



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:03 PM BST

PDB ID : 4V5P  
Title : The crystal structure of EF-Tu and A9C-tRNA-Trp bound to a near- 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](mailto:validation@mail.wwpdb.org)

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

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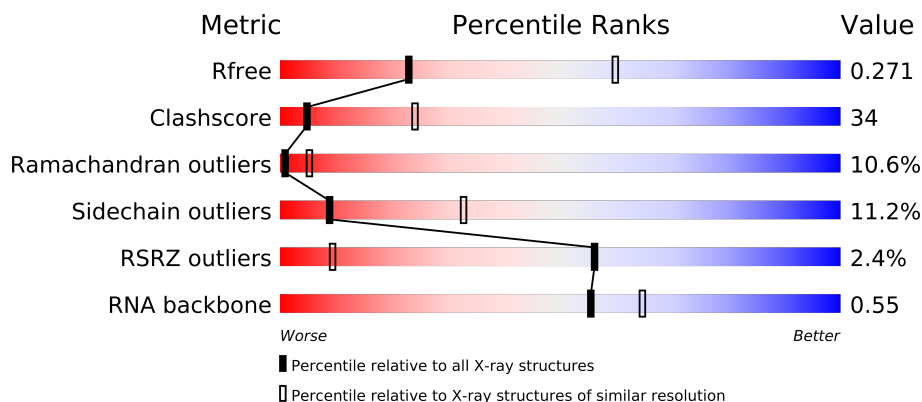
The following versions of software and data (see [references](#)) were used in the production of this report:

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  $\geq 3$ , 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	135	
12	CL	135	
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 307322 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			

There are 8 discrepancies between the modelled and reference sequences:

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

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			361	164	68	113	16			
23	CX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			

- Molecule 24 is a RNA chain called A-SITE TRNA A9C TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total 1643	C 741	N 287	O 537	P 76	S 2	0	0	0
24	CY	77	Total 1643	C 741	N 287	O 537	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
			2983	1886	522	563	12			
25	CZ	385	Total	C	N	O	S	0	0	0
			2983	1886	522	563	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	6	ILE	VAL	CONFLICT	UNP Q5SHN6
AZ	264	LYS	ARG	CONFLICT	UNP Q5SHN6
CZ	6	ILE	VAL	CONFLICT	UNP Q5SHN6
CZ	264	LYS	ARG	CONFLICT	UNP Q5SHN6

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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				

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

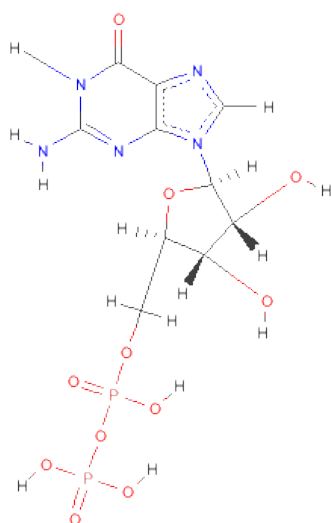
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		

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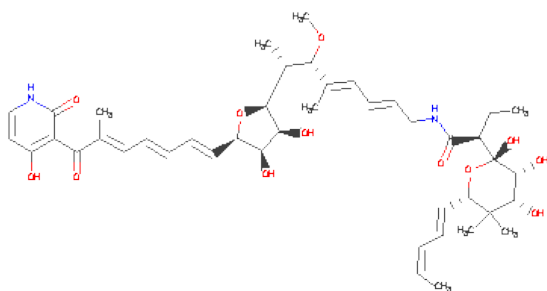
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- 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:  $C_{43}H_{60}N_2O_{12}$ ).



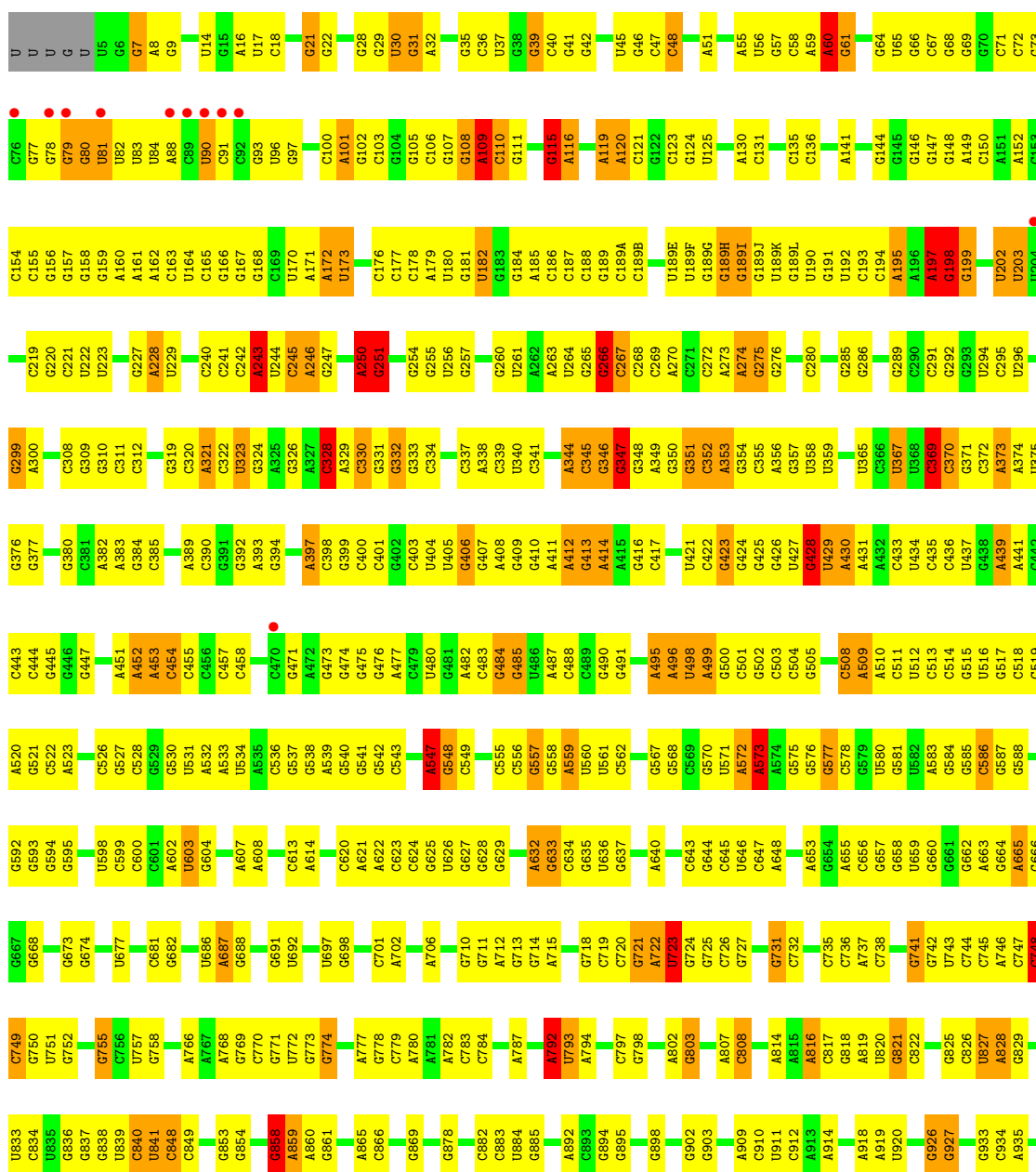
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
61	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

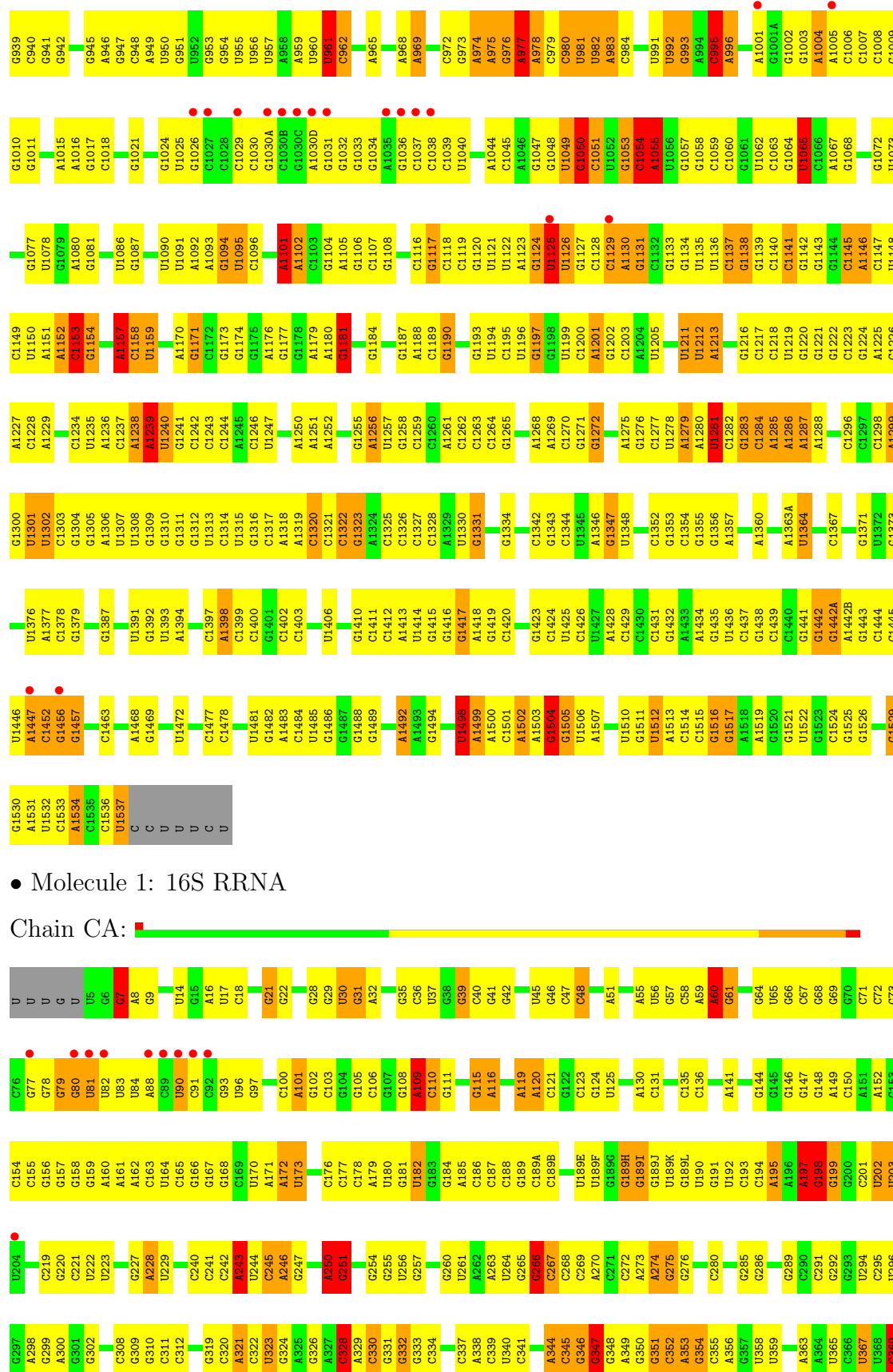
### 3 Residue-property plots

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

Chain AA: 

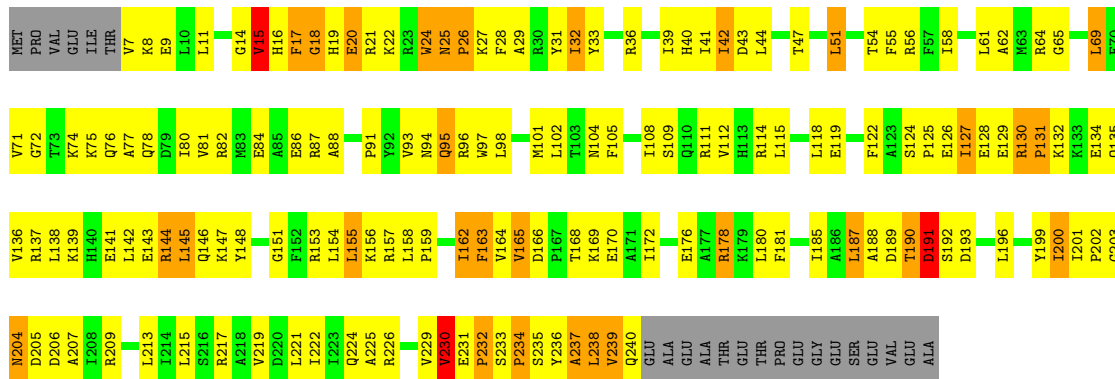




U1506	G1421	U1345	A1204	G1131	A1055	A983	A913	A819	C738	G561	G584	G515	C436	C370
A1507	G1422	A1346	U1205	C1132	U1056	C984	A914	U820	G741	G662	G585	U516	U437	G371
G1508	G1423	G1347	G1206	G1133	G1057	U991	A918	G1057	C822	A663	C586	C517	A438	C372
C1509	C1424	U1348	U1211	G1134	C1059	U992	A919	U992	U743	A664	G587	C518	A439	A373
U1510	U1425	U1352	U1212	U1135	C1060	U993	U920	G825	C744	A665	G588	C519	A441	A374
U1512	A1428	G1353	A1213	U1137	G1061	A994	U921	C826	C745	G666	G592	A520	U442	U375
A1513	C1429	C1354	G1216	G1138	U1062	C995	A923	U827	A746	G667	G593	G521	C443	G376
C1514	C1430	G1355	C1217	G1139	C1063	C996	C924	A828	C747	G668	G594	C522	C444	G377
C1515	G1431	G1356	C1218	C1140	U1065	C997	G925	G829	C748	G673	G595	A523	C445	
G1516	G1432	A1357	U1219	C1141	U1066	A1001	G926	G829	C749	G674	G596	C524	C446	G380
U1517			U1220	G1142	U1067	G1001A	G927	U833	G750	G675	U598	C526	U447	C381
A1518	G1435	A1360	G1221	G1143	A1067	G1002	G927	C834	U751	U677	C599	G527	A451	A382
A1519	U1436	G1361	G1222	G1144	G1003	G1003		U835			C600	C528	A452	A383
			G1223	C1145	A1004	G836	C934	G836	G755		G601	G529	A453	G384
U1522	G1442	C1363	C1224	A1146	A1005	G837	A935	A1005	C756	C681	A602	G530	A454	C385
G1523	G1442A	U1363A	G1224	A1147	C1006	G838	C936	C1006	U757	G682	U603	U531	C454	
C1524	A1442B	A1364	A1225	U1148	C1007	G839	A937	U839	G758	U686	G604	A532	C455	A389
G1525	G1443	G1365	C1226	C1149	C1008	A938	G938	C840		A687	G604	A533	C456	C390
G1526	C1444	C1366	A1227	U1150	G1009	G939	C939	U841	A766	G688	A607	U534	C457	G391
	C1445	C1367	A1228	U1151	U1078	G940	C940	U842			A608	A535	C458	C392
G1530	A1447	U1301	A1229	A1152	U1079	G1010	G941	C849	C770	U691	C613	C536	C471	A393
A1531	C1452	U1302	C1234	C1153	A1080	G1011	G942	G853	U771	U692	A614	G537	A472	G394
U1532	G1456	G1303	U1235	G1154	U1086	A1015	G945	G854	U772	U697		G540	G473	A397
C1533		C1304	A1236	A1157	G1087	G1016	A946		G773	G698	A621	G541	G474	C398
A1534	C1459	A1306	C1237	C1158	U1090	G858	G947	A859	G774		A622	G542	G475	C399
C1535	U1376	U1307	U1238	U1159	U1091	A860	A949	A860	A777	C701	C623	C543	C476	C400
C1536	A1377	U1308	A1239	A1170	U1092	G861	U950	G861	C778	A702	C624	C543	C477	C401
U1537	G1378	G1309	U1240	G1171	U1025	C862	G951	C862	C779	A706	G625	A547	C479	G402
C	C1463	G1310	G1241	G1172	U1094		U952			C707	U626	G548	G481	U404
U		C1311	C1242	G1173	U1095	A865	G953	A865	A761	C708	G627	C549	U480	U405
C	C1466	G1312	C1243	G1174	C1096	C866	G954	C866	C783	C709	G628	G550	A482	G406
U	G1467	A1313	A1244	G1175	A1101	G1030	U955	U955	U782	G710	G629	U551	C483	A408
U	C1468	C1314	A1245	G1176	A1102	C1030A	U956	G869	C784	G711	A632	U552	U486	G409
C	G1469	U1315	C1246	G1177	G1103	G1030C	U957	U870		A712	G633	C555	A487	G410
U		G1316	U1247	G1178	G1104	A1030D	A958		A787	G713	C634	C556	C488	A411
	C1479	C1317	A1250	A1179	A1105	G1031	A959	G878		G714	G635	C557	C489	A412
		A1318	A1251	A1180	G1106	G1032	U960		A782	A715	U636	G558	C490	A413
	G1482	A1319	A1252	G1181	C1107	G1033	U961	C882	U783	A716	G637	A559	G491	A414
		C1320	A1253	G1182	G1108	C962	C962	C883	A794	C717	G638	U560		A415
U1485		C1321	G1255	G1184	G1109	A1035	G963	U884		G718	G639	U561	A495	G416
G1486		G1322	A1256	G1185	A1110	G1036	A964	G885	C797	C719	A640	C562	A496	C417
G1487		C1323	U1257	G1187	C1116	C1037	A965		G798	C720	C643	G567	U498	
G1488		A1324	G1258	A1188	G1117	C1038	A968	G894	A802	G721	G644	G568	A499	U421
G1489		C1325	C1259	A1189	C1118	C1039	A969	G895	U803	A722	C645	C501	G500	C422
C1490		C1327	G1260	G1190	C1119	U1040		C896	U804	U723	G646	G502	C501	G423
G1491		C1328	A1261	G1191	C1120	G903	C972	G897		G724	U646	G503	G502	G424
A1492		U1329	C1262	G1193	U1121	C899	G973	G898	A807	G725	C647	C504	C503	G425
A1493		U1330	C1263	U1194	U1122	C899	G974		C808	G727	A648	G505	G504	G426
		G1331	C1264	U1195	A1123	A900	A974				A653	G575	G505	U427
			G1265	C1196	G1047	A901	A975		C811	G731	G654	G576	C508	G428
		G1334	G1266	U1197	G1124	G902	G976	G902		C732	A655	C578	A509	A430
			G1267	G1198	U1125	U1049	A977	G903		C733	C656	G579	A510	A431
		G1338	U1268	U1199	U1126	G1050	A978		A814	A730	C657	U580	A511	A432
			A1269	C1200	G1127	C1051	C979	A909	A815	G734	G657	U581	C511	A433
		C1342	C1270	A1201	C1128	U1052	C980	C910	A816	C735	G658	U582	U512	C433
			G1271	G1202	C1129	U1053	U981	U911	C817	C736	G659	U583	C513	U434
			G1272	C1203	A1130	C1054	U982	C912	G818	A737	G660		C514	C435

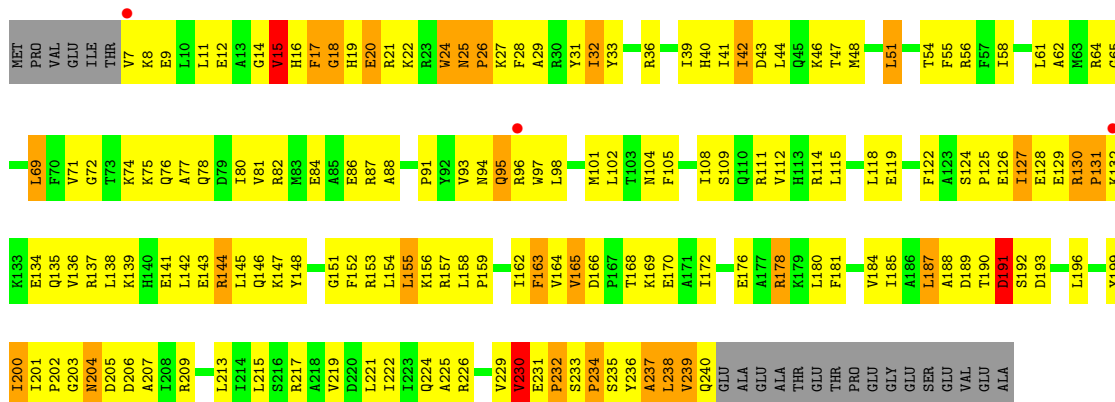
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



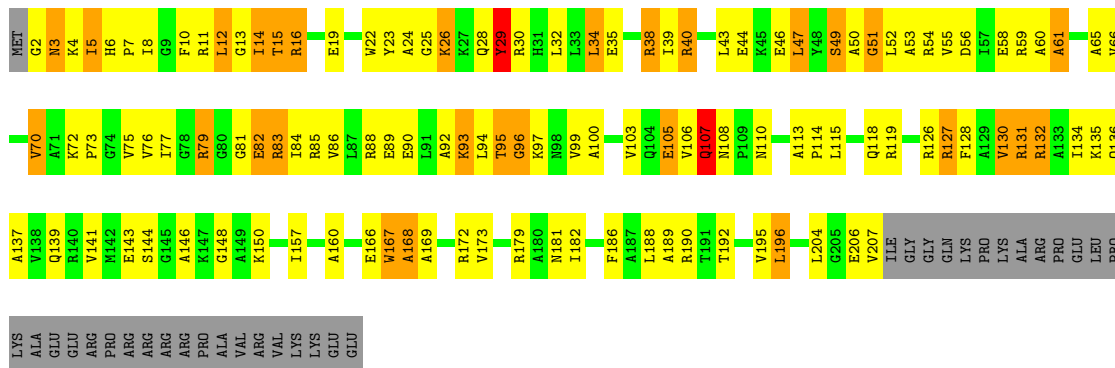
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



- Molecule 3: 30S RIBOSOMAL PROTEIN S3

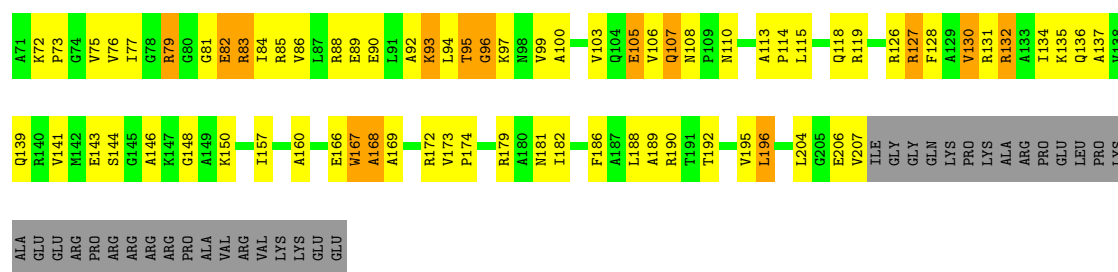
Chain AC:



- Molecule 3: 30S RIBOSOMAL PROTEIN S3

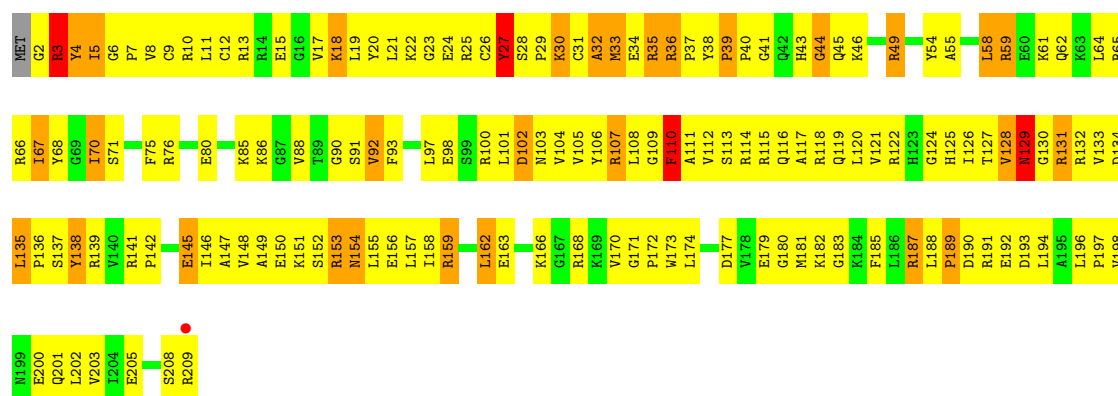
Chain CC:





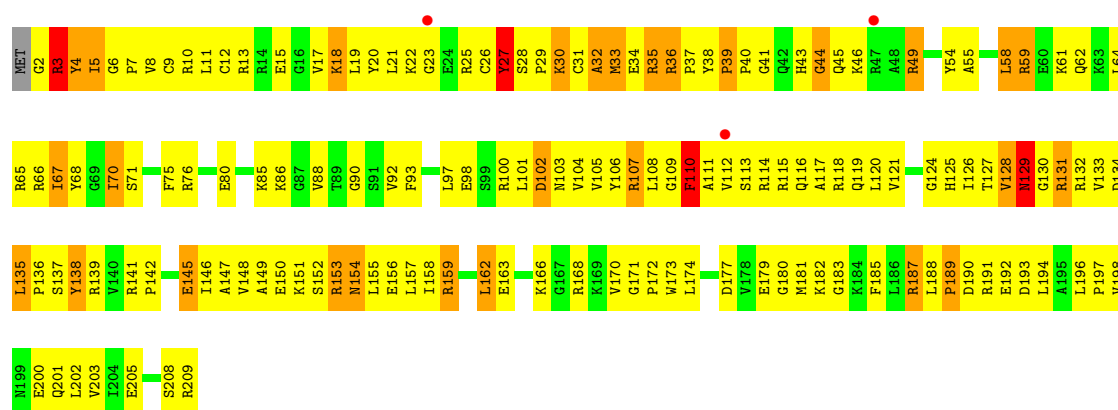
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



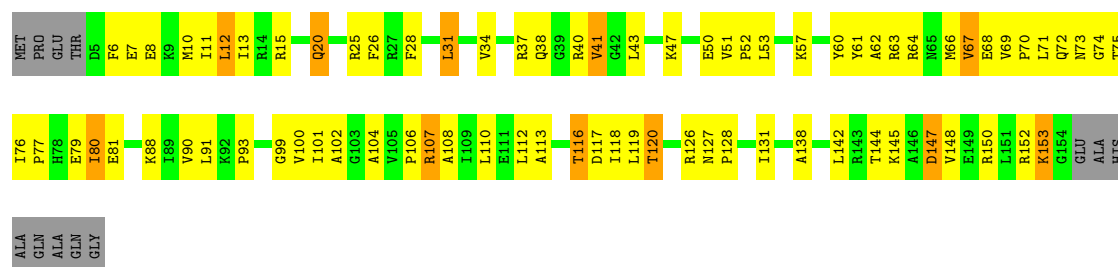
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

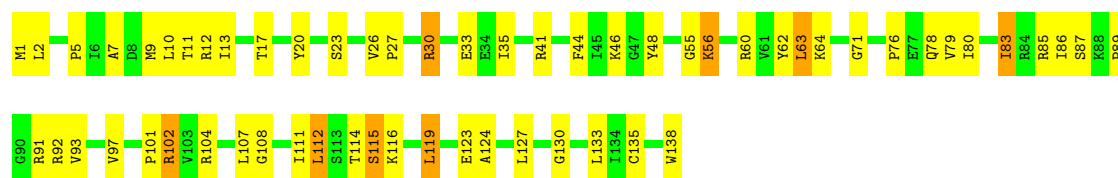
Chain AE:





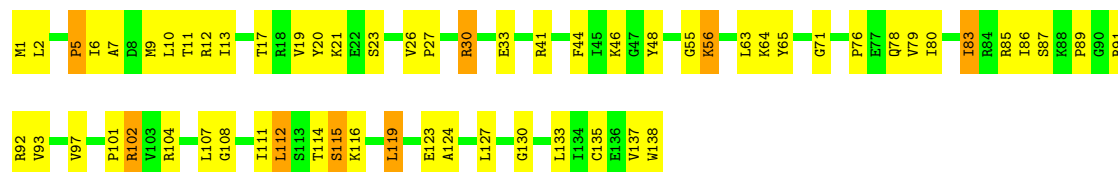


Chain AH:



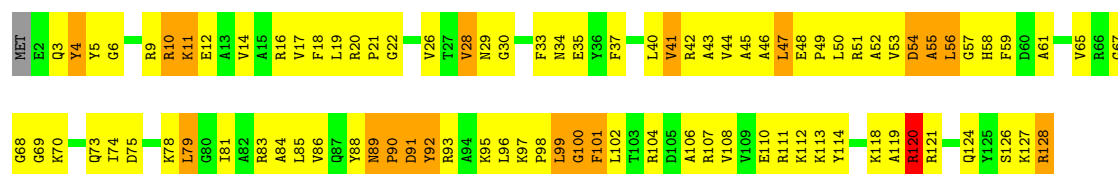
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



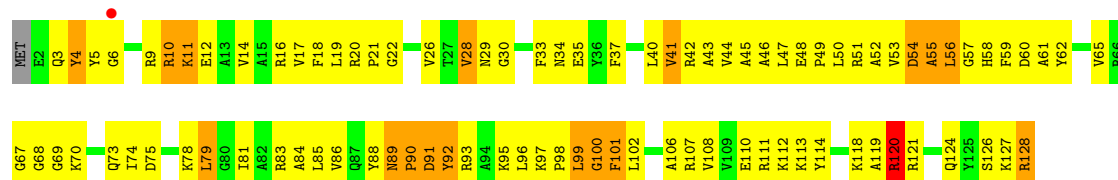
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



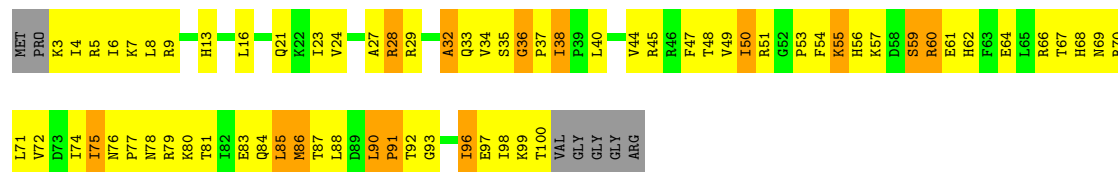
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

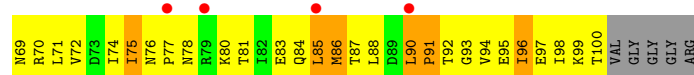
Chain AJ:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:





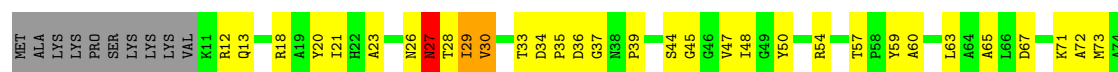
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



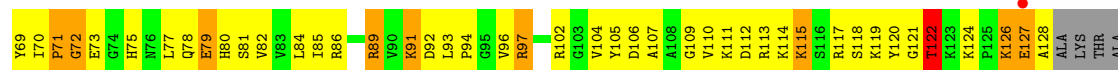
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



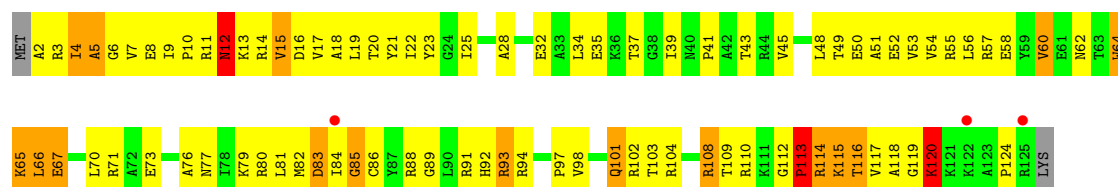
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



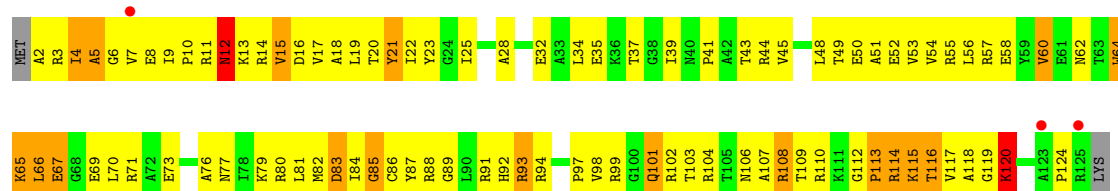
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



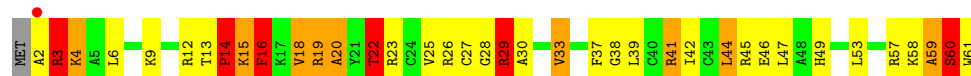
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



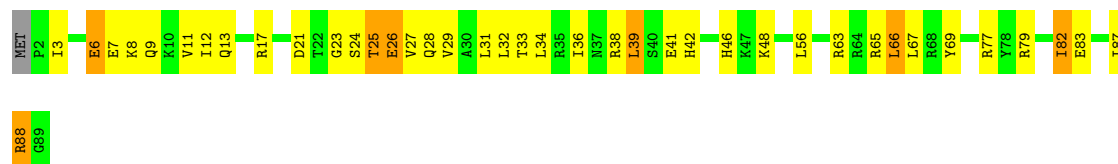
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



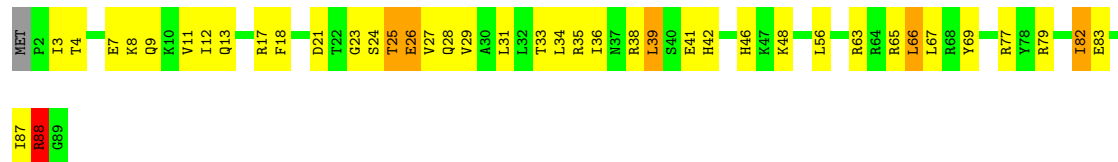
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



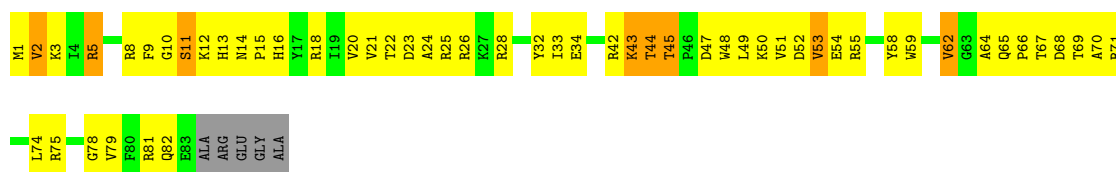
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



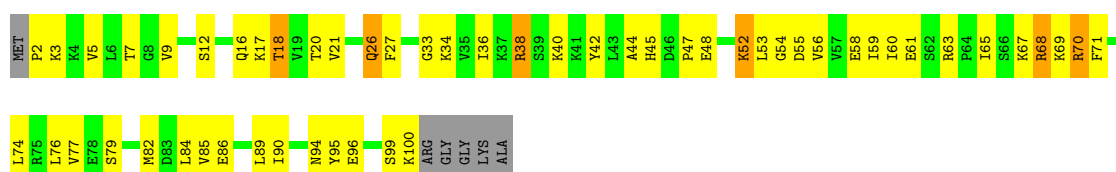
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



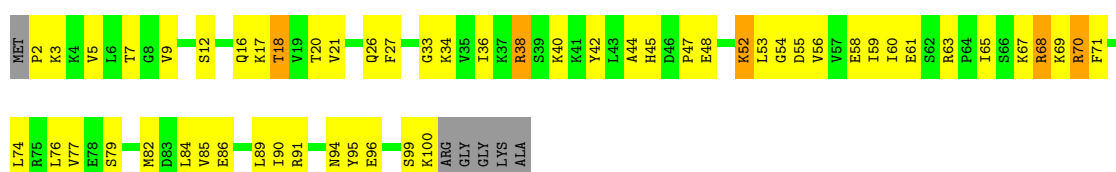
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



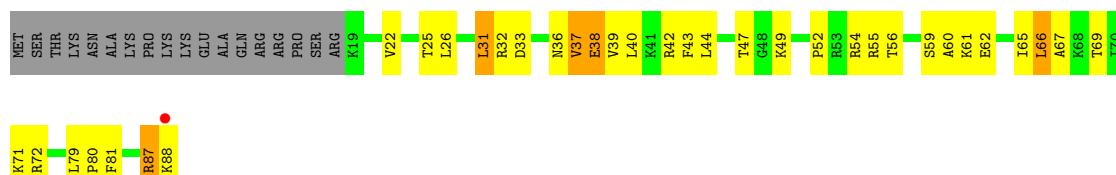
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:

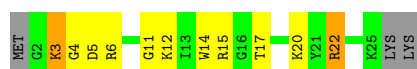


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:







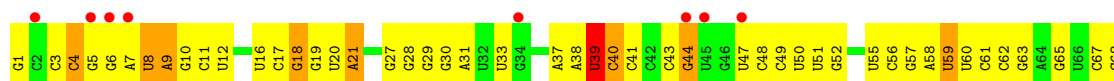
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

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:



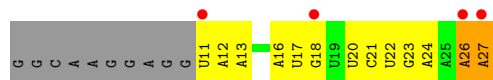
- Molecule 23: MRNA

Chain AX:



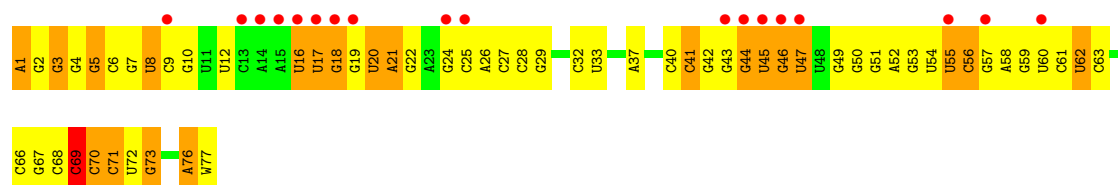
- Molecule 23: MRNA

Chain CX:



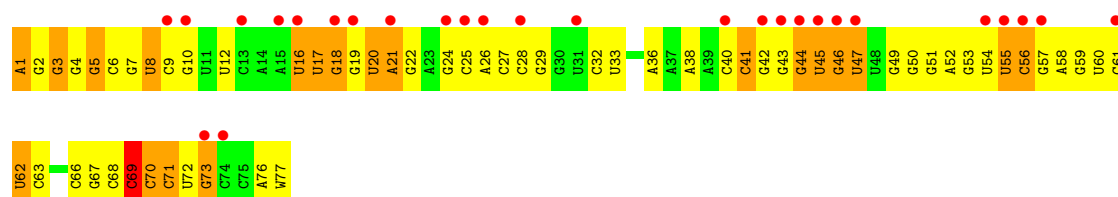
- Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP

Chain AY:



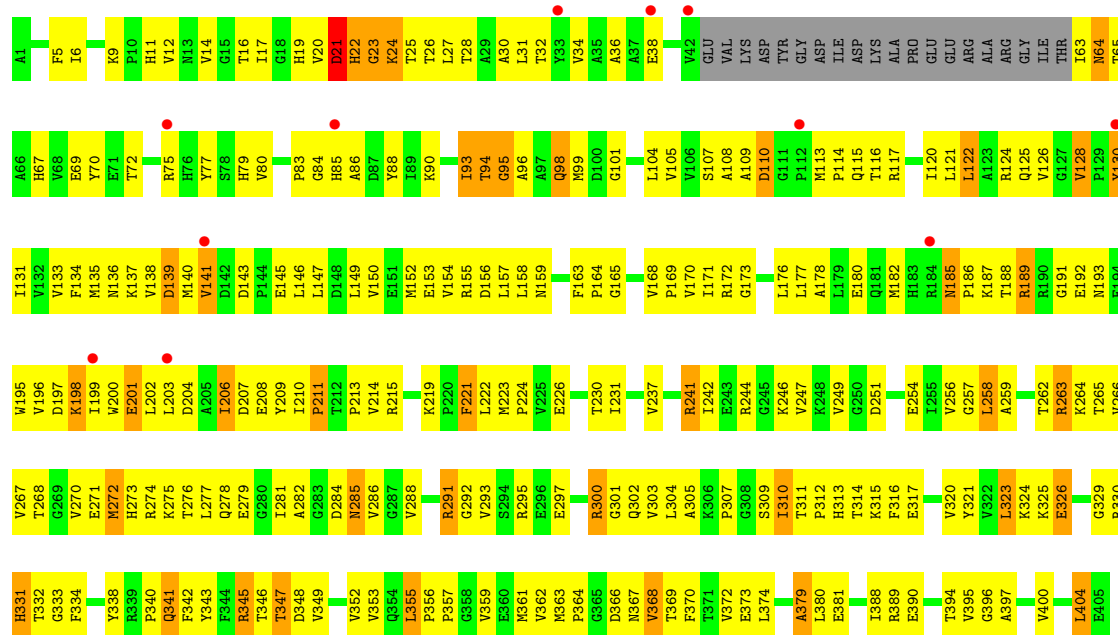
• Molecule 24: A-SITE TRNA A9C TRP-TRNA TRP

Chain CY:



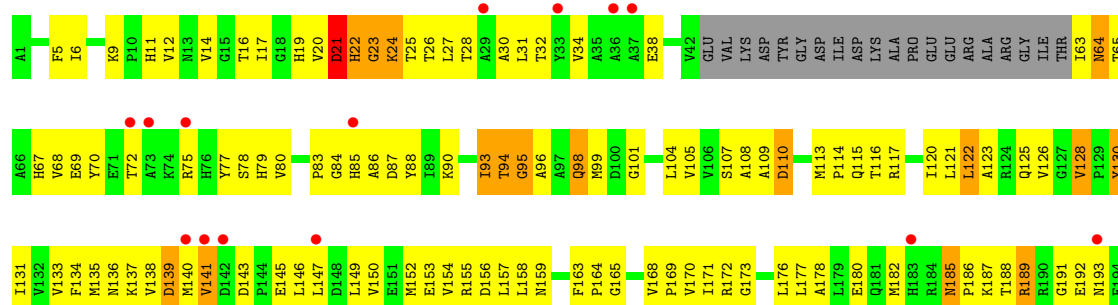
• Molecule 25: ELONGATION FACTOR TU

Chain AZ:

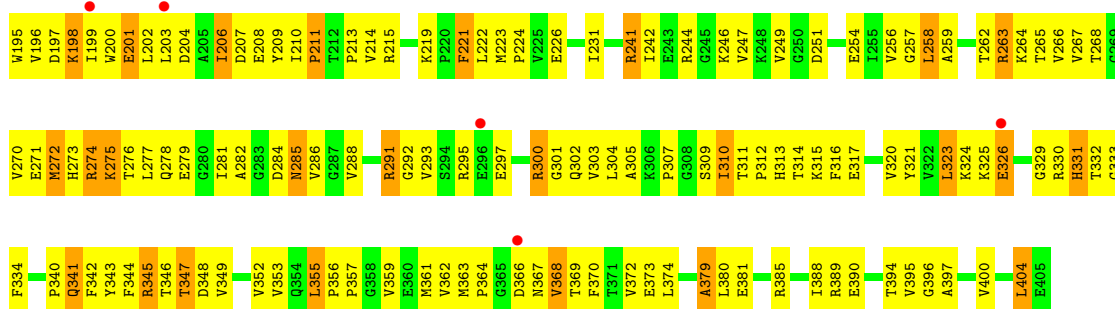


• Molecule 25: ELONGATION FACTOR TU

Chain CZ:

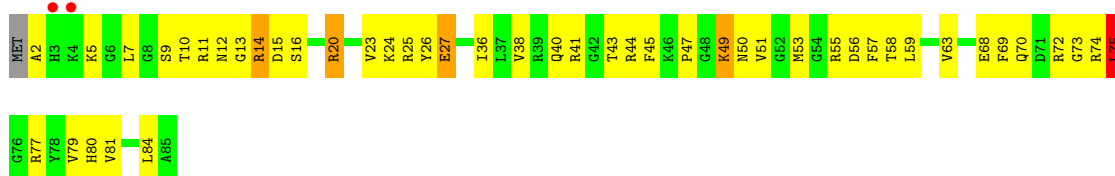






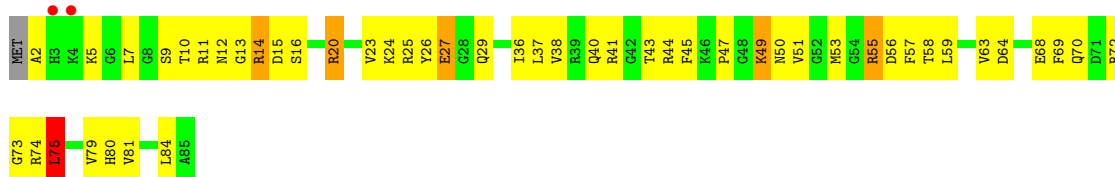
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



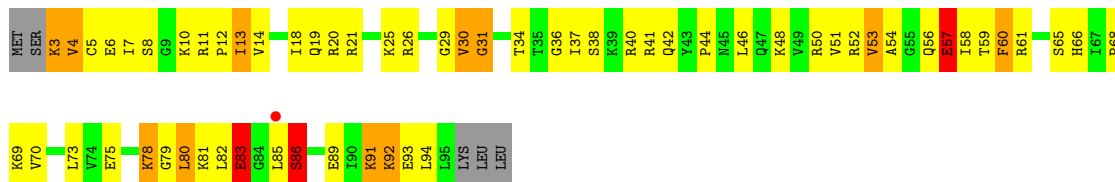
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



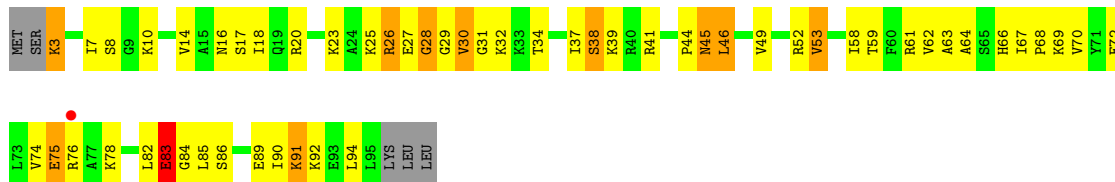
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



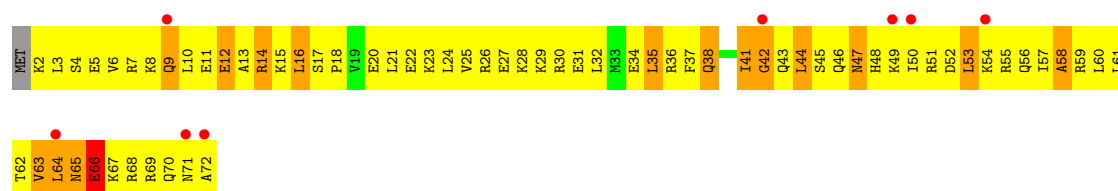
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



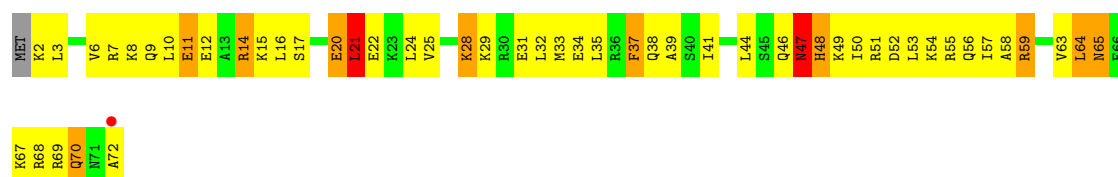
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



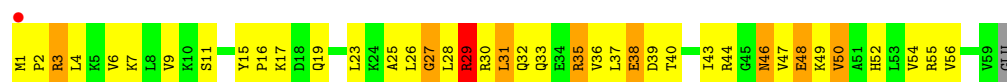
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



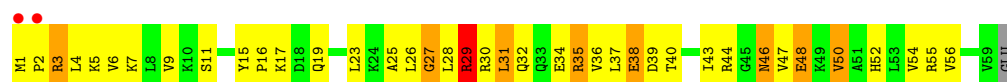
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



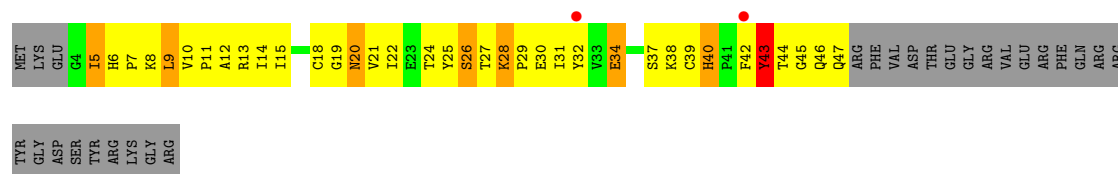
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



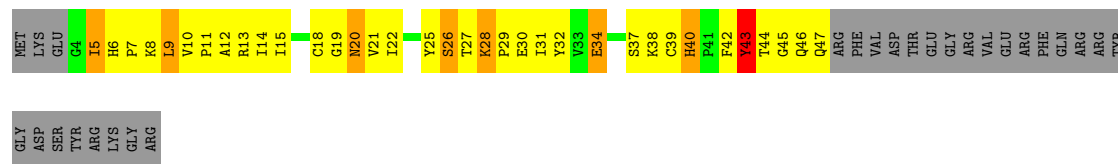
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



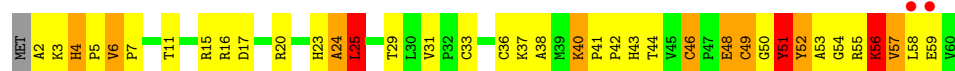
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:



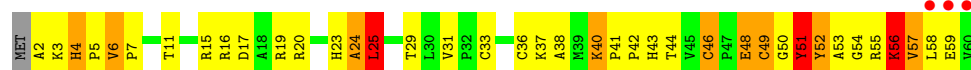
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

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:



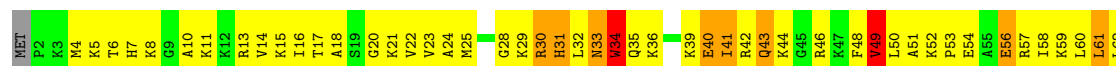
• Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:



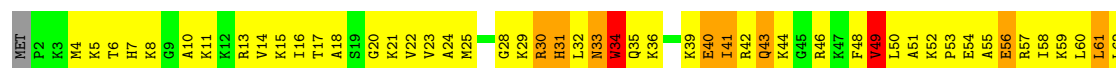
• Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



• Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8:





• Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



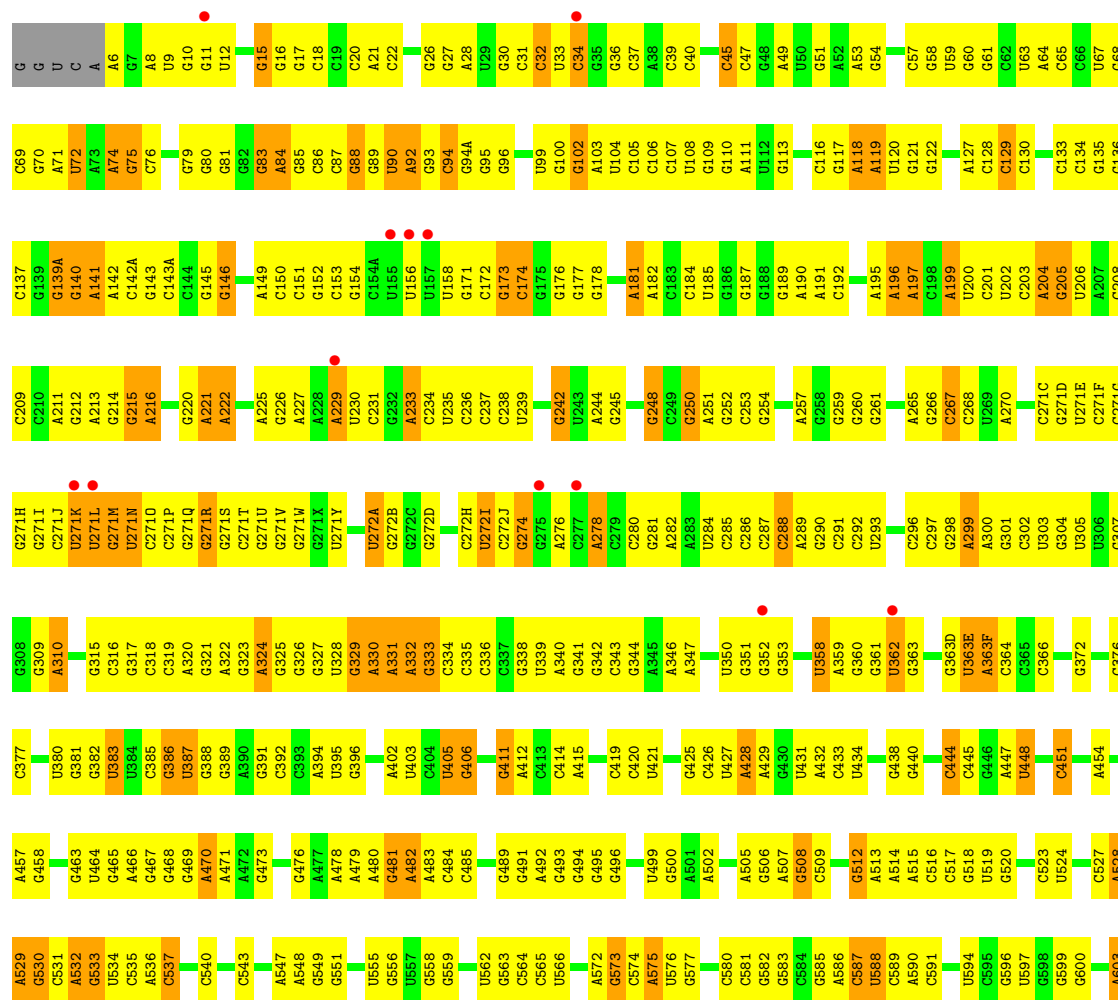
• Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



• Molecule 36: 23S RIBOSOMAL RNA

Chain BA:



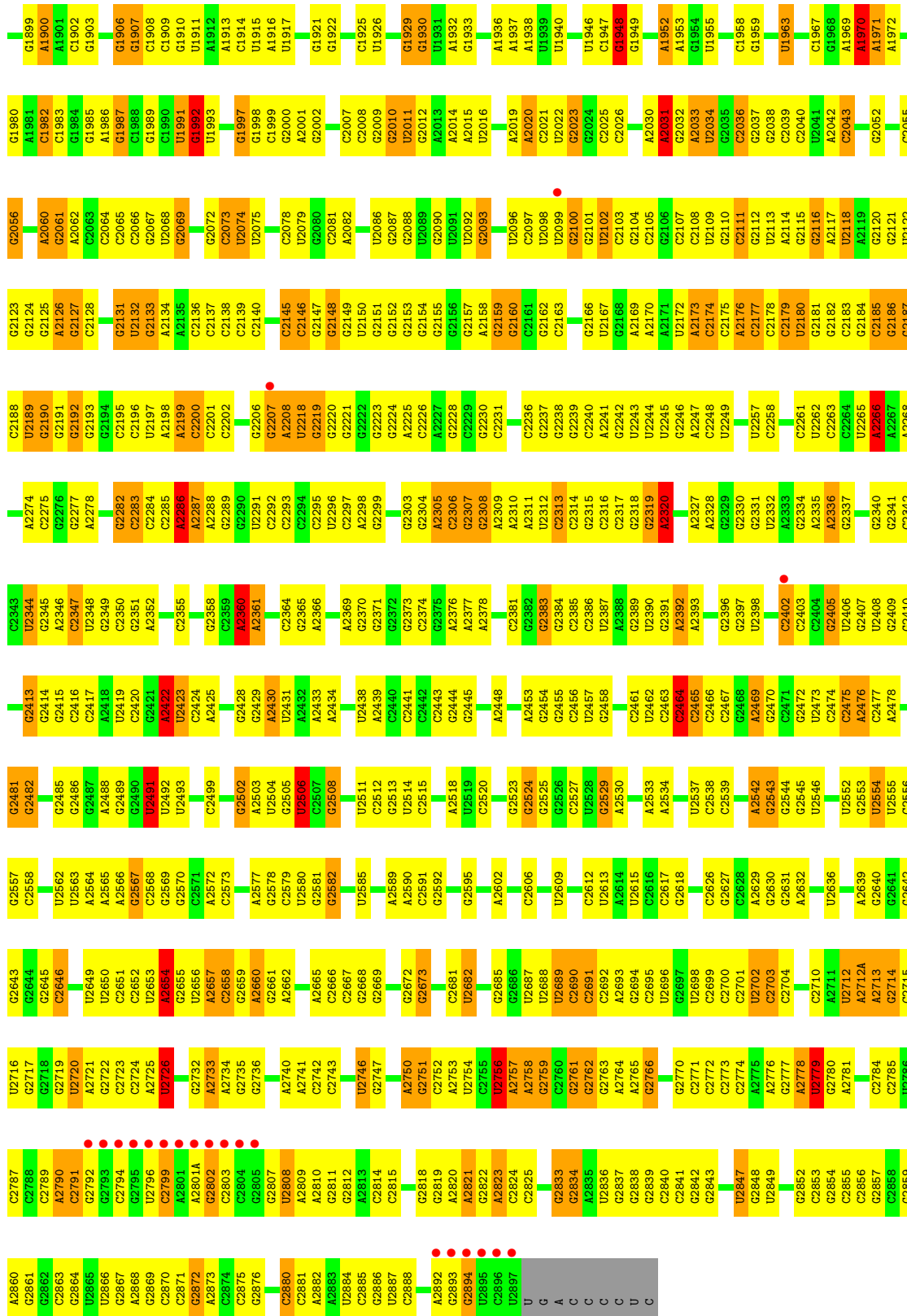
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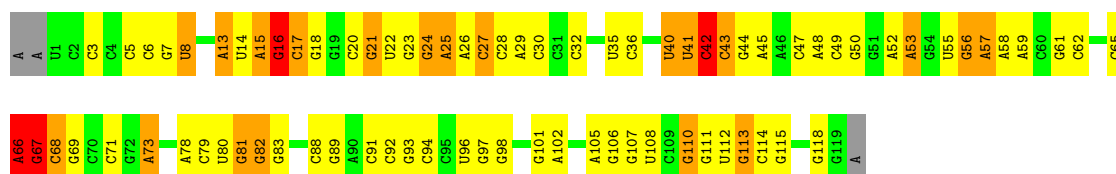
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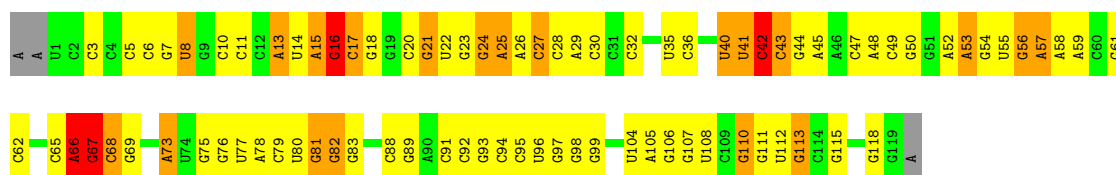






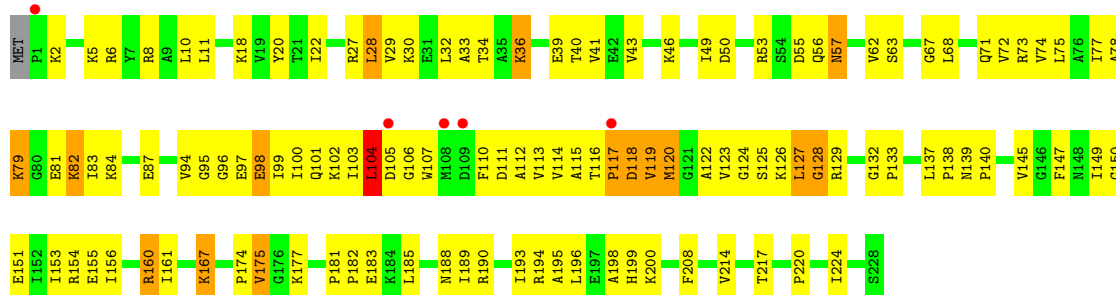
• Molecule 37: 5S RIBOSOMAL RNA

Chain DB:



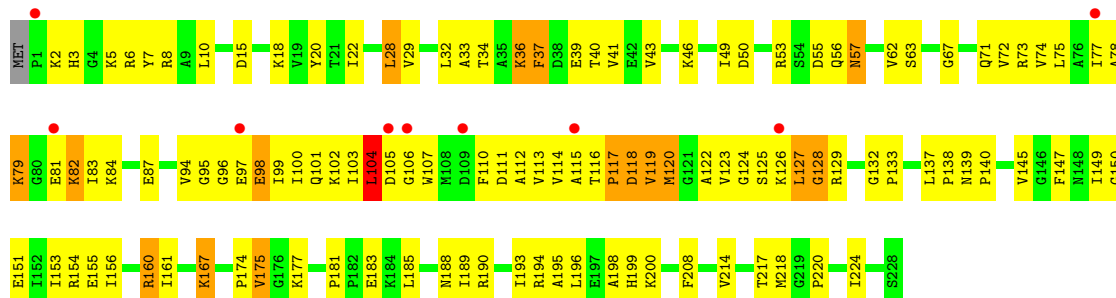
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC:



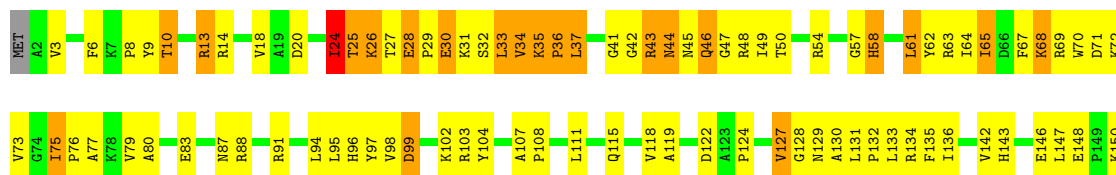
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

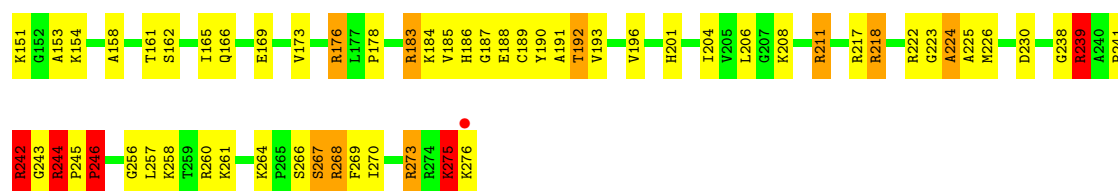
Chain DC:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

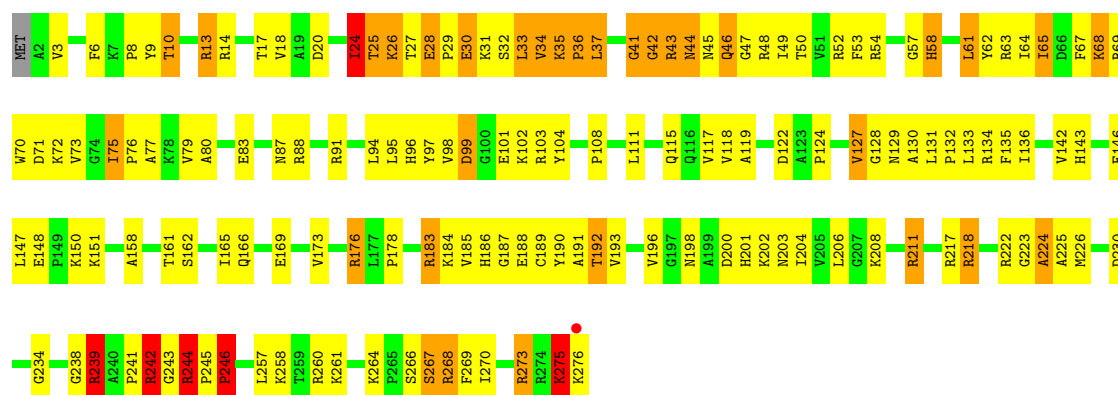
Chain BD:





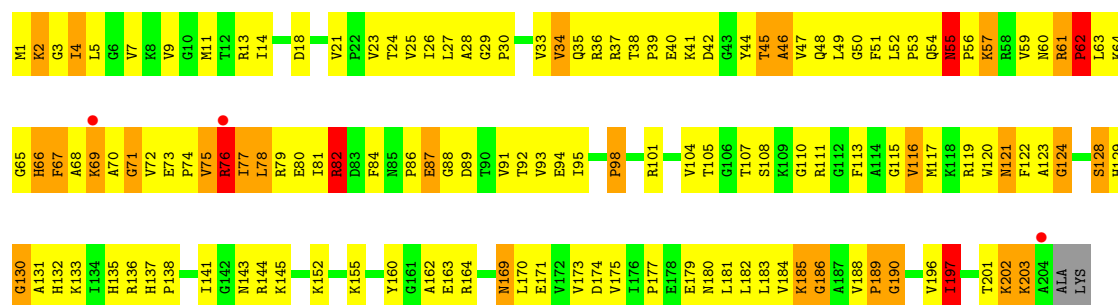
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD:



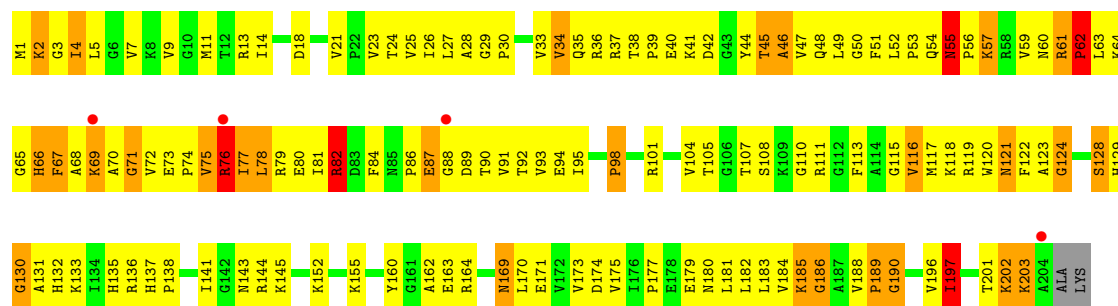
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE:



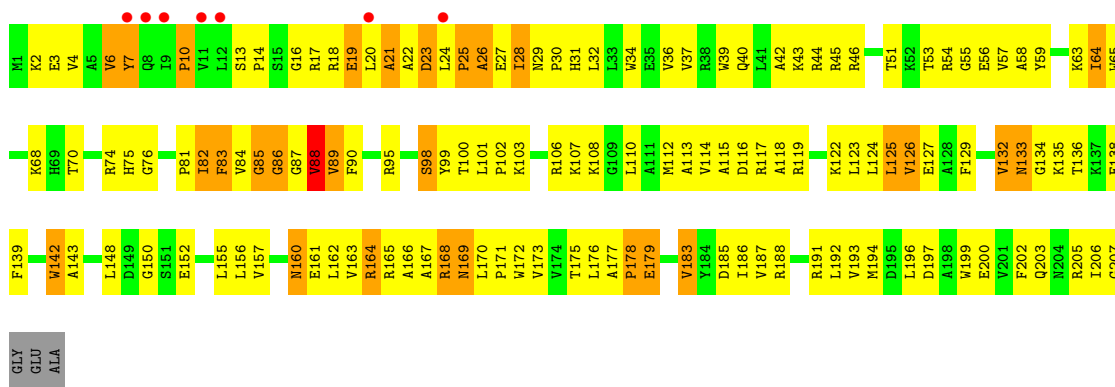
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE:



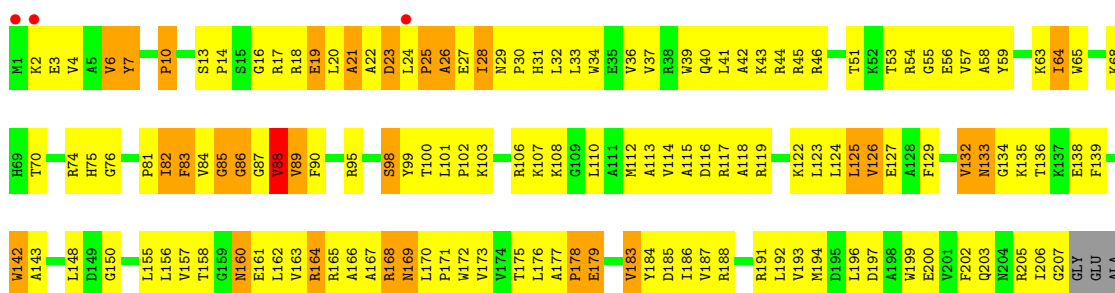
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF:



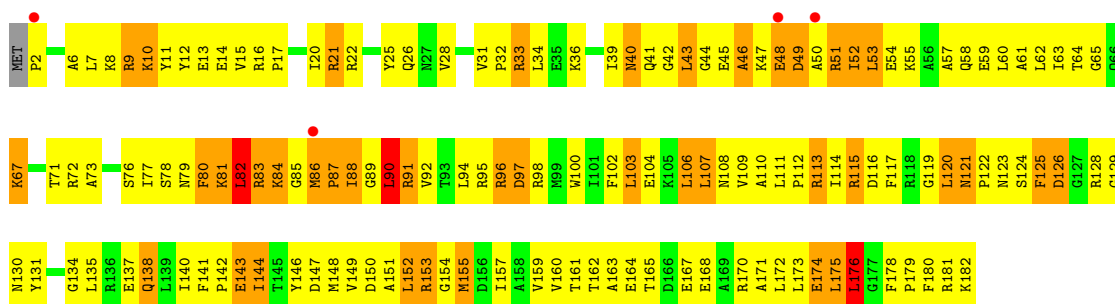
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:



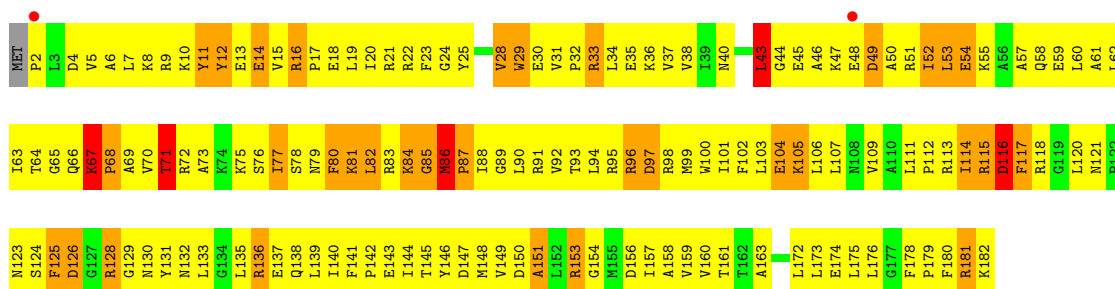
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain BG:

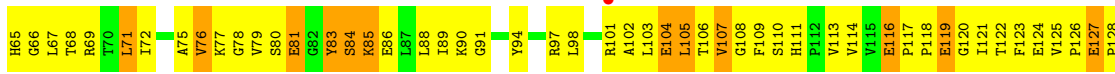


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

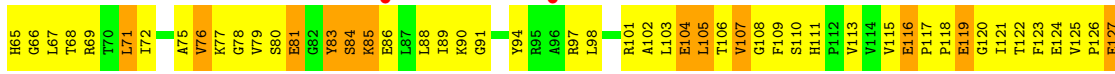
Chain DG:



• Molecule 43: 50S RIBOSOMAL PROTEIN L6



- Molecule 43: 50S RIBOSOMAL PROTEIN L6



- Molecule 44: 50S RIBOSOMAL PROTEIN L10

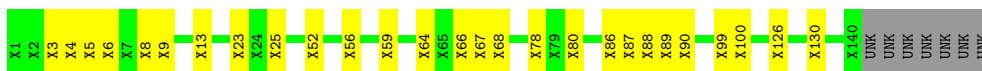


- Molecule 44: 50S RIBOSOMAL PROTEIN L10

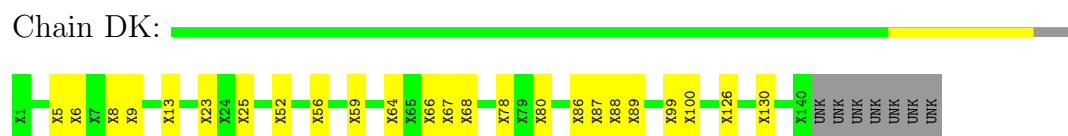


- Molecule 45: 50S RIBOSOMAL PROTEIN L11

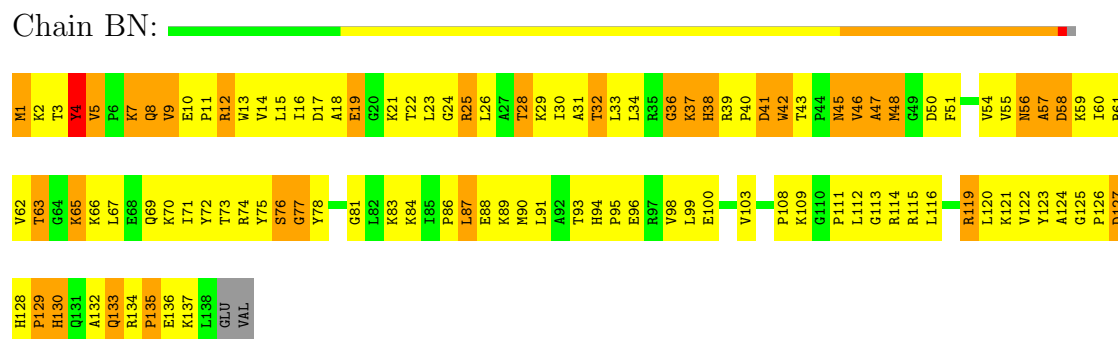
Age Group	Percentage
18-24	15%
25-34	20%
35-44	25%
45-54	20%
55-64	15%
65-74	10%
75-84	5%
85+	5%



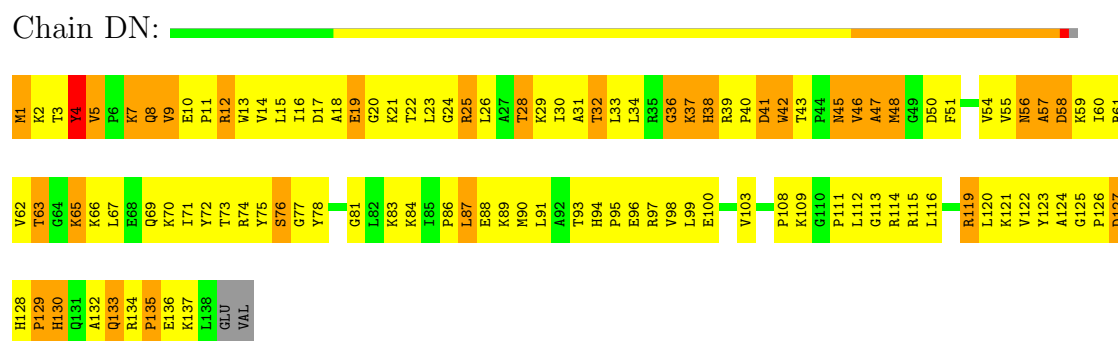
- Molecule 45: 50S RIBOSOMAL PROTEIN L11



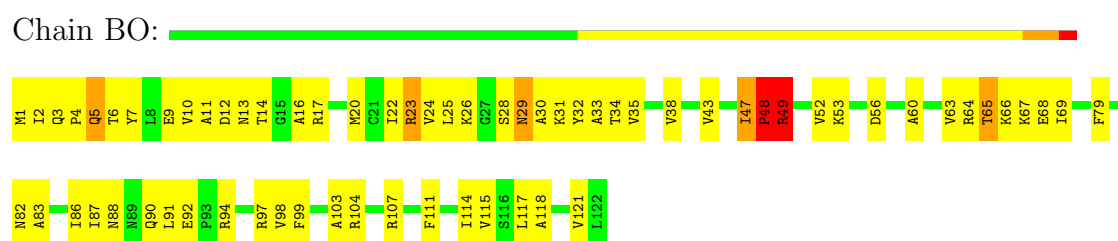
- Molecule 46: 50S RIBOSOMAL PROTEIN L13



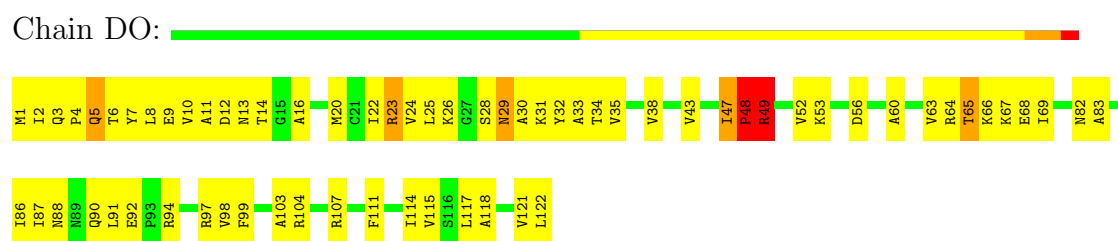
- Molecule 46: 50S RIBOSOMAL PROTEIN L13



- Molecule 47: 50S RIBOSOMAL PROTEIN L14

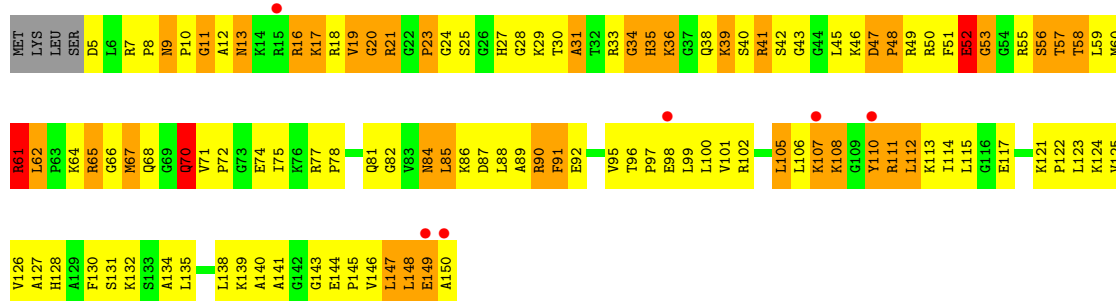


- Molecule 47: 50S RIBOSOMAL PROTEIN L14



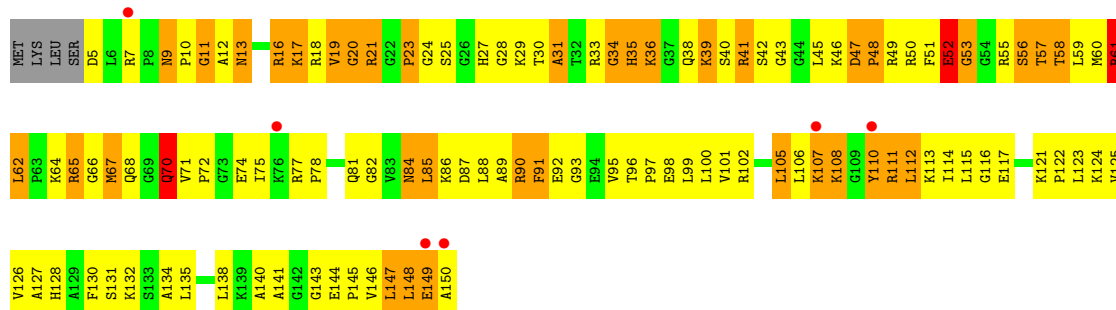
- Molecule 48: 50S RIBOSOMAL PROTEIN L15





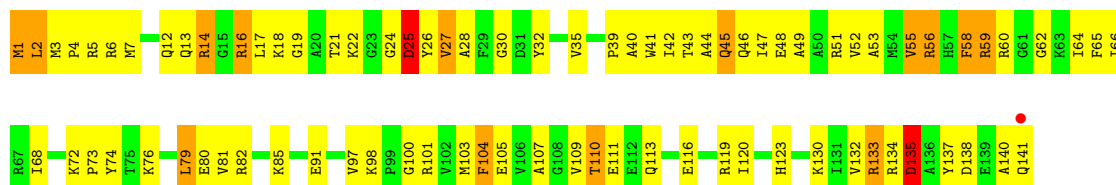
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



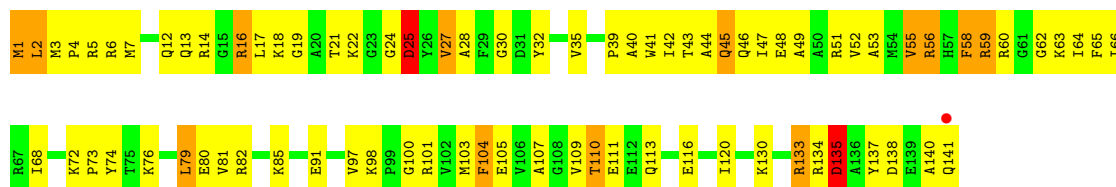
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



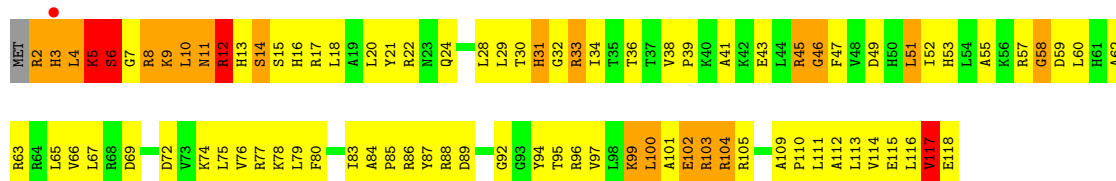
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



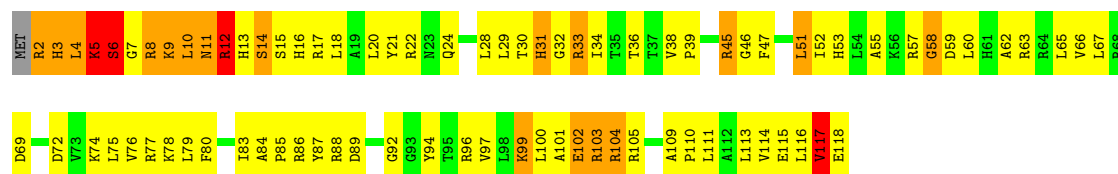
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



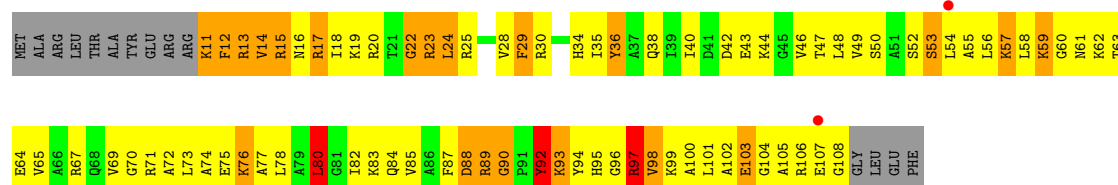
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



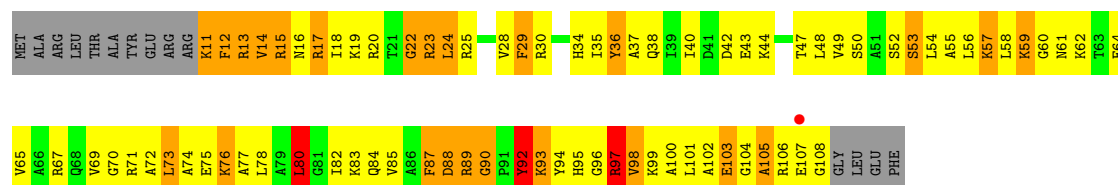
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



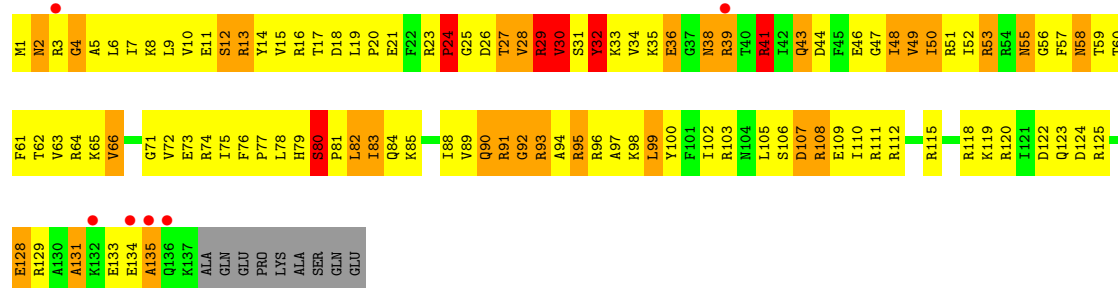
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:

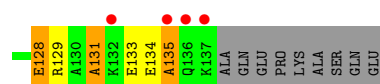


- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:

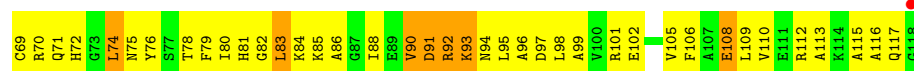
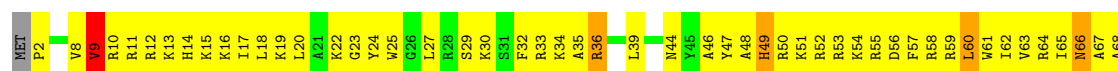






• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



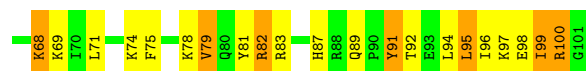
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



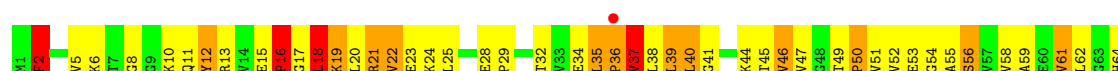
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



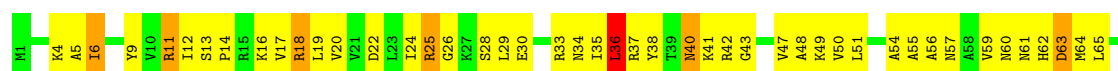
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



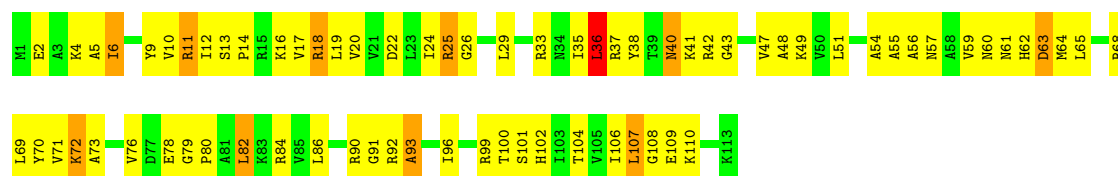
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



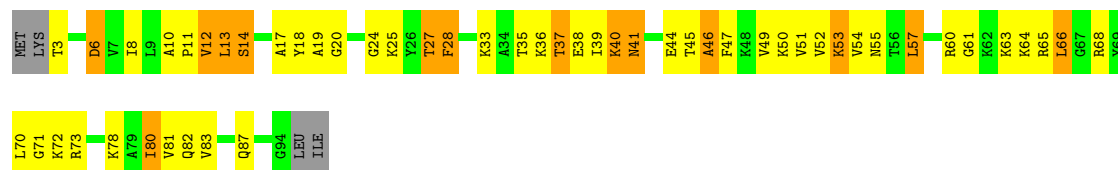
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



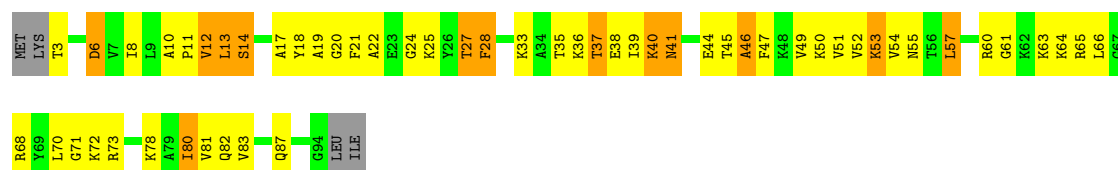
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



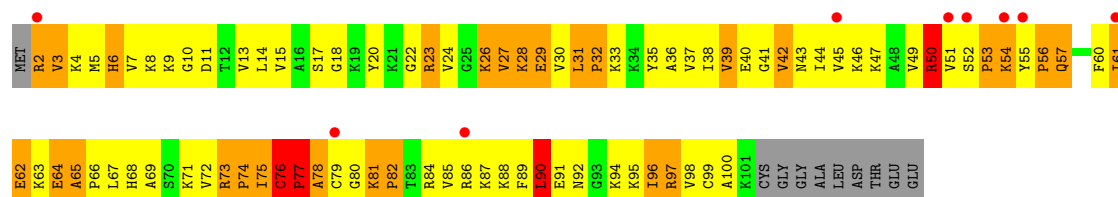
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

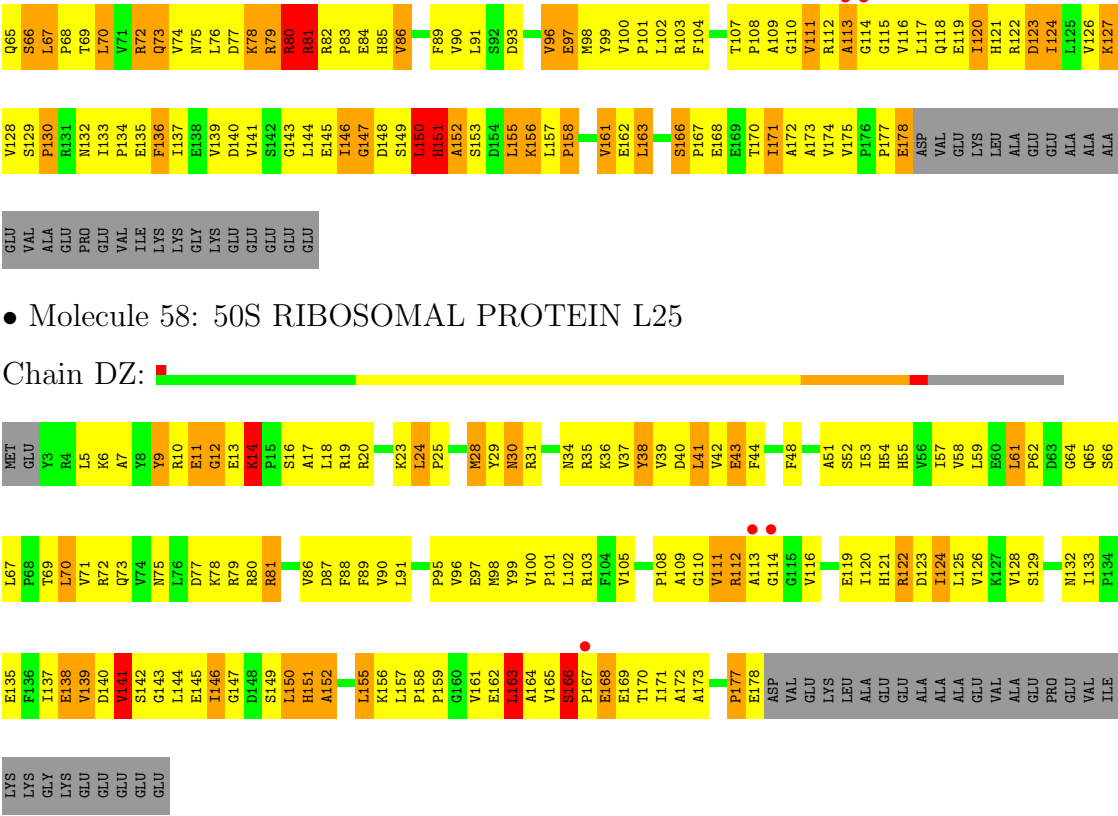
Chain DX:



- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.90Å 268.50Å 403.60Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.92 – 2.93	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-3.10) 90.5 (49.92-2.93)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.243 , 0.267 0.248 , 0.271	Depositor DCC
$R_{free}$ test set	59600 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.0	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1195890 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	307322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	4/36325 (0.0%)	0.75	46/56695 (0.1%)
1	CA	0.52	2/36325 (0.0%)	0.74	36/56695 (0.1%)
2	AB	0.44	0/1935	0.68	0/2609
2	CB	0.43	0/1935	0.69	0/2609
3	AC	0.49	0/1636	0.73	1/2205 (0.0%)
3	CC	0.45	0/1636	0.72	1/2205 (0.0%)
4	AD	0.39	0/1733	0.63	0/2318
4	CD	0.39	0/1733	0.63	0/2318
5	AE	0.54	0/1162	0.77	0/1564
5	CE	0.52	0/1162	0.76	0/1564
6	AF	0.39	0/856	0.65	0/1154
6	CF	0.39	0/856	0.66	0/1154
7	AG	0.45	0/1276	0.63	0/1709
7	CG	0.42	0/1276	0.63	1/1709 (0.1%)
8	AH	0.49	0/1136	0.73	0/1527
8	CH	0.45	0/1136	0.73	0/1527
9	AI	0.44	0/1029	0.68	0/1379
9	CI	0.42	0/1029	0.68	0/1379
10	AJ	0.41	0/807	0.68	0/1085
10	CJ	0.39	0/807	0.67	0/1085
11	AK	0.50	0/900	0.70	0/1213
11	CK	0.47	0/900	0.70	0/1213
12	AL	0.42	0/986	0.72	0/1320
12	CL	0.41	0/986	0.71	0/1320
13	AM	0.41	0/998	0.71	1/1336 (0.1%)
13	CM	0.38	0/998	0.71	1/1336 (0.1%)
14	AN	0.46	0/501	0.78	0/664
14	CN	0.45	0/501	0.79	0/664
15	AO	0.42	0/745	0.64	0/992
15	CO	0.43	0/745	0.64	0/992
16	AP	0.36	0/716	0.64	0/963
16	CP	0.35	0/716	0.64	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.45	0/836	0.67	0/1117
17	CQ	0.44	0/836	0.67	0/1117
18	AR	0.45	0/579	0.66	0/768
18	CR	0.46	0/579	0.67	0/768
19	AS	0.44	0/642	0.69	0/865
19	CS	0.41	0/642	0.69	0/865
20	AT	0.35	0/765	0.65	0/1007
20	CT	0.34	0/765	0.65	0/1007
21	AU	0.45	0/212	0.67	0/277
21	CU	0.50	0/212	0.66	0/277
22	AV	0.55	0/1809	0.73	1/2819 (0.0%)
22	AW	0.36	0/1809	0.73	2/2819 (0.1%)
22	CV	0.53	0/1809	0.73	1/2819 (0.0%)
22	CW	0.36	0/1809	0.73	2/2819 (0.1%)
23	AX	0.50	0/405	0.71	0/629
23	CX	0.49	0/405	0.70	0/629
24	AY	0.43	1/1616 (0.1%)	0.70	1/2511 (0.0%)
24	CY	0.45	1/1616 (0.1%)	0.70	1/2511 (0.0%)
25	AZ	0.31	0/3041	0.56	0/4127
25	CZ	0.32	0/3041	0.57	0/4127
26	B0	0.39	0/671	0.69	0/892
26	D0	0.41	0/671	0.70	0/892
27	B1	0.47	0/738	0.73	0/981
27	D1	0.40	0/738	0.68	0/981
28	B2	0.35	0/600	0.66	0/793
28	D2	0.33	0/600	0.64	1/793 (0.1%)
29	B3	0.37	0/472	0.61	0/634
29	D3	0.35	0/472	0.61	0/634
30	B4	0.38	0/349	0.65	0/474
30	D4	0.37	0/349	0.65	0/474
31	B5	0.38	0/473	0.72	0/639
31	D5	0.38	0/473	0.71	0/639
32	B6	0.60	0/440	0.82	0/586
32	D6	0.54	0/440	0.80	0/586
33	B7	0.42	0/426	0.68	0/561
33	D7	0.42	0/426	0.69	0/561
34	B8	0.56	0/515	0.87	1/679 (0.1%)
34	D8	0.53	0/515	0.87	1/679 (0.1%)
35	B9	0.42	0/310	0.65	0/407
35	D9	0.41	0/310	0.65	0/407
36	BA	0.51	3/69976 (0.0%)	0.72	33/109244 (0.0%)
36	DA	0.49	2/69976 (0.0%)	0.72	32/109244 (0.0%)
37	BB	0.43	0/2853	0.75	2/4451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DB	0.46	0/2853	0.75	2/4451 (0.0%)
38	BC	0.39	1/1774 (0.1%)	0.60	0/2391
38	DC	0.40	2/1774 (0.1%)	0.60	0/2391
39	BD	0.51	0/2195	0.81	1/2955 (0.0%)
39	DD	0.50	0/2195	0.80	1/2955 (0.0%)
40	BE	0.43	0/1596	0.75	0/2153
40	DE	0.43	0/1596	0.74	0/2153
41	BF	0.36	0/1658	0.65	0/2244
41	DF	0.37	0/1658	0.65	0/2244
42	BG	0.40	0/1499	0.74	1/2016 (0.0%)
42	DG	0.38	0/1499	0.68	0/2016
43	BH	0.32	0/1245	0.66	0/1682
43	DH	0.32	0/1245	0.66	0/1682
46	BN	0.37	0/1131	0.70	0/1525
46	DN	0.37	0/1131	0.69	0/1525
47	BO	0.47	0/943	0.68	0/1269
47	DO	0.46	0/943	0.67	0/1269
48	BP	0.43	0/1131	0.91	2/1504 (0.1%)
48	DP	0.42	0/1131	0.91	2/1504 (0.1%)
49	BQ	0.50	0/1143	0.71	0/1527
49	DQ	0.49	0/1143	0.72	0/1527
50	BR	0.38	0/974	0.71	1/1302 (0.1%)
50	DR	0.38	0/974	0.70	1/1302 (0.1%)
51	BS	0.36	0/778	0.76	0/1036
51	DS	0.37	0/778	0.75	0/1036
52	BT	0.43	0/1155	0.76	2/1542 (0.1%)
52	DT	0.41	0/1155	0.76	2/1542 (0.1%)
53	BU	0.41	0/975	0.68	0/1297
53	DU	0.43	0/975	0.68	0/1297
54	BV	0.37	0/790	0.68	0/1057
54	DV	0.39	0/790	0.68	0/1057
55	BW	0.35	0/907	0.67	0/1216
55	DW	0.36	0/907	0.67	0/1216
56	BX	0.40	0/739	0.65	0/993
56	DX	0.40	0/739	0.65	0/993
57	BY	0.36	0/788	0.73	1/1051 (0.1%)
57	DY	0.36	0/788	0.73	1/1051 (0.1%)
58	BZ	0.46	0/1435	0.81	1/1949 (0.1%)
58	DZ	0.44	0/1435	0.74	0/1949
All	All	0.49	16/330268 (0.0%)	0.72	183/493444 (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	5	49
1	CA	4	49
22	AW	1	1
22	CW	1	1
24	AY	2	0
24	CY	2	0
36	BA	2	66
36	DA	2	67
37	BB	0	6
37	DB	0	6
All	All	19	245

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	761	A	C5-C6	-10.36	1.31	1.41
36	DA	761	A	C5-C6	-10.14	1.31	1.41
36	BA	2506	U	N1-C2	8.65	1.46	1.38
36	DA	2506	U	N1-C2	8.34	1.46	1.38
1	AA	858	G	C5-C6	-7.88	1.34	1.42

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	BD	244	ARG	C-N-CD	-11.04	96.32	120.60
39	DD	244	ARG	C-N-CD	-10.91	96.59	120.60
1	CA	1498	U	C2'-C3'-O3'	10.87	133.42	109.50
1	AA	1498	U	C2'-C3'-O3'	10.68	132.99	109.50
1	AA	508	C	C2'-C3'-O3'	9.74	130.93	109.50

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1239	A	C3'
1	AA	1498	U	C3'
1	AA	1504	G	C3'
1	AA	1531	A	C3'

5 of 245 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	14	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	21	G	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	1017	0
1	CA	32451	0	16382	1043	0
2	AB	1900	0	1951	209	0
2	CB	1900	0	1951	211	0
3	AC	1612	0	1677	148	0
3	CC	1612	0	1677	155	0
4	AD	1703	0	1764	221	0
4	CD	1703	0	1763	226	0
5	AE	1146	0	1207	78	0
5	CE	1146	0	1207	89	0
6	AF	843	0	857	78	0
6	CF	843	0	857	77	0
7	AG	1257	0	1296	94	0
7	CG	1257	0	1296	89	0
8	AH	1116	0	1177	50	0
8	CH	1116	0	1177	52	0
9	AI	1010	0	1037	143	0
9	CI	1010	0	1037	142	0
10	AJ	794	0	840	113	0
10	CJ	794	0	840	118	0
11	AK	885	0	904	59	0
11	CK	885	0	904	61	0
12	AL	970	0	1057	112	0
12	CL	970	0	1057	111	0
13	AM	987	0	1059	136	0
13	CM	987	0	1059	139	0
14	AN	492	0	529	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	61	0
15	AO	734	0	771	42	0
15	CO	734	0	771	43	0
16	AP	700	0	720	72	0
16	CP	700	0	720	73	0
17	AQ	823	0	891	56	0
17	CQ	823	0	891	58	0
18	AR	574	0	644	35	0
18	CR	574	0	644	39	0
19	AS	629	0	652	77	0
19	CS	629	0	652	79	0
20	AT	763	0	861	78	0
20	CT	763	0	861	79	0
21	AU	208	0	221	12	0
21	CU	208	0	221	13	0
22	AV	1619	0	822	60	0
22	AW	1619	0	822	67	0
22	CV	1619	0	822	63	0
22	CW	1619	0	822	71	0
23	AX	361	0	184	7	0
23	CX	361	0	184	11	0
24	AY	1643	0	853	75	0
24	CY	1643	0	853	74	0
25	AZ	2983	0	2999	284	0
25	CZ	2983	0	2999	287	0
26	B0	662	0	688	63	0
26	D0	662	0	688	65	0
27	B1	731	0	808	69	0
27	D1	731	0	808	69	0
28	B2	598	0	653	158	0
28	D2	598	0	653	67	0
29	B3	467	0	523	49	0
29	D3	467	0	523	47	0
30	B4	340	0	336	51	0
30	D4	340	0	336	53	0
31	B5	459	0	480	62	0
31	D5	459	0	480	65	0
32	B6	433	0	461	135	0
32	D6	433	0	461	133	0
33	B7	418	0	467	29	0
33	D7	418	0	467	28	0
34	B8	507	0	576	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D8	507	0	576	123	0
35	B9	307	0	336	39	0
35	D9	307	0	335	42	0
36	BA	62477	0	31497	2141	0
36	DA	62477	0	31497	2212	0
37	BB	2551	0	1295	85	0
37	DB	2551	0	1295	97	0
38	BC	1742	0	1800	141	0
38	DC	1742	0	1800	132	0
39	BD	2145	0	2234	221	0
39	DD	2145	0	2234	234	0
40	BE	1563	0	1629	225	0
40	DE	1563	0	1629	222	0
41	BF	1623	0	1677	193	0
41	DF	1623	0	1677	197	0
42	BG	1474	0	1535	247	0
42	DG	1474	0	1535	232	0
43	BH	1222	0	1282	178	0
43	DH	1222	0	1282	184	0
44	BJ	651	0	164	27	0
44	DJ	651	0	164	31	0
45	BK	700	0	173	18	0
45	DK	700	0	173	15	0
46	BN	1104	0	1180	176	0
46	DN	1104	0	1180	171	0
47	BO	933	0	996	77	0
47	DO	933	0	996	78	0
48	BP	1114	0	1187	263	0
48	DP	1114	0	1187	265	0
49	BQ	1122	0	1179	112	0
49	DQ	1122	0	1179	106	0
50	BR	960	0	1021	133	0
50	DR	960	0	1021	128	0
51	BS	770	0	832	152	0
51	DS	770	0	832	150	0
52	BT	1141	0	1202	229	0
52	DT	1141	0	1202	223	0
53	BU	958	0	1015	132	0
53	DU	958	0	1015	130	0
54	BV	779	0	852	117	0
54	DV	779	0	852	120	0
55	BW	896	0	953	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	86	0
56	BX	725	0	778	82	0
56	DX	725	0	778	84	0
57	BY	775	0	870	162	0
57	DY	775	0	870	156	0
58	BZ	1403	0	1432	216	0
58	DZ	1403	0	1432	200	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	0	0
60	AZ	28	0	12	2	0
60	CZ	28	0	12	6	0
61	AZ	57	0	58	3	0
61	CZ	57	0	59	2	0
All	All	307322	0	208715	17683	0

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 17683 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:DC:123:VAL:CG2	38:DC:127:LEU:HD23	1.33	1.53
38:BC:123:VAL:CG2	38:BC:127:LEU:HD23	1.33	1.51
38:DC:123:VAL:HG23	38:DC:127:LEU:CD2	1.50	1.42
38:BC:123:VAL:HG23	38:BC:127:LEU:CD2	1.50	1.41
36:DA:1899:G:N2	36:DA:1902:C:H41	1.34	1.24

There are no symmetry-related clashes.

## 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%)	175 (75%)	39 (17%)	18 (8%)	1	11
2	CB	232/256 (91%)	173 (75%)	41 (18%)	18 (8%)	1	11
3	AC	204/239 (85%)	161 (79%)	23 (11%)	20 (10%)	1	6
3	CC	204/239 (85%)	159 (78%)	28 (14%)	17 (8%)	1	9
4	AD	206/209 (99%)	134 (65%)	46 (22%)	26 (13%)	0	3
4	CD	206/209 (99%)	133 (65%)	48 (23%)	25 (12%)	1	4
5	AE	148/162 (91%)	138 (93%)	5 (3%)	5 (3%)	6	32
5	CE	148/162 (91%)	138 (93%)	6 (4%)	4 (3%)	8	39
6	AF	99/101 (98%)	80 (81%)	12 (12%)	7 (7%)	2	12
6	CF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	2	12
7	AG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	3	21
7	CG	153/156 (98%)	123 (80%)	22 (14%)	8 (5%)	3	21
8	AH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	30	76
8	CH	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	30	76
9	AI	125/128 (98%)	85 (68%)	23 (18%)	17 (14%)	0	2
9	CI	125/128 (98%)	84 (67%)	24 (19%)	17 (14%)	0	2
10	AJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	1	7
10	CJ	96/105 (91%)	75 (78%)	12 (12%)	9 (9%)	1	7
11	AK	117/129 (91%)	100 (86%)	10 (8%)	7 (6%)	2	17
11	CK	117/129 (91%)	101 (86%)	9 (8%)	7 (6%)	2	17
12	AL	122/135 (90%)	94 (77%)	15 (12%)	13 (11%)	1	5
12	CL	122/135 (90%)	91 (75%)	18 (15%)	13 (11%)	1	5
13	AM	122/126 (97%)	82 (67%)	26 (21%)	14 (12%)	1	4
13	CM	122/126 (97%)	84 (69%)	24 (20%)	14 (12%)	1	4
14	AN	58/61 (95%)	41 (71%)	6 (10%)	11 (19%)	0	0
14	CN	58/61 (95%)	40 (69%)	7 (12%)	11 (19%)	0	0
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	CO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	19	62
16	AP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	1	9
16	CP	81/88 (92%)	52 (64%)	22 (27%)	7 (9%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	11	48
17	CQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	11	48
18	AR	68/88 (77%)	56 (82%)	11 (16%)	1 (2%)	15	57
18	CR	68/88 (77%)	57 (84%)	10 (15%)	1 (2%)	15	57
19	AS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	2
19	CS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	2
20	AT	97/106 (92%)	64 (66%)	24 (25%)	9 (9%)	1	7
20	CT	97/106 (92%)	62 (64%)	26 (27%)	9 (9%)	1	7
21	AU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	4	24
21	CU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	4	24
25	AZ	381/405 (94%)	269 (71%)	82 (22%)	30 (8%)	1	11
25	CZ	381/405 (94%)	268 (70%)	83 (22%)	30 (8%)	1	11
26	B0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	5	31
26	D0	82/85 (96%)	69 (84%)	10 (12%)	3 (4%)	5	31
27	B1	91/98 (93%)	70 (77%)	10 (11%)	11 (12%)	1	4
27	D1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	2	15
28	B2	69/72 (96%)	40 (58%)	15 (22%)	14 (20%)	0	0
28	D2	69/72 (96%)	44 (64%)	18 (26%)	7 (10%)	1	6
29	B3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	8
29	D3	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1	8
30	B4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	1	4
30	D4	42/71 (59%)	20 (48%)	17 (40%)	5 (12%)	1	4
31	B5	57/60 (95%)	39 (68%)	8 (14%)	10 (18%)	0	0
31	D5	57/60 (95%)	39 (68%)	8 (14%)	10 (18%)	0	0
32	B6	48/54 (89%)	24 (50%)	8 (17%)	16 (33%)	0	0
32	D6	48/54 (89%)	24 (50%)	8 (17%)	16 (33%)	0	0
33	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	10	46
33	D7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	10	46
34	B8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	1	6
34	D8	61/65 (94%)	34 (56%)	21 (34%)	6 (10%)	1	6
35	B9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	9
38	BC	226/229 (99%)	170 (75%)	45 (20%)	11 (5%)	3	23
38	DC	226/229 (99%)	171 (76%)	43 (19%)	12 (5%)	3	21
39	BD	273/276 (99%)	219 (80%)	31 (11%)	23 (8%)	1	9
39	DD	273/276 (99%)	217 (80%)	31 (11%)	25 (9%)	1	7
40	BE	202/206 (98%)	134 (66%)	39 (19%)	29 (14%)	0	2
40	DE	202/206 (98%)	134 (66%)	39 (19%)	29 (14%)	0	2
41	BF	205/210 (98%)	148 (72%)	35 (17%)	22 (11%)	1	5
41	DF	205/210 (98%)	149 (73%)	34 (17%)	22 (11%)	1	5
42	BG	179/182 (98%)	118 (66%)	33 (18%)	28 (16%)	0	1
42	DG	179/182 (98%)	119 (66%)	31 (17%)	29 (16%)	0	0
43	BH	157/180 (87%)	93 (59%)	34 (22%)	30 (19%)	0	0
43	DH	157/180 (87%)	94 (60%)	33 (21%)	30 (19%)	0	0
46	BN	136/140 (97%)	93 (68%)	20 (15%)	23 (17%)	0	0
46	DN	136/140 (97%)	93 (68%)	20 (15%)	23 (17%)	0	0
47	BO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	3	22
47	DO	120/122 (98%)	106 (88%)	8 (7%)	6 (5%)	3	22
48	BP	144/150 (96%)	78 (54%)	36 (25%)	30 (21%)	0	0
48	DP	144/150 (96%)	77 (54%)	37 (26%)	30 (21%)	0	0
49	BQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	5	31
49	DQ	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	5	31
50	BR	115/118 (98%)	83 (72%)	16 (14%)	16 (14%)	0	2
50	DR	115/118 (98%)	83 (72%)	17 (15%)	15 (13%)	0	3
51	BS	96/112 (86%)	50 (52%)	24 (25%)	22 (23%)	0	0
51	DS	96/112 (86%)	49 (51%)	23 (24%)	24 (25%)	0	0
52	BT	135/146 (92%)	82 (61%)	30 (22%)	23 (17%)	0	0
52	DT	135/146 (92%)	82 (61%)	30 (22%)	23 (17%)	0	0
53	BU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	2	16
53	DU	115/118 (98%)	83 (72%)	25 (22%)	7 (6%)	2	16
54	BV	99/101 (98%)	61 (62%)	23 (23%)	15 (15%)	0	1
54	DV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BW	111/113 (98%)	87 (78%)	12 (11%)	12 (11%)	1	5
55	DW	111/113 (98%)	85 (77%)	14 (13%)	12 (11%)	1	5
56	BX	90/96 (94%)	64 (71%)	20 (22%)	6 (7%)	2	14
56	DX	90/96 (94%)	65 (72%)	19 (21%)	6 (7%)	2	14
57	BY	98/110 (89%)	41 (42%)	31 (32%)	26 (26%)	0	0
57	DY	98/110 (89%)	43 (44%)	29 (30%)	26 (26%)	0	0
58	BZ	174/206 (84%)	109 (63%)	27 (16%)	38 (22%)	0	0
58	DZ	174/206 (84%)	109 (63%)	47 (27%)	18 (10%)	1	6
All	All	12256/13106 (94%)	8858 (72%)	2104 (17%)	1294 (11%)	1	5

5 of 1294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	18	GLY
2	AB	190	THR
2	AB	191	ASP
2	AB	230	VAL

### 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%)	178 (88%)	24 (12%)	8	27
2	CB	202/220 (92%)	180 (89%)	22 (11%)	9	34
3	AC	160/188 (85%)	143 (89%)	17 (11%)	10	35
3	CC	160/188 (85%)	144 (90%)	16 (10%)	11	38
4	AD	180/181 (99%)	157 (87%)	23 (13%)	6	24
4	CD	180/181 (99%)	157 (87%)	23 (13%)	6	24
5	AE	115/123 (94%)	104 (90%)	11 (10%)	12	42
5	CE	115/123 (94%)	105 (91%)	10 (9%)	15	49
6	AF	90/90 (100%)	81 (90%)	9 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CF	90/90 (100%)	82 (91%)	8 (9%)	14	47
7	AG	126/127 (99%)	116 (92%)	10 (8%)	18	55
7	CG	126/127 (99%)	116 (92%)	10 (8%)	18	55
8	AH	119/119 (100%)	109 (92%)	10 (8%)	16	52
8	CH	119/119 (100%)	109 (92%)	10 (8%)	16	52
9	AI	98/99 (99%)	89 (91%)	9 (9%)	13	45
9	CI	98/99 (99%)	89 (91%)	9 (9%)	13	45
10	AJ	88/92 (96%)	80 (91%)	8 (9%)	14	45
10	CJ	88/92 (96%)	80 (91%)	8 (9%)	14	45
11	AK	90/99 (91%)	81 (90%)	9 (10%)	11	38
11	CK	90/99 (91%)	82 (91%)	8 (9%)	14	47
12	AL	104/111 (94%)	95 (91%)	9 (9%)	15	49
12	CL	104/111 (94%)	97 (93%)	7 (7%)	23	63
13	AM	99/101 (98%)	86 (87%)	13 (13%)	6	23
13	CM	99/101 (98%)	86 (87%)	13 (13%)	6	23
14	AN	49/50 (98%)	39 (80%)	10 (20%)	2	8
14	CN	49/50 (98%)	39 (80%)	10 (20%)	2	8
15	AO	79/80 (99%)	70 (89%)	9 (11%)	8	31
15	CO	79/80 (99%)	71 (90%)	8 (10%)	11	38
16	AP	72/74 (97%)	66 (92%)	6 (8%)	16	53
16	CP	72/74 (97%)	66 (92%)	6 (8%)	16	53
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	20	59
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	20	59
18	AR	61/77 (79%)	54 (88%)	7 (12%)	8	31
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%)	56 (81%)	13 (19%)	2	9
20	AT	76/82 (93%)	71 (93%)	5 (7%)	24	64
20	CT	76/82 (93%)	71 (93%)	5 (7%)	24	64
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	72
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AZ	322/338 (95%)	299 (93%)	23 (7%)	21	61
25	CZ	322/338 (95%)	299 (93%)	23 (7%)	21	61
26	B0	66/67 (98%)	58 (88%)	8 (12%)	7	27
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%)	71 (91%)	7 (9%)	14	47
28	B2	66/67 (98%)	61 (92%)	5 (8%)	19	58
28	D2	66/67 (98%)	60 (91%)	6 (9%)	14	45
29	B3	51/52 (98%)	44 (86%)	7 (14%)	5	21
29	D3	51/52 (98%)	44 (86%)	7 (14%)	5	21
30	B4	39/63 (62%)	32 (82%)	7 (18%)	2	10
30	D4	39/63 (62%)	32 (82%)	7 (18%)	2	10
31	B5	51/52 (98%)	43 (84%)	8 (16%)	4	14
31	D5	51/52 (98%)	43 (84%)	8 (16%)	4	14
32	B6	49/52 (94%)	36 (74%)	13 (26%)	1	2
32	D6	49/52 (94%)	37 (76%)	12 (24%)	1	4
33	B7	41/42 (98%)	35 (85%)	6 (15%)	5	18
33	D7	41/42 (98%)	35 (85%)	6 (15%)	5	18
34	B8	53/55 (96%)	45 (85%)	8 (15%)	4	16
34	D8	53/55 (96%)	45 (85%)	8 (15%)	4	16
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%)	170 (94%)	10 (6%)	30	70
38	DC	180/181 (99%)	171 (95%)	9 (5%)	34	75
39	BD	217/218 (100%)	187 (86%)	30 (14%)	5	21
39	DD	217/218 (100%)	186 (86%)	31 (14%)	5	19
40	BE	165/166 (99%)	148 (90%)	17 (10%)	10	36
40	DE	165/166 (99%)	148 (90%)	17 (10%)	10	36
41	BF	165/166 (99%)	150 (91%)	15 (9%)	14	45
41	DF	165/166 (99%)	150 (91%)	15 (9%)	14	45
42	BG	155/156 (99%)	132 (85%)	23 (15%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DG	155/156 (99%)	138 (89%)	17 (11%)	9	34
43	BH	132/148 (89%)	116 (88%)	16 (12%)	7	27
43	DH	132/148 (89%)	116 (88%)	16 (12%)	7	27
46	BN	117/119 (98%)	102 (87%)	15 (13%)	6	24
46	DN	117/119 (98%)	102 (87%)	15 (13%)	6	24
47	BO	100/100 (100%)	95 (95%)	5 (5%)	34	75
47	DO	100/100 (100%)	95 (95%)	5 (5%)	34	75
48	BP	112/116 (97%)	97 (87%)	15 (13%)	6	22
48	DP	112/116 (97%)	97 (87%)	15 (13%)	6	22
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	6	22
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	7	24
50	BR	100/101 (99%)	89 (89%)	11 (11%)	9	34
50	DR	100/101 (99%)	90 (90%)	10 (10%)	11	38
51	BS	77/88 (88%)	68 (88%)	9 (12%)	8	29
51	DS	77/88 (88%)	68 (88%)	9 (12%)	8	29
52	BT	120/127 (94%)	97 (81%)	23 (19%)	2	9
52	DT	120/127 (94%)	98 (82%)	22 (18%)	2	10
53	BU	92/94 (98%)	83 (90%)	9 (10%)	12	40
53	DU	92/94 (98%)	84 (91%)	8 (9%)	15	49
54	BV	82/82 (100%)	66 (80%)	16 (20%)	2	8
54	DV	82/82 (100%)	66 (80%)	16 (20%)	2	8
55	BW	91/92 (99%)	86 (94%)	5 (6%)	30	71
55	DW	91/92 (99%)	86 (94%)	5 (6%)	30	71
56	BX	74/78 (95%)	64 (86%)	10 (14%)	6	22
56	DX	74/78 (95%)	64 (86%)	10 (14%)	6	22
57	BY	84/91 (92%)	70 (83%)	14 (17%)	3	11
57	DY	84/91 (92%)	70 (83%)	14 (17%)	3	11
58	BZ	155/179 (87%)	126 (81%)	29 (19%)	2	9
58	DZ	155/179 (87%)	135 (87%)	20 (13%)	6	24
All	All	10338/10860 (95%)	9176 (89%)	1162 (11%)	9	33

5 of 1162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	18	LEU
4	CD	138	TYR
52	DT	38	ASN
55	BW	82	LEU
58	BZ	127	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 301 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	94	ASN
6	CF	32	ASN
50	DR	24	GLN
55	BW	57	ASN
2	CB	78	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1509/1522 (99%)	240 (15%)	49 (3%)
1	CA	1509/1522 (99%)	234 (15%)	47 (3%)
22	AV	75/76 (98%)	19 (25%)	2 (2%)
22	AW	75/76 (98%)	17 (22%)	0
22	CV	75/76 (98%)	19 (25%)	1 (1%)
22	CW	75/76 (98%)	17 (22%)	0
23	AX	16/27 (59%)	6 (37%)	0
23	CX	16/27 (59%)	6 (37%)	0
24	AY	74/77 (96%)	25 (33%)	5 (6%)
24	CY	74/77 (96%)	25 (33%)	5 (6%)
36	BA	2900/2915 (99%)	510 (17%)	46 (1%)
36	DA	2900/2915 (99%)	508 (17%)	46 (1%)
37	BB	118/122 (96%)	25 (21%)	2 (1%)
37	DB	118/122 (96%)	25 (21%)	2 (1%)
All	All	9534/9630 (99%)	1676 (17%)	205 (2%)

5 of 1676 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

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Mol	Chain	Res	Type
1	AA	39	G

5 of 205 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2126	A
1	CA	250	A
36	DA	1970	A
36	BA	2282	G
1	CA	30	U

## 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	1.11	2 (10%)	27,30,33	1.74	4 (14%)
24	H2U	AY	17	24	19,21,22	1.11	1 (5%)	27,30,33	1.92	5 (18%)
24	H2U	AY	20	24	19,21,22	1.06	2 (10%)	27,30,33	1.84	5 (18%)
24	OMC	AY	32	24	20,22,23	1.20	3 (15%)	25,31,34	0.95	2 (8%)
24	MIA	AY	37	24	29,31,32	1.18	3 (10%)	41,44,47	1.57	5 (12%)
24	7MG	AY	46	24	24,26,27	2.27	4 (16%)	34,39,42	2.33	5 (14%)
24	5MU	AY	54	24	20,22,23	1.11	3 (15%)	25,32,35	1.47	2 (8%)
24	PSU	AY	55	24	19,21,22	1.12	2 (10%)	23,30,33	1.06	2 (8%)
24	4SU	AY	8	24	19,21,22	1.45	5 (26%)	23,30,33	24.72	1 (4%)
24	H2U	CY	16	24	19,21,22	1.15	3 (15%)	27,30,33	1.75	4 (14%)
24	H2U	CY	17	24	19,21,22	1.08	1 (5%)	27,30,33	1.94	5 (18%)
24	H2U	CY	20	24	19,21,22	1.05	2 (10%)	27,30,33	1.83	5 (18%)
24	OMC	CY	32	24	20,22,23	1.24	3 (15%)	25,31,34	0.92	2 (8%)
24	MIA	CY	37	24	29,31,32	1.07	3 (10%)	41,44,47	1.56	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	7MG	CY	46	24	24,26,27	2.27	4 (16%)	34,39,42	2.33	6 (17%)
24	5MU	CY	54	24	20,22,23	1.13	3 (15%)	25,32,35	1.42	3 (12%)
24	PSU	CY	55	24	19,21,22	1.12	2 (10%)	23,30,33	1.06	2 (8%)
24	4SU	CY	8	24	19,21,22	1.48	5 (26%)	23,30,33	24.71	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	1/1/5/5	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
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	1/1/5/5	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 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-9.67	1.38	1.46
24	AY	46	7MG	C8-N9	-9.66	1.38	1.46
24	CY	8	4SU	C5-C4	3.75	1.42	1.38
24	AY	8	4SU	C5-C4	3.73	1.42	1.38
24	AY	37	MIA	C2-S10	3.34	1.78	1.75

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	8	4SU	C4-N3-C2	118.52	126.67	121.60
24	CY	8	4SU	C4-N3-C2	118.48	126.67	121.60
24	AY	46	7MG	C6-N1-C2	9.14	125.36	120.20
24	CY	46	7MG	C6-N1-C2	9.09	125.33	120.20
24	CY	46	7MG	N7-C8-N9	7.32	112.85	103.13

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	CY	55	PSU	C3'
24	AY	55	PSU	C3'

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	1.47	6 (20%)	45,47,47	1.74	10 (22%)
61	KIR	AZ	502	-	59,59,59	3.62	24 (40%)	82,84,84	1.68	17 (20%)
60	GDP	CZ	501	-	30,30,30	1.43	6 (20%)	45,47,47	1.88	10 (22%)
61	KIR	CZ	502	-	59,59,59	3.59	24 (40%)	82,84,84	1.66	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 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-13.94	1.22	1.44
61	CZ	502	KIR	O18-C17	-13.68	1.22	1.44
61	AZ	502	KIR	O30-C30	-11.83	1.17	1.42
61	CZ	502	KIR	O30-C30	-11.77	1.17	1.42
61	AZ	502	KIR	O34-C33	-11.14	1.29	1.44

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	C2-N3-C4	5.67	122.10	115.30
60	CZ	501	GDP	C2-N3-C4	5.40	121.77	115.30
61	AZ	502	KIR	O29-C29-O34	-4.89	102.25	110.32
61	CZ	502	KIR	O29-C29-O34	-4.76	102.48	110.32
61	AZ	502	KIR	C45-C28-C27	4.75	113.05	108.38

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1510/1522 (99%)	-0.08	29 (1%) 64 13	17, 54, 143, 200	0
1	CA	1510/1522 (99%)	-0.26	20 (1%) 74 19	26, 58, 145, 200	0
2	AB	234/256 (91%)	-0.13	0 100 100	34, 64, 130, 141	0
2	CB	234/256 (91%)	-0.12	3 (1%) 74 19	36, 65, 130, 142	0
3	AC	206/239 (86%)	-0.23	0 100 100	27, 48, 81, 86	0
3	CC	206/239 (86%)	-0.30	0 100 100	32, 52, 82, 88	0
4	AD	208/209 (99%)	0.14	1 (0%) 88 39	55, 89, 119, 122	0
4	CD	208/209 (99%)	0.09	3 (1%) 72 17	55, 90, 119, 122	0
5	AE	150/162 (92%)	-0.33	0 100 100	23, 41, 62, 84	0
5	CE	150/162 (92%)	-0.31	0 100 100	30, 44, 64, 86	0
6	AF	101/101 (100%)	-0.18	0 100 100	48, 72, 88, 94	0
6	CF	101/101 (100%)	-0.02	0 100 100	52, 74, 90, 95	0
7	AG	155/156 (99%)	-0.13	0 100 100	40, 64, 100, 115	0
7	CG	155/156 (99%)	-0.10	1 (0%) 86 36	45, 67, 101, 115	0
8	AH	138/138 (100%)	-0.29	0 100 100	30, 44, 61, 71	0
8	CH	138/138 (100%)	-0.35	0 100 100	31, 47, 62, 72	0
9	AI	127/128 (99%)	0.10	0 100 100	33, 73, 113, 120	0
9	CI	127/128 (99%)	0.15	1 (0%) 83 28	40, 77, 114, 120	0
10	AJ	98/105 (93%)	0.22	0 100 100	41, 80, 133, 136	0
10	CJ	98/105 (93%)	0.39	4 (4%) 35 5	44, 84, 134, 137	0
11	AK	119/129 (92%)	-0.13	1 (0%) 83 28	28, 49, 80, 104	0
11	CK	119/129 (92%)	-0.13	0 100 100	32, 53, 82, 104	0
12	AL	124/135 (91%)	-0.06	1 (0%) 83 28	28, 66, 87, 125	0
12	CL	124/135 (91%)	0.02	1 (0%) 83 28	30, 67, 88, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	0.00	3 (2%) 56 9	50, 73, 100, 137	0
13	CM	124/126 (98%)	0.04	3 (2%) 56 9	53, 76, 101, 137	0
14	AN	60/61 (98%)	-0.08	1 (1%) 67 15	33, 48, 76, 79	0
14	CN	60/61 (98%)	-0.17	1 (1%) 67 15	39, 53, 76, 80	0
15	AO	88/89 (98%)	-0.25	0 100 100	36, 51, 73, 81	0
15	CO	88/89 (98%)	-0.18	0 100 100	37, 53, 73, 81	0
16	AP	83/88 (94%)	0.11	0 100 100	62, 78, 99, 125	0
16	CP	83/88 (94%)	0.15	0 100 100	62, 80, 100, 124	0
17	AQ	99/105 (94%)	-0.19	0 100 100	33, 55, 72, 83	0
17	CQ	99/105 (94%)	-0.17	0 100 100	39, 56, 73, 83	0
18	AR	70/88 (79%)	-0.18	1 (1%) 72 17	37, 55, 87, 99	0
18	CR	70/88 (79%)	-0.15	0 100 100	43, 59, 88, 99	0
19	AS	78/93 (83%)	0.18	1 (1%) 74 19	61, 81, 116, 125	0
19	CS	78/93 (83%)	0.26	1 (1%) 74 19	63, 83, 117, 125	0
20	AT	99/106 (93%)	0.05	0 100 100	49, 77, 112, 115	0
20	CT	99/106 (93%)	0.12	1 (1%) 79 23	52, 78, 113, 115	0
21	AU	24/27 (88%)	0.16	1 (4%) 35 5	43, 55, 76, 93	0
21	CU	24/27 (88%)	0.40	0 100 100	46, 59, 78, 92	0
22	AV	76/76 (100%)	-0.22	0 100 100	34, 64, 95, 113	0
22	AW	76/76 (100%)	0.71	8 (10%) 7 1	60, 165, 193, 200	0
22	CV	76/76 (100%)	-0.29	0 100 100	38, 66, 97, 114	0
22	CW	76/76 (100%)	0.84	11 (14%) 3 1	63, 166, 193, 200	0
23	AX	17/27 (62%)	0.65	2 (11%) 5 1	27, 87, 137, 139	0
23	CX	17/27 (62%)	0.68	4 (23%) 1 0	32, 89, 137, 140	0
24	AY	76/77 (98%)	1.36	18 (23%) 1 0	70, 149, 176, 179	0
24	CY	76/77 (98%)	1.61	27 (35%) 1 0	72, 149, 176, 179	0
25	AZ	385/405 (95%)	0.44	11 (2%) 49 7	84, 129, 155, 177	0
25	CZ	385/405 (95%)	0.49	19 (4%) 28 4	85, 129, 155, 177	0
26	B0	84/85 (98%)	0.09	2 (2%) 56 9	47, 64, 95, 108	0
26	D0	84/85 (98%)	0.19	2 (2%) 56 9	50, 66, 95, 108	0
27	B1	93/98 (94%)	-0.04	1 (1%) 77 22	38, 55, 114, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	0.12	1 (1%) 77 22	54, 71, 121, 129	0
28	B2	71/72 (98%)	0.80	8 (11%) 6 1	108, 136, 147, 149	0
28	D2	71/72 (98%)	0.27	1 (1%) 72 17	88, 107, 126, 142	0
29	B3	59/60 (98%)	0.08	1 (1%) 67 15	50, 71, 91, 116	0
29	D3	59/60 (98%)	0.28	2 (3%) 43 6	51, 72, 91, 116	0
30	B4	44/71 (61%)	0.55	2 (4%) 32 5	109, 148, 172, 176	0
30	D4	44/71 (61%)	0.29	0 100 100	110, 148, 172, 176	0
31	B5	59/60 (98%)	0.05	2 (3%) 43 6	45, 71, 131, 148	0
31	D5	59/60 (98%)	0.10	3 (5%) 27 4	46, 73, 130, 148	0
32	B6	50/54 (92%)	0.55	3 (6%) 21 3	50, 80, 106, 112	0
32	D6	50/54 (92%)	0.47	2 (4%) 36 5	54, 82, 106, 114	0
33	B7	48/49 (97%)	-0.02	0 100 100	45, 53, 90, 110	0
33	D7	48/49 (97%)	-0.07	0 100 100	47, 55, 89, 110	0
34	B8	63/65 (96%)	0.13	0 100 100	49, 63, 79, 101	0
34	D8	63/65 (96%)	0.14	1 (1%) 68 15	51, 65, 80, 101	0
35	B9	37/37 (100%)	0.20	1 (2%) 52 8	62, 75, 96, 98	0
35	D9	37/37 (100%)	0.34	2 (5%) 25 4	61, 77, 96, 98	0
36	BA	2901/2915 (99%)	0.02	101 (3%) 42 6	21, 65, 173, 200	0
36	DA	2901/2915 (99%)	-0.04	93 (3%) 45 7	26, 67, 173, 200	0
37	BB	119/122 (97%)	-0.24	0 100 100	52, 81, 104, 123	0
37	DB	119/122 (97%)	-0.33	0 100 100	55, 82, 104, 123	0
38	BC	228/229 (99%)	0.06	5 (2%) 59 11	47, 78, 152, 166	0
38	DC	228/229 (99%)	0.31	9 (3%) 37 5	51, 80, 152, 167	0
39	BD	275/276 (99%)	-0.21	1 (0%) 90 45	27, 44, 71, 96	0
39	DD	275/276 (99%)	-0.22	1 (0%) 90 45	29, 46, 71, 96	0
40	BE	204/206 (99%)	0.03	3 (1%) 70 16	40, 65, 114, 124	0
40	DE	204/206 (99%)	0.02	4 (1%) 62 12	41, 65, 114, 124	0
41	BF	207/210 (98%)	0.13	7 (3%) 43 6	45, 96, 152, 159	0
41	DF	207/210 (98%)	0.19	3 (1%) 72 17	45, 97, 152, 159	0
42	BG	181/182 (99%)	-0.09	4 (2%) 59 11	50, 73, 111, 132	0
42	DG	181/182 (99%)	0.07	2 (1%) 77 22	78, 100, 124, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	0.58	10 (6%) 19 3	84, 119, 144, 150	0
43	DH	159/180 (88%)	0.49	7 (4%) 33 5	83, 119, 144, 151	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	-0.03	0 100 100	51, 74, 118, 123	0
46	DN	138/140 (98%)	-0.03	0 100 100	51, 75, 118, 123	0
47	BO	122/122 (100%)	-0.24	0 100 100	35, 49, 62, 66	0
47	DO	122/122 (100%)	-0.28	0 100 100	35, 50, 62, 65	0
48	BP	146/150 (97%)	0.42	6 (4%) 35 5	47, 93, 118, 139	0
48	DP	146/150 (97%)	0.48	6 (4%) 35 5	49, 95, 118, 139	0
49	BQ	141/141 (100%)	-0.09	1 (0%) 84 32	35, 54, 75, 117	0
49	DQ	141/141 (100%)	-0.10	1 (0%) 84 32	39, 54, 76, 117	0
50	BR	117/118 (99%)	0.03	1 (0%) 81 25	51, 70, 88, 93	0
50	DR	117/118 (99%)	0.03	0 100 100	52, 71, 89, 93	0
51	BS	98/112 (87%)	0.21	2 (2%) 62 12	69, 89, 114, 118	0
51	DS	98/112 (87%)	0.41	1 (1%) 79 23	71, 90, 114, 117	0
52	BT	137/146 (93%)	0.10	6 (4%) 33 5	50, 71, 133, 164	0
52	DT	137/146 (93%)	0.08	6 (4%) 33 5	51, 72, 134, 164	0
53	BU	117/118 (99%)	-0.04	1 (0%) 81 25	51, 68, 90, 112	0
53	DU	117/118 (99%)	-0.07	0 100 100	52, 69, 89, 112	0
54	BV	101/101 (100%)	0.18	1 (0%) 79 23	52, 98, 113, 116	0
54	DV	101/101 (100%)	0.21	1 (0%) 79 23	52, 98, 113, 116	0
55	BW	113/113 (100%)	-0.05	0 100 100	56, 71, 102, 133	0
55	DW	113/113 (100%)	0.06	0 100 100	56, 72, 103, 134	0
56	BX	92/96 (95%)	0.14	0 100 100	64, 83, 101, 111	0
56	DX	92/96 (95%)	0.11	0 100 100	65, 84, 102, 112	0
57	BY	100/110 (90%)	0.73	9 (9%) 10 2	93, 114, 151, 160	0
57	DY	100/110 (90%)	0.85	9 (9%) 10 2	93, 114, 151, 160	0
58	BZ	176/206 (85%)	-0.00	2 (1%) 77 22	44, 71, 117, 123	0
58	DZ	176/206 (85%)	0.08	3 (1%) 67 15	56, 78, 111, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	22010/23376 (94%)	0.02	518 (2%) 56 9	17, 69, 146, 200	0

The worst 5 of 518 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BA	2802	G	10.4
36	DA	2802	G	8.6
36	BA	654(K)	C	8.4
36	DA	654(K)	C	8.2
1	CA	89	C	8.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	5MU	CY	54	21/22	0.41	-	144,149,151,153	0
24	MIA	AY	37	29/30	0.31	-	71,88,103,104	0
24	7MG	CY	46	24/25	0.44	-	170,172,175,176	0
24	4SU	AY	8	20/21	0.33	-	145,147,149,149	0
24	OMC	CY	32	21/22	0.51	-	107,112,121,122	0
24	PSU	CY	55	20/21	0.44	-	154,160,160,160	0
24	7MG	AY	46	24/25	0.39	-	170,172,175,176	0
24	H2U	CY	20	20/21	0.43	-	178,179,179,180	0
24	5MU	AY	54	21/22	0.34	-	145,149,150,153	0
24	MIA	CY	37	29/30	0.24	-	74,88,101,102	0
24	H2U	AY	20	20/21	0.48	-	178,179,179,179	0
24	H2U	CY	16	20/21	0.60	-	170,173,173,174	0
24	H2U	AY	17	20/21	0.64	-	170,174,175,176	0
24	OMC	AY	32	21/22	0.30	-	107,112,120,121	0
24	PSU	AY	55	20/21	0.40	-	154,159,160,161	0
24	H2U	CY	17	20/21	0.51	-	170,173,175,176	0
24	H2U	AY	16	20/21	0.59	-	169,173,173,174	0
24	4SU	CY	8	20/21	0.34	-	146,147,148,149	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
60	GDP	AZ	501	28/28	0.29	-	130,136,140,141	0
59	ZN	D9	101	1/1	0.11	-	81,81,81,81	0
59	ZN	D4	101	1/1	0.10	-	115,115,115,115	0
59	ZN	CD	301	1/1	0.26	-	72,72,72,72	0
59	ZN	AN	101	1/1	0.15	-	34,34,34,34	0
59	ZN	CN	101	1/1	0.16	-	60,60,60,60	0
59	ZN	B4	101	1/1	0.17	-	90,90,90,90	0
59	ZN	AD	301	1/1	0.25	-	59,59,59,59	0
61	KIR	AZ	502	57/57	0.33	-	117,119,121,122	0
59	ZN	B9	101	1/1	0.11	-	82,82,82,82	0
61	KIR	CZ	502	57/57	0.37	-	118,120,121,123	0
60	GDP	CZ	501	28/28	0.17	-	129,136,140,140	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.