



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:57 PM BST

PDB ID : 4V8U  
Title : Crystal Structure of 70S Ribosome with Both Cognate tRNAs in the E and P Sites Representing an Authentic Elongation Complex.  
Authors : GAO, Y.G.; FENG, S.; CHEN, Y.  
Deposited on : 2012-08-28  
Resolution : 3.70 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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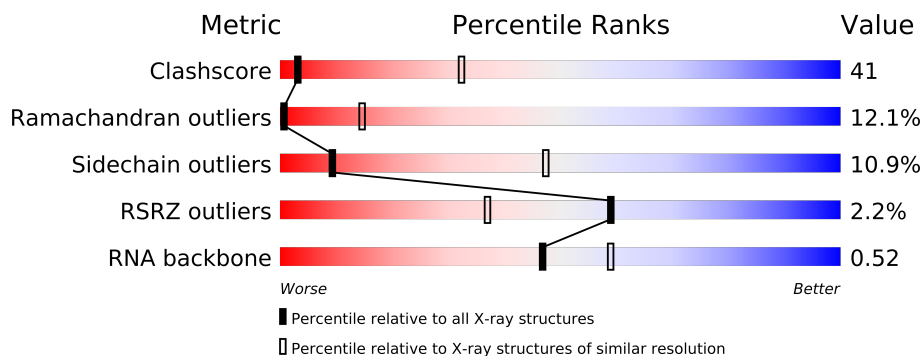
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.70 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))
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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	
7	AG	156	
7	CG	156	

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Mol	Chain	Length	Quality of chain
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	CV	76	
23	AW	77	
23	CW	77	
24	AX	25	
24	CX	25	
25	AY	691	
25	CY	691	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	

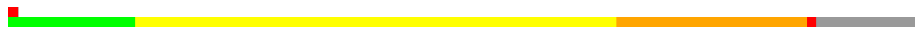
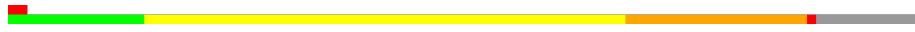


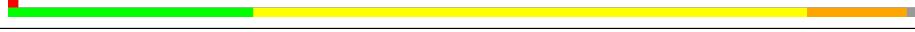
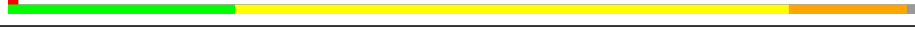
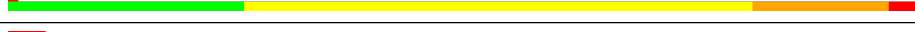


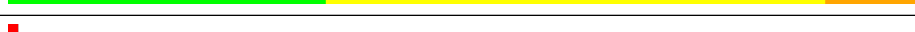

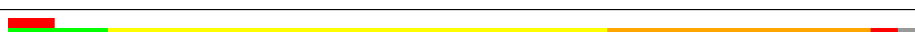
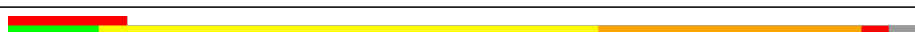
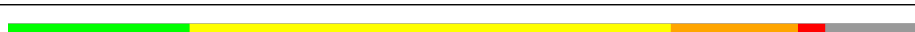
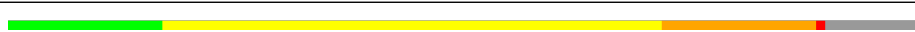

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Mol	Chain	Length	Quality of chain
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	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	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	
49	BR	118	
49	DR	118	

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Mol	Chain	Length	Quality of chain
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	
52	DU	118	
53	BV	101	
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	DZ	206	

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307606 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 RIBOSOMAL RNA.

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	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	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	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	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	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

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

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

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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	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	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	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			

- Molecule 23 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 24 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			257	116	49	80	12			
24	CX	12	Total	C	N	O	P	0	0	0
			257	116	49	80	12			

- Molecule 25 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			
25	CY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	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	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
30	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
31	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
33	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	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
			62474	27806	11681	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	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	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
40	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			
43	DH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				
44	DJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
50	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
51	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
55	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			
56	DY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
57	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B4	1	Total	Zn	0	0
			1	1		

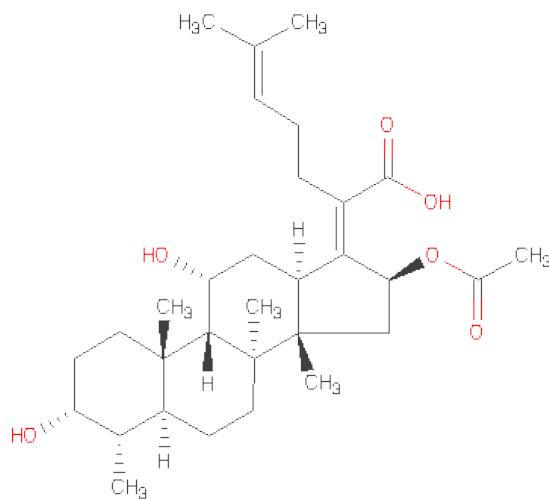
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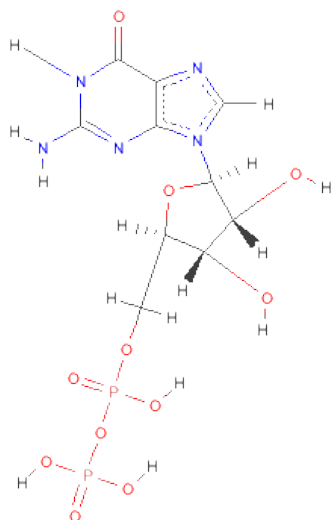
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CN	1	Total	Zn	0	0
			1	1		
58	AN	1	Total	Zn	0	0
			1	1		
58	B9	1	Total	Zn	0	0
			1	1		
58	D9	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		
58	CD	1	Total	Zn	0	0
			1	1		
58	AD	1	Total	Zn	0	0
			1	1		

- Molecule 59 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AY	1	Total	C	O	0	0
			37	31	6		
59	CY	1	Total	C	O	0	0
			37	31	6		

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



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

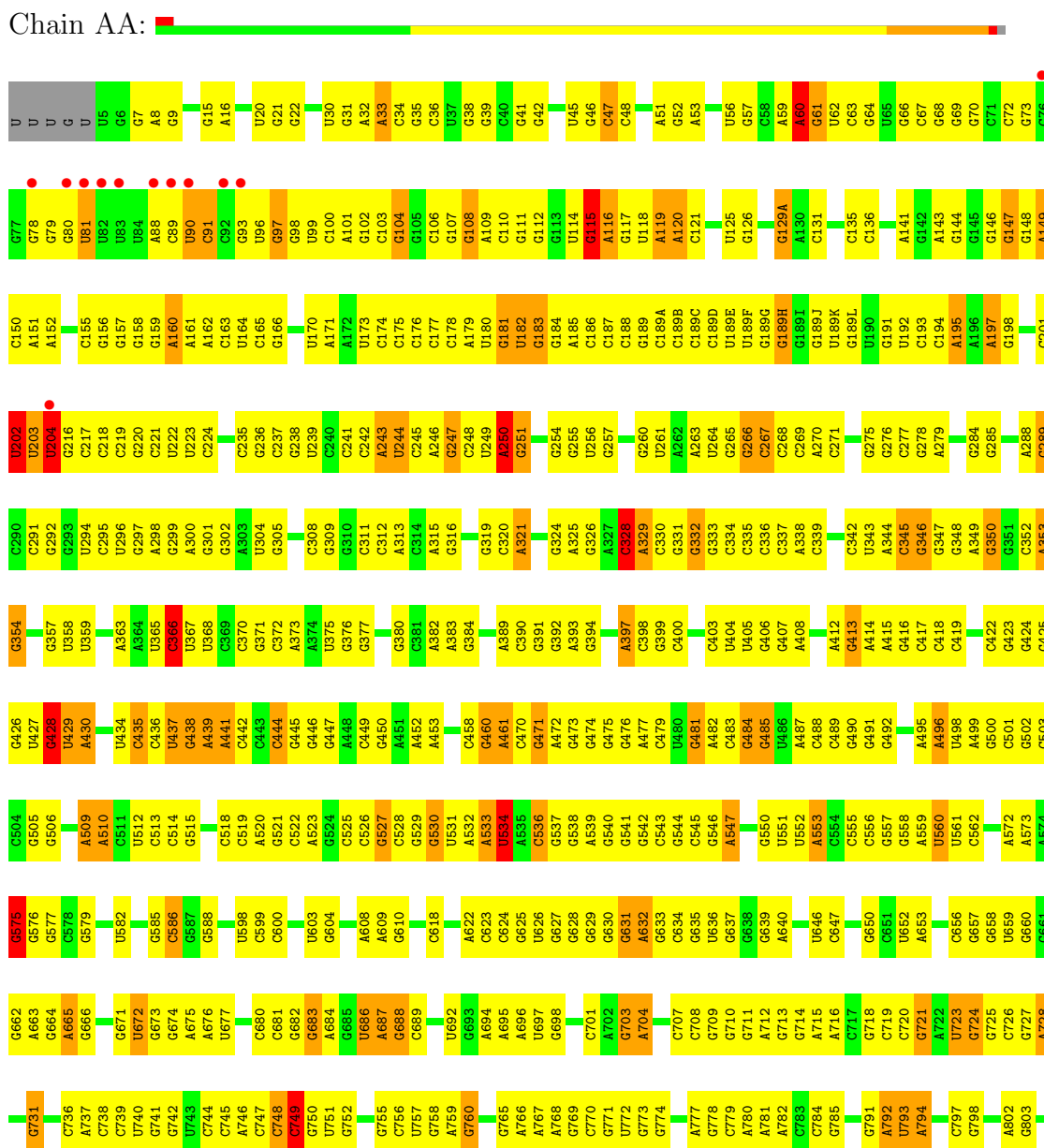
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

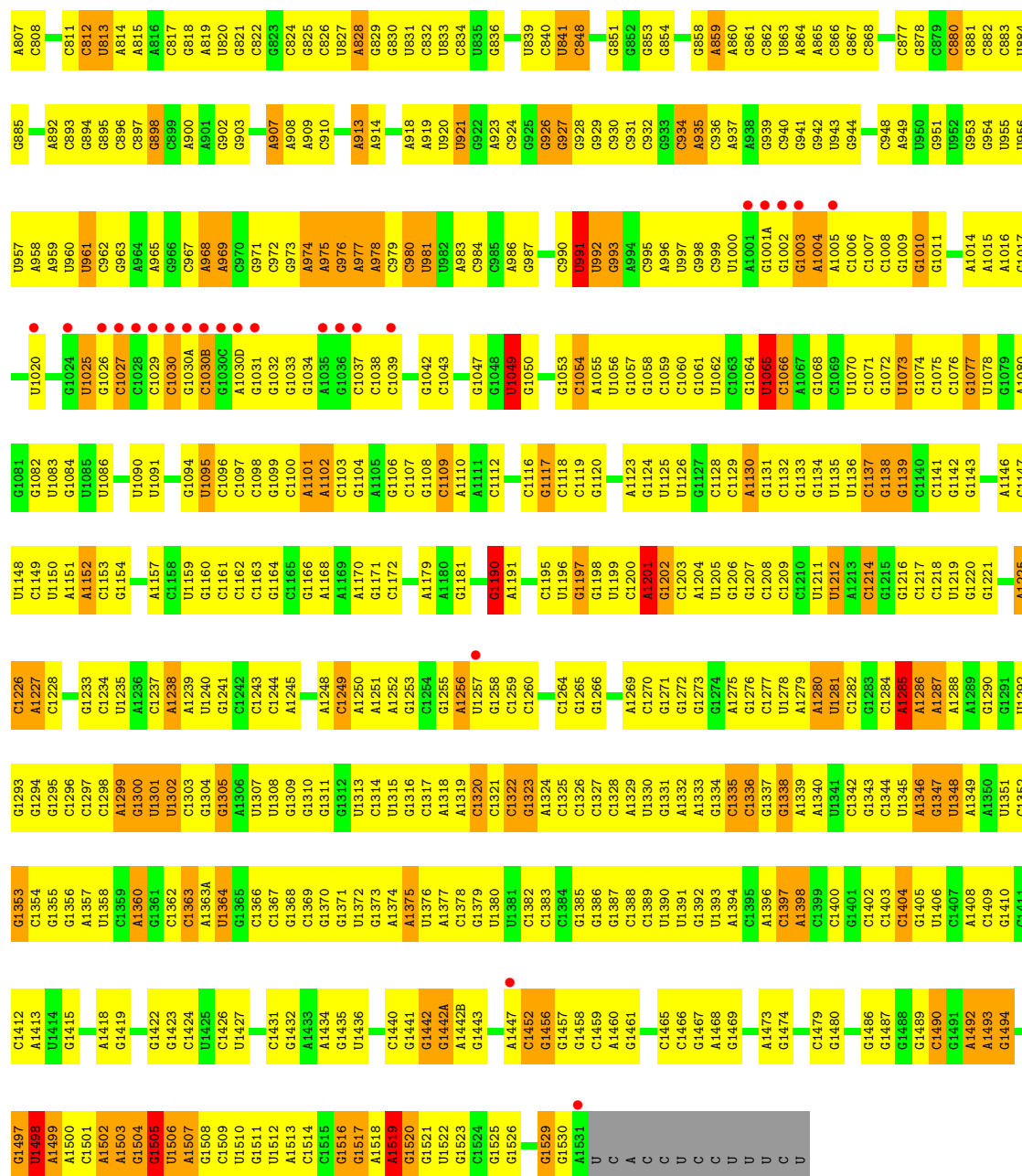
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	1	Total	Mg	0	0
			1	1		
61	CY	1	Total	Mg	0	0
			1	1		

### 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.

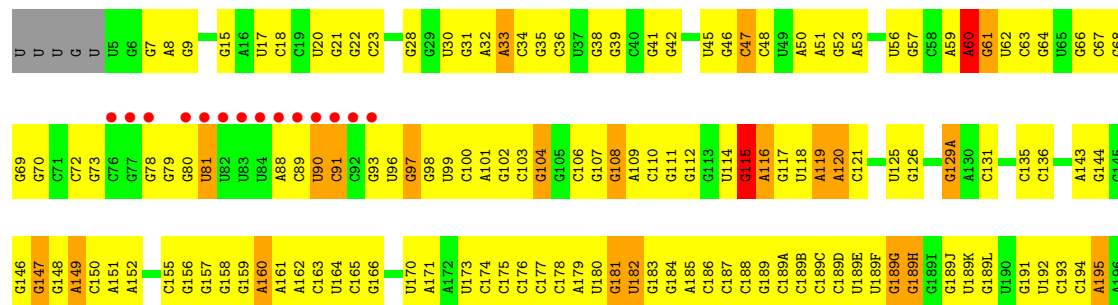
#### • Molecule 1: 16S RIBOSOMAL RNA



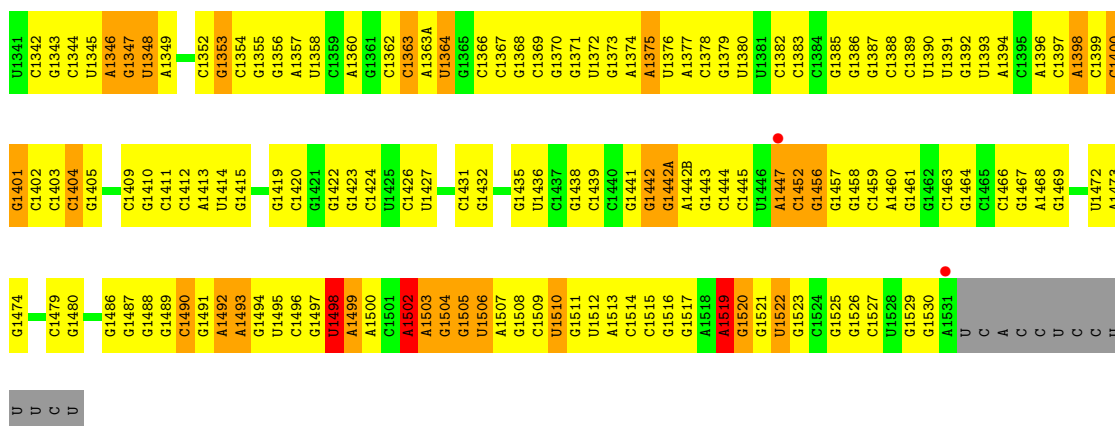


# Molecule 1: 16S RIBOSOMAL RNA

Chain CA:

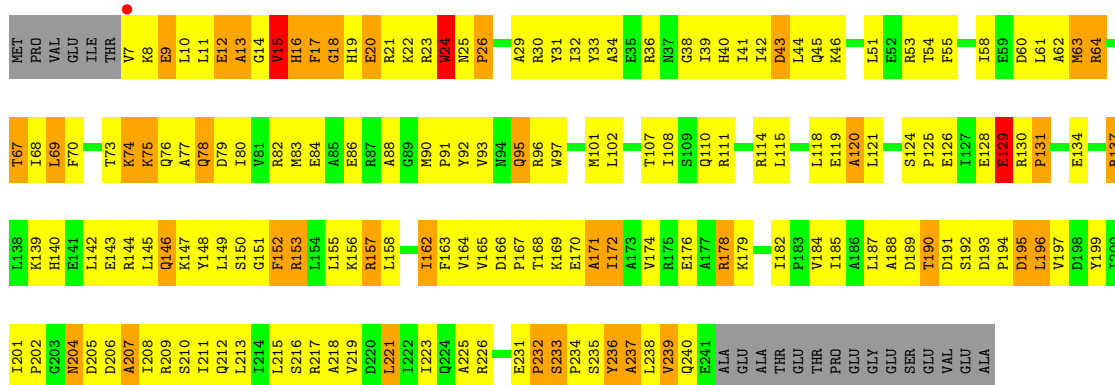


U1281	U1282	G1283	G1284	G1285	G1286	U1287	U1288	U1289	G1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340																																																																																																																																																																																																																		
U1212	A1213	C1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	U1235	U1236	U1237	U1238	A1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281																																																																																																																																																																																																								
U1135	U1136	U1137	G1138	G1139	G1140	G1141	G1142	G1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	A1151	A1152	C1153	G1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211																																																																																																																																																																																																	
C1089	U1070	C1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	G1079	U1080	G1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134																																																																																																																																																																																																												
A1004	A1005	C1006	C1007	C1008	U1009	G1010	G1011	U1012	A1013	A1014	A1015	A1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	C1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134																																																																																																																																											
G942	U943	G944	G945	G946	G947	G948	A949	U950	U951	U952	G953	G954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134																																																																													
A865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	U884	C885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134
G791	A792	U793	A794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1																																							



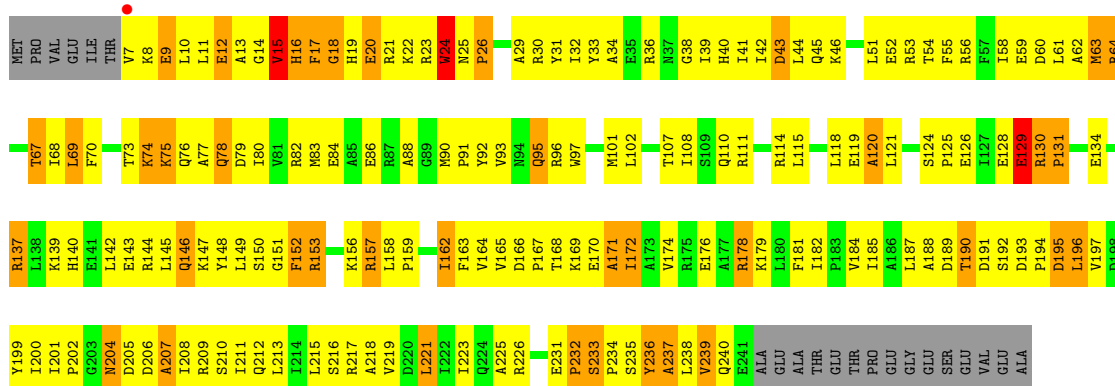
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



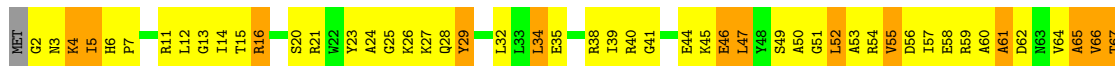
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

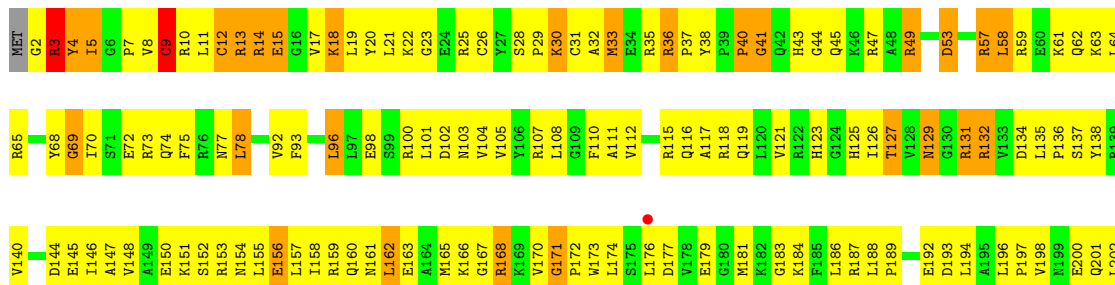
Chain AC:



Chain CC:

Chain AD:

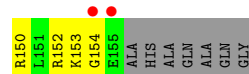
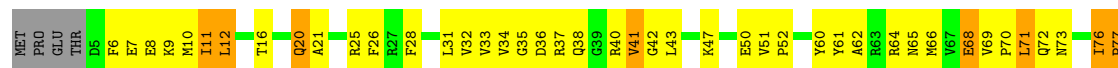
Chain CD:





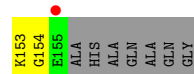
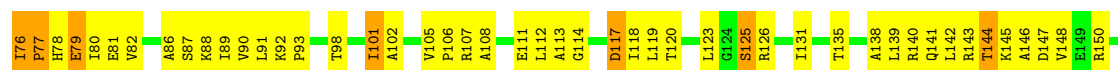
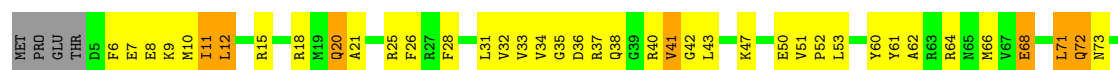
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



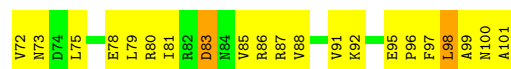
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



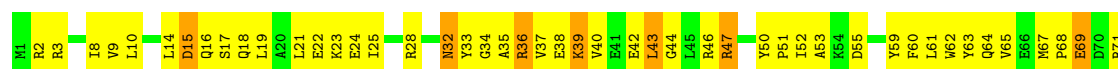
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

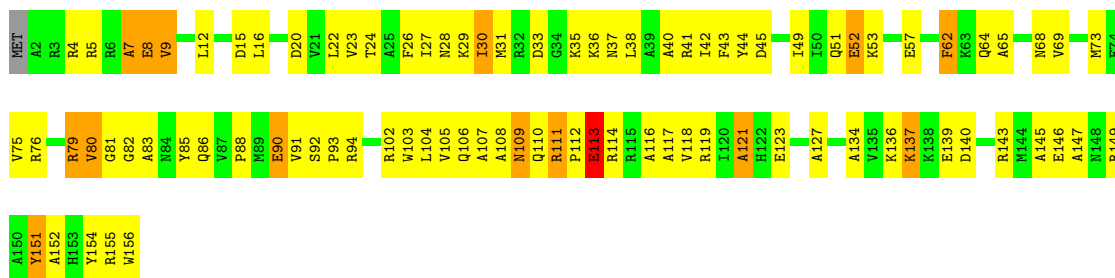
Chain CF:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:





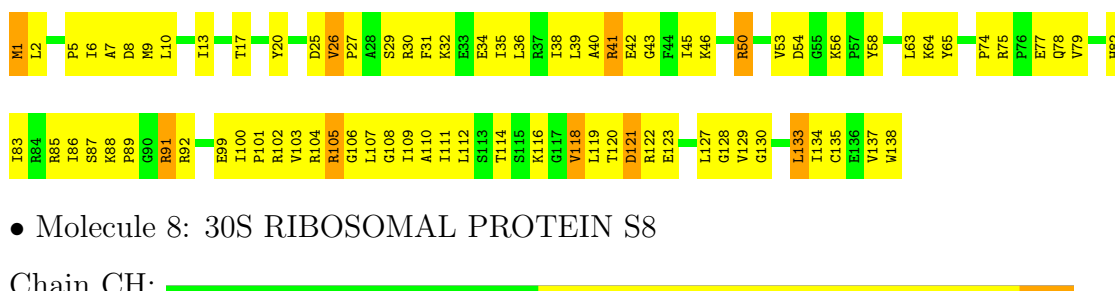
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



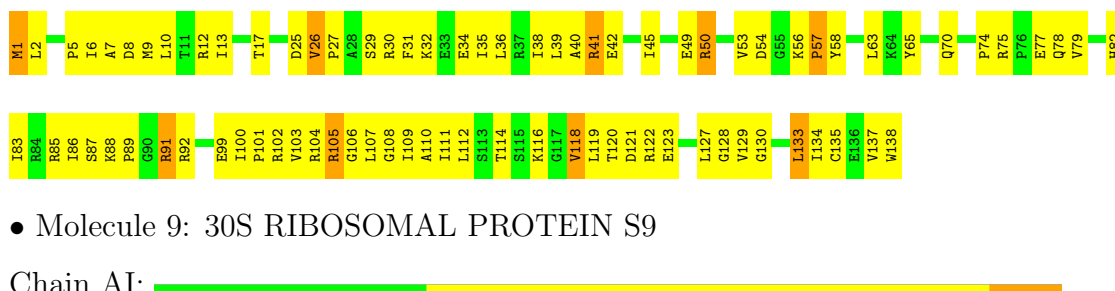
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



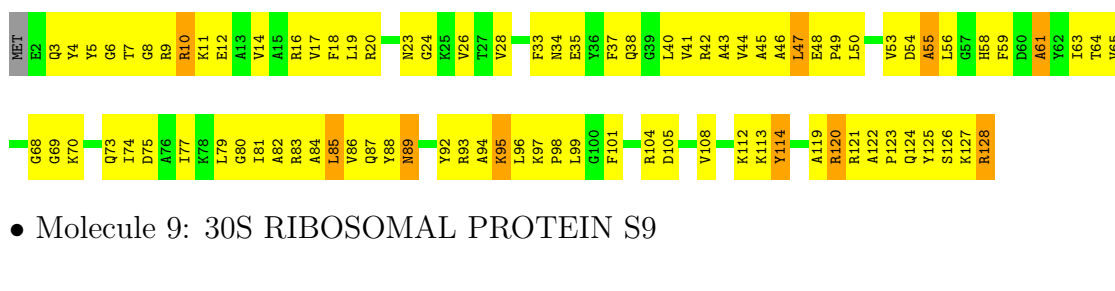
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



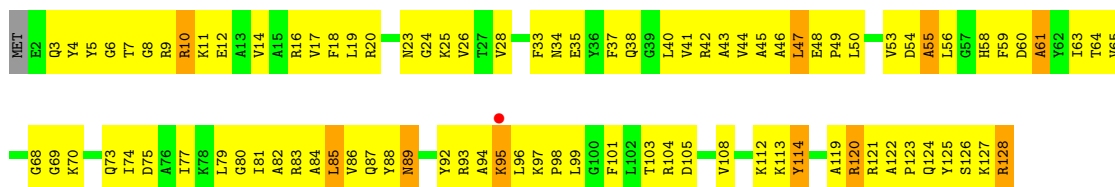
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



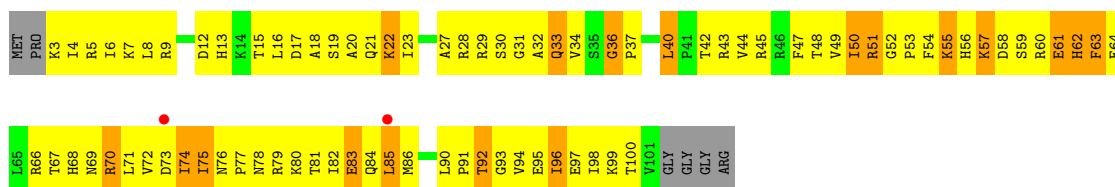
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



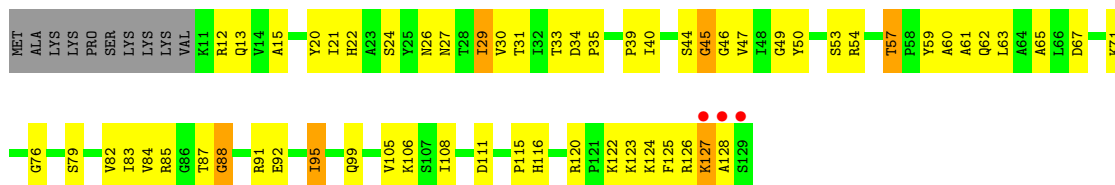
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



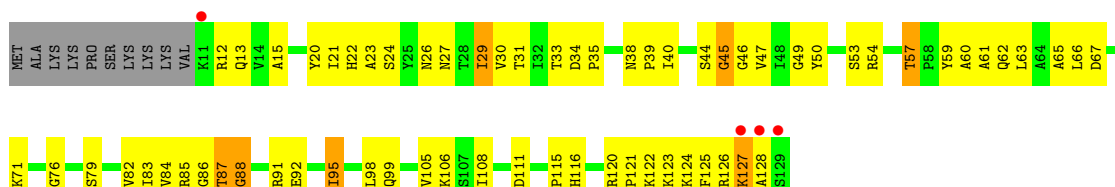
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

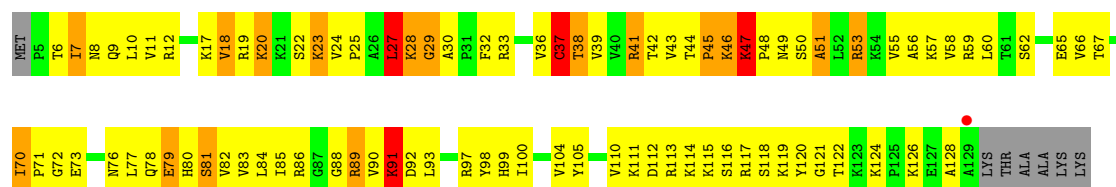
Chain CK:



- Molecule 12: 30S RIBOSOMAL PROTEIN S12

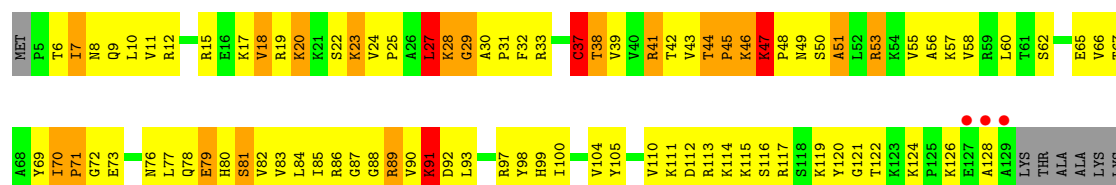
Chain AL:





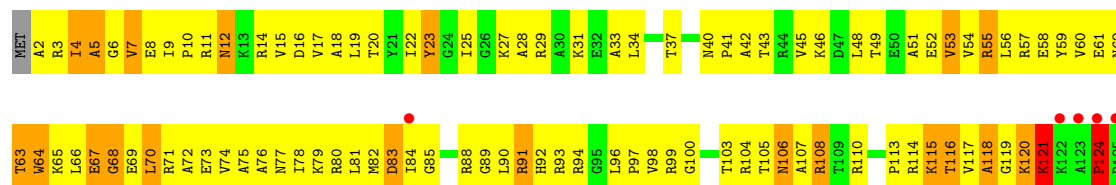
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



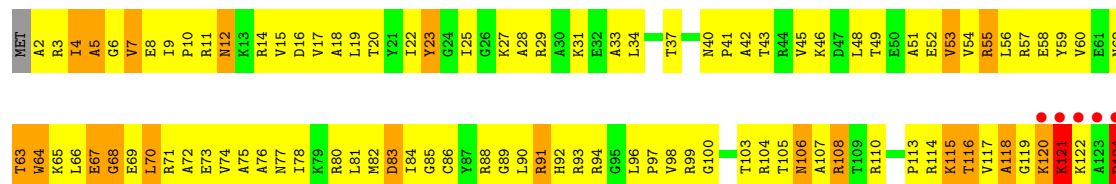
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



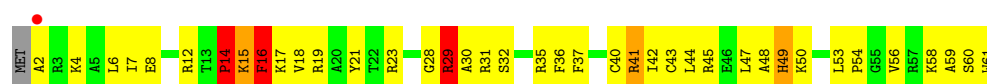
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



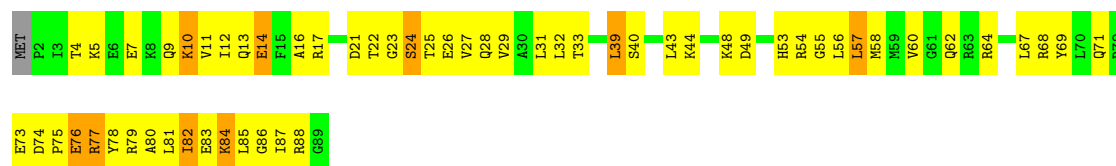
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



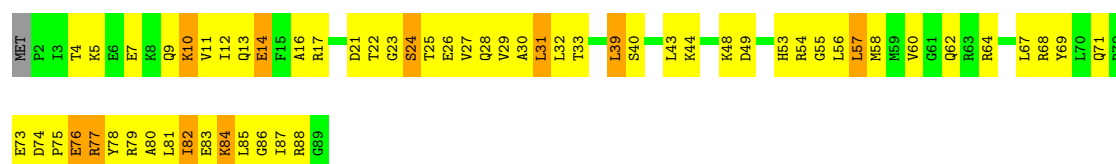
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



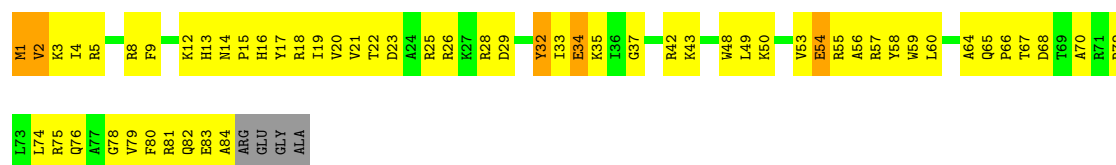
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



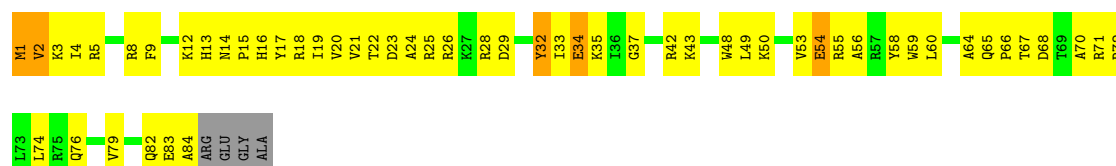
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



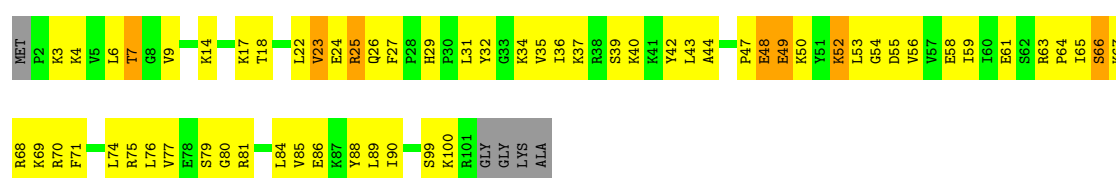
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



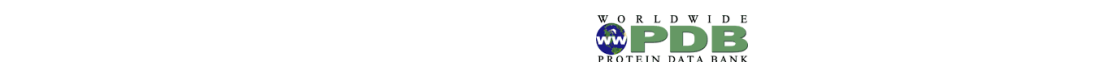
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

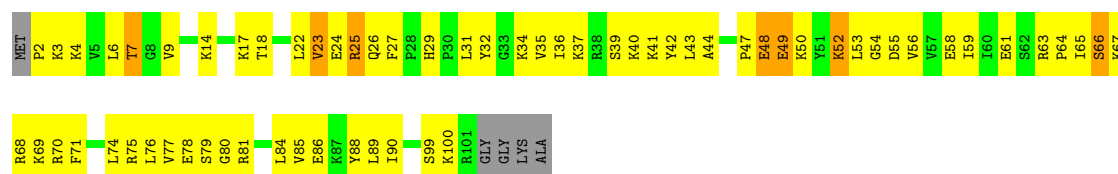
Chain AQ:



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:





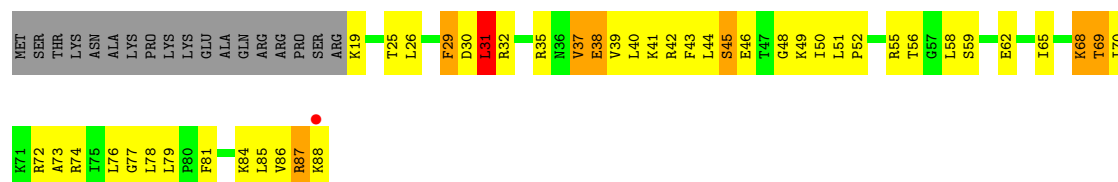
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



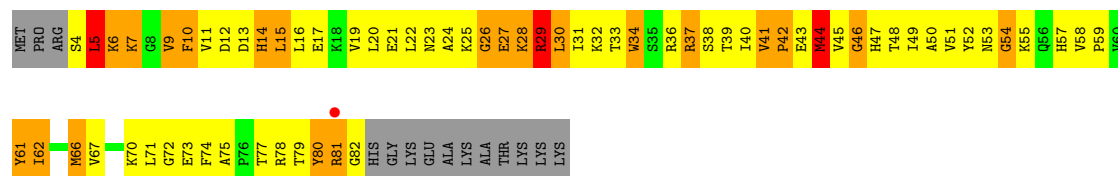
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



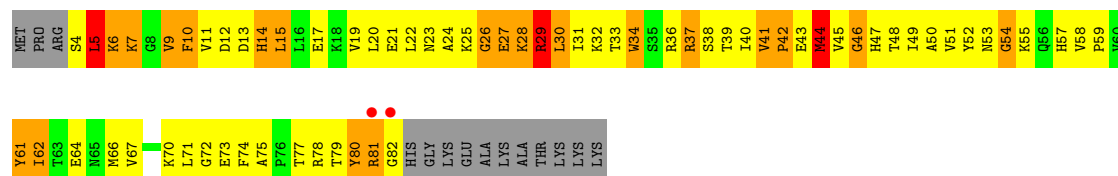
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

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:



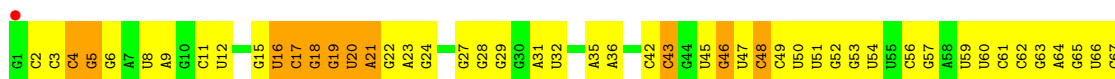
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



• Molecule 22: MRNA

Chain AV:



• Molecule 22: MRNA

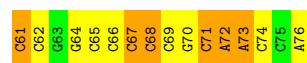
Chain CV:



• Molecule 23: RNA

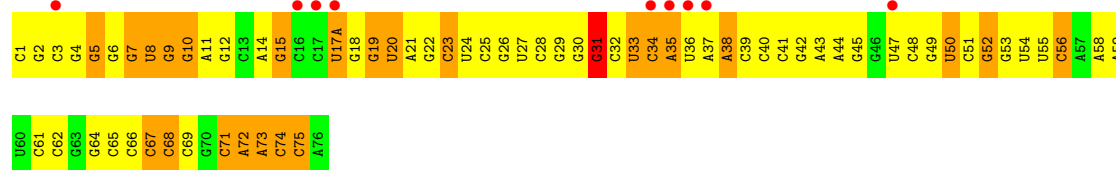
Chain AW:





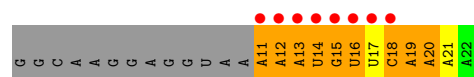
• Molecule 23: RNA

Chain CW:



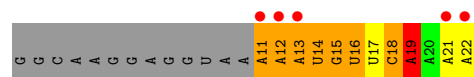
• Molecule 24: RNA

Chain AX:



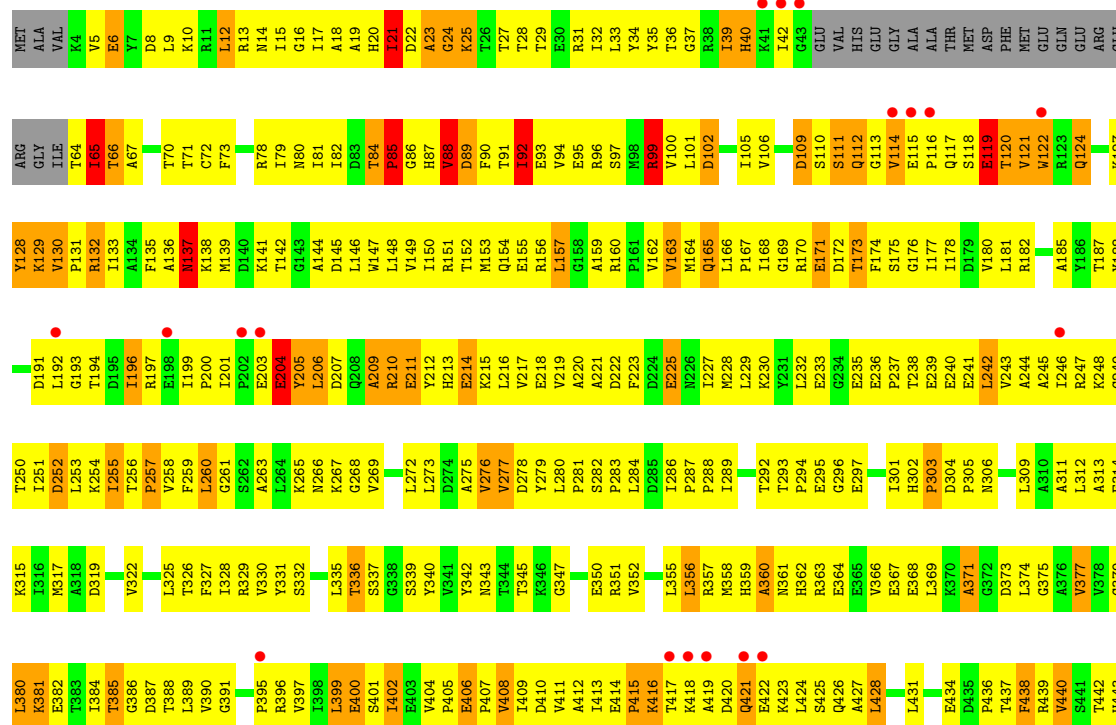
• Molecule 24: RNA

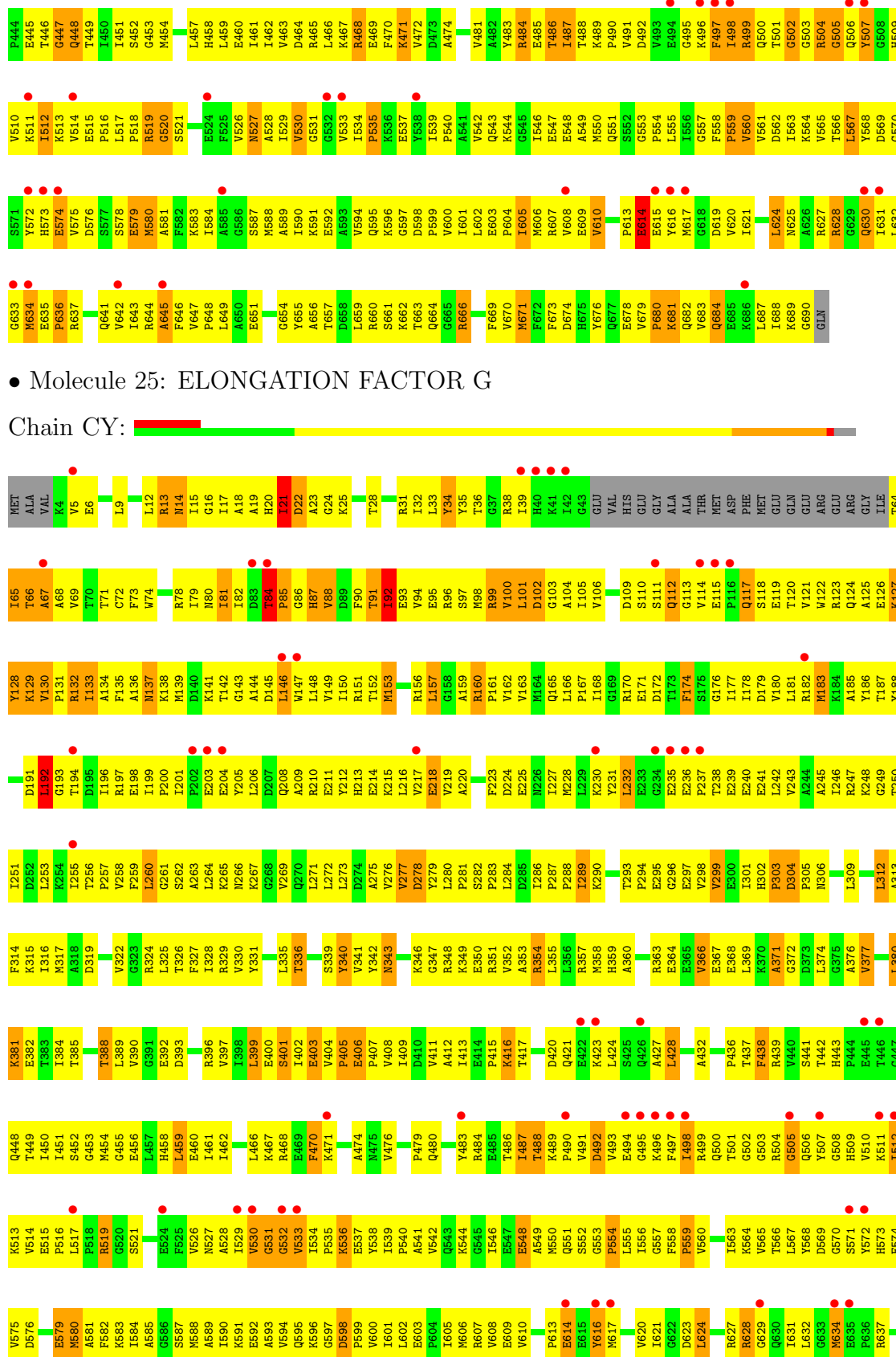
Chain CX:



• Molecule 25: ELONGATION FACTOR G

Chain AY:



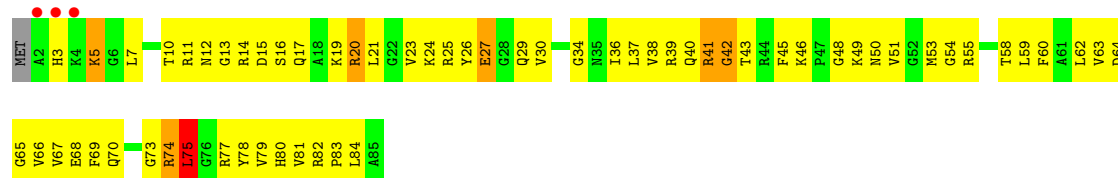






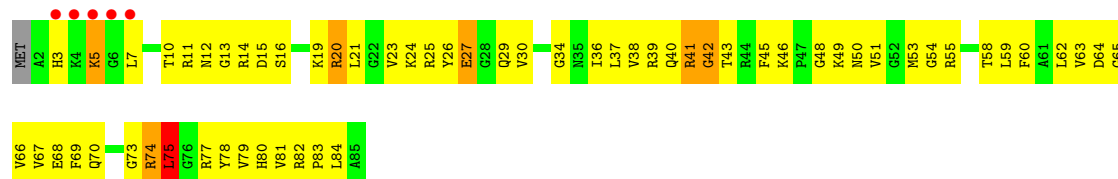
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



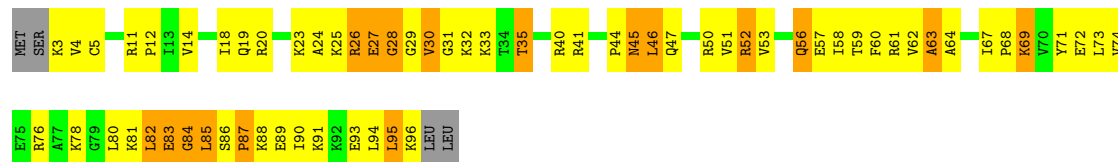
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



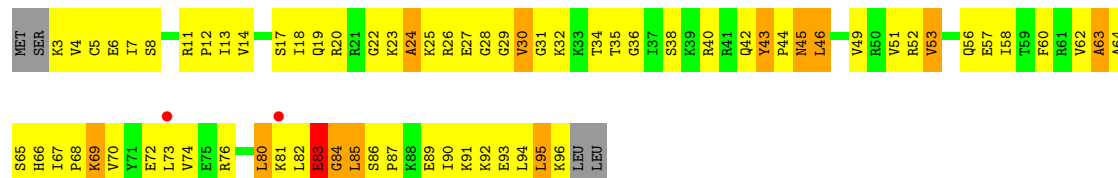
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



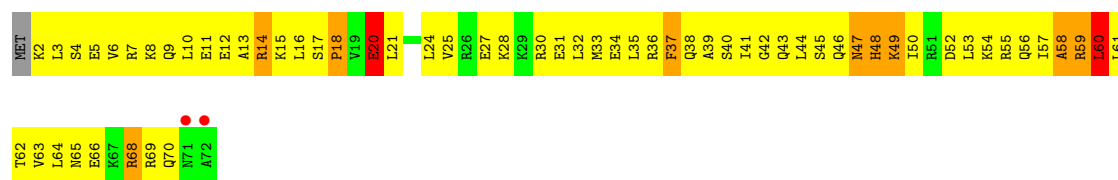
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



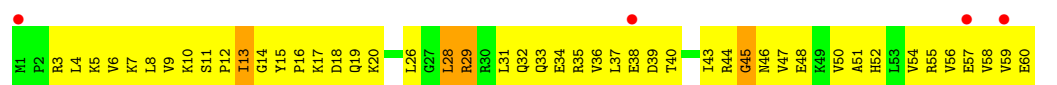
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



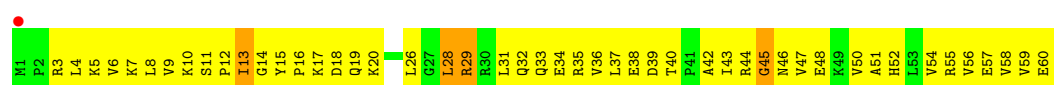
- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



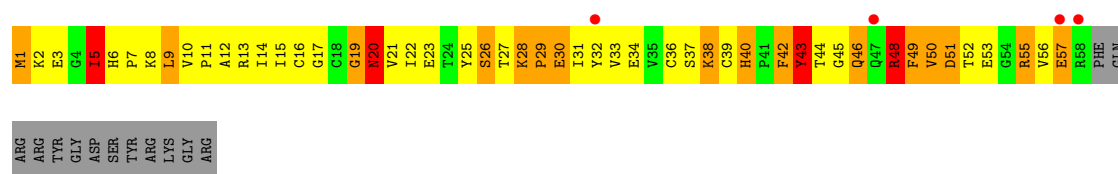
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



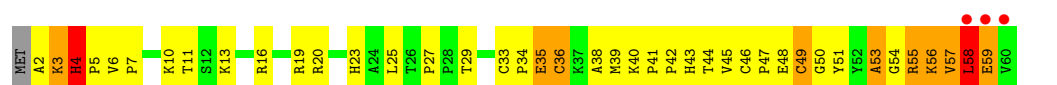
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

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:



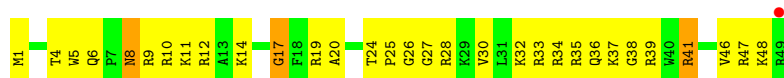
- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:



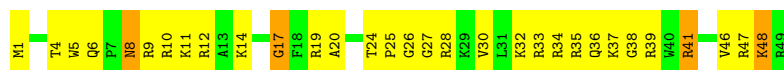
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



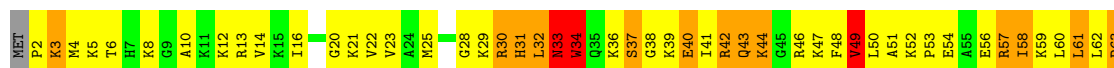
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

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:



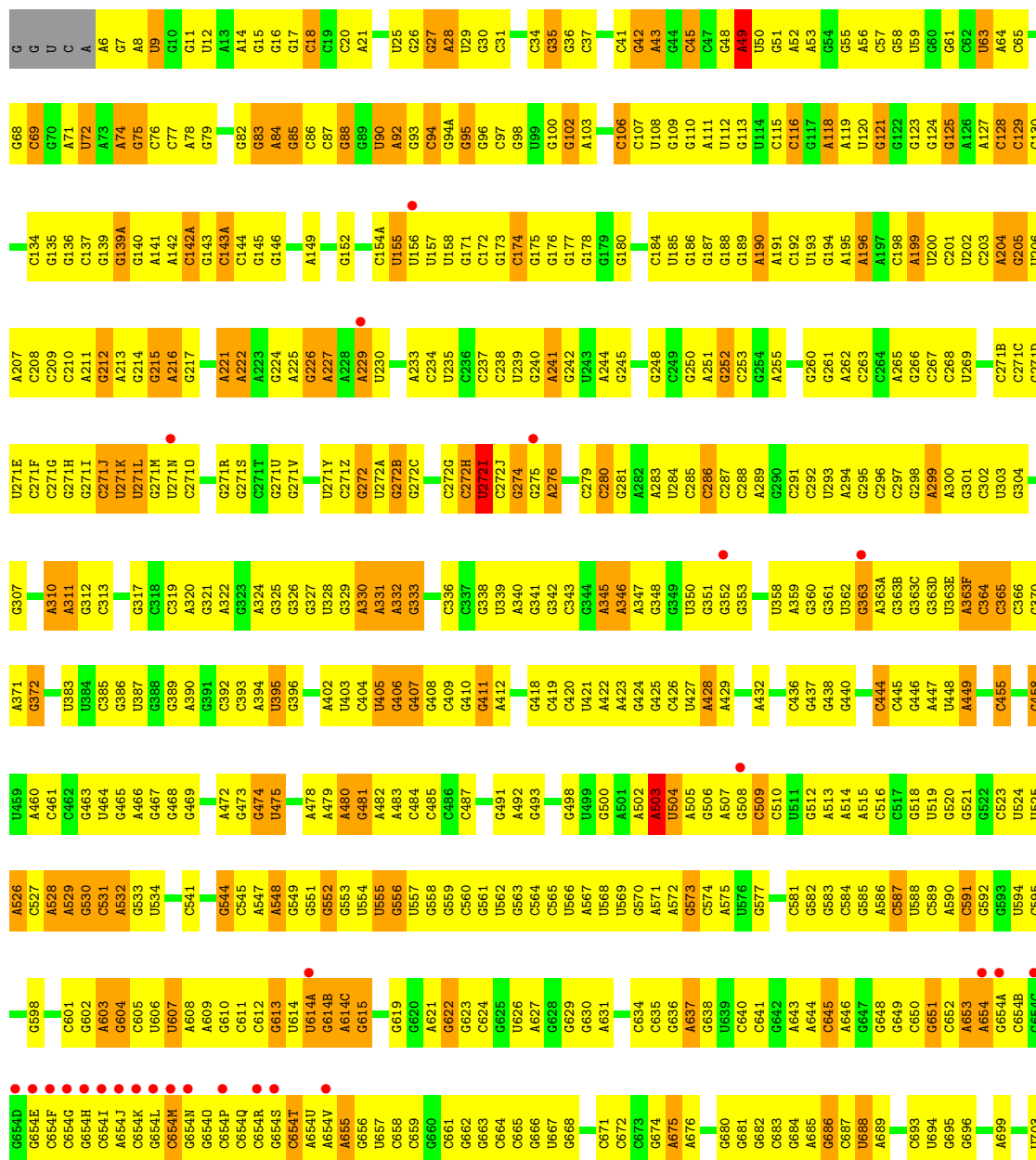
• Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



• Molecule 36: 23S RIBOSOMAL RNA

Chain BA:





C2715	C2651	C2575	C2510	G2446	G2383	C2313	A2241	U2167	G2029	U1955	G1878	U1798	G1714
U2716	C2652	G2576	U2511	G2447	G2384	C2314	G2242	G2168	A2030	U1956	C1878	G1799	G1717
G2717	G2655	A2577	C2512	U2448	C2385	G2315	U2243	A2169	A2031	G1959	C1882	G1800	G1718
U2720	U2656	G2578	G2513	U2449	C2386	C2316	U2244	G2170	G2032	A1960	C1883	G1801	G1719
A2721	U2657	C2579	U2514	A2450	U2387	C2317	U2245	A2171	A2033	G1963	A1885	A1802	U1720
G2722	C2658	G2580	C2515	A2451	A2388	G2318	G2246	U2172	U2034	U1964	C1886	C1804	G1721
C2723	G2659	G2581	G2516	G2452	G2389	G2319	A2247	A2173	G2035	G1967	C1887	A1805	A1722
C2724	A2660	G2582	C2517	G2453	U2390	A2320	U2248	G2174	G2036	G1968	C1888	U1739	U1740
A2725	G2661	U2584	A2518	G2454	G2391	G2321	U2249	C2175	C2037	C1967	A1889	A1741	A1741
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G2727	G2663	C2586	G2523	G2456	A2393	G2323	U2257	G2182	C2039	A1969	A1900	G1810	C1745
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A2731	G2667	U2463	U2527	U2464	G2397	A2327	U2261	G2186	G2043	G1973	G1903	A1814	G1748
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A2733	G2669	C2465	U2529	C2466	U2401	G2329	U2263	G2188	G2049	G1977	G1907	G1816	C1754
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G2735	G2671	G2467	G2531	C2468	G2403	U2331	A2265	U2189	A2051	G1985	G1909	U1820	A1756
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G2752	G2688	G2483	U2546	U2483	U2418	C2346	U2280	G2204	A2071	C2001	C1928	G1842	C1774
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G2758	G2694	U2489	U2552	G2489	A2424	A2360	U2286	G2210	U2077	G2007	G1934	A1848	A1780
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G2765	G2701	U2496	U2559	G2496	A2431	U2367	U2293	G2217	C2084	G2018	U1944	G1858	C1789
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A2777	U2713	U2645	C2571	U2508	C2443	A2378	U2305	G2229	G2096	G2031	U2031	C1882	A1803
U2778	A2714	U2646	A2572	C2509	U2444	A2379	U2306	G2230	G2097	G2032	U2032	C1883	A1804
G2779	G2715	U2647	U2573	U2510	G2445	A2380	U2307	G2231	G2098	G2033	U2033	C1884	A1805
U2780	C2716	U2648	C2574	G2509	G2446	C2381	U2308	G2232	G2099	G2034	U2034	C1885	A1806
G2781	G2717	U2649	U2575	G2511	U2447	G2382	U2309	G2233	G2100	U2035	U2035	C1886	A1807
U2782	U2718	U2650	U2576	U2512	G2448	G2383	U2310	G2234	G2101	U2036	U2036	C1887	A1808
C2783	G2719	U2651	U2577	U2513	U2449	U2384	U2311	G2235	G2102	U2037	U2037	C1888	A1809
A2784	U2720	U2652	U2578	U2514	U2450	U2385	U2312	G2236	G2103	U2038	U2038	C1889	A1810
G2785	G2721	U2653	U2579	U2515	U2451	U2386	U2313	G2237	G2104	U2039	U2039	C1890	A1811
U2786	U2722	U2654	U2580	U2516	U2452	U2387	U2314	G2238	G2105	U2040	U2040	C1891	A1812
C2787	G2723	U2655	U2581	U2517	U2453	U2388	U2315	G2239	G2106	U2041	U2041	C1892	A1813
U2788	A2724	U2656	U2582	U2518	U2454	U2389	U2316	G2240	G2107	U2042	U2042	C1893	A1814
G2789	U2725	U2657	U2583	U2519	U2455	U2390	U2317	G2241	G2108	U2043	U2043	C1894	A1815
A2790	A2726	U2658	U2584	U2520	U2456	U2391	U2318	G2242	G2109	U2044	U2044	C1895	A1816
C2791	G2727	U2659	U2585	U2521	U2457	U2392	U2319	G2243	G2110	U2045	U2045	C1896	A1817
U2792	U2728	U2660	U2586	U2522	U2458	U2393	U2320	G2244	G2111	U2046	U2046	C1897	A1818
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A2794	C2730	U2662	U2588	U2524	U2460	U2395	U2322	G2246	G2113	U2048	U2048	C1899	A1820
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C2798	G2734	U2666	U2592	U2528	U2464	U2399	U2326	G2250	G2117	U2052	U2052	C1903	A1824
U2799	A2735	G2667	U2593	U2529	U2465	U2400	U2327	G2251	G2118	U2053	U2053	C1904	A1825
G2800	G2736	U2668	U2594	U2530	U2466	U2401	U2328	G2252	G2119	U2054	U2054	C1905	A1826
U2801	U2737	U2669	U2595	U2531	U2467	U2402	U2329	G2253	G2120	U2055	U2055	C1906	A1827
G2802	A2738	G2670	U2596	U2532	U2468	U2403	U2330	G2254	G2121	U2056	U2056	C1907	A1828
U2803	G2739	U2671	U2597	U2533	U2469	U2404	U2331	G2255	G2122	U2057	U2057	C1908	A1829
A2804	G2740	U2672	U2598	U2534	U2470	U2405	U2332	G2256	G2123	U2058	U2058	C1909	A1830
C2805	U2741	C2673	U2599	U2535	U2471	U2406	U2333	G2257	G2124	U2059	U2059	C1910	A1831
U2806	G2742	G2674	U2600	U2536	U2472	U2407	U2334	G2258	G2125	U2060	U2060	C1911	A1832
G2807	C2743	U2675	U2601	U2537	U2473	U2408	U2335	G2259	G2126	U2061	U2061	C1912	A1833
U2808	A2744	G2676	U2602	U2538	U2474	U2409	U2336	G2260	G2127	U2062	U2062	C1913	A1834
C2809	G2745	U2677	U2603	U2539	U2475	U2410	U2						

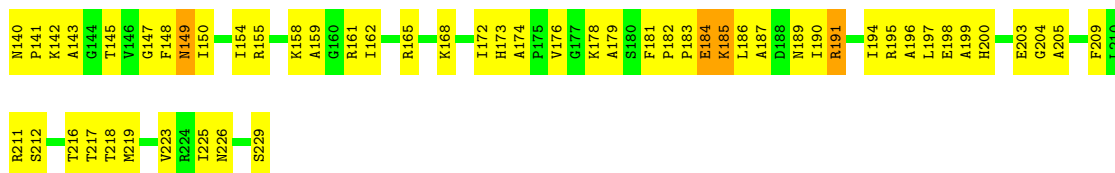


G1681	A1609	C1536	C1467	G1401	G1332	U1267	C1207	A1143	U1081	C1018	G955	C894	C818	G755
G1682	A1610	G1537	A1472	C1402	C1333	A1268	C1208	G1144	U1082	U1019	G956	C885	C756	G757
G1683	C1611	G1538	C1473	C1403	G1334	A1269	G1209	C1145	U1083	A1020	A957	C886	A821	U757
C1684		G1539	C1474	C1404	U1335	C1270	A1210	C1146	A1086	A1021	U958	A887	U822	G758
A1614		U1540	C1474	U1405	G1336	G1271	U1211	C1147	A1087	G1022	A959	C888	G823	G759
C1615		G1541	G1475	U1406	G1337	A1272	G1212	A1148	C1087	U1023	A960	C889	A824	G760
A1616		A1542	C1476	C1407	G1338	C1273	A1213	G1149	A1088	G1024	C961	A890	C825	A761
C1617	A1618	C1543	A1477	C1408	G1339	A1274	A1214	C1150	U1089	G1025	G962	C892	U826	
A1694	G1619	A1544	G1478	C1409	U1340	A1275	G1215	G1151	U1090	U1026	U963	C893	U827	
G1695		A1545	G1479	G1410	U1341	A1276	G1216	G1152	G1091	A1027	G964	C894	U828	
G1696		C1546	G1480	C1411		G1277	C1217	C1153	G1092	A1028	C965	U895	A829	
G1697	G1623		U1481		G1344	A1278	C1218	G1154	G1093	A1029	G966	A896	G830	
A1698	G1624	C1549	G1482	U1415	C1345	A1279	G1219	A1155	U1094	G1030		C897	G831	
G1699	C1625		G1484	C1416	G1346	G1280	A1220	A1156	A0995	U1033	U969	C898	G769	
		A1553	G1485	C1417	G1347	G1281	C1221	G1157	A1096	C970	C899	A899	U833	G770
U1629		A1554	A1486		G1348	G1285	C1221A	U1097	G1034	A900	C971	A900	C834	
G1630		C1555	G1487	U1420	A1349	A1286	G1222	U1159	A1098	U1035	G972	A901	A835	U773
		C1556	G1488	G1421	C1350	A1287	G1223	G1160	C1099	G1036	A973	C902	G836	A774
A1632		C1557	U1489	G1422	C1351	A1288		C1161	U1100	G1037	G974	C903	C837	G775
G1633		A1558	U1490	G1423	U1352	C1289	G1227	G1162	C1101	U1038	C975	C904	C838	G776
G1634		G1559	G1491	G1424	A1353	C1290	G1228	G1163	C1102	G1039	G975A	U839	U839	
G1635		G1492	G1493		A1354	C1291	G1229	G1164	A1103	C1040	C976	G906	C840	G778
G1636		C1565	C1493	A1427		C1292	C1230	U1165	C1104	C1041	G977	U907	A841	
G1637		A1566	A1494	C1428	G1358	U1291	G1231	C1166	U1105	G1042			A781	
C1638		C1567	U1495	G1429	A1359	C1293	G1232	U1167	U1106	C1043	G979	A910	C844	A782
U1639		G1568	A1496	C1430	A1360	U1294	G1233	G1168	G1107	A1044	A980	C914	C846	A783
C1640		A1569	U1497	U1431	G1361	C1295	G1233	G1169	U1108	A1045	A981	C914	C846	A784
				G1432	C1362	G1296	U1234	G1170	C1109	A1046	C982	C915	U847	
					C1363	C1297	G1235	G1171	G1110	G1047	A983	G916	G848	G786
					G1364	C1298	G1236	G1173	A1111	A1048	A984	A917	A849	U787
					A1365	G1299	A1237	A1174	G1112	C1049	C985	A918	C850	
					G1366	U1300	G1238	U1175	U1113	A1050	C986	U851	C851	A789
					A1367	A1301	G1239	G1176	G1114	G1051	C987	C924	C852	G790
					G1368	A1302	U1240	A1177	G1115	C1052	A988	C925	C853	G791
					G1369	A1241	A1241	C1178	G1116	C1053	G989	A926	G854	G792
						C1306	G1242	G1179	G1117	A1054	A990	G927	C855	A793
						A1307	G1243	C1180	C1118	G1055	C991	G928	C856	A794
						A1308	G1244	C1181	G1119	A1056	C992	C932	C857	G795
						G1309	G1245	G1183	G1120	A1057	G993	G932	U858	C796
						G1310	A1246	G1184	C1121	G1058	A933	A933	C859	C797
						G1311	G1247	C1185	G1122	G1059	G934	G934	U860	G798
						U1312	G1248	G1186	C1123	U1060	C997	C935	A861	G799
						C1313	U1249	G1187	G1124	U1061	C998	C936	G862	A800
						G1314	G1250	U1188	C1125	G1062	U999	U937	A863	G801
						C1315	G1251	A1189	A1126	G1063	A1000	G938	C864	A802
						G1252	C1252	G1190	A1127	C1064	A1001	G939	C865	U803
						A1316	A1253	G1191	A1128		G1002	G940	A866	A804
						C1317	A1254	G1192		A1067		A941		G805
						G1318	G1255	G1193		G1068	C1005	G942	C869	G806
						C1319	U1256	G1193	G1131	A1069	C1006	U943	A870	C807
						C1320	G1257	C1196	U1132	A1070		G944	U871	G808
						A1321	C1257	G1197	U1133	G1071	A1009	C944	G809	G809
						A1322	G1258	G1197	C1135	A1071	A945	G946	G810	
						U1390	G1259	U1198	G1136	A1072	A1010	G947	U811	
						U1391	G1260	U1199	G1137	A1073	G1011	C947	U877	U810
						G1325	C1261	C1200	G1138	G1074	U1012	G948	A878	U811
						U1326	A1262	G1203	G1139	G1075	C1013	C949	U879	C812
						C1327	G1263	A1204	U1140	C1076	U1014	G950	C880	U813
						G1328	U1263	G1203	C1141	A1077	G1015	C949	C881	C814
						U1329	G1264	A1204	U1141	C1077	C1016	G950	C881	C815
						C1330	A1265	U1205	U1142		G1017	A953	C882	C816
						A1331	G1266	U1206	A1142A		C1018	C954	C882	C817
							C1266							



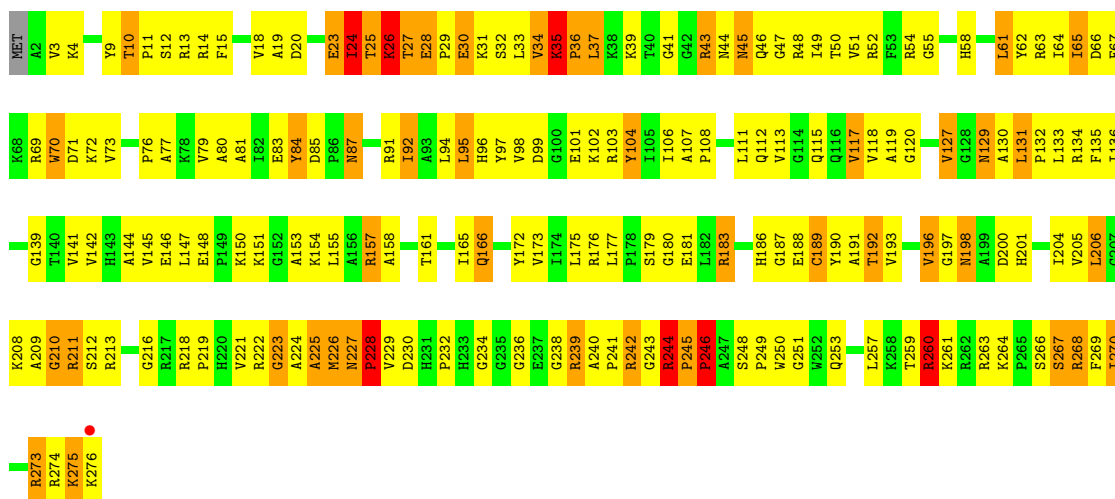


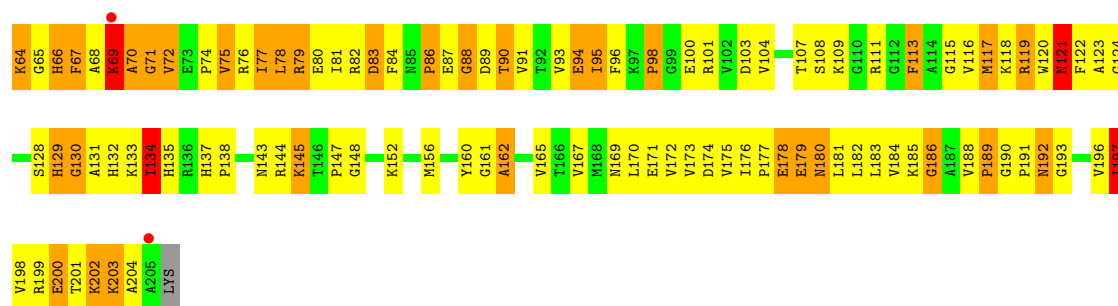




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

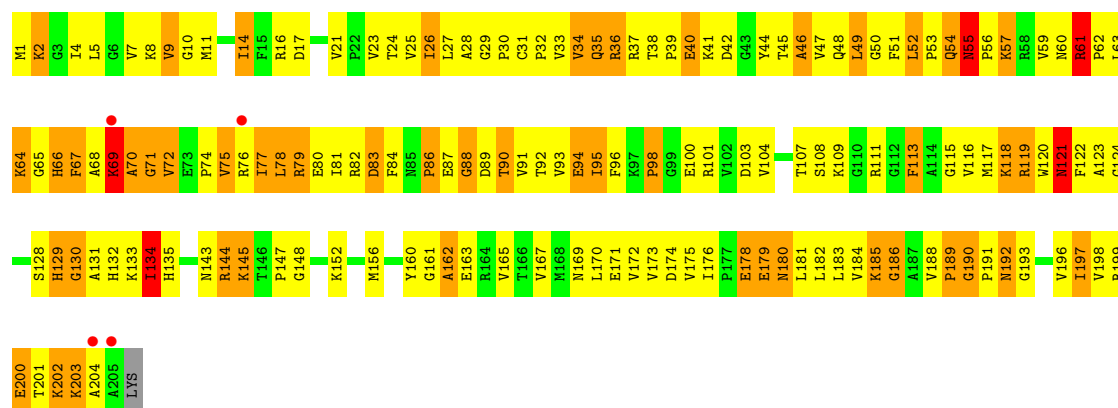
Chain BD:





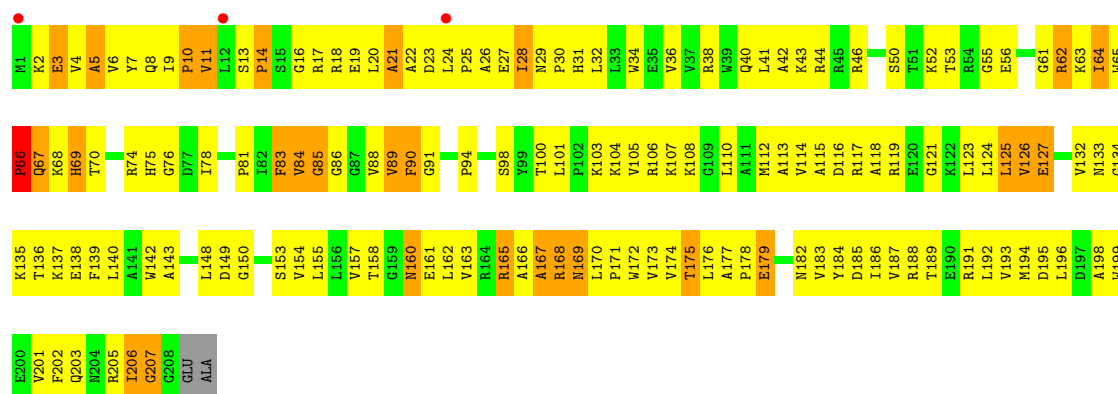
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE:



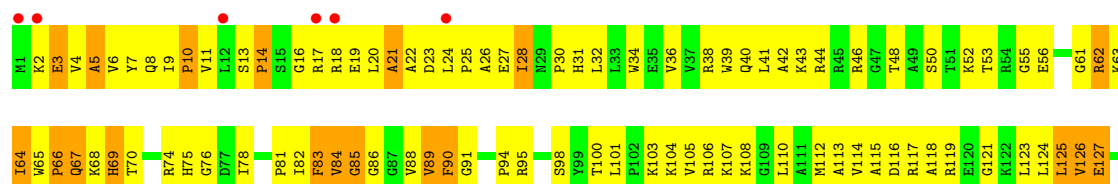
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF:

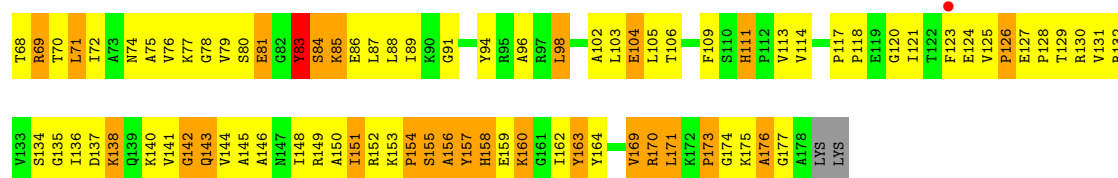


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:

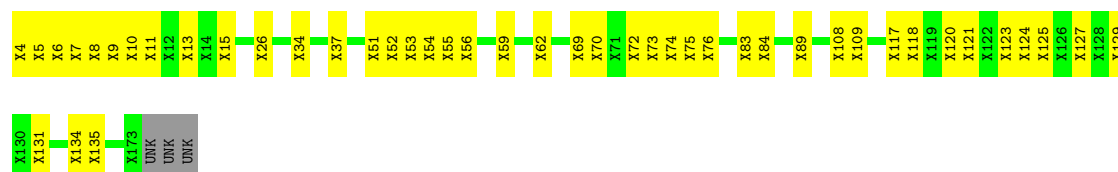






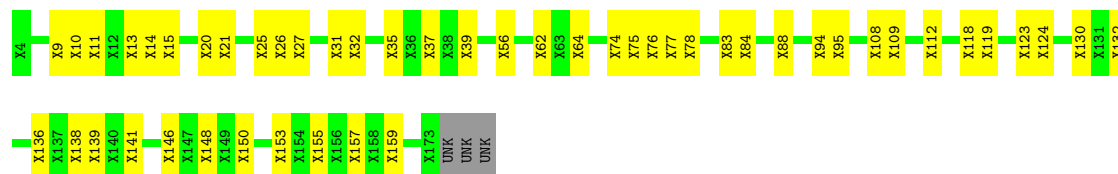
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



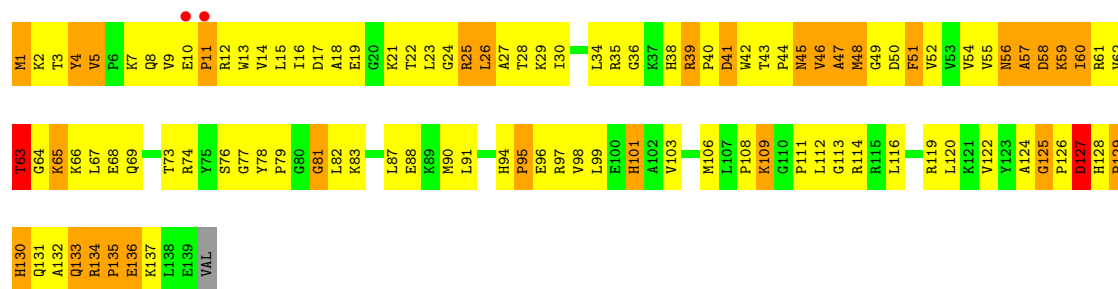
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN:



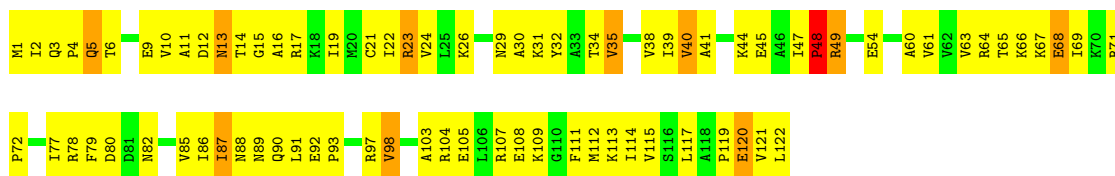
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain DN:



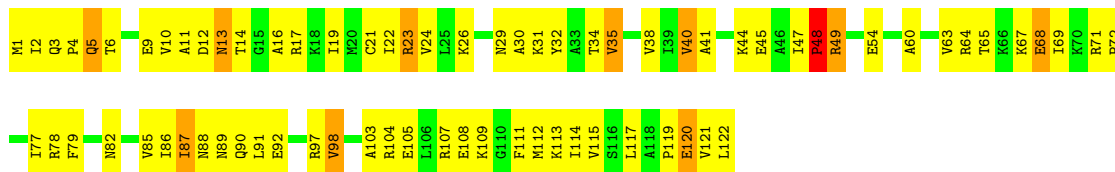
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:



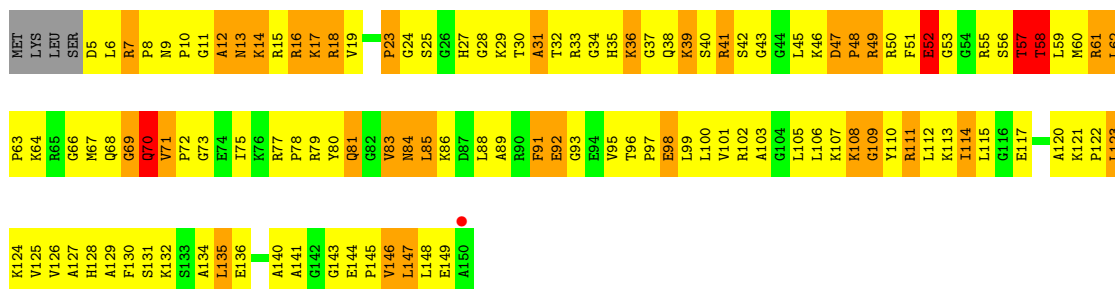
- Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain DO:



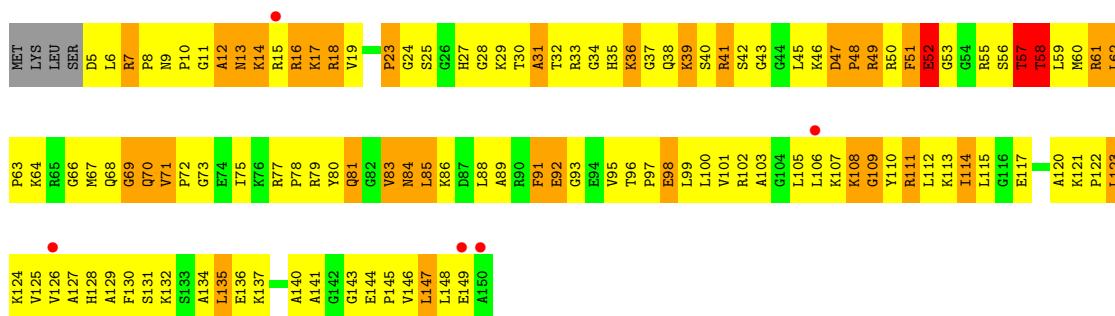
- Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain BP:



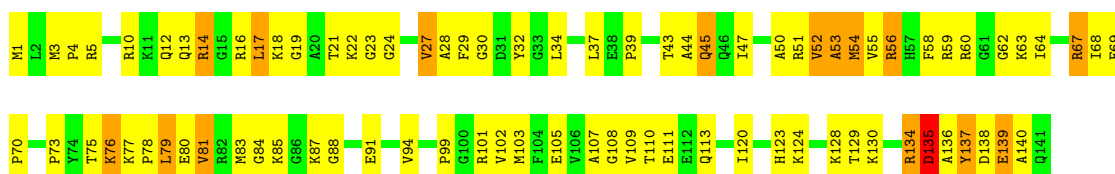
- Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain DP:



- Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



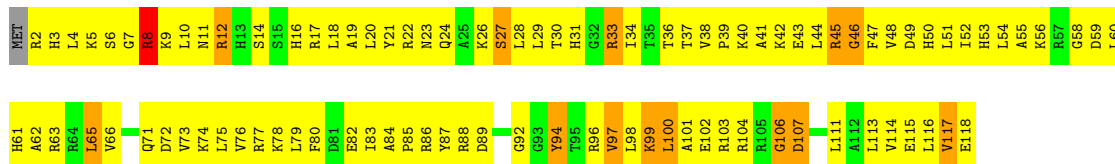
## • Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



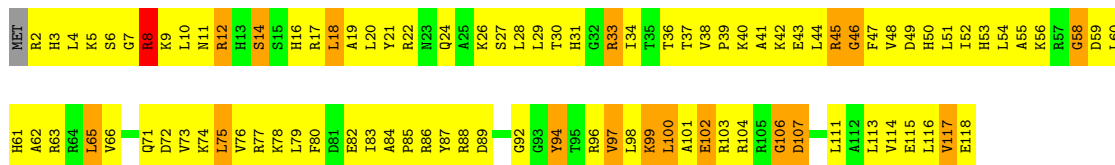
## • Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR:



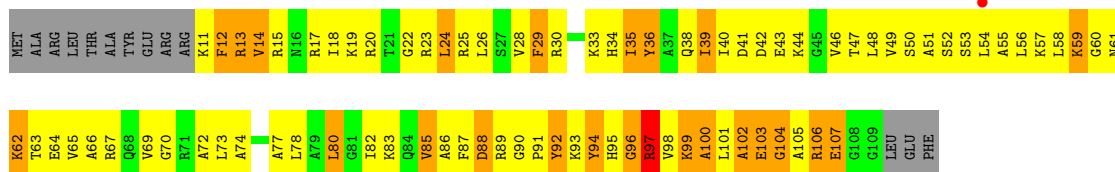
## • Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain DR:



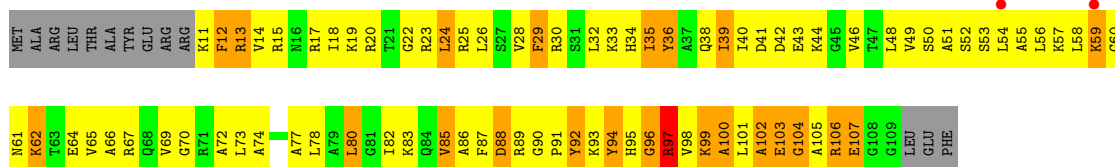
## • Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain BS:



## • Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain DS:

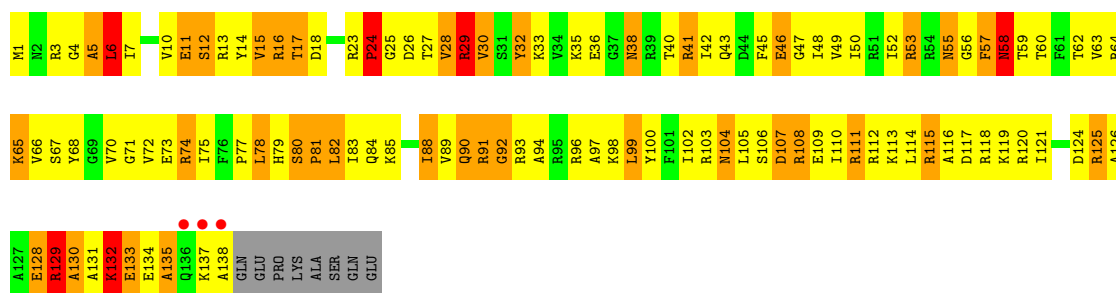


## • Molecule 51: 50S RIBOSOMAL PROTEIN L19

Chain BT:

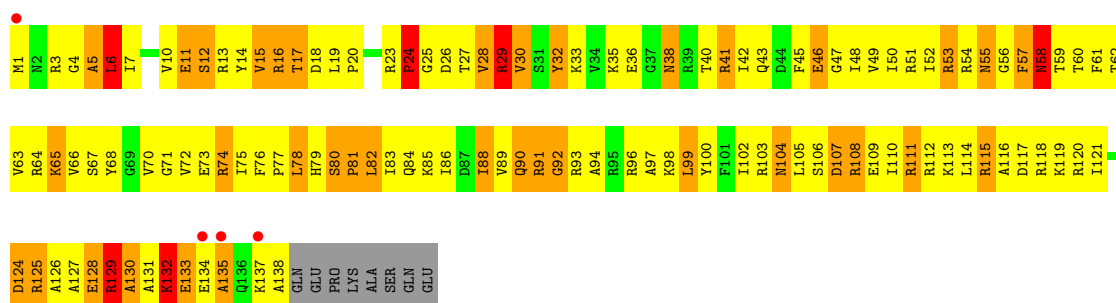






• Molecule 51: 50S RIBOSOMAL PROTEIN L19

Chain DT:



• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:



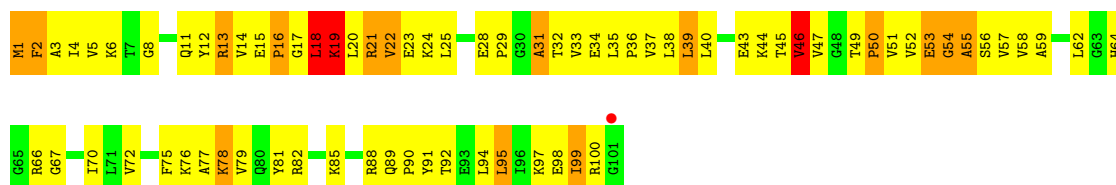
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain DU:



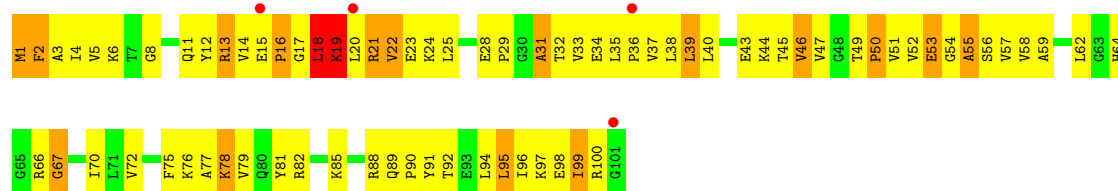
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain BV:



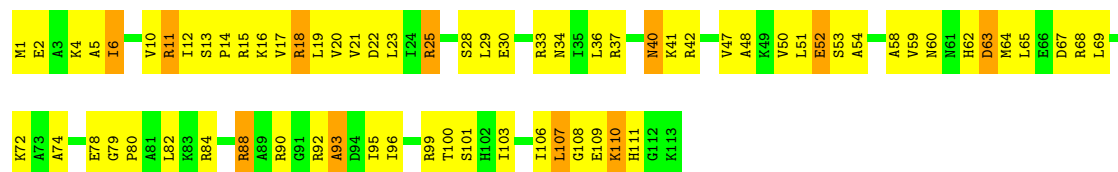
- Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain DV:



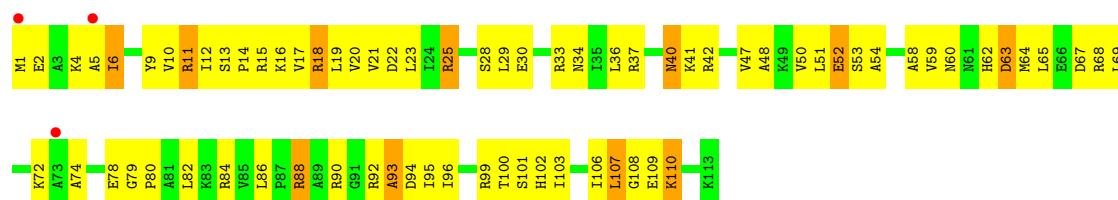
- Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain BW:



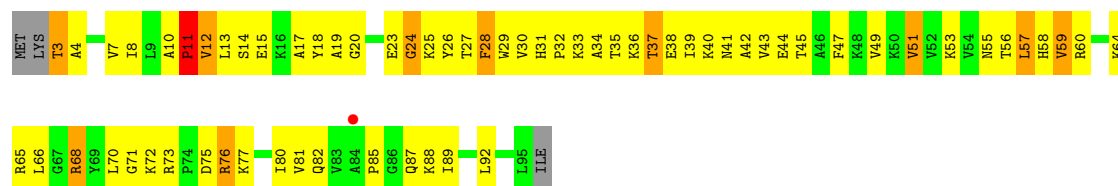
- Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain DW:



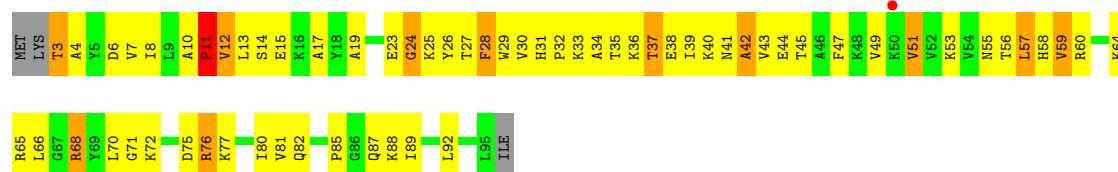
- Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain BX:



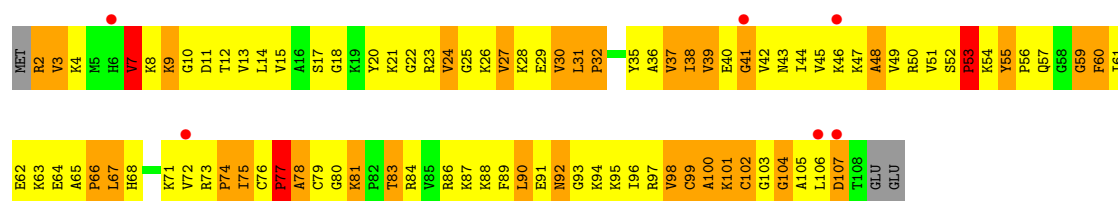
- Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain DX:



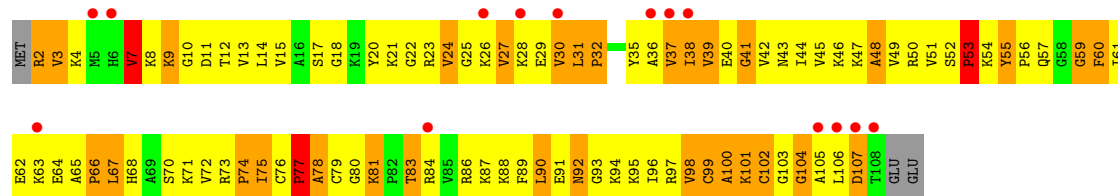
- Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY:



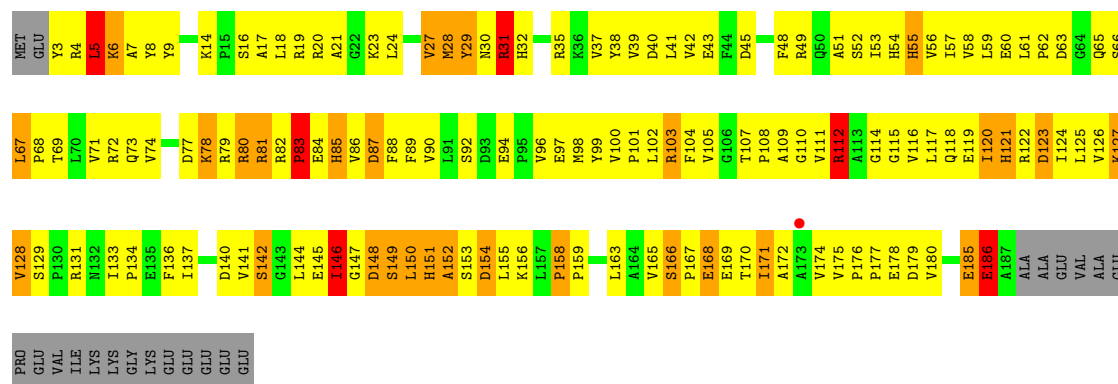
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain DY:



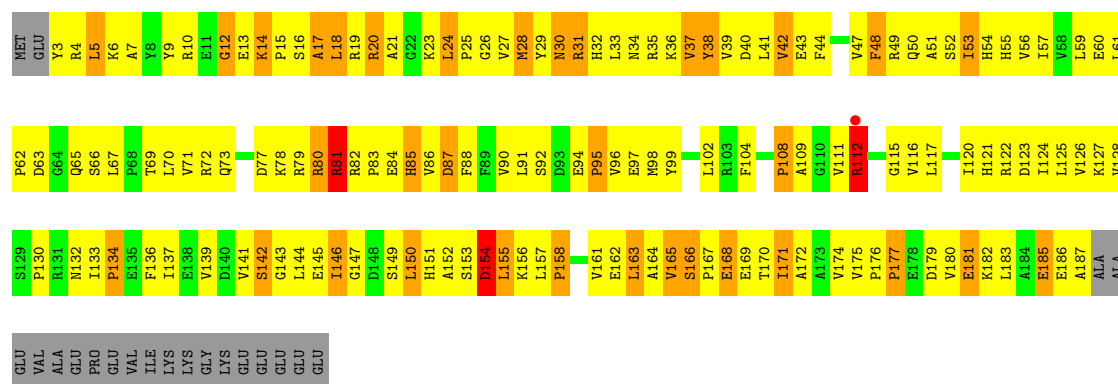
• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



• Molecule 57: 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, $\alpha$ , $\beta$ , $\gamma$	291.36Å 269.43Å 401.95Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	49.75 – 3.70 49.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-3.70) 99.8 (49.75-3.40)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.214 , 0.249 0.239 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	84.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 53.6	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 846438 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	307606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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: GDP, 5MU, ZN, MG, FUA

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	0.54	0/36190	0.74	23/56486 (0.0%)
1	CA	0.51	0/36190	0.74	16/56486 (0.0%)
2	AB	0.44	0/1936	0.67	0/2611
2	CB	0.41	0/1936	0.68	0/2611
3	AC	0.48	0/1637	0.64	0/2207
3	CC	0.43	0/1637	0.64	0/2207
4	AD	0.39	0/1733	0.65	0/2318
4	CD	0.39	0/1733	0.65	0/2318
5	AE	0.49	0/1163	0.68	0/1566
5	CE	0.50	0/1163	0.68	0/1566
6	AF	0.40	0/856	0.63	0/1154
6	CF	0.38	0/856	0.64	0/1154
7	AG	0.40	0/1276	0.60	0/1709
7	CG	0.38	0/1276	0.61	0/1709
8	AH	0.45	0/1136	0.71	0/1527
8	CH	0.43	0/1136	0.70	0/1527
9	AI	0.42	0/1027	0.67	0/1373
9	CI	0.40	0/1027	0.66	0/1373
10	AJ	0.45	0/808	0.69	0/1087
10	CJ	0.42	0/808	0.69	0/1087
11	AK	0.45	0/900	0.70	0/1213
11	CK	0.41	0/900	0.69	0/1213
12	AL	0.47	0/987	0.71	0/1322
12	CL	0.45	0/987	0.70	0/1322
13	AM	0.39	0/999	0.67	0/1338
13	CM	0.38	0/999	0.67	0/1338
14	AN	0.47	0/501	0.67	0/664
14	CN	0.45	0/501	0.67	0/664
15	AO	0.40	0/745	0.62	0/992
15	CO	0.39	0/745	0.62	0/992
16	AP	0.39	0/717	0.63	0/965
16	CP	0.40	0/717	0.62	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.47	0/837	0.66	0/1119
17	CQ	0.44	0/837	0.66	0/1119
18	AR	0.45	0/579	0.67	0/768
18	CR	0.46	0/579	0.68	0/768
19	AS	0.43	0/643	0.68	1/867 (0.1%)
19	CS	0.41	0/643	0.68	1/867 (0.1%)
20	AT	0.38	0/765	0.64	0/1007
20	CT	0.36	0/765	0.65	0/1007
21	AU	0.47	0/213	0.61	0/279
21	CU	0.46	0/213	0.62	0/279
22	AV	0.52	0/1809	0.70	0/2819
22	CV	0.46	0/1809	0.69	0/2819
23	AW	0.36	0/1810	0.70	0/2821
23	CW	0.95	2/1810 (0.1%)	0.68	0/2821
24	AX	0.38	0/288	0.72	0/446
24	CX	0.69	1/288 (0.3%)	0.85	1/446 (0.2%)
25	AY	0.47	0/5313	0.69	0/7195
25	CY	0.45	0/5313	0.68	0/7195
26	B0	0.40	0/671	0.66	0/892
26	D0	0.40	0/671	0.66	0/892
27	B1	0.42	0/739	0.71	0/983
27	D1	0.41	0/739	0.67	0/983
28	B2	0.32	0/600	0.64	0/793
28	D2	0.33	0/600	0.61	0/793
29	B3	0.40	0/473	0.59	0/636
29	D3	0.40	0/473	0.60	0/636
30	B4	0.47	0/461	0.83	1/623 (0.2%)
30	D4	0.48	0/461	0.83	1/623 (0.2%)
31	B5	0.37	0/473	0.69	0/639
31	D5	0.39	0/473	0.69	0/639
32	B6	0.62	0/440	0.94	2/586 (0.3%)
32	D6	0.56	0/440	0.93	2/586 (0.3%)
33	B7	0.43	0/427	0.68	0/563
33	D7	0.44	0/427	0.67	0/563
34	B8	0.54	0/516	0.83	0/681
34	D8	0.51	0/516	0.82	0/681
35	B9	0.42	0/310	0.65	0/407
35	D9	0.43	0/310	0.66	0/407
36	BA	0.50	3/69972 (0.0%)	0.74	35/109237 (0.0%)
36	DA	0.49	3/69972 (0.0%)	0.73	36/109237 (0.0%)
37	BB	0.41	0/2853	0.72	1/4451 (0.0%)
37	DB	0.41	0/2853	0.72	1/4451 (0.0%)
38	BC	0.55	1/1774 (0.1%)	0.61	0/2391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DC	0.41	0/1774	0.60	0/2391
39	BD	0.47	0/2195	0.77	1/2955 (0.0%)
39	DD	0.46	0/2195	0.76	1/2955 (0.0%)
40	BE	0.44	0/1597	0.70	0/2155
40	DE	0.44	0/1597	0.70	0/2155
41	BF	0.37	0/1659	0.62	0/2246
41	DF	0.36	0/1659	0.62	0/2246
42	BG	0.41	0/1498	0.74	1/2013 (0.0%)
42	DG	0.38	0/1498	0.69	0/2013
43	BH	0.36	0/1293	0.67	0/1746
43	DH	0.36	0/1293	0.67	0/1746
45	BN	0.35	0/1132	0.68	0/1527
45	DN	0.35	0/1132	0.68	0/1527
46	BO	0.44	0/943	0.66	0/1269
46	DO	0.44	0/943	0.66	0/1269
47	BP	0.41	0/1131	0.87	3/1504 (0.2%)
47	DP	0.40	0/1131	0.87	3/1504 (0.2%)
48	BQ	0.43	0/1143	0.63	0/1527
48	DQ	0.43	0/1143	0.63	0/1527
49	BR	0.37	0/974	0.66	0/1302
49	DR	0.36	0/974	0.66	0/1302
50	BS	0.39	0/779	0.68	0/1038
50	DS	0.37	0/779	0.67	0/1038
51	BT	0.45	0/1156	0.77	1/1544 (0.1%)
51	DT	0.45	0/1156	0.77	1/1544 (0.1%)
52	BU	0.39	0/975	0.64	0/1297
52	DU	0.40	0/975	0.64	0/1297
53	BV	0.36	0/790	0.67	0/1057
53	DV	0.35	0/790	0.68	0/1057
54	BW	0.36	0/907	0.62	0/1216
54	DW	0.35	0/907	0.62	0/1216
55	BX	0.40	0/740	0.65	0/995
55	DX	0.41	0/740	0.64	0/995
56	BY	0.39	0/824	0.62	0/1100
56	DY	0.39	0/824	0.62	0/1100
57	BZ	0.44	0/1500	0.67	0/2037
57	DZ	0.41	0/1500	0.70	0/2037
All	All	0.48	10/331626 (0.0%)	0.72	132/494526 (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	26
1	CA	1	21
22	AV	0	1
36	BA	2	39
36	DA	2	37
All	All	6	124

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	38	A	O3'-P	37.35	2.06	1.61
38	BC	54	ARG	C-N	-15.66	0.98	1.34
24	CX	19	A	O3'-P	-9.03	1.50	1.61
36	BA	272(I)	U	N1-C2	7.87	1.45	1.38
36	DA	272(I)	U	N1-C2	7.37	1.45	1.38

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BA	1992	G	C2'-C3'-O3'	10.46	132.51	109.50
36	DA	1992	G	C2'-C3'-O3'	10.39	132.37	109.50
1	AA	1498	U	C2'-C3'-O3'	9.73	130.91	109.50
1	CA	1498	U	C2'-C3'-O3'	9.60	130.62	109.50
36	BA	1799	G	C2'-C3'-O3'	9.35	130.07	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1498	U	C3'
36	BA	1799	G	C3'
36	BA	1992	G	C3'
1	CA	1498	U	C3'
36	DA	1799	G	C3'

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	118	U	Sidechain
1	AA	202	U	Sidechain
1	AA	250	A	Sidechain
1	AA	436	C	Sidechain



## 5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1170	0
1	CA	32329	0	16318	1209	0
2	AB	1901	0	1951	223	0
2	CB	1901	0	1951	225	0
3	AC	1613	0	1677	185	0
3	CC	1613	0	1677	191	0
4	AD	1703	0	1763	171	0
4	CD	1703	0	1763	178	0
5	AE	1147	0	1207	115	0
5	CE	1147	0	1207	112	0
6	AF	843	0	857	76	0
6	CF	843	0	857	79	0
7	AG	1257	0	1296	89	0
7	CG	1257	0	1296	93	0
8	AH	1116	0	1177	89	0
8	CH	1116	0	1177	88	0
9	AI	1010	0	1035	139	0
9	CI	1010	0	1035	137	0
10	AJ	795	0	840	154	0
10	CJ	795	0	840	159	0
11	AK	885	0	904	56	0
11	CK	885	0	904	63	0
12	AL	971	0	1057	142	0
12	CL	971	0	1057	145	0
13	AM	988	0	1059	156	0
13	CM	988	0	1059	154	0
14	AN	492	0	529	64	0
14	CN	492	0	529	63	0
15	AO	734	0	771	69	0
15	CO	734	0	771	73	0
16	AP	701	0	720	66	0
16	CP	701	0	720	67	0
17	AQ	824	0	891	57	0
17	CQ	824	0	891	65	0
18	AR	574	0	644	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CR	574	0	644	79	0
19	AS	630	0	652	106	0
19	CS	630	0	652	108	0
20	AT	763	0	861	97	0
20	CT	763	0	861	94	0
21	AU	209	0	221	18	0
21	CU	209	0	221	17	0
22	AV	1619	0	822	60	0
22	CV	1619	0	822	58	0
23	AW	1641	0	839	126	0
23	CW	1641	0	840	115	0
24	AX	257	0	130	45	0
24	CX	257	0	130	50	0
25	AY	5215	0	5288	857	0
25	CY	5215	0	5287	809	0
26	B0	662	0	688	98	0
26	D0	662	0	688	99	0
27	B1	732	0	808	126	0
27	D1	732	0	808	112	0
28	B2	598	0	653	84	0
28	D2	598	0	653	113	0
29	B3	468	0	523	59	0
29	D3	468	0	523	64	0
30	B4	451	0	449	93	0
30	D4	451	0	449	88	0
31	B5	459	0	480	101	0
31	D5	459	0	480	99	0
32	B6	433	0	461	150	0
32	D6	433	0	461	149	0
33	B7	419	0	467	38	0
33	D7	419	0	467	36	0
34	B8	508	0	576	96	0
34	D8	508	0	576	101	0
35	B9	307	0	335	30	0
35	D9	307	0	335	27	0
36	BA	62474	0	31497	2600	0
36	DA	62474	0	31497	2637	0
37	BB	2551	0	1295	132	0
37	DB	2551	0	1295	139	0
38	BC	1742	0	1797	158	0
38	DC	1742	0	1798	160	0
39	BD	2145	0	2234	304	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DD	2145	0	2234	315	0
40	BE	1564	0	1629	249	0
40	DE	1564	0	1629	244	0
41	BF	1624	0	1677	237	0
41	DF	1624	0	1677	232	0
42	BG	1474	0	1534	241	0
42	DG	1474	0	1534	261	0
43	BH	1269	0	1337	178	0
43	DH	1269	0	1337	176	0
44	BJ	851	0	194	31	0
44	DJ	851	0	195	32	0
45	BN	1105	0	1180	183	0
45	DN	1105	0	1180	184	0
46	BO	933	0	996	109	0
46	DO	933	0	996	102	0
47	BP	1114	0	1187	296	0
47	DP	1114	0	1187	297	0
48	BQ	1122	0	1179	134	0
48	DQ	1122	0	1179	123	0
49	BR	960	0	1021	150	0
49	DR	960	0	1021	152	0
50	BS	771	0	832	153	0
50	DS	771	0	832	146	0
51	BT	1142	0	1202	242	0
51	DT	1142	0	1202	241	0
52	BU	958	0	1015	133	0
52	DU	958	0	1015	139	0
53	BV	779	0	852	140	0
53	DV	779	0	852	140	0
54	BW	896	0	953	100	0
54	DW	896	0	953	99	0
55	BX	726	0	778	79	0
55	DX	726	0	778	83	0
56	BY	811	0	901	175	0
56	DY	811	0	901	179	0
57	BZ	1468	0	1492	200	0
57	DZ	1468	0	1492	219	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B9	1	0	0	0	0
58	CD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D9	1	0	0	0	0
59	AY	37	0	47	15	0
59	CY	37	0	47	26	0
60	AY	28	0	12	13	0
60	CY	28	0	12	10	0
61	AY	1	0	0	0	0
61	CY	1	0	0	0	0
All	All	307606	0	211582	21259	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 41.

The worst 5 of 21259 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:BC:121:MET:CE	38:BC:121:MET:SD	2.02	1.48
23:CW:34:C:C3'	23:CW:35:A:H5''	1.42	1.47
38:DC:121:MET:CE	38:DC:121:MET:SD	2.02	1.46
38:DC:109:MET:CE	38:DC:109:MET:SD	2.03	1.44
23:AW:34:C:C3'	23:AW:35:A:H5''	1.42	1.44

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	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	10
2	CB	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	10
3	AC	205/239 (86%)	146 (71%)	32 (16%)	27 (13%)	0	12
3	CC	205/239 (86%)	148 (72%)	31 (15%)	26 (13%)	0	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	47 (23%)	21 (10%)	1	19
4	CD	206/209 (99%)	138 (67%)	49 (24%)	19 (9%)	1	24
5	AE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	5	50
5	CE	149/162 (92%)	118 (79%)	26 (17%)	5 (3%)	6	56
6	AF	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	5	50
6	CF	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	5	50
7	AG	153/156 (98%)	112 (73%)	27 (18%)	14 (9%)	1	24
7	CG	153/156 (98%)	112 (73%)	29 (19%)	12 (8%)	1	29
8	AH	136/138 (99%)	106 (78%)	26 (19%)	4 (3%)	7	60
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	7	60
9	AI	121/128 (94%)	85 (70%)	27 (22%)	9 (7%)	2	31
9	CI	121/128 (94%)	87 (72%)	25 (21%)	9 (7%)	2	31
10	AJ	97/105 (92%)	67 (69%)	19 (20%)	11 (11%)	1	16
10	CJ	97/105 (92%)	68 (70%)	18 (19%)	11 (11%)	1	16
11	AK	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	29
11	CK	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	29
12	AL	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	7
12	CL	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	7
13	AM	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	10
13	CM	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	10
14	AN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	25
14	CN	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	1	25
15	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	27
15	CO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	27
16	AP	82/88 (93%)	62 (76%)	15 (18%)	5 (6%)	2	37
16	CP	82/88 (93%)	63 (77%)	14 (17%)	5 (6%)	2	37
17	AQ	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	7	59
17	CQ	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	7	59
18	AR	68/88 (77%)	47 (69%)	13 (19%)	8 (12%)	1	15
18	CR	68/88 (77%)	48 (71%)	12 (18%)	8 (12%)	1	15
19	AS	77/93 (83%)	42 (54%)	17 (22%)	18 (23%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CS	77/93 (83%)	40 (52%)	19 (25%)	18 (23%)	0	2
20	AT	97/106 (92%)	57 (59%)	28 (29%)	12 (12%)	1	14
20	CT	97/106 (92%)	57 (59%)	27 (28%)	13 (13%)	0	12
21	AU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	13
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	13
25	AY	663/691 (96%)	458 (69%)	126 (19%)	79 (12%)	1	15
25	CY	663/691 (96%)	482 (73%)	125 (19%)	56 (8%)	1	26
26	B0	82/85 (96%)	63 (77%)	15 (18%)	4 (5%)	3	44
26	D0	82/85 (96%)	63 (77%)	15 (18%)	4 (5%)	3	44
27	B1	92/98 (94%)	74 (80%)	8 (9%)	10 (11%)	1	17
27	D1	92/98 (94%)	71 (77%)	12 (13%)	9 (10%)	1	21
28	B2	69/72 (96%)	40 (58%)	21 (30%)	8 (12%)	1	15
28	D2	69/72 (96%)	34 (49%)	26 (38%)	9 (13%)	0	13
29	B3	58/60 (97%)	35 (60%)	19 (33%)	4 (7%)	2	33
29	D3	58/60 (97%)	35 (60%)	19 (33%)	4 (7%)	2	33
30	B4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	1
30	D4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	1
31	B5	57/60 (95%)	37 (65%)	10 (18%)	10 (18%)	0	6
31	D5	57/60 (95%)	37 (65%)	10 (18%)	10 (18%)	0	6
32	B6	48/54 (89%)	21 (44%)	13 (27%)	14 (29%)	0	0
32	D6	48/54 (89%)	21 (44%)	13 (27%)	14 (29%)	0	0
33	B7	47/49 (96%)	38 (81%)	8 (17%)	1 (2%)	11	67
33	D7	47/49 (96%)	38 (81%)	8 (17%)	1 (2%)	11	67
34	B8	62/65 (95%)	30 (48%)	18 (29%)	14 (23%)	0	2
34	D8	62/65 (95%)	30 (48%)	18 (29%)	14 (23%)	0	2
35	B9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	1	16
35	D9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	1	16
38	BC	226/229 (99%)	175 (77%)	42 (19%)	9 (4%)	5	50
38	DC	226/229 (99%)	176 (78%)	40 (18%)	10 (4%)	4	48
39	BD	273/276 (99%)	184 (67%)	54 (20%)	35 (13%)	0	13
39	DD	273/276 (99%)	185 (68%)	53 (19%)	35 (13%)	0	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BE	203/206 (98%)	123 (61%)	39 (19%)	41 (20%)	0	3
40	DE	203/206 (98%)	122 (60%)	39 (19%)	42 (21%)	0	3
41	BF	206/210 (98%)	138 (67%)	45 (22%)	23 (11%)	1	16
41	DF	206/210 (98%)	138 (67%)	44 (21%)	24 (12%)	1	15
42	BG	177/182 (97%)	116 (66%)	39 (22%)	22 (12%)	1	14
42	DG	177/182 (97%)	112 (63%)	44 (25%)	21 (12%)	1	15
43	BH	165/180 (92%)	89 (54%)	40 (24%)	36 (22%)	0	2
43	DH	165/180 (92%)	90 (54%)	40 (24%)	35 (21%)	0	3
45	BN	137/140 (98%)	87 (64%)	26 (19%)	24 (18%)	0	6
45	DN	137/140 (98%)	88 (64%)	25 (18%)	24 (18%)	0	6
46	BO	120/122 (98%)	97 (81%)	13 (11%)	10 (8%)	1	27
46	DO	120/122 (98%)	97 (81%)	13 (11%)	10 (8%)	1	27
47	BP	144/150 (96%)	79 (55%)	38 (26%)	27 (19%)	0	4
47	DP	144/150 (96%)	79 (55%)	39 (27%)	26 (18%)	0	5
48	BQ	139/141 (99%)	106 (76%)	25 (18%)	8 (6%)	3	39
48	DQ	139/141 (99%)	107 (77%)	25 (18%)	7 (5%)	3	44
49	BR	115/118 (98%)	81 (70%)	23 (20%)	11 (10%)	1	22
49	DR	115/118 (98%)	81 (70%)	22 (19%)	12 (10%)	1	18
50	BS	97/112 (87%)	42 (43%)	32 (33%)	23 (24%)	0	1
50	DS	97/112 (87%)	41 (42%)	34 (35%)	22 (23%)	0	2
51	BT	136/146 (93%)	77 (57%)	32 (24%)	27 (20%)	0	3
51	DT	136/146 (93%)	78 (57%)	31 (23%)	27 (20%)	0	3
52	BU	115/118 (98%)	78 (68%)	30 (26%)	7 (6%)	2	37
52	DU	115/118 (98%)	76 (66%)	31 (27%)	8 (7%)	2	33
53	BV	99/101 (98%)	69 (70%)	17 (17%)	13 (13%)	0	13
53	DV	99/101 (98%)	68 (69%)	18 (18%)	13 (13%)	0	13
54	BW	111/113 (98%)	78 (70%)	23 (21%)	10 (9%)	1	24
54	DW	111/113 (98%)	76 (68%)	25 (22%)	10 (9%)	1	24
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	1	20
55	DX	91/96 (95%)	55 (60%)	26 (29%)	10 (11%)	1	17
56	BY	105/110 (96%)	44 (42%)	32 (30%)	29 (28%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	DY	105/110 (96%)	44 (42%)	32 (30%)	29 (28%)	0	1
57	BZ	183/206 (89%)	116 (63%)	39 (21%)	28 (15%)	0	8
57	DZ	183/206 (89%)	118 (64%)	34 (19%)	31 (17%)	0	6
All	All	12924/13672 (94%)	8641 (67%)	2723 (21%)	1560 (12%)	1	14

5 of 1560 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	13	ALA
2	AB	15	VAL
2	AB	74	LYS
2	AB	75	LYS

### 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%)	184 (91%)	18 (9%)	14	59
2	CB	202/220 (92%)	183 (91%)	19 (9%)	13	55
3	AC	160/188 (85%)	139 (87%)	21 (13%)	6	37
3	CC	160/188 (85%)	139 (87%)	21 (13%)	6	37
4	AD	180/181 (99%)	160 (89%)	20 (11%)	9	46
4	CD	180/181 (99%)	160 (89%)	20 (11%)	9	46
5	AE	115/123 (94%)	104 (90%)	11 (10%)	12	54
5	CE	115/123 (94%)	104 (90%)	11 (10%)	12	54
6	AF	90/90 (100%)	83 (92%)	7 (8%)	18	65
6	CF	90/90 (100%)	83 (92%)	7 (8%)	18	65
7	AG	126/127 (99%)	117 (93%)	9 (7%)	21	70
7	CG	126/127 (99%)	118 (94%)	8 (6%)	25	75
8	AH	119/119 (100%)	110 (92%)	9 (8%)	19	67
8	CH	119/119 (100%)	110 (92%)	9 (8%)	19	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	98/99 (99%)	91 (93%)	7 (7%)	21	70
9	CI	98/99 (99%)	91 (93%)	7 (7%)	21	70
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	7	40
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	5	35
11	AK	90/99 (91%)	87 (97%)	3 (3%)	50	89
11	CK	90/99 (91%)	87 (97%)	3 (3%)	50	89
12	AL	104/109 (95%)	93 (89%)	11 (11%)	10	49
12	CL	104/109 (95%)	93 (89%)	11 (11%)	10	49
13	AM	99/101 (98%)	90 (91%)	9 (9%)	14	57
13	CM	99/101 (98%)	90 (91%)	9 (9%)	14	57
14	AN	49/50 (98%)	44 (90%)	5 (10%)	11	51
14	CN	49/50 (98%)	44 (90%)	5 (10%)	11	51
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	67
15	CO	79/80 (99%)	73 (92%)	6 (8%)	19	67
16	AP	72/74 (97%)	68 (94%)	4 (6%)	30	78
16	CP	72/74 (97%)	68 (94%)	4 (6%)	30	78
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	32	80
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	25	74
18	AR	61/77 (79%)	58 (95%)	3 (5%)	35	82
18	CR	61/77 (79%)	58 (95%)	3 (5%)	35	82
19	AS	69/80 (86%)	60 (87%)	9 (13%)	6	37
19	CS	69/80 (86%)	60 (87%)	9 (13%)	6	37
20	AT	76/82 (93%)	66 (87%)	10 (13%)	6	36
20	CT	76/82 (93%)	67 (88%)	9 (12%)	8	42
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	80
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	80
25	AY	563/582 (97%)	495 (88%)	68 (12%)	7	41
25	CY	563/582 (97%)	498 (88%)	65 (12%)	8	44
26	B0	66/67 (98%)	59 (89%)	7 (11%)	10	49
26	D0	66/67 (98%)	59 (89%)	7 (11%)	10	49
27	B1	78/83 (94%)	68 (87%)	10 (13%)	6	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D1	78/83 (94%)	72 (92%)	6 (8%)	18	66
28	B2	66/67 (98%)	60 (91%)	6 (9%)	14	57
28	D2	66/67 (98%)	61 (92%)	5 (8%)	19	67
29	B3	51/52 (98%)	48 (94%)	3 (6%)	28	76
29	D3	51/52 (98%)	48 (94%)	3 (6%)	28	76
30	B4	51/63 (81%)	39 (76%)	12 (24%)	1	9
30	D4	51/63 (81%)	39 (76%)	12 (24%)	1	9
31	B5	51/52 (98%)	47 (92%)	4 (8%)	18	65
31	D5	51/52 (98%)	47 (92%)	4 (8%)	18	65
32	B6	49/52 (94%)	39 (80%)	10 (20%)	2	13
32	D6	49/52 (94%)	39 (80%)	10 (20%)	2	13
33	B7	41/42 (98%)	36 (88%)	5 (12%)	7	40
33	D7	41/42 (98%)	36 (88%)	5 (12%)	7	40
34	B8	53/55 (96%)	45 (85%)	8 (15%)	4	29
34	D8	53/55 (96%)	44 (83%)	9 (17%)	3	22
35	B9	34/34 (100%)	32 (94%)	2 (6%)	28	76
35	D9	34/34 (100%)	32 (94%)	2 (6%)	28	76
38	BC	180/181 (99%)	169 (94%)	11 (6%)	26	75
38	DC	180/181 (99%)	168 (93%)	12 (7%)	23	72
39	BD	217/218 (100%)	182 (84%)	35 (16%)	3	26
39	DD	217/218 (100%)	182 (84%)	35 (16%)	3	26
40	BE	165/166 (99%)	140 (85%)	25 (15%)	4	29
40	DE	165/166 (99%)	140 (85%)	25 (15%)	4	29
41	BF	165/166 (99%)	154 (93%)	11 (7%)	23	72
41	DF	165/166 (99%)	154 (93%)	11 (7%)	23	72
42	BG	155/156 (99%)	127 (82%)	28 (18%)	2	18
42	DG	155/156 (99%)	126 (81%)	29 (19%)	2	16
43	BH	136/148 (92%)	125 (92%)	11 (8%)	17	64
43	DH	136/148 (92%)	125 (92%)	11 (8%)	17	64
45	BN	117/119 (98%)	103 (88%)	14 (12%)	7	41
45	DN	117/119 (98%)	103 (88%)	14 (12%)	7	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BO	100/100 (100%)	94 (94%)	6 (6%)	27	76
46	DO	100/100 (100%)	94 (94%)	6 (6%)	27	76
47	BP	112/116 (97%)	93 (83%)	19 (17%)	3	22
47	DP	112/116 (97%)	92 (82%)	20 (18%)	2	19
48	BQ	111/111 (100%)	101 (91%)	10 (9%)	14	58
48	DQ	111/111 (100%)	101 (91%)	10 (9%)	14	58
49	BR	100/101 (99%)	89 (89%)	11 (11%)	9	47
49	DR	100/101 (99%)	87 (87%)	13 (13%)	6	37
50	BS	77/88 (88%)	69 (90%)	8 (10%)	10	50
50	DS	77/88 (88%)	69 (90%)	8 (10%)	10	50
51	BT	120/127 (94%)	96 (80%)	24 (20%)	2	13
51	DT	120/127 (94%)	96 (80%)	24 (20%)	2	13
52	BU	92/94 (98%)	82 (89%)	10 (11%)	9	47
52	DU	92/94 (98%)	81 (88%)	11 (12%)	7	41
53	BV	82/82 (100%)	72 (88%)	10 (12%)	7	40
53	DV	82/82 (100%)	73 (89%)	9 (11%)	9	47
54	BW	91/92 (99%)	86 (94%)	5 (6%)	30	79
54	DW	91/92 (99%)	86 (94%)	5 (6%)	30	79
55	BX	74/78 (95%)	65 (88%)	9 (12%)	7	40
55	DX	74/78 (95%)	65 (88%)	9 (12%)	7	40
56	BY	87/91 (96%)	76 (87%)	11 (13%)	7	39
56	DY	87/91 (96%)	76 (87%)	11 (13%)	7	39
57	BZ	162/179 (90%)	137 (85%)	25 (15%)	4	28
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	10	49
All	All	10872/11344 (96%)	9687 (89%)	1185 (11%)	9	47

5 of 1185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BU	108	GLU
5	CE	79	GLU
50	DS	67	ARG
54	BW	107	LEU
2	CB	36	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
53	BV	11	GLN
7	CG	13	GLN
48	DQ	45	GLN
55	BX	82	GLN
3	CC	110	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	254 (16%)	36 (2%)
1	CA	1503/1522 (98%)	252 (16%)	34 (2%)
22	AV	75/76 (98%)	13 (17%)	1 (1%)
22	CV	75/76 (98%)	15 (20%)	1 (1%)
23	AW	76/77 (98%)	27 (35%)	1 (1%)
23	CW	76/77 (98%)	27 (35%)	1 (1%)
24	AX	12/25 (48%)	8 (66%)	2 (16%)
24	CX	12/25 (48%)	7 (58%)	2 (16%)
36	BA	2900/2915 (99%)	588 (20%)	61 (2%)
36	DA	2900/2915 (99%)	585 (20%)	63 (2%)
37	BB	118/122 (96%)	25 (21%)	0
37	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9474 (98%)	1826 (19%)	202 (2%)

5 of 1826 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A

5 of 202 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2345	G
1	CA	429	U
36	DA	2198	A
36	BA	2481	G
1	CA	60	A

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

2 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	$\# Z  > 2$
23	5MU	AW	54	23	20,22,23	1.07	3 (15%)	25,32,35	1.33	2 (8%)
23	5MU	CW	54	23	20,22,23	1.05	3 (15%)	25,32,35	1.35	3 (12%)

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
23	5MU	AW	54	23	-	0/6/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/6/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	54	5MU	C6-N1	2.33	1.38	1.34
23	CW	54	5MU	C6-C5	-2.22	1.34	1.40
23	CW	54	5MU	C6-N1	2.20	1.38	1.34
23	CW	54	5MU	P-OP1	2.19	1.49	1.46
23	AW	54	5MU	P-OP1	2.16	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	54	5MU	C6-N1-C2	-4.94	121.00	122.41
23	CW	54	5MU	C6-N1-C2	-4.87	121.02	122.41
23	CW	54	5MU	C5-C6-N1	2.12	123.92	122.02
23	AW	54	5MU	C5M-C5-C6	2.05	122.88	118.61
23	CW	54	5MU	C5M-C5-C6	2.05	122.87	118.61

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 14 ligands modelled in this entry, 10 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
59	FUA	AY	701	-	40,40,40	1.70	8 (20%)	64,64,64	1.69	10 (15%)
60	GDP	AY	702	61	30,30,30	1.62	6 (20%)	45,47,47	2.44	9 (20%)
59	FUA	CY	701	-	40,40,40	1.69	8 (20%)	64,64,64	1.51	10 (15%)
60	GDP	CY	702	61	30,30,30	1.54	6 (20%)	45,47,47	1.81	9 (20%)

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
59	FUA	AY	701	-	-	0/18/92/92	0/4/4/4
60	GDP	AY	702	61	-	0/16/32/32	0/3/3/3
59	FUA	CY	701	-	-	0/18/92/92	0/4/4/4
60	GDP	CY	702	61	-	0/16/32/32	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AY	702	GDP	C5-N7	-4.74	1.32	1.38
59	AY	701	FUA	C29-C22	4.52	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CY	701	FUA	C23-C22	-4.34	1.39	1.51
59	CY	701	FUA	C29-C22	4.23	1.53	1.47
59	AY	701	FUA	C23-C22	-4.22	1.39	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AY	702	GDP	C6-C5-N7	-11.74	132.56	134.14
60	AY	702	GDP	C2-N3-C4	5.13	121.45	115.30
60	CY	702	GDP	C6-C5-N7	-5.12	133.45	134.14
59	AY	701	FUA	C23-C22-C17	-5.05	117.04	123.78
60	AY	702	GDP	C5-C4-N3	-5.03	120.28	126.07

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	AI	2
9	CI	2
42	DG	1
42	BG	1
23	CW	1
38	BC	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BG	112:PRO	C	113:ARG	N	3.28
1	DG	112:PRO	C	113:ARG	N	3.21
1	CI	53:VAL	C	54:ASP	N	3.01

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AI	53:VAL	C	54:ASP	N	3.00
1	CI	104:ARG	C	105:ASP	N	2.58



## 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%)	-0.07	36 (2%) 56 35	34, 72, 165, 200	0
1	CA	1504/1522 (98%)	-0.06	30 (1%) 62 39	43, 89, 174, 200	0
2	AB	235/256 (91%)	-0.13	1 (0%) 90 78	40, 82, 172, 191	0
2	CB	235/256 (91%)	-0.01	1 (0%) 90 78	53, 102, 164, 194	0
3	AC	207/239 (86%)	-0.25	0 100 100	23, 69, 122, 174	0
3	CC	207/239 (86%)	-0.15	0 100 100	45, 93, 143, 190	0
4	AD	208/209 (99%)	0.01	0 100 100	46, 95, 144, 166	0
4	CD	208/209 (99%)	0.04	1 (0%) 88 73	48, 107, 157, 188	0
5	AE	151/162 (93%)	-0.19	2 (1%) 74 50	27, 62, 107, 187	0
5	CE	151/162 (93%)	-0.07	1 (0%) 84 66	45, 76, 117, 200	0
6	AF	101/101 (100%)	-0.18	0 100 100	44, 85, 125, 174	0
6	CF	101/101 (100%)	0.14	1 (0%) 79 57	72, 115, 152, 183	0
7	AG	155/156 (99%)	-0.15	0 100 100	36, 80, 126, 182	0
7	CG	155/156 (99%)	-0.01	1 (0%) 86 69	63, 108, 150, 193	0
8	AH	138/138 (100%)	-0.21	0 100 100	35, 65, 111, 136	0
8	CH	138/138 (100%)	-0.14	0 100 100	45, 79, 117, 147	0
9	AI	127/128 (99%)	0.04	0 100 100	41, 79, 135, 157	0
9	CI	127/128 (99%)	0.15	1 (0%) 83 63	68, 111, 151, 175	0
10	AJ	99/105 (94%)	0.22	3 (3%) 48 29	33, 87, 180, 193	0
10	CJ	99/105 (94%)	0.37	2 (2%) 62 39	60, 127, 179, 190	0
11	AK	119/129 (92%)	-0.01	3 (2%) 54 34	27, 62, 109, 171	0
11	CK	119/129 (92%)	0.12	4 (3%) 43 27	48, 89, 126, 181	0
12	AL	125/132 (94%)	-0.09	1 (0%) 83 63	37, 76, 118, 180	0
12	CL	125/132 (94%)	0.09	3 (2%) 56 35	42, 82, 124, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	125/126 (99%)	0.21	5 (4%)	36	23	52, 98, 165, 200	0
13	CM	125/126 (99%)	0.32	7 (5%)	24	15	63, 126, 171, 200	0
14	AN	60/61 (98%)	-0.11	0	100	100	35, 62, 103, 131	0
14	CN	60/61 (98%)	0.02	1 (1%)	67	44	58, 91, 127, 146	0
15	AO	88/89 (98%)	-0.14	0	100	100	27, 71, 116, 144	0
15	CO	88/89 (98%)	-0.04	0	100	100	31, 82, 119, 141	0
16	AP	84/88 (95%)	0.12	0	100	100	36, 85, 130, 160	0
16	CP	84/88 (95%)	0.22	0	100	100	58, 95, 126, 166	0
17	AQ	100/105 (95%)	-0.07	0	100	100	40, 78, 112, 139	0
17	CQ	100/105 (95%)	0.04	0	100	100	60, 84, 120, 147	0
18	AR	70/88 (79%)	-0.08	1 (1%)	72	48	38, 72, 119, 167	0
18	CR	70/88 (79%)	-0.02	1 (1%)	72	48	60, 95, 142, 167	0
19	AS	79/93 (84%)	0.08	1 (1%)	74	50	63, 95, 174, 182	0
19	CS	79/93 (84%)	0.37	2 (2%)	54	34	74, 117, 181, 199	0
20	AT	99/106 (93%)	0.25	0	100	100	55, 95, 147, 176	0
20	CT	99/106 (93%)	0.20	0	100	100	72, 103, 153, 173	0
21	AU	25/27 (92%)	0.38	1 (4%)	36	23	33, 84, 132, 167	0
21	CU	25/27 (92%)	0.80	3 (12%)	5	6	77, 115, 145, 164	0
22	AV	76/76 (100%)	-0.05	1 (1%)	74	50	51, 94, 154, 200	0
22	CV	76/76 (100%)	-0.03	2 (2%)	53	33	67, 107, 165, 200	0
23	AW	77/77 (100%)	0.72	8 (10%)	7	7	97, 182, 200, 200	0
23	CW	77/77 (100%)	0.79	9 (11%)	5	6	97, 190, 200, 200	0
24	AX	12/25 (48%)	2.69	8 (66%)	0	1	52, 114, 167, 193	0
24	CX	12/25 (48%)	2.18	5 (41%)	1	1	52, 114, 172, 193	0
25	AY	667/691 (96%)	0.61	45 (6%)	17	13	71, 142, 179, 200	0
25	CY	667/691 (96%)	0.72	65 (9%)	8	8	84, 151, 186, 200	0
26	B0	84/85 (98%)	0.32	3 (3%)	41	26	61, 87, 134, 191	0
26	D0	84/85 (98%)	0.77	5 (5%)	21	15	78, 109, 144, 172	0
27	B1	94/98 (95%)	0.10	0	100	100	50, 88, 142, 151	0
27	D1	94/98 (95%)	0.31	2 (2%)	60	38	59, 99, 153, 181	0
28	B2	71/72 (98%)	0.22	2 (2%)	50	31	79, 127, 176, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	D2	71/72 (98%)	0.31	2 (2%) 50 31	82, 134, 172, 186	0
29	B3	60/60 (100%)	0.57	4 (6%) 17 13	55, 95, 148, 180	0
29	D3	60/60 (100%)	0.59	1 (1%) 67 44	61, 105, 145, 174	0
30	B4	58/71 (81%)	0.44	3 (5%) 26 17	90, 141, 200, 200	0
30	D4	58/71 (81%)	0.50	4 (6%) 17 12	106, 166, 200, 200	0
31	B5	59/60 (98%)	0.19	3 (5%) 27 17	46, 96, 175, 192	0
31	D5	59/60 (98%)	0.30	3 (5%) 27 17	50, 104, 167, 200	0
32	B6	50/54 (92%)	0.48	0 100 100	55, 97, 142, 173	0
32	D6	50/54 (92%)	0.54	1 (2%) 62 39	71, 111, 153, 178	0
33	B7	49/49 (100%)	0.27	1 (2%) 62 39	51, 79, 117, 200	0
33	D7	49/49 (100%)	0.21	0 100 100	64, 91, 127, 166	0
34	B8	64/65 (98%)	0.15	2 (3%) 47 29	51, 81, 124, 148	0
34	D8	64/65 (98%)	0.26	1 (1%) 68 45	67, 104, 137, 168	0
35	B9	37/37 (100%)	0.24	1 (2%) 52 32	66, 89, 127, 141	0
35	D9	37/37 (100%)	0.40	2 (5%) 25 16	65, 91, 151, 187	0
36	BA	2901/2915 (99%)	-0.01	56 (1%) 64 41	36, 88, 184, 200	0
36	DA	2901/2915 (99%)	0.01	56 (1%) 64 41	42, 102, 186, 200	0
37	BB	119/122 (97%)	-0.28	1 (0%) 83 63	68, 101, 129, 160	0
37	DB	119/122 (97%)	-0.21	0 100 100	83, 126, 154, 189	0
38	BC	228/229 (99%)	0.13	3 (1%) 74 50	44, 101, 163, 195	0
38	DC	228/229 (99%)	0.38	6 (2%) 53 33	66, 125, 187, 199	0
39	BD	275/276 (99%)	-0.12	1 (0%) 90 78	31, 64, 106, 155	0
39	DD	275/276 (99%)	-0.08	1 (0%) 90 78	40, 74, 115, 163	0
40	BE	205/206 (99%)	0.12	2 (0%) 79 57	37, 88, 146, 184	0
40	DE	205/206 (99%)	0.18	4 (1%) 62 39	50, 97, 157, 200	0
41	BF	208/210 (99%)	0.17	3 (1%) 72 48	53, 111, 183, 200	0
41	DF	208/210 (99%)	0.33	7 (3%) 43 27	58, 131, 186, 200	0
42	BG	181/182 (99%)	-0.01	4 (2%) 59 37	51, 99, 144, 194	0
42	DG	181/182 (99%)	0.15	4 (2%) 59 37	67, 122, 168, 192	0
43	BH	167/180 (92%)	0.57	7 (4%) 35 22	87, 131, 174, 185	0
43	DH	167/180 (92%)	0.48	2 (1%) 75 52	76, 133, 175, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	0.06	0 100 100	60, 99, 148, 177	0
45	DN	139/140 (99%)	0.15	2 (1%) 72 48	64, 108, 162, 176	0
46	BO	122/122 (100%)	-0.01	0 100 100	34, 72, 107, 128	0
46	DO	122/122 (100%)	0.01	0 100 100	40, 79, 108, 156	0
47	BP	146/150 (97%)	0.39	1 (0%) 84 66	48, 104, 158, 195	0
47	DP	146/150 (97%)	0.60	5 (3%) 43 27	52, 127, 173, 195	0
48	BQ	141/141 (100%)	-0.03	0 100 100	39, 77, 122, 173	0
48	DQ	141/141 (100%)	-0.01	1 (0%) 84 66	52, 86, 127, 185	0
49	BR	117/118 (99%)	0.08	0 100 100	36, 89, 128, 177	0
49	DR	117/118 (99%)	0.15	0 100 100	46, 95, 135, 181	0
50	BS	99/112 (88%)	0.14	1 (1%) 79 57	53, 109, 156, 191	0
50	DS	99/112 (88%)	0.48	2 (2%) 62 39	51, 121, 164, 192	0
51	BT	138/146 (94%)	0.06	3 (2%) 59 37	53, 95, 168, 200	0
51	DT	138/146 (94%)	0.03	4 (2%) 49 31	56, 103, 172, 200	0
52	BU	117/118 (99%)	-0.05	1 (0%) 81 61	55, 91, 138, 200	0
52	DU	117/118 (99%)	0.02	1 (0%) 81 61	66, 104, 147, 191	0
53	BV	101/101 (100%)	0.24	1 (0%) 79 57	43, 112, 158, 177	0
53	DV	101/101 (100%)	0.46	4 (3%) 36 23	64, 126, 171, 193	0
54	BW	113/113 (100%)	0.19	0 100 100	56, 95, 150, 195	0
54	DW	113/113 (100%)	0.41	3 (2%) 52 32	73, 106, 158, 194	0
55	BX	93/96 (96%)	0.23	1 (1%) 77 54	61, 101, 133, 176	0
55	DX	93/96 (96%)	0.17	1 (1%) 77 54	63, 111, 141, 154	0
56	BY	107/110 (97%)	0.73	6 (5%) 24 15	93, 138, 178, 187	0
56	DY	107/110 (97%)	1.08	14 (13%) 4 4	87, 147, 182, 200	0
57	BZ	185/206 (89%)	0.20	1 (0%) 88 73	50, 108, 163, 190	0
57	DZ	185/206 (89%)	0.30	1 (0%) 88 73	54, 122, 170, 199	0
All	All	22518/23492 (95%)	0.11	506 (2%) 59 37	23, 98, 175, 200	0

The worst 5 of 506 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	CW	17	C	12.0
1	AA	89	C	11.6
23	AW	17	C	11.3
36	DA	654(E)	G	11.0
36	BA	654(D)	G	10.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
23	5MU	AW	54	21/22	0.27	-	200,200,200,200	0
23	5MU	CW	54	21/22	0.14	-	200,200,200,200	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
59	FUA	AY	701	37/37	0.62	-	98,102,110,111	0
58	ZN	D9	1000	1/1	0.09	-	123,123,123,123	0
61	MG	CY	703	1/1	0.23	-	46,46,46,46	0
58	ZN	AN	101	1/1	0.23	-	84,84,84,84	0
58	ZN	CD	301	1/1	0.23	-	69,69,69,69	0
59	FUA	CY	701	37/37	0.62	-	102,104,107,109	0
58	ZN	D4	1000	1/1	0.14	-	200,200,200,200	0
58	ZN	AD	301	1/1	0.30	-	78,78,78,78	0
58	ZN	CN	101	1/1	0.14	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	ZN	B4	101	1/1	0.07	-	172,172,172,172	0
61	MG	AY	703	1/1	0.31	-	55,55,55,55	0
60	GDP	CY	702	28/28	0.17	-	96,102,109,110	0
58	ZN	B9	101	1/1	0.10	-	93,93,93,93	0
60	GDP	AY	702	28/28	0.23	-	93,97,99,99	0

## 6.5 Other polymers

There are no such residues in this entry.