



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 10:06 PM BST

PDB ID : 4V5Q  
Title : The crystal structure of EF-Tu and G24A-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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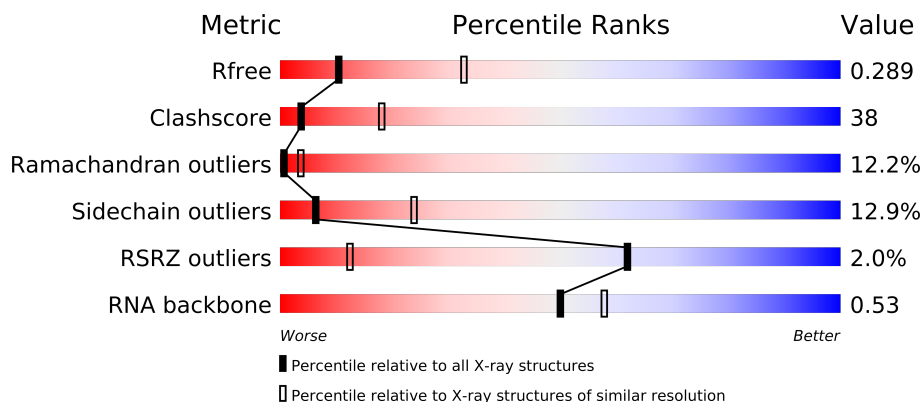
The following versions of software and data (see [references](#)) were used in the production of this report:

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	132	
12	CL	132	
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 307194 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

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

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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
			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 G24A TRP-TRNA TRP.

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

- Molecule 25 is a protein called ELONGATION FACTOR TU.

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

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

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

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

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

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

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

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

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

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

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

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

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

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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.

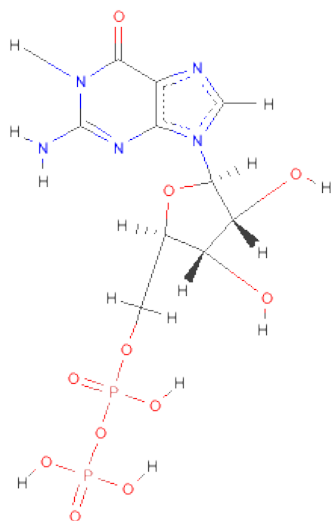


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			
58	DZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			

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

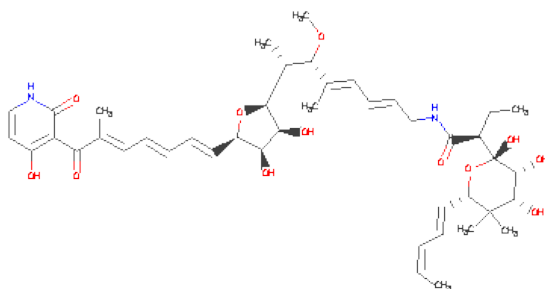
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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



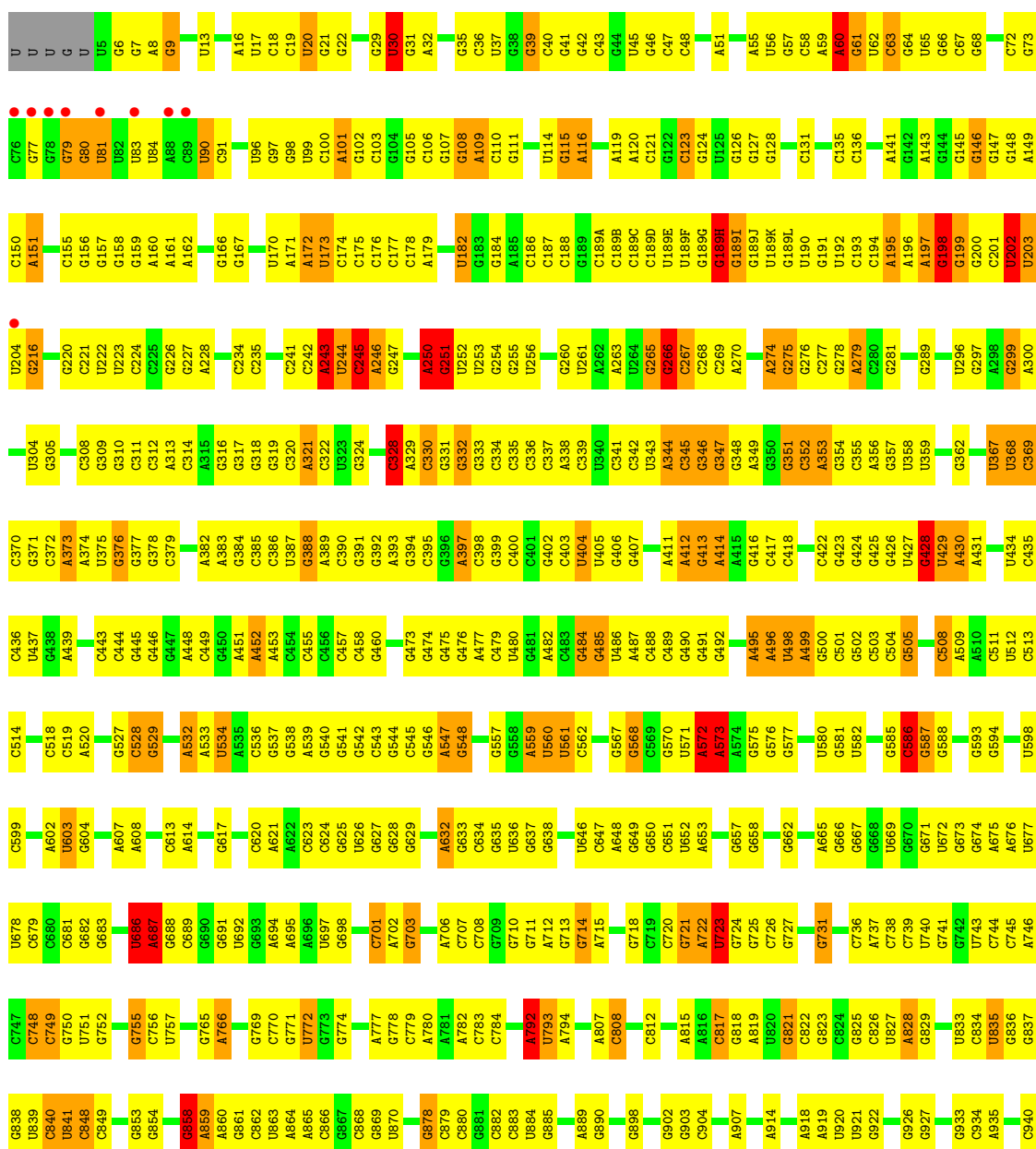
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
61	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

### 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.

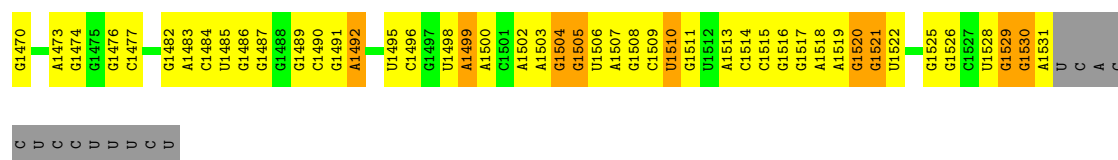
#### • Molecule 1: 16S rRNA

Chain AA: 



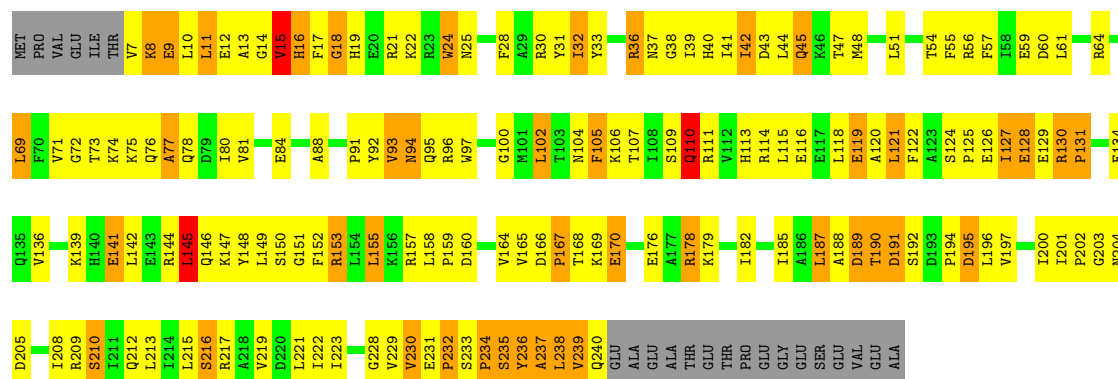


A1398	C1327	G1203	A1067	G10014	G939	G854	G776	A704	U636	U561	A495	A411	C341
C1328	A1268	A1204	G1068	G1002	C940	G854	A777	U705	G637	C562	A496	A412	C342
A1329	A1269	U1205	C1069	G1003	G941	G858	G778	A706	G638	G566	U496	G413	U343
U1330	C1270	G1206	U1070	A1004	G942	A859	C779	C707	G639	G566	U499	A414	A344
C1401	G1271	C1207	C1141	A1005	U943	A860	A780	C708	A640	G566	U499	A415	C345
A1332	G1272	C1208	G1072	C1006	G945	G861	A781	G709	U641	A572	G500	A416	G346
A1333	G1273	C1209	U1073	C1007	G946	G864	A782	G710	A642	A573	G501	C417	G347
G1405	G1274	G1210	C1074	G1008	A947	A865	C783	G711	C643	A574	G502	C418	G348
A1408	C1335	U1211	C1075	G1009	G948	G866	C784	A712	G644	G575	C503	G422	A349
C1409	G1336	U1212	G1076	G1010	C948	G866	C785	A713	C645	G576	G504	G423	G351
A1412	G1337	U1213	G1077	G1011	A949	G869	C786	G714	U646	G577	G505	G424	C352
C1413	G1338	C1214	A1080	U1012	U950	U870	C787	G715	C647	G578	G506	G425	A353
U1414	G1339	G1215	U1086	G1013	G951	U870	C788	G716	A648	G579	C507	G426	G354
G1415	C1340	G1216	G1087	A1014	U952	G874	C789	C719	G649	U580	C508	U427	G355
G1416	C1341	C1217	U1088	A1015	G953	G874	A792	C720	G650	G581	A509	G428	C356
U1417	G1342	C1218	G1088	A1016	G954	G877	U793	G721	C651	U582	A510	U429	A356
A1418	U1345	U1219	C1089	G1017	U955	C877	A794	A722	G652	A583	C511	A430	G357
C1426	A1346	G1220	U1090	C1018	U956	G878	C795	U723	A653	G584	U512	A431	U358
G1419	G1347	G1221	U1090	C1019	U957	G882	C796	G724	G656	G585	C518	A432	U359
U1348	U1348	G1222	G1094	G1024	A958	C882	C797	G725	C657	U591	C519	C433	A360
A1423	A1287	C1223	U1095	U1025	A959	C883	C797	G726	G658	G592	A520	U434	G361
C1424	A1288	G1224	C1096	U1025	U960	U884	A802	C727	U659	G592	C521	C436	U367
U1425	A1289	A1225	C1097	G1026	U961	U885	G803	G727	U659	G592	C522	C437	U368
C1426	C1352	G1226	C1098	G1026	G962	G885	A803	G727	U659	G592	C522	C438	C369
U1427	G1353	A1227	G1099	G1030	G963	G890	A807	G731	G660	G596	A523	G439	C370
A1428	U1292	C1228	G1100	G1030A	A964	U891	C808	A733	A663	G597	A524	U439	G371
C1429	G1293	A1229	A1101	A1030D	A965	A892	C811	C736	G664	C599	C525	C443	C372
C1430	G1294	C1230	A1102	G1031	G966	A892	C811	C736	A665	C600	C526	C444	A373
C1431	G1295	G1231	C1103	G1032	C967	G895	A814	A737	G666	C601	C527	G445	A374
U1358	C1296	G1231	G1104	G1033	A968	C896	A815	C738	G667	A602	G530	G446	U375
C1359	C1297	U1360	A1105	G1033	A969	C897	A816	C739	G673	U603	G531	G447	C376
A1360	C1298	U1235	G1106	G1036	C970	C898	A816	U740	G674	G604	U532	A448	G377
U1436	A1299	U1236	C1107	C1037	G971	C899	C817	G741	G675	U605	A533	U449	G378
C1362	G1300	C1237	G1108	C1038	C972	A900	G818	C744	A676	G606	U534	C450	C381
C1363	U1301	A1238	C1111	C1039	A974	G906	U820	C745	U677	A608	A535	A451	A382
U1364	C1302	U1239	C1112	U1040	A975	A907	G821	A746	U678	A609	C536	A452	A383
U1365	G1303	G1241	C1113	A1041	G976	A908	C822	C747	C679	G610	C537	A453	G384
C1366	C1304	G1242	C1114	A1044	A977	A909	C822	C748	C680	C613	A538	C458	C385
C1367	G1305	C1243	C1115	C1045	C979	A913	C826	C749	G683	A614	A540	G460	C386
G1368	A1179	A1180	C1116	A1046	C980	A914	U827	G755	A684	C615	G541	G471	G387
C1369	G1177	G1178	C1117	G1047	U981	A915	A828	C756	G685	G616	G542	G472	A388
U1370	G1181	G1182	C1118	U1048	U982	A916	G829	U757	U686	G617	C543	G473	C390
C1371	G1185	G1186	C1119	U1049	A983	G917	G830	G758	A687	C620	G544	G474	A389
U1372	G1188	G1189	G1120	G1050	U984	A918	U831	A759	G688	A621	C545	G475	C391
A1447	C1312	C1313	U1121	C1051	C985	A919	C832	G760	C689	A622	A547	G476	A393
C1452	U1196	C1314	U1122	U1052	A986	U920	C832	G761	G691	C623	G548	A477	G394
U1456	G1197	C1315	G1123	G1053	G987	U920	C832	G762	G692	C624	C549	C479	A397
G1457	G1190	A1191	G1124	G1054	C988	C924	G836	C764	U692	C625	G550	U480	C398
G1458	C1316	C1192	U1125	A1055	C989	G925	G837	G765	G693	G626	G551	G484	G402
U1461	C1317	C1193	U1126	U1056	C990	G926	G838	A766	A694	U627	G552	G485	C403
G1462	A1318	C1319	G1127	U1057	U991	G927	C839	A768	A695	G627	U552	U486	U404
C1463	C1320	U1196	C1128	G1058	U992	G927	C840	G769	A696	G628	C555	A487	U405
G1464	C1321	G1197	C1129	G1059	U993	G933	U841	C770	U697	G629	C556	G488	G406
U1391	C1322	G1198	A1130	C1059	G993	G933	C848	C771	G698	G629	C557	C489	G406
C1392	A1261	U1199	C1332	G1060	C985	A935	U850	U772	C701	A632	G558	G490	U405
U1393	C1262	C1263	C1132	G1061	A996	C936	G851	G773	A702	G633	A559	G491	G406
G1468	A1201	C1325	G1133	U1065	A1001	A937	G852	G774	A703	G634	U560	G491	G406
G1469	G1202	U1136	U1136	C1066	A1001	A938	G853	G775	G703	G635	U560	G491	G406



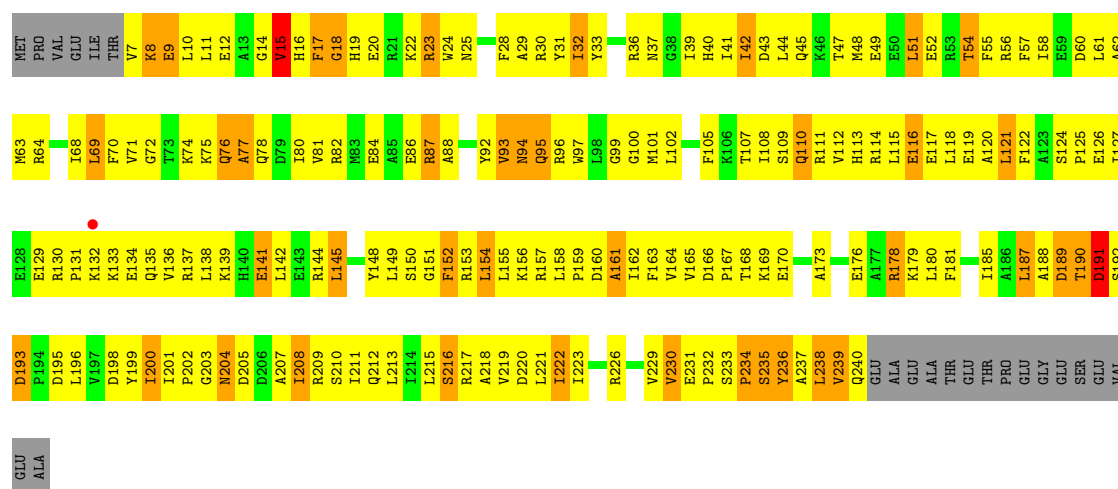
## • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



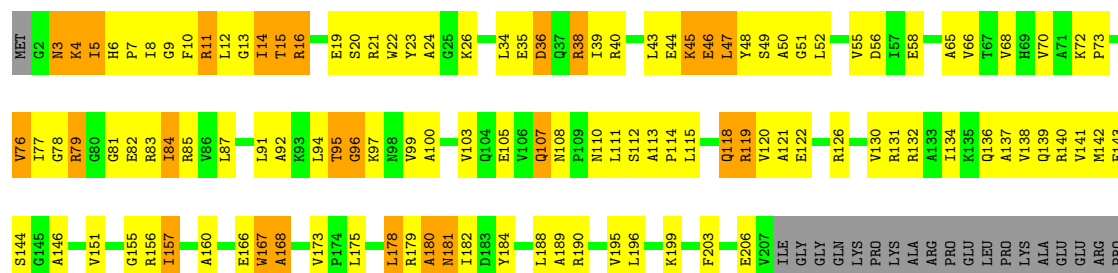
## • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



## • Molecule 3: 30S RIBOSOMAL PROTEIN S3

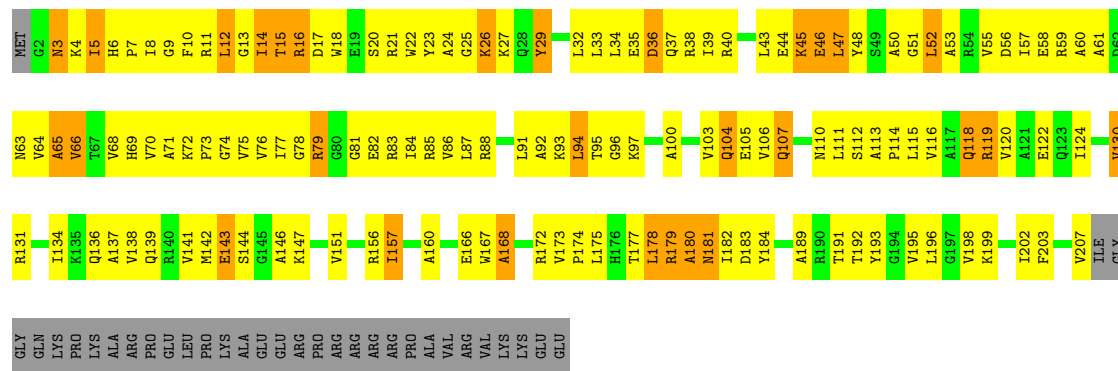
Chain AC:



ARG  
ARG  
ARG  
ARG  
PRO  
ALA  
VAL  
VAL  
LYS  
GLU  
GLU

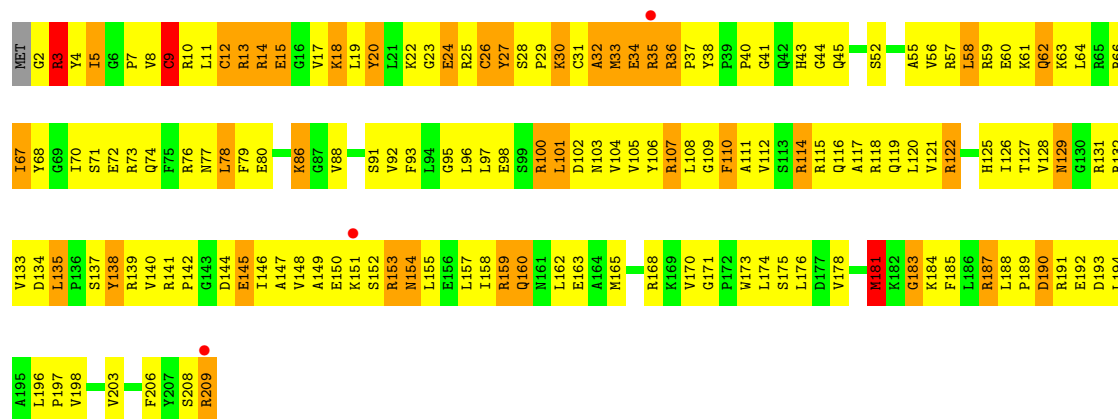
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



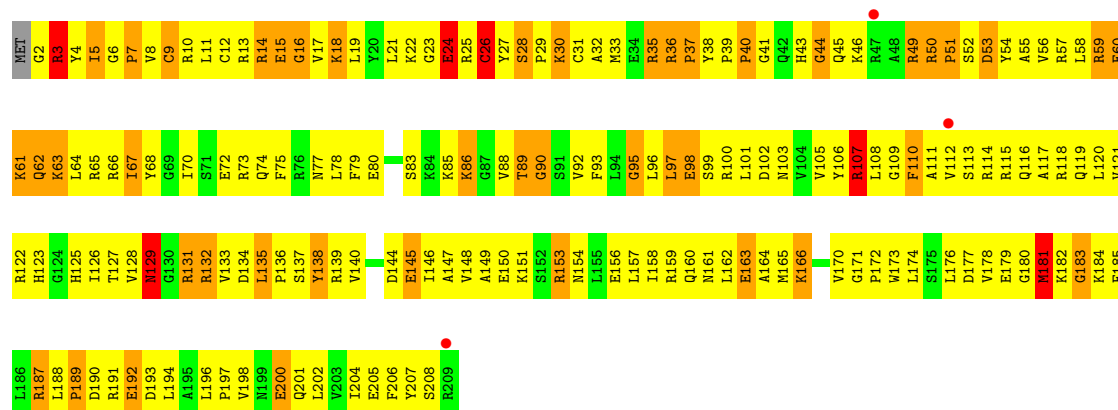
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



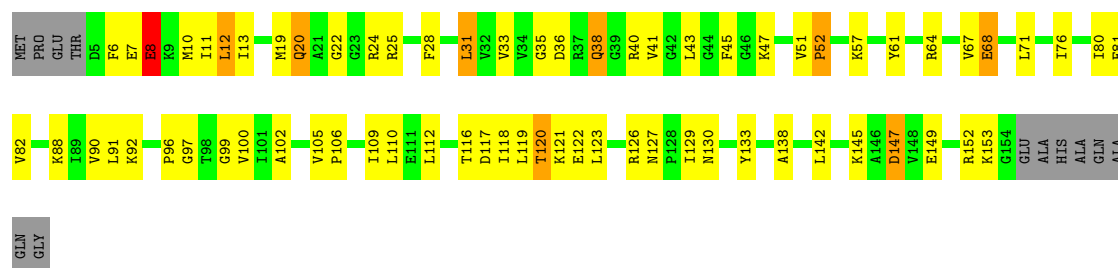
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



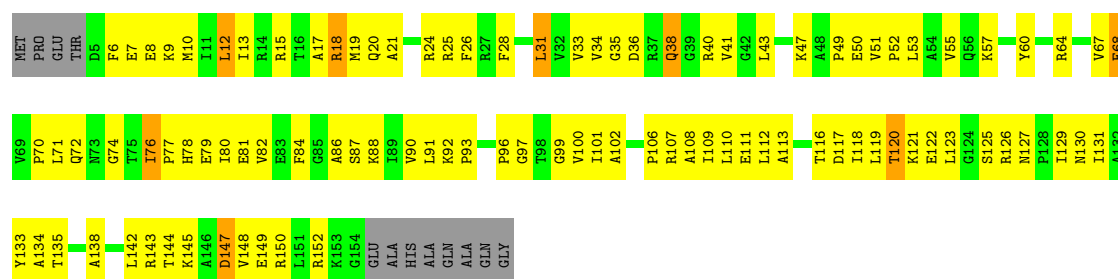
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



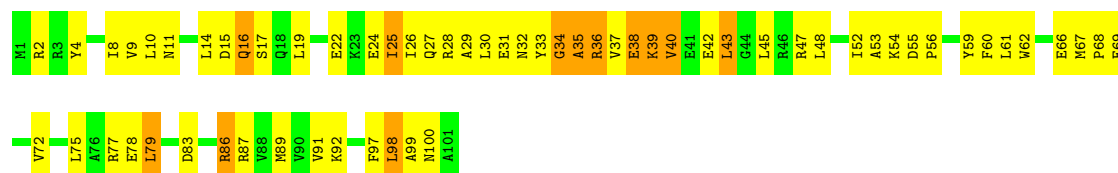
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



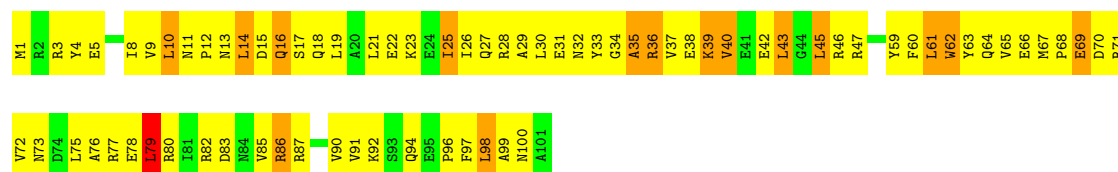
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



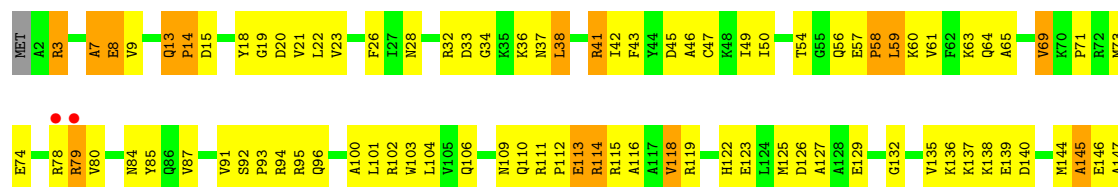
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:

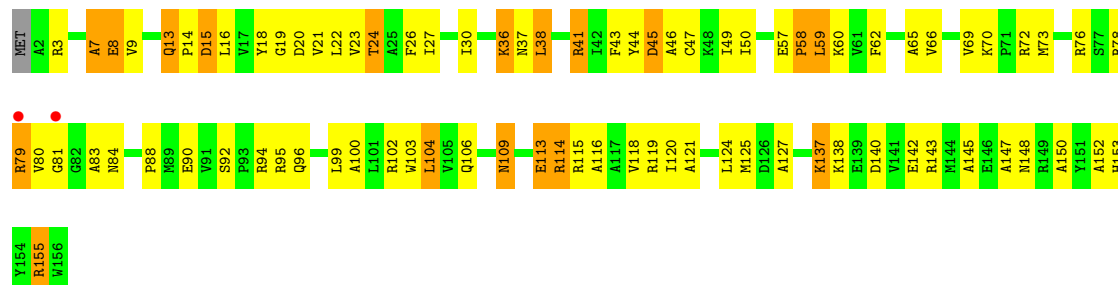






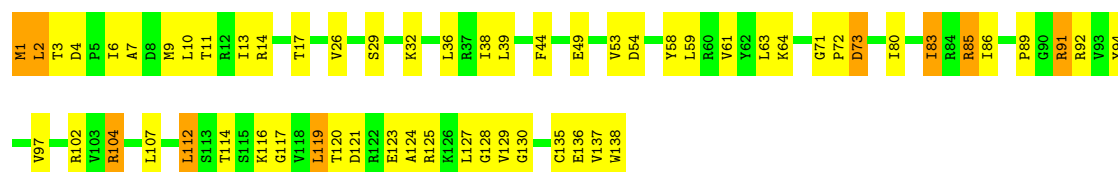
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



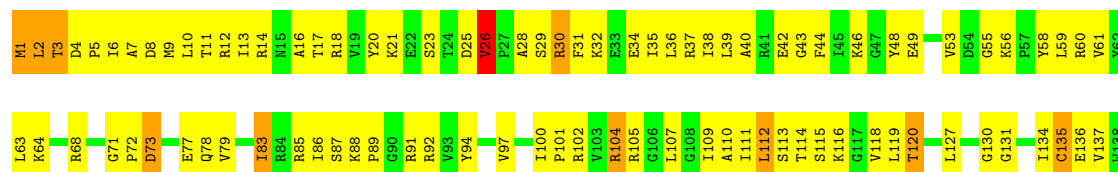
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



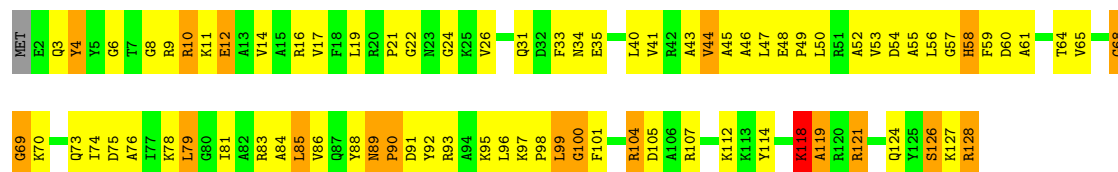
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

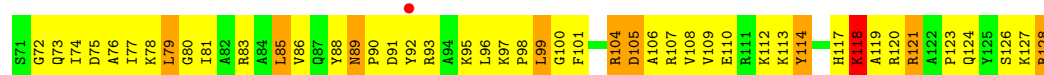
Chain AI:



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:





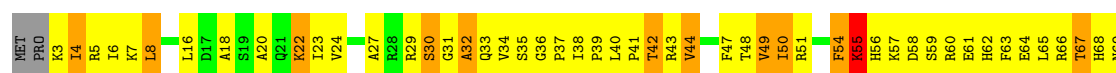
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



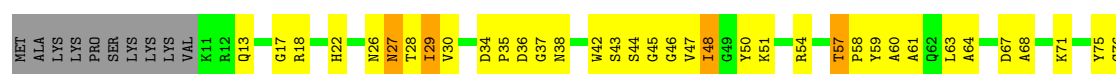
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



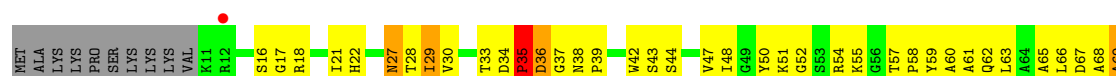
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



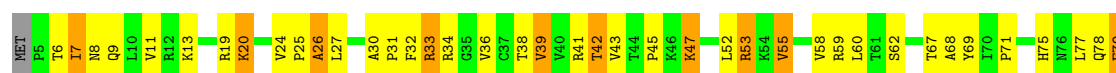
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



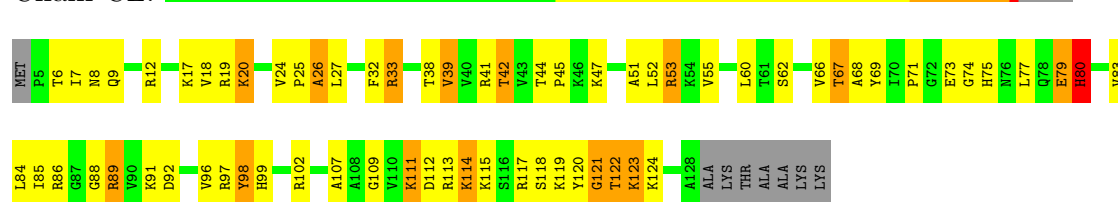
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



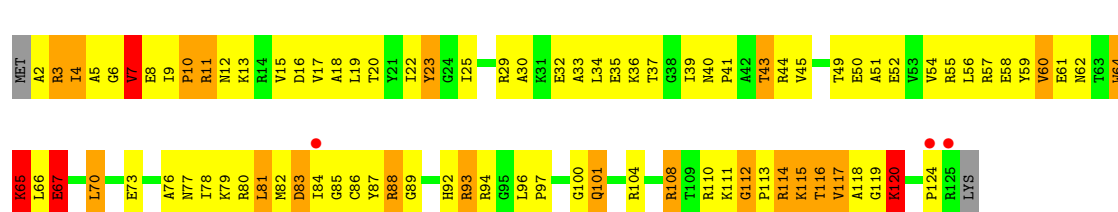
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



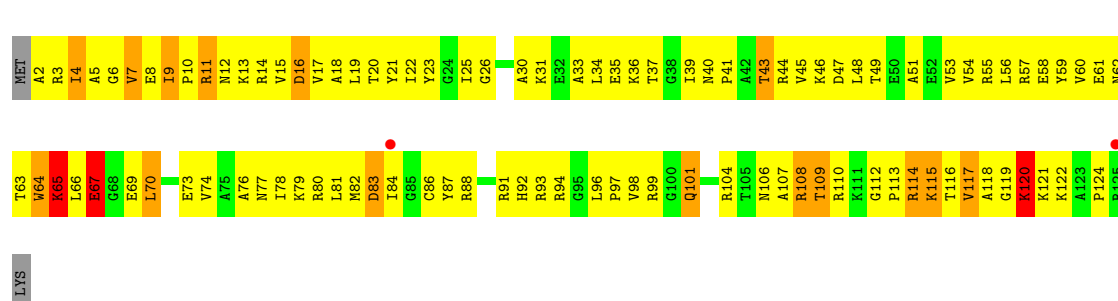
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



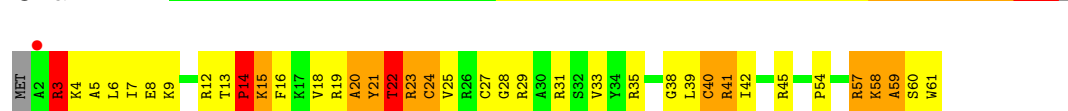
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



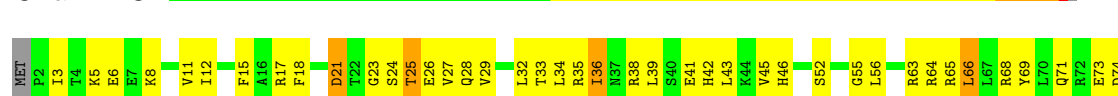
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

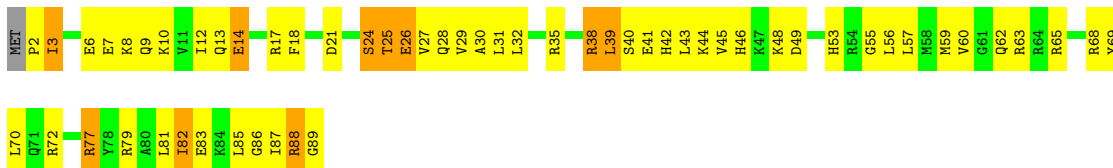
Chain AO:





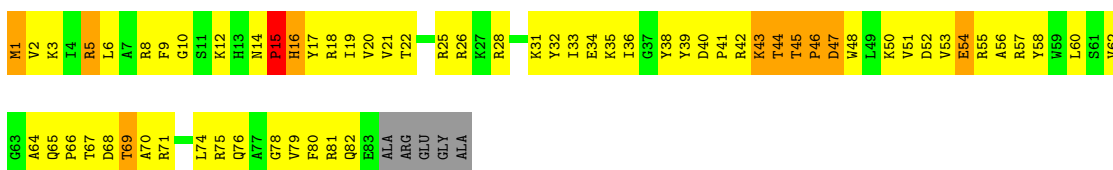
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



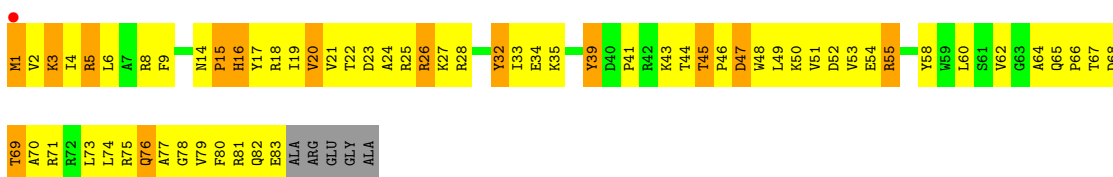
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



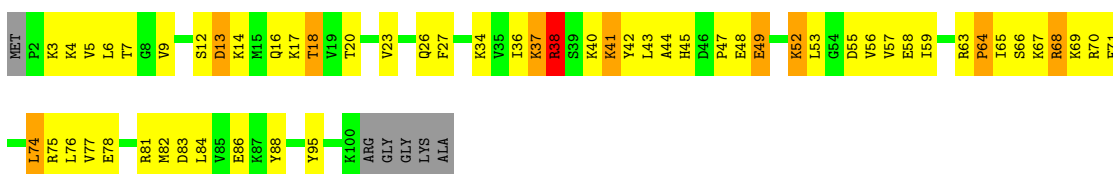
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



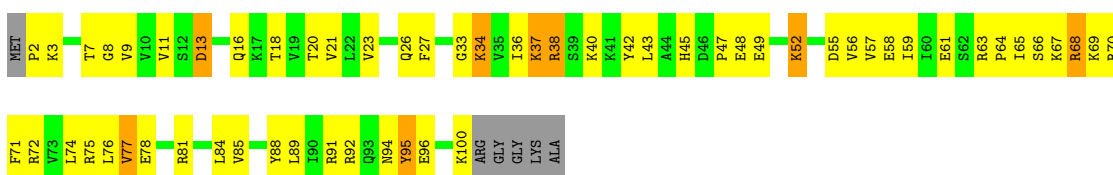
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



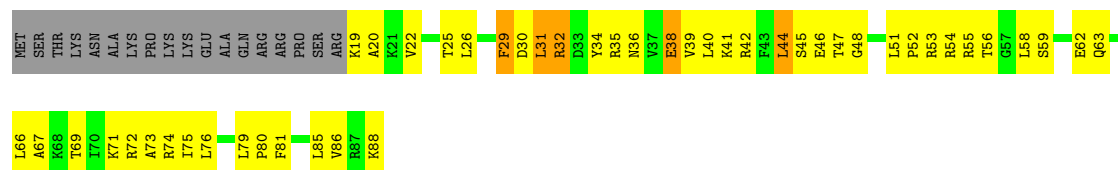
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



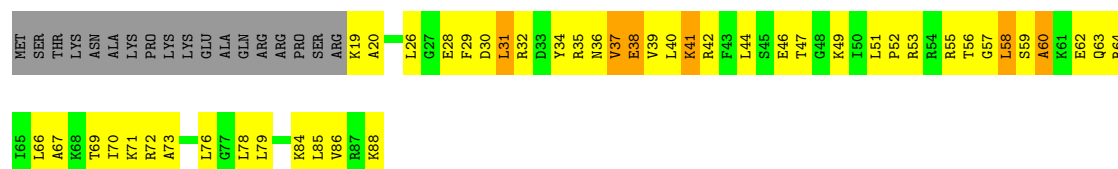
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



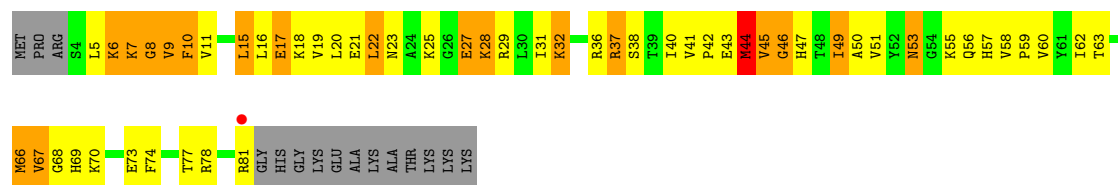
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



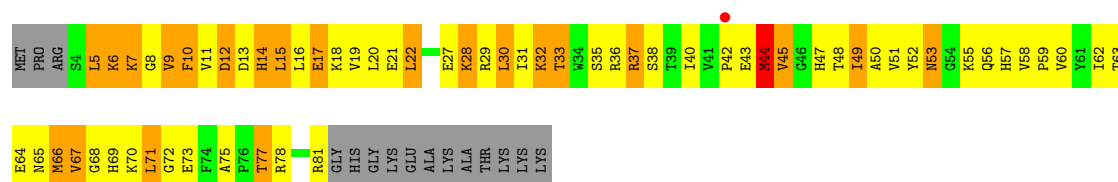
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



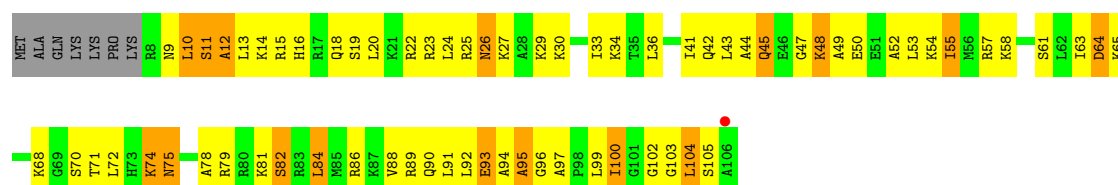
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



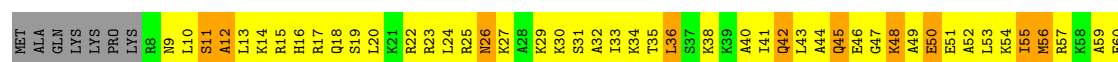
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

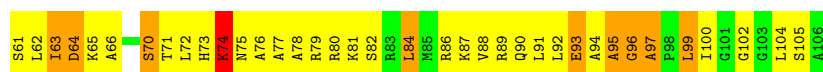
Chain AT:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:





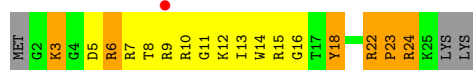
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



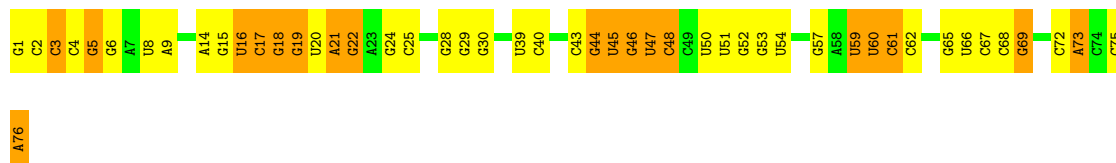
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



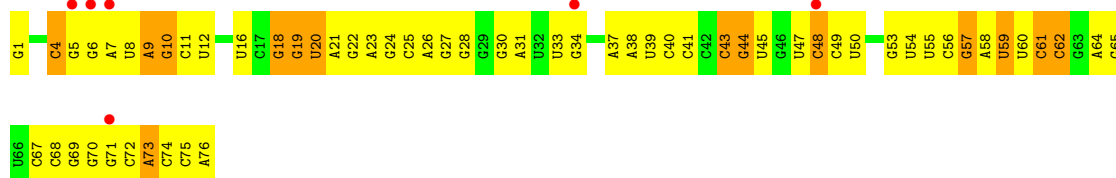
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



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

Chain AW:



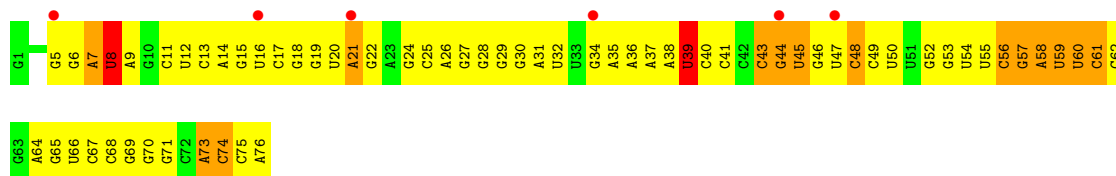
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CV:



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

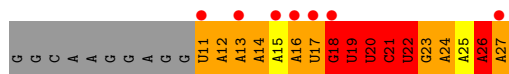
Chain CW:



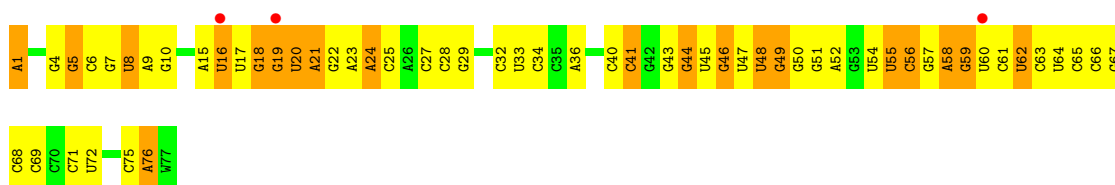
- Molecule 23: MRNA

G	G	C	A	A	G	G	A	G	U11	A12	A13	A14	A15	A16	U17	G18	U19	U20	C21	U22	G23	A24	A25	A26	A27
---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

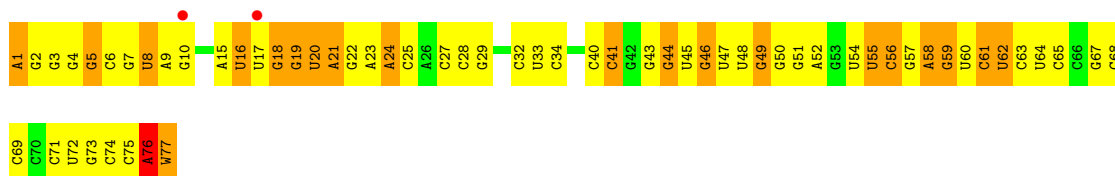
- Chain CX:



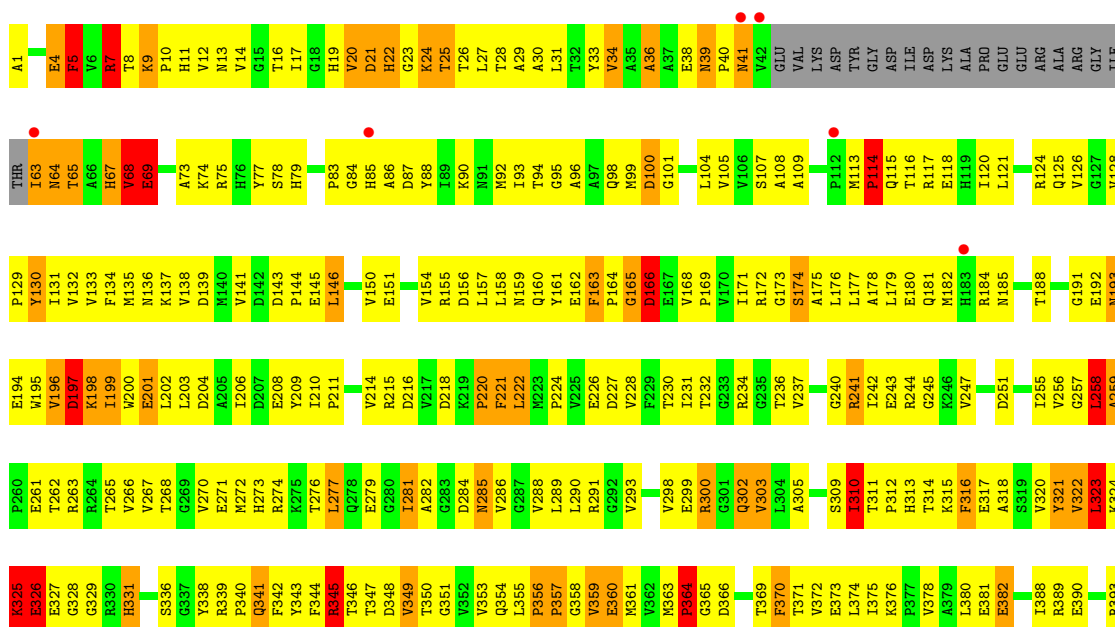
- Chain AY: 

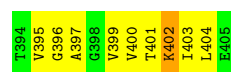


- Chain CY:



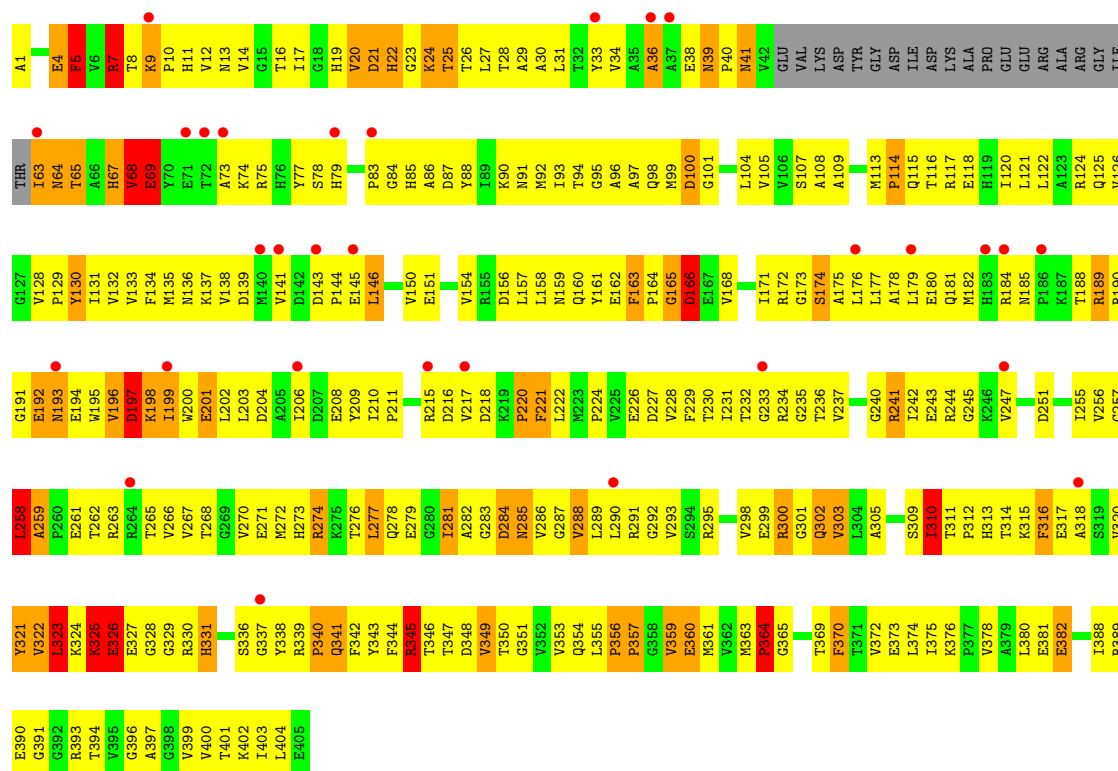
- Chain AZ: 





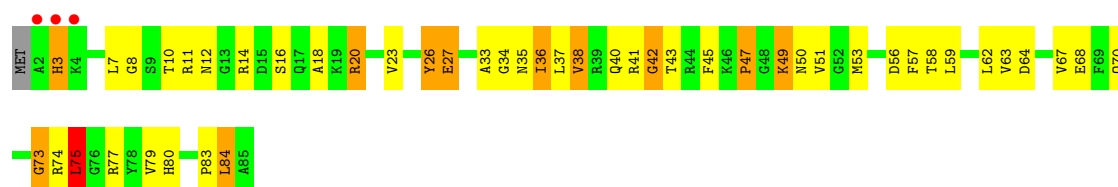
• Molecule 25: ELONGATION FACTOR TU

Chain CZ:



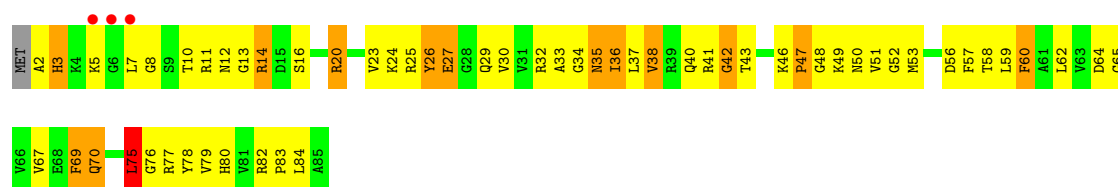
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:

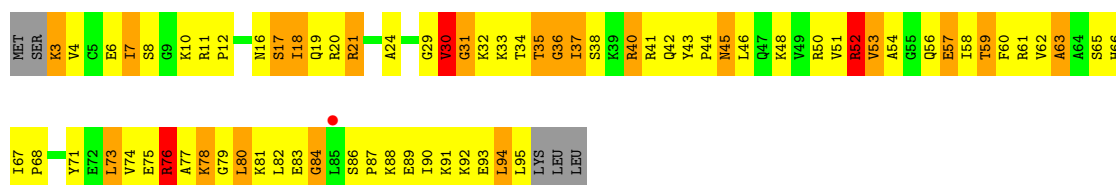


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:

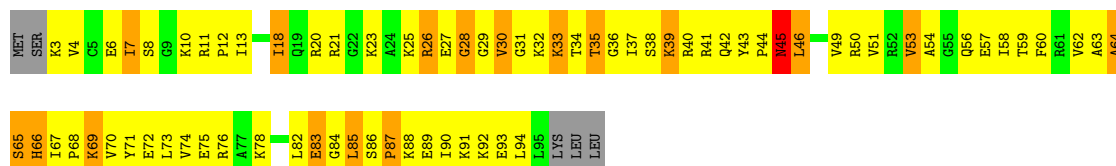






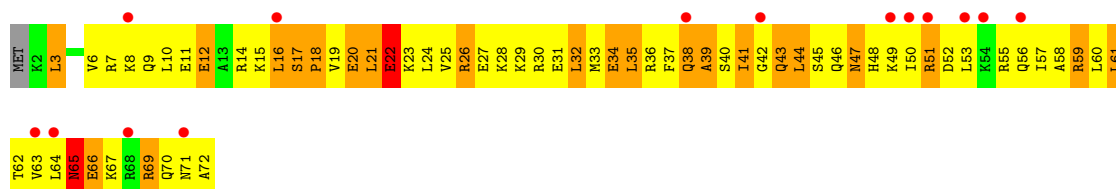
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



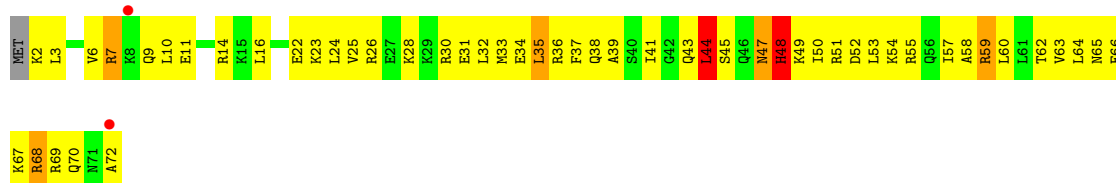
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



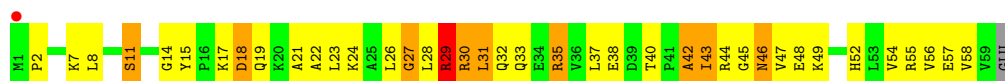
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



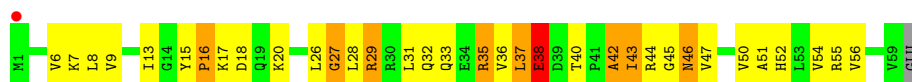
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



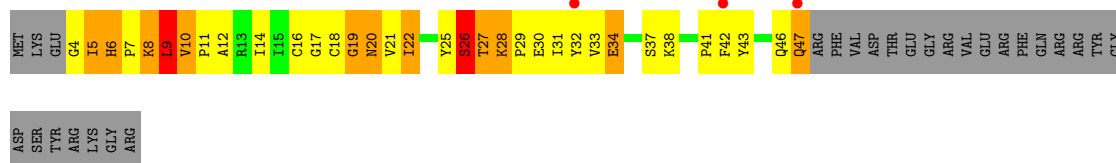
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



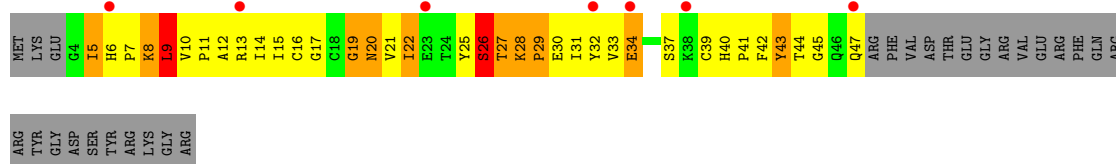
• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:



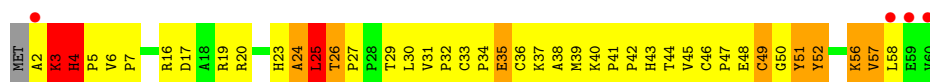
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:



• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5:



• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:



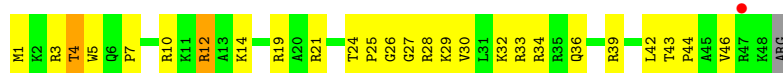
• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:



• Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



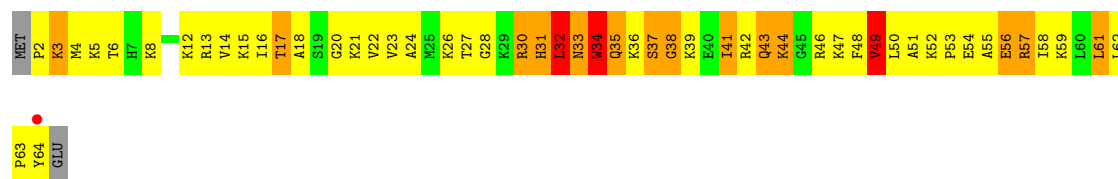
• Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:



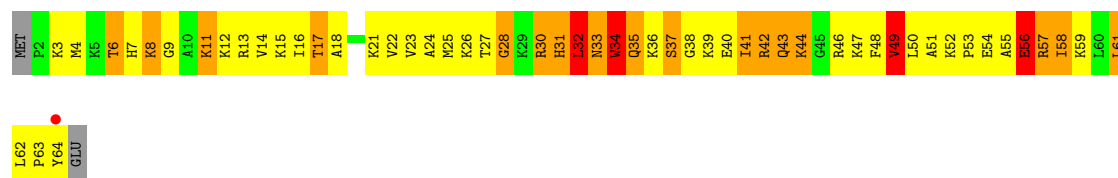
• Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



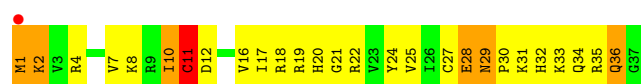
• Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8:



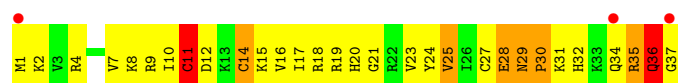
• Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



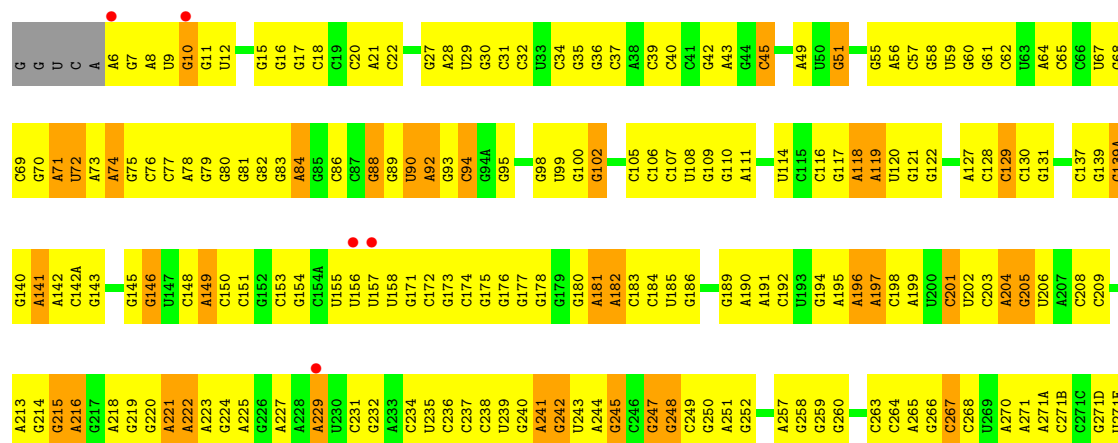
• Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



• Molecule 36: 23S RIBOSOMAL RNA

Chain BA:





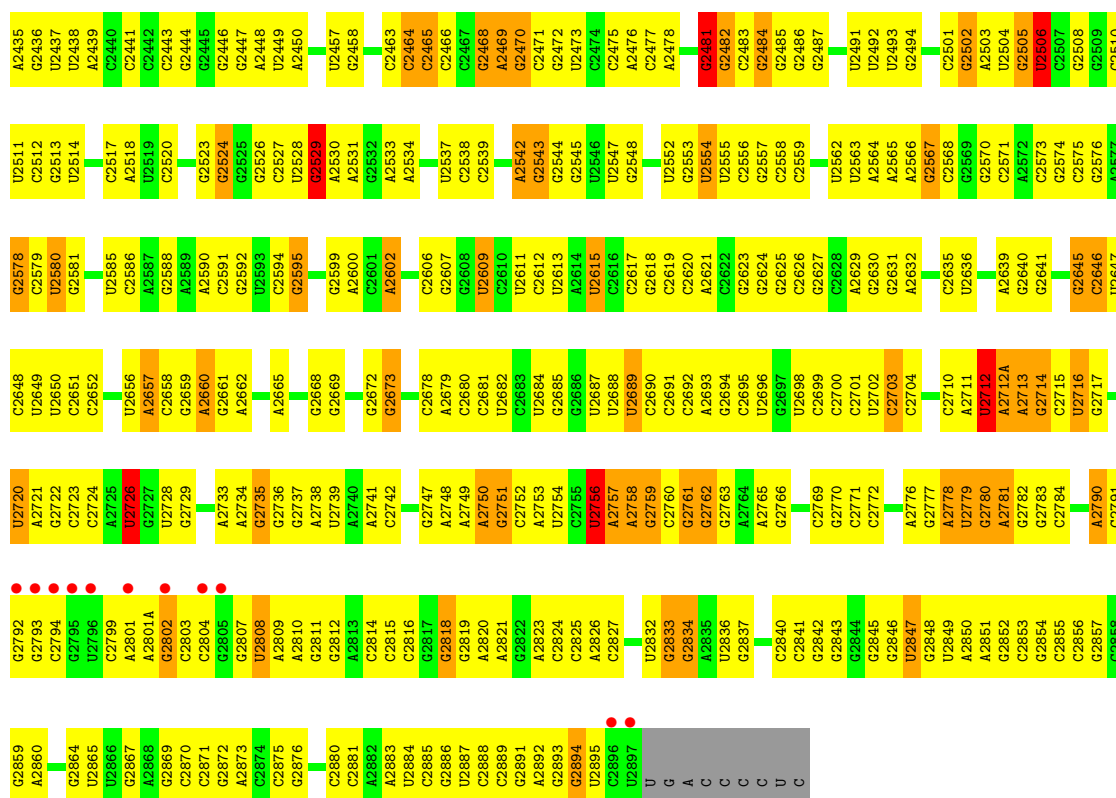




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G1315	G1245	A1177	G1107	G1047	A980	A900	U828	U757	A676	C634	C574	A506	G438	C364
G1316	A1246	C1178	U1108	A1048	A981	A901	A829	C758	A677	C635	C575	A507	G439	C365
G1317	G1248	G1183	C1109	C1049	C982	C902	A830	U759	C678	C636	U576	A508	G440	C366
G1318	G1249	G1184	G1110	A1050	A983	C903	G831	G760	C679	A637	U577	G509	U441	G370
G1319	G1250	C1185	G1112	G1052	A984	C904	G832	A761	A685	C638	A578	G512	G442	A371
G1320	C1251	G1186	U1113	C1053	C985	U905	U833	U762	G686	U639	C579	A513	A443	G372
G1321	G1252	G1187	U1114	G1054	C986	G906	C834	G763	C687	C640	C580	A514	C444	U373
A1322	A1253	U1188	G1115	G1055	G987	U907	A835	A764	U688	A645	C581	A515	C445	A374
G1323	A1254	A1189	G1116	G1056	G988	C908	C837	C765	A689	A646	C582	C516	G447	C375
G1324	G1255	G1190	C1116	G1057	G989	A909	C838	U767	G690	G647	C584	C517	A448	C376
	G1256	G1191	G1120	A1058	C991	A910	U839	G768	G691	A648	C585	G518	U449	C377
	C1257	G1192	C1121	U1059	C992	C912	C840	G769	C692	G648	A586	U519	A450	G378
G1327	C1258	G1193	G1125	U1060	G993	U913		G770	C693	G649	C587	G520	G451	G379
U1329	G1259		G1126	U1061	C994	C914	G845	G771	U694	C650	U588	G521	C452	U380
C1330	C1261	C1196	A1127	G1062	A995	C915	U846	U772	U695	G651	C589	G522	C453	G382
A1331	A1262	G1197	G1063	G1063	A996	G916	U847	C773	G696	C652	C590	G523	A454	U383
G1332	U1263	U1198	C1064	A1069	G997	A917	G848	A774	C697	A653	C591	U524	C455	U384
	U1263	U1199	U1065	A1070	C998	A918	A849	G775	C708	C654F	C592		C456	C385
G1336	G1264	C1200	U1066	U1066	U999		C850	G776	U703	G654A	G593	C527	A457	G386
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G1338		C1196	G1068	G1068	A1001	C925	G852	A782	A705	C654C	C595	A529	U459	G388
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	A1269	U1199	U1065	A1070	C998	A918	A849	G775	C708	C654F	C598	A532	G463	G391
G1344	G1271	C1200	U1066	U1066	U999		C850	G776	U703	G654A	G593	C527	U464	C392
C1345	A1272	U1061	U1067	U1068	A1001	C925	U851	A782	A705	C654B	U594	A528	G465	G396
G1346	U1273	C1201	G1068	G1068	A1001	C925	G852	A783	A706	G654C	C595	A529	G466	G397
G1347	G1274	G1197	G1069	A1069	A996	A926	U847	A784	A707	G654D	C596	G530	G467	G398
G1348	A1275	U1210	A142A	G1076	U1012	G940	A861	C790	G713	G654E	A603	G537	G468	G399
A1349	G1276	U1211	A143	G1077	U1013	A941	G862	C791	C720	G654L	C604	C540	G469	G400
C1350	G1277	U1212	G144	U1078	U1014	A942	G863	G792	C721	C654M	C605	C541	A470	A401
G1278	A1278	A1213	C145	U1079	G1013	G944	G864	A793	A722	G654N	U606	C543	A471	A402
G1279		G1214		C1080	C1018		A866	C796	G723	G654O	A608	C543	U477	U403
A1286	A1286	G1215	G1149	U1081	U1018	G945	G874	C797	U724	C654Q	A609	A547	A478	C404
A1287	U1286	C1216	C1150	U1082	A1020	A953	G875	A802	C730	C654R	C610	A548	A479	U405
G1288	C1289	G1217	G1151	U1083	A1021	G954	U876	U803	G729	G654S	C611	G549	A480	G406
G1290	G1290	C1218	C1152	A1084	U1022	G954	U877	U804	C730	G654T	C612	G551	G481	G407
C1291	C1291	C1221A	G1154	A1085	G1024	A957	U878	G805	G733	A654U	G613	G553	A482	G408
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A1300	U1300		G1164	A1095	U1033	C964	A887	C814	G745			G562	G491	C419
A1301	A1301	G1231	U1165	U1096	G1034	C965	C888	C815	A746	C661	A621	U562	A492	C420
A1302	G1302	G1232	C1166	U1097	U1035	U969	C889	C816	U747		G622	G563	G493	U421
C1303	C1303		U1167	A1098	G1036	C970	A890	C817	G748		G623	C564	G494	C422
G1304	G1304	A1237	G1168	G1099	C1038	C971	G892	A819	C749	G668	C624	C565	G495	A423
C1306	C1306	G1238	G1170	U1100	G1039	G972	C894	A820	A750	A670	A627	U566	A497	G427
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A1378	A1378	A1241	A1173	C1104	G1042	C975	A896	G823	C753	C672	G630	U569	G500	G432
A1379	A1379	A1242	A1174	C1105	A1045	G978	C897	A824	C754	C673	A631	G570	A501	A432
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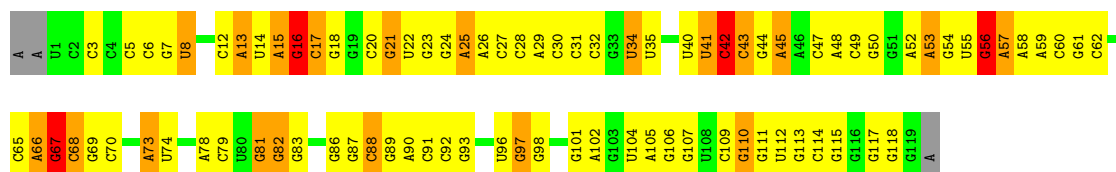






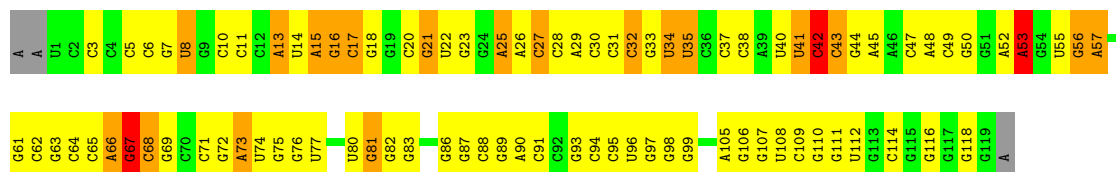
### • Molecule 37: 5S RIBOSOMAL RNA

Chain BB:



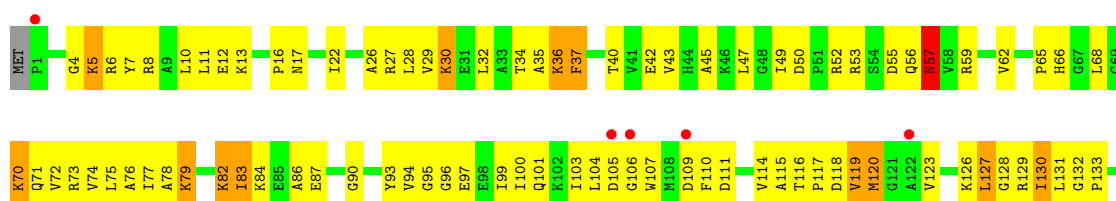
### • Molecule 37: 5S RIBOSOMAL RNA

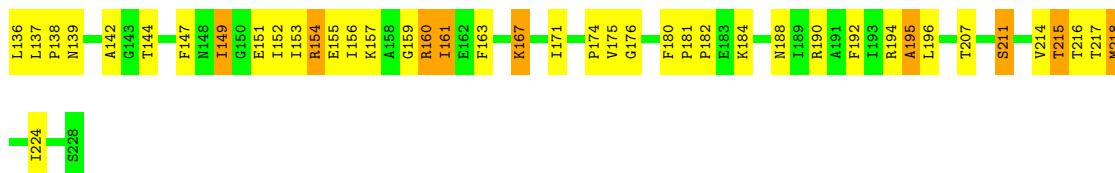
Chain DB:



### • Molecule 38: 50S RIBOSOMAL PROTEIN L1

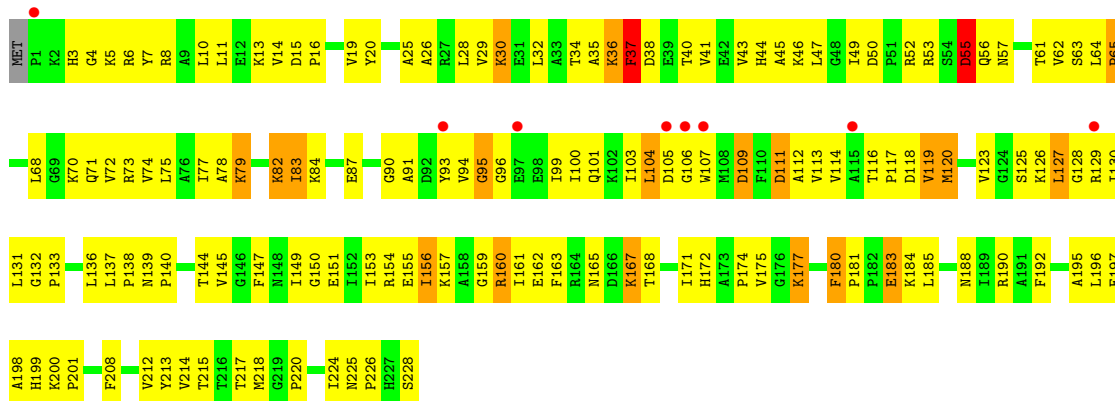
Chain BC:





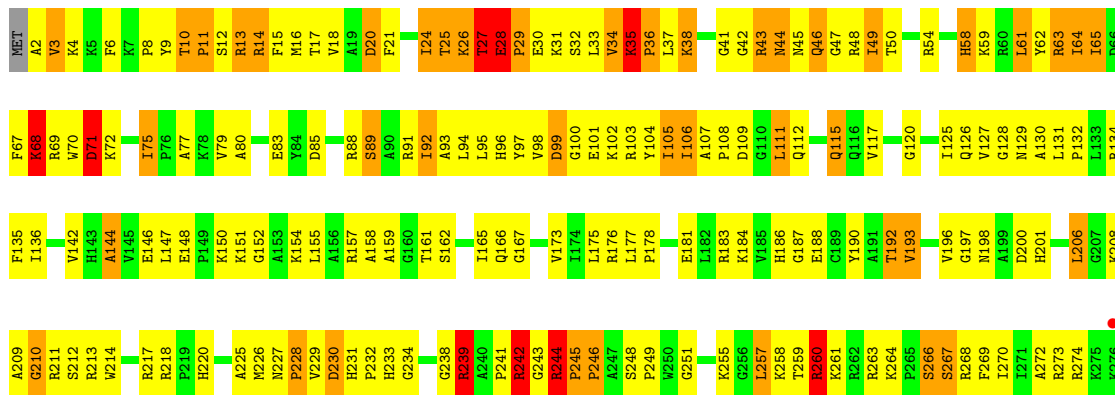
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain DC:



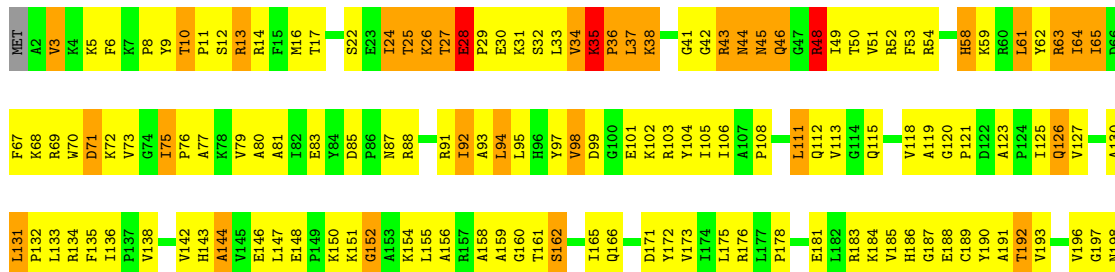
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

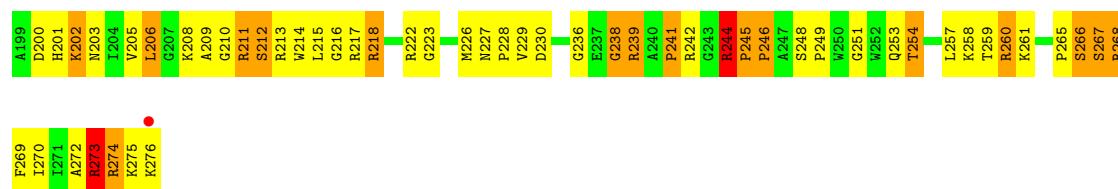
Chain BD:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

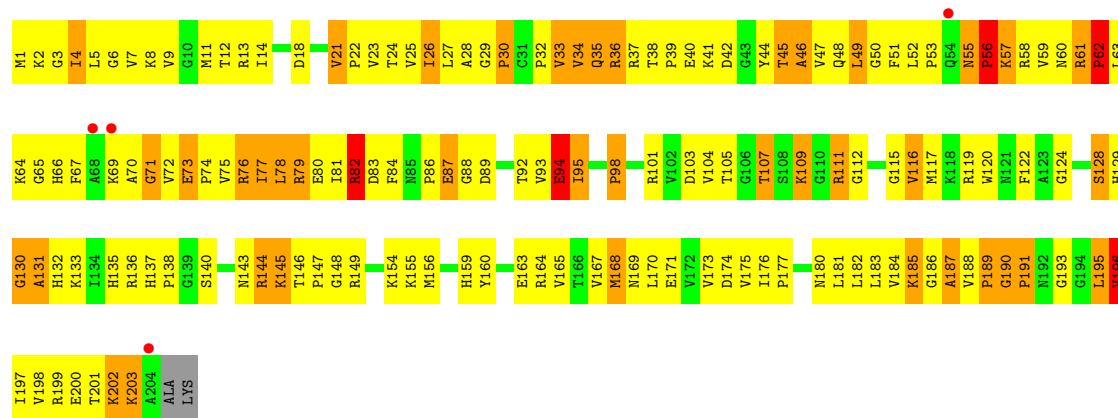
Chain DD:





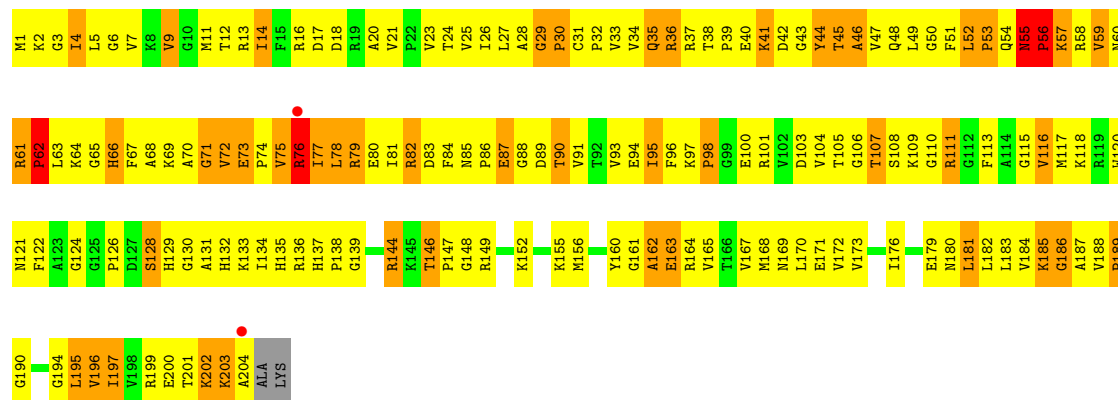
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE:



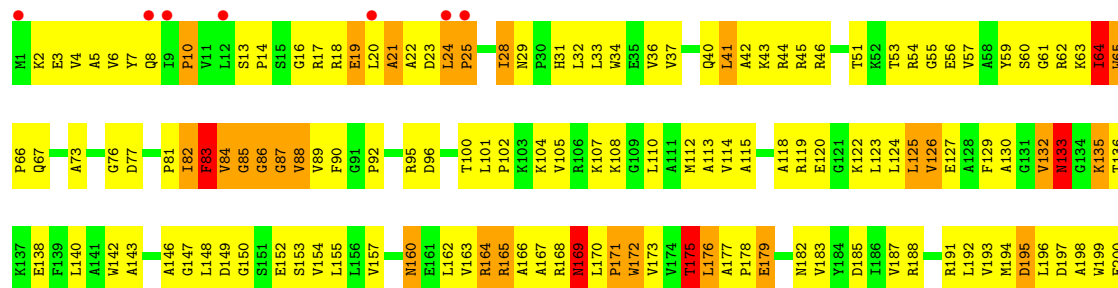
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE:



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

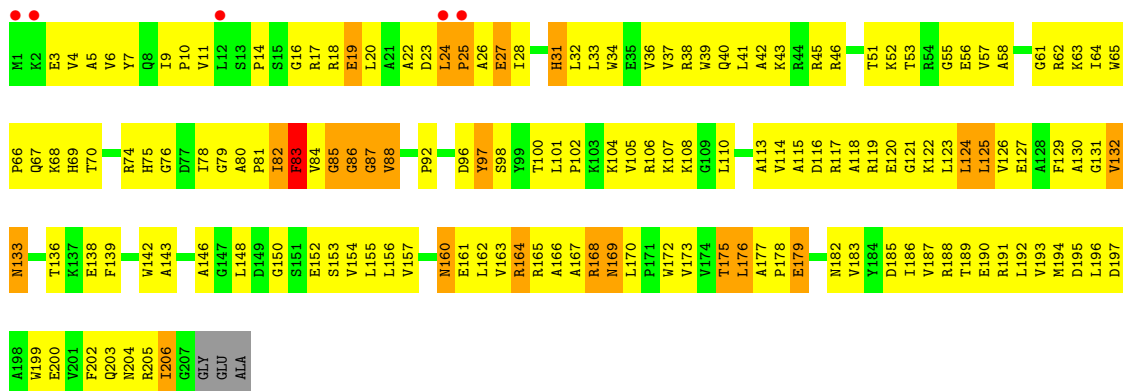
Chain BF:





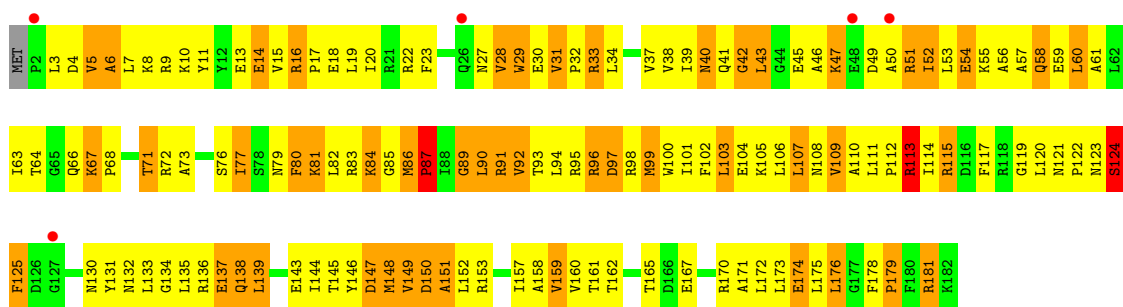
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:



• Molecule 42: 50S RIBOSOMAL PROTEIN L5

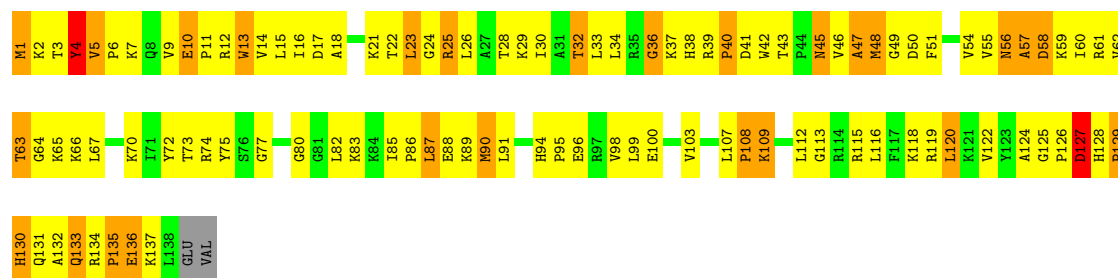
Chain BG:





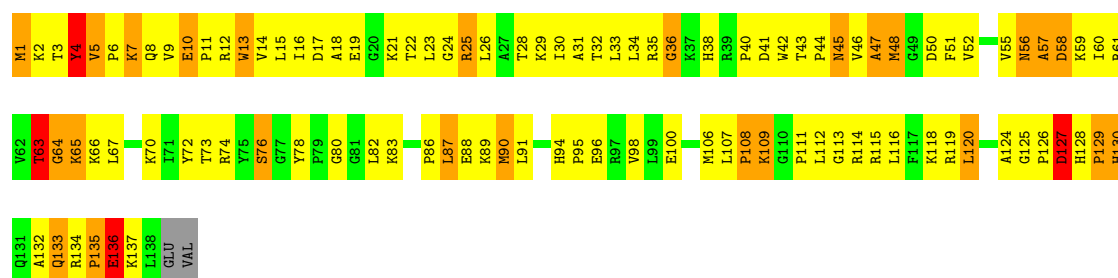
## • Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



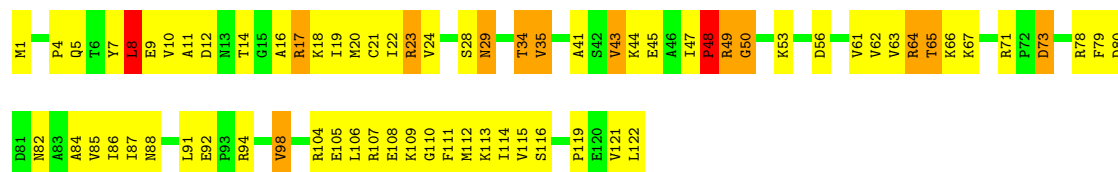
## • Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



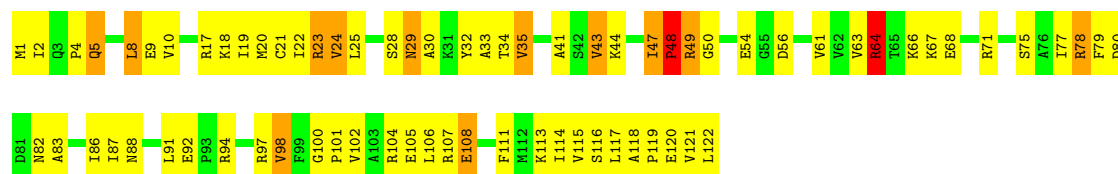
## • Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



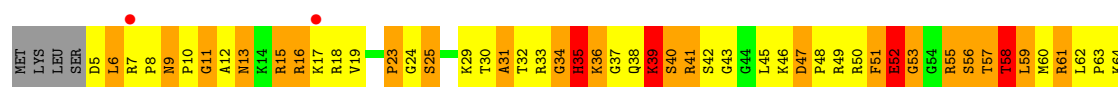
## • Molecule 47: 50S RIBOSOMAL PROTEIN L14

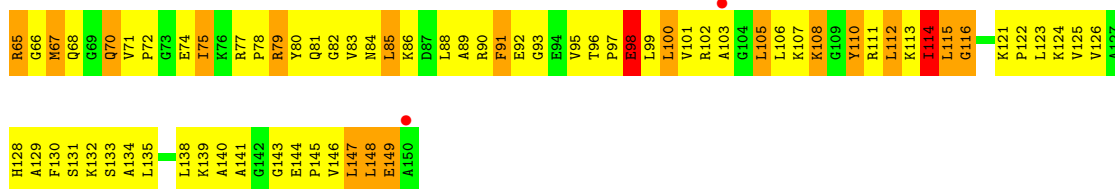
Chain DO:



## • Molecule 48: 50S RIBOSOMAL PROTEIN L15

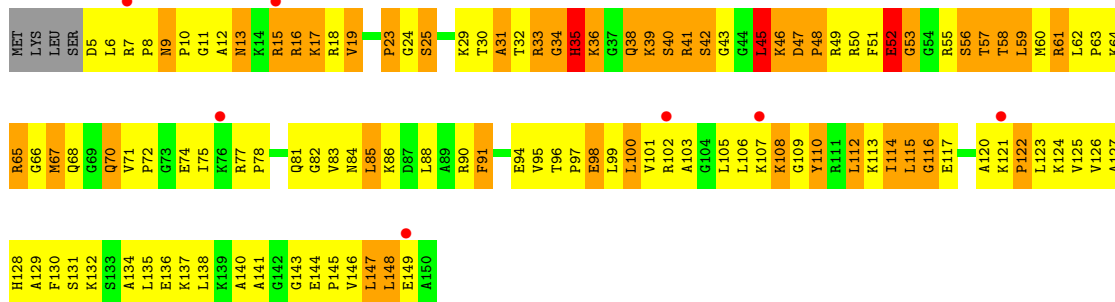
Chain BP:





• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



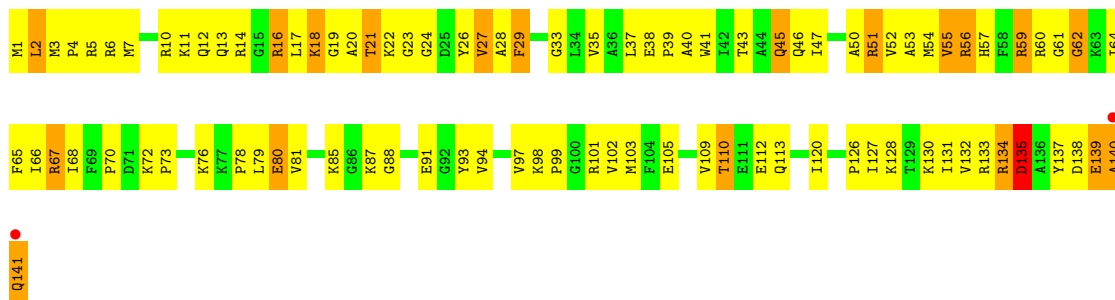
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



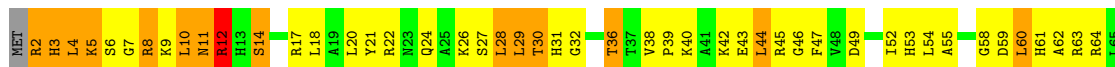
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

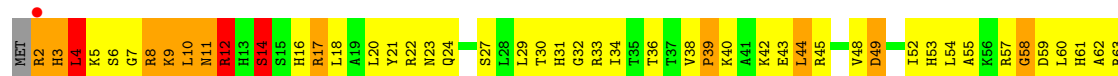
Chain BR:





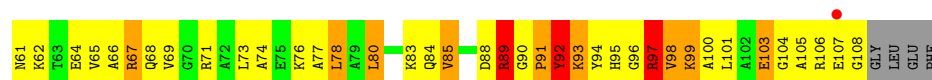
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



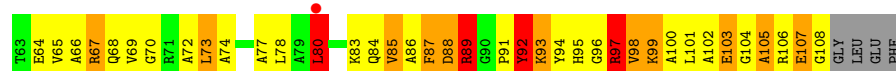
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



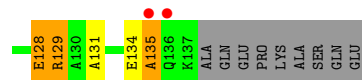
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:

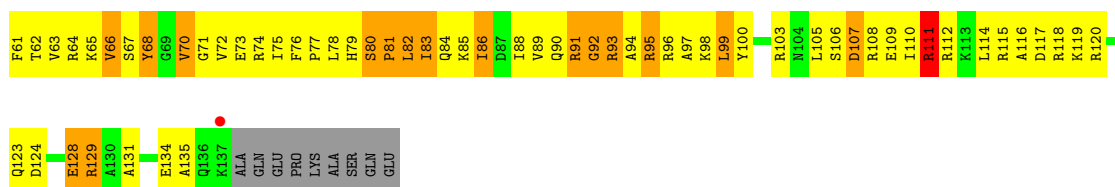


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:

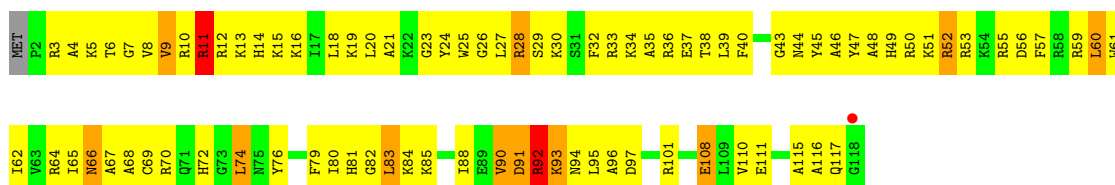






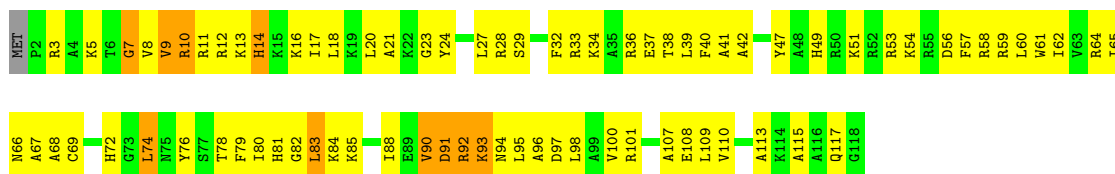
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



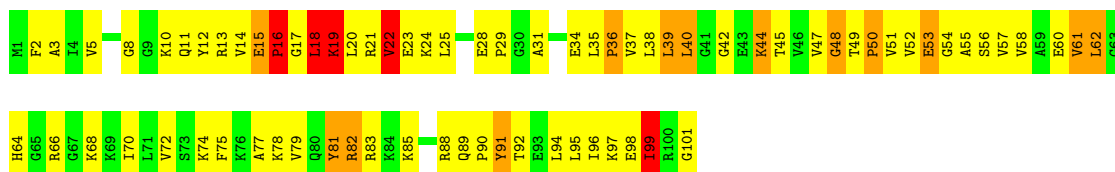
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



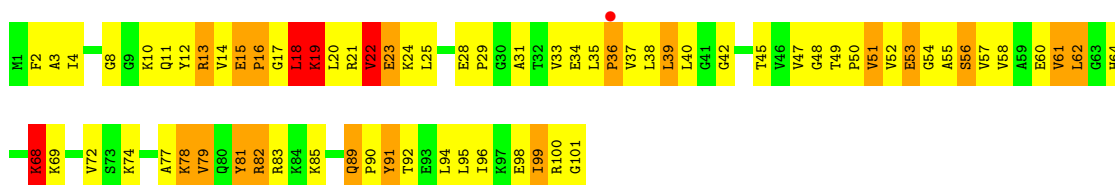
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



• Molecule 54: 50S RIBOSOMAL PROTEIN L21

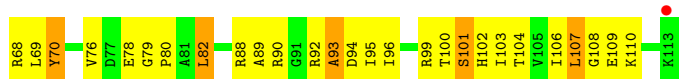
Chain DV:



• Molecule 55: 50S RIBOSOMAL PROTEIN L22

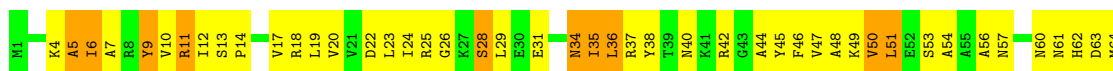
Chain BW:





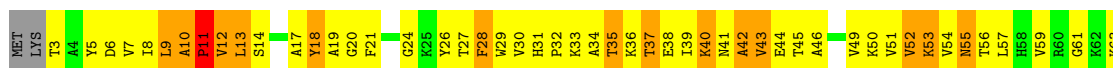
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



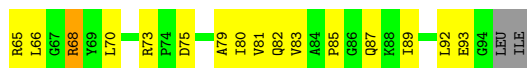
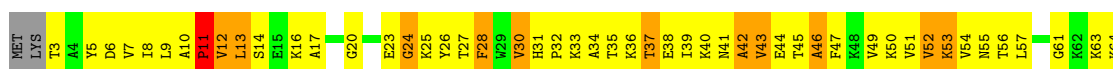
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



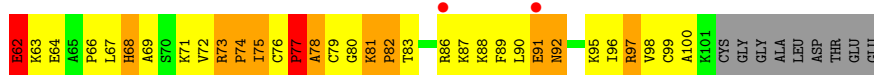
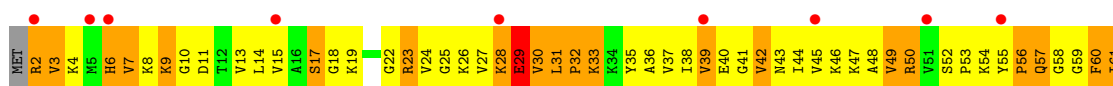
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



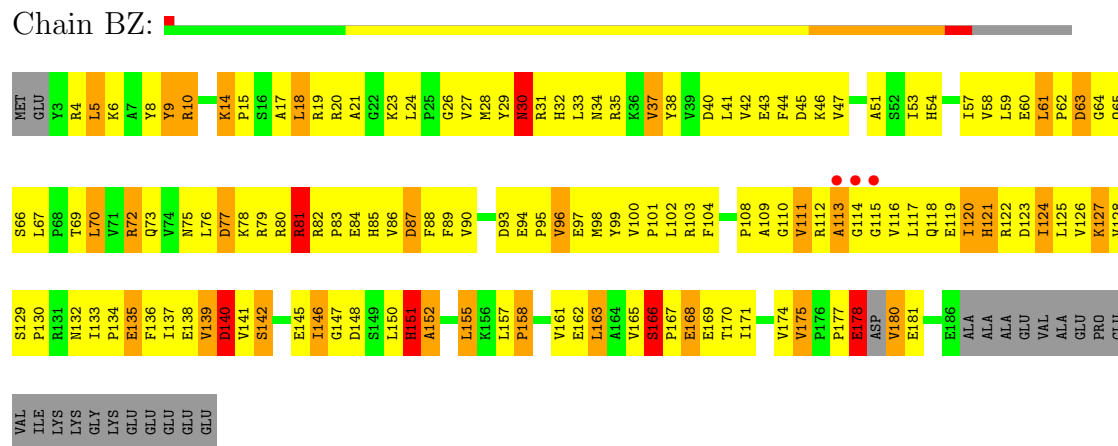
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:



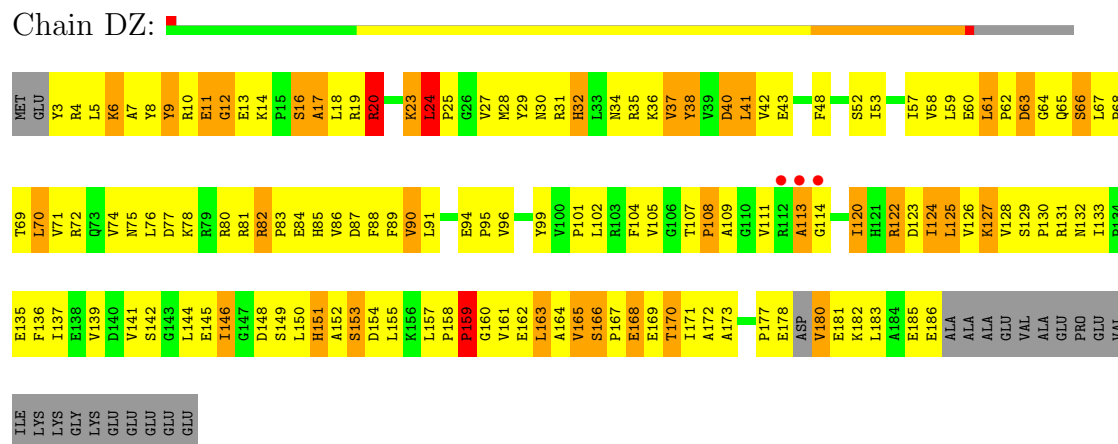
● Molecule 58: 50S RIBOSOMAL PROTEIN L25

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, $\alpha$ , $\beta$ , $\gamma$	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-3.10) 91.8 (49.22-2.80)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.238 , 0.275 0.254 , 0.289	Depositor DCC
$R_{free}$ test set	69565 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 44.9	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 1394902 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	307194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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	0.67	10/36190 (0.0%)	0.79	44/56486 (0.1%)
1	CA	0.54	3/36190 (0.0%)	0.74	25/56486 (0.0%)
2	AB	0.55	0/1935	0.76	0/2609
2	CB	0.43	0/1935	0.70	0/2609
3	AC	0.65	1/1636 (0.1%)	0.83	0/2205
3	CC	0.43	0/1636	0.70	0/2205
4	AD	0.48	1/1733 (0.1%)	0.75	1/2318 (0.0%)
4	CD	0.44	1/1733 (0.1%)	0.71	0/2318
5	AE	0.65	1/1162 (0.1%)	0.81	0/1564
5	CE	0.52	0/1162	0.77	0/1564
6	AF	0.50	0/856	0.70	1/1154 (0.1%)
6	CF	0.38	0/856	0.67	0/1154
7	AG	0.52	0/1276	0.73	1/1709 (0.1%)
7	CG	0.39	0/1276	0.63	0/1709
8	AH	0.57	0/1136	0.80	0/1527
8	CH	0.49	0/1136	0.79	0/1527
9	AI	0.55	0/1029	0.82	0/1379
9	CI	0.41	0/1029	0.68	0/1379
10	AJ	0.55	0/807	0.85	0/1085
10	CJ	0.40	0/807	0.75	1/1085 (0.1%)
11	AK	0.60	1/900 (0.1%)	0.80	0/1213
11	CK	0.46	0/900	0.76	1/1213 (0.1%)
12	AL	0.52	0/986	0.82	1/1320 (0.1%)
12	CL	0.44	0/986	0.77	0/1320
13	AM	0.51	0/998	0.80	0/1336
13	CM	0.39	0/998	0.74	0/1336
14	AN	0.70	1/501 (0.2%)	0.98	1/664 (0.2%)
14	CN	0.53	1/501 (0.2%)	0.86	1/664 (0.2%)
15	AO	0.52	0/745	0.77	0/992
15	CO	0.44	0/745	0.66	0/992
16	AP	0.46	0/716	0.74	0/963
16	CP	0.40	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.54	0/836	0.76	0/1117
17	CQ	0.45	0/836	0.76	0/1117
18	AR	0.56	0/579	0.73	0/768
18	CR	0.46	0/579	0.72	0/768
19	AS	0.55	0/642	0.76	0/865
19	CS	0.40	0/642	0.76	0/865
20	AT	0.42	0/765	0.69	0/1007
20	CT	0.36	0/765	0.71	0/1007
21	AU	0.55	0/212	0.87	0/277
21	CU	0.48	0/212	0.80	0/277
22	AV	0.68	0/1809	0.79	0/2819
22	AW	0.47	0/1809	0.74	0/2819
22	CV	0.92	5/1809 (0.3%)	0.90	7/2819 (0.2%)
22	CW	0.41	0/1809	0.73	0/2819
23	AX	0.79	0/405	0.91	2/629 (0.3%)
23	CX	1.78	13/405 (3.2%)	1.64	16/629 (2.5%)
24	AY	0.49	1/1618 (0.1%)	0.71	0/2514
24	CY	0.64	2/1618 (0.1%)	0.76	0/2514
25	AZ	0.84	12/3042 (0.4%)	0.99	15/4129 (0.4%)
25	CZ	0.90	14/3042 (0.5%)	1.02	17/4129 (0.4%)
26	B0	0.47	0/671	0.78	0/892
26	D0	0.42	0/671	0.74	0/892
27	B1	0.51	0/738	0.81	1/981 (0.1%)
27	D1	0.42	0/738	0.76	0/981
28	B2	0.38	0/600	0.73	0/793
28	D2	0.35	0/600	0.60	0/793
29	B3	0.40	0/472	0.67	0/634
29	D3	0.38	0/472	0.68	0/634
30	B4	0.46	0/349	0.66	0/474
30	D4	0.51	0/349	0.62	0/474
31	B5	0.44	0/473	0.73	0/639
31	D5	0.43	0/473	0.74	0/639
32	B6	0.70	0/440	0.94	0/586
32	D6	0.58	0/440	0.85	0/586
33	B7	0.49	0/426	0.73	0/561
33	D7	0.44	0/426	0.74	1/561 (0.2%)
34	B8	0.58	0/515	0.89	1/679 (0.1%)
34	D8	0.52	0/515	0.87	1/679 (0.1%)
35	B9	0.56	0/310	0.73	0/407
35	D9	0.69	1/310 (0.3%)	0.81	0/407
36	BA	0.56	7/69976 (0.0%)	0.74	36/109244 (0.0%)
36	DA	0.51	3/69976 (0.0%)	0.73	25/109244 (0.0%)
37	BB	0.51	0/2853	0.77	3/4451 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DB	0.48	0/2853	0.76	0/4451
38	BC	0.46	2/1774 (0.1%)	0.65	0/2391
38	DC	0.41	2/1774 (0.1%)	0.61	0/2391
39	BD	0.62	0/2195	0.93	3/2955 (0.1%)
39	DD	0.51	0/2195	0.86	1/2955 (0.0%)
40	BE	0.46	0/1596	0.77	1/2153 (0.0%)
40	DE	0.45	0/1596	0.75	1/2153 (0.0%)
41	BF	0.40	0/1658	0.65	0/2244
41	DF	0.40	0/1658	0.64	0/2244
42	BG	0.48	0/1499	0.78	0/2016
42	DG	0.40	0/1499	0.70	0/2016
43	BH	0.37	0/1245	0.66	0/1682
43	DH	0.35	0/1245	0.66	0/1682
46	BN	0.39	0/1131	0.72	0/1525
46	DN	0.39	0/1131	0.70	0/1525
47	BO	0.53	0/943	0.74	1/1269 (0.1%)
47	DO	0.51	1/943 (0.1%)	0.74	0/1269
48	BP	0.46	0/1131	0.96	4/1504 (0.3%)
48	DP	0.42	0/1131	0.93	4/1504 (0.3%)
49	BQ	0.52	0/1143	0.73	0/1527
49	DQ	0.51	0/1143	0.69	0/1527
50	BR	0.41	0/974	0.81	2/1302 (0.2%)
50	DR	0.38	0/974	0.77	2/1302 (0.2%)
51	BS	0.45	0/778	0.79	0/1036
51	DS	0.41	0/778	0.76	1/1036 (0.1%)
52	BT	0.48	0/1155	0.78	1/1542 (0.1%)
52	DT	0.44	0/1155	0.77	1/1542 (0.1%)
53	BU	0.42	0/975	0.69	0/1297
53	DU	0.44	0/975	0.69	0/1297
54	BV	0.38	0/790	0.68	0/1057
54	DV	0.37	0/790	0.67	0/1057
55	BW	0.39	0/907	0.76	0/1216
55	DW	0.39	0/907	0.68	0/1216
56	BX	0.45	0/739	0.70	0/993
56	DX	0.41	0/739	0.67	0/993
57	BY	0.36	0/788	0.69	0/1051
57	DY	0.38	0/788	0.70	0/1051
58	BZ	0.50	0/1491	0.75	0/2024
58	DZ	0.46	0/1491	0.72	0/2024
All	All	0.55	83/330116 (0.0%)	0.75	224/493186 (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	1	90
1	CA	2	54
5	AE	0	1
22	AV	0	1
22	CV	0	2
22	CW	0	2
23	AX	0	2
23	CX	0	6
24	CY	0	1
25	AZ	0	2
25	CZ	0	2
36	BA	2	87
36	DA	0	79
37	BB	0	4
37	DB	0	3
39	BD	0	1
46	BN	0	1
All	All	5	338

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	34	G	C5-C6	-23.91	1.18	1.42
25	CZ	69	GLU	CB-CG	17.54	1.85	1.52
25	AZ	69	GLU	CB-CG	16.36	1.83	1.52
25	AZ	68	VAL	CA-C	12.52	1.85	1.52
25	CZ	68	VAL	CA-C	11.51	1.82	1.52

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AZ	356	PRO	C-N-CD	-26.29	62.77	120.60
25	CZ	356	PRO	C-N-CD	-25.87	63.68	120.60
25	AZ	197	ASP	CB-CG-OD2	-14.50	105.25	118.30
25	AZ	69	GLU	N-CA-CB	-13.90	85.58	110.60
25	CZ	69	GLU	N-CA-CB	-13.63	86.07	110.60

All (5) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
36	BA	1300	U	C3'
36	BA	1820	U	C3'
1	CA	508	C	C3'
1	CA	1399	C	C3'

5 of 338 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	123	C	Sidechain
1	AA	13	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	20	U	Sidechain

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1034	0
1	CA	32329	0	16318	1281	0
2	AB	1900	0	1951	204	0
2	CB	1900	0	1951	237	0
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	183	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	75	0
5	CE	1146	0	1207	108	0
6	AF	843	0	857	71	0
6	CF	843	0	857	94	0
7	AG	1257	0	1296	88	0
7	CG	1257	0	1296	87	0
8	AH	1116	0	1177	64	0
8	CH	1116	0	1177	92	0
9	AI	1010	0	1037	111	0
9	CI	1010	0	1037	117	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	794	0	840	126	0
10	CJ	794	0	840	169	0
11	AK	885	0	904	67	0
11	CK	885	0	904	77	0
12	AL	970	0	1057	112	0
12	CL	970	0	1057	87	0
13	AM	987	0	1059	122	0
13	CM	987	0	1059	139	0
14	AN	492	0	531	62	0
14	CN	492	0	530	77	0
15	AO	734	0	771	47	0
15	CO	734	0	771	56	0
16	AP	700	0	720	92	0
16	CP	700	0	720	102	0
17	AQ	823	0	891	70	0
17	CQ	823	0	891	76	0
18	AR	574	0	644	51	0
18	CR	574	0	644	54	0
19	AS	629	0	652	81	0
19	CS	629	0	652	104	0
20	AT	763	0	861	105	0
20	CT	763	0	861	110	0
21	AU	208	0	221	32	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	74	0
22	AW	1619	0	822	75	0
22	CV	1619	0	822	78	0
22	CW	1619	0	822	90	0
23	AX	361	0	184	27	0
23	CX	361	0	184	30	0
24	AY	1644	0	853	71	0
24	CY	1644	0	853	130	0
25	AZ	2984	0	2997	433	0
25	CZ	2984	0	2997	513	0
26	B0	662	0	688	75	0
26	D0	662	0	688	96	0
27	B1	731	0	808	88	0
27	D1	731	0	808	116	0
28	B2	598	0	653	179	0
28	D2	598	0	653	81	0
29	B3	467	0	523	57	0
29	D3	467	0	523	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B4	340	0	336	51	0
30	D4	340	0	335	55	0
31	B5	459	0	480	82	0
31	D5	459	0	480	86	0
32	B6	433	0	461	143	0
32	D6	433	0	461	147	0
33	B7	418	0	467	35	0
33	D7	418	0	467	40	0
34	B8	507	0	576	118	0
34	D8	507	0	576	134	0
35	B9	307	0	335	35	0
35	D9	307	0	336	49	0
36	BA	62477	0	31497	2272	0
36	DA	62477	0	31497	2491	0
37	BB	2551	0	1295	108	0
37	DB	2551	0	1295	108	0
38	BC	1742	0	1800	152	0
38	DC	1742	0	1800	181	0
39	BD	2145	0	2234	297	0
39	DD	2145	0	2234	321	0
40	BE	1563	0	1629	227	0
40	DE	1563	0	1629	256	0
41	BF	1623	0	1677	197	0
41	DF	1623	0	1677	209	0
42	BG	1474	0	1535	241	0
42	DG	1474	0	1535	275	0
43	BH	1222	0	1282	171	0
43	DH	1222	0	1282	159	0
44	BJ	651	0	170	19	0
44	DJ	651	0	162	25	0
45	BK	700	0	175	15	0
45	DK	700	0	171	13	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	159	0
47	BO	933	0	996	92	0
47	DO	933	0	996	100	0
48	BP	1114	0	1187	291	0
48	DP	1114	0	1187	301	0
49	BQ	1122	0	1179	141	0
49	DQ	1122	0	1179	138	0
50	BR	960	0	1021	131	0
50	DR	960	0	1021	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BS	770	0	832	166	0
51	DS	770	0	832	159	0
52	BT	1141	0	1202	234	0
52	DT	1141	0	1202	211	0
53	BU	958	0	1015	141	0
53	DU	958	0	1015	152	0
54	BV	779	0	852	135	0
54	DV	779	0	852	124	0
55	BW	896	0	953	100	0
55	DW	896	0	953	97	0
56	BX	725	0	778	98	0
56	DX	725	0	778	107	0
57	BY	775	0	870	176	0
57	DY	775	0	870	164	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	206	0
59	AD	1	0	0	0	0
59	AN	1	0	0	2	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	1	0
60	AZ	28	0	12	12	0
60	CZ	28	0	12	13	0
61	AZ	57	0	59	11	0
61	CZ	57	0	59	14	0
All	All	307194	0	208701	19683	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 38.

The worst 5 of 19683 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:CZ:69:GLU:CG	25:CZ:69:GLU:CB	1.85	1.54
25:AZ:69:GLU:CB	25:AZ:69:GLU:CG	1.83	1.52
25:CZ:68:VAL:C	25:CZ:68:VAL:CA	1.82	1.46
25:AZ:68:VAL:C	25:AZ:68:VAL:CA	1.85	1.45
25:CZ:198:LYS:HE3	25:CZ:201:GLU:OE1	1.33	1.29

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%)	168 (72%)	35 (15%)	29 (12%)	1	3
2	CB	232/256 (91%)	154 (66%)	50 (22%)	28 (12%)	1	4
3	AC	204/239 (85%)	161 (79%)	29 (14%)	14 (7%)	2	13
3	CC	204/239 (85%)	147 (72%)	40 (20%)	17 (8%)	1	9
4	AD	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	1	5
4	CD	206/209 (99%)	128 (62%)	44 (21%)	34 (16%)	0	0
5	AE	148/162 (91%)	138 (93%)	8 (5%)	2 (1%)	16	58
5	CE	148/162 (91%)	122 (82%)	25 (17%)	1 (1%)	30	76
6	AF	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	2	16
6	CF	99/101 (98%)	75 (76%)	13 (13%)	11 (11%)	1	5
7	AG	153/156 (98%)	121 (79%)	20 (13%)	12 (8%)	1	11
7	CG	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	3	21
8	AH	136/138 (99%)	124 (91%)	8 (6%)	4 (3%)	7	38
8	CH	136/138 (99%)	117 (86%)	12 (9%)	7 (5%)	3	22
9	AI	125/128 (98%)	85 (68%)	26 (21%)	14 (11%)	1	5
9	CI	125/128 (98%)	79 (63%)	31 (25%)	15 (12%)	1	4
10	AJ	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	1	7
10	CJ	96/105 (91%)	71 (74%)	16 (17%)	9 (9%)	1	7
11	AK	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	25	71
11	CK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	3	22
12	AL	122/132 (92%)	97 (80%)	15 (12%)	10 (8%)	1	10
12	CL	122/132 (92%)	92 (75%)	22 (18%)	8 (7%)	2	15
13	AM	122/126 (97%)	75 (62%)	31 (25%)	16 (13%)	0	3
13	CM	122/126 (97%)	72 (59%)	35 (29%)	15 (12%)	1	3
14	AN	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	34 (59%)	15 (26%)	9 (16%)	0	1
15	AO	86/89 (97%)	68 (79%)	13 (15%)	5 (6%)	3	18
15	CO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	6	32
16	AP	81/88 (92%)	50 (62%)	21 (26%)	10 (12%)	1	3
16	CP	81/88 (92%)	49 (60%)	22 (27%)	10 (12%)	1	3
17	AQ	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	4	27
17	CQ	97/105 (92%)	80 (82%)	11 (11%)	6 (6%)	2	16
18	AR	68/88 (77%)	52 (76%)	12 (18%)	4 (6%)	2	17
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	2	11
19	AS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	2
19	CS	76/93 (82%)	45 (59%)	20 (26%)	11 (14%)	0	2
20	AT	97/106 (92%)	62 (64%)	24 (25%)	11 (11%)	1	4
20	CT	97/106 (92%)	64 (66%)	19 (20%)	14 (14%)	0	2
21	AU	22/27 (82%)	16 (73%)	3 (14%)	3 (14%)	0	2
21	CU	22/27 (82%)	14 (64%)	5 (23%)	3 (14%)	0	2
25	AZ	381/405 (94%)	272 (71%)	66 (17%)	43 (11%)	1	4
25	CZ	381/405 (94%)	270 (71%)	68 (18%)	43 (11%)	1	4
26	B0	82/85 (96%)	65 (79%)	10 (12%)	7 (8%)	1	9
26	D0	82/85 (96%)	62 (76%)	12 (15%)	8 (10%)	1	6
27	B1	91/98 (93%)	58 (64%)	18 (20%)	15 (16%)	0	0
27	D1	91/98 (93%)	64 (70%)	12 (13%)	15 (16%)	0	0
28	B2	69/72 (96%)	34 (49%)	20 (29%)	15 (22%)	0	0
28	D2	69/72 (96%)	44 (64%)	19 (28%)	6 (9%)	1	9
29	B3	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1	5
29	D3	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	2
30	B4	42/71 (59%)	25 (60%)	10 (24%)	7 (17%)	0	0
30	D4	42/71 (59%)	17 (40%)	17 (40%)	8 (19%)	0	0
31	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	0
31	D5	57/60 (95%)	40 (70%)	8 (14%)	9 (16%)	0	1
32	B6	48/54 (89%)	20 (42%)	10 (21%)	18 (38%)	0	0
32	D6	48/54 (89%)	20 (42%)	14 (29%)	14 (29%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	B7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
33	D7	46/49 (94%)	40 (87%)	6 (13%)	0	100	100
34	B8	61/65 (94%)	31 (51%)	18 (30%)	12 (20%)	0	0
34	D8	61/65 (94%)	27 (44%)	19 (31%)	15 (25%)	0	0
35	B9	35/37 (95%)	19 (54%)	11 (31%)	5 (14%)	0	2
35	D9	35/37 (95%)	17 (49%)	13 (37%)	5 (14%)	0	2
38	BC	226/229 (99%)	176 (78%)	33 (15%)	17 (8%)	2	11
38	DC	226/229 (99%)	170 (75%)	37 (16%)	19 (8%)	1	9
39	BD	273/276 (99%)	199 (73%)	46 (17%)	28 (10%)	1	6
39	DD	273/276 (99%)	197 (72%)	43 (16%)	33 (12%)	1	4
40	BE	202/206 (98%)	125 (62%)	45 (22%)	32 (16%)	0	1
40	DE	202/206 (98%)	129 (64%)	38 (19%)	35 (17%)	0	0
41	BF	205/210 (98%)	145 (71%)	34 (17%)	26 (13%)	0	3
41	DF	205/210 (98%)	129 (63%)	54 (26%)	22 (11%)	1	5
42	BG	179/182 (98%)	110 (62%)	33 (18%)	36 (20%)	0	0
42	DG	179/182 (98%)	99 (55%)	53 (30%)	27 (15%)	0	1
43	BH	157/180 (87%)	97 (62%)	31 (20%)	29 (18%)	0	0
43	DH	157/180 (87%)	99 (63%)	27 (17%)	31 (20%)	0	0
46	BN	136/140 (97%)	91 (67%)	27 (20%)	18 (13%)	0	2
46	DN	136/140 (97%)	89 (65%)	27 (20%)	20 (15%)	0	2
47	BO	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	2	14
47	DO	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	2	14
48	BP	144/150 (96%)	77 (54%)	36 (25%)	31 (22%)	0	0
48	DP	144/150 (96%)	78 (54%)	34 (24%)	32 (22%)	0	0
49	BQ	139/141 (99%)	112 (81%)	20 (14%)	7 (5%)	3	22
49	DQ	139/141 (99%)	112 (81%)	17 (12%)	10 (7%)	2	12
50	BR	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
50	DR	115/118 (98%)	73 (64%)	27 (24%)	15 (13%)	0	3
51	BS	96/112 (86%)	44 (46%)	29 (30%)	23 (24%)	0	0
51	DS	96/112 (86%)	44 (46%)	22 (23%)	30 (31%)	0	0
52	BT	135/146 (92%)	76 (56%)	28 (21%)	31 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	DT	135/146 (92%)	71 (53%)	35 (26%)	29 (22%)	0	0
53	BU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
53	DU	115/118 (98%)	74 (64%)	34 (30%)	7 (6%)	2	16
54	BV	99/101 (98%)	65 (66%)	21 (21%)	13 (13%)	0	3
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	3
55	BW	111/113 (98%)	78 (70%)	17 (15%)	16 (14%)	0	2
55	DW	111/113 (98%)	72 (65%)	23 (21%)	16 (14%)	0	2
56	BX	90/96 (94%)	63 (70%)	15 (17%)	12 (13%)	0	2
56	DX	90/96 (94%)	58 (64%)	22 (24%)	10 (11%)	1	5
57	BY	98/110 (89%)	43 (44%)	28 (29%)	27 (28%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	117 (65%)	38 (21%)	26 (14%)	0	2
58	DZ	181/206 (88%)	114 (63%)	42 (23%)	25 (14%)	0	2
All	All	12270/13100 (94%)	8441 (69%)	2326 (19%)	1503 (12%)	1	4

5 of 1503 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	127	ILE
2	AB	131	PRO

### 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%)	177 (88%)	25 (12%)	7	25
3	AC	160/188 (85%)	142 (89%)	18 (11%)	9	32
3	CC	160/188 (85%)	144 (90%)	16 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	180/181 (99%)	151 (84%)	29 (16%)	3	13
4	CD	180/181 (99%)	153 (85%)	27 (15%)	4	17
5	AE	115/123 (94%)	106 (92%)	9 (8%)	18	57
5	CE	115/123 (94%)	105 (91%)	10 (9%)	15	49
6	AF	90/90 (100%)	79 (88%)	11 (12%)	7	26
6	CF	90/90 (100%)	77 (86%)	13 (14%)	5	19
7	AG	126/127 (99%)	113 (90%)	13 (10%)	10	36
7	CG	126/127 (99%)	116 (92%)	10 (8%)	18	55
8	AH	119/119 (100%)	108 (91%)	11 (9%)	13	45
8	CH	119/119 (100%)	112 (94%)	7 (6%)	28	68
9	AI	98/99 (99%)	89 (91%)	9 (9%)	13	45
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	37
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	7	25
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	4	13
11	AK	90/99 (91%)	77 (86%)	13 (14%)	5	19
11	CK	90/99 (91%)	77 (86%)	13 (14%)	5	19
12	AL	104/109 (95%)	91 (88%)	13 (12%)	7	25
12	CL	104/109 (95%)	93 (89%)	11 (11%)	10	35
13	AM	99/101 (98%)	85 (86%)	14 (14%)	5	20
13	CM	99/101 (98%)	85 (86%)	14 (14%)	5	20
14	AN	49/50 (98%)	42 (86%)	7 (14%)	5	19
14	CN	49/50 (98%)	43 (88%)	6 (12%)	7	26
15	AO	79/80 (99%)	69 (87%)	10 (13%)	6	24
15	CO	79/80 (99%)	69 (87%)	10 (13%)	6	24
16	AP	72/74 (97%)	68 (94%)	4 (6%)	30	70
16	CP	72/74 (97%)	65 (90%)	7 (10%)	12	41
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	20	59
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	66	92
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%)	58 (84%)	11 (16%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	69/80 (86%)	54 (78%)	15 (22%)	1	6
20	AT	76/82 (93%)	66 (87%)	10 (13%)	6	23
20	CT	76/82 (93%)	67 (88%)	9 (12%)	8	29
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	35
21	CU	19/22 (86%)	16 (84%)	3 (16%)	4	14
25	AZ	322/338 (95%)	282 (88%)	40 (12%)	7	25
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	6	24
26	B0	66/67 (98%)	53 (80%)	13 (20%)	2	8
26	D0	66/67 (98%)	55 (83%)	11 (17%)	3	11
27	B1	78/83 (94%)	68 (87%)	10 (13%)	6	24
27	D1	78/83 (94%)	70 (90%)	8 (10%)	10	36
28	B2	66/67 (98%)	55 (83%)	11 (17%)	3	11
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%)	45 (88%)	6 (12%)	8	29
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	29 (74%)	10 (26%)	1	2
31	B5	51/52 (98%)	44 (86%)	7 (14%)	5	21
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%)	36 (74%)	13 (26%)	1	2
33	B7	41/42 (98%)	37 (90%)	4 (10%)	12	40
33	D7	41/42 (98%)	35 (85%)	6 (15%)	5	18
34	B8	53/55 (96%)	43 (81%)	10 (19%)	2	9
34	D8	53/55 (96%)	43 (81%)	10 (19%)	2	9
35	B9	34/34 (100%)	28 (82%)	6 (18%)	3	10
35	D9	34/34 (100%)	29 (85%)	5 (15%)	4	18
38	BC	180/181 (99%)	168 (93%)	12 (7%)	23	63
38	DC	180/181 (99%)	165 (92%)	15 (8%)	16	53
39	BD	217/218 (100%)	176 (81%)	41 (19%)	2	9
39	DD	217/218 (100%)	185 (85%)	32 (15%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BE	165/166 (99%)	137 (83%)	28 (17%)	3	11
40	DE	165/166 (99%)	137 (83%)	28 (17%)	3	11
41	BF	165/166 (99%)	147 (89%)	18 (11%)	9	34
41	DF	165/166 (99%)	152 (92%)	13 (8%)	18	55
42	BG	155/156 (99%)	130 (84%)	25 (16%)	3	13
42	DG	155/156 (99%)	127 (82%)	28 (18%)	2	10
43	BH	132/148 (89%)	122 (92%)	10 (8%)	19	58
43	DH	132/148 (89%)	123 (93%)	9 (7%)	22	62
46	BN	117/119 (98%)	102 (87%)	15 (13%)	6	24
46	DN	117/119 (98%)	99 (85%)	18 (15%)	4	15
47	BO	100/100 (100%)	92 (92%)	8 (8%)	17	55
47	DO	100/100 (100%)	90 (90%)	10 (10%)	11	38
48	BP	112/116 (97%)	89 (80%)	23 (20%)	2	8
48	DP	112/116 (97%)	92 (82%)	20 (18%)	2	10
49	BQ	111/111 (100%)	94 (85%)	17 (15%)	4	15
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	7	24
50	BR	100/101 (99%)	88 (88%)	12 (12%)	7	27
50	DR	100/101 (99%)	89 (89%)	11 (11%)	9	34
51	BS	77/88 (88%)	65 (84%)	12 (16%)	4	14
51	DS	77/88 (88%)	61 (79%)	16 (21%)	2	7
52	BT	120/127 (94%)	101 (84%)	19 (16%)	4	14
52	DT	120/127 (94%)	102 (85%)	18 (15%)	4	17
53	BU	92/94 (98%)	84 (91%)	8 (9%)	15	49
53	DU	92/94 (98%)	85 (92%)	7 (8%)	19	58
54	BV	82/82 (100%)	69 (84%)	13 (16%)	4	13
54	DV	82/82 (100%)	66 (80%)	16 (20%)	2	8
55	BW	91/92 (99%)	85 (93%)	6 (7%)	24	64
55	DW	91/92 (99%)	85 (93%)	6 (7%)	24	64
56	BX	74/78 (95%)	65 (88%)	9 (12%)	7	26
56	DX	74/78 (95%)	68 (92%)	6 (8%)	17	53
57	BY	84/91 (92%)	72 (86%)	12 (14%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	DY	84/91 (92%)	73 (87%)	11 (13%)	6	23
58	BZ	161/179 (90%)	134 (83%)	27 (17%)	3	11
58	DZ	161/179 (90%)	138 (86%)	23 (14%)	5	19
All	All	10350/10856 (95%)	9014 (87%)	1336 (13%)	6	24

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BT	99	LEU
4	CD	163	GLU
51	DS	12	PHE
54	BV	40	LEU
58	BZ	148	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
55	BW	57	ASN
7	CG	84	ASN
49	DQ	45	GLN
56	BX	87	GLN
3	CC	3	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	227 (15%)	50 (3%)
1	CA	1503/1522 (98%)	229 (15%)	41 (2%)
22	AV	75/76 (98%)	20 (26%)	0
22	AW	75/76 (98%)	20 (26%)	0
22	CV	75/76 (98%)	19 (25%)	2 (2%)
22	CW	75/76 (98%)	22 (29%)	2 (2%)
23	AX	17/27 (62%)	8 (47%)	1 (5%)
23	CX	17/27 (62%)	9 (52%)	1 (5%)
24	AY	74/77 (96%)	24 (32%)	1 (1%)
24	CY	74/77 (96%)	25 (33%)	1 (1%)
36	BA	2900/2915 (99%)	511 (17%)	48 (1%)
36	DA	2900/2915 (99%)	513 (17%)	43 (1%)
37	BB	118/122 (96%)	26 (22%)	4 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	DB	118/122 (96%)	26 (22%)	4 (3%)
All	All	9524/9630 (98%)	1679 (17%)	198 (2%)

5 of 1679 RNA backbone outliers are listed below:

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

5 of 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2145	C
1	CA	197	A
36	DA	1970	A
36	BA	2464	C
37	BB	16	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	1.09	1 (5%)	27,30,33	1.70	4 (14%)
24	H2U	AY	17	24	19,21,22	1.01	1 (5%)	27,30,33	1.80	6 (22%)
24	H2U	AY	20	24	19,21,22	1.05	1 (5%)	27,30,33	1.94	6 (22%)
24	OMC	AY	32	24	20,22,23	1.45	3 (15%)	25,31,34	0.94	2 (8%)
24	MIA	AY	37	24	29,31,32	1.30	3 (10%)	41,44,47	1.65	5 (12%)
24	7MG	AY	46	24	24,26,27	2.40	4 (16%)	34,39,42	2.33	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	1.08	2 (10%)	25,32,35	1.33	3 (12%)
24	PSU	AY	55	24	19,21,22	1.06	2 (10%)	23,30,33	1.03	2 (8%)
24	4SU	AY	8	24	19,21,22	2.12	6 (31%)	23,30,33	20.48	3 (13%)
24	H2U	CY	16	24	19,21,22	1.09	2 (10%)	27,30,33	1.72	4 (14%)
24	H2U	CY	17	24	19,21,22	1.06	1 (5%)	27,30,33	1.86	7 (25%)
24	H2U	CY	20	24	19,21,22	1.07	1 (5%)	27,30,33	1.97	7 (25%)
24	OMC	CY	32	24	20,22,23	1.57	3 (15%)	25,31,34	0.95	2 (8%)
24	MIA	CY	37	24	29,31,32	1.54	5 (17%)	41,44,47	1.41	5 (12%)
24	7MG	CY	46	24	24,26,27	2.48	3 (12%)	34,39,42	2.33	6 (17%)
24	5MU	CY	54	24	20,22,23	1.17	4 (20%)	25,32,35	1.28	2 (8%)
24	PSU	CY	55	24	19,21,22	1.16	2 (10%)	23,30,33	1.07	2 (8%)
24	4SU	CY	8	24	19,21,22	2.21	6 (31%)	23,30,33	20.31	3 (13%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-10.14	1.38	1.46
24	CY	46	7MG	C8-N9	-9.91	1.38	1.46
24	CY	46	7MG	P-OP1	5.17	1.52	1.46
24	CY	37	MIA	C2-S10	5.17	1.80	1.75
24	CY	8	4SU	C5-C4	4.92	1.44	1.38

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	8	4SU	C4-N3-C2	98.04	125.79	121.60
24	CY	8	4SU	C4-N3-C2	97.27	125.76	121.60
24	AY	46	7MG	C6-N1-C2	9.04	125.30	120.20
24	CY	46	7MG	C6-N1-C2	8.95	125.25	120.20
24	CY	46	7MG	N7-C8-N9	7.64	113.28	103.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	GDP	AZ	501	-	30,30,30	1.24	4 (13%)	45,47,47	2.92	9 (20%)
61	KIR	AZ	502	-	59,59,59	3.69	24 (40%)	82,84,84	1.77	18 (21%)
60	GDP	CZ	501	-	30,30,30	1.23	4 (13%)	45,47,47	2.93	9 (20%)
61	KIR	CZ	502	-	59,59,59	3.69	25 (42%)	82,84,84	1.72	19 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-14.05	1.22	1.44
61	CZ	502	KIR	O18-C17	-13.38	1.23	1.44
61	CZ	502	KIR	O30-C30	-11.57	1.18	1.42
61	AZ	502	KIR	O30-C30	-11.38	1.18	1.42
61	AZ	502	KIR	O34-C33	-10.33	1.30	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	C6-C5-N7	-15.38	132.07	134.14
60	CZ	501	GDP	C6-C5-N7	-15.38	132.07	134.14
60	AZ	501	GDP	PA-O3A-PB	-5.54	116.58	131.93
60	CZ	501	GDP	PA-O3A-PB	-5.34	117.13	131.93
60	CZ	501	GDP	C2-N3-C4	5.15	121.48	115.30

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	1504/1522 (98%)	-0.34	22 (1%)	70	16	22, 58, 151, 200	0
1	CA	1504/1522 (98%)	-0.30	18 (1%)	75	20	39, 79, 157, 200	0
2	AB	234/256 (91%)	-0.22	0	100	100	33, 66, 135, 154	0
2	CB	234/256 (91%)	-0.20	1 (0%)	90	45	50, 89, 142, 150	0
3	AC	206/239 (86%)	-0.39	0	100	100	25, 49, 78, 88	0
3	CC	206/239 (86%)	-0.28	0	100	100	53, 80, 106, 113	0
4	AD	208/209 (99%)	0.05	3 (1%)	72	17	59, 88, 122, 126	0
4	CD	208/209 (99%)	0.09	3 (1%)	72	17	79, 105, 125, 135	0
5	AE	150/162 (92%)	-0.41	0	100	100	30, 45, 71, 97	0
5	CE	150/162 (92%)	-0.31	0	100	100	48, 63, 85, 102	0
6	AF	101/101 (100%)	-0.32	0	100	100	48, 74, 94, 105	0
6	CF	101/101 (100%)	-0.12	0	100	100	79, 98, 111, 119	0
7	AG	155/156 (99%)	-0.26	2 (1%)	74	19	39, 65, 96, 117	0
7	CG	155/156 (99%)	-0.04	2 (1%)	74	19	71, 95, 115, 127	0
8	AH	138/138 (100%)	-0.37	0	100	100	32, 49, 69, 74	0
8	CH	138/138 (100%)	-0.31	0	100	100	46, 64, 80, 87	0
9	AI	127/128 (99%)	-0.15	0	100	100	32, 68, 111, 124	0
9	CI	127/128 (99%)	0.23	3 (2%)	56	9	66, 106, 132, 139	0
10	AJ	98/105 (93%)	-0.08	0	100	100	33, 70, 112, 125	0
10	CJ	98/105 (93%)	0.27	1 (1%)	79	23	66, 109, 144, 148	0
11	AK	119/129 (92%)	-0.28	1 (0%)	83	28	32, 50, 92, 118	0
11	CK	119/129 (92%)	-0.13	1 (0%)	83	28	52, 76, 100, 120	0
12	AL	124/132 (93%)	-0.21	1 (0%)	83	28	33, 61, 85, 124	0
12	CL	124/132 (93%)	-0.13	0	100	100	47, 72, 99, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	-0.09	3 (2%)	56	9	43, 72, 103, 131	0
13	CM	124/126 (98%)	-0.01	2 (1%)	68	15	76, 99, 122, 142	0
14	AN	60/61 (98%)	-0.23	1 (1%)	67	15	30, 53, 78, 84	0
14	CN	60/61 (98%)	-0.02	1 (1%)	67	15	65, 83, 102, 105	0
15	AO	88/89 (98%)	-0.31	0	100	100	36, 54, 82, 88	0
15	CO	88/89 (98%)	-0.21	0	100	100	44, 68, 90, 98	0
16	AP	83/88 (94%)	-0.02	0	100	100	61, 74, 98, 133	0
16	CP	83/88 (94%)	0.10	1 (1%)	75	20	74, 90, 110, 132	0
17	AQ	99/105 (94%)	-0.26	0	100	100	40, 60, 79, 89	0
17	CQ	99/105 (94%)	-0.16	0	100	100	53, 71, 91, 102	0
18	AR	70/88 (79%)	-0.28	0	100	100	39, 60, 90, 99	0
18	CR	70/88 (79%)	-0.16	0	100	100	56, 81, 108, 118	0
19	AS	78/93 (83%)	-0.04	1 (1%)	74	19	52, 73, 117, 127	0
19	CS	78/93 (83%)	0.08	1 (1%)	74	19	81, 97, 126, 132	0
20	AT	99/106 (93%)	0.08	1 (1%)	79	23	55, 80, 126, 130	0
20	CT	99/106 (93%)	0.04	0	100	100	74, 90, 120, 122	0
21	AU	24/27 (88%)	-0.03	1 (4%)	35	5	41, 55, 79, 99	0
21	CU	24/27 (88%)	0.45	1 (4%)	35	5	74, 92, 105, 113	0
22	AV	76/76 (100%)	-0.50	0	100	100	35, 72, 107, 124	0
22	AW	76/76 (100%)	0.24	6 (7%)	13	2	64, 140, 185, 199	0
22	CV	76/76 (100%)	-0.32	0	100	100	51, 86, 120, 137	0
22	CW	76/76 (100%)	0.30	6 (7%)	13	2	94, 170, 191, 200	0
23	AX	17/27 (62%)	0.35	2 (11%)	5	1	31, 91, 142, 143	0
23	CX	17/27 (62%)	1.96	7 (41%)	1	0	69, 122, 155, 157	0
24	AY	76/77 (98%)	0.26	3 (3%)	37	5	57, 142, 190, 200	0
24	CY	76/77 (98%)	0.34	2 (2%)	53	8	73, 145, 192, 200	0
25	AZ	385/405 (95%)	0.34	6 (1%)	68	15	87, 124, 151, 169	0
25	CZ	385/405 (95%)	0.77	30 (7%)	13	2	111, 133, 156, 170	0
26	B0	84/85 (98%)	0.05	3 (3%)	41	6	58, 73, 107, 122	0
26	D0	84/85 (98%)	0.26	3 (3%)	41	6	69, 86, 113, 123	0
27	B1	93/98 (94%)	0.01	1 (1%)	77	22	45, 69, 129, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	0.06	0 100 100	59, 86, 133, 139	0
28	B2	71/72 (98%)	0.77	14 (19%) 2 0	130, 143, 155, 158	0
28	D2	71/72 (98%)	0.24	2 (2%) 50 8	100, 122, 136, 143	0
29	B3	59/60 (98%)	0.03	1 (1%) 67 15	65, 81, 106, 122	0
29	D3	59/60 (98%)	0.17	1 (1%) 67 15	60, 93, 106, 126	0
30	B4	44/71 (61%)	0.34	3 (6%) 17 3	111, 140, 167, 173	0
30	D4	44/71 (61%)	0.67	7 (15%) 3 1	136, 163, 184, 186	0
31	B5	59/60 (98%)	0.04	3 (5%) 27 4	62, 87, 148, 163	0
31	D5	59/60 (98%)	0.11	4 (6%) 17 3	63, 92, 145, 154	0
32	B6	50/54 (92%)	0.26	3 (6%) 21 3	57, 84, 103, 110	0
32	D6	50/54 (92%)	0.52	6 (12%) 5 1	73, 97, 116, 122	0
33	B7	48/49 (97%)	0.09	1 (2%) 60 11	51, 64, 101, 121	0
33	D7	48/49 (97%)	0.11	1 (2%) 60 11	64, 73, 104, 125	0
34	B8	63/65 (96%)	0.11	1 (1%) 68 15	56, 73, 91, 115	0
34	D8	63/65 (96%)	0.21	1 (1%) 68 15	72, 85, 101, 120	0
35	B9	37/37 (100%)	0.30	1 (2%) 52 8	73, 85, 103, 104	0
35	D9	37/37 (100%)	0.64	3 (8%) 12 2	67, 96, 107, 120	0
36	BA	2901/2915 (99%)	-0.21	69 (2%) 56 9	26, 77, 181, 200	0
36	DA	2901/2915 (99%)	-0.17	69 (2%) 56 9	37, 87, 180, 200	0
37	BB	119/122 (97%)	-0.53	0 100 100	59, 85, 112, 132	0
37	DB	119/122 (97%)	-0.48	0 100 100	69, 101, 126, 132	0
38	BC	228/229 (99%)	-0.03	5 (2%) 59 11	50, 79, 160, 173	0
38	DC	228/229 (99%)	0.24	8 (3%) 42 6	68, 103, 170, 180	0
39	BD	275/276 (99%)	-0.29	1 (0%) 90 45	30, 49, 83, 105	0
39	DD	275/276 (99%)	-0.21	1 (0%) 90 45	42, 61, 91, 111	0
40	BE	204/206 (99%)	-0.02	4 (1%) 62 12	50, 79, 128, 140	0
40	DE	204/206 (99%)	-0.00	2 (0%) 79 23	47, 84, 133, 138	0
41	BF	207/210 (98%)	0.19	7 (3%) 43 6	53, 112, 162, 170	0
41	DF	207/210 (98%)	0.26	5 (2%) 56 9	62, 118, 161, 170	0
42	BG	181/182 (99%)	-0.02	5 (2%) 50 8	63, 86, 117, 130	0
42	DG	181/182 (99%)	-0.00	3 (1%) 67 15	89, 108, 136, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	0.44	6 (3%)	38	5	93, 134, 152, 156	0
43	DH	159/180 (88%)	0.33	4 (2%)	54	9	87, 129, 146, 154	0
44	BJ	0/173	-	-	-	-	-	-
44	DJ	0/173	-	-	-	-	-	-
45	BK	0/147	-	-	-	-	-	-
45	DK	0/147	-	-	-	-	-	-
46	BN	138/140 (98%)	-0.08	0	100	100	63, 89, 125, 134	0
46	DN	138/140 (98%)	-0.14	0	100	100	69, 90, 125, 133	0
47	BO	122/122 (100%)	-0.28	0	100	100	46, 63, 77, 85	0
47	DO	122/122 (100%)	-0.24	0	100	100	47, 67, 83, 89	0
48	BP	146/150 (97%)	0.35	4 (2%)	52	8	55, 103, 133, 150	0
48	DP	146/150 (97%)	0.43	7 (4%)	29	4	64, 115, 137, 153	0
49	BQ	141/141 (100%)	-0.17	1 (0%)	84	32	46, 64, 86, 128	0
49	DQ	141/141 (100%)	-0.17	2 (1%)	72	17	51, 66, 90, 126	0
50	BR	117/118 (99%)	0.00	1 (0%)	81	25	60, 85, 107, 126	0
50	DR	117/118 (99%)	0.04	1 (0%)	81	25	57, 90, 105, 123	0
51	BS	98/112 (87%)	0.10	3 (3%)	47	7	63, 90, 116, 126	0
51	DS	98/112 (87%)	0.28	2 (2%)	62	12	77, 102, 126, 128	0
52	BT	137/146 (93%)	-0.04	2 (1%)	70	16	58, 84, 142, 167	0
52	DT	137/146 (93%)	-0.04	2 (1%)	70	16	63, 90, 147, 169	0
53	BU	117/118 (99%)	-0.05	1 (0%)	81	25	64, 79, 111, 128	0
53	DU	117/118 (99%)	-0.03	0	100	100	63, 86, 110, 124	0
54	BV	101/101 (100%)	0.11	0	100	100	62, 116, 129, 136	0
54	DV	101/101 (100%)	0.21	1 (0%)	79	23	71, 115, 134, 136	0
55	BW	113/113 (100%)	0.04	1 (0%)	81	25	65, 90, 116, 141	0
55	DW	113/113 (100%)	0.13	1 (0%)	81	25	73, 93, 123, 145	0
56	BX	92/96 (95%)	0.11	0	100	100	75, 95, 110, 118	0
56	DX	92/96 (95%)	0.08	0	100	100	82, 100, 116, 120	0
57	BY	100/110 (90%)	0.70	11 (11%)	6	1	108, 134, 162, 168	0
57	DY	100/110 (90%)	0.66	10 (10%)	8	2	107, 136, 160, 169	0
58	BZ	183/206 (88%)	-0.10	3 (1%)	68	15	56, 83, 120, 132	0
58	DZ	183/206 (88%)	-0.06	3 (1%)	68	15	62, 88, 120, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	22012/23370 (94%)	-0.08	437 (1%) 62 12	22, 84, 152, 200	0

The worst 5 of 437 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BA	654(K)	C	9.1
36	BA	654(T)	C	8.6
36	DA	1077	A	8.0
36	BA	1077	A	8.0
41	BF	24	LEU	7.5

## 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	MIA	AY	37	29/30	0.25	-	64,78,89,98	0
24	H2U	AY	16	20/21	0.55	-	196,198,199,200	0
24	OMC	AY	32	21/22	0.19	-	101,105,115,115	0
24	PSU	AY	55	20/21	0.24	-	156,161,162,162	0
24	H2U	AY	20	20/21	0.42	-	186,189,193,193	0
24	5MU	CY	54	21/22	0.26	-	139,149,151,155	0
24	MIA	CY	37	29/30	0.21	-	80,87,95,99	0
24	PSU	CY	55	20/21	0.29	-	158,161,162,162	0
24	H2U	CY	17	20/21	0.57	-	199,199,200,200	0
24	OMC	CY	32	21/22	0.26	-	108,114,121,121	0
24	7MG	AY	46	24/25	0.29	-	145,150,151,151	0
24	7MG	CY	46	24/25	0.29	-	148,153,154,154	0
24	5MU	AY	54	21/22	0.20	-	139,150,152,154	0
24	4SU	AY	8	20/21	0.25	-	142,144,146,146	0
24	H2U	CY	20	20/21	0.37	-	188,191,192,192	0
24	H2U	CY	16	20/21	0.46	-	194,198,199,199	0
24	H2U	AY	17	20/21	0.39	-	199,199,200,200	0
24	4SU	CY	8	20/21	0.31	-	143,145,147,148	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	0.30	-	129,133,138,138	0
59	ZN	CD	301	1/1	0.28	-	79,79,79,79	0
59	ZN	D4	101	1/1	0.13	-	196,196,196,196	0
59	ZN	D9	101	1/1	0.18	-	141,141,141,141	0
59	ZN	B9	101	1/1	0.13	-	113,113,113,113	0
61	KIR	CZ	502	57/57	0.65	-	122,131,140,141	0
59	ZN	AD	301	1/1	0.27	-	74,74,74,74	0
61	KIR	AZ	502	57/57	0.37	-	115,122,129,130	0
60	GDP	CZ	501	28/28	0.27	-	137,140,141,141	0
59	ZN	B4	101	1/1	0.13	-	112,112,112,112	0
59	ZN	CN	101	1/1	0.17	-	77,77,77,77	0
59	ZN	AN	101	1/1	0.18	-	48,48,48,48	0

### 6.5 Other polymers

There are no such residues in this entry.