0	2
9	CI	125/128 (98%)	81 (65%)	25 (20%)	19 (15%)	0	1
10	AJ	96/105 (91%)	69 (72%)	19 (20%)	8 (8%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	96/105 (91%)	71 (74%)	17 (18%)	8 (8%)	1	9
11	AK	117/129 (91%)	98 (84%)	13 (11%)	6 (5%)	3	22
11	CK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	17
12	AL	122/131 (93%)	93 (76%)	17 (14%)	12 (10%)	1	6
12	CL	122/131 (93%)	86 (70%)	19 (16%)	17 (14%)	0	2
13	AM	122/126 (97%)	70 (57%)	34 (28%)	18 (15%)	0	2
13	CM	122/126 (97%)	72 (59%)	36 (30%)	14 (12%)	1	4
14	AN	58/61 (95%)	39 (67%)	8 (14%)	11 (19%)	0	0
14	CN	58/61 (95%)	29 (50%)	14 (24%)	15 (26%)	0	0
15	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	6	32
15	CO	86/89 (97%)	64 (74%)	18 (21%)	4 (5%)	4	23
16	AP	81/88 (92%)	63 (78%)	14 (17%)	4 (5%)	3	23
16	CP	81/88 (92%)	60 (74%)	15 (18%)	6 (7%)	2	11
17	AQ	97/105 (92%)	82 (84%)	11 (11%)	4 (4%)	4	27
17	CQ	97/105 (92%)	77 (79%)	13 (13%)	7 (7%)	2	12
18	AR	68/88 (77%)	45 (66%)	19 (28%)	4 (6%)	2	17
18	CR	68/88 (77%)	49 (72%)	15 (22%)	4 (6%)	2	17
19	AS	76/93 (82%)	47 (62%)	20 (26%)	9 (12%)	1	4
19	CS	76/93 (82%)	41 (54%)	25 (33%)	10 (13%)	0	2
20	AT	97/106 (92%)	65 (67%)	20 (21%)	12 (12%)	1	3
20	CT	97/106 (92%)	67 (69%)	19 (20%)	11 (11%)	1	4
21	AU	22/27 (82%)	19 (86%)	2 (9%)	1 (4%)	4	24
21	CU	22/27 (82%)	15 (68%)	6 (27%)	1 (4%)	4	24
25	AZ	381/405 (94%)	268 (70%)	74 (19%)	39 (10%)	1	6
25	CZ	381/405 (94%)	275 (72%)	61 (16%)	45 (12%)	1	4
26	B0	82/85 (96%)	61 (74%)	16 (20%)	5 (6%)	2	16
26	D0	82/85 (96%)	63 (77%)	16 (20%)	3 (4%)	5	31
27	B1	91/98 (93%)	60 (66%)	19 (21%)	12 (13%)	0	2
27	D1	91/98 (93%)	62 (68%)	15 (16%)	14 (15%)	0	1
28	B2	69/72 (96%)	36 (52%)	14 (20%)	19 (28%)	0	0
28	D2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B3	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	2
29	D3	57/60 (95%)	43 (75%)	7 (12%)	7 (12%)	1	3
30	B4	42/71 (59%)	24 (57%)	10 (24%)	8 (19%)	0	0
30	D4	42/71 (59%)	19 (45%)	13 (31%)	10 (24%)	0	0
31	B5	57/60 (95%)	33 (58%)	14 (25%)	10 (18%)	0	0
31	D5	57/60 (95%)	35 (61%)	13 (23%)	9 (16%)	0	1
32	B6	48/54 (89%)	20 (42%)	11 (23%)	17 (35%)	0	0
32	D6	48/54 (89%)	23 (48%)	13 (27%)	12 (25%)	0	0
33	B7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	10	46
33	D7	46/49 (94%)	31 (67%)	14 (30%)	1 (2%)	10	46
34	B8	61/65 (94%)	39 (64%)	15 (25%)	7 (12%)	1	4
34	D8	61/65 (94%)	40 (66%)	12 (20%)	9 (15%)	0	2
35	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	2
35	D9	35/37 (95%)	18 (51%)	10 (29%)	7 (20%)	0	0
38	BC	226/229 (99%)	159 (70%)	52 (23%)	15 (7%)	2	15
38	DC	226/229 (99%)	153 (68%)	54 (24%)	19 (8%)	1	9
39	BD	273/276 (99%)	194 (71%)	51 (19%)	28 (10%)	1	6
39	DD	273/276 (99%)	200 (73%)	47 (17%)	26 (10%)	1	7
40	BE	202/206 (98%)	133 (66%)	41 (20%)	28 (14%)	0	2
40	DE	202/206 (98%)	134 (66%)	37 (18%)	31 (15%)	0	1
41	BF	205/210 (98%)	137 (67%)	40 (20%)	28 (14%)	0	2
41	DF	205/210 (98%)	140 (68%)	37 (18%)	28 (14%)	0	2
42	BG	179/182 (98%)	109 (61%)	44 (25%)	26 (14%)	0	2
42	DG	179/182 (98%)	103 (58%)	40 (22%)	36 (20%)	0	0
43	BH	157/180 (87%)	94 (60%)	40 (26%)	23 (15%)	0	2
43	DH	157/180 (87%)	94 (60%)	39 (25%)	24 (15%)	0	1
46	BN	136/140 (97%)	85 (62%)	29 (21%)	22 (16%)	0	0
46	DN	136/140 (97%)	89 (65%)	27 (20%)	20 (15%)	0	2
47	BO	120/122 (98%)	102 (85%)	10 (8%)	8 (7%)	2	14
47	DO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	3	18
48	BP	144/150 (96%)	66 (46%)	39 (27%)	39 (27%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DP	144/150 (96%)	68 (47%)	39 (27%)	37 (26%)	0	0
49	BQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	6
49	DQ	139/141 (99%)	102 (73%)	29 (21%)	8 (6%)	3	18
50	BR	115/118 (98%)	79 (69%)	17 (15%)	19 (16%)	0	0
50	DR	115/118 (98%)	69 (60%)	24 (21%)	22 (19%)	0	0
51	BS	96/112 (86%)	53 (55%)	24 (25%)	19 (20%)	0	0
51	DS	96/112 (86%)	52 (54%)	23 (24%)	21 (22%)	0	0
52	BT	135/146 (92%)	79 (58%)	32 (24%)	24 (18%)	0	0
52	DT	135/146 (92%)	77 (57%)	34 (25%)	24 (18%)	0	0
53	BU	115/118 (98%)	75 (65%)	27 (24%)	13 (11%)	1	4
53	DU	115/118 (98%)	76 (66%)	25 (22%)	14 (12%)	1	4
54	BV	99/101 (98%)	63 (64%)	23 (23%)	13 (13%)	0	3
54	DV	99/101 (98%)	61 (62%)	26 (26%)	12 (12%)	1	4
55	BW	111/113 (98%)	79 (71%)	21 (19%)	11 (10%)	1	6
55	DW	111/113 (98%)	81 (73%)	20 (18%)	10 (9%)	1	8
56	BX	90/96 (94%)	64 (71%)	21 (23%)	5 (6%)	3	19
56	DX	90/96 (94%)	64 (71%)	19 (21%)	7 (8%)	1	11
57	BY	98/110 (89%)	39 (40%)	27 (28%)	32 (33%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	114 (63%)	39 (22%)	28 (16%)	0	1
58	DZ	181/206 (88%)	106 (59%)	34 (19%)	41 (23%)	0	0
All	All	12270/13098 (94%)	8296 (68%)	2465 (20%)	1509 (12%)	1	3

5 of 1509 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	18	GLY
2	AB	77	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	174 (86%)	28 (14%)	5	21
2	CB	202/220 (92%)	173 (86%)	29 (14%)	5	19
3	AC	160/188 (85%)	139 (87%)	21 (13%)	6	23
3	CC	160/188 (85%)	141 (88%)	19 (12%)	8	27
4	AD	180/181 (99%)	150 (83%)	30 (17%)	3	11
4	CD	180/181 (99%)	151 (84%)	29 (16%)	3	13
5	AE	115/123 (94%)	104 (90%)	11 (10%)	12	42
5	CE	115/123 (94%)	103 (90%)	12 (10%)	10	36
6	AF	90/90 (100%)	76 (84%)	14 (16%)	4	14
6	CF	90/90 (100%)	77 (86%)	13 (14%)	5	19
7	AG	126/127 (99%)	116 (92%)	10 (8%)	18	55
7	CG	126/127 (99%)	118 (94%)	8 (6%)	25	66
8	AH	119/119 (100%)	105 (88%)	14 (12%)	8	29
8	CH	119/119 (100%)	106 (89%)	13 (11%)	9	34
9	AI	98/99 (99%)	84 (86%)	14 (14%)	5	19
9	CI	98/99 (99%)	86 (88%)	12 (12%)	7	26
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	8	31
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	11	37
11	AK	90/99 (91%)	84 (93%)	6 (7%)	23	63
11	CK	90/99 (91%)	81 (90%)	9 (10%)	11	38
12	AL	104/108 (96%)	84 (81%)	20 (19%)	2	9
12	CL	104/108 (96%)	84 (81%)	20 (19%)	2	9
13	AM	99/101 (98%)	85 (86%)	14 (14%)	5	20
13	CM	99/101 (98%)	90 (91%)	9 (9%)	14	45
14	AN	49/50 (98%)	41 (84%)	8 (16%)	3	12
14	CN	49/50 (98%)	40 (82%)	9 (18%)	2	9
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CO	79/80 (99%)	69 (87%)	10 (13%)	6	24
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	33
16	CP	72/74 (97%)	66 (92%)	6 (8%)	16	53
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	12	42
18	AR	61/77 (79%)	55 (90%)	6 (10%)	12	40
18	CR	61/77 (79%)	54 (88%)	7 (12%)	8	31
19	AS	69/80 (86%)	56 (81%)	13 (19%)	2	9
19	CS	69/80 (86%)	57 (83%)	12 (17%)	3	11
20	AT	76/82 (93%)	70 (92%)	6 (8%)	18	55
20	CT	76/82 (93%)	69 (91%)	7 (9%)	13	45
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	72
21	CU	19/22 (86%)	17 (90%)	2 (10%)	10	35
25	AZ	322/338 (95%)	281 (87%)	41 (13%)	6	24
25	CZ	322/338 (95%)	284 (88%)	38 (12%)	8	29
26	B0	66/67 (98%)	57 (86%)	9 (14%)	5	21
26	D0	66/67 (98%)	56 (85%)	10 (15%)	4	16
27	B1	78/83 (94%)	67 (86%)	11 (14%)	5	20
27	D1	78/83 (94%)	64 (82%)	14 (18%)	2	10
28	B2	66/67 (98%)	54 (82%)	12 (18%)	2	10
28	D2	66/67 (98%)	60 (91%)	6 (9%)	14	45
29	B3	51/52 (98%)	46 (90%)	5 (10%)	12	40
29	D3	51/52 (98%)	47 (92%)	4 (8%)	18	57
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	28 (72%)	11 (28%)	0	1
31	B5	51/52 (98%)	48 (94%)	3 (6%)	28	68
31	D5	51/52 (98%)	45 (88%)	6 (12%)	8	29
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	6
32	D6	49/52 (94%)	40 (82%)	9 (18%)	2	9
33	B7	41/42 (98%)	34 (83%)	7 (17%)	3	11
33	D7	41/42 (98%)	34 (83%)	7 (17%)	3	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	B8	53/55 (96%)	43 (81%)	10 (19%)	2	9
34	D8	53/55 (96%)	44 (83%)	9 (17%)	3	11
35	B9	34/34 (100%)	28 (82%)	6 (18%)	3	10
35	D9	34/34 (100%)	31 (91%)	3 (9%)	14	49
38	BC	180/181 (99%)	164 (91%)	16 (9%)	14	47
38	DC	180/181 (99%)	167 (93%)	13 (7%)	21	60
39	BD	217/218 (100%)	185 (85%)	32 (15%)	4	18
39	DD	217/218 (100%)	185 (85%)	32 (15%)	4	18
40	BE	165/166 (99%)	142 (86%)	23 (14%)	5	21
40	DE	165/166 (99%)	139 (84%)	26 (16%)	4	14
41	BF	165/166 (99%)	156 (94%)	9 (6%)	30	71
41	DF	165/166 (99%)	158 (96%)	7 (4%)	40	81
42	BG	155/156 (99%)	133 (86%)	22 (14%)	5	20
42	DG	155/156 (99%)	131 (84%)	24 (16%)	4	14
43	BH	132/148 (89%)	117 (89%)	15 (11%)	8	31
43	DH	132/148 (89%)	115 (87%)	17 (13%)	6	24
46	BN	117/119 (98%)	102 (87%)	15 (13%)	6	24
46	DN	117/119 (98%)	104 (89%)	13 (11%)	9	33
47	BO	100/100 (100%)	88 (88%)	12 (12%)	7	27
47	DO	100/100 (100%)	90 (90%)	10 (10%)	11	38
48	BP	112/116 (97%)	95 (85%)	17 (15%)	4	16
48	DP	112/116 (97%)	90 (80%)	22 (20%)	2	8
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	7	24
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	7	24
50	BR	100/101 (99%)	86 (86%)	14 (14%)	5	21
50	DR	100/101 (99%)	86 (86%)	14 (14%)	5	21
51	BS	77/88 (88%)	66 (86%)	11 (14%)	5	19
51	DS	77/88 (88%)	66 (86%)	11 (14%)	5	19
52	BT	120/127 (94%)	98 (82%)	22 (18%)	2	10
52	DT	120/127 (94%)	99 (82%)	21 (18%)	3	11
53	BU	92/94 (98%)	82 (89%)	10 (11%)	9	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	DU	92/94 (98%)	83 (90%)	9 (10%)	12	40
54	BV	82/82 (100%)	66 (80%)	16 (20%)	2	8
54	DV	82/82 (100%)	69 (84%)	13 (16%)	4	13
55	BW	91/92 (99%)	80 (88%)	11 (12%)	7	27
55	DW	91/92 (99%)	81 (89%)	10 (11%)	9	34
56	BX	74/78 (95%)	65 (88%)	9 (12%)	7	26
56	DX	74/78 (95%)	68 (92%)	6 (8%)	17	53
57	BY	84/91 (92%)	71 (84%)	13 (16%)	4	14
57	DY	84/91 (92%)	71 (84%)	13 (16%)	4	14
58	BZ	161/179 (90%)	137 (85%)	24 (15%)	4	17
58	DZ	161/179 (90%)	133 (83%)	28 (17%)	3	11
All	All	10350/10854 (95%)	9007 (87%)	1343 (13%)	6	23

5 of 1343 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	13	ARG
4	CD	179	GLU
51	DS	99	LYS
55	BW	39	THR
2	CB	32	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	66	ASN
5	CE	78	HIS
48	DP	38	GLN
54	BV	64	HIS
2	CB	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	236 (15%)	51 (3%)
1	CA	1503/1522 (98%)	237 (15%)	46 (3%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AV	75/76 (98%)	17 (22%)	1 (1%)
22	AW	75/76 (98%)	21 (28%)	0
22	CV	75/76 (98%)	21 (28%)	0
22	CW	75/76 (98%)	21 (28%)	2 (2%)
23	AX	16/27 (59%)	5 (31%)	0
23	CX	17/27 (62%)	6 (35%)	1 (5%)
24	AY	74/77 (96%)	29 (39%)	4 (5%)
24	CY	74/77 (96%)	27 (36%)	3 (4%)
36	BA	2900/2915 (99%)	525 (18%)	49 (1%)
36	DA	2900/2915 (99%)	520 (17%)	46 (1%)
37	BB	118/122 (96%)	26 (22%)	2 (1%)
37	DB	118/122 (96%)	24 (20%)	3 (2%)
All	All	9523/9630 (98%)	1715 (18%)	208 (2%)

5 of 1715 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2036	C
1	CA	266	G
36	DA	2033	A
36	BA	2131	G
37	BB	56	G

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

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

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

the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	H2U	AY	16	24	19,21,22	1.07	1 (5%)	27,30,33	1.77	4 (14%)
24	H2U	AY	17	24	19,21,22	0.97	1 (5%)	27,30,33	1.87	7 (25%)
24	H2U	AY	20	24	19,21,22	1.14	2 (10%)	27,30,33	1.90	7 (25%)
24	OMC	AY	32	24	20,22,23	1.13	2 (10%)	25,31,34	0.91	2 (8%)
24	MIA	AY	37	24	29,31,32	1.39	5 (17%)	41,44,47	2.00	7 (17%)
24	7MG	AY	46	24	24,26,27	2.21	4 (16%)	34,39,42	2.37	6 (17%)
24	5MU	AY	54	24	20,22,23	1.05	2 (10%)	25,32,35	1.37	3 (12%)
24	PSU	AY	55	24	19,21,22	1.10	3 (15%)	23,30,33	1.30	4 (17%)
24	4SU	AY	8	24	19,21,22	1.55	5 (26%)	23,30,33	24.22	1 (4%)
24	H2U	CY	16	24	19,21,22	1.08	1 (5%)	27,30,33	1.74	4 (14%)
24	H2U	CY	17	24	19,21,22	1.04	2 (10%)	27,30,33	1.87	6 (22%)
24	H2U	CY	20	24	19,21,22	1.22	3 (15%)	27,30,33	1.92	7 (25%)
24	OMC	CY	32	24	20,22,23	1.35	3 (15%)	25,31,34	0.89	2 (8%)
24	MIA	CY	37	24	29,31,32	1.97	5 (17%)	41,44,47	1.89	6 (14%)
24	7MG	CY	46	24	24,26,27	2.34	3 (12%)	34,39,42	2.39	6 (17%)
24	5MU	CY	54	24	20,22,23	1.06	2 (10%)	25,32,35	1.38	2 (8%)
24	PSU	CY	55	24	19,21,22	0.99	2 (10%)	23,30,33	1.34	4 (17%)
24	4SU	CY	8	24	19,21,22	1.59	4 (21%)	23,30,33	24.89	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	16	24	-	0/8/38/39	0/2/2/2
24	H2U	AY	17	24	-	0/8/38/39	0/2/2/2
24	H2U	AY	20	24	-	0/8/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/8/27/28	0/2/2/2
24	MIA	AY	37	24	-	0/16/33/34	0/3/3/3
24	7MG	AY	46	24	-	0/8/37/38	0/3/3/3
24	5MU	AY	54	24	-	0/6/25/26	0/2/2/2
24	PSU	AY	55	24	-	0/8/25/26	0/2/2/2
24	4SU	AY	8	24	-	0/6/25/26	0/2/2/2
24	H2U	CY	16	24	-	0/8/38/39	0/2/2/2
24	H2U	CY	17	24	-	0/8/38/39	0/2/2/2
24	H2U	CY	20	24	-	0/8/38/39	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OMC	CY	32	24	-	0/8/27/28	0/2/2/2
24	MIA	CY	37	24	-	0/16/33/34	0/3/3/3
24	7MG	CY	46	24	-	0/8/37/38	0/3/3/3
24	5MU	CY	54	24	-	0/6/25/26	0/2/2/2
24	PSU	CY	55	24	-	0/8/25/26	0/2/2/2
24	4SU	CY	8	24	-	0/6/25/26	0/2/2/2

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-10.29	1.38	1.46
24	AY	46	7MG	C8-N9	-9.50	1.38	1.46
24	CY	37	MIA	C2-S10	7.77	1.82	1.75
24	CY	8	4SU	C5-C4	4.39	1.43	1.38
24	AY	8	4SU	C5-C4	3.84	1.43	1.38

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	8	4SU	C4-N3-C2	119.32	126.70	121.60
24	AY	8	4SU	C4-N3-C2	116.12	126.57	121.60
24	AY	37	MIA	C11-S10-C2	9.20	108.91	102.23
24	AY	46	7MG	C6-N1-C2	9.09	125.33	120.20
24	CY	46	7MG	C6-N1-C2	9.03	125.30	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
60	GDP	AZ	501	-	30,30,30	1.80	5 (16%)	45,47,47	2.50	11 (24%)
61	KIR	AZ	502	-	59,59,59	3.65	23 (38%)	82,84,84	1.70	17 (20%)
60	GDP	CZ	501	-	30,30,30	1.85	7 (23%)	45,47,47	4.73	8 (17%)
61	KIR	CZ	502	-	59,59,59	3.80	26 (44%)	82,84,84	1.63	16 (19%)

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
60	GDP	AZ	501	-	-	0/16/32/32	0/3/3/3
61	KIR	AZ	502	-	-	0/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/16/32/32	0/3/3/3
61	KIR	CZ	502	-	-	0/54/98/98	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-13.60	1.22	1.44
61	AZ	502	KIR	O18-C17	-13.44	1.23	1.44
61	CZ	502	KIR	O30-C30	-12.01	1.17	1.42
61	AZ	502	KIR	O30-C30	-11.97	1.17	1.42
61	AZ	502	KIR	O34-C33	-11.27	1.29	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CZ	501	GDP	C6-C5-N7	-30.05	130.09	134.14
60	AZ	501	GDP	C5-C4-N3	-7.40	117.55	126.07
60	AZ	501	GDP	C4-C5-N7	-6.85	102.80	109.41
61	AZ	502	KIR	C45-C28-C27	5.79	114.07	108.38
61	CZ	502	KIR	O29-C29-O34	-5.40	101.42	110.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	-0.33	10 (0%) 84 32	21, 54, 143, 200	0
1	CA	1504/1522 (98%)	-0.40	9 (0%) 86 36	31, 70, 146, 200	0
2	AB	234/256 (91%)	-0.14	1 (0%) 90 45	31, 60, 136, 149	0
2	CB	234/256 (91%)	-0.10	1 (0%) 90 45	46, 81, 139, 148	0
3	AC	206/239 (86%)	-0.24	0 100 100	20, 46, 78, 89	0
3	CC	206/239 (86%)	-0.13	0 100 100	49, 74, 96, 100	0
4	AD	208/209 (99%)	0.03	2 (0%) 79 23	45, 83, 112, 119	0
4	CD	208/209 (99%)	0.12	2 (0%) 79 23	64, 95, 118, 126	0
5	AE	150/162 (92%)	-0.31	0 100 100	25, 42, 69, 86	0
5	CE	150/162 (92%)	-0.23	0 100 100	43, 58, 82, 100	0
6	AF	101/101 (100%)	-0.15	1 (0%) 79 23	44, 70, 86, 94	0
6	CF	101/101 (100%)	-0.12	0 100 100	64, 86, 97, 101	0
7	AG	155/156 (99%)	-0.19	0 100 100	37, 66, 97, 113	0
7	CG	155/156 (99%)	-0.04	2 (1%) 74 19	67, 87, 107, 122	0
8	AH	138/138 (100%)	-0.30	0 100 100	31, 47, 68, 75	0
8	CH	138/138 (100%)	-0.25	0 100 100	41, 61, 75, 84	0
9	AI	127/128 (99%)	-0.12	0 100 100	32, 72, 111, 123	0
9	CI	127/128 (99%)	0.10	2 (1%) 68 15	59, 97, 119, 124	0
10	AJ	98/105 (93%)	0.06	0 100 100	30, 73, 126, 129	0
10	CJ	98/105 (93%)	0.44	6 (6%) 21 3	57, 102, 133, 137	0
11	AK	119/129 (92%)	-0.23	0 100 100	29, 45, 78, 105	0
11	CK	119/129 (92%)	-0.19	0 100 100	43, 66, 91, 106	0
12	AL	124/131 (94%)	-0.29	0 100 100	24, 49, 70, 103	0
12	CL	124/131 (94%)	-0.25	0 100 100	38, 54, 78, 111	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	-0.07	1 (0%) 83 28	46, 82, 106, 147	0
13	CM	124/126 (98%)	-0.01	4 (3%) 45 7	67, 92, 114, 148	0
14	AN	60/61 (98%)	-0.20	1 (1%) 67 15	28, 51, 84, 90	0
14	CN	60/61 (98%)	0.04	1 (1%) 67 15	65, 78, 98, 105	0
15	AO	88/89 (98%)	-0.29	0 100 100	31, 51, 79, 85	0
15	CO	88/89 (98%)	-0.23	0 100 100	41, 63, 85, 92	0
16	AP	83/88 (94%)	-0.20	0 100 100	48, 67, 85, 123	0
16	CP	83/88 (94%)	-0.20	0 100 100	62, 77, 92, 122	0
17	AQ	99/105 (94%)	-0.30	0 100 100	40, 58, 77, 85	0
17	CQ	99/105 (94%)	-0.26	0 100 100	44, 65, 85, 93	0
18	AR	70/88 (79%)	-0.24	0 100 100	35, 55, 88, 104	0
18	CR	70/88 (79%)	-0.15	0 100 100	47, 73, 100, 113	0
19	AS	78/93 (83%)	-0.02	0 100 100	48, 75, 119, 122	0
19	CS	78/93 (83%)	0.03	0 100 100	71, 91, 120, 124	0
20	AT	99/106 (93%)	-0.12	1 (1%) 79 23	65, 83, 117, 119	0
20	CT	99/106 (93%)	-0.15	0 100 100	64, 84, 117, 118	0
21	AU	24/27 (88%)	-0.31	0 100 100	45, 61, 75, 90	0
21	CU	24/27 (88%)	-0.04	0 100 100	67, 79, 92, 94	0
22	AV	76/76 (100%)	-0.43	0 100 100	35, 70, 102, 112	0
22	AW	76/76 (100%)	-0.13	0 100 100	63, 136, 178, 190	0
22	CV	76/76 (100%)	-0.46	0 100 100	48, 76, 115, 128	0
22	CW	76/76 (100%)	-0.10	2 (2%) 53 8	71, 165, 186, 196	0
23	AX	17/27 (62%)	-0.01	0 100 100	30, 82, 132, 133	0
23	CX	17/27 (62%)	0.21	0 100 100	36, 99, 145, 145	0
24	AY	76/77 (98%)	-0.35	0 100 100	37, 110, 177, 190	0
24	CY	76/77 (98%)	-0.33	0 100 100	45, 113, 178, 193	0
25	AZ	385/405 (95%)	0.17	3 (0%) 83 28	63, 105, 134, 163	0
25	CZ	385/405 (95%)	0.80	42 (10%) 6 1	93, 117, 143, 169	0
26	B0	84/85 (98%)	-0.10	2 (2%) 56 9	62, 73, 100, 114	0
26	D0	84/85 (98%)	-0.00	1 (1%) 75 20	66, 79, 101, 111	0
27	B1	93/98 (94%)	-0.11	1 (1%) 77 22	47, 63, 120, 125	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	-0.12	0 100 100	51, 74, 115, 120	0
28	B2	71/72 (98%)	0.86	13 (18%) 2 0	122, 140, 151, 153	0
28	D2	71/72 (98%)	0.06	1 (1%) 72 17	90, 106, 126, 139	0
29	B3	59/60 (98%)	-0.06	1 (1%) 67 15	59, 79, 101, 116	0
29	D3	59/60 (98%)	0.04	1 (1%) 67 15	58, 80, 97, 114	0
30	B4	44/71 (61%)	0.73	4 (9%) 9 2	102, 156, 180, 186	0
30	D4	44/71 (61%)	0.89	5 (11%) 6 1	113, 165, 186, 187	0
31	B5	59/60 (98%)	0.23	3 (5%) 27 4	52, 86, 150, 164	0
31	D5	59/60 (98%)	0.09	5 (8%) 11 2	55, 80, 148, 161	0
32	B6	50/54 (92%)	0.17	2 (4%) 36 5	55, 88, 106, 112	0
32	D6	50/54 (92%)	0.14	0 100 100	57, 95, 107, 113	0
33	B7	48/49 (97%)	-0.15	1 (2%) 60 11	47, 61, 95, 116	0
33	D7	48/49 (97%)	-0.26	0 100 100	47, 61, 91, 109	0
34	B8	63/65 (96%)	-0.11	0 100 100	55, 72, 84, 112	0
34	D8	63/65 (96%)	-0.15	0 100 100	56, 73, 85, 109	0
35	B9	37/37 (100%)	0.30	1 (2%) 52 8	79, 98, 112, 116	0
35	D9	37/37 (100%)	0.62	2 (5%) 25 4	84, 104, 115, 119	0
36	BA	2901/2915 (99%)	-0.33	43 (1%) 70 16	25, 74, 176, 200	0
36	DA	2901/2915 (99%)	-0.35	38 (1%) 74 19	32, 76, 175, 200	0
37	BB	119/122 (97%)	-0.46	0 100 100	54, 97, 123, 144	0
37	DB	119/122 (97%)	-0.52	0 100 100	61, 104, 128, 140	0
38	BC	228/229 (99%)	0.15	11 (4%) 29 4	40, 73, 163, 176	0
38	DC	228/229 (99%)	0.31	12 (5%) 25 4	64, 87, 166, 174	0
39	BD	275/276 (99%)	-0.26	0 100 100	28, 48, 78, 93	0
39	DD	275/276 (99%)	-0.24	0 100 100	28, 53, 80, 94	0
40	BE	204/206 (99%)	-0.09	1 (0%) 88 39	46, 73, 120, 129	0
40	DE	204/206 (99%)	-0.10	2 (0%) 79 23	39, 72, 122, 132	0
41	BF	207/210 (98%)	0.20	8 (3%) 37 5	42, 102, 155, 162	0
41	DF	207/210 (98%)	0.18	7 (3%) 43 6	47, 105, 155, 161	0
42	BG	181/182 (99%)	0.04	3 (1%) 67 15	66, 85, 120, 134	0
42	DG	181/182 (99%)	0.17	3 (1%) 67 15	89, 108, 130, 139	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	0.47	9 (5%)	23	3	85, 123, 148, 152	0
43	DH	159/180 (88%)	0.30	3 (1%)	64	13	85, 123, 145, 150	0
44	BJ	0/173	-	-	-	-	-	-
44	DJ	0/173	-	-	-	-	-	-
45	BK	0/147	-	-	-	-	-	-
45	DK	0/147	-	-	-	-	-	-
46	BN	138/140 (98%)	-0.07	0	100	100	56, 86, 130, 138	0
46	DN	138/140 (98%)	-0.06	0	100	100	61, 83, 132, 136	0
47	BO	122/122 (100%)	-0.24	0	100	100	43, 60, 73, 82	0
47	DO	122/122 (100%)	-0.24	0	100	100	40, 60, 73, 77	0
48	BP	146/150 (97%)	0.17	1 (0%)	84	32	49, 98, 124, 145	0
48	DP	146/150 (97%)	0.15	2 (1%)	72	17	47, 102, 126, 141	0
49	BQ	141/141 (100%)	-0.16	1 (0%)	84	32	47, 61, 84, 125	0
49	DQ	141/141 (100%)	-0.19	1 (0%)	84	32	43, 60, 87, 122	0
50	BR	117/118 (99%)	-0.06	0	100	100	55, 84, 101, 108	0
50	DR	117/118 (99%)	-0.12	0	100	100	52, 79, 97, 106	0
51	BS	98/112 (87%)	0.12	0	100	100	69, 101, 122, 126	0
51	DS	98/112 (87%)	0.27	1 (1%)	79	23	86, 106, 124, 126	0
52	BT	137/146 (93%)	0.06	4 (2%)	49	7	54, 84, 135, 163	0
52	DT	137/146 (93%)	0.04	5 (3%)	41	6	56, 81, 137, 160	0
53	BU	117/118 (99%)	-0.16	0	100	100	60, 74, 102, 111	0
53	DU	117/118 (99%)	-0.20	0	100	100	52, 74, 100, 108	0
54	BV	101/101 (100%)	0.12	2 (1%)	62	12	61, 102, 117, 121	0
54	DV	101/101 (100%)	0.18	2 (1%)	62	12	50, 102, 117, 119	0
55	BW	113/113 (100%)	-0.04	2 (1%)	65	14	60, 83, 111, 140	0
55	DW	113/113 (100%)	-0.04	1 (0%)	81	25	59, 76, 112, 143	0
56	BX	92/96 (95%)	0.04	0	100	100	69, 86, 109, 120	0
56	DX	92/96 (95%)	-0.01	0	100	100	60, 88, 108, 121	0
57	BY	100/110 (90%)	0.43	7 (7%)	16	3	103, 121, 153, 159	0
57	DY	100/110 (90%)	0.46	7 (7%)	16	3	99, 119, 153, 162	0
58	BZ	183/206 (88%)	0.09	3 (1%)	68	15	53, 85, 129, 139	0
58	DZ	183/206 (88%)	0.10	3 (1%)	68	15	59, 85, 124, 132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22012/23368 (94%)	-0.15	316 (1%) 72 17	20, 77, 144, 200	0

The worst 5 of 316 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BA	654(K)	C	11.2
38	DC	97	GLU	7.8
41	DF	1	MET	7.7
38	BC	106	GLY	7.5
1	CA	88	A	7.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	7MG	CY	46	24/25	0.19	-	125,128,129,130	0
24	H2U	AY	17	20/21	0.34	-	186,190,190,191	0
24	7MG	AY	46	24/25	0.19	-	121,123,124,124	0
24	OMC	CY	32	21/22	0.17	-	78,83,93,94	0
24	4SU	CY	8	20/21	0.19	-	115,116,119,119	0
24	H2U	AY	16	20/21	0.51	-	172,183,184,185	0
24	H2U	CY	17	20/21	0.44	-	186,194,196,196	0
24	OMC	AY	32	21/22	0.15	-	61,66,79,80	0
24	MIA	CY	37	29/30	0.23	-	52,66,80,85	0
24	H2U	CY	16	20/21	0.27	-	171,181,183,185	0
24	H2U	AY	20	20/21	0.24	-	174,177,179,179	0
24	5MU	CY	54	21/22	0.18	-	113,125,126,129	0
24	PSU	AY	55	20/21	0.17	-	130,139,140,140	0
24	PSU	CY	55	20/21	0.16	-	131,134,135,136	0
24	H2U	CY	20	20/21	0.26	-	176,177,180,180	0
24	MIA	AY	37	29/30	0.23	-	42,52,67,76	0
24	4SU	AY	8	20/21	0.18	-	110,113,114,115	0
24	5MU	AY	54	21/22	0.15	-	108,122,123,127	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
61	KIR	AZ	502	57/57	0.37	-	100,107,118,119	0
59	ZN	D9	101	1/1	0.18	-	87,87,87,87	0
59	ZN	CD	301	1/1	0.29	-	75,75,75,75	0
61	KIR	CZ	502	57/57	0.66	-	115,117,122,122	0
60	GDP	AZ	501	28/28	0.18	-	114,118,123,123	0
59	ZN	D4	101	1/1	0.12	-	103,103,103,103	0
59	ZN	AN	101	1/1	0.20	-	42,42,42,42	0
59	ZN	CN	101	1/1	0.18	-	69,69,69,69	0
60	GDP	CZ	501	28/28	0.23	-	114,131,139,140	0
59	ZN	AD	301	1/1	0.29	-	61,61,61,61	0
59	ZN	B4	101	1/1	0.19	-	91,91,91,91	0
59	ZN	B9	101	1/1	0.16	-	103,103,103,103	0

6.5 Other polymers

There are no such residues in this entry.