



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:36 PM BST

PDB ID : 4V5R
Title : The crystal structure of EF-Tu and Trp-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>

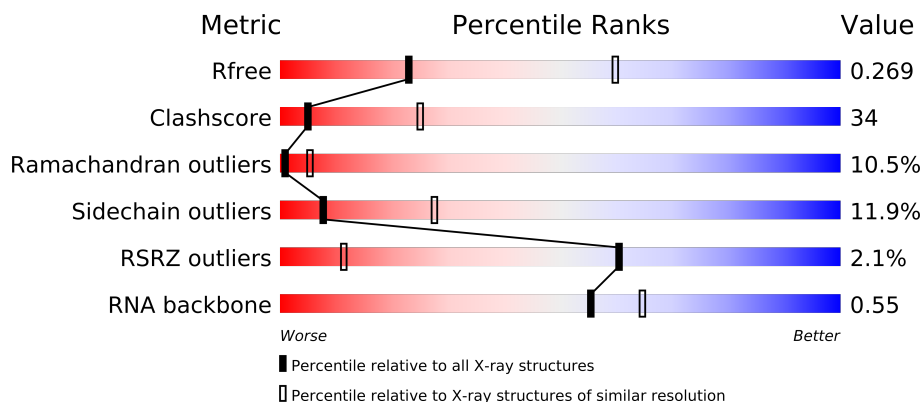
The following versions of software and data (see [references](#)) were used in the production of this report:

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	

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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	

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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	

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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 307330 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	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			
1	CA	1510	Total	C	N	O	P	0	0	0
			32451	14445	6010	10487	1509			

- 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			

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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 TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1645	742	289	536	76	2			

- 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			

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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			

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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			

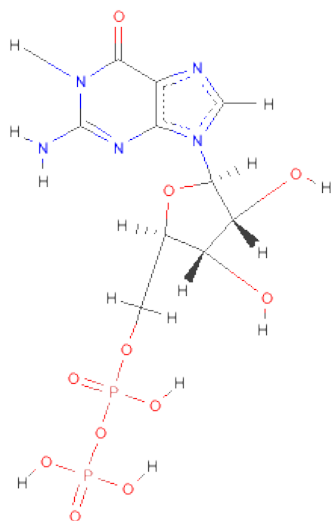
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

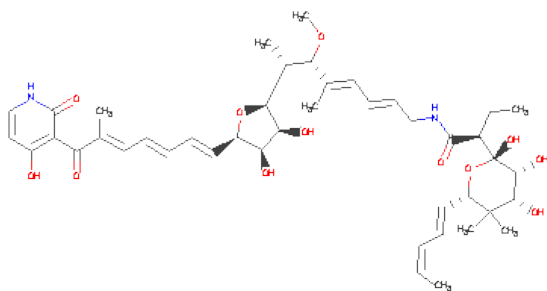
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

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

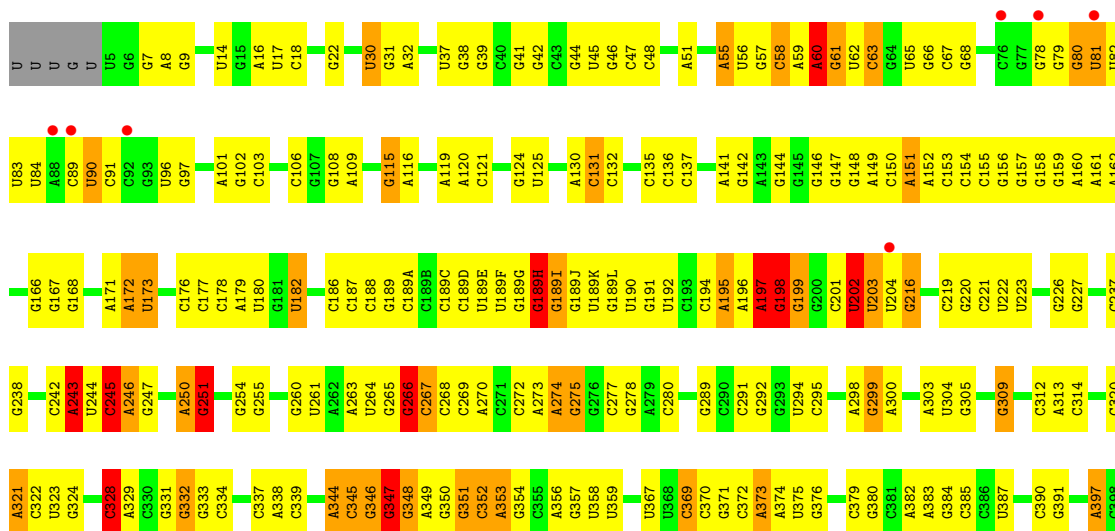


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
60	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

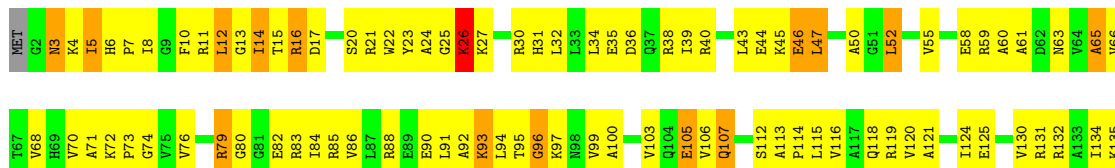
- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).



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		







M1	R2	R3	V6	R7	I8	M11	P12	M13	I14	D15	G16	S17	D18	I19	A20	L21	E22	F23	I25	T26	Q27	R28	A29	L30	E31	M32	A35	E38	K39	V40	E41	E42	L43	G44	L45	R46	R47	A53	K54	D55	P56	Q57	G58	Y59	F60	L61	R62	P63	Q64	V65	E66	M67	R68
E69	D70	R71	V72	L75	A76	R77	E78	L79	R80	I81	R82	D83	M84	V85	R86	R87	V91	K92	F97	L98	A99	M100	A101																														

[illegible][illegible]

V80	G81	G82	A83	P86	M89	E90	V91	R94	G96	A100	L101	R102	A103	L104	V105	Q106	E113	R114	R115	A116	A117	V118	R119	M125	D126	A127	G132	K136	K137	K138	V141	M144	A145	V151	A152	R155	V156														
ME1	A2	R3	R6	A7	E8	D15	L16	V17	Y18	G19	D20	V21	L22	V23	T24	A25	F26	T27	N28	V29	T30	K36	N37	L38	R41	I42	F43	Y44	D45	A46	G47	K48	L49	S50	O51	E52	K53	T54	O55	O56	E57	P58	L59	K60	A65	N68	V69	K70	V75	R78	E70

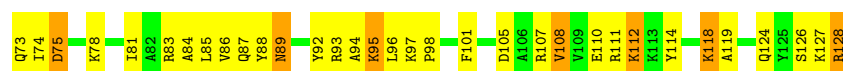
R105	G106	L107	G108	I109	A110	L111	L112	S113	T114	S115	L119	T120	D121	R122	E123	A124	R125	K126	L127	G128	V129	G130	L133	I134	G135	E136	V137	W138	M1	L2	T3	D4	P5	I6	D8	M9	L10	L13	L17	R18	V19	Y20	K21	V26	R30	F31	K32	R41	E42	G43	F44	D52	V53	D54	G55	K56	P57	Y58	L59	E77	Q78	R83	R84	R85	I86	S87	K88	P89	G90	R91	R92	V93	Y94	V97	R102	V103	E104
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

M1	L2	T3	P4	P5	I6	A7	D8	M9	L10	L13	T17	R18	V19	Y20	K21	V26	R30	F31	K32	R41	E42	G43	F44	D52	V53	D54	G55	K56	F57	Y58	L59	G71	P72	E77	K78	R83	R84	R85	S87	K88	P89	G90	R91	R92	V93	Y94	V97
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• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



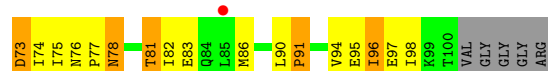
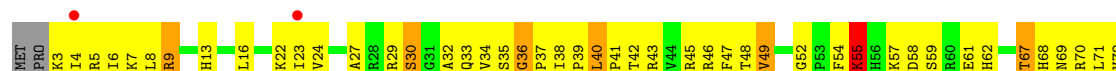
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



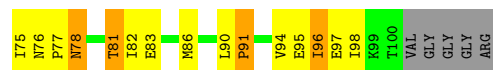
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



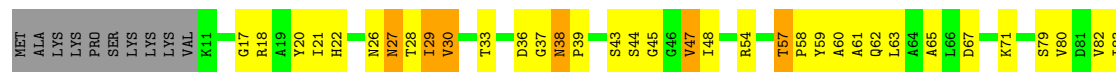
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



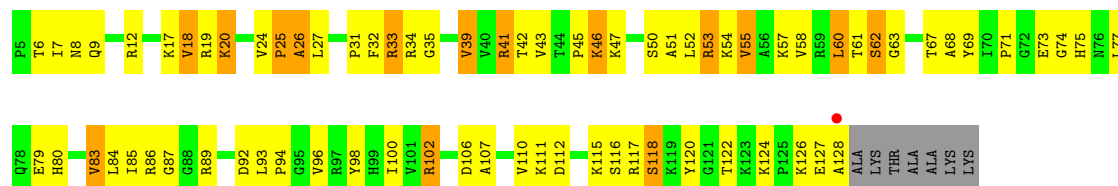
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



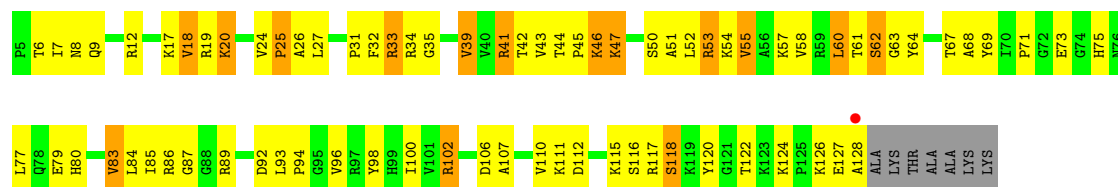
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



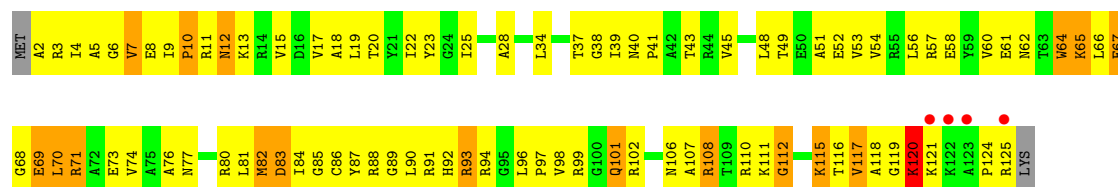
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



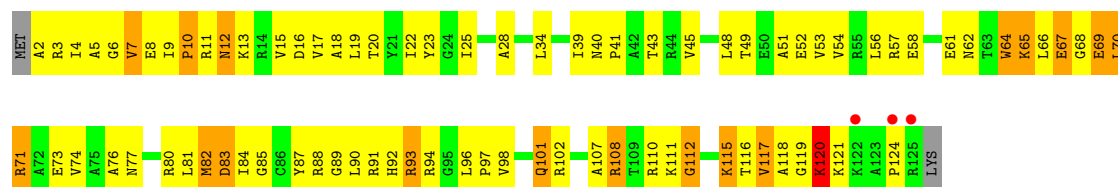
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

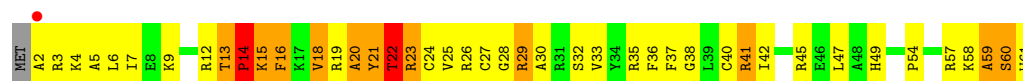
Chain AN:





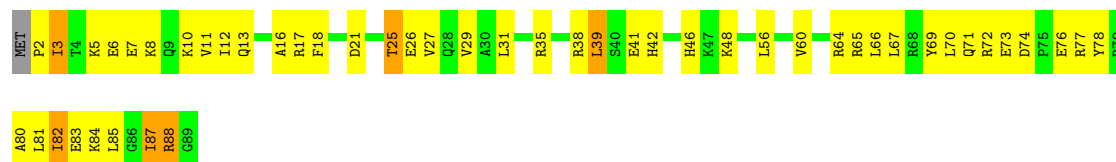
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



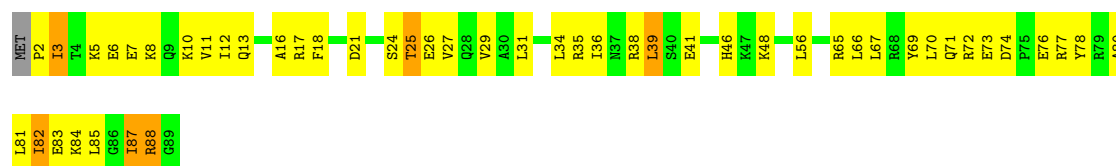
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



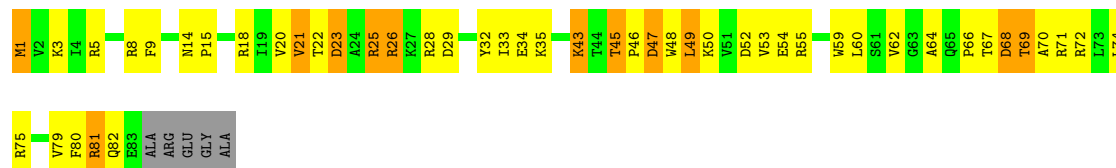
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



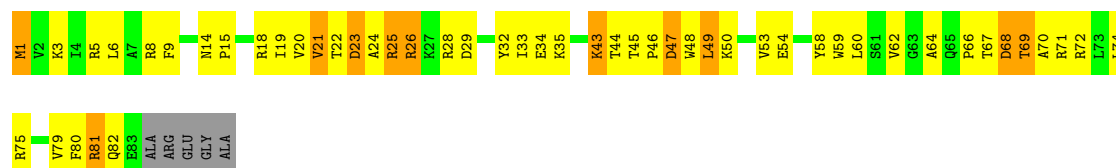
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



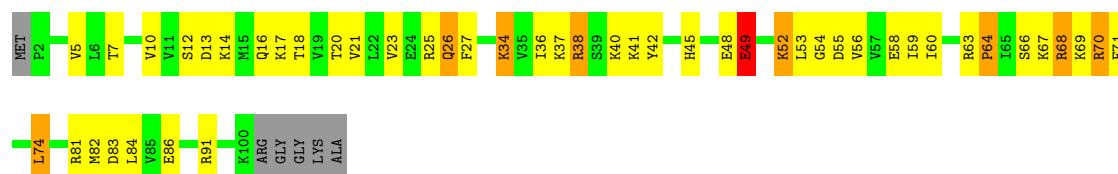
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



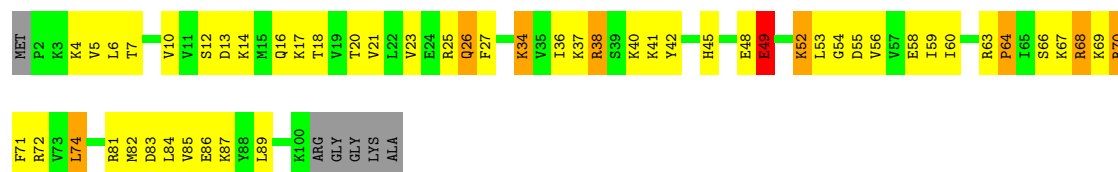
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



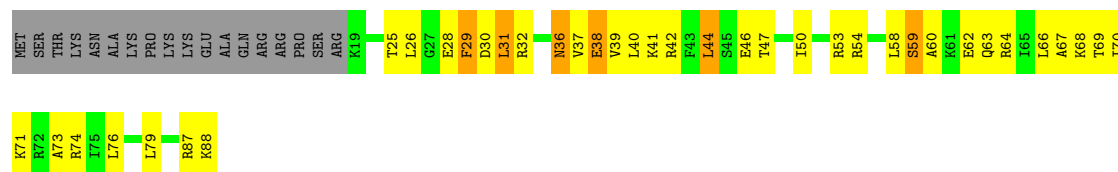
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



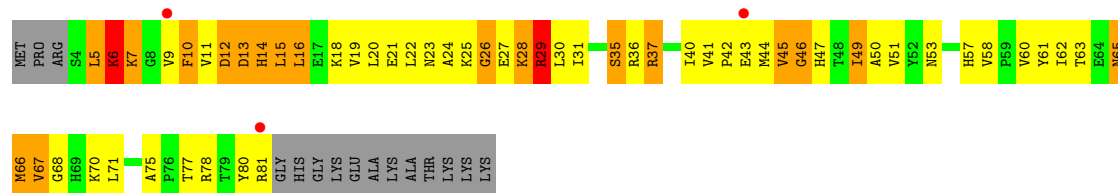
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



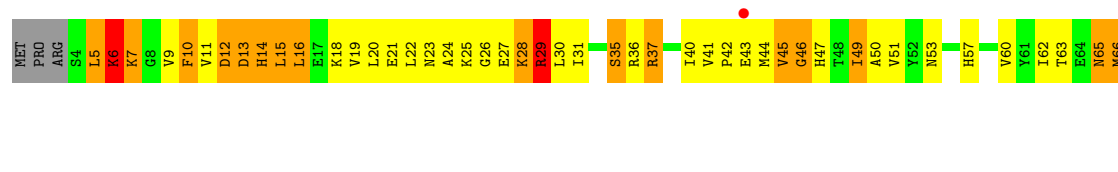
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

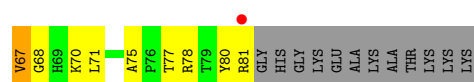
Chain AS:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

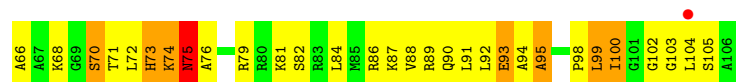
Chain CS:





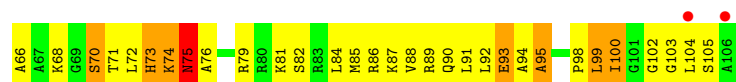
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



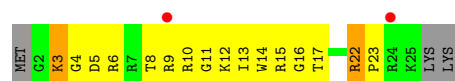
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



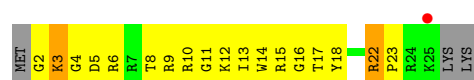
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



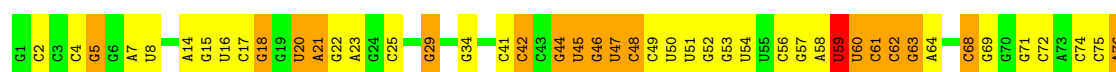
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



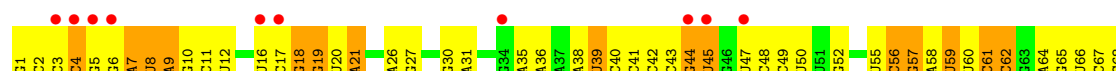
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



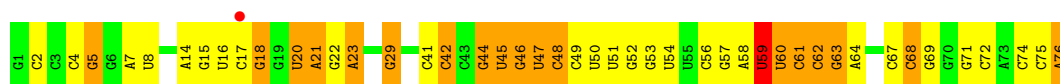
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

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:



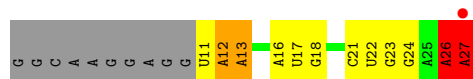
- Molecule 23: MRNA

Chain AX:



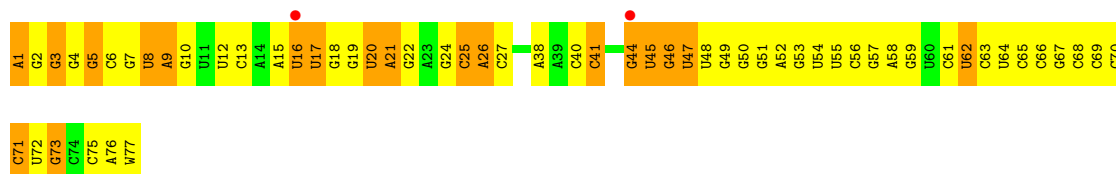
- Molecule 23: MRNA

Chain CX:



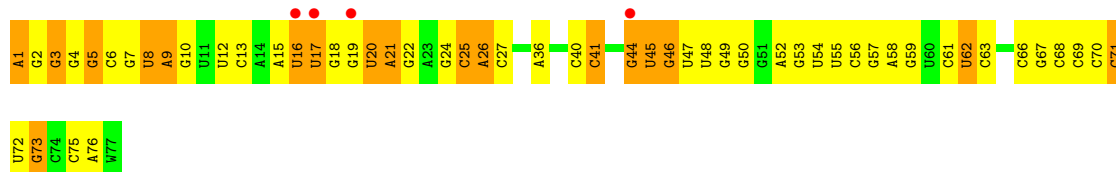
- Molecule 24: A-SITE TRNA TRP-TRNA TRP

Chain AY:



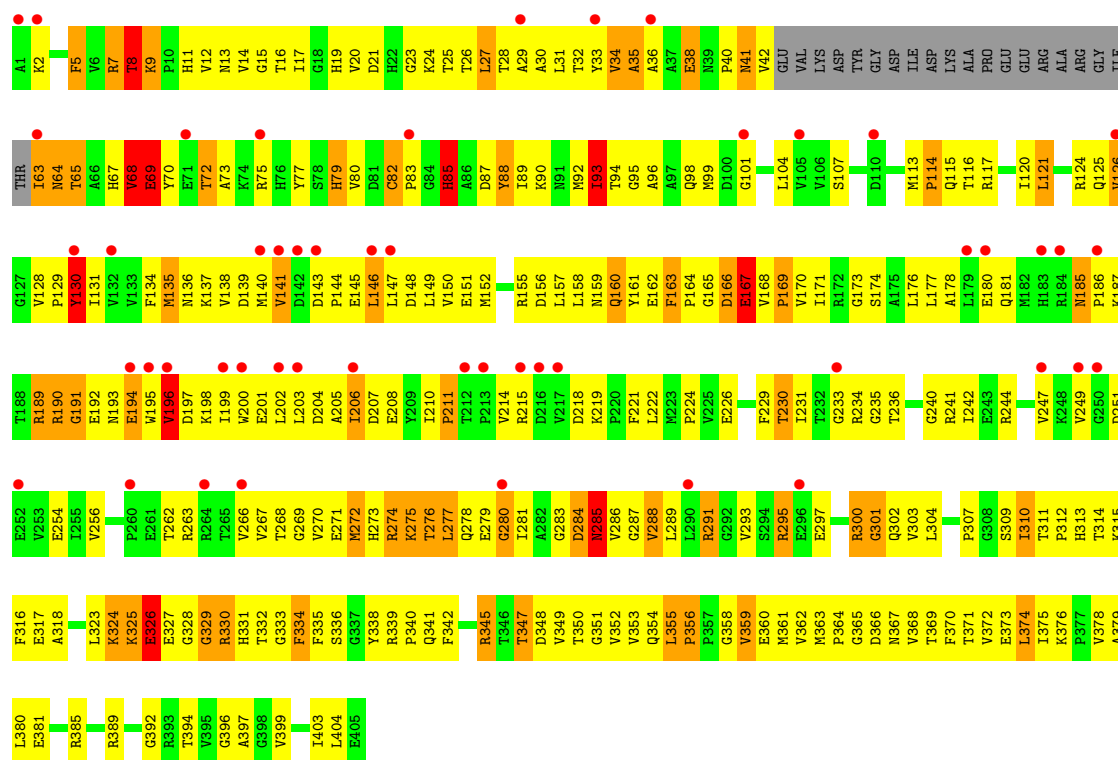
- Molecule 24: A-SITE TRNA TRP-TRNA TRP

Chain CY:



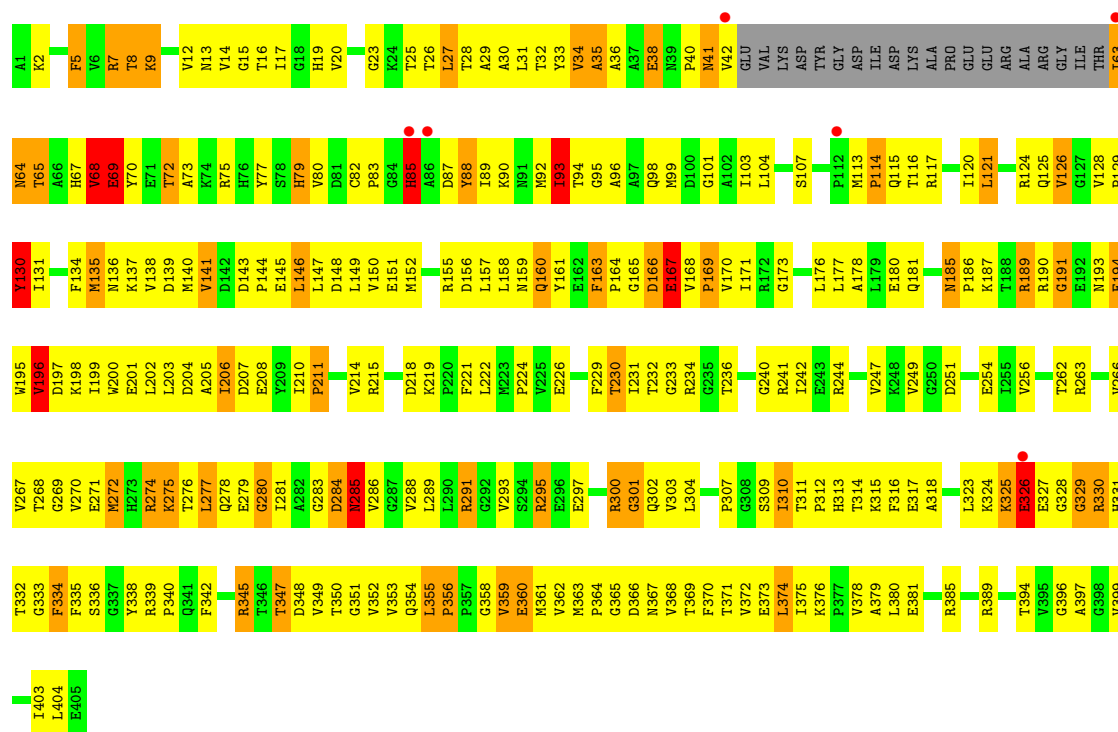
- Molecule 25: ELONGATION FACTOR TU

Chain AZ:



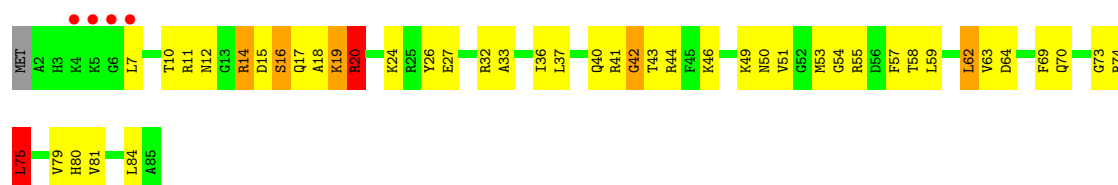
• Molecule 25: ELONGATION FACTOR TU

Chain CZ:



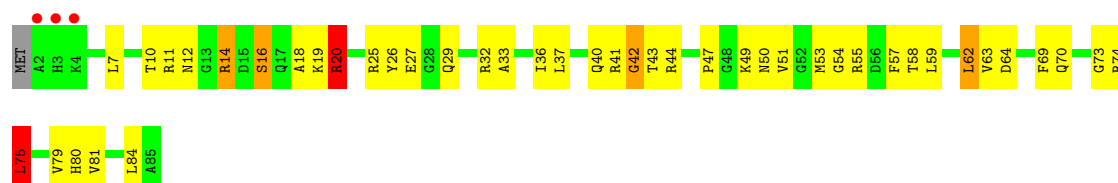
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



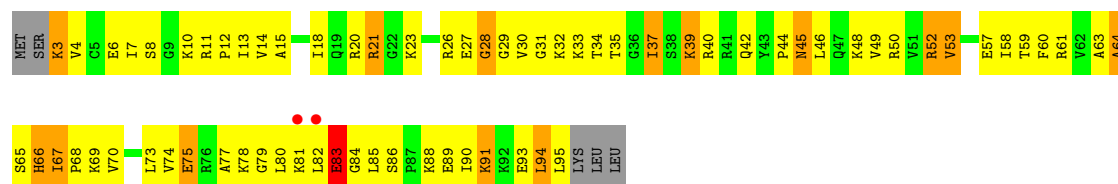
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



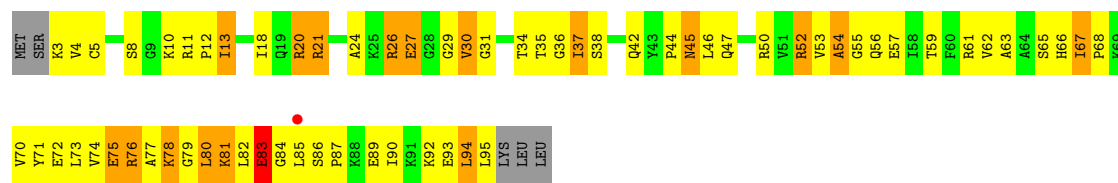
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



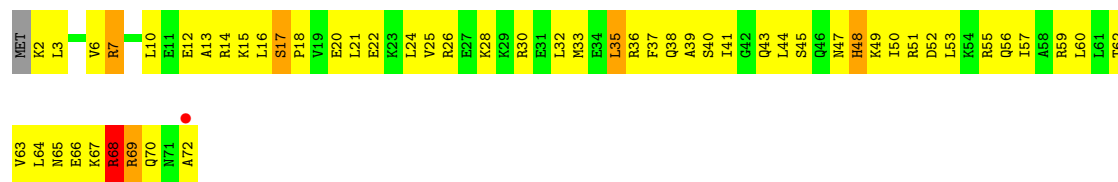
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



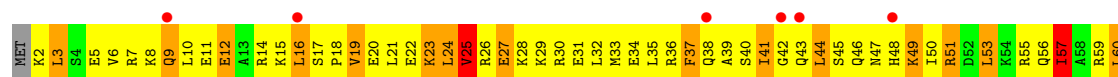
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

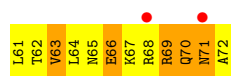
Chain B2:



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

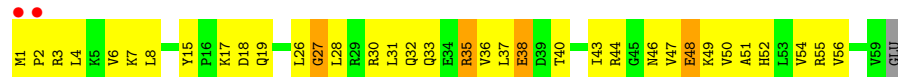
Chain D2:





• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



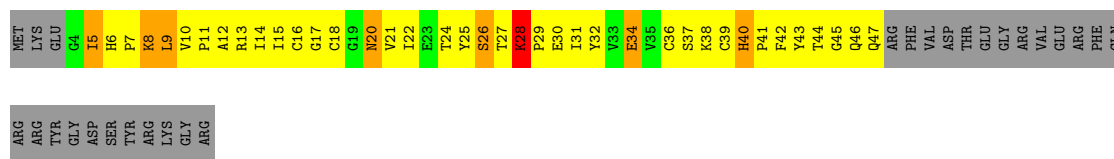
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



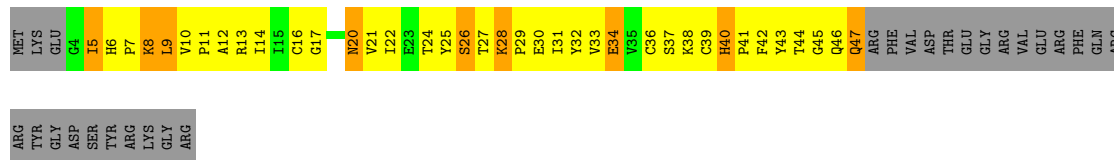
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:



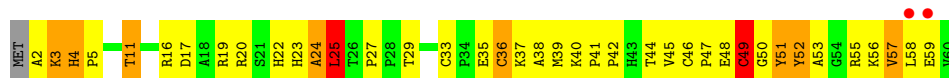
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:



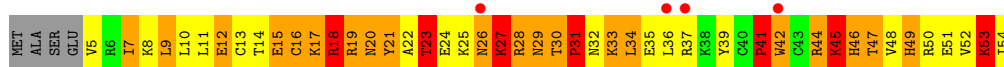
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

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:



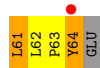
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:



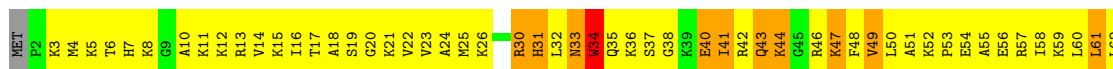
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



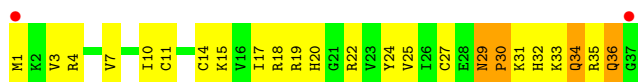
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8:



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



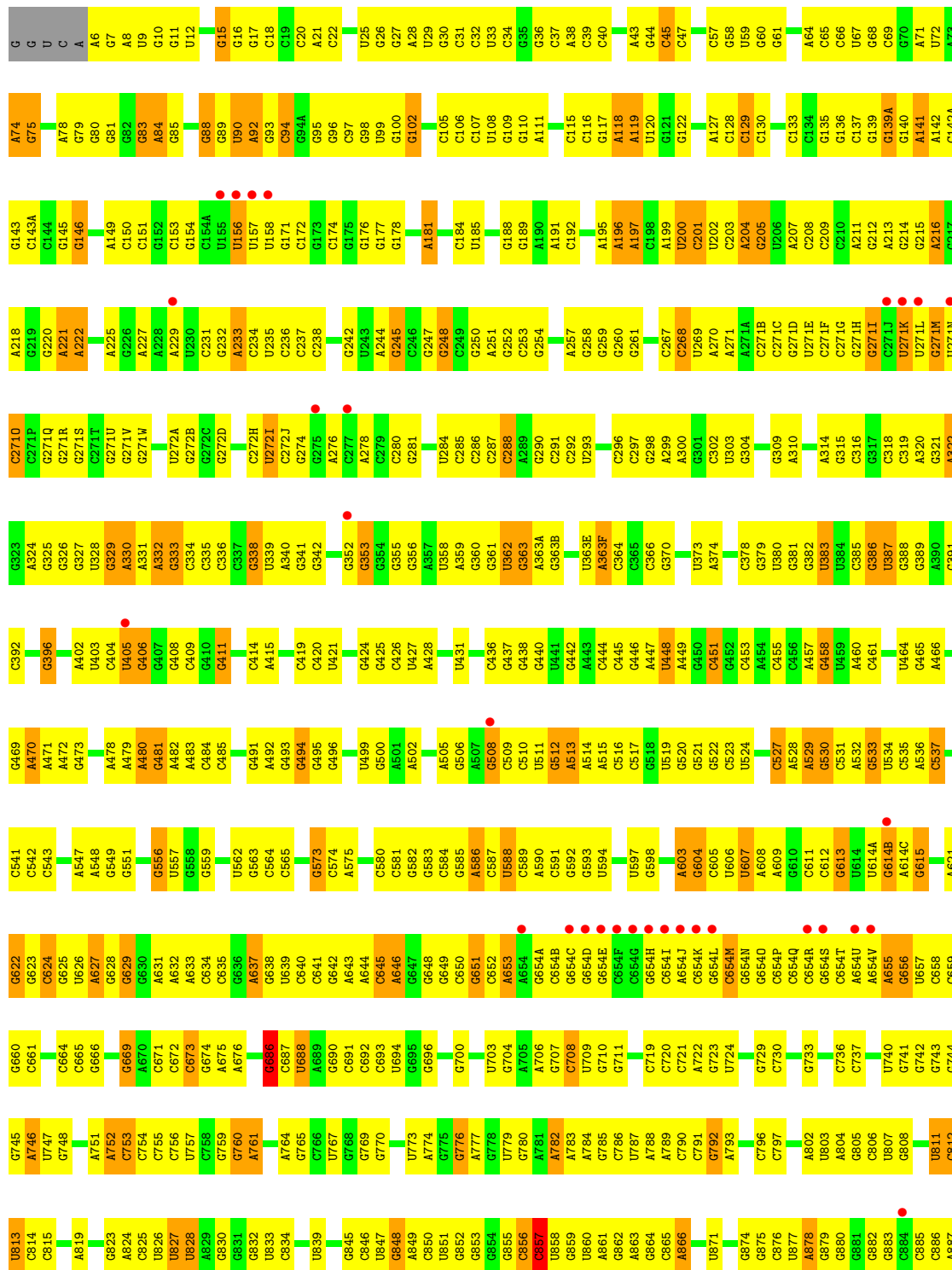
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



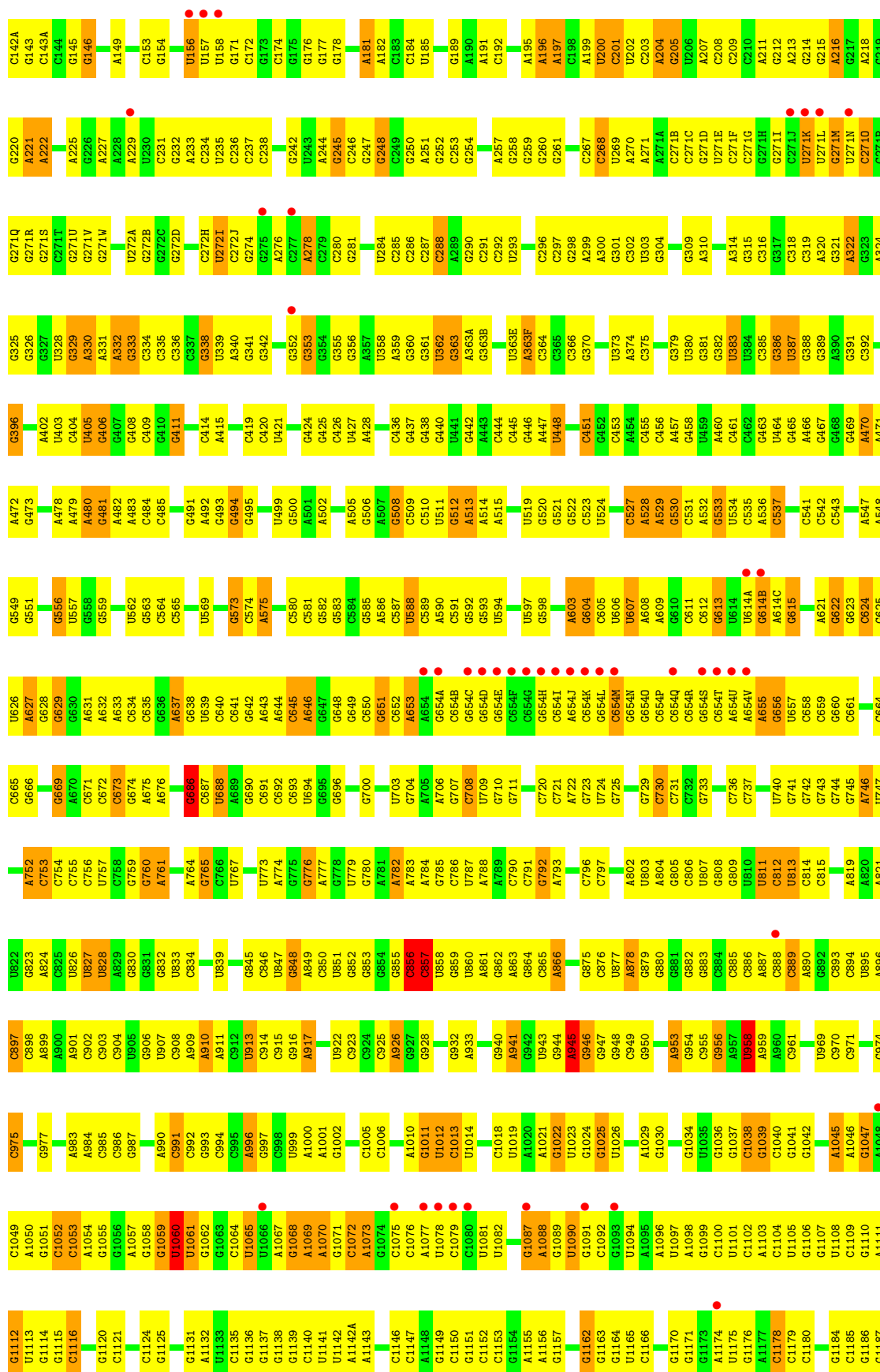
• Molecule 36: 23S RIBOSOMAL RNA

Chain BA:

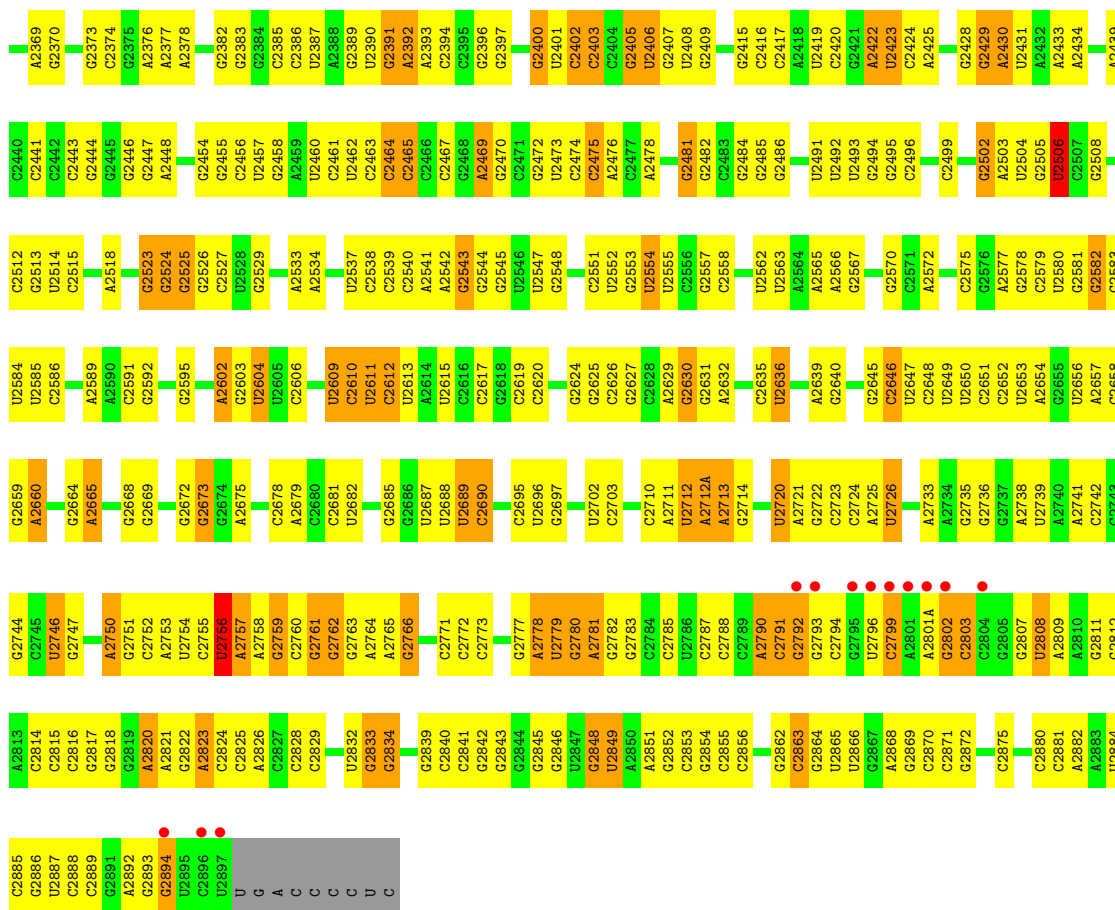


A1981	A1884	C1806	A1722	C1636	G1546	G1480	G1413	G1339	C1261	G1186	G1041	C961	C888
C1982	A1885	G1807	U1739	A1637	C1547	U1481	G1416	U1340	G1264	G1187	G1042	U969	C889
G1983	C1886	C1638	C1548	C1639	C1549	G1484	G1417	U1341	A1265	U1188	A1045	C970	A890
G1984	C1887	A1810	A1741	U1639	C1549	G1485	G1418	G1344	A1268	G1190	A1046	C971	C892
G1987	A1889	G1811	G1742	C1640	G1552	G1486	G1419	G1348	A1269	G1191	G1047	G972	C893
C1988	G1899	G1813	C1744	G1642	A1553	U1420	U1420	A1349	C1270	G1192	A1048	A973	C894
G1989	A1900	G1816	C1745	G1643	A1554	G1424	G1424	G1349	G1271	G1193	C1049	C974	U895
U1992	C1901	G1817	G1747A	G1647	C1557	G1491	G1425	U1352	A1272	U1199	G1051	C975	C897
U1993	C1902	G1818	G1748	G1648	C1558	C1492	G1426	A1353	A1273	C1200	A0582	A983	C898
C1996	G1906	A1819	A1749	G1649	G1559	A1494	A1427	A1354	A1274	G1203	C1053	A984	A900
G1997	C1907	G1820	C1751	G1651	A1567	A1496	G1428	G1355	A1276	A1204	C1054	C985	A901
G1998	C1908	G1822	C1752	G1652	C1568	U1497	G1429	G1357	G1279	U1205	G1055	C986	C902
G1999	C1909	G1826	G1753	A1653	A1569	C1498	C1430	G1358	A1277	G1206	G1056	G987	C903
G2000	G1910	G1827	C1754	A1654	A1570	C1499	G1432	A1359	A1278	G1207	C1057	C988	C904
A2001	U1911	G1828	G1755	A1571	A1571	G1500	U1433	A1360	A1279	G1208	A0588	A990	U905
U2011	A1912	G1831	G1756	C1657	U1578	C1501	A1434	G1361	A1286	C1209	G1059	C991	G906
C2006	A1913	G1832	U1757	C1658	A1579	U1503	G1436	A1362	A1287	A1210	U1060	C992	U907
C2007	C1914	G1835	G1758	A1665	A1580	C1504	C1437	G1363	A1288	G1211	U1061	G993	C908
C2008	U1915	G1836	A1762	G1666	G1581	C1505	U1438	G1364	U1289	G1212	G1063	C994	A910
C2009	A1916	C1837	G1763	G1667	C1582	C1506	U1439	A1365	C1291	A1213	C1064	A996	A911
G2010	U1917	C1838	G1764	A1668	C1583	A1507	G1440	A1366	C1293	G1215	U1065	C997	C912
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C2012	G1921	G1840	C1670	C1670	A1586	C1509	G1441	G1368	C1297	C1221A	G1068	U999	C914
A2013	G1922	G1841	U1673	U1673	A1587	A1509A	A1445	G1374	C1298	G1222	A1069	A1000	C915
A2014	C1923	U1842	G1674	C1674	C1588	A1509B	C1446A	C1375	G1299	G1223	A1070	G1002	A917
U2022	G1929	G1843	C1771	U1675	C1589	G1510	C1446	C1376	U1300	G1227	G1071	G1005	U922
G2023	U1931	C1844	G1772	U1676	C1590	C1511	G1447	G1377	A1301	G1231	C1072	C1006	C925
G2024	A1932	G1845	A1773	A1677	G1591	U1512	G1448	A1378	G1303	G1232	A1073	A1009	A926
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C2026	A1936	A1847	U1777	U1679	G1593	G1514	G1450	G1380	C1305	G1235	A1077	G1011	G928
G2027	C1937	A1848	U1778	U1680	G1594	G1515	C1450A	A1385	C1306	G1236	U1078	U1012	G932
U2028	A1938	U1849	U1779	G1681	G1595	C1516	U1453	A1386	G1311	A1247	C1079	C1013	A933
G2029	U1939	U1851	A1780	C1683	A1597	G1517	G1455	C1387	U1312	G1238	G1087	U1014	G940
A2030	U1946	A1854	C1781	C1684	C1598	U1523	C1458	G1388	U1313	U1239	A1088	C1018	G941
A2031	C1947	G1855	G1782	U1688	C1599	G1524	G1459	G1389	C1314	G1240	G1089	U1019	A941
G2032	G1954	G1856	A1783	U1689	C1600	G1525	A1460	U1390	C1315	A1241	U1090	A1020	G943
U2033	C1949	G1857	A1785	A1689	G1601	G1526	G1461	A1316	C1316	A1242	G1091	G1021	U943
G2035	A1952	G1858	A1786	G1697	U1602	G1527	C1464	A1393	C1317	G1243	C1092	G1022	G944
C2036	A1953	A1859	A1698	A1698	A1603	A1528	G1466	U1396	C1318	G1244	G1093	U1023	A945
C2039	U1955	G1860	C1699	C1699	C1607	A1529	C1467	G1400	C1320	U1246	U1094	G1024	G946
C2040	G1960	G1861	A1700	A1608	A1608	G1529	C1467	G1401	C1327	A1247	A1096	U1026	G947
C2043	A1963	G1862	A1701	A1609	A1609	U1534	C1468	C1402	G1328	G1248	U1097	C949	G948
C2044	A1964	U1863	U1709	A1610	A1610	A1535	A1469	G1403	U1329	G1170	A1098	A1029	C949
G2045	U1965	G1865	C1710	A1614	A1614	C1536	G1470	C1404	U1329	G1171	G1099	G1030	G950
C2050	C1967	C1877	C1711	G1615	G1615	G1537	A1471	U1405	C1330	G1252	C1100	U1039	A953
A2051	G1968	G1878	U1712	A1616	C1616	G1538	A1472	U1406	A1331	A1174	G1101	G1034	G954
G2052	A1969	G1879	U1713	C1617	C1617	G1539	A1473	U1407	G1332	U1175	C1102	U1035	C955
C2053	G1970	C1880	G1714	A1618	U1540	U1540	C1474	C1408	C1333	G1176	A1103	G1036	G956
A2054	A1971	G1881	G1717	G1619	G1619	G1541	G1475	C1409	G1334	G1177	C1104	G1037	A957
G2055	C1972	C1882	G1718	G1620	G1620	A1542	G1476	G1409	U1335	G1178	U1105	G1038	U958
C2056	A1973	A1634	U1719	C1621	C1621	C1543	A1477	G1411	G1337	C1179	G1106	G1039	A959
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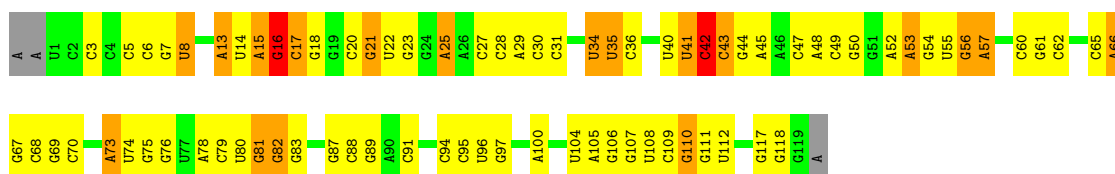


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G2207	U2214	G2207	A2208	U2218	G2219	G2220	G2223	U2215	C2224	A2225	G2228	C2229	G2230	C2231	G2238	G2239	C2240	A2241	G2242		U2245	U2246	U2247	A2248	U2249	G2250	U2257	C2258		U2262	C2263	C2264	U2265	A2266	A2267	A2268		U2272		C2275	G2276	G2277	A2278	G2279		G2282	C2283	C2284	C2285	A2286	A2287	A2288	G2289	G2290	U2291	C2292	C2293	C2296		
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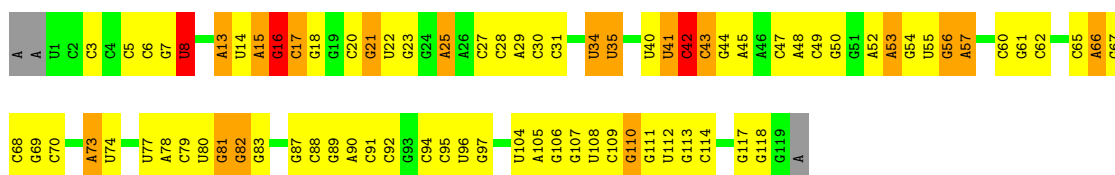
• Molecule 37: 5S RIBOSOMAL RNA

Chain BB:



• Molecule 37: 5S RIBOSOMAL RNA

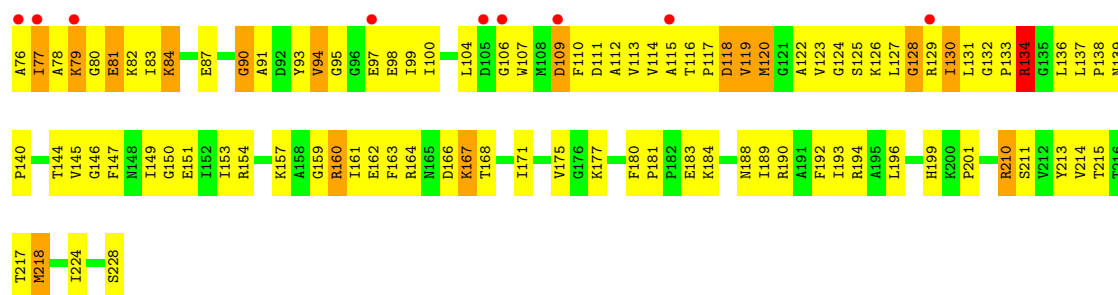
Chain DB:



• Molecule 38: 50S RIBOSOMAL PROTEIN L1

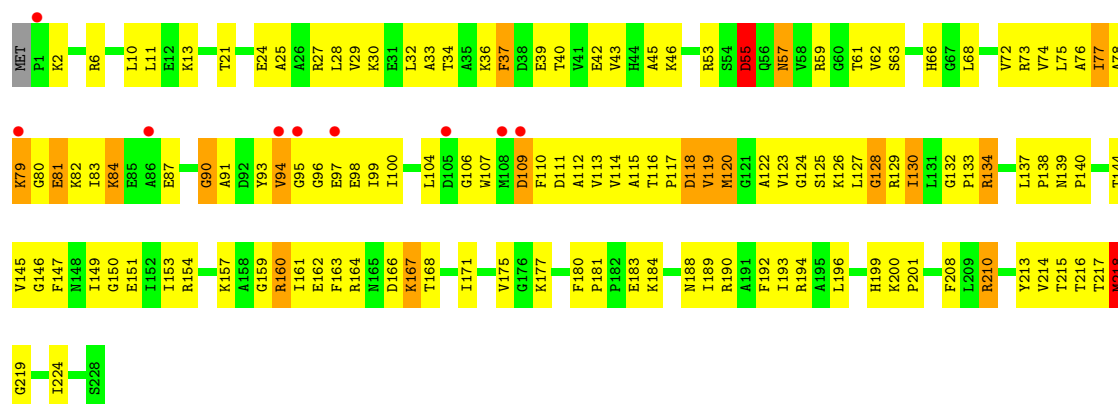
Chain BC:





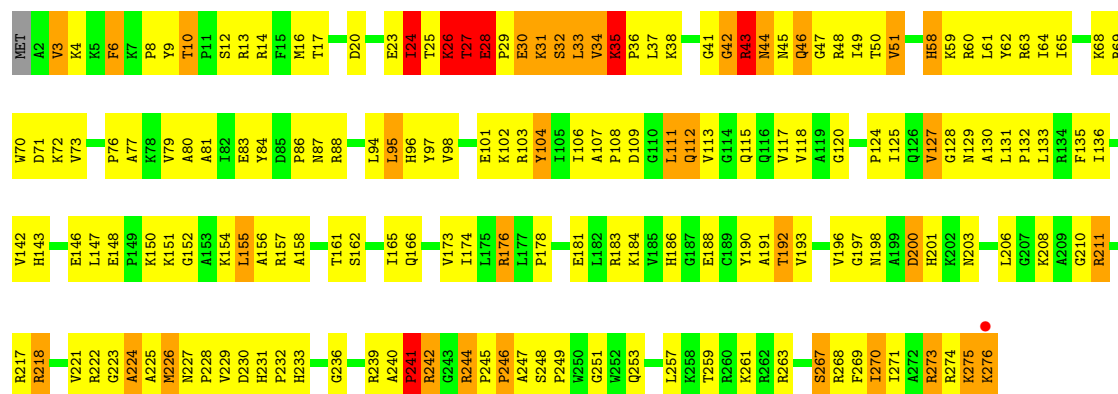
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain DC:



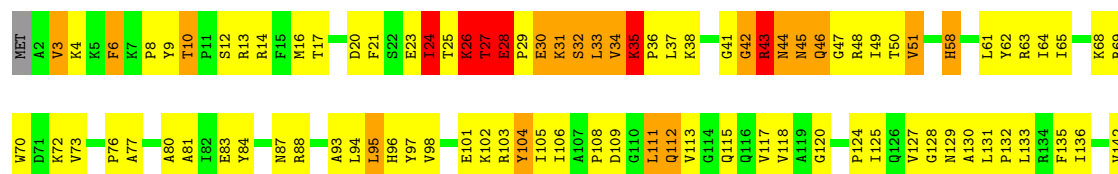
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

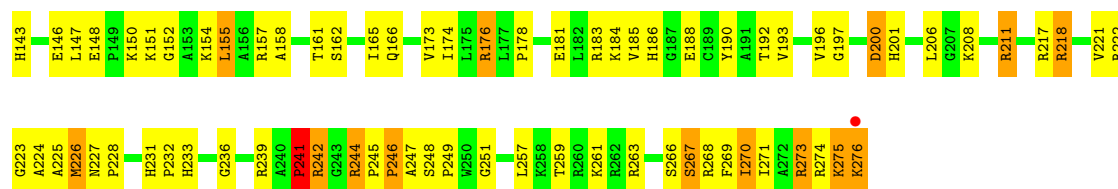
Chain BD:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

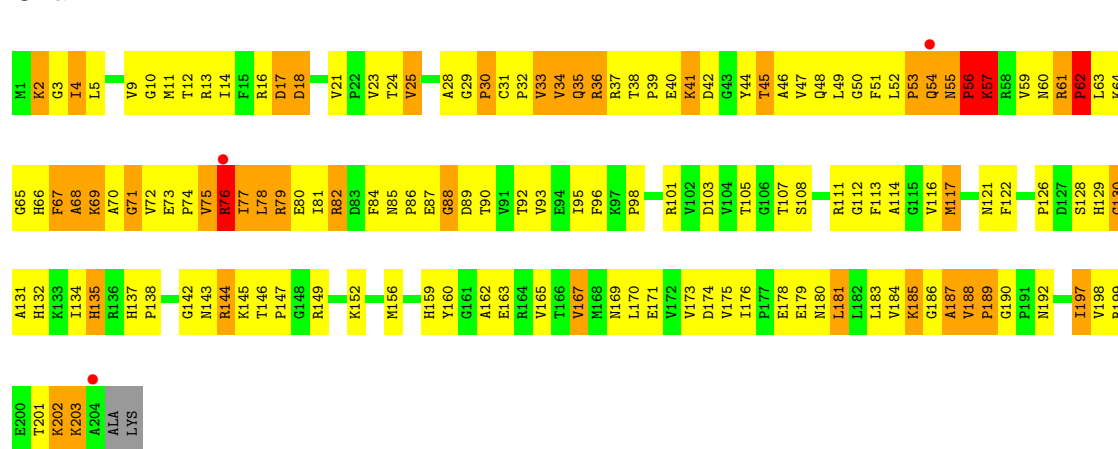
Chain DD:





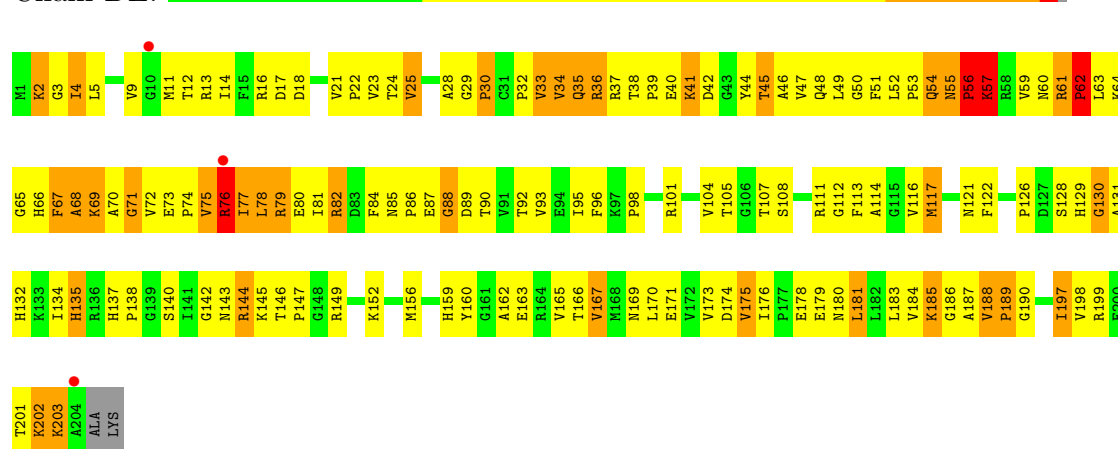
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE:



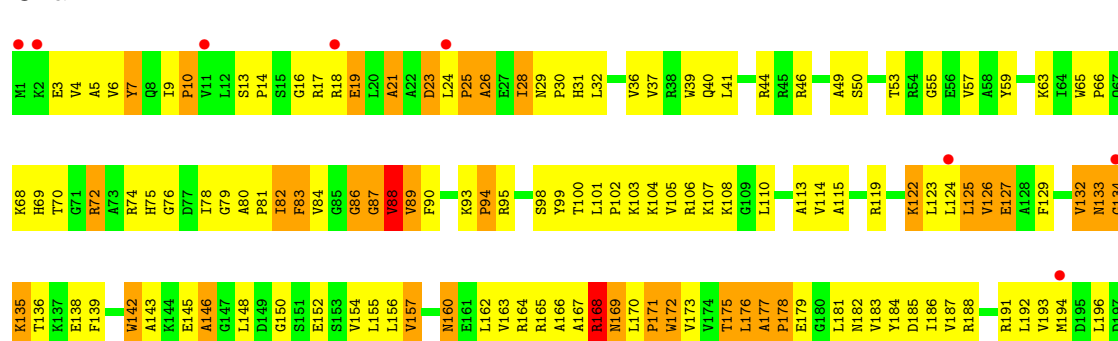
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

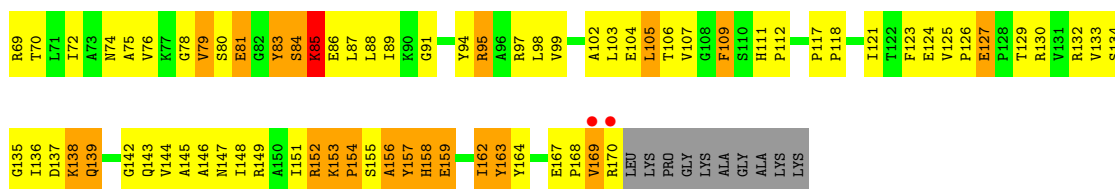
Chain DE:



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

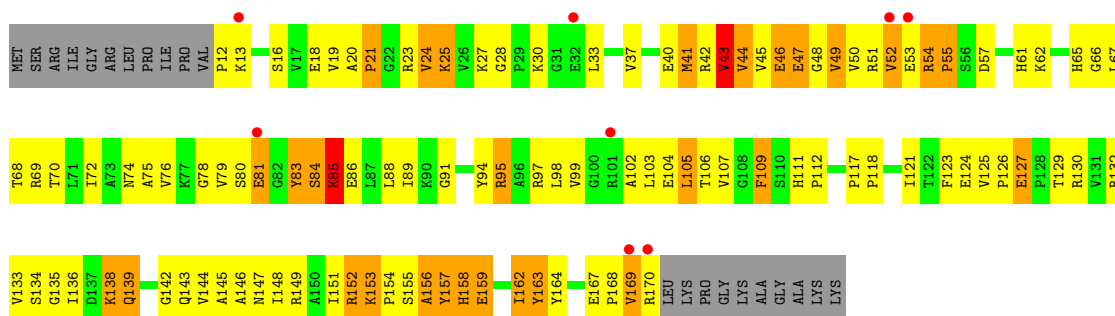
Chain BF:





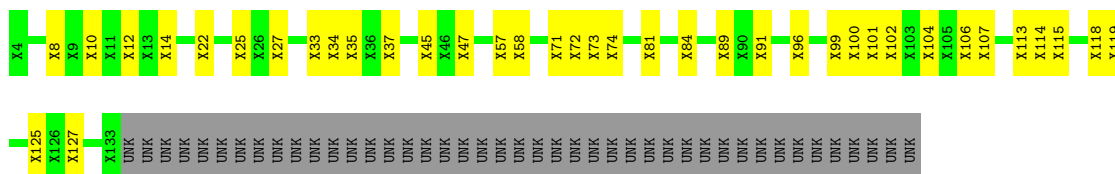
• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain DH:



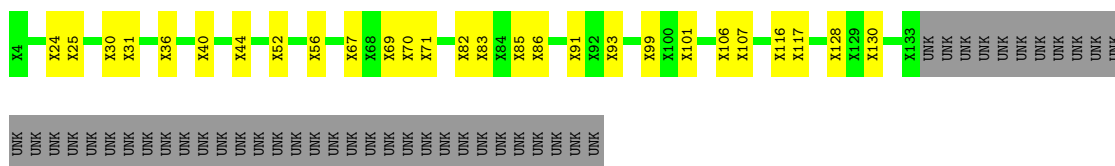
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:



• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK:



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



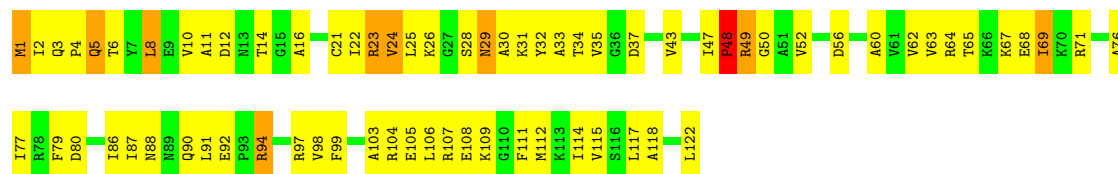
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



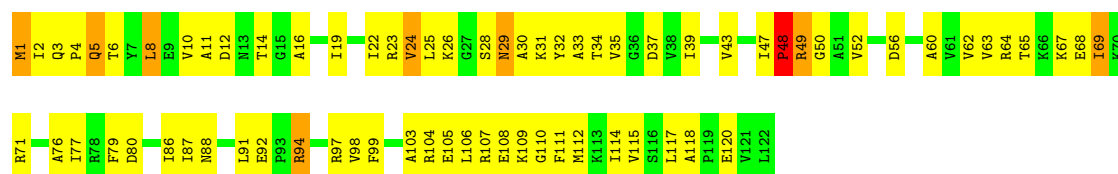
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



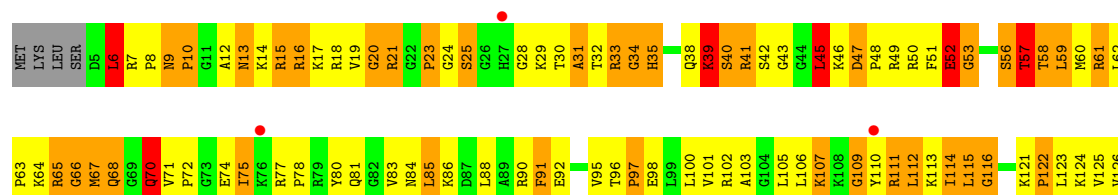
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO:



- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:





• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



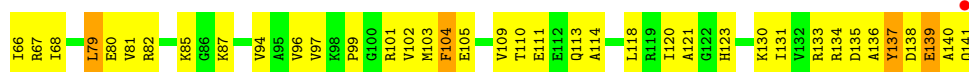
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



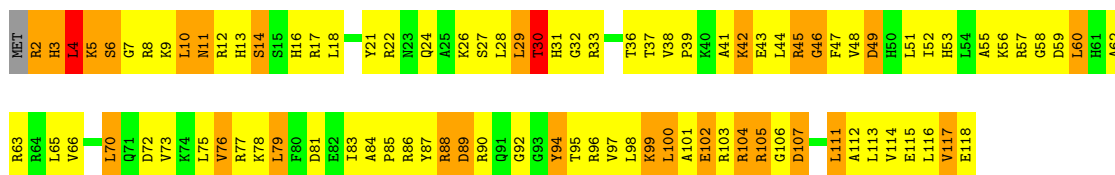
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



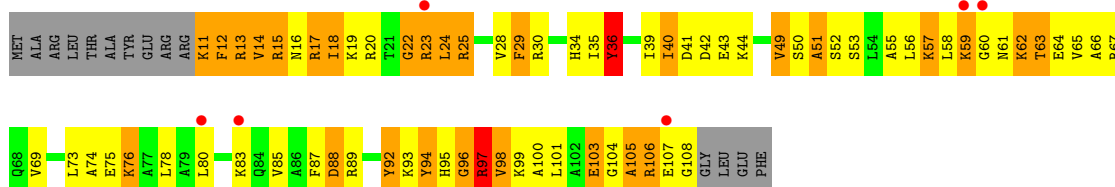
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



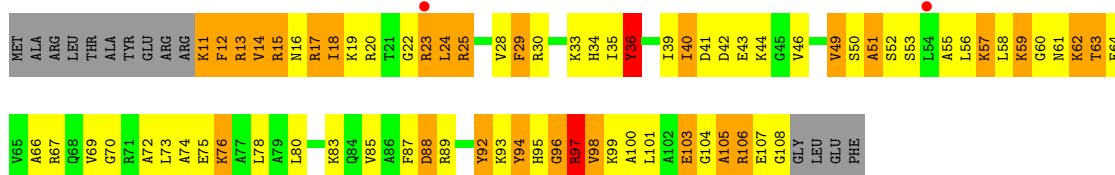
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



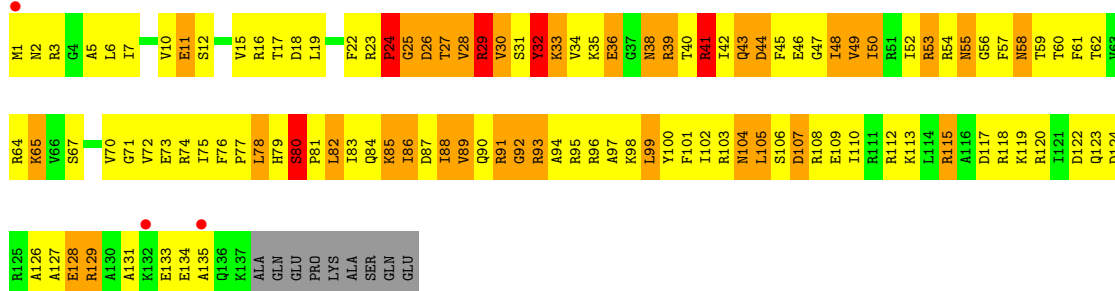
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



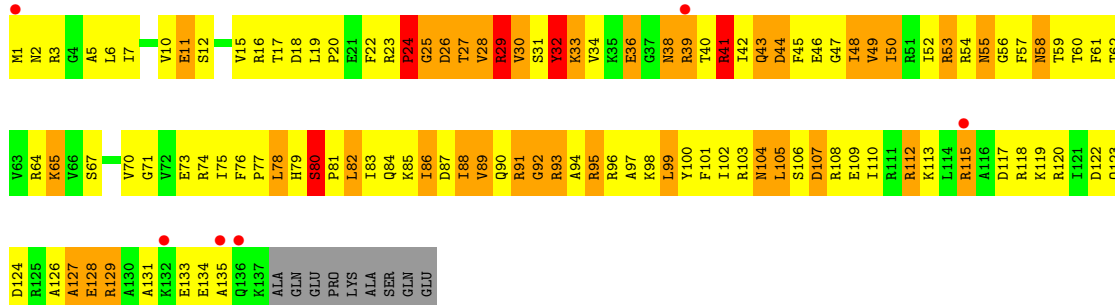
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:

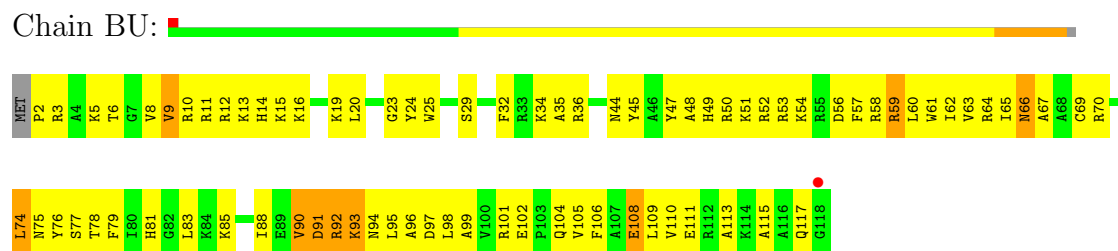


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

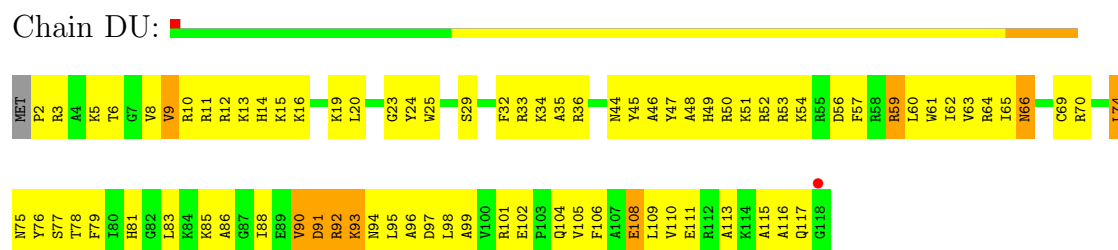
Chain DT:



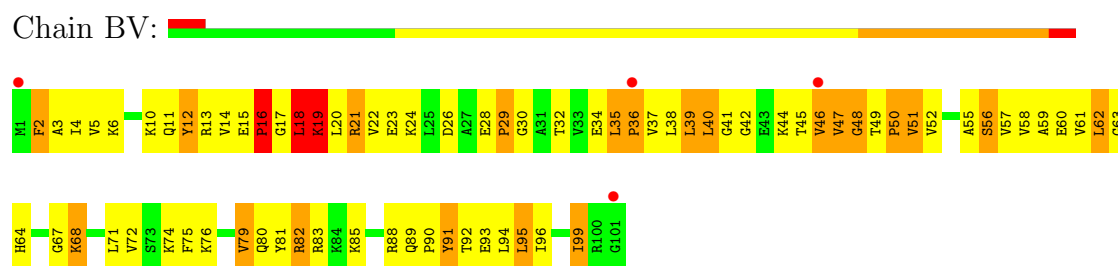
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



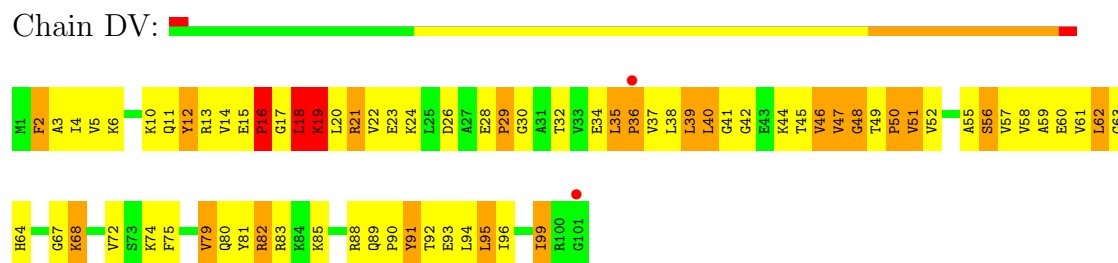
- Molecule 53: 50S RIBOSOMAL PROTEIN L20



- Molecule 54: 50S RIBOSOMAL PROTEIN L21



- Molecule 54: 50S RIBOSOMAL PROTEIN L21

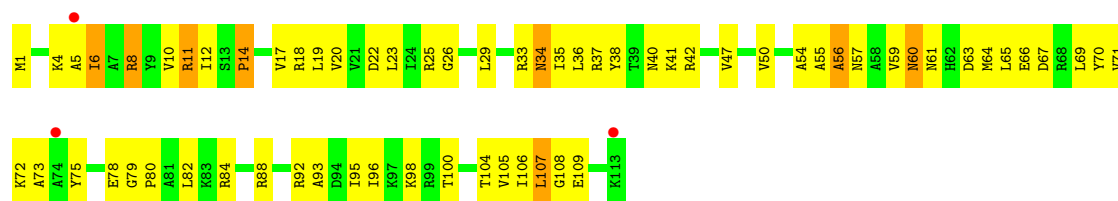


- Molecule 55: 50S RIBOSOMAL PROTEIN L22



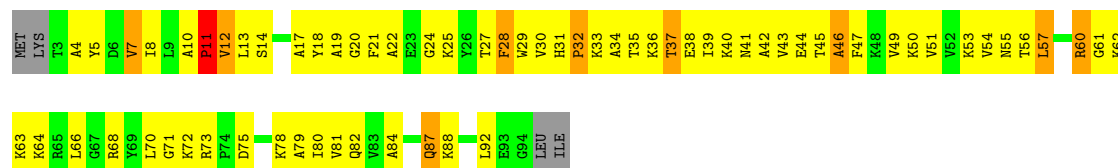
- Molecule 55: 50S RIBOSOMAL PROTEIN L22





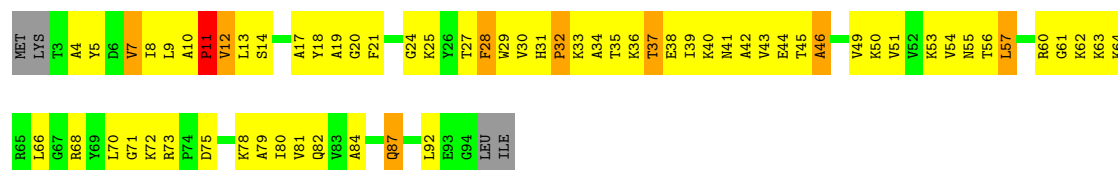
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



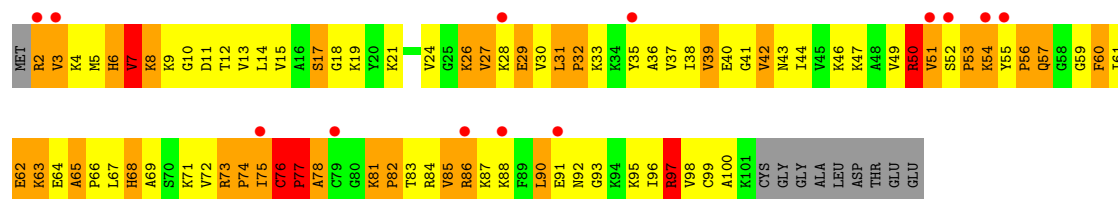
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



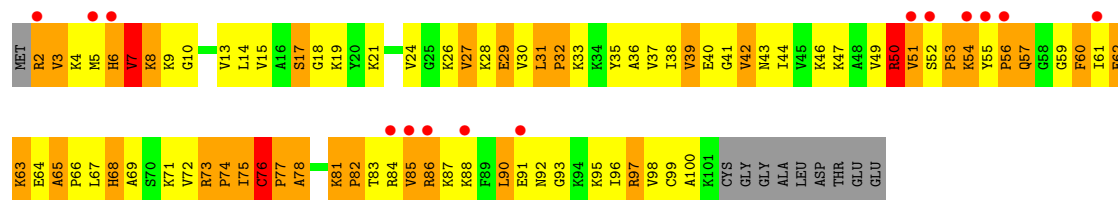
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

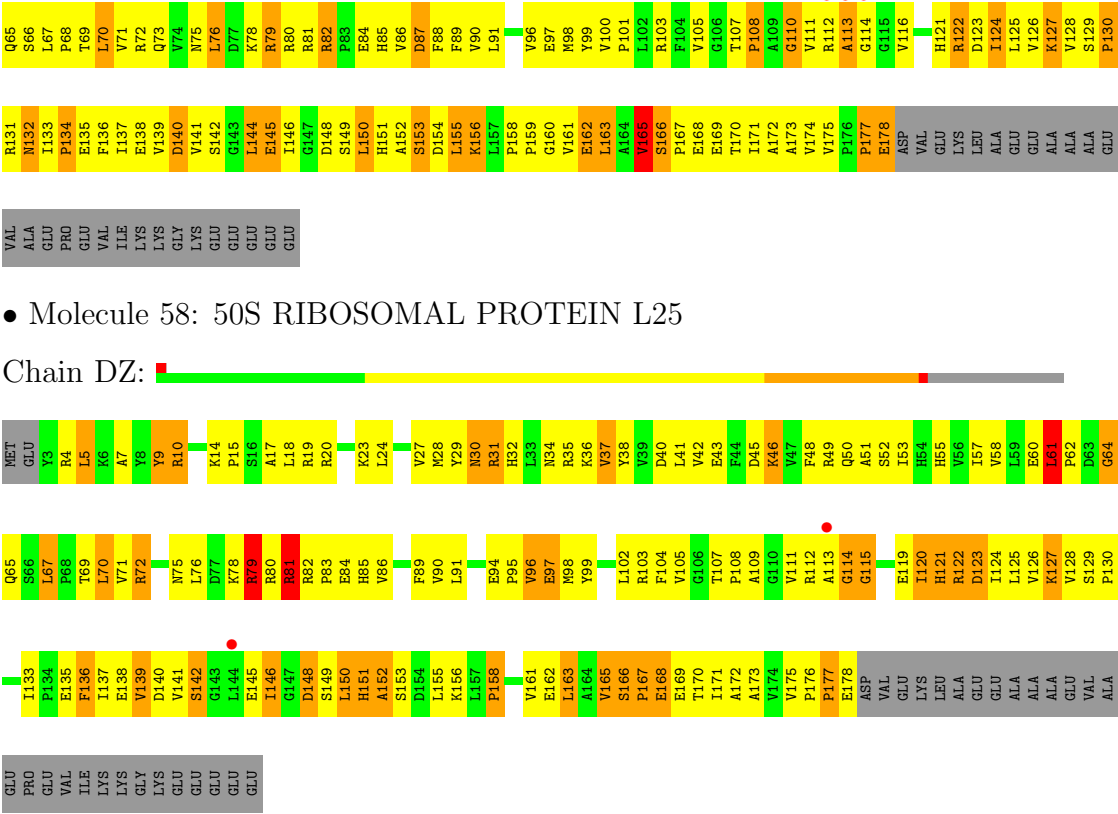
Chain DY:



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:





• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	290.20Å 269.20Å 404.00Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.10) 92.4 (49.51-2.90)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.264 0.244 , 0.269	Depositor DCC
R_{free} test set	62894 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.8	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 1263345 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	307330	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% 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	0.57	6/36325 (0.0%)	0.75	35/56695 (0.1%)
1	CA	0.64	11/36325 (0.0%)	0.76	45/56695 (0.1%)
2	AB	0.49	0/1935	0.69	0/2609
2	CB	0.49	0/1935	0.69	0/2609
3	AC	0.53	0/1636	0.72	1/2205 (0.0%)
3	CC	0.58	0/1636	0.73	1/2205 (0.0%)
4	AD	0.45	0/1733	0.69	1/2318 (0.0%)
4	CD	0.43	0/1733	0.68	1/2318 (0.0%)
5	AE	0.56	0/1162	0.75	0/1564
5	CE	0.59	0/1162	0.76	0/1564
6	AF	0.43	0/856	0.68	0/1154
6	CF	0.42	0/856	0.67	0/1154
7	AG	0.45	0/1276	0.64	0/1709
7	CG	0.47	0/1276	0.64	0/1709
8	AH	0.48	0/1136	0.73	0/1527
8	CH	0.49	0/1136	0.75	0/1527
9	AI	0.45	0/1029	0.68	0/1379
9	CI	0.46	0/1029	0.68	0/1379
10	AJ	0.44	0/807	0.73	0/1085
10	CJ	0.47	0/807	0.74	0/1085
11	AK	0.49	0/900	0.72	0/1213
11	CK	0.52	0/900	0.72	0/1213
12	AL	0.49	0/986	0.77	0/1320
12	CL	0.51	0/986	0.78	0/1320
13	AM	0.45	0/998	0.73	0/1336
13	CM	0.46	0/998	0.73	0/1336
14	AN	0.62	0/501	0.81	0/664
14	CN	0.56	0/501	0.80	0/664
15	AO	0.47	0/745	0.67	0/992
15	CO	0.47	0/745	0.67	0/992
16	AP	0.43	0/716	0.70	0/963
16	CP	0.43	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.50	0/836	0.70	0/1117
17	CQ	0.50	0/836	0.70	0/1117
18	AR	0.50	0/579	0.66	0/768
18	CR	0.47	0/579	0.65	0/768
19	AS	0.47	0/642	0.71	0/865
19	CS	0.49	0/642	0.72	0/865
20	AT	0.40	0/765	0.66	0/1007
20	CT	0.42	0/765	0.67	0/1007
21	AU	0.51	0/212	0.65	0/277
21	CU	0.47	0/212	0.64	0/277
22	AV	0.66	0/1809	0.83	1/2819 (0.0%)
22	AW	0.55	0/1809	0.75	0/2819
22	CV	0.72	0/1809	0.82	1/2819 (0.0%)
22	CW	0.57	1/1809 (0.1%)	0.76	0/2819
23	AX	0.69	0/406	0.87	2/631 (0.3%)
23	CX	0.80	0/406	0.90	3/631 (0.5%)
24	AY	0.49	1/1619 (0.1%)	0.70	0/2516
24	CY	0.50	1/1619 (0.1%)	0.70	0/2516
25	AZ	0.67	3/3042 (0.1%)	0.76	7/4129 (0.2%)
25	CZ	0.65	4/3042 (0.1%)	0.76	6/4129 (0.1%)
26	B0	0.45	0/671	0.70	0/892
26	D0	0.44	0/671	0.70	0/892
27	B1	0.43	0/738	0.72	0/981
27	D1	0.51	0/738	0.83	0/981
28	B2	0.35	0/600	0.63	0/793
28	D2	0.40	0/600	0.82	0/793
29	B3	0.35	0/472	0.60	0/634
29	D3	0.36	0/472	0.61	0/634
30	B4	0.41	0/349	0.64	0/474
30	D4	0.42	0/349	0.65	0/474
31	B5	0.40	0/473	0.64	0/639
31	D5	0.39	0/473	0.63	0/639
32	B6	0.62	0/440	0.95	0/586
32	D6	0.67	0/440	0.97	0/586
33	B7	0.45	0/426	0.71	0/561
33	D7	0.43	0/426	0.72	0/561
34	B8	0.55	0/515	0.77	0/679
34	D8	0.58	0/515	0.77	0/679
35	B9	0.53	0/310	0.70	0/407
35	D9	0.50	0/310	0.69	0/407
36	BA	0.52	5/69976 (0.0%)	0.72	27/109244 (0.0%)
36	DA	0.53	5/69976 (0.0%)	0.72	35/109244 (0.0%)
37	BB	0.49	0/2853	0.74	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.44	0/2853	0.74	1/4451 (0.0%)
38	BC	0.42	1/1774 (0.1%)	0.74	3/2391 (0.1%)
38	DC	0.43	2/1774 (0.1%)	0.75	3/2391 (0.1%)
39	BD	0.52	0/2195	0.88	4/2955 (0.1%)
39	DD	0.54	0/2195	0.90	4/2955 (0.1%)
40	BE	0.43	0/1596	0.71	0/2153
40	DE	0.44	0/1596	0.71	0/2153
41	BF	0.38	0/1658	0.74	3/2244 (0.1%)
41	DF	0.36	0/1658	0.74	3/2244 (0.1%)
42	BG	0.39	0/1499	0.70	1/2016 (0.0%)
42	DG	0.47	0/1499	0.80	0/2016
43	BH	0.35	0/1245	0.67	0/1682
43	DH	0.35	0/1245	0.67	0/1682
46	BN	0.39	0/1131	0.71	1/1525 (0.1%)
46	DN	0.39	0/1131	0.71	1/1525 (0.1%)
47	BO	0.52	1/943 (0.1%)	0.71	0/1269
47	DO	0.51	0/943	0.72	0/1269
48	BP	0.43	0/1131	0.89	3/1504 (0.2%)
48	DP	0.44	0/1131	0.90	4/1504 (0.3%)
49	BQ	0.51	0/1143	0.72	1/1527 (0.1%)
49	DQ	0.54	0/1143	0.72	1/1527 (0.1%)
50	BR	0.38	0/974	0.72	1/1302 (0.1%)
50	DR	0.39	0/974	0.72	1/1302 (0.1%)
51	BS	0.43	0/778	0.75	0/1036
51	DS	0.41	0/778	0.75	0/1036
52	BT	0.44	0/1155	0.76	2/1542 (0.1%)
52	DT	0.45	0/1155	0.77	2/1542 (0.1%)
53	BU	0.44	0/975	0.67	0/1297
53	DU	0.42	0/975	0.67	0/1297
54	BV	0.38	0/790	0.67	0/1057
54	DV	0.36	0/790	0.67	0/1057
55	BW	0.38	0/907	0.64	0/1216
55	DW	0.37	0/907	0.65	0/1216
56	BX	0.43	0/739	0.91	3/993 (0.3%)
56	DX	0.42	0/739	0.89	3/993 (0.3%)
57	BY	0.37	0/788	0.68	1/1051 (0.1%)
57	DY	0.37	0/788	0.68	1/1051 (0.1%)
58	BZ	0.46	0/1435	0.74	0/1949
58	DZ	0.49	0/1435	0.79	3/1949 (0.2%)
All	All	0.53	41/330278 (0.0%)	0.73	216/493462 (0.0%)

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	4	59
1	CA	4	49
22	AV	0	3
22	CV	0	2
23	AX	0	2
23	CX	0	1
36	BA	2	63
36	DA	2	72
37	BB	0	2
37	DB	0	2
49	BQ	0	1
49	DQ	0	1
All	All	12	257

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CZ	68	VAL	C-O	-20.43	0.84	1.23
25	AZ	68	VAL	C-O	-19.95	0.85	1.23
36	DA	761	A	C5-C6	-10.79	1.31	1.41
36	BA	761	A	C5-C6	-10.15	1.31	1.41
1	CA	858	G	C5-C6	-10.08	1.32	1.42

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	DC	134	ARG	NE-CZ-NH2	-14.36	113.12	120.30
39	DD	43	ARG	NE-CZ-NH1	14.15	127.37	120.30
41	BF	168	ARG	NE-CZ-NH2	-13.66	113.47	120.30
38	DC	134	ARG	NE-CZ-NH1	13.54	127.07	120.30
38	BC	134	ARG	NE-CZ-NH2	-13.34	113.63	120.30

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1363(A)	A	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
36	BA	1819	A	C3'

5 of 257 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	30	U	Sidechain
1	AA	37	U	Sidechain
1	AA	60	A	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	32451	0	16382	929	0
1	CA	32451	0	16382	850	0
2	AB	1900	0	1951	185	2
2	CB	1900	0	1951	176	2
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	141	0
4	AD	1703	0	1765	168	0
4	CD	1703	0	1765	156	0
5	AE	1146	0	1207	69	0
5	CE	1146	0	1207	69	0
6	AF	843	0	857	64	0
6	CF	843	0	857	59	0
7	AG	1257	0	1296	70	0
7	CG	1257	0	1296	63	0
8	AH	1116	0	1177	55	0
8	CH	1116	0	1177	49	0
9	AI	1010	0	1037	109	0
9	CI	1010	0	1037	109	0
10	AJ	794	0	840	116	0
10	CJ	794	0	840	116	0
11	AK	885	0	904	58	0
11	CK	885	0	904	57	0
12	AL	970	0	1057	99	0
12	CL	970	0	1057	97	0
13	AM	987	0	1059	116	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	CM	987	0	1059	116	0
14	AN	492	0	530	57	0
14	CN	492	0	530	62	0
15	AO	734	0	771	44	0
15	CO	734	0	771	43	0
16	AP	700	0	720	75	0
16	CP	700	0	720	80	0
17	AQ	823	0	891	60	0
17	CQ	823	0	891	62	0
18	AR	574	0	644	46	0
18	CR	574	0	644	50	0
19	AS	629	0	652	76	0
19	CS	629	0	652	73	0
20	AT	763	0	861	97	0
20	CT	763	0	861	99	0
21	AU	208	0	221	25	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	59	0
22	AW	1619	0	822	82	0
22	CV	1619	0	822	58	0
22	CW	1619	0	822	76	0
23	AX	362	0	184	15	0
23	CX	362	0	184	14	0
24	AY	1645	0	853	132	0
24	CY	1645	0	853	89	0
25	AZ	2984	0	2997	475	0
25	CZ	2984	0	2997	384	0
26	B0	662	0	688	66	0
26	D0	662	0	688	65	0
27	B1	731	0	808	84	0
27	D1	731	0	808	80	0
28	B2	598	0	653	87	0
28	D2	598	0	653	215	0
29	B3	467	0	523	35	0
29	D3	467	0	523	35	0
30	B4	340	0	337	53	0
30	D4	340	0	336	58	0
31	B5	459	0	480	84	0
31	D5	459	0	480	76	0
32	B6	433	0	461	123	0
32	D6	433	0	461	121	0
33	B7	418	0	467	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	D7	418	0	467	37	0
34	B8	507	0	576	130	0
34	D8	507	0	576	128	0
35	B9	307	0	337	33	0
35	D9	307	0	335	31	0
36	BA	62477	0	31497	2071	0
36	DA	62477	0	31497	2074	0
37	BB	2551	0	1295	93	0
37	DB	2551	0	1295	101	0
38	BC	1742	0	1800	162	2
38	DC	1742	0	1800	153	2
39	BD	2145	0	2234	254	0
39	DD	2145	0	2234	240	0
40	BE	1563	0	1629	237	0
40	DE	1563	0	1629	235	0
41	BF	1623	0	1677	214	0
41	DF	1623	0	1677	216	0
42	BG	1474	0	1535	236	0
42	DG	1474	0	1535	269	0
43	BH	1222	0	1282	159	0
43	DH	1222	0	1282	155	0
44	BJ	651	0	156	23	0
44	DJ	651	0	166	16	0
45	BK	700	0	167	9	0
45	DK	700	0	167	9	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	157	0
47	BO	933	0	996	86	0
47	DO	933	0	996	88	0
48	BP	1114	0	1187	267	0
48	DP	1114	0	1187	264	0
49	BQ	1122	0	1179	119	0
49	DQ	1122	0	1179	128	0
50	BR	960	0	1021	151	0
50	DR	960	0	1021	150	0
51	BS	770	0	832	135	0
51	DS	770	0	832	138	0
52	BT	1141	0	1202	207	0
52	DT	1141	0	1202	207	0
53	BU	958	0	1015	129	0
53	DU	958	0	1015	132	0
54	BV	779	0	852	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DV	779	0	852	141	0
55	BW	896	0	953	84	0
55	DW	896	0	953	84	0
56	BX	725	0	778	100	0
56	DX	725	0	778	92	0
57	BY	775	0	870	177	0
57	DY	775	0	870	169	0
58	BZ	1403	0	1432	211	0
58	DZ	1403	0	1432	189	0
59	AD	1	0	0	1	0
59	AN	1	0	0	1	0
59	B4	1	0	0	1	0
59	B9	1	0	0	1	0
59	CD	1	0	0	1	0
59	CN	1	0	0	1	0
59	D4	1	0	0	0	0
59	D9	1	0	0	0	0
60	AZ	28	0	12	15	0
60	CZ	28	0	12	8	0
61	AZ	57	0	58	13	0
61	CZ	57	0	58	9	0
All	All	307330	0	208699	17315	4

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 34.

The worst 5 of 17315 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:AZ:355:LEU:CD2	25:AZ:370:PHE:HB3	1.63	1.28
25:CZ:355:LEU:CD2	25:CZ:370:PHE:HB3	1.63	1.24
39:DD:35:LYS:HG3	39:DD:104:TYR:CE2	1.73	1.23
25:AZ:2:LYS:O	25:AZ:275:LYS:HE3	1.42	1.20
25:CZ:355:LEU:HD23	25:CZ:370:PHE:CB	1.73	1.19

All (4) 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_445]	1.97	0.23
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_646]	2.02	0.18
2:CB:66:GLY:CA	38:DC:27:ARG:NH2[2_445]	2.09	0.11
2:AB:66:GLY:CA	38:BC:27:ARG:NH2[2_646]	2.18	0.02

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%)	161 (69%)	48 (21%)	23 (10%)	1	6
2	CB	232/256 (91%)	164 (71%)	45 (19%)	23 (10%)	1	6
3	AC	204/239 (85%)	169 (83%)	22 (11%)	13 (6%)	2	15
3	CC	204/239 (85%)	171 (84%)	21 (10%)	12 (6%)	2	17
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	9
4	CD	206/209 (99%)	149 (72%)	38 (18%)	19 (9%)	1	7
5	AE	148/162 (91%)	136 (92%)	10 (7%)	2 (1%)	16	58
5	CE	148/162 (91%)	136 (92%)	9 (6%)	3 (2%)	11	49
6	AF	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1	8
6	CF	99/101 (98%)	73 (74%)	17 (17%)	9 (9%)	1	8
7	AG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	8	41
7	CG	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	11	49
8	AH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	15	57
8	CH	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	15	57
9	AI	125/128 (98%)	83 (66%)	34 (27%)	8 (6%)	2	15
9	CI	125/128 (98%)	83 (66%)	35 (28%)	7 (6%)	3	19
10	AJ	96/105 (91%)	69 (72%)	21 (22%)	6 (6%)	2	16
10	CJ	96/105 (91%)	71 (74%)	19 (20%)	6 (6%)	2	16
11	AK	117/129 (91%)	98 (84%)	18 (15%)	1 (1%)	25	71
11	CK	117/129 (91%)	99 (85%)	17 (14%)	1 (1%)	25	71
12	AL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	2	15
12	CL	122/131 (93%)	104 (85%)	10 (8%)	8 (7%)	2	15
13	AM	122/126 (97%)	85 (70%)	27 (22%)	10 (8%)	1	10
13	CM	122/126 (97%)	85 (70%)	28 (23%)	9 (7%)	2	11
14	AN	58/61 (95%)	42 (72%)	9 (16%)	7 (12%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	43 (74%)	7 (12%)	8 (14%)	0	2
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	10	45
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	10	45
16	AP	81/88 (92%)	58 (72%)	17 (21%)	6 (7%)	2	11
16	CP	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	2	11
17	AQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	3	21
17	CQ	97/105 (92%)	85 (88%)	7 (7%)	5 (5%)	3	21
18	AR	68/88 (77%)	55 (81%)	11 (16%)	2 (3%)	7	38
18	CR	68/88 (77%)	56 (82%)	10 (15%)	2 (3%)	7	38
19	AS	76/93 (82%)	48 (63%)	15 (20%)	13 (17%)	0	0
19	CS	76/93 (82%)	47 (62%)	16 (21%)	13 (17%)	0	0
20	AT	97/106 (92%)	67 (69%)	22 (23%)	8 (8%)	1	10
20	CT	97/106 (92%)	67 (69%)	21 (22%)	9 (9%)	1	7
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	4	24
21	CU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	4	24
25	AZ	381/405 (94%)	263 (69%)	80 (21%)	38 (10%)	1	6
25	CZ	381/405 (94%)	266 (70%)	77 (20%)	38 (10%)	1	6
26	B0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	3	23
26	D0	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	3	23
27	B1	91/98 (93%)	68 (75%)	13 (14%)	10 (11%)	1	5
27	D1	91/98 (93%)	63 (69%)	10 (11%)	18 (20%)	0	0
28	B2	69/72 (96%)	46 (67%)	17 (25%)	6 (9%)	1	9
28	D2	69/72 (96%)	37 (54%)	16 (23%)	16 (23%)	0	0
29	B3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	8
29	D3	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	8
30	B4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0
30	D4	42/71 (59%)	24 (57%)	11 (26%)	7 (17%)	0	0
31	B5	57/60 (95%)	41 (72%)	7 (12%)	9 (16%)	0	1
31	D5	57/60 (95%)	40 (70%)	8 (14%)	9 (16%)	0	1
32	B6	48/54 (89%)	23 (48%)	8 (17%)	17 (35%)	0	0
32	D6	48/54 (89%)	23 (48%)	8 (17%)	17 (35%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
33	D7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
34	B8	61/65 (94%)	43 (70%)	12 (20%)	6 (10%)	1	6
34	D8	61/65 (94%)	45 (74%)	10 (16%)	6 (10%)	1	6
35	B9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	9
35	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	9
38	BC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	2	12
38	DC	226/229 (99%)	170 (75%)	40 (18%)	16 (7%)	2	12
39	BD	273/276 (99%)	214 (78%)	33 (12%)	26 (10%)	1	7
39	DD	273/276 (99%)	214 (78%)	34 (12%)	25 (9%)	1	7
40	BE	202/206 (98%)	125 (62%)	46 (23%)	31 (15%)	0	1
40	DE	202/206 (98%)	125 (62%)	47 (23%)	30 (15%)	0	1
41	BF	205/210 (98%)	153 (75%)	23 (11%)	29 (14%)	0	2
41	DF	205/210 (98%)	153 (75%)	23 (11%)	29 (14%)	0	2
42	BG	179/182 (98%)	103 (58%)	45 (25%)	31 (17%)	0	0
42	DG	179/182 (98%)	111 (62%)	40 (22%)	28 (16%)	0	1
43	BH	157/180 (87%)	105 (67%)	28 (18%)	24 (15%)	0	1
43	DH	157/180 (87%)	105 (67%)	29 (18%)	23 (15%)	0	2
46	BN	136/140 (97%)	85 (62%)	32 (24%)	19 (14%)	0	2
46	DN	136/140 (97%)	86 (63%)	32 (24%)	18 (13%)	0	2
47	BO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	4	27
47	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	4	27
48	BP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0	0
48	DP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
49	BQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	4	26
49	DQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	4	26
50	BR	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
50	DR	115/118 (98%)	82 (71%)	14 (12%)	19 (16%)	0	0
51	BS	96/112 (86%)	44 (46%)	31 (32%)	21 (22%)	0	0
51	DS	96/112 (86%)	44 (46%)	32 (33%)	20 (21%)	0	0
52	BT	135/146 (92%)	85 (63%)	24 (18%)	26 (19%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	DT	135/146 (92%)	85 (63%)	24 (18%)	26 (19%)	0	0
53	BU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	4	26
53	DU	115/118 (98%)	82 (71%)	28 (24%)	5 (4%)	4	26
54	BV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	3
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	3
55	BW	111/113 (98%)	82 (74%)	23 (21%)	6 (5%)	3	20
55	DW	111/113 (98%)	84 (76%)	21 (19%)	6 (5%)	3	20
56	BX	90/96 (94%)	63 (70%)	16 (18%)	11 (12%)	1	4
56	DX	90/96 (94%)	64 (71%)	15 (17%)	11 (12%)	1	4
57	BY	98/110 (89%)	32 (33%)	36 (37%)	30 (31%)	0	0
57	DY	98/110 (89%)	32 (33%)	37 (38%)	29 (30%)	0	0
58	BZ	174/206 (84%)	111 (64%)	36 (21%)	27 (16%)	0	1
58	DZ	174/206 (84%)	119 (68%)	31 (18%)	24 (14%)	0	2
All	All	12256/13098 (94%)	8805 (72%)	2168 (18%)	1283 (10%)	1	5

5 of 1283 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	18	GLY
2	AB	130	ARG
2	AB	234	PRO
3	AC	12	LEU

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%)	181 (90%)	21 (10%)	10	36
2	CB	202/220 (92%)	180 (89%)	22 (11%)	9	34
3	AC	160/188 (85%)	141 (88%)	19 (12%)	8	27
3	CC	160/188 (85%)	142 (89%)	18 (11%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	180/181 (99%)	162 (90%)	18 (10%)	11	38
4	CD	180/181 (99%)	162 (90%)	18 (10%)	11	38
5	AE	115/123 (94%)	102 (89%)	13 (11%)	9	32
5	CE	115/123 (94%)	102 (89%)	13 (11%)	9	32
6	AF	90/90 (100%)	80 (89%)	10 (11%)	9	33
6	CF	90/90 (100%)	80 (89%)	10 (11%)	9	33
7	AG	126/127 (99%)	118 (94%)	8 (6%)	25	66
7	CG	126/127 (99%)	118 (94%)	8 (6%)	25	66
8	AH	119/119 (100%)	107 (90%)	12 (10%)	11	38
8	CH	119/119 (100%)	107 (90%)	12 (10%)	11	38
9	AI	98/99 (99%)	90 (92%)	8 (8%)	17	53
9	CI	98/99 (99%)	89 (91%)	9 (9%)	13	45
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	7	25
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	7	25
11	AK	90/99 (91%)	80 (89%)	10 (11%)	9	33
11	CK	90/99 (91%)	80 (89%)	10 (11%)	9	33
12	AL	104/108 (96%)	92 (88%)	12 (12%)	8	31
12	CL	104/108 (96%)	92 (88%)	12 (12%)	8	31
13	AM	99/101 (98%)	88 (89%)	11 (11%)	9	33
13	CM	99/101 (98%)	88 (89%)	11 (11%)	9	33
14	AN	49/50 (98%)	42 (86%)	7 (14%)	5	19
14	CN	49/50 (98%)	42 (86%)	7 (14%)	5	19
15	AO	79/80 (99%)	70 (89%)	9 (11%)	8	31
15	CO	79/80 (99%)	70 (89%)	9 (11%)	8	31
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	33
16	CP	72/74 (97%)	65 (90%)	7 (10%)	12	41
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	25	65
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	25	65
18	AR	61/77 (79%)	51 (84%)	10 (16%)	3	12
18	CR	61/77 (79%)	51 (84%)	10 (16%)	3	12
19	AS	69/80 (86%)	56 (81%)	13 (19%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	69/80 (86%)	56 (81%)	13 (19%)	2	9
20	AT	76/82 (93%)	68 (90%)	8 (10%)	10	35
20	CT	76/82 (93%)	68 (90%)	8 (10%)	10	35
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	72
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	72
25	AZ	322/338 (95%)	279 (87%)	43 (13%)	6	22
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	6	24
26	B0	66/67 (98%)	59 (89%)	7 (11%)	10	35
26	D0	66/67 (98%)	59 (89%)	7 (11%)	10	35
27	B1	78/83 (94%)	67 (86%)	11 (14%)	5	20
27	D1	78/83 (94%)	68 (87%)	10 (13%)	6	24
28	B2	66/67 (98%)	64 (97%)	2 (3%)	53	87
28	D2	66/67 (98%)	57 (86%)	9 (14%)	5	21
29	B3	51/52 (98%)	45 (88%)	6 (12%)	8	29
29	D3	51/52 (98%)	45 (88%)	6 (12%)	8	29
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	10
30	D4	39/63 (62%)	33 (85%)	6 (15%)	4	15
31	B5	51/52 (98%)	45 (88%)	6 (12%)	8	29
31	D5	51/52 (98%)	45 (88%)	6 (12%)	8	29
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	31 (63%)	18 (37%)	0	0
33	B7	41/42 (98%)	38 (93%)	3 (7%)	20	59
33	D7	41/42 (98%)	38 (93%)	3 (7%)	20	59
34	B8	53/55 (96%)	44 (83%)	9 (17%)	3	11
34	D8	53/55 (96%)	44 (83%)	9 (17%)	3	11
35	B9	34/34 (100%)	31 (91%)	3 (9%)	14	49
35	D9	34/34 (100%)	31 (91%)	3 (9%)	14	49
38	BC	180/181 (99%)	172 (96%)	8 (4%)	39	79
38	DC	180/181 (99%)	172 (96%)	8 (4%)	39	79
39	BD	217/218 (100%)	186 (86%)	31 (14%)	5	19
39	DD	217/218 (100%)	187 (86%)	30 (14%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BE	165/166 (99%)	145 (88%)	20 (12%)	7	27
40	DE	165/166 (99%)	143 (87%)	22 (13%)	6	22
41	BF	165/166 (99%)	152 (92%)	13 (8%)	18	55
41	DF	165/166 (99%)	152 (92%)	13 (8%)	18	55
42	BG	155/156 (99%)	135 (87%)	20 (13%)	6	24
42	DG	155/156 (99%)	124 (80%)	31 (20%)	2	8
43	BH	132/148 (89%)	118 (89%)	14 (11%)	10	35
43	DH	132/148 (89%)	118 (89%)	14 (11%)	10	35
46	BN	117/119 (98%)	101 (86%)	16 (14%)	5	21
46	DN	117/119 (98%)	101 (86%)	16 (14%)	5	21
47	BO	100/100 (100%)	93 (93%)	7 (7%)	21	61
47	DO	100/100 (100%)	93 (93%)	7 (7%)	21	61
48	BP	112/116 (97%)	93 (83%)	19 (17%)	3	11
48	DP	112/116 (97%)	93 (83%)	19 (17%)	3	11
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	14	47
49	DQ	111/111 (100%)	101 (91%)	10 (9%)	14	47
50	BR	100/101 (99%)	87 (87%)	13 (13%)	6	23
50	DR	100/101 (99%)	85 (85%)	15 (15%)	4	17
51	BS	77/88 (88%)	65 (84%)	12 (16%)	4	14
51	DS	77/88 (88%)	65 (84%)	12 (16%)	4	14
52	BT	120/127 (94%)	97 (81%)	23 (19%)	2	9
52	DT	120/127 (94%)	97 (81%)	23 (19%)	2	9
53	BU	92/94 (98%)	86 (94%)	6 (6%)	24	65
53	DU	92/94 (98%)	86 (94%)	6 (6%)	24	65
54	BV	82/82 (100%)	67 (82%)	15 (18%)	2	10
54	DV	82/82 (100%)	67 (82%)	15 (18%)	2	10
55	BW	91/92 (99%)	87 (96%)	4 (4%)	39	79
55	DW	91/92 (99%)	86 (94%)	5 (6%)	30	71
56	BX	74/78 (95%)	67 (90%)	7 (10%)	12	42
56	DX	74/78 (95%)	68 (92%)	6 (8%)	17	53
57	BY	84/91 (92%)	71 (84%)	13 (16%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	DY	84/91 (92%)	72 (86%)	12 (14%)	5 19
58	BZ	155/179 (87%)	130 (84%)	25 (16%)	3 13
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	4 14
All	All	10338/10854 (95%)	9112 (88%)	1226 (12%)	8 27

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	95	LEU
7	CG	24	THR
51	DS	97	ARG
57	BY	7	VAL
2	CB	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 325 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	49	HIS
5	CE	20	GLN
49	DQ	141	GLN
55	BW	57	ASN
2	CB	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	227 (15%)	43 (2%)
1	CA	1509/1522 (99%)	222 (14%)	46 (3%)
22	AV	75/76 (98%)	22 (29%)	1 (1%)
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	23 (30%)	1 (1%)
22	CW	75/76 (98%)	21 (28%)	3 (4%)
23	AX	16/27 (59%)	6 (37%)	1 (6%)
23	CX	16/27 (59%)	5 (31%)	1 (6%)
24	AY	74/77 (96%)	25 (33%)	3 (4%)
24	CY	74/77 (96%)	25 (33%)	3 (4%)
36	BA	2900/2915 (99%)	494 (17%)	45 (1%)
36	DA	2900/2915 (99%)	492 (16%)	45 (1%)
37	BB	118/122 (96%)	22 (18%)	3 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	DB	118/122 (96%)	22 (18%)	3 (2%)
All	All	9534/9630 (99%)	1627 (17%)	200 (2%)

5 of 1627 RNA backbone outliers are listed below:

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

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2689	U
1	CA	353	A
36	DA	2033	A
36	BA	2762	G
1	CA	115	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	1.16	3 (15%)	27,30,33	1.79	4 (14%)
24	H2U	AY	17	24	19,21,22	1.24	3 (15%)	27,30,33	1.83	5 (18%)
24	H2U	AY	20	24	19,21,22	0.97	1 (5%)	27,30,33	1.82	5 (18%)
24	OMC	AY	32	24	20,22,23	1.39	3 (15%)	25,31,34	0.93	2 (8%)
24	MIA	AY	37	24	29,31,32	1.08	2 (6%)	41,44,47	1.56	6 (14%)
24	7MG	AY	46	24	24,26,27	2.39	4 (16%)	34,39,42	2.36	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	5MU	AY	54	24	20,22,23	1.16	2 (10%)	25,32,35	1.38	3 (12%)
24	PSU	AY	55	24	19,21,22	0.99	1 (5%)	23,30,33	1.16	4 (17%)
24	4SU	AY	8	24	19,21,22	1.48	4 (21%)	23,30,33	24.53	1 (4%)
24	H2U	CY	16	24	19,21,22	1.17	3 (15%)	27,30,33	1.76	4 (14%)
24	H2U	CY	17	24	19,21,22	1.26	4 (21%)	27,30,33	1.83	5 (18%)
24	H2U	CY	20	24	19,21,22	0.95	2 (10%)	27,30,33	1.83	5 (18%)
24	OMC	CY	32	24	20,22,23	1.27	3 (15%)	25,31,34	0.93	2 (8%)
24	MIA	CY	37	24	29,31,32	1.11	4 (13%)	41,44,47	1.57	5 (12%)
24	7MG	CY	46	24	24,26,27	2.85	4 (16%)	34,39,42	2.37	6 (17%)
24	5MU	CY	54	24	20,22,23	1.22	4 (20%)	25,32,35	1.37	3 (12%)
24	PSU	CY	55	24	19,21,22	0.95	1 (5%)	23,30,33	1.18	4 (17%)
24	4SU	CY	8	24	19,21,22	1.38	5 (26%)	23,30,33	24.09	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	-	1/8/38/39	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	-	1/8/38/39	0/2/2/2
24	H2U	CY	20	24	-	0/8/38/39	0/2/2/2
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 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-10.36	1.38	1.46
24	AY	46	7MG	C8-N9	-10.27	1.38	1.46
24	CY	46	7MG	P-OP1	7.59	1.55	1.46
24	AY	8	4SU	C5-C4	3.82	1.42	1.38
24	AY	32	OMC	C2-N1	3.61	1.42	1.38

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	8	4SU	C4-N3-C2	117.61	126.63	121.60
24	CY	8	4SU	C4-N3-C2	115.48	126.54	121.60
24	CY	46	7MG	C6-N1-C2	9.04	125.31	120.20
24	AY	46	7MG	C6-N1-C2	8.92	125.24	120.20
24	AY	46	7MG	N7-C8-N9	7.54	113.14	103.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	CY	17	H2U	P-O5'-C5'-C4'
24	AY	17	H2U	P-O5'-C5'-C4'

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	1.35	3 (10%)	45,47,47	2.16	8 (17%)
61	KIR	AZ	502	-	59,59,59	3.56	24 (40%)	82,84,84	1.65	19 (23%)
60	GDP	CZ	501	-	30,30,30	1.36	4 (13%)	45,47,47	3.53	8 (17%)
61	KIR	CZ	502	-	59,59,59	3.55	25 (42%)	82,84,84	1.68	20 (24%)

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 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-13.62	1.22	1.44
61	AZ	502	KIR	O18-C17	-13.36	1.23	1.44
61	AZ	502	KIR	O30-C30	-11.90	1.17	1.42
61	CZ	502	KIR	O30-C30	-11.58	1.18	1.42
61	CZ	502	KIR	O34-C33	-11.07	1.29	1.44

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CZ	501	GDP	C6-C5-N7	-19.52	131.51	134.14
60	AZ	501	GDP	C6-C5-N7	-9.83	132.82	134.14
60	CZ	501	GDP	C5-C4-N3	-6.62	118.45	126.07
60	CZ	501	GDP	C2-N3-C4	5.55	121.96	115.30
61	AZ	502	KIR	O29-C29-O34	-5.24	101.68	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	1510/1522 (99%)	-0.37	15 (0%) 79 23	44, 78, 160, 200	0
1	CA	1510/1522 (99%)	-0.17	23 (1%) 70 16	37, 73, 161, 200	0
2	AB	234/256 (91%)	-0.12	2 (0%) 81 25	58, 88, 152, 164	0
2	CB	234/256 (91%)	-0.17	1 (0%) 90 45	54, 86, 151, 164	0
3	AC	206/239 (86%)	-0.25	0 100 100	52, 75, 101, 110	0
3	CC	206/239 (86%)	-0.23	0 100 100	46, 70, 100, 109	0
4	AD	208/209 (99%)	-0.03	1 (0%) 88 39	71, 97, 124, 132	0
4	CD	208/209 (99%)	-0.02	1 (0%) 88 39	67, 96, 123, 131	0
5	AE	150/162 (92%)	-0.28	0 100 100	53, 65, 89, 110	0
5	CE	150/162 (92%)	-0.29	0 100 100	49, 63, 88, 109	0
6	AF	101/101 (100%)	-0.05	0 100 100	71, 99, 115, 122	0
6	CF	101/101 (100%)	-0.13	1 (0%) 79 23	68, 97, 114, 121	0
7	AG	155/156 (99%)	0.02	1 (0%) 86 36	66, 89, 113, 130	0
7	CG	155/156 (99%)	-0.12	1 (0%) 86 36	59, 86, 112, 129	0
8	AH	138/138 (100%)	-0.20	0 100 100	54, 70, 87, 95	0
8	CH	138/138 (100%)	-0.22	0 100 100	52, 67, 87, 94	0
9	AI	127/128 (99%)	0.32	3 (2%) 56 9	62, 96, 128, 139	0
9	CI	127/128 (99%)	0.06	0 100 100	54, 93, 127, 139	0
10	AJ	98/105 (93%)	0.37	3 (3%) 47 7	59, 99, 141, 145	0
10	CJ	98/105 (93%)	0.11	0 100 100	54, 95, 140, 144	0
11	AK	119/129 (92%)	-0.07	1 (0%) 83 28	55, 73, 107, 134	0
11	CK	119/129 (92%)	-0.10	2 (1%) 67 15	51, 68, 108, 133	0
12	AL	124/131 (94%)	-0.05	1 (0%) 83 28	55, 70, 94, 132	0
12	CL	124/131 (94%)	-0.14	1 (0%) 83 28	51, 68, 93, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	0.11	4 (3%)	45	7	71, 97, 124, 152	0
13	CM	124/126 (98%)	0.00	3 (2%)	56	9	67, 95, 123, 152	0
14	AN	60/61 (98%)	-0.16	1 (1%)	67	15	57, 72, 93, 96	0
14	CN	60/61 (98%)	-0.07	1 (1%)	67	15	49, 66, 91, 96	0
15	AO	88/89 (98%)	-0.13	0	100	100	57, 75, 99, 105	0
15	CO	88/89 (98%)	-0.09	0	100	100	56, 74, 98, 104	0
16	AP	83/88 (94%)	0.11	0	100	100	74, 91, 109, 135	0
16	CP	83/88 (94%)	0.13	0	100	100	72, 89, 108, 136	0
17	AQ	99/105 (94%)	-0.09	0	100	100	60, 79, 95, 108	0
17	CQ	99/105 (94%)	-0.14	0	100	100	57, 78, 93, 107	0
18	AR	70/88 (79%)	-0.11	0	100	100	58, 82, 106, 119	0
18	CR	70/88 (79%)	-0.22	0	100	100	56, 79, 105, 118	0
19	AS	78/93 (83%)	0.18	3 (3%)	38	5	75, 99, 137, 139	0
19	CS	78/93 (83%)	0.17	2 (2%)	53	8	71, 99, 136, 139	0
20	AT	99/106 (93%)	0.18	1 (1%)	79	23	75, 97, 131, 135	0
20	CT	99/106 (93%)	0.16	2 (2%)	62	12	71, 96, 132, 135	0
21	AU	24/27 (88%)	0.48	2 (8%)	11	2	66, 84, 103, 115	0
21	CU	24/27 (88%)	0.20	1 (4%)	35	5	64, 78, 99, 115	0
22	AV	76/76 (100%)	-0.38	0	100	100	56, 91, 128, 148	0
22	AW	76/76 (100%)	0.64	10 (13%)	4	1	103, 172, 200, 200	0
22	CV	76/76 (100%)	-0.31	1 (1%)	74	19	50, 89, 128, 147	0
22	CW	76/76 (100%)	0.59	8 (10%)	7	1	100, 172, 200, 200	0
23	AX	17/27 (62%)	0.44	2 (11%)	5	1	50, 97, 156, 157	0
23	CX	17/27 (62%)	0.43	1 (5%)	22	3	45, 95, 156, 157	0
24	AY	76/77 (98%)	0.03	2 (2%)	53	8	61, 141, 187, 195	0
24	CY	76/77 (98%)	-0.01	4 (5%)	25	4	57, 141, 187, 195	0
25	AZ	385/405 (95%)	0.93	50 (12%)	4	1	116, 142, 165, 183	0
25	CZ	385/405 (95%)	0.16	6 (1%)	68	15	113, 141, 165, 183	0
26	B0	84/85 (98%)	0.37	4 (4%)	29	4	77, 91, 118, 131	0
26	D0	84/85 (98%)	0.26	3 (3%)	41	6	76, 90, 119, 131	0
27	B1	93/98 (94%)	0.19	2 (2%)	59	11	74, 95, 134, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	0.08	1 (1%) 77 22	56, 76, 130, 142	0
28	B2	71/72 (98%)	0.17	1 (1%) 72 17	110, 133, 148, 157	0
28	D2	71/72 (98%)	0.75	8 (11%) 6 1	134, 154, 174, 175	0
29	B3	59/60 (98%)	0.27	2 (3%) 43 6	81, 99, 120, 142	0
29	D3	59/60 (98%)	0.20	1 (1%) 67 15	80, 97, 120, 142	0
30	B4	44/71 (61%)	0.11	0 100 100	124, 149, 160, 163	0
30	D4	44/71 (61%)	0.18	0 100 100	123, 147, 158, 163	0
31	B5	59/60 (98%)	0.19	4 (6%) 17 3	73, 105, 158, 176	0
31	D5	59/60 (98%)	0.05	2 (3%) 43 6	72, 104, 158, 176	0
32	B6	50/54 (92%)	0.43	4 (8%) 12 2	74, 106, 116, 125	0
32	D6	50/54 (92%)	0.40	3 (6%) 21 3	73, 104, 115, 123	0
33	B7	48/49 (97%)	0.21	0 100 100	70, 79, 119, 139	0
33	D7	48/49 (97%)	0.28	2 (4%) 35 5	68, 78, 119, 140	0
34	B8	63/65 (96%)	0.21	1 (1%) 68 15	80, 90, 104, 131	0
34	D8	63/65 (96%)	0.19	1 (1%) 68 15	78, 88, 104, 131	0
35	B9	37/37 (100%)	0.34	2 (5%) 25 4	76, 90, 104, 108	0
35	D9	37/37 (100%)	0.19	0 100 100	76, 90, 104, 107	0
36	BA	2901/2915 (99%)	-0.18	62 (2%) 60 11	49, 95, 190, 200	0
36	DA	2901/2915 (99%)	-0.12	63 (2%) 59 11	46, 93, 190, 200	0
37	BB	119/122 (97%)	-0.50	0 100 100	78, 108, 134, 157	0
37	DB	119/122 (97%)	-0.42	0 100 100	75, 107, 133, 157	0
38	BC	228/229 (99%)	0.29	12 (5%) 25 4	69, 99, 177, 187	0
38	DC	228/229 (99%)	0.10	9 (3%) 37 5	67, 97, 177, 187	0
39	BD	275/276 (99%)	-0.15	1 (0%) 90 45	50, 68, 98, 123	0
39	DD	275/276 (99%)	-0.15	1 (0%) 90 45	47, 66, 97, 123	0
40	BE	204/206 (99%)	0.09	3 (1%) 70 16	64, 93, 141, 152	0
40	DE	204/206 (99%)	0.04	3 (1%) 70 16	64, 93, 141, 152	0
41	BF	207/210 (98%)	0.33	9 (4%) 34 5	73, 128, 176, 184	0
41	DF	207/210 (98%)	0.32	8 (3%) 37 5	71, 127, 176, 184	0
42	BG	181/182 (99%)	0.07	4 (2%) 59 11	97, 125, 147, 157	0
42	DG	181/182 (99%)	-0.01	4 (2%) 59 11	75, 96, 125, 146	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	0.30	2 (1%) 74 19	106, 142, 163, 165	0
43	DH	159/180 (88%)	0.52	8 (5%) 28 4	106, 142, 163, 165	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.03	2 (1%) 72 17	78, 104, 145, 148	0
46	DN	138/140 (98%)	0.00	0 100 100	77, 104, 144, 147	0
47	BO	122/122 (100%)	-0.19	0 100 100	58, 76, 90, 97	0
47	DO	122/122 (100%)	-0.13	0 100 100	57, 76, 89, 97	0
48	BP	146/150 (97%)	0.45	4 (2%) 52 8	73, 121, 146, 162	0
48	DP	146/150 (97%)	0.52	4 (2%) 52 8	72, 120, 145, 162	0
49	BQ	141/141 (100%)	-0.05	2 (1%) 72 17	61, 78, 107, 138	0
49	DQ	141/141 (100%)	-0.01	1 (0%) 84 32	60, 77, 107, 139	0
50	BR	117/118 (99%)	0.11	2 (1%) 67 15	76, 98, 114, 129	0
50	DR	117/118 (99%)	0.08	0 100 100	75, 98, 115, 129	0
51	BS	98/112 (87%)	0.50	6 (6%) 21 3	89, 112, 137, 141	0
51	DS	98/112 (87%)	0.25	2 (2%) 62 12	88, 111, 136, 140	0
52	BT	137/146 (93%)	0.05	3 (2%) 59 11	74, 97, 155, 179	0
52	DT	137/146 (93%)	0.11	6 (4%) 33 5	73, 97, 154, 179	0
53	BU	117/118 (99%)	0.04	1 (0%) 81 25	81, 98, 125, 142	0
53	DU	117/118 (99%)	0.04	1 (0%) 81 25	78, 97, 125, 142	0
54	BV	101/101 (100%)	0.28	4 (3%) 36 5	79, 130, 146, 150	0
54	DV	101/101 (100%)	0.26	2 (1%) 62 12	79, 129, 146, 150	0
55	BW	113/113 (100%)	0.21	2 (1%) 65 14	85, 100, 133, 165	0
55	DW	113/113 (100%)	0.12	3 (2%) 52 8	82, 100, 133, 165	0
56	BX	92/96 (95%)	0.25	0 100 100	83, 109, 125, 134	0
56	DX	92/96 (95%)	0.17	0 100 100	83, 108, 124, 134	0
57	BY	100/110 (90%)	0.89	13 (13%) 4 1	127, 146, 179, 187	0
57	DY	100/110 (90%)	0.88	14 (14%) 3 1	126, 146, 179, 187	0
58	BZ	176/206 (85%)	-0.00	3 (1%) 67 15	75, 103, 135, 144	0
58	DZ	176/206 (85%)	-0.01	2 (1%) 77 22	64, 94, 140, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22010/23368 (94%)	-0.02	468 (2%) 60 11	37, 93, 163, 200	0

The worst 5 of 468 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	DH	170	ARG	8.7
1	AA	89	C	8.6
49	DQ	141	GLN	8.2
36	DA	654(K)	C	8.1
57	BY	2	ARG	7.7

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	MIA	CY	37	29/30	0.28	-	60,80,107,108	0
24	5MU	AY	54	21/22	0.20	-	143,153,153,156	0
24	H2U	CY	20	20/21	0.36	-	185,186,187,187	0
24	MIA	AY	37	29/30	0.25	-	63,84,108,108	0
24	7MG	AY	46	24/25	0.35	-	166,169,171,171	0
24	4SU	CY	8	20/21	0.22	-	140,141,142,142	0
24	PSU	AY	55	20/21	0.19	-	157,166,168,168	0
24	7MG	CY	46	24/25	0.22	-	166,168,170,170	0
24	OMC	AY	32	21/22	0.32	-	98,106,112,113	0
24	H2U	AY	20	20/21	0.31	-	186,186,188,188	0
24	5MU	CY	54	21/22	0.17	-	142,153,154,156	0
24	PSU	CY	55	20/21	0.19	-	158,166,168,168	0
24	H2U	CY	17	20/21	0.58	-	194,195,195,195	0
24	OMC	CY	32	21/22	0.17	-	96,103,108,109	0
24	H2U	AY	16	20/21	0.64	-	181,191,192,193	0
24	H2U	AY	17	20/21	0.51	-	194,195,195,195	0
24	H2U	CY	16	20/21	0.65	-	181,191,191,193	0
24	4SU	AY	8	20/21	0.29	-	140,143,144,144	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
60	GDP	CZ	501	28/28	0.24	-	141,145,153,153	0
59	ZN	B9	101	1/1	0.15	-	200,200,200,200	0
59	ZN	B4	101	1/1	0.08	-	200,200,200,200	0
59	ZN	AD	301	1/1	0.30	-	99,99,99,99	0
59	ZN	CN	101	1/1	0.17	-	63,63,63,63	0
59	ZN	AN	101	1/1	0.16	-	84,84,84,84	0
59	ZN	D4	101	1/1	0.14	-	129,129,129,129	0
59	ZN	CD	301	1/1	0.31	-	85,85,85,85	0
61	KIR	CZ	502	57/57	0.36	-	139,145,150,151	0
59	ZN	D9	101	1/1	0.11	-	133,133,133,133	0
61	KIR	AZ	502	57/57	0.60	-	139,147,150,150	0
60	GDP	AZ	501	28/28	0.24	-	151,157,158,158	0

6.5 Other polymers

There are no such residues in this entry.